Supporting information

Synthesis of Cyclopentacarbazolones via Palladium-Catalyzed Annulation of Internal Alkynes

Devanga K. Sreenivas, Jatoth Sandhyarani and Rajagopal Nagarajan

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Table of contents

<table>
<thead>
<tr>
<th>Table of contents</th>
<th>page number</th>
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</thead>
<tbody>
<tr>
<td>1H NMR, 13C NMR, DEPT, LCMS and CHN analysis of all compounds</td>
<td>S2-S112</td>
</tr>
<tr>
<td>2D NOESY of 3r</td>
<td>S96</td>
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<tr>
<td>Check/cif Platron of compounds 3a, 3r, and 3s</td>
<td>S113-S121</td>
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</table>
$^1$H NMR of 5-ethyl-8-methyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
$^{13}$C NMR of 5-ethyl-8-methyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
DEPT of 5-ethyl-8-methyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
LCMS of 5-ethyl-8-methyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
Elemental analysis of 5-ethyl-8-methyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
$^1$H NMR of 5-butyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
$^{13}$C NMR of 5-butyl-2,3-diphenylcyclopenta[b]carbazol-1(5$H$)-one
DEPT of 5-butyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
LCMS of 5-butyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
Elemental analysis of 5-butyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
$^1$H NMR of 8-methyl-5-pentyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
$^{13}$C NMR of 8-methyl-5-pentyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
DEPT of 8-methyl-5-pentyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
LCMS of 8-methyl-5-pentyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
Elemental analysis of 8-methyl-5-pentyl-2,3-diphenylcyclopenta[\textit{b}]carbazol-1(5\textit{H})-one
$^1$H NMR of 5-benzyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
$^{13}$C NMR of 5-benzyl-2,3-diphenylcyclopenta[b]carbazol-1(5$H$)-one
DEPT of 5-benzyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
LCMS of 5-benzyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
Elemental analysis of 5-benzyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
$^1$H NMR of 8-tert-butyl-5-ethyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
$^{13}$C NMR of 8-tert-butyl-5-ethyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
DEPT of 8-tert-butyl-5-ethyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
LCMS of 8-tert-butyl-5-ethyl-2,3-diphenylcyclopenta[\(b\)]carbazol-1(5\(H\))-one
Elemental analysis of 8-tert-butyl-5-ethyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one

FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

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DEPT of 5-ethyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
LCMS of 5-ethyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
Elemental analysis of 5-ethyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one.
$^1$H NMR of 7-bromo-5-butyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
$^{13}$C NMR of 7-bromo-5-butyl-2,3-diphenycyclopenta[b]carbazol-1(5H)-one
DEPT of 7-bromo-5-butyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
LCMS of 7-bromo-5-butyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
Elemental analysis of 7-bromo-5-butyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
$^1$H NMR of 5-ethyl-6,8-dimethyl-2,3-diphenylcyclopenta[b]carbazol-1(5$H$)$-one
$^{13}$C NMR of 5-ethyl-6,8-dimethyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
DEPT of 5-ethyl-6,8-dimethyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
LCMS of 5-ethyl-6,8-dimethyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
Elemental analysis of 5-ethyl-6,8-dimethyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
$^1$H NMR of 5-hexyl-2,3-diphenylcyclopenta[b]carbazol-1(5$H$)-one
$^{13}$C NMR of 5-hexyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
DEPT of 5-hexyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
LCMS of 5-hexyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
Elemental analysis of 5-hexyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
$^1$HNMR of 5-benzyl-8-methyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
$^{13}$C NMR of 5-benzyl-8-methyl-2,3-diphenylcyclopenta[\(b\)]carbazol-1(5\(H\))one
DEPT of 5-benzyl-8-methyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
LC-MS of 5-benzyl-8-methyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
Elemental analysis of 5-benzyl-8-methyl-2,3-diphenylcyclopenta[b]carbazol-1(5H)-one
$^1$H NMR of 2,3-dibutyl-8-methyl-5-pentylcyclopenta[b]carbazol-1(5$H$)-one
$^{13}$CNMR of 2,3-dibutyl-8-methyl-5-pentylcyclopenta[b]carbazol-1(5H)-one
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LCMS of 2,3-dibutyl-8-methyl-5-pentylcyclopenta[b]carbazol-1(5H)-one
Elemental analysis of 2,3-dibutyl-8-methyl-5-pentylcyclopenta[b]carbazol-1(5H)-one
$^1$H NMR of 2,3,5-tributylcyclopenta[b]carbazol-1(5$H$)-one
$^{13}$C NMR of 2,3,5-tributylcyclopenta\([b]\)carbazol-1(5\(H\))-one
DEPT of 2,3,5-tributylylcyclopenta[b]carbazol-1(5H)-one
LCMS of 2,3,5-tributylcyclopenta[b]carbazol-1(5H)-one
Elemental analysis of 2,3,5-tributylcyclopenta[b]carbazol-1(5H)-one
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Elemental analysis of 2,3-dibutyl-8-methyl-5-pentylcyclopenta[b]carbazol-1(5H)-one
$^1$H NMR of 5-benzyl-2,3-dipropylcyclopenta[b]carbazol-1(5H)-one
$^{13}$C NMR of 5-benzyl-2,3-dipropylcyclopenta[b]carbazol-1(5$H$)-one
DEPT of 5-benzyl-2,3-dipropylcyclopenta[b]carbazol-1(5H)-one
LCMS of 5-benzyl-2,3-dipropylcyclopenta[\textit{b}]carbazol-1(5\textit{H})-one
Elemental analysis of 5-benzyl-2,3-dipropylcyclopenta[b]carbazol-1(5H)-one
$^1$HNMR of 5-ethyl-2,3-dip-tolycyclopenta[b]carbazol-1(5\textit{H})-one
$^{13}$C NMR of 5-ethyl-2,3-dip-tolyclopenta[b]carbazol-1(5H)-one
DEPT of 5-ethyl-2,3-dip-tolycyclopenta[\textit{b}]carbazol-1(\textit{5H})-one
LCMS of 5-ethyl-2,3-dip-tolycyclopenta[b]carbazol-1(5H)-one
Elemental analysis of 5-ethyl-2,3-dip-tolycyclopenta[b]carbazol-1(5H)-one
$^{1}$HNMR of 7-bromo-5-butyl-2,3-dip-tolylcyclopenta[b]carbazol-1(5H)-one

![HNMR Spectrogram](image)
$^{13}$CNMR of 7-bromo-5-butyl-2,3-dip-tolylcyclopenta[b]carbazol-1(5H)-one
DEPT of 7-bromo-5-butyl-2,3-dip-tolycyclopenta[b]carbazol-1(5H)-one
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Elemental analysis of 7-bromo-5-butyl-2,3-dip-tolylcyclopenta[b]carbazol-1(5H)-one
$^1$H NMR of 2-(4-chlorophenyl)-5-ethyl-3-phenylcyclopenta[b]carbazol-1(5H)-one
$^{13}$C NMR of 2-(4-chlorophenyl)-5-ethyl-3-phenylcyclopenta[b]carbazol-1(5$H$)-one
DEPT of 2-(4-chlorophenyl)-5-ethyl-3-phenylcyclopenta[b]carbazol-1(5H)-one
LCMS of 2-(4-chlorophenyl)-5-ethyl-3-phenylcyclopenta[b]carbazol-1(5H)-one
Elemental analysis of 2-(4-chlorophenyl)-5-ethyl-3-phenylcyclopenta[b]carbazol-1(5H)-one

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![Chemical structure image]

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Elemental analysis of 3-(4-chlorophenyl)-5-ethyl-2-phenylcyclopenta[b]carbazol-1(5H)-one
$^1$HNMR of 2,5-diethyl-8-methyl-3-phenylcyclopenta[b]carbazol-1(5H)-one
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Elemental analysis of 5-ethyl-2-methyl-3-phenylcyclopenta[\textit{b}]carbazol-1(5\textit{H})-one
Compound 3a

checkCIF/PLATON (standard)

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

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Please wait while processing ....

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Click on the hyperlinks for more details of the test.

Alert level C

THETM01_ALERT_3_C The value of sin(theta_max)/wavelength is less than 0.590

Calculated sin(theta_max)/wavelength = 0.5882

Alert level G
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.

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**PLATON version of 18/07/2011; check.def file version of 04/07/2011**

**Datablock rn63 - ellipsoid plot**
Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Compound 3r

checkCIF/PLATON (standard)

You have not supplied any structure factors. As a result the full set of tests cannot be run.
No syntax errors found. Please wait while processing ....

**Datablock: rn100_m**

**Bond precision:**  
C-C = 0.0028 Å  
Wavelength=0.71073

**Cell:**  
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alpha=76.514(3) beta=78.141(3) gamma=75.769(3)

**Temperature:** 298 K

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EMPIRICAL

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Npar= 256

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 G**

**PLAT005_ALERT_5_G** No _iucr_refine_instructions_details in CIF ....

**PLAT154_ALERT_1_G** The su's on the Cell Angles are Equal ..........  
0.00300 Deg.

0 **Alert level A** = Most likely a serious problem – resolve or explain
0 ALERT level B = A potentially serious problem, consider carefully
0 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
1 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
0 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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Publication of your CIF in other journals

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Datablock rn100_m - ellipsoid plot
Download CIF editor (pubICIF) from the IUCr
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Test a new CIF entry
Compound 3s

**Test a new CIF entry** checkCIF/PLATON (standard)

You have not supplied any structure factors. As a result the full set of tests cannot be run.
No syntax errors found. Please wait while processing ....

**Datablock: rn70**

<table>
<thead>
<tr>
<th>Bond precision:</th>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>C-C = 0.0027 A</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wavelength=0.71073</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Cell:</th>
<th>a=7.9184(6)</th>
<th>b=10.4371(7)</th>
<th>c=12.1136(10)</th>
</tr>
</thead>
<tbody>
<tr>
<td>alpha=76.338(6)</td>
<td>beta=83.212(7)</td>
<td>gamma=77.905(6)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Temperature: 298 K</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Volume</th>
<th>948.72(13)</th>
<th>948.72(12)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Space group</td>
<td>P -1</td>
<td>P -1</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 1</td>
<td>?</td>
</tr>
<tr>
<td>Mr</td>
<td>351.43</td>
<td>351.43</td>
</tr>
<tr>
<td>Dx,g cm-3</td>
<td>1.230</td>
<td>1.230</td>
</tr>
<tr>
<td>Z</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>Mu (mm-1)</td>
<td>0.074</td>
<td>0.074</td>
</tr>
<tr>
<td>F000</td>
<td>372.0</td>
<td>372.0</td>
</tr>
<tr>
<td>F000'</td>
<td>372.14</td>
<td></td>
</tr>
<tr>
<td>h,k,lmax</td>
<td>9,12,14</td>
<td>9,12,14</td>
</tr>
<tr>
<td>Nref</td>
<td>3357</td>
<td>3352</td>
</tr>
<tr>
<td>Tmin,Tmax</td>
<td>0.984,0.991</td>
<td>0.982,0.991</td>
</tr>
<tr>
<td>Tmin'</td>
<td>0.982</td>
<td></td>
</tr>
</tbody>
</table>

Correction method= MULTI-SCAN

<table>
<thead>
<tr>
<th>Data completeness= 0.999</th>
<th>Theta(max)= 25.000</th>
</tr>
</thead>
<tbody>
<tr>
<td>R(reflections)= 0.0462( 2212)</td>
<td>wr2(reflections)= 0.1245( 3352)</td>
</tr>
<tr>
<td>S = 1.046</td>
<td>Npar= 247</td>
</tr>
</tbody>
</table>

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 G**

**PLAT005_ALERT_5_G** No _iucr_refine_instructions_details in CIF ....
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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