

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: _____, 2018; your sample code: _____

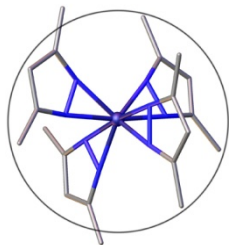
- I will keep the sample in my lab until a diffractometer is available I will need my sample back
 Air-stable Air- and moisture-sensitive Temperature-sensitive May contain solvent in the lattice Toxic
Other analyses performed? EA IR NMR Mass Spec MP Color: _____

Indicate all solvents the compound has been exposed to: acetone / MeCN / benzene / CHCl₃ / CH₂Cl₂ / Dichloroethane / DMF / DMSO / EtOH / ether / EtOAc / heptane / hexane / MeOH / pentane / THF / toluene / H₂O / 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 = _____ Å³, Estimated molecular volume = _____ Å³, 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 ₂ Cl ₂	42.52
EtOH	26.72
Ether	42.120
EtOAc	48.124
Hexane	50.154
MeOH	18.48
Toluene	50.138