Information for Single Crystal Analysis

filled out by AKS-staff only

Date of data collection	Name of data set
Data recipient & sending date	Crystal description

Sample identifier

Elemental composition ($C_xH_yN_z$...)(no abbrevations like *Me* or *Cp*)

Location of sample (laboratory bench, freezer, ...)

Preparation (including all reagents, solvents, expected structure and crystallization method)

Lattice parameters of all starting material, by- and side-products, related compounds (a, b, c, α, β, γ, V, Z and space group)

Name	Date
Tel.	E-mail
AK	Signature of group leader (mandatory)

Important information (default value)

Storage temperature (25 °C)	Stability towards air ☒ minutes ☐ seconds
Additional molecules in the lattice/solvents (none)	Additional information (none)

Please provide information from earlier structure solution/refinement attempts overleaf.

What do you want to achieve?

- ☒ I want crystal data meeting the requirements for publication in common inorganic journals. (default)
- ☐ I just want a picture of my structure. I am aware that the result will probably not be publishable.
- ☐ I want raw frame data. I will care for integration myself.
- ☐ I want a high resolution dataset to resolve a special problem:

To obtain the best crystal structure it is important that we know all details about the synthesis and storing conditions. These conditions influence the selection of the crystal, such as size and the measurement's parameters. Information about additional molecules in the lattice may be obtained by ^{1}H NMR spectroscopy. The tube of the samples ought to be well labeled with paper using the identifier and name on this sheet, **NOT** with Edding! Schlenk tubes will not be stored longer than four weeks. Please do not put snap-on lids in Schlenk tubes.
We will not provide long term data storage!

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Information from earlier studies