**Single Crystal X-Ray Diffraction Submission Form**

Email completed form to Prof. Christine McKenzie ([mckenzie@sdu.dk](mailto:mckenzie@sdu.dk)) with ***cc to your supervisor.***

If your crystals are stable, place the sample in the labelled SCXRD submission cupboard in the X-ray laboratory along with a ***print out of this form***. If not, state any special arrangement needed in the email and box below. ***Note -*** usually crystals are best stored in their mother liquor.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Research group:** |  |  | **Internal ref. code:** |  |
| **Name:** |  |  | **Submission date:** |  |
| **E-mail:** |  |  | Data Collection date: |  |
|  |  |  |  |  |

|  |  |  |  |
| --- | --- | --- | --- |
| **Label on vial:** |  | **Proposed total element count** [e.g. C6H16O8]: |  |
| **Save crystal?** | **Yes** ☐ **No** ☐ | **Colour:** |  |

|  |  |
| --- | --- |
| **Proposed structure.**  Please indicate a preferred atom numbering scheme if you have one. | If a crystal structure of your compound is **known**, please provide a reference and justification for new data collection. E.g. Do you just want a unit cell check? |
| If the proposed molecule is chiral - is the sample a single enantiomer or a racemic mixture? |
| **Known or suspected hazards** (e.g. toxic, explosive) |
| **Is any special handling required?** (e.g. air/light sensitive). Other comments. |
| **Preparation/Crystallization route** include **ALL** solvents, precursors/reactants, spectator molecules and ions. | |

**DATA COLLECTION RECORD & REPORT**

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Crystal information** | | | | | | **Final Unit cell** | | | **Crystal system** | | | | **Centering** | |
| Color, Habit | | |  | | | a (Å) |  | | ☐ | Triclinic | | | ☐ | P |
| Size | | | x x mm | | | b (Å) |  | | ☐ | Monoclinic | | | ☐ | A |
| **Collection** | | | | | | c (Å) |  | | ☐ | Orthorhombic | | | ☐ | B |
| Radiation | | | Cu ☐ Mo☐ | | | α (°) |  | | ☐ | Tetragonal | | | ☐ | C |
| Temperature (K) | | |  | | | β (°) |  | | ☐ | Hexagonal | | | ☐ | I |
| Exposure time/frame | | |  | | | ϒ (°) |  | | ☐ | Trigonal | | | ☐ | F |
| Strategy | | |  | | | Vol. (Å3) |  | | ☐ | Cubic | | |  |  |
| Data collection time | | |  | | | | | | | | | | | |
| **Integration and scaling**   |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | | Resolution cut off | Å | Abs. correction | ☐ | Multi-scan | ☐ | Faces | ☐ | None | | Initial *R*(int) |  | Final *R*(int) |  | | | | | |   **Solution and refinement** | | | | | | | | | | | | | | | |
| Software | ☐ | SHELXS | | ☐ | SHELXT | | ☐ | OLEX report | | | ☐ | publcif | | | |
| Methods | ☐ | SHELXL | | ☐ | SQUEEZE | | ☐ | Mercury | | | ☐ | other | | | |
| Comments (e.g. twinning) | | | | | | | | | | | | | | | |
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| **Final results** | | | | | Notes: |
| Space group |  | | | |
| *R1* / *wR*2 | / | | | |
| Completeness / GooF | / | | | |
| Flack parameter |  | | | |
| Structure | ☐ | As proposed | ☐ | Other |
| Status | ☐ | Completed | ☐ | Abandoned |