

# Crystal Structure Service

## Request for Determination

Structure Code

Date: \_\_\_\_\_ Applicant: \_\_\_\_\_ Supervisor: \_\_\_\_\_

Room No: \_\_\_\_\_ Tel. № \_\_\_\_\_ e-mail \_\_\_\_\_

Probable molecular formula(e), e.g.  $C_{22}H_{14}Cu_0S_4$ : \_\_\_\_\_ Mol.weight \_\_\_\_\_

Possible structural formula(e) with numbering scheme(s) if appropriate

1. State *specifically* what information you require (e.g. connectivity, H-atom location, absolute configuration) and the scientific case to justify the determination:

2. State preferred temperature (78-375K) for the determination and reason(s) for requiring this temperature:

Room Temp.  Low Temp

3. Outline the preparative scheme for your compound, including all the solvents you used:

4. Describe how the crystals were grown, including which solvents were used:

Crystallised from: \_\_\_\_\_ Soluble in: \_\_\_\_\_ Insoluble in: \_\_\_\_\_

5. List any relevant spectroscopic data and qualitative or quantitative analytical data (CHN, etc):

6. Provide physical data on the actual sample submitted:

Crystal colour: \_\_\_\_\_ Shape: \_\_\_\_\_ Melting point: \_\_\_\_\_

Other properties: \_\_\_\_\_

**Sensitivity to:** Dry air  Moist air  Water  Light  Solvent loss  Other \_\_\_\_\_

How long do the crystals survive unprotected in air? \_\_\_\_\_

7. Specify any hazards associated with the sample, including those from any solvents present:

Inflammable:  Pyrophoric:  Explosive:  Carcinogenic:  Toxic (give details): \_\_\_\_\_

Other hazards: \_\_\_\_\_

8. Storage of crystals in diffractometer room: ambient  fridge  freezer

Other location (in exceptional cases only): \_\_\_\_\_

**PLEASE RETURN THIS FORM DULY COMPLETED**

**ENSURE THAT YOUR SAMPLE IS CLEARLY LABELLED WITH THE NUMBER SHOWN ABOVE.**