ANNEXURE-A

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) BS_RR

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: BS_RR

Bond precision:	C-C = 0.0065 A	Wavelength=0	.71073
Cell:	a=10.240(7) alpha=90		c=13.274(9) gamma=90
Temperature:	100 K	2000 10/ 120 (1)	gannia yo
	Calculated	Reported	
Volume	1101.5(13)	1101.5(12)	
Space group		P 21/n	
Hall group		-P 2yn	
Moiety formula	C14 H28 Cu2 N4 O10) ?	
Sum formula	C14 H28 Cu2 N4 O10	C14 H28 Cu2	N4 010
Mr	539.50	539.48	
Dx,g cm-3	1.627	1.627	
Z	2	2	
Mu (mm-1)	1.987	1.987	
F000	556.0	556.0	
F000′	557.52		
h,k,lmax	12,10,16	12,10,16	
Nref	2179	2038	
Tmin,Tmax	0.543,0.699	0.542,0.697	
Tmin'	0.514		
Correction method= # Reported T Limits: Tmin=0.542 Tmax=0.697 AbsCorr = MULTI-SCAN			
Data completenes	ss= 0.935	Theta(max) = 25.999	
R(reflections)=	0.0453(1240)		R2(reflections)= .0878(2038)
S = 0.852	Npar= 14		/

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 B PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 140 Report 🍛 Alert level C RINTA01_ALERT_3_C The value of Rint is greater than 0.12 Rint given 0.140 PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.1 Ratio PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C4 Check 'MainMol' Ueq as Compared to Neighbors of PLAT242_ALERT_2_C Low C6 Check PLAT245_ALERT_2_C U(iso) H1 Smaller than U(eq) N1 by 0.024 Ang**2 PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.0065 Ang. Alert level G PLAT019_ALERT_1_G _diffrn_measured_fraction_theta_full/*_max < 1.0 0.991 Report PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 0.140 Report

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.19 Ratio PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 2.15 Info (II) . 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 1 Note PLAT963 ALERT 2 G Both SHELXL WEIGHT Parameter Values Zero Please Check PLAT967 ALERT 5 G Note: Two-Theta Cutoff Value in Embedded .res .. 52.0 Degree PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

0 ALERT level A = Most likely a serious problem - resolve or explain 1 ALERT level B = A potentially serious problem, consider carefully 6 ALERT level C = Check. Ensure it is not caused by an omission or oversight 11 ALERT level G = General information/check it is not something unexpected 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data 5 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 2 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

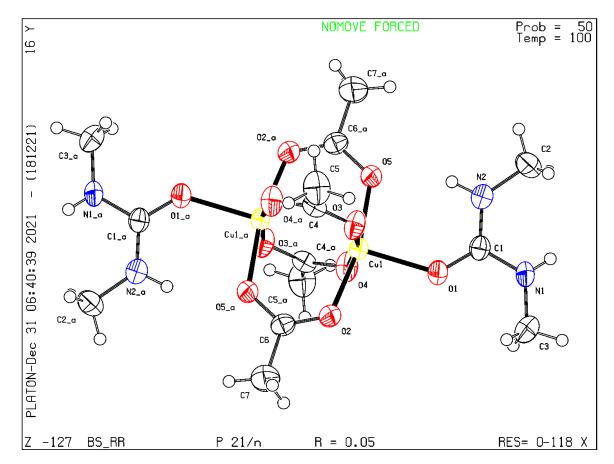
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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.

PLATON version of 18/12/2021; check.def file version of 18/12/2021

Datablock BS_RR - ellipsoid plot



ANNEXURE-B

List of Publications

Journals:

- [1] Saikia, R., Dey Baruah, S., Deka, R. C., Thakur, A. J. and Bora, U. An insight into nitromethane as an organic nitrile alternative source towards the synthesis of aryl nitriles. *European Journal of Organic Chemistry*, 2019(36):6211-6216, 2019.
- [2] Saikia, R., Park, K., Masuda, H., Itoh, M., Yamada, T., Sajiki, H., Mahanta, S. P., Thakur, A. J. and Bora, U. Revisiting the synthesis of aryl nitriles: A pivotal role of CAN. Organic & Biomolecular Chemistry, 19(6):1344-1351, 2021.
- [3] Saikia R., Boruah, P. K., Ahmed, S. M., Das, M. R., Thakur, A. J. and Bora, U. An Avenue to Chan-Lam N-arylation by Cu(0) nanoparticles immobilized graphitic carbon-nitride oxide surface. Applied Catalysis A: General, 643:118767, 2022.
- [4] Sarmah, D., Saikia, R. and Bora, U. An attractive avenue to Chan-Lam cross-coupling: Scope and developments under Ni-catalysis. *Tetrahedron*, 104:132567, 2022.
- [5] Das, S. K., Dewan, A., Deka, P., Saikia, R., Thakuria, S., Deka, R. C., Thakur, A. J. and Bora, U. Biogenic palladium nanostructures for Suzuki-Miyaura and Sonogashira cross-coupling reaction under mild reaction conditions. *Current Research in Green and Sustainable Chemistry*, 5:100301, 2022.

Book Chapter:

[1] Saikia, R. and Saikia, R. A. A study on organic solvents: Its necessity, its impact on the environment and sustainable alternatives, In Narzary, A., Begum, P. and Bhagawati, C., editors, *Environment: Climate Change and Natural Challenges*, Gargaon College Publication Cell & Purbayon Publication, 2021.

List of Conferences

As Abstract

Oral Presentation:

- [1] Saikia R., Baruah, S. D., Thakur, A. J. and Bora U. *Cu(I)-catalyzed synthesis of aryl/heteryl nitriles with nitromethane as the in situ cyanide generating source*. Regional Seminar on Science for Sustainable Development (SSD-2019), Organized by Department of Chemistry, B. Borooah College, Guwahati, 9th January, 2019.
- [2] Saikia, R., Baruah, S. D., Deka, R. C., Thakur, A. J. and Bora, U. Nitromethane as an organic nitrile surrogate towards the synthesis of aryl nitriles. International Conference on Emerging Trends in Chemical Sciences (ETCS 2020), Organized by Department of Chemistry, Gauhati University, Guwahati, 13th-15th February, 2020.

Poster Presentation:

- [1] Saikia, R., Thakur, A. J. and Bora, U. $Cu/g-C_3N_4$ catalyzed Chan-Lam coupling: An expedient, on water approach at room temperature. Frontiers in Chemical Sciences (FICS), Organized by Department of Chemistry, Indian Institute of Technology, Guwahati, 6th-8th December 2018.
- [2] Saikia, R., Thakur, A. J. and Bora, U. An expedient, on water approach to Chan-Lam coupling at room temperature. OrganiX-2018: An International Conference in Chemistry, Organized by Department of Chemical Sciences, Tezpur University, 20th-21st December, 2018.
- [3] Saikia, R., Baruah, S. D., Deka, R. C., Thakur, A. J. and Bora, U. Unwinding the role of nitromethane in the synthesis of aromatic nitriles. First virtual J-NOST symposium; XVI-J-NOST, Organized by Indian Institute of Science, Bangalore, 31st October-1st November, 2020.