

_____ Molecular Structure Laboratory Sample Submission Form

Date _____ Professor _____

Name _____ Your Sample Code _____

Phone # : _____ Room # _____ E-mail _____

Air-stable _____ Air- and Moisture Sensitive _____ Solvent dependent _____

What analyses have been performed ? EA _____; NMR _____; IR _____; MP _____

Mark or write-in all solvents the compound has been in contact with: _____

Hexane/pentane/ether/DMSO/CH₂Cl₂/CHCl₃/benzene/toluene/EtOH/MeOH/MeCN/H₂O

Synthetic route :

Proposed structure(s):

Molecular formula _____

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Date _____	Bruker CCD-1000 Bruker APEXII _____ kV / _____ mA
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Space group _____

a = _____ (____) Å

b = _____ (____) Å

c = _____ (____) Å

α = _____ (____) °

β = _____ (____) °

γ = _____ (____) °

V = _____ (____) Å³

Z = _____

T = _____ K

Lattice _____

Size _____

Color _____

Habit _____

CSD check

Reciprocal Net

Data Collection Parameters

Run	Start	2 θ	ω	ϕ	γ	Axis	Width	Number	Exposure
0	001	-28.0	-28.0	0	54.86	2	-	_____	_____
0	001	-28.0	-28.0	_____	54.86	2	-	_____	_____
0	001	-28.0	-28.0	_____	54.86	2	-	_____	_____
0	001	-28.0	-28.0	_____	54.86	-	-	_____	_____
0	001	-28.0	-28.0	_____	54.86	-	-	_____	_____

Data Reduction Parameters

SADABS R(int) before parameter refinement _____	Series 0 # of reflections _____
SADABS R(int) after parameter refinement _____	Series 1 # of reflections _____
Initial CELL on _____ Final CELL on _____	Series 2 # of reflections _____
# of reflections _____ I/ σ _____	Series 3 # of reflections _____

Structure solution and refinement

R(int) _____ R(σ) _____

TREF Patterson

R = _____ GOF _____

e/Å³ _____ / - _____

PLATON

of e/cell _____

Volume _____

Solvents _____

F(000)

MW

D(calc.)