Appendix

Annexure A

Check CIF Reports

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

```
Bond precision:   C-C = 0.0034 A          Wavelength=0.71073

Cell:               a=7.383(3)      b=12.408(5)      c=12.784(5)
                    alpha=90        beta=90          gamma=90
Temperature:        100 K

                 Calculated                  Reported
Volume           1171.1(8)                   1171.1(8)
Space group      P 21 21 21                  P 21 21 21
Hall group       P 2ac 2ab                   P 2ac 2ab
Moiety formula   C14 H13 N O2                ?
Sum formula      C14 H13 N O2                C14 H13 N O2
Mr               227.25                      227.25
Dx,g cm-3        1.289                       1.289
Z                4                           4
Mu (mm-1)        0.087                       0.087
F000             480.0                       480.0
F000'            480.22
h,k,lmax         9,16,17                     9,16,17
Nref             2943[ 1702]                 2937
Tmin,Tmax        0.985,0.990
Tmin'            0.984

Correction method= Not given

Data completeness= 1.73/1.00        Theta(max)= 28.416

R(reflections)= 0.0459( 2005)                wR2(reflections)=
                                             0.1243( 2937)
S = 1.012                  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 C

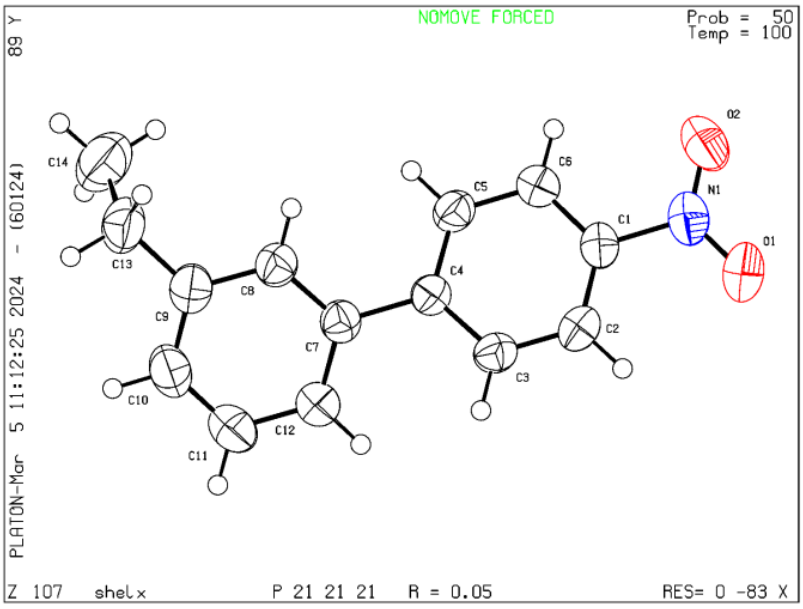
```
STRVA01_ALERT_4_C           Flack test results are meaningless.
          From the CIF: _refine_ls_abs_structure_Flack    0.000
          From the CIF: _refine_ls_abs_structure_Flack_su    2.000
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
             C14 H13 N O2
```

Alert level G

```
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High .      2.000 Report
PLAT850_ALERT_4_G Check Flack Parameter Exact Value 0.00 with s.u.       2.00 Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL     2019/3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          2 Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by .       0.40 Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       3.42 Note
             Predicted wR2: Based on SigI**2  3.63 or SHELX Weight 12.63
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
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 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
1 ALERT type 5 Informative message, check



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: shelx

Bond precision: C-C = 0.0060 A Wavelength=0.71073

Cell: a=33.45(2) b=33.45(2) c=5.541(4)
alpha=90 beta=90 gamma=120
Temperature: 100 K

	Calculated	Reported
Volume	5369(8)	5369(7)
Space group	R -3	R -3 :H
Hall group	-R 3	-R 3
Moiety formula	C12 H11 N O4	?
Sum formula	C12 H11 N O4	C12 H11 N O4
Mr	233.22	233.22
Dx,g cm-3	1.298	1.298
Z	18	18
Mu (mm-1)	0.099	0.099
F000	2196.0	2196.0
F000'	2197.26	
h,k,lmax	41,41,6	41,41,6
Nref	2347	2342
Tmin,Tmax	0.985,0.990	0.527,0.746
Tmin'	0.973	

Correction method= # Reported T Limits: Tmin=0.527 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 25.993

R(reflections)= 0.0781(1481) wR2(reflections)= 0.2473(2342)

S = 1.071 Npar= 159

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

PLAT601_ALERT_2_A Unit Cell Contains Solvent Accessible VOIDS of . 231 Ang**3

Alert level B

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.247
PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 ..... 0.247 Report

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

PLAT031_ALERT_4_C	Refined Extinction Parameter Within Range of ...	3.000 Sigma
PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density	0.75 eA-3
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C9 Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.006 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	5.482 Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	5 Note
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..	1 Check

Alert level G

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	6.25 Why ?
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	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

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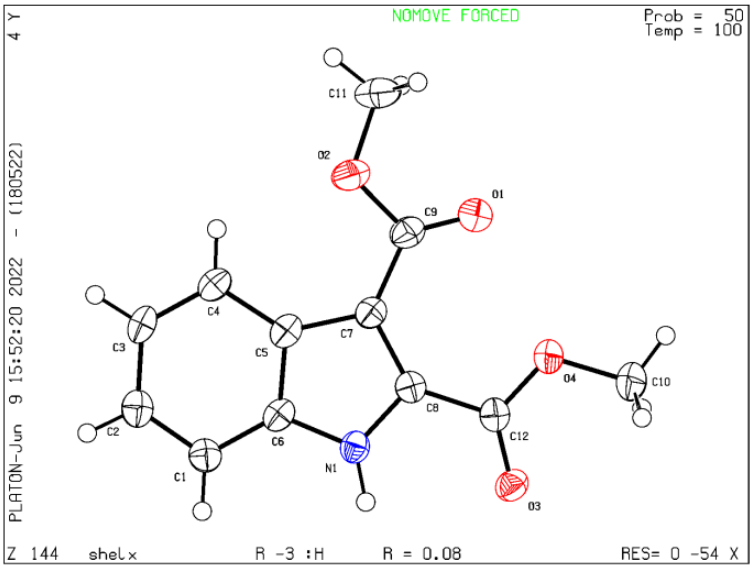

Annexure B

List of Publications

Journal Articles

Included in the thesis

(i) Sarmah, M., **Sarmah, D.,** Dewan, A., Bora, P., Boruah, P. K., Das, M. R., Bharali, P. and Bora, U. Dual Responsive Sustainable Cu_2O/Cu Nanocatalyst for Sonogashira and Chan-Lam Cross-Coupling Reactions. *Catalysis Letters*, *153*(5):1423-1437, 2023.

(ii) **Sarmah, D.**, Choudhury, A., and Bora, U. Palladium nanoparticle catalyzed synthesis of indoles *via* intramolecular Heck cyclisation. *Organic and Biomolecular Chemistry*, 22(31):6419-6431, 2024.

(iii) **Sarmah, D**., Bora, P., Guha, A. K., Gour, N. K., Choudhury, A., and Bora, U. Palladium (II) Catalyzed Synthesis of Meta-Substituted Biphenyls via Carboxylate Directed *Ortho*-Arylation Decarboxylation Cascade: Experimental and Theoretical Insights. *Applied Organometallic Chemistry*, *39*(4):e70066, 2025.

Not included in the thesis

(i) Eldiehy, K. S., Daimary, N., Borah, D., **Sarmah, D.**, Bora, U., Mandal, M., and Deka, D Towards biodiesel sustainability: Waste sweet potato leaves as a green heterogeneous catalyst for biodiesel production using microalgal oil and waste cooking oil. *Industrial Crops and Products*, 187(B): 115467, 2022.

(ii) **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.

(iii) **Sarmah, D.**, Tahu, M., and Bora, U. Recent advances in the synthesis of indoles via C–H activation aided by N–N and N–S cleavage in the directing group. *Applied Organometallic Chemistry*, 35(11): e6390, 2021.

(iv) **Sarmah, D.**, Borah, K. K., and Bora, U. Aqueous extracts of biomass ash as an alternative class of Green Solvents for organic transformations: A review update. *Sustainable Chemistry and Pharmacy*,24:100551, 2021.

(v) **Sarmah, D.**, and Bora, U. Methylene Surrogates for the Synthesis of 3, 3'-Diindolylmethanes. *ChemistrySelect*, 5(28):8577-8603, 2020.

Book Chapters

(i) Saikia, R., **Sarmah, D.**, Dewan, A., Thakur, A. J. and Bora, U. (2022) Nanocellulose: A Biogenic Answer to Sustainable Heterogeneous Catalysis. In Taylor, J. C., editor, *Advances in Chemistry Research,*Nova Science Publishers, 73:189 – 220, 2022.

List of Conferences Attended

(i) **Poster presentation** at National Conference on Sustainability, Medicine and Clean Energy, Organised by the Department of Chemical Sciences, Tezpur University on 1st March 2022. Topic of Presentation: Biogenic Cu_2O/Cu nanomaterial catalysed *N*-arylation of Imidazoles and Benzimidazoles with Arylboronic acids.

(ii) **Poster Presentation** at International Conference on Frontier Areas of Science and Technology, Organised by Indian JSPS alumni association at IIT Guwahati from 9th to 10th September 2024.Topic of Presentation: Pd (II)-PEG System for the synthesis of indoles *via* Intramolecular Heck Cyclisation.

(iii) **Oral Presentation** at National Conference in Recent Development in Science and Technology, organised by the Department of Chemistry, Karimganj College from 17th to 18th February 2024. Topic of Presentation: *N*-arylation of Imidazoles and Benzimidazoles with Arylboronic acids catalyzed by biogenic Cu_2O/Cu nanomaterial.

(iv) **Oral Presentation** at International Conference on Advances and Innovations in Chemical Sciences, organised by the Department of Chemistry. Cotton University from 24th to 25th January 2025. Topic of Presentation: Pd (II)- PEG System for the synthesis of indoles *via* Intramolecular Heck Cyclisation.