



# Mercury

01 基础操作

02 画透明背景与带景深图

03 画文献中晶体图

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The screenshot displays the CSD Python API software interface. The main window shows a black area with the text "No coordinates available" in yellow. The interface includes a menu bar with options like File, Edit, Selection, Display, Calculate, CSD-Community, CSD-Core, CSD-Materials, CSD-Discovery, CSD Python API, and Help. Below the menu bar is a toolbar with various icons and dropdown menus. The "Display Options" panel at the bottom left contains checkboxes for "Packing", "Asymmetric Unit", "Auto centre", "Short Contact", "H-Bond", "Show hydrogens", "Show cell axes", "Label atoms", "Depth cue", "Z-Clipping", and "Stereo". The "Structure Navigator" panel on the right shows a tree view of databases and structures.

File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API Help

Picking Mode: Pick Atoms Clear Measurements Show Labels for All atoms with Atom Label

Style: Ellipsoid Colour: by Element Manage Styles... Work Atom selections: Select by SMARTS:[c]

Animate... Default view: b a b c a\* b\* c\* x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90 ← → ↓ ↑ zoom- zoom+

No coordinates available

Display Options

Display

Packing  Short Contact < (sum of vdW radii) Contacts...

Asymmetric Unit  H-Bond Default definition More Info

Auto centre Reset Powder...

Options

Show hydrogens  Depth cue

Show cell axes  Z-Clipping

Label atoms  Stereo

Structure Navigator

Databases Find

Crystal Structures Spacegroup

Databases

Structures

Refcode Lists

ConQuest Hits

Mercury Files

Tree View

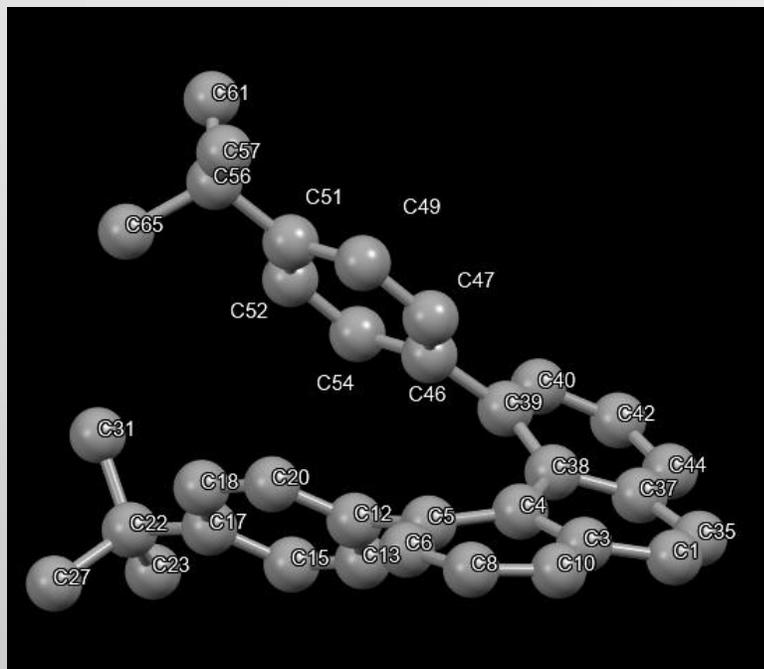
Multiple Structures

Structures...

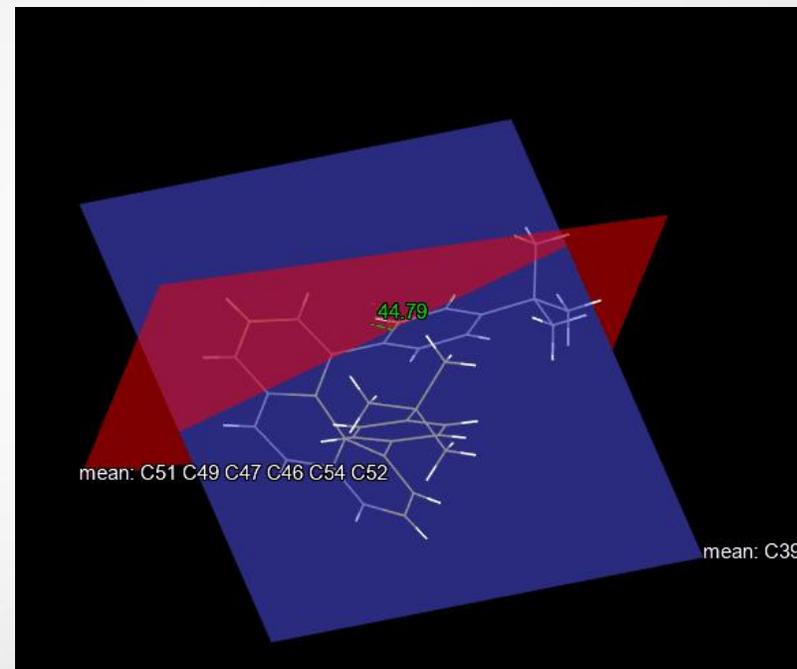
Structure Navigator Searches

Select 'Open' from the File menu to read a structure file or database

## 1.1 原子标签位置设置

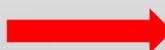


## 1.2 二面角



本公众号(Tokyo)全文链接  
mp.weixin.qq.com

[https://mp.weixin.qq.com/s/li2glrEdSC\\_IrLdpxb3mfw](https://mp.weixin.qq.com/s/li2glrEdSC_IrLdpxb3mfw)

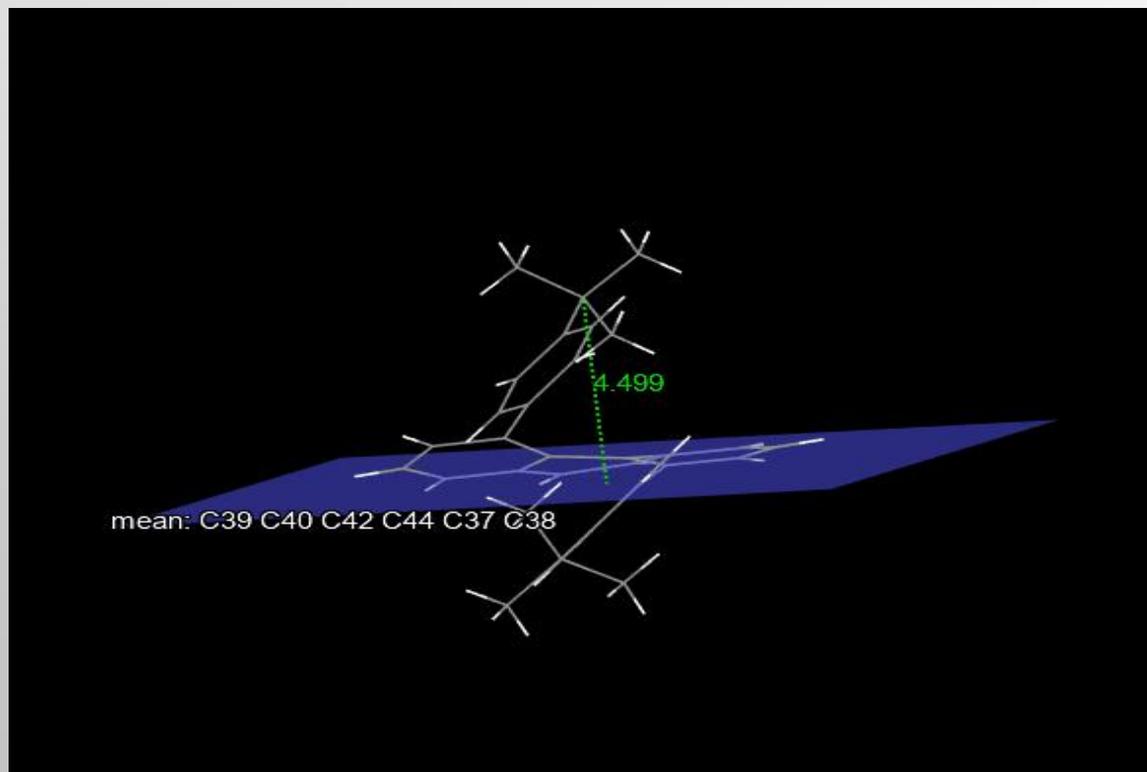


**Mercury**

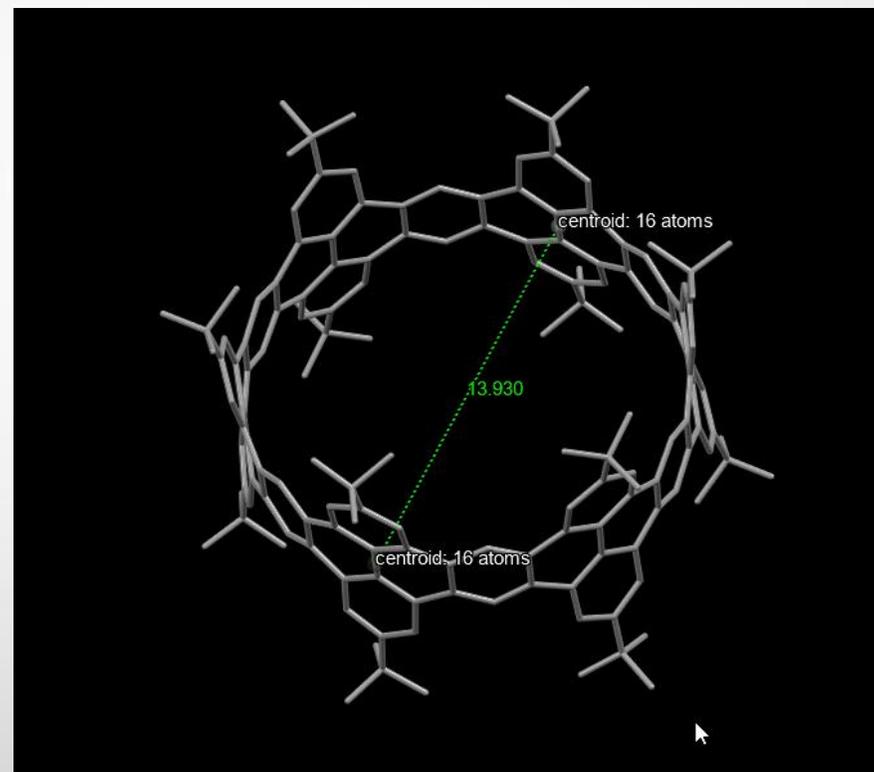
1. Mercury的下载与安装
2. Mercury中原子标签位置设置
3. 使用Mercury计算二面角及点面距离操作步骤
4. Mercury中如何绘制无序组分

公众号文章链接[https://mp.weixin.qq.com/s/li2glrEdSC\\_IrLdpxb3mfw](https://mp.weixin.qq.com/s/li2glrEdSC_IrLdpxb3mfw)

### 1.3 点到面的距离

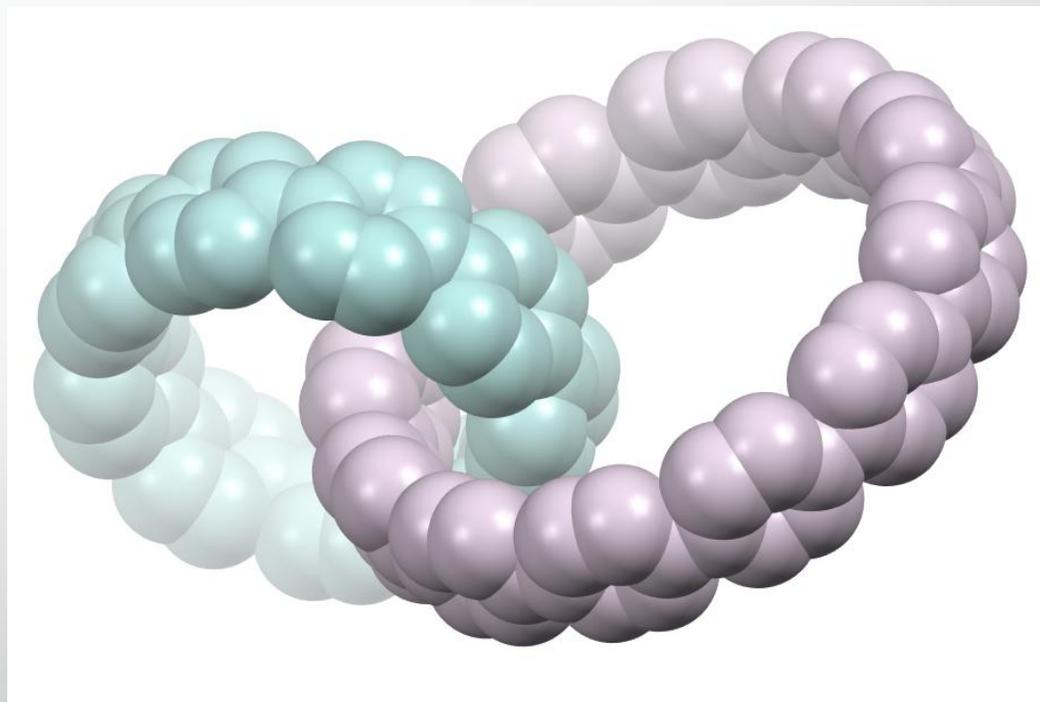
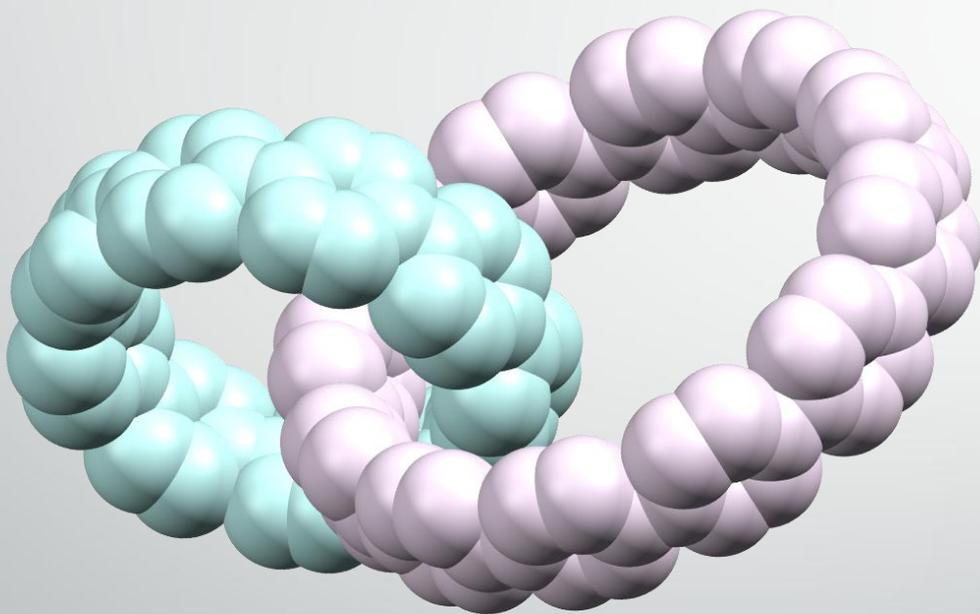


### 1.4 面到面的距离

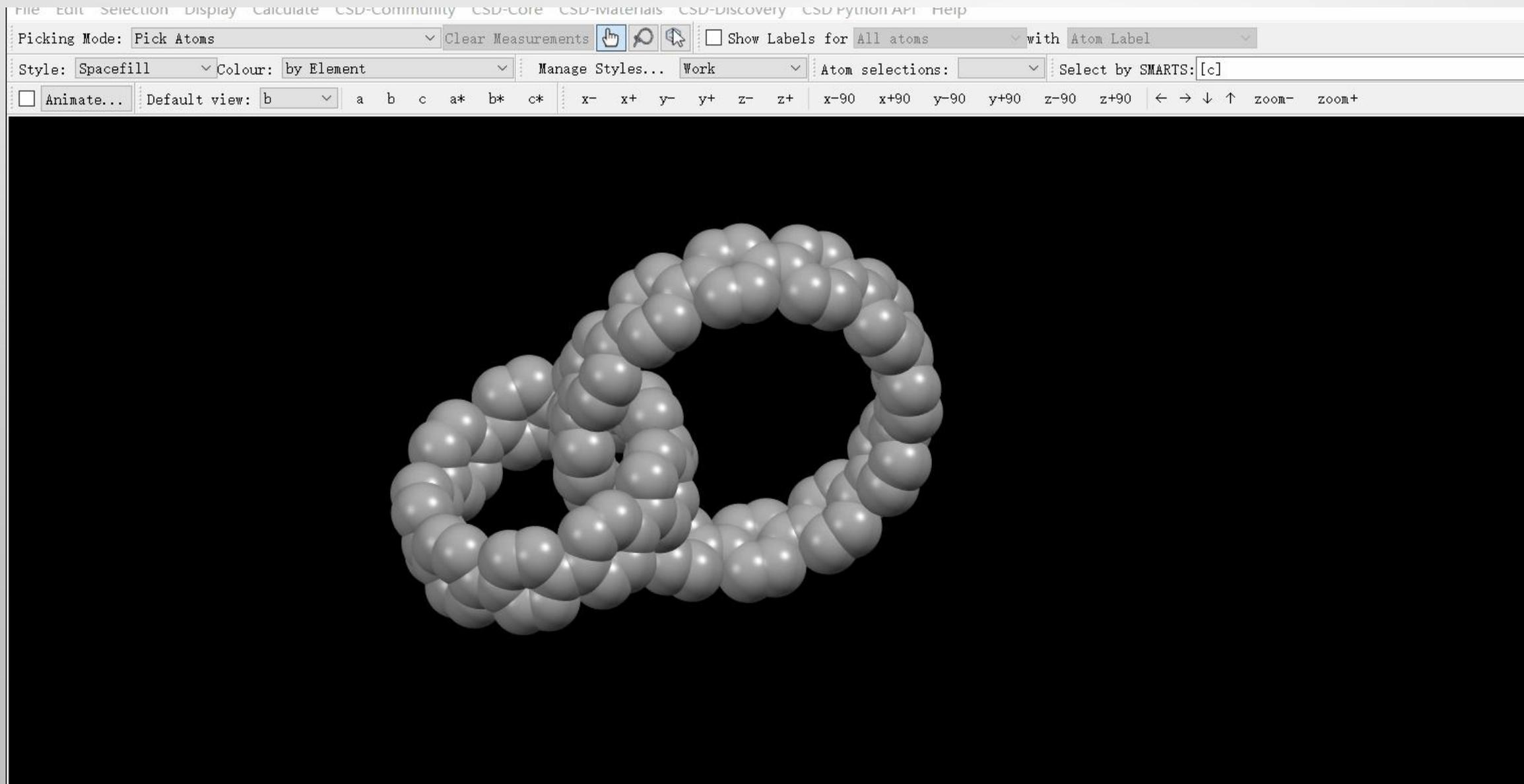


02

## 画透明背景与景深图



## 2.1 打开File找到POV-Ray Image选项,在这里面可以设置透明背景, 同时也能通过material properties变换不同风格



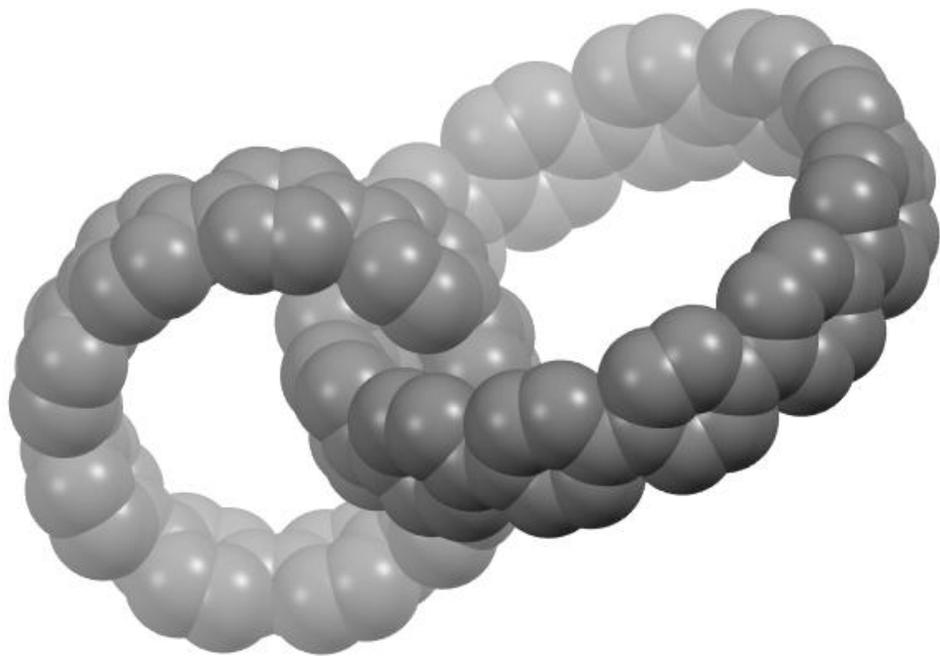
## 2.2 打开Display找到Display Options选项，可以从中获得不同景深的图片

File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API Help

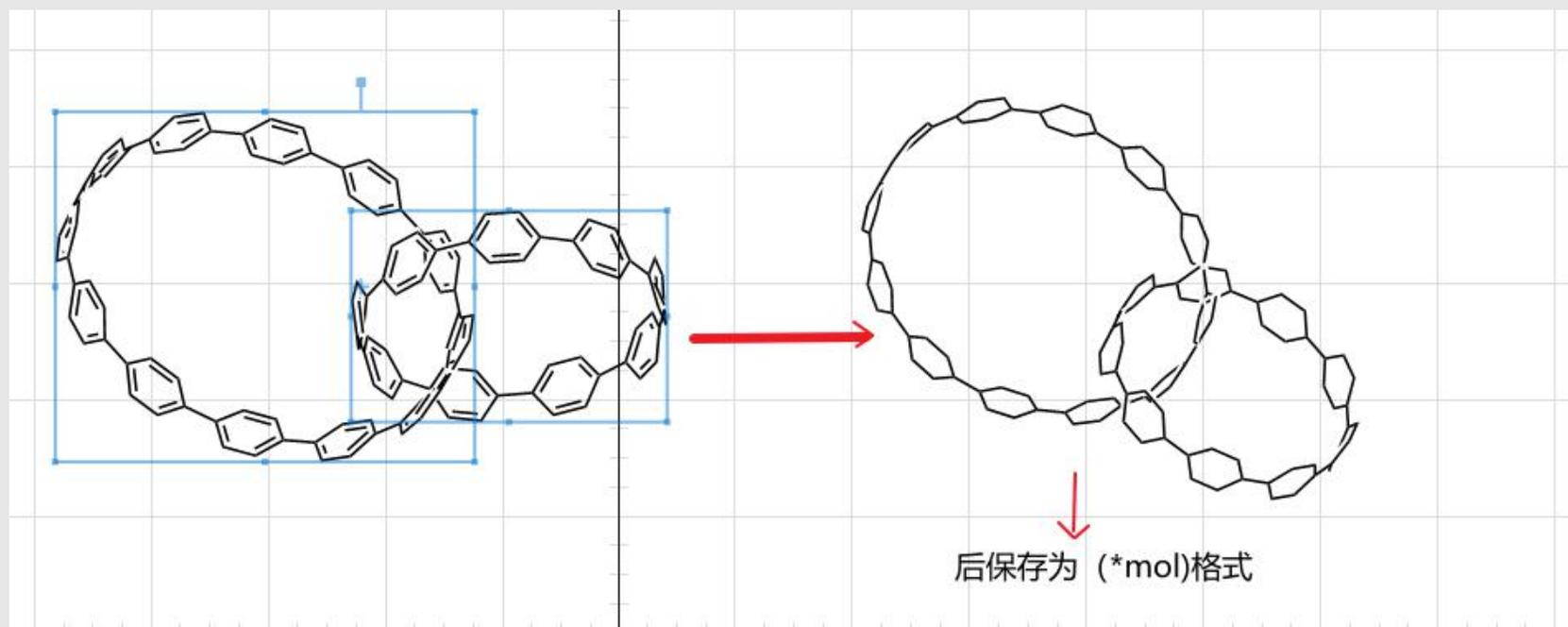
Picking Mode: Pick Atoms Clear Measurements     Show Labels for All atoms with Atom Label

Style: Spacefill Colour: by Element Manage Styles... 3D Print Atom selections: Select by SMARTS: [c]

Animate... Default view: b a b c a\* b\* c\* x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90 ← → ↓ ↑ zoom- zoom+

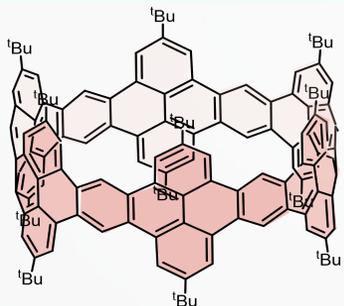


注意：用Mercury画分子图时，有时我们需要把原来在chemdraw中得到的优化图（cdx格式）稍作处理，如当我们选用capped sticks格式时，为了图片更为美观简洁要把分子中的双键修成单键，并保存为\*.mol格式，后在Mercury中打开。



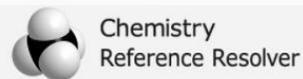
03

## 画文献中晶体图



锁定晶体分子

找文献



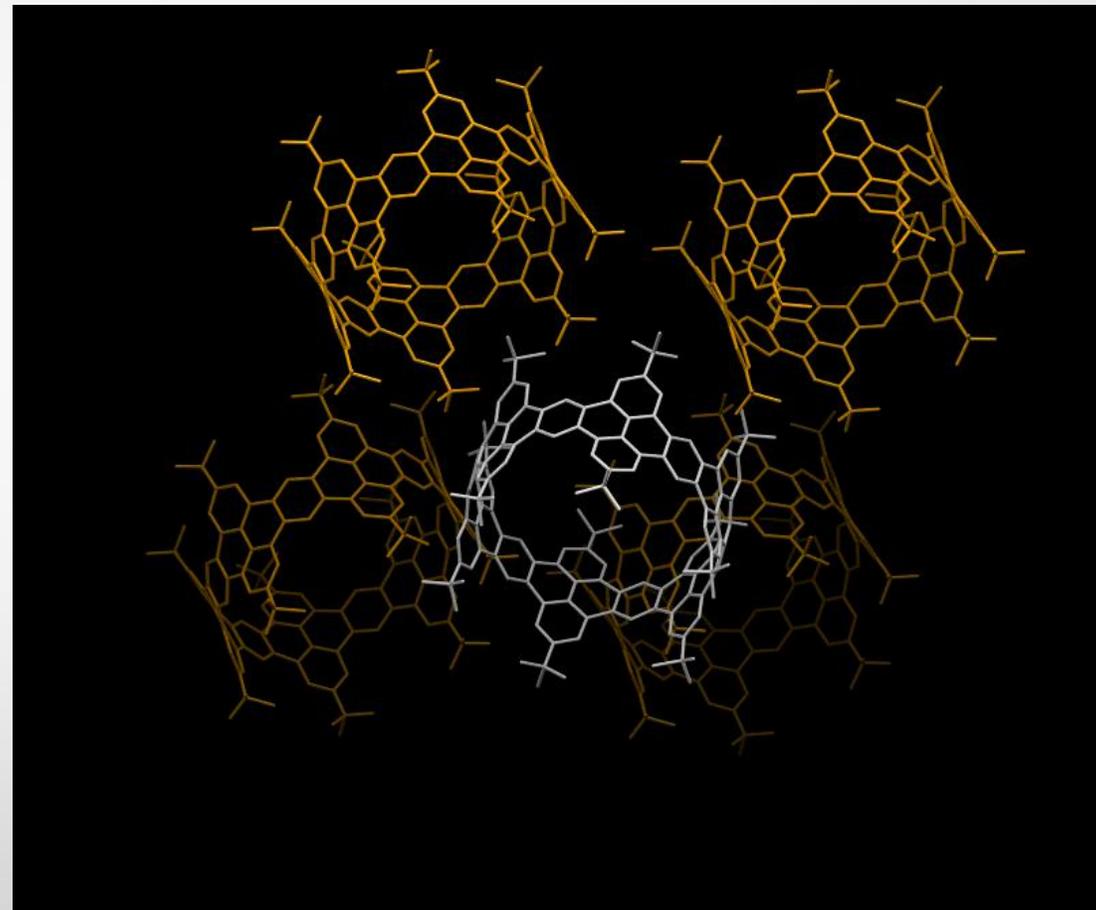
SCI-HUB

下载为cif格式

41557\_2020\_627\_MOESM30\_ESM.cif

找晶体支撑材料

流程：在Mercury中打开cif格式文件,删去多余的溶剂分子，对照文献所示晶体，改变晶体分子的风格及其颜色，选好展示角度，保存图片。



## 3.1 视频

The screenshot shows a software interface with a menu bar at the top: File, Edit, Selection, Display, Calculate, CSD-Community, CSD-Core, CSD-Materials, CSD-Discovery, CSD-Python API, Help. Below the menu bar is a toolbar with various icons and dropdown menus. The main display area is black and contains the text "No coordinates available" in yellow. At the bottom, there is a "Display Options" panel with several sections: "Display" with checkboxes for Packing, Asymmetric Unit, Auto centre, Short Contact, and H-Bond; "Options" with checkboxes for Show hydrogens, Show cell axes, Label atoms, Depth cue, Z-Clipping, and Stereo; and buttons for Contacts..., More Info, and Powder... A status bar at the very bottom reads "Select 'Open' from the File menu to read a structure file or database."

File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD-Python API Help

Picking Mode: Pick Atoms Clear Measurements Show Labels for All atoms with Atom Label

Style: Capped Sticks Colour: by Element Manage Styles... Work Atom selections: Select by SMARTS: [c]

Animate... Default view: b a b c a\* b\* c\* x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90 ← → ↓ ↑ zoom- zoom+

No coordinates available

Display Options

Display

Packing  Short Contact < (sum of vdW radii)  Asymmetric Unit  H-Bond Default definition  Auto centre

Reset

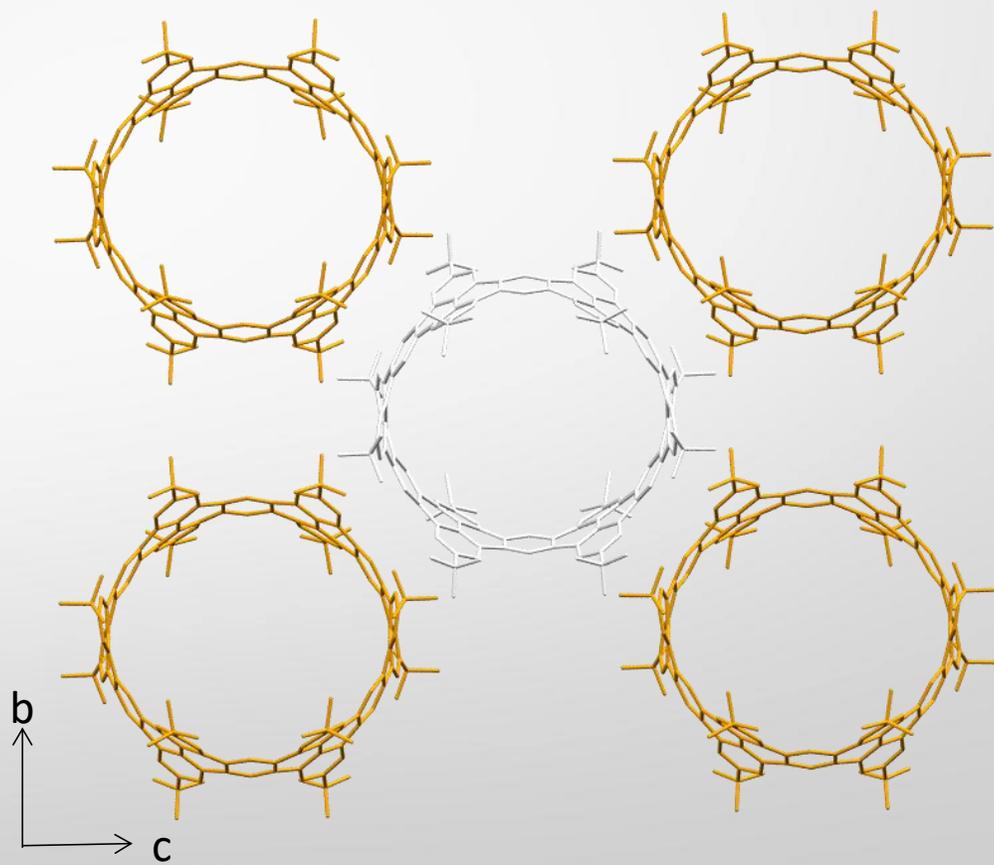
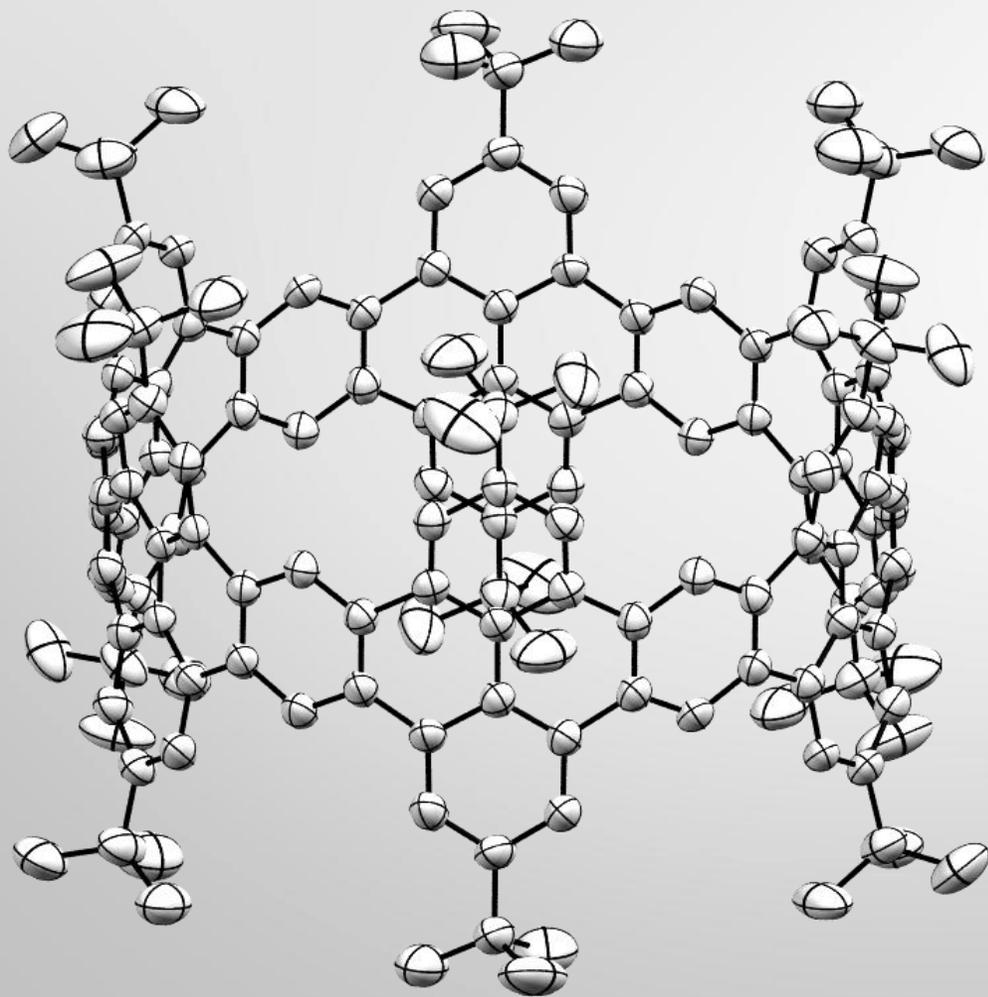
Options

Show hydrogens  Depth cue  Show cell axes  Z-Clipping  Label atoms  Stereo

Contacts... More Info Powder...

Select 'Open' from the File menu to read a structure file or database.

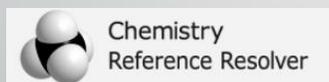
### 3.2 例图



## 文献检索与下载



<https://cn.bing.com/?ensearch=1&FORM=BEHPTB>



<https://chemsearch.kovsky.net/>



<https://sci-hub.se/> 当所需文献没下载版权时，输入DOI号查找下载