

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) lb202201

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: lb202201

Bond precision:	C-C = 0.0227 Å	Wavelength=0.67012
Cell:	a=25.1985(11)	b=15.1525(7) c=19.7180(9)
	alpha=90	beta=95.339(2) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	7496.1(6)	7496.1(6)
Space group	C 2/m	C 2/m
Hall group	-C 2y	-C 2y
Moiety formula	2(C80), 2(C36 H44 N4 Ni), 2(Dy2 N V), C6 H6, 4(C3 H3) N4 Ni, 3(C6 H6)	2(Dy2 V N C80), 2(C36 H44 N4 Ni), 3(C6 H6)
Sum formula	C250 H106 Dy4 N10 Ni2 V2	C250 H106 Dy4 N10 Ni2 V2
Mr	4118.71	4118.74
Dx, g cm ⁻³	1.825	1.825
Z	2	2
Mu (mm ⁻¹)	2.053	2.095
F000	4084.0	4084.0
F000'	4086.18	
h,k,lmax	30,18,23	30,18,23
Nref	7177	7133
Tmin,Tmax	0.691,0.730	0.502,0.646
Tmin'	0.626	

Correction method= # Reported T Limits: Tmin=0.502 Tmax=0.646
AbsCorr = ?

Data completeness= 0.994 Theta(max)= 23.835

R(reflections)= 0.1348(6094)	wR2(reflections)= 0.3972(7133)
S = 1.066	Npar= 684

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

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Ni1 3.41 eA-3

Author Response: The alert was mainly due to there is q peak that not assigned to any element. However, when observed closely, the electron density appears near to the metal nickel. Thus, such residual density is likely not from unaccounted atom types.

Alert level B

PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25)	0.40	Report
PLAT212_ALERT_2_B ADP of Atom C84 is N.P.D. or (nearly) 2D .		Please Check
PLAT213_ALERT_2_B Atom C21 has ADP max/min Ratio	4.2	oblate
PLAT214_ALERT_2_B Atom C100 (Anion/Solvent) ADP max/min Ratio	5.9	oblate
PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds	0.0227	Ang.
PLAT369_ALERT_2_B Long C(sp2)-C(sp2) Bond C17 - C22 .	1.60	Ang.
PLAT369_ALERT_2_B Long C(sp2)-C(sp2) Bond C26 - C32 .	1.64	Ang.
PLAT939_ALERT_3_B Large Value of Not (SHELXL) Weight Optimized S .	468.77	Check
PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.01Ang From Dy5	2.90	eA-3
PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.22Ang From C5S	2.81	eA-3
PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.20Ang From C7	2.78	eA-3
PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.92Ang From C43	2.71	eA-3
PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.20Ang From C2	2.54	eA-3
PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on Dy1	1.69	eA-3

Author Response: The alert was mainly due to there is q peak that not assigned to any element. However, when observed closely, the electron density appears near to the metal nickel. Thus, such residual density is likely not from unaccounted atom types.

Alert level C

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .	2.01	%
PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given		Please Do !
PLAT082_ALERT_2_C High R1 Value	0.13	Report
PLAT213_ALERT_2_C Atom C6 has ADP max/min Ratio	3.2	oblate
PLAT213_ALERT_2_C Atom C26 has ADP max/min Ratio	3.1	oblate
PLAT213_ALERT_2_C Atom C32 has ADP max/min Ratio	3.2	oblate
PLAT213_ALERT_2_C Atom C34 has ADP max/min Ratio	3.1	oblate
PLAT213_ALERT_2_C Atom C43 has ADP max/min Ratio	3.3	oblate
PLAT221_ALERT_2_C Solv./Anion Resd 3 V Ueq(max)/Ueq(min) Range	4.7	Ratio
PLAT223_ALERT_4_C Solv./Anion Resd 2 H Ueq(max)/Ueq(min) Range	4.3	Ratio
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C100		Check

PLAT244_ALERT_4_C	Low	'Solvent' Ueq as Compared to Neighbors of	N1	Check
PLAT244_ALERT_4_C	Low	'Solvent' Ueq as Compared to Neighbors of	C102	Check
PLAT250_ALERT_2_C	Large	U3/U1 Ratio for Average U(i,j) Tensor	2.5	Note
PLAT369_ALERT_2_C	Long	C(sp2)-C(sp2) Bond C28 - C29 .	1.56	Ang.
PLAT369_ALERT_2_C	Long	C(sp2)-C(sp2) Bond C31 - C37 .	1.54	Ang.
PLAT369_ALERT_2_C	Long	C(sp2)-C(sp2) Bond C36 - C38 .	1.53	Ang.
PLAT369_ALERT_2_C	Long	C(sp2)-C(sp2) Bond C43 - C43_c .	1.55	Ang.
PLAT906_ALERT_3_C	Large	K Value in the Analysis of Variance	4.725	Check
PLAT911_ALERT_3_C	Missing	FCF Refl Between Thmin & STh/L= 0.600	30	Report
PLAT918_ALERT_3_C	Reflection(s)	with I(obs) much Smaller I(calc) .	57	Check
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens. 1.00Ang From C31	2.38	eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens. 0.99Ang From C20	2.33	eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens. 0.95Ang From C30	2.23	eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens. 0.85Ang From C21	1.94	eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens. 1.02Ang From C5	1.86	eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens. 0.32Ang From C5S	1.86	eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens. 0.62Ang From C43	1.78	eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens. 0.89Ang From C11	1.75	eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens. 0.78Ang From C5	1.72	eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens. 1.11Ang From C28	1.67	eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens. 1.00Ang From C9	1.66	eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens. 1.04Ang From C25	1.65	eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens. 0.75Ang From C7	1.61	eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens. 1.22Ang From C27	1.61	eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens. 1.18Ang From C26	1.58	eA-3
PLAT972_ALERT_2_C	Check	Calcd Resid. Dens. 0.37Ang From V2	-2.28	eA-3
PLAT977_ALERT_2_C	Check	Negative Difference Density on H92A .	-0.41	eA-3
PLAT977_ALERT_2_C	Check	Negative Difference Density on H100 .	-0.46	eA-3

Alert level G

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu			
	not performed for this radiation type.			
PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	23	Note	
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	55	Report	
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	451.04	Why ?	
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.67012	Ang.	
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	3	Report	
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report	
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	1	Report	
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	9	Report	
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	2	Report	
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	3	Report	
PLAT300_ALERT_4_G	Atom Site Occupancy of Dy1 Constrained at	0.4276	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Dy2 Constrained at	0.1566	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Dy3 Constrained at	0.1184	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Dy4 Constrained at	0.0543	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Dy5 Constrained at	0.1502	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Dy6 Constrained at	0.0929	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of V1 Constrained at	0.4408	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of V2 Constrained at	0.2796	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of ClS Constrained at	0.5	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of C2S Constrained at	0.5	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of C5S Constrained at	0.5	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of H1S Constrained at	0.5	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of H2S Constrained at	0.5	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of H5S Constrained at	0.5	Check	

PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	77% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100% Note
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C2 -C3_c .	1.45 Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C4 -C7 .	1.43 Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C16 -C18_c .	1.43 Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C19 -C21 .	1.44 Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C20 -C19_c .	1.44 Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C26 -C32 .	1.46 Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C7 -C7_c	0.17 Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C12 -C15	0.22 Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C15 -C12_c	0.22 Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C26 -C32	0.30 Ang.
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C1 Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C13 Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C23 Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C25 Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C24 - C25 .	1.51 Ang.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	37.90 Deg.
	DY2 -N1 -DY5 1_555 1_555 1_555 #	56 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	37.90 Deg.
	DY2 -N1 -DY5 6_565 1_555 6_565 #	58 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	28.00 Deg.
	DY5 -N1 -DY3 1_555 1_555 1_555 #	65 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	28.00 Deg.
	DY5 -N1 -DY3 6_565 1_555 6_565 #	71 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	26.10 Deg.
	DY5 -N1 -DY1 6_565 1_555 6_565 #	92 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	33.00 Deg.
	DY3 -N1 -DY1 6_565 1_555 6_565 #	94 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	36.20 Deg.
	V2 -N1 -DY1 1_555 1_555 6_565 #	96 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	26.10 Deg.
	DY5 -N1 -DY1 1_555 1_555 1_555 #	100 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	33.00 Deg.
	DY3 -N1 -DY1 1_555 1_555 1_555 #	102 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	36.20 Deg.
	V2 -N1 -DY1 6_565 1_555 1_555 #	104 Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Ni1 (II) .	1.97 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	713 Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min) .	1 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	14 Note
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1 Info
PLAT984_ALERT_1_G	The Dy-f' = -0.1397 Deviates from the B&C-Value	-0.1359 Check
PLAT984_ALERT_1_G	The Ni-f' = 0.3450 Deviates from the B&C-Value	0.3430 Check
PLAT985_ALERT_1_G	The Dy-f" = 4.0369 Deviates from the B&C-Value	4.0100 Check
PLAT985_ALERT_1_G	The Ni-f" = 1.0093 Deviates from the B&C-Value	1.0059 Check
PLAT985_ALERT_1_G	The V-f" = 0.4805 Deviates from the B&C-Value	0.4775 Check
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	2 Check

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

10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
62 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
38 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

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.

