checkCIF/PLATON report

Structure factors have been supplied for datablock(s) kv836_1_kv

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.

No syntax errors found.　　　CIF dictionary　　　Interpreting this report

Datablock: kv836_1_kv

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Bond precision:   C-C = 0.0131 A          Wavelength=0.71073

Cell:          a=13.8130(3)        b=15.0609(3)       c=30.1361(7)
               alpha=94.447(1)   beta=93.223(1)   gamma=94.144(1)
Temperature:   150 K
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	Calculated	Reported
Volume	6222.1(2)	6222.1(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C118.50 H112 Mn6 N22.50 O14 Re1.50), F6 P, 2(Cl0.50), 2(Cl0.2	2(C118.5 H112 Mn6 N22.5 O14 Re1.5), 2(Cl0.25 O0.5), 1.5(Cl), F6
Sum formula	C237 H224 Cl2 F6 Mn12 N45 O30 P Re3	C237 H224 Cl2 F6 Mn12 N45 O30 P Re3
Mr	5616.41	5616.35
Dx,g cm-3	1.499	1.499
Z	1	1
Mu (mm-1)	2.143	2.143
F000	2829.0	2829.0
F000'	2831.33	
h,k,lmax	16,17,35	16,17,35
Nref	22125	22053
Tmin,Tmax	0.773,0.918	0.645,0.745
Tmin'	0.598	

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Correction method= # Reported T Limits: Tmin=0.645 Tmax=0.745
AbsCorr = MULTI-SCAN


Data completeness= 0.997          Theta(max)= 25.083


R(reflections)= 0.0570( 13745)     wR2(reflections)= 0.1331( 22053)


S = 0.978                Npar= 1593
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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
PLAT430_ALERT_2_A Short Inter D...A Contact O1S   .. N815   ..   1.37 Ang.

**Author Response: These atoms are from different parts of disordered CN
ligand and solvent H2O molecule**

Alert level C
PLAT220_ALERT_2_C Non-Solvent Resd 1   C   Ueq(max)/Ueq(min) Range   5.1 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 1   N   Ueq(max)/Ueq(min) Range   5.7 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1   H Uiso(max)/Uiso(min) Range   4.5 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C524 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C619 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C225 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C525 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds .... 0.01309 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......   2.112 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min)   7 Note
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.596   65 Report
PLAT971_ALERT_2_C Check Calcd Residual Density 0.78A From   C813   1.54 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Residual Density on   Re1   1.01 eA-3
PLAT975_ALERT_2_C Check Calcd Residual Density 0.57A From   O2S   0.57 eA-3
PLAT975_ALERT_2_C Check Calcd Residual Density 0.97A From   O2S   0.53 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on   H512   -0.32 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.   0 Note

Alert level G
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   15 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension   2 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   4 Report
PLAT012_ALERT_1_G No   _shelx_res_checksum found in CIF .... Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)   0.001 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records   11 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records   7 Report
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of   P1 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Re2   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N810   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N811   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N812   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N813   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N814   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N815   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N816   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C810   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C811   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C812   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C813   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C814   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C815   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C816   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1   is Constrained at   0.5 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of Cl2      is Constrained at        0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3      is Constrained at        0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1S      is Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2S      is Constrained at         0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1)..           5 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3)..        100 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4)..        100 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5)..        100 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6)..        100 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  7)..        100 % Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....        O1S Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....        O2S Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C326 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C514 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1S    .. C815    ..       2.50 Ang.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         14 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5 Note
          Cl0.25
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         27 Note
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) Still         35 % Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         12 Note
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  1 ALERT level A = Most likely a serious problem - resolve or explain
  0 ALERT level B = A potentially serious problem, consider carefully
 17 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 45 ALERT level G = General information/check it is not something unexpected

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

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