University of Zurich[UZH]

Winterthurerstrasse 190
CH-8057 Zurich
Phone +41 44 635 42 28
Fax +41 44 635 68 12
www.chem.uzh.ch/linden

Department of Chemistry
X-ray Crystallography Facility

REQUEST FOR A CRYSTAL STRUCTURE DETERMINATION

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

Company: ..... Tel. Nr: .....

Address: .....

E-mail: ..... Signature: .....

Sample code or name: .....

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

Solvent: ..... Colour: .....

Safety precautions & hazards: .....

Are you confident of the structure of your molecule?

☐ yes ☐ some doubt ☐ structure completely unknown

Spectra done: ☐ ^{1}H-NMR ☐ ^{13}C-NMR ☐ MS ☐ IR ☐ Microanalysis

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 ☐ O_2 sensitive

☐ loses solvent ☐ thermally unstable at ..... °C

Speed of decomposition: ☐ instant ☐ minutes ☐ hours

Special requirements:

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

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

☐ torsion angles involving H atoms

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

☐ other: .....

Diagrams:

You will normally receive the following diagrams:
One thermal ellipsoid (ORTEP) plot of the molecule in black ink ready for publication.
A packing diagram if intermolecular hydrogen bonds are present.
Diagrams will be also available as colour TIFF files
If you are interested in the packing, it is best to visualise this yourself using Mercury and the provided CIF

Indicate additional requirements below:

☐ stereoview of single molecule

☐ molecular packing

☐ special requirements (colours, views, style, etc.): .....

.....

Format of report & data files:

Report & tables document: ☐ Word

File of atomic coordinates: ☐ PDB format ☐ CIF (for structure visualisation with Mercury)

☐ other: .....

Structural formula:

Clearly show chirality, if known. If the composition is uncertain, give the reaction starting materials and all likely products.

Please indicate the desired atom numbering. Renumbering at a later date makes significant extra work!

7.1.2014 AL