

Supplementary data for article:

Milenković, M. R.; Bacchi, A.; Cantoni, G.; Radulović, S. S.; Gligorijević, N.; Arandžević, S.; Sladić, D.; Vujčić, M.; Mitić, D.; Anđelković, K. K. Synthesis, Characterisation and Biological Activity of Co(III) Complex with the Condensation Product of 2-(Diphenylphosphino)Benzaldehyde and Ethyl Carbazate. *Inorganica Chimica Acta* **2013**, *395*, 33–43. <https://doi.org/10.1016/j.ica.2012.09.043>

Alert level B

PLAT220 ALERT 2 B	Large Non-Solvent	C	Ueq(max)/Ueq(min) ...	4.4	Ratio
PLAT230 ALERT 2 B	Hirshfeld Test Diff for	C9	-- C10 ..	7.3	su

Alert level C

PLAT048 ALERT 1 C	MoietyFormula Not Given				?
PLAT125 ALERT 4 C	No '_symmetry_space_group_name_Hall' Given				?
PLAT220 ALERT 2 C	Large Non-Solvent	C	Ueq(max)/Ueq(min) ...	3.3	Ratio
PLAT222 ALERT 3 C	Large Non-Solvent	H	Uiso(max)/Uiso(min) ..	5.6	Ratio
PLAT230 ALERT 2 C	Hirshfeld Test Diff for	C18	-- C19 ..	5.7	su
PLAT230 ALERT 2 C	Hirshfeld Test Diff for	C19	-- C20 ..	7.0	su
PLAT242 ALERT 2 C	Check Low		Ueq as Compared to Neighbors for		C31

Alert level G

PLAT005 ALERT 5 G	No _iucr_refine_instructions_details in CIF				?
PLAT128 ALERT 4 G	Alternate Setting of Space-group C2/c			I2/a	
PLAT199 ALERT 1 G	Check the Reported _cell_measurement_temperature			293	K
PLAT200 ALERT 1 G	Check the Reported _diffrn_ambient_temperature			293	K
PLAT790 ALERT 4 G	Centre of Gravity not Within Unit Cell: Resd. #				2

C22 H21 N2 O2 P

- 2 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
7 **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

- 5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Datablock: 2

Bond precision: C-C = 0.0028 A

Wavelength=0.71073

Cell: a=15.677(1) b=13.403(1) c=19.949(2)
alpha=90 beta=93.012(1) gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	4185.9(6)	4185.9(6)
Space group	P 21/n	P21/n
Hall group	-P 2yn	?
Moiety formula	C44 H40 Co N4 O4 P2, B F4	?
Sum formula	C44 H40 B Co F4 N4 O4 P2	C44 H40 B Co F4 N4 O4 P2
Mr	896.48	896.48
Dx,g cm-3	1.423	1.423
Z	4	4
Mu (mm-1)	0.553	0.553
F000	1848.0	1848.0
F000'	1851.04	
h,k,lmax	23,19,29	23,19,29
Nref	14520	13805
Tmin,Tmax	0.961,0.984	0.800,1.000
Tmin'	0.957	

Correction method= MULTI-SCAN

Data completeness= 0.951

Theta(max)= 31.990

R(reflections)= 0.0386(10766)

wR2(reflections)= 0.1150(13805)

S = 1.029

Npar= 569

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 A

PLAT761_ALERT_1_A	CIF Contains no X-H Bonds	?
PLAT762_ALERT_1_A	CIF Contains no X-Y-H or H-Y-H Angles	?

Alert level B

PLAT029_ALERT_3_B	_diffrn_measured_fraction_theta_full Low	0.951
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Alert level C

PLAT048_ALERT_1_C	MoietyFormula Not Given	?
PLAT125_ALERT_4_C	No '_symmetry_space_group_name_Hall' Given	?
PLAT234_ALERT_4_C	Large Hirshfeld Difference F1 -- B1 ..	0.17 Ang.
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	B1
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.1

Alert level G

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in CIF	?
PLAT128_ALERT_4_G	Alternate Setting of Space-group P21/c	P21/n
PLAT199_ALERT_1_G	Check the Reported _cell_measurement_temperature	293 K
PLAT200_ALERT_1_G	Check the Reported _diffrn_ambient_temperature	293 K
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Col -- N1 ..	5.2 su

<u>PLAT232 ALERT 2 G</u>	Hirshfeld Test Diff (M-X) Col -- N3 ..	6.8 su
<u>PLAT302 ALERT 4 G</u>	Note: Anion/Solvent Disorder	60 Perc.
<u>PLAT779 ALERT 4 G</u>	Suspect or Irrelevant (Bond) Angle in CIF #	103
	F31 -B1 -F3 1.555 1.555 1.555	44.00 Deg.

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1 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

PUBL004 ALERT 1 A The contact author's name and address are missing,
_publ_contact_author_name and _publ_contact_author_address.
PUBL005 ALERT 1 A _publ_contact_author_email, _publ_contact_author_fax and
_publ_contact_author_phone are all missing.
At least one of these should be present.
PUBL006 ALERT 1 A _publ_requested_journal is missing
e.g. 'Acta Crystallographica Section C'
PUBL008 ALERT 1 A _publ_section_title is missing. Title of paper.
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).
PUBL012 ALERT 1 A _publ_section_abstract is missing.
Abstract of paper in English.

Alert level G

PUBL013 ALERT 1 G The _publ_section_comment (discussion of study) is
missing. This is required for a full paper submission (but is
optional for an electronic paper).
PUBL017 ALERT 1 G The _publ_section_references section is missing or
empty.

7 **ALERT level A** = Data missing that is essential or data in wrong format
2 **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 Acta Crystallographica Section C or Section E, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. Your explanation will be considered as part of the review process.

If you intend to submit to another section of Acta Crystallographica or Journal of Applied Crystallography or Journal of Synchrotron Radiation, you should make sure that at least a **basic structural check** is run on the final version of your CIF prior to submission.

```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
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: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
```

```
RESPONSE: ...
;
_vrf_PLAT761_1
;
PROBLEM: CIF Contains no X-H Bonds ..... ?
RESPONSE: ...
;
_vrf_PLAT762_1
;
PROBLEM: CIF Contains no X-Y-H or H-Y-H Angles ..... ?
RESPONSE: ...
;
_vrf_PLAT761_2
;
PROBLEM: CIF Contains no X-H Bonds ..... ?
RESPONSE: ...
;
_vrf_PLAT762_2
;
PROBLEM: CIF Contains no X-Y-H or H-Y-H Angles ..... ?
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 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 19/04/2012; check.def file version of 14/04/2012



