Phosphanegold(I) Thiolates: Intramolecular Au···O vs Au···π Interactions

Chien Ing YEO
Research Centre for Crystalline Materials
Faculty of Science and Technology
Sunway University (Kuala Lumpur)

Gold

?????
You

Gold

Jewelry?
Investment?
Drugs?

Gold

Phosphanegold(I) thiolates:

- Au···π Interactions
- Au···O Interactions

Auranofin

- Treatment of rheumatoid arthritis

Thiocarbamides
Phosphanegold(I) Thiolates

Thiocarbamides

<table>
<thead>
<tr>
<th>Bond</th>
<th>Bond length (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C = S</td>
<td>1.6679 (19)</td>
</tr>
<tr>
<td>C – N</td>
<td>1.337 (2)</td>
</tr>
</tbody>
</table>

Phosphanegold(I) Thiolates

<table>
<thead>
<tr>
<th>Bond</th>
<th>Bond length (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Au – P</td>
<td>2.2561 (7)</td>
</tr>
<tr>
<td>Au – S</td>
<td>2.3171 (7)</td>
</tr>
<tr>
<td>C – S</td>
<td>1.776 (3)</td>
</tr>
<tr>
<td>C = N</td>
<td>1.269 (4)</td>
</tr>
</tbody>
</table>

Phosphanegold(I) Thiolates

Au…O

P1-Au-S1 ~175°
Ph$_3$PAu[SC(OEt)=NPh]: Au…O vs Au…π

Dichloromethane/Methanol

Chloroform

Au…O vs Au…π

At rotation angles = 0 and 360° about the C-S bond, the conformation features an intramolecular Au…π(aryl) interaction while that at 180° has an Au…O interaction.

Binuclear Phosphanegold(I) Thiolates

R = Et, Ph and Cy
Binuclear Phosphanegold(I) Thiolates

**Summary**

- Au...O interactions predominate in mononuclear phosphanegold(I) thiolates, Au...π Interactions are however more stable!
- Au...π Interactions impart higher stability to binuclear phosphanegold(I) thiolates

**Binuclear Phosphanegold(I) Thiolates**

- **Au...π wins!**
- **Au...π and Au...O**
- **Au...O**

**One Au...π and one Au...O interactions >** Two Au...π interactions >

- 12.2 kcal mol⁻¹
- 23.6 kcal mol⁻¹

Two Au...O interactions
Acknowledgement

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