

IdentCode

Gerät / Temperatur

Datum

## *X-Ray crystal structure analysis*

Requester \_\_\_\_\_ Research group \_\_\_\_\_ Telephone \_\_\_\_\_

Sample ID \_\_\_\_\_ Mol. weight \_\_\_\_\_ g/mol Melting point \_\_\_\_\_ °C

Empirical formula \_\_\_\_\_ Date \_\_\_\_\_

e-mail-Address \_\_\_\_\_ Signature \_\_\_\_\_  
Requester Research group leader

Sensitivities  Light  Air  Moisture  Heat

Crystal colour \_\_\_\_\_ Crystal shape \_\_\_\_\_

Analytical findings (EA, NMR, MS, ...) \_\_\_\_\_

Synthesis route:

Which solvents might be included in the sample:

Method of crystallisation:

Structural proposal: Provide numbering of atoms if needed.

Other elements which might be present.

Please complete every field.

**p.t.o.**

If isotypic samples have been measured already or in the case of recurrence – fill in the IdentCode and the unit cell parameters of that measurement.

The measurement is:  a recurrent measurement  possibly isotypic

to:

IdentCode of data collection

Unit cell:

Crystal system / Space group: \_\_\_\_\_

Unit cell:  $a =$   $b =$   $c =$   $V =$

$\alpha =$   $\beta =$   $\gamma =$

Please give the unit cells of concurrent side products or starting materials:

Substance:	$a$	$b$	$c$	$\alpha$	$\beta$	$\gamma$	space grp.

Kristallfarbe:

Kristallform:

Größe:

Zentrierung:

0	90
180	270
Ø	

Generatoreinstellungen:

\_\_\_\_\_ kV \_\_\_\_\_ mA

Meßbedingungen:

\_\_\_\_\_ sets \_\_\_\_\_ frames \_\_\_\_\_ ° p.f. \_\_\_\_\_ sec.

Abskor.:

Lösung:

Erste Zelle: a: b: c:  $\alpha$ :  $\beta$ :  $\gamma$ : V:

Meßparameter & Notizen: