Supporting information

Y(OTf)$_3$-Catalyzed Diastereoselective [3+2] Cycloaddition of N-Tosylaziridines and Imines: Efficient Synthesis of Multisubstituted Imidazolidines.

Xingxing Wu$^{[a]}$, Junliang Zhang$^{[a, b]}$

$^a$ Shanghai Key Laboratory of Green Chemistry and Chemical Processes, Department of Chemistry, East China Normal University, 3663 N. Zhongshan Road, Shanghai 200062

$^b$ State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 354 Fenglin Road, Shanghai 200032 (P. R. China)

E-mail: jlzhang@chem.ecnu.edu.cn

Fax: (+86)-021-6223-5039; e-mail: jlzhang@chem.ecnu.edu.cn
Structure of compound 3aa:

Figure 1. ORTEP representation of 3aa.

Table 1. Crystal data and structure refinement for 3aa.

<table>
<thead>
<tr>
<th>Bond precision:</th>
<th>C-C = 0.0049 Å</th>
<th>Wavelength=0.71073</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell:</td>
<td>a=14.7367(4)</td>
<td>b=13.5062(3)</td>
</tr>
<tr>
<td></td>
<td>c=16.6193(4)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>α=90°</td>
<td>β=103.935(1)</td>
</tr>
<tr>
<td></td>
<td>γ=90°</td>
<td></td>
</tr>
<tr>
<td>Temperature</td>
<td>296 K</td>
<td></td>
</tr>
<tr>
<td>Volume</td>
<td>3210.50(14)</td>
<td>3210.50(14)</td>
</tr>
<tr>
<td>Space group</td>
<td>P 21/n</td>
<td>P 21/n</td>
</tr>
<tr>
<td>Hall group</td>
<td>Z=1</td>
<td>Z=1</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C33 H30 Br Cl N2 O6 S</td>
<td>?</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C33 H30 Br Cl N2 O6 S</td>
<td>C33 H30 Br Cl N2 O6 S</td>
</tr>
<tr>
<td>Mr</td>
<td>698.01</td>
<td>698.01</td>
</tr>
<tr>
<td>D, g cm⁻³</td>
<td>1.444</td>
<td>1.444</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>Mu (mm⁻¹)</td>
<td>1.475</td>
<td>1.475</td>
</tr>
<tr>
<td>F000</td>
<td>1432.0</td>
<td>1432.0</td>
</tr>
<tr>
<td>F000'</td>
<td>1432.52</td>
<td></td>
</tr>
<tr>
<td>h,k,lmax</td>
<td>17,16,19</td>
<td>17,16,19</td>
</tr>
<tr>
<td>Nref</td>
<td>5665</td>
<td>5665</td>
</tr>
<tr>
<td>Tmin,Tmax</td>
<td>0.338,0.681</td>
<td>0.338,0.700</td>
</tr>
<tr>
<td>Correction method</td>
<td>MULTI-SOFT</td>
<td></td>
</tr>
<tr>
<td>Data completeness</td>
<td>0.998</td>
<td>θ-max=25.010</td>
</tr>
<tr>
<td>R(reflections)</td>
<td>0.0457(3886)</td>
<td>wR2(reflections)=0.1100(5656)</td>
</tr>
<tr>
<td>S = 1.025</td>
<td>Npar=39</td>
<td></td>
</tr>
</tbody>
</table>
$\text{Br} \quad \text{Ts} \quad \text{CO}_2\text{Me} \quad \text{CO}_2\text{Me}$

$\text{Bn} \quad \text{N}$

$\text{Cl}$

3aa
### 166 2-140DH75250830

<table>
<thead>
<tr>
<th>序号</th>
<th>保留时间 (min)</th>
<th>峰名称</th>
<th>峰高 (mAU)</th>
<th>峰面积 (mAU*min)</th>
<th>相对峰面积 (%)</th>
<th>样品量</th>
<th>类型</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>13.25</td>
<td>n.a.</td>
<td>69.104</td>
<td>65.798</td>
<td>49.62</td>
<td>n.a.</td>
<td>BMb</td>
</tr>
<tr>
<td>2</td>
<td>16.13</td>
<td>n.a.</td>
<td>41.516</td>
<td>66.803</td>
<td>50.38</td>
<td>n.a.</td>
<td>bMB</td>
</tr>
<tr>
<td>总和</td>
<td></td>
<td></td>
<td>110.620</td>
<td>132.601</td>
<td>100.00</td>
<td>0.000</td>
<td></td>
</tr>
</tbody>
</table>

- **样品名**: 2-140DH75250830
- **进样量**: 20.0
- **瓶序号**: 264
- **波长**: 254
- **通道**: UV_VIS_1
- **控制程序**: 程序文件-公用-08
- **定量方法**: 方法-公用
- **记录时间**: 2012-2-6 21:53
- **样品重量**: 1.0000
- **运行时间 (min)**: 25.81

![UV_VIS_1 Waveform](attachment:image.png)

- **WVL**: 254 nm
- **Racemic 3ac**
### 样品信息

<table>
<thead>
<tr>
<th>样品名</th>
<th>7-1-01DH75250830</th>
<th>进样量 (μL)</th>
<th>20.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>通道</td>
<td>UV_VIS_1</td>
<td>压纸:</td>
<td>UV_VIS_1</td>
</tr>
<tr>
<td>波长</td>
<td>254</td>
<td>带宽:</td>
<td>n.a.</td>
</tr>
<tr>
<td>定量方法</td>
<td>方法-公用</td>
<td>稀释因子:</td>
<td>1.0000</td>
</tr>
<tr>
<td>记录时间</td>
<td>2012-2-6 22:20</td>
<td>样品重量:</td>
<td>1.0000</td>
</tr>
<tr>
<td>运行时间 (min)</td>
<td>29.59</td>
<td>样品量:</td>
<td>1.0000</td>
</tr>
</tbody>
</table>

### 色谱图

- **保留时间 (min):** 13.09, 16.19
- **峰名称:** BMb
- **波长:** 254 nm
- **积分:**
  - 峰高 (mAU): 123.628, 27.919
  - 峰面积 (mAU*min): 117.166, 40.105
  - 相对峰面积 (%): 74.50, 25.50
  - 样品量 (μL): n.a., n.a.

### 总和:

- 峰高 (mAU): **151.548**
- 峰面积 (mAU*min): **157.270**
- 相对峰面积 (%): **100.00**
- 样品量 (μL): **0.000**

### 峰信息

<table>
<thead>
<tr>
<th>序号</th>
<th>保留时间 (min)</th>
<th>峰名称</th>
<th>峰高 (mAU)</th>
<th>峰面积 (mAU*min)</th>
<th>相对峰面积 (%)</th>
<th>样品量 (μL)</th>
<th>类型</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>13.09</td>
<td>n.a.</td>
<td>123.628</td>
<td>117.166</td>
<td>74.50</td>
<td>n.a.</td>
<td>BMb</td>
</tr>
<tr>
<td>2</td>
<td>16.19</td>
<td>n.a.</td>
<td>27.919</td>
<td>40.105</td>
<td>25.50</td>
<td>n.a.</td>
<td>bMB</td>
</tr>
<tr>
<td>总和</td>
<td></td>
<td></td>
<td><strong>151.548</strong></td>
<td><strong>157.270</strong></td>
<td><strong>100.00</strong></td>
<td><strong>0.000</strong></td>
<td></td>
</tr>
</tbody>
</table>
Br

Br

3ad

Br

N

Ts

CO₂Me

CO₂Me

F

N

BnN

1.07

7.28

4.06

2.11

1.00

3.04

3.07

1.01

1.00

3.05

ppm
trans-3ak
<table>
<thead>
<tr>
<th>Protons</th>
<th>ppm</th>
</tr>
</thead>
<tbody>
<tr>
<td>200</td>
<td>180</td>
</tr>
<tr>
<td>160</td>
<td>140</td>
</tr>
<tr>
<td>120</td>
<td>100</td>
</tr>
</tbody>
</table>

**Diagram:**

[Chemical structure image]

**Legend:**

- **3ca:** Compound Identifier

**Note:**

- ppm values for specific protons are marked in the diagram.

**Additional Details:**

- The structure includes elements such as F, Ts, CO₂Me, Bn, and Cl.

**Analysis:**

- The data indicates the presence of multiple functional groups and atoms with specific ppm values.

**Image Description:**

- The image contains a detailed chemical structure with annotated ppm values.

**Context:**

- The data is likely from a spectroscopic analysis, possibly an NMR spectrum, given the ppm scale and the structure's complexity.
wux−3−4C

Me

Ts

Bn

CO₂Me

CO₂Me

3ea

Cl