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Department of Chemistry
X-ray Crystallography Facility

Fill in ALL sections. **Label your sample clearly with your name and sample code.**

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

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

E-mail: ....
    a UZH e-mail address is preferred

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: ☐ ^{1}H-NMR   ☐ ^{13}C-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   ☐ O_2 sensitive

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

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:

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.

25.4.2020 AL