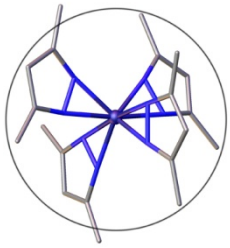


# MOLECULAR STRUCTURE LABORATORY SAMPLE SUBMISSION FORM

_____

## CONTACT INFORMATION

Name: _____; e-mail: _____; phone #: _____;

Advisor: _____.

## DESIRED CRYSTALLOGRAPHIC INFORMATION

□ Unit cell only □ Data collection only □ Complete structural characterization

□ Absolute configuration □ Relative configuration □ Other? Specify: _____

## SAMPLE INFORMATION

Date submitted: _____, 2016; your sample code: _____

□ I will keep the sample in my lab until a diffractometer is available □ I will need my sample back

□ Air-stable □ Air- and moisture-sensitive □ Temperature-sensitive □ May contain solvent in the lattice □ Toxic

Other analyses performed? □ EA □ IR □ NMR □ Mass Spec □ MP □ Color: _____

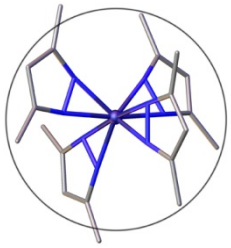
Indicate all solvents the compound has been exposed to: acetone / MeCN / benzene / $CHCl_3$ / $CH_2Cl_2$ / Dichloroethane / DMF / DMSO / EtOH / ether / EtOAc / heptane / hexane / MeOH / pentane / THF / toluene / $H_2O$ / or specify:

_____

## SYNTHETIC ROUTE (Show the reaction, indicate the synthons, desired compound, and byproducts if known):

## PROPOSED STRUCTURE:

Proposed molecular formula: _____



# MOLECULAR STRUCTURE LABORATORY SAMPLE SUBMISSION FORM

_____ Date examined: _____, 2018

## DIFFRACTOMETER INFORMATION

□ Gromit □ Bucky Power: _____ kV / _____ mA Temp _____ K

## CRYSTAL INFORMATION

Size: _____ x _____ x _____ mm; color: _____; habit _____; mosaicity = _____°

## CRYSTALLOGRAPHIC INFORMATION

Crystal system: □ triclinic □ monoclinic □ orthorhombic □ tetragonal □ cubic □ trigonal □ hexagonal

Centering: _____; a = _____ Å, b = _____ Å, c = _____ Å, α = _____°, β = _____°, γ = _____°.

Unit cell volume = _____ $Å^3$, Estimated molecular volume = _____ $Å^3$, Z = ____ μ = _____ $mm^{-1}$ Friedif = _____

## USUAL CHECKS

□ Cambridge Structural Database □ Reciprocal Net □ Cell_now

## DATA COLLECTION PARAMETERS

### UNIT CELL

# of reflections _____ Scan width _____° Exposure time _____sec

### DATA COLLECTION

ω runs _____, φ runs _____, Scan width _____°, Exposure time(s) _____sec

## DATA REDUCTION PARAMETERS

□ Video acquired □ Crystal faces indexed

Absorption correct type: □ Analytical □ Multi-scan □ No correction.

## NOTES:

| SOLVENT | ELECTRONS, VOLUME $Å^3$ |
|---|---|
| Acetone | 32, 86 |
| MeCN | 22, 57 |
| Benzene | 42, 144 |
| $CHCl_3$ | 58, 61 |
| $CH_2Cl_2$ | 42, 52 |
| EtOH | 26, 72 |
| Ether | 42, 120 |
| EtOAc | 48, 124 |
| Hexane | 50, 154 |
| MeOH | 18, 48 |
| Toluene | 50, 138 |