checkCIF () running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait . .
++ + SHELXL - CRYSTAL STRUCTURE REFINEMENT - MULTI-CPU VERSION + + Copyright(C) George M. Sheldrick 1993-2014 Version 2014/7 + + infile_sx started at 05:18:56 on 04-Aug-2016 + ++
Command line parameters: infile_sx -a50000 -b3000 -c624 -t8 -a sets the approximate maximum number of atoms including hydrogens. -b sets the maximum number of full-matrix parameters (leave unchanged for CGLS). For example -b9000 allows refinement of 1000 anisotropic atoms or 3000 with BLOC 1. For a 32-bit version, -b times the square root of the number of threads should not exceed about 65500. -c sets the reflection buffer size. This depends on the CPU cache size but will rarely need changing. -t sets the number of threads, otherwise the multi-CPU version sets this equal to the number of available CPUs. For optimal performance on systems with hyperthreading, usually the hyperthreading should be switched off or -t used to halve the number of threads; e.g. -t4 rather than -t8 for an Intel i7 processor. Running 8 threads on 8 processors Read instructions and data ** ATOM NAMES NOT ALLOWED **
++ + infile_sx finished at 05:18:56 Total elapsed time: 0.00 secs +
++ . Create .fcf from SHELXL .ins & .hkl. Substituted SHELXL Instruction:LS. 1 Inserted SHELXL Instruction:BLOC ** PROBLEM to Recreate FCF for this ENTRY ** Entry # 1 - 0A, 0B, 1C, 1G-Alerts, BP C-C = 0.0038 :: CheckCIF out on :infile.chk . . . . . .
. . . . . .
. . . . . .

checkCIF/PLATON (full publication check)

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found.
Please wait while processing ....

CIF dictionary
Interpreting this report

Datablock: I

Bond precision: C-C = 0.0038 A Wavelength=0.71073

Cell: a=8.717(3) b=16.325(5) c=21.043(7)
alpha=90 beta=90 gamma=90

Temperature: 90 K

	Calculated	Reported
Volume	2994.5(17)	2994.5(17)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C36 H30 S4	C36 H30 S4
Sum formula	C36 H30 S4	C36 H30 S4
Mr	590.84	590.84
Dx,g cm-3	1.311	1.311
Z	4	4
Mu (mm-1)	0.342	0.342
F000	1240.0	1240.0
F000'	1242.35	
h,k,lmax	10,19,25	10,19,25
Nref	2646	2641
Tmin,Tmax	0.902,0.934	0.659,0.934
Tmin'	0.887	

Correction method= # Reported T Limits: Tmin=0.659 Tmax=0.934 AbsCorr = EMPIRICAL

Data completeness= 0.998 Theta(max)= 25.020

R(reflections)= 0.0433(2172) wR2(reflections)= 0.1298(2641)
S = 1.156 Npar= 181

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 C

PLAT373_ALERT_2_C	Long	C(sp)-C(sp)	Bond	C18	-	C18_a	..	1.37 Ang.

Alert level G

PLAT371_ALERT_2_G	Long	C(sp2)-C(sp1)	Bond	C12	-	C17	..	1.43 Ang.

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
1 **ALERT level G** = General information/check it is not something unexpected

0 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
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

PUBL006_ALERT_1_A	_publ_requested_journal is missing
	e.g. 'Acta Crystallographica Section C'
PUBL009_ALERT_1_A	_publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A	_publ_author_address is missing. Author(s) address(es).

3 **ALERT level A** = Data missing that is essential or data in wrong format
0 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF
You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.
If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form
Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

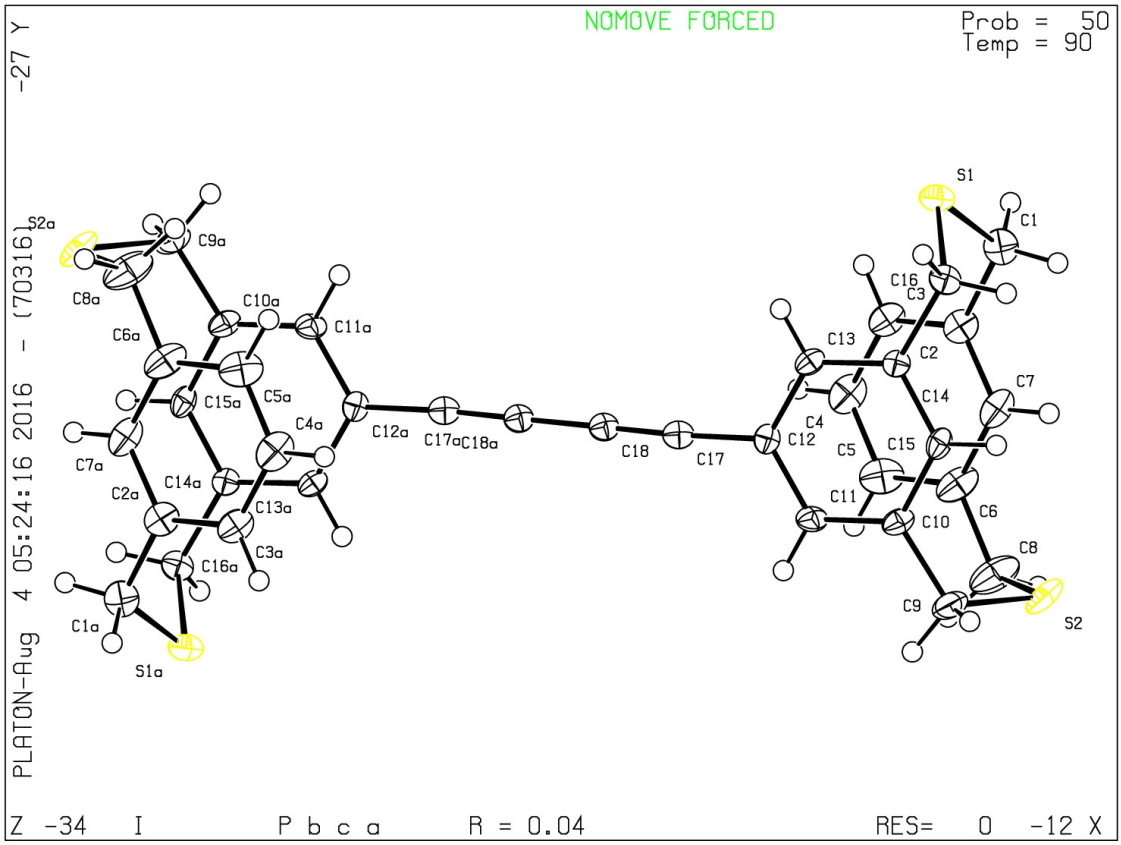
```
# start Validation Reply Form
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
```

;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
end Validation Reply Form

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 08/07/2016; check.def file version of 05/07/2016

Datablock I – ellipsoid plot



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Test a new CIF entry