

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: aa

Bond precision: C-C = 0.0039 Å

Wavelength=0.71073

Cell: a=8.0530(16) b=10.533(2) c=13.076(3)
 alpha=66.93(3) beta=80.25(3) gamma=68.36(3)
Temperature: 293 K

	Calculated	Reported
Volume	948.1(4)	948.1(3)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C20 H15 Co N5 O5	?
Sum formula	C20 H15 Co N5 O5	C20 H15 Co N5 O5
Mr	464.30	464.30
Dx, g cm-3	1.626	1.626
Z	2	2
Mu (mm-1)	0.951	0.951
F000	474.0	588.0
F000'	474.89	
h, k, lmax	10, 13, 16	10, 13, 16
Nref	4341	4271
Tmin, Tmax	0.604, 0.804	0.604, 0.804
Tmin'	0.592	

Correction method= MULTI-SCAN

Data completeness= 0.984

Theta(max)= 27.460

R(reflections)= 0.0442(3558)

wR2(reflections)= 0.0975(4271)

S = 1.110

Npar= 343

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

PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X) Co1 -- O5 ..	7.49 su
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...	?
PLAT152_ALERT_1_C	Supplied and Calc Volume s.u. Inconsistent	?
PLAT194_ALERT_1_C	Missing _cell_measurement_reflms_used datum	?
PLAT195_ALERT_1_C	Missing _cell_measurement_theta_max datum	?
PLAT196_ALERT_1_C	Missing _cell_measurement_theta_min datum	?

● Alert level G

PLAT066_ALERT_1_G	Predicted and Reported Transmissions Identical .	?
PLAT154_ALERT_1_G	The su's on the Cell Angles are Equal (x 10000)	3000 Deg.
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	12
PLAT199_ALERT_1_G	Check the Reported _cell_measurement_temperature	293 K
PLAT200_ALERT_1_G	Check the Reported _diffrn_ambient_temperature .	293 K
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	6
01	-C01 -01 -C1	2.00 0.00 2.665 1.555 1.555 1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	13
02	-C02 -02 -C1	7.00 0.00 2.675 1.555 1.555 1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	16
04	-C02 -04 -C4	0.00 0.00 2.675 1.555 1.555 1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	29
N1	-C02 -N1 -C9	0.00 0.00 2.675 1.555 1.555 1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	34
N1	-C02 -N1 -C13	0.00 0.00 2.675 1.555 1.555 1.555

0 **ALERT level A** = In general: serious problem

0 **ALERT level B** = Potentially serious problem

6 **ALERT level C** = Check and explain

10 **ALERT level G** = General alerts; check

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

1 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

6 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

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*, 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 19/05/2009; check.def file version of 13/05/2009

