



Supporting Information

for

Base-promoted deacylation of 2-acetyl-2,5-dihydrothiophenes and their oxygen-mediated hydroxylation

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Beilstein J. Org. Chem. **2026**, 22, 192–204. doi:10.3762/bjoc.22.13

CheckCIF-file for compound 5g

Datablock: exp_166

Bond precision:	C-C = 0.0035 A	Wavelength=0.71073
Cell:	a=9.3076(5) b=9.3243(5) c=10.1072(4)	
	alpha=102.086(4) beta=102.480(4) gamma=108.253(5)	
Temperature:	295 K	
	Calculated	Reported
Volume	776.19(8)	776.19(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C17 H18 N2 O2 S	C17 H18 N2 O2 S
Sum formula	C17 H18 N2 O2 S	C17 H18 N2 O2 S
Mr	314.39	314.39
Dx,g cm-3	1.345	1.345
Z	2	2
Mu (mm-1)	0.217	0.217
F000	332.0	332.0
F000'	332.38	
h,k,lmax	13,13,14	12,13,14
Nref	4745	4252
Tmin,Tmax	0.906,0.953	0.711,1.000
Tmin'	0.899	
Correction method=	# Reported T Limits: Tmin=0.711 Tmax=1.000	
AbsCorr =	MULTI-SCAN	
Data completeness=	0.896	Theta(max)= 30.500
R(reflections)=	0.0596(2973)	wR2(reflections)= 0.1768(4252)
S =	1.060	Npar= 208

The following ALERTS were generated. Each ALERT has the format
[test-name_ALERT_alert-type_alert-level](#).
Click on the hyperlinks for more details of the test.

Alert level G

PLAT012_ALERT_1_G	No	_shelx_res_checksum Found in CIF	Please Check
PLAT398_ALERT_2_G	Deviating	C-O-C Angle From 120 for O1	110.0 Degree
PLAT793_ALERT_4_G	Model has Chirality at C4	(Centro SpGr)	R Verify
PLAT793_ALERT_4_G	Model has Chirality at C5	(Centro SpGr)	R Verify
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		4 Note
	-3 5 11, 1 11 0, -4-10 6, 4 -3 1,		

- 0

ALERT level A

= Most likely a serious problem - resolve or explain
- 0

ALERT level B

= A potentially serious problem, consider carefully
- 0

ALERT level C

= Check. Ensure it is not caused by an omission or oversight
- 5

ALERT level G

= General information/check it is not something unexpected
- 1

ALERT type 1

CIF construction/syntax error, inconsistent or missing data
- 2

ALERT type 2

Indicator that the structure model may be wrong or deficient
- 0

ALERT type 3

Indicator that the structure quality may be low
- 2

ALERT type 4

Improvement, methodology, query or suggestion
- 0

ALERT type 5

Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON-NOV 22 13:28:43 2025 - (VERSION=260925)

exp_166

P -1

$$R = 0.06$$

RES= 0 88 X

NOMOVE FORCED

Prob = 50%
Temp = 295K

