

No syntax errors found.
Please wait while processing

[CIF dictionary](#)
[Interpreting this report](#)

Datablock: TH41_01new

Bond precision: C-C = 0.0030 Å Wavelength=0.71073
Cell: a=6.0106 (3) b=12.0412 (6) c=16.2062 (9)
alpha=90 beta=90 gamma=90
Temperature: 123 K

	Calculated	Reported
Volume	1172.92 (11)	1172.92 (11)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C15 H14 O2	C15 H14 O2
Sum formula	C15 H14 O2	C15 H14 O2
Mr	226.26	226.26
Dx, g cm ⁻³	1.281	1.281
Z	4	4
Mu (mm ⁻¹)	0.084	0.084
F000	480.0	480.0
F000'	480.23	
h, k, lmax	7, 14, 19	7, 14, 19
Nref	2306 [1358]	2304
Tmin, Tmax	0.982, 0.997	
Tmin'	0.963	
Correction method	Not given	
Data completeness	1.70/1.00	Theta(max) = 25.994
R(reflections) = 0.0301 (2106)		wR2(reflections) = 0.0695 (2304)
S = 1.150	Npar = 162	

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

PLAT002 ALERT 2 G	Number of Distance or Angle Restraints on AtSite	4	Note
PLAT032 ALERT 4 G	Std. Uncertainty on Flack Parameter Value High .	0.500	
Report			
PLAT172 ALERT 4 G	The CIF-Embedded .res File Contains DFIX Records	2	
Report			
PLAT860 ALERT 3 G	Number of Least-Squares Restraints	2	Note
PLAT883 ALERT 1 G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT899 ALERT 4 G	SHELXL2018 is Outdated and Succeeded by SHELXL	2019/3	Note
PLAT910 ALERT 3 G	Missing # of FCF Reflection(s) Below Theta(Min). 0 1 1, 0 0 2,	2	Note
PLAT967 ALERT 5 G	Note: Two-Theta Cutoff Value in Embedded .res ..	52.0	
Degree			
PLAT969 ALERT 5 G	The 'Henn et al.' R-Factor-gap value	4.263	Note
	Predicted wR2: Based on SigI**2 1.63 or SHELX Weight	6.04	
PLAT978 ALERT 2 G	Number C-C Bonds with Positive Residual Density.	4	Info

- 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
10 **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
2 ALERT type 3 Indicator that the structure quality may be low

3 ALERT type 4 Improvement, methodology, query or suggestion
2 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. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that [full publication checks](#) are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 22/08/2024; check.def file version of 21/08/2024

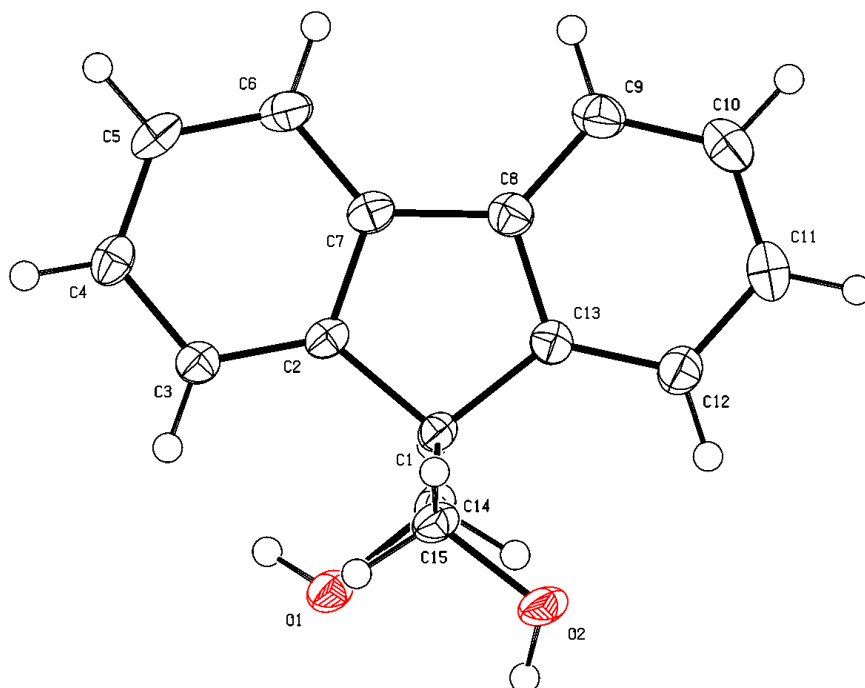
Datablock TH41_01new - ellipsoid plot

-40 Y

PLATON-Oct 21 12:55:24 2024 - (220824)

NOMOVE FORCED

Prob = 50
Temp = 123



Z -169 TH41_01new

P 21 21 21 R = 0.03

RES= 0-134 X