checkCIF/PLATON report (publication check)

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Datablock: ver89

Bond precision: C-C = 0.0027 A Wavelength=0.71073

Cell: a=11.7638(15) b=11.7638(15) c=11.7638(15)
alpha=76.338(2) beta=76.338(2) gamma=76.338(2)

	Calculated	Reported
Volume	1508.8(3)	1508.8(3)
Space group	R -3 r	R-3
Hall group	-P 3*	?
Moiety formula	C33.93 H30 Al N O4	?
Sum formula	C33.93 H30 Al N O4	C34 H36 AL N O4
Mr	542.73	549.62
Dx,g cm-3	1.195	1.210
Z	2	2
Mu (mm-1)	0.104	0.105
F000	571.2	584.0
F000'	571.52	
h,k,lmax	15,15,15	15,15,15
Nref	2517	2434
Tmin,Tmax	0.963,0.969	0.740,1.000
Tmin'	0.959	

Correction method= 'MULTI-SCAN'

Data completeness= Ratio = 0.97 Theta(max)= 28.34

R(reflections)= 0.0528(1988) wR2(reflections)= 0.1513(2434)

S = 1.056 Npar= 156

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

PLAT432_ALERT_2_A Short Inter X...Y Contact C13 .. C14 .. 1.96 Ang.

Author Response: Those atoms belong to disordered by 3-fold axis O=C-Ph moiety

PLAT432_ALERT_2_A Short Inter X...Y Contact C13 .. C15 .. 2.77 Ang.

Author Response: Those atoms belong to disordered by 3-fold axis O=C-Ph moiety

PLAT432_ALERT_2_A Short Inter X...Y Contact C14 .. C14 .. 2.04 Ang.

Author Response: Those atoms belong to disordered by 3-fold axis O=C-Ph moiety

PLAT432_ALERT_2_A Short Inter X...Y Contact C14 .. C14 .. 2.04 Ang.

Author Response: Those atoms belong to disordered by 3-fold axis O=C-Ph moiety

PLAT432_ALERT_2_A Short Inter X...Y Contact C14 .. C15 .. 2.23 Ang.

Author Response: Those atoms belong to disordered by 3-fold axis O=C-Ph moiety

PLAT762_ALERT_1_A CIF Contains no X-Y-H or H-Y-H Angles ..... ?

Author Response: The angles were omitted because of high disorder in a molecule

PLAT773_ALERT_2_A Suspect C-C Bond in CIF: C10 -C11 .. 1.72 Ang.

Author Response: Those atoms belong to disordered by 3-fold axis O=C-Ph moiety

PLAT773_ALERT_2_A Suspect C-C Bond in CIF: C10 -C12A .. 2.00 Ang.

Author Response: Those atoms belong to disordered by 3-fold axis O=C-Ph moiety

PLAT773_ALERT_2_A Suspect C-C Bond in CIF: C11 -C10 .. 1.72 Ang.

Author Response: Those atoms belong to disordered by 3-fold axis O=C-Ph moiety

PLAT773_ALERT_2_A Suspect C-C Bond in CIF: C11 -C12 .. 2.01 Ang.

Author Response: Those atoms belong to disordered by 3-fold axis O=C-Ph moiety

PLAT773_ALERT_2_A Suspect C-C Bond in CIF: C12 -C11 .. 2.01 Ang.

Author Response: Those atoms belong to disordered by 3-fold axis O=C-Ph moiety

PLAT773_ALERT_2_A Suspect C-C Bond in CIF: C13 -C12A .. 1.86 Ang.

Author Response: Those atoms belong to disordered by 3-fold axis O=C-Ph moiety

PLAT773_ALERT_2_A Suspect C-C Bond in CIF: C13 -C14 .. 1.96 Ang.

Author Response: Those atoms belong to disordered by 3-fold axis O=C-Ph moiety

PLAT773_ALERT_2_A Suspect C-C Bond in CIF: C14 -C13 .. 1.96 Ang.

Author Response: Those atoms belong to disordered by 3-fold axis O=C-Ph moiety

PLAT773_ALERT_2_A Suspect C-C Bond in CIF: C12A -C13 .. 1.86 Ang.

Author Response: Those atoms belong to disordered by 3-fold axis O=C-Ph moiety

PLAT773_ALERT_2_A Suspect C-C Bond in CIF: C12A -C10 .. 2.00 Ang.

Author Response: Those atoms belong to disordered by 3-fold axis O=C-Ph moiety

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Alert level B

ABSTM02_ALERT_3_B The ratio of expected to reported Tmax/Tmin(RR') is < 0.75

```
Tmin and Tmax reported:      0.740     1.000
Tmin(prime) and Tmax expected:      0.958     0.969
RR(prime) =      0.748
Please check that your absorption correction is
```

appropriate.

PLAT061_ALERT_3_B Tmax/Tmin Range Test RR' too Large 0.75

PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C10

PLAT432_ALERT_2_B Short Inter X...Y Contact C13 .. C13 .. 3.03 Ang.

Author Response: Those atoms belong to disordered by 3-fold axis O=C-Ph moiety

PLAT432_ALERT_2_B Short Inter X...Y Contact C13 .. C13 .. 3.03 Ang.

Author Response: Those atoms belong to disordered by 3-fold axis O=C-Ph moiety

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Alert level C

CHEMW03_ALERT_2_C The ratio of given/expected molecular weight as calculated from the _atom_site* data lies outside the range 0.99 <> 1.01

```
From the CIF: _cell_formula_units_Z                  2
From the CIF: _chemical_formula_weight          549.62
TEST: Calculate formula weight from _atom_site_*
atom     mass    num     sum
C        12.01   33.93  407.53
H         1.01   30.00   30.24
N        14.01    1.00   14.01
O        16.00    4.00   64.00
Al       26.98    1.00   26.98
Calculated formula weight             542.76
```

HYDTR01_ALERT_1_C The hydrogen treatment should only be one of the following
keywords
* refall
* refxyz
* refU
* noref
* undef
* constr
* none
* mixed
Hydrogen treatment given as const
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low 0.97
PLAT041_ALERT_1_C Calc. and Rep. SumFormula Strings Differ .... ?
PLAT043_ALERT_1_C Check Reported Molecular Weight 549.62
PLAT044_ALERT_1_C Calculated and Reported Dx Differ ..... ?
PLAT048_ALERT_1_C MoietyFormula Not Given ..... ?
PLAT062_ALERT_4_C Rescale T(min) & T(max) by 0.97
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... ?
PLAT120_ALERT_1_C Reported SPGR R-3 Inconsistent with Explicit R-3R
PLAT125_ALERT_4_C No _symmetry_space_group_name_Hall Given ..... ?
PLAT128_ALERT_4_C Non-standard setting of Space group R-3 .... R-3r
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.22 Ratio
PLAT222_ALERT_3_C Large Non-Solvent H Ueq(max)/Ueq(min) ... 3.79 Ratio
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for O2
PLAT301_ALERT_3_C Main Residue Disorder ..... 13.00 Perc.
PLAT391_ALERT_3_C Deviating Methyl C6 H-C-H Bond Angle ..... 101.00 Deg.
PLAT432_ALERT_2_C Short Inter X...Y Contact C12 .. C14 .. 3.19 Ang.

Author Response: Those atoms belong to disordered by 3-fold axis O=C-Ph moiety

PLAT731_ALERT_1_C Bond Calc 1.7449(13), Rep 1.745(3) ..... 2.31 su-Rat
AL1 -O1 1.555 2.555
PLAT731_ALERT_1_C Bond Calc 1.7449(12), Rep 1.745(4) ..... 3.33 su-Rat
AL1 -O1 1.555 3.555
PLAT731_ALERT_1_C Bond Calc 2.099(4), Rep 2.0984(15) ..... 2.67 su-Rat
AL1 -N1 1.555 1.555

PLAT732_ALERT_1_C Angle Calc 109.8(3), Rep 109.76(14) ..... 2.14 su-Rat
C9 -N1 -AL1 1.555 1.555 1.555
PLAT764_ALERT_4_C Overcomplete CIF Bond List Detected (Rep/Expd) . 1.35 Ratio
PLAT779_ALERT_2_C Suspect or Irrelevant (Bond) Angle in CIF ..... 33.00 Deg.
C11 -C10 -C12A 1.555 1.555 3.555
PLAT779_ALERT_2_C Suspect or Irrelevant (Bond) Angle in CIF ..... 43.12 Deg.
C11 -C10 -C12A 3.555 1.555 3.555
PLAT779_ALERT_2_C Suspect or Irrelevant (Bond) Angle in CIF ..... 26.80 Deg.
C12A -C11 -C12 3.555 1.555 1.555
PLAT779_ALERT_2_C Suspect or Irrelevant (Bond) Angle in CIF ..... 43.49 Deg.
C11 -C11 -C12 2.555 1.555 2.555
PLAT779_ALERT_2_C Suspect or Irrelevant (Bond) Angle in CIF ..... 5.60 Deg.
C12A -C11 -C12 1.555 1.555 2.555
PLAT779_ALERT_2_C Suspect or Irrelevant (Bond) Angle in CIF ..... 12.10 Deg.
C12A -C12 -C11 3.555 1.555 3.555
PLAT779_ALERT_2_C Suspect or Irrelevant (Bond) Angle in CIF ..... 41.28 Deg.
C11 -C12 -C11 1.555 1.555 3.555
PLAT779_ALERT_2_C Suspect or Irrelevant (Bond) Angle in CIF ..... 15.51 Deg.
C12 -C13 -C12A 1.555 1.555 3.555
PLAT779_ALERT_2_C Suspect or Irrelevant (Bond) Angle in CIF ..... 27.50 Deg.
C12 -C15 -C12A 2.555 1.555 1.555
PLAT779_ALERT_2_C Suspect or Irrelevant (Bond) Angle in CIF ..... 35.38 Deg.
C12 -C12A -C13 2.555 1.555 2.555
PLAT779_ALERT_2_C Suspect or Irrelevant (Bond) Angle in CIF ..... 37.80 Deg.
C15 -C12A -C13 1.555 1.555 2.555

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C34 H36 Al1 N1 O4
Atom count from the _atom_site data: C33.93 H30 Al1 N1 O4
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_sum C34 H36 Al N O4
TEST: Compare cell contents of formula and atom_site data

atom Z*formula cif sites diff
C 68.00 67.86 0.14

```
          H          72.00      60.00    12.00
          Al          2.00       2.00     0.00
          N           2.00       2.00     0.00
          O           8.00       8.00     0.00
```

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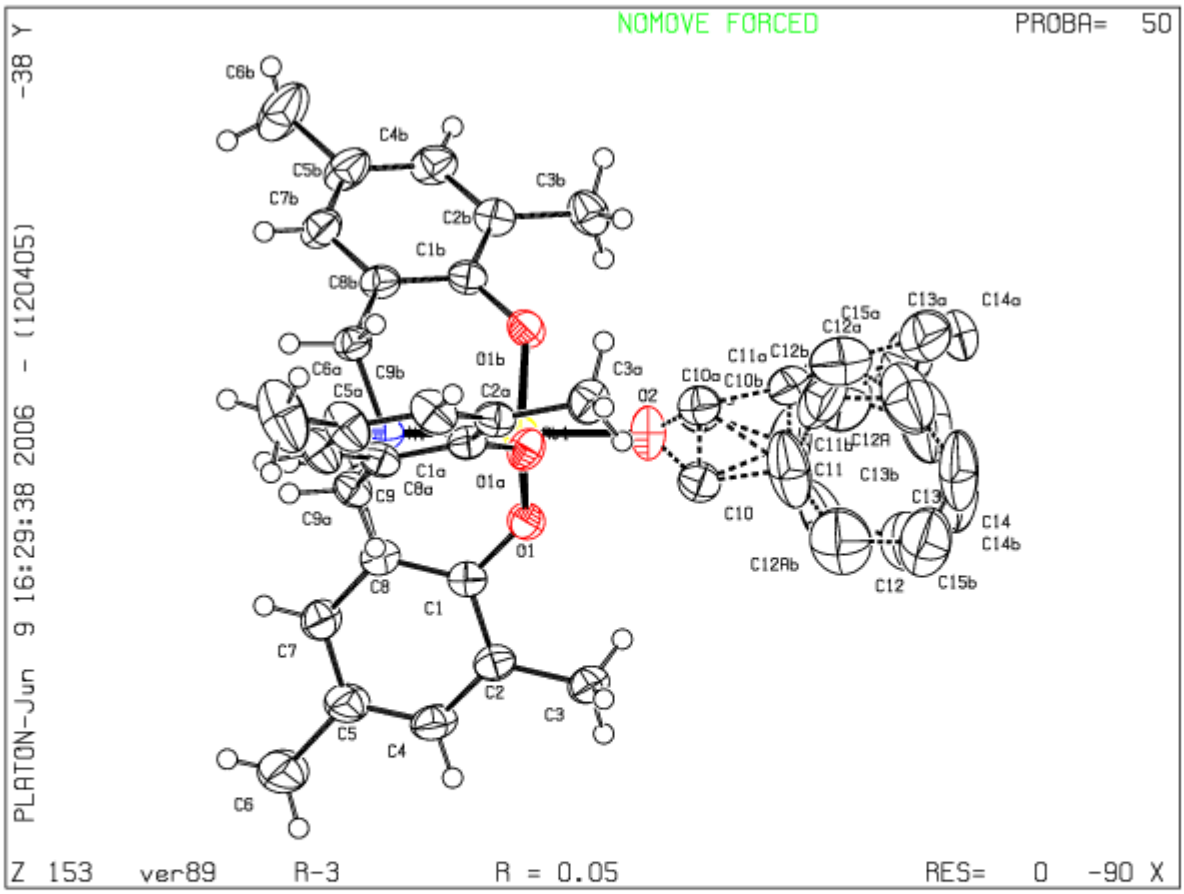
  16 ALERT level A = In general: serious problem
   5 ALERT level B = Potentially serious problem
  34 ALERT level C = Check and explain
   3 ALERT level G = General alerts; check

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

PLATON version of 12/04/2005; check.def file version of 22/03/2005

Datablock ver89 - ellipsoid plot



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