University of Zurich[UZH]

Department of Chemistry
X-ray Crystallography Facility

University of Zurich
Department of Chemistry
X-ray Crystallography Facility
Winterthurerstrasse 190
CH-8057 Zurich

www.chem.uzh.ch/en/research/services/xray.html

Request Form

Prof. Dr. Bernhard Spingler
spingler@chem.uzh.ch
044 635 46 56

Fill in all sections. **Please label your sample clearly with your name and sample code.**

Name: ..... Date: .....

Group: ..... Laboratory: .....

E-mail: .....

Sample code or name: .....

Molecular formula: ..... Melting point: .....°C

Solvent(s): ..... Colour: .....

Safety precautions & hazards: .....

Are you confident of the structure of your molecule?

☐ yes ☐ some doubt ☐ structure completely unknown

Spectra done: ☐ 1H-NMR ☐ 13C-NMR ☐ MS ☐ IR ☐ Elemental analysis

Chirality

☐ none ☐ racemic single ☐ enantiomer

If chiral: ☐ all sites known ☐ all sites unknown ☐ some sites unknown

➔ Clearly indicate the chirality of known sites on your diagram opposite.

Crystal stability

☐ stable ☐ moisture sensitive ☐ light sensitive

☐ keep cold ☐ hygroscopic

☐ loses solvent ☐ thermally unstable at …….°C ☐ O_2 sensitive

Speed of decomposition: ☐ instant ☐ minutes ☐hours

Special requirements

☐ temperature of study: ……..K (160 K is normally used)

☐ investigation of classic hydrogen bonding interactions (e.g. N–H···O, etc.)

☐ torsion angles involving H atoms

☐ determine absolute configuration (possible only if an element heavier than N is present)

☐ other: .....

Diagrams: (these will be e-mailed to you)

You will normally receive the following diagrams:

- One displacement ellipsoid plot of the molecule ready for publication.
- A packing diagram if intermolecular hydrogen bonds are present.
- If you are interested in the packing, it is often best to visualise this yourself using Mercury and the provided CIF.

➔ Indicate additional requirements below (e.g. stereoview, view directions, style, etc.):

Format of report & data files: (these will be e-mailed to you)

Report & tables document: ☒ Word

File of atomic coordinates: ☒ CIF (for structure visualisation with Mercury, Diamond, etc. Suitable for deposition in the CSD or with a publication)

☐ other file formats, tables, calculations, special needs:

Structural formula:

Paste a sketch of the expected structure onto the dot below.
If the composition is uncertain, give the reaction starting materials and all likely products.

➔ **Please indicate the desired atom numbering if it is important to you. Clearly show chirality, if known.**

➔ **Please indicate what you hope to learn from this analysis.**

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Comments: