Supplementary Material

Synthesis of 2-aroyl-(4 or 5)-aryl-1H-imidazoles and 2-hydroxy-3,6-diaryl-pyrazines via a cascade process

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**Note for NMR spectra:** The NMR signals of some compounds (like 3p) are very weak. The reason is that their solubility in DMSO-\(d_6\) is extremely low, and even lower in other deuterated reagents. The signals of deuterated solvent DMSO-\(d_6\) at \(\delta\) 2.45-2.55 (ppm) in respective \(^1\text{H}-\text{NMR}\) spectrum and at \(\delta\) 39.4-39.6 (ppm) for DMSO-\(d_6\) in respective \(^13\text{C}-\text{NMR}\) spectrum were observed. The signals of water (DMSO-\(d_6\) absorbs water easily) around \(\delta\) 3.33 (ppm) in respective \(^1\text{H}-\text{NMR}\) spectrum were observed. The signals of residual acetone around 2.09 (ppm) in \(^1\text{H}-\text{NMR}\) spectrum and around 30.6 (ppm) in \(^13\text{C}-\text{NMR}\) spectrum were observed in some compounds like 2n and 2n'.

Single-crystal data for compounds 2j (CCDC 920522), 2k (CCDC 873930) and 3p (CCDC 920523) have been deposited in the Cambridge Crystallographic Data Centre. These data can be obtained free of charge via [http://www.ccdc.ac.uk/data_request/cif](http://www.ccdc.ac.uk/data_request/cif).
checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 2j

Bond precision: C-C = 0.0020 A  Wavelength=0.71073

Cell:
   a=7.264(3)  b=8.306(3)  c=21.005(7)
   alpha=90  beta=97.327(4)  gamma=90

Temperature: 133 K

Calculated Reported
Volume 1257.0(8) 1256.9(7)
Space group P 21/c P 21/c
Hall group - P 2ybc ?
Molety formula C14 H10 N4 O, H2 O C14 H12 N4 O2
Sum formula C14 H12 N4 O2 C14 H12 N4 O2
Mr 268.28 268.28
Dx, g cm-3 1.418 1.418
Z 4 4
Mu (mm-1) 0.099 0.099
F000 560.0 560.0
F000’ 560.23
h,k,lmax 9,11,28 9,11,28
Nref 3281 3290
Tmin,Tmax 0.978,0.994 0.947,0.994
Tmin’ 0.946

Correction method: MULTI-SCANS

Data completeness= 0.973  Theta(max)= 29.140
R(reflections)= 0.0545( 3024)  wR2(reflections)= 0.1272( 3290)
S = 0.999  Npar= 193

The following ALERTS were generated. Each ALERT has the format
<test-name>_<alert_type>_<alert-level>.
Click on the hyperlinks for more details of the test.

* Alert level C
ABSTYD_ALERT_1_0: An _exp1_absorプ_m_correction_type has been without
a literature citation. This should be contained in the
_exp1 absorbsorption process details field.
Absorption correction given as Multi-scans
Alert level G

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

Alert type 1 CIF construction/syntax error, inconsistent or missing data
Alert type 2 Indicator that the structure model may be wrong or deficient
Alert type 3 Indicator that the structure quality may be low
Alert type 4 Improvement, methodology, query or suggestion
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, 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 24/04/2013; check.def file version of 23/04/2013
checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 2k

Bond precision: C-C = 0.0030 Å Wavelength=0.71073

Cell:

- a=4.417(3)
- b=25.392(14)
- c=10.491(6)
- alpha=90
- beta=101.058(8)
- gamma=90

Temperature: 153 K

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<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
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</thead>
<tbody>
<tr>
<td>Volume</td>
<td>1154.8(12)</td>
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<tr>
<td>Space group</td>
<td>C c</td>
</tr>
<tr>
<td>Hall group</td>
<td>C -2yc</td>
</tr>
<tr>
<td>Molely formula</td>
<td>C14 H10 N4 O</td>
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<tr>
<td>Mr</td>
<td>250.26</td>
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<tr>
<td>Dx, g cm-3</td>
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<tr>
<td>P000</td>
<td>520.0</td>
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<tr>
<td>P000'</td>
<td>520.19</td>
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<tr>
<td>h,k,lmax</td>
<td>6,34,14</td>
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<tr>
<td>Bref</td>
<td>3123 [1570]</td>
</tr>
<tr>
<td>Tmin, Tmax</td>
<td>0.991,0.997</td>
</tr>
</tbody>
</table>

Correction method: Not given

Data completeness= 1.55/0.78 Theta(max) = 29.160

R(reflections) = 0.0353 (2051) \[\text{wR2(reflections)} = 0.0840 (2435)\]

\[S = 1.001, \text{Npar} = 176\]

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**

STRENGTH ALERT C

- Flack parameter is too small

From the CIF: _refine_ls_abs_structure_Plaekk -1.800

From the CIF: _refine_ls_abs_structure_Plaekk au 1.400
Alert level G

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 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
2 ALERT type 4 Improvement, methodology, query or suggestion
1 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.

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checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

**Datablock: 3p**

- **Bond precision:** C-C = 0.0035 Å
- **Wavelength:** 0.71073 Å

**Cell:**
- \(a=19.908(8)\)
- \(b=10.770(4)\)
- \(c=13.126(5)\)
- \(\alpha=90^\circ\)
- \(\beta=130.374(4)\)
- \(\gamma=90^\circ\)

**Temperature:** 153 K

**Volume:** 2144.1(14) Å³

- **Space group:** C 2/c
- **Hall group:** -C 2yc
- **Moloty formula:** C\(_{10}\) H\(_6\) N\(_4\) O S\(_2\)
- **Sum formula:** C\(_{10}\) H\(_6\) N\(_4\) O S\(_2\)
- **Mr:** 262.33
- **Dx,g cm\(^{-3}\):** 1.625
- **Z:** 8
- **Mu (mm\(^{-1}\):** 0.403
- **F(000):** 1072.0
- **F(000)':** 1074.29
- **h,k,lmax:** 27,14,17
- **Rint:** 0.966, 0.976
- **Tmin, Tmax:** 0.796, 0.974

**Correction method:** MULTI-SCANS

- **Data completeness:** 0.999
- **Theta(max):** 28.990°
- **R(reflections):** 0.0474(2388)
- **wR2(reflections):** 0.1267(2847)
- **S:** 1.002
- **Npar:** 172

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**
  - ABSTY02 ALERT 1 الإسلام An _exptl_absorp_correction_type has been given without a literature citation. This should be contained in the _exptl_absorp_correction_type field.
  - Absorption correction given as Multi-scans
Alert level G

Alert level G Extra text has been found in the _exptl_absorp_correction_type field, which should be only a single keyword. A literature citation should be included in the _exptl_absorp_process_details field.

PLAT03_ALERT_2_G Number of Distance or Angle Restraints on AtSite 6
PLAT05_ALERT_2_G No _lucr_refine_instructions_details in the CIF 7
PLAT06_ALERT_2_G Note: Main Residue Disorder 18 4
PLAT09_ALERT_2_G Number of Unusual/Non-Standard Labels 1
PLAT06_ALERT_2_G No ADDSYM Analysis: Too Many Excluded Atoms 1
PLAT060_ALERT_2_G Note: Number of Least-Squares Restraints 5

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7 ALERT Level G = General information/check it is not something unexpected

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