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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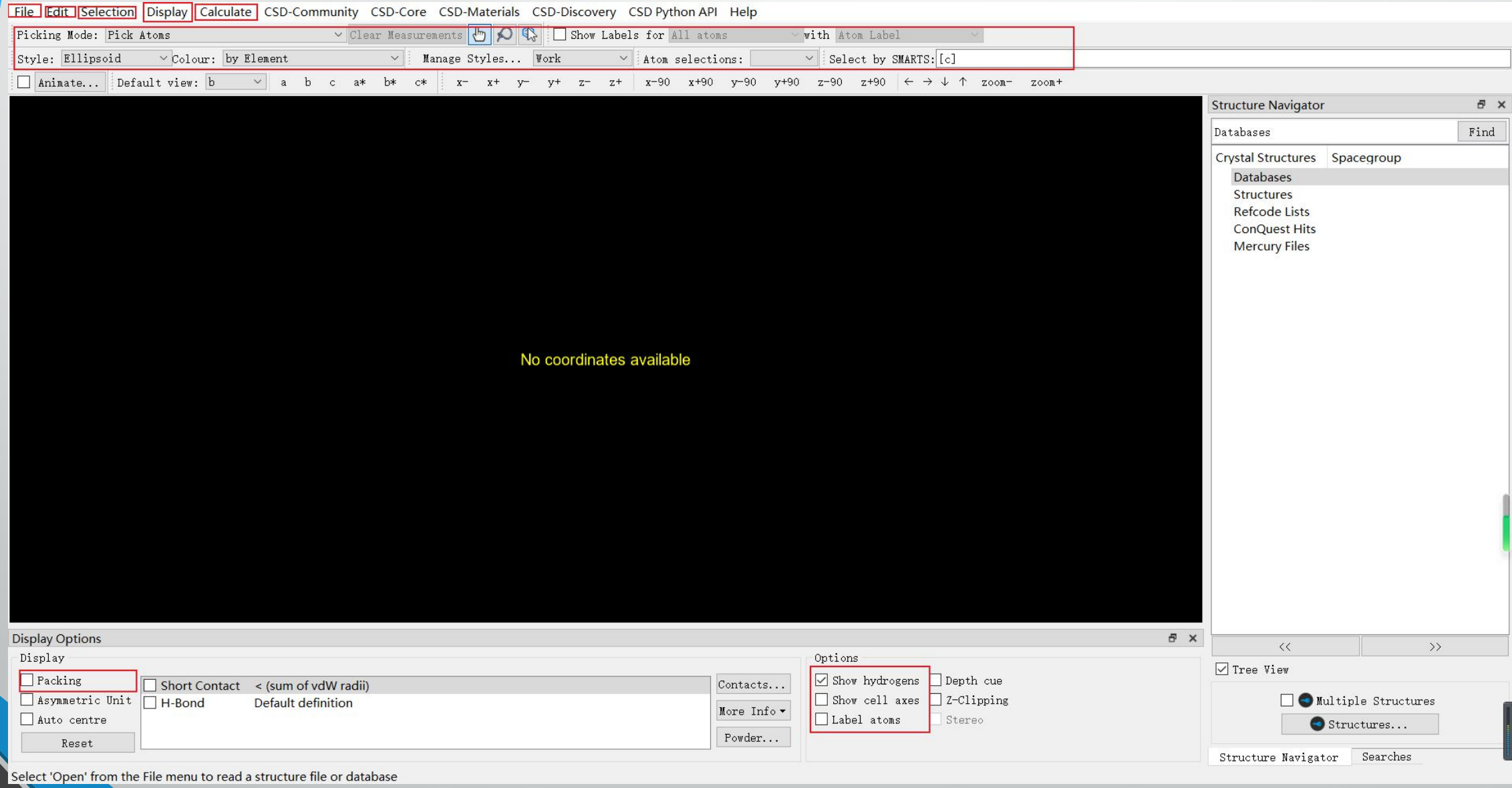
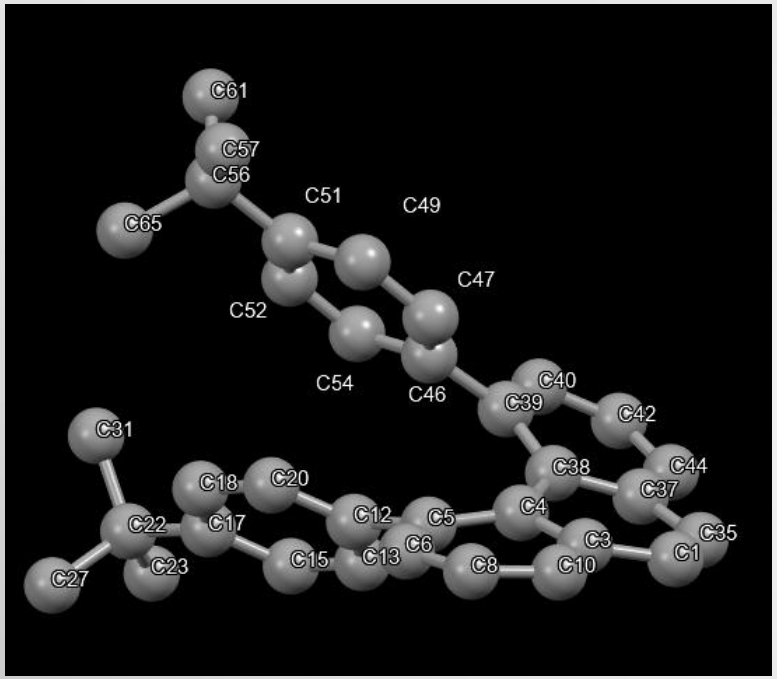
指导老师：李远明 教授
日　　期：20210919

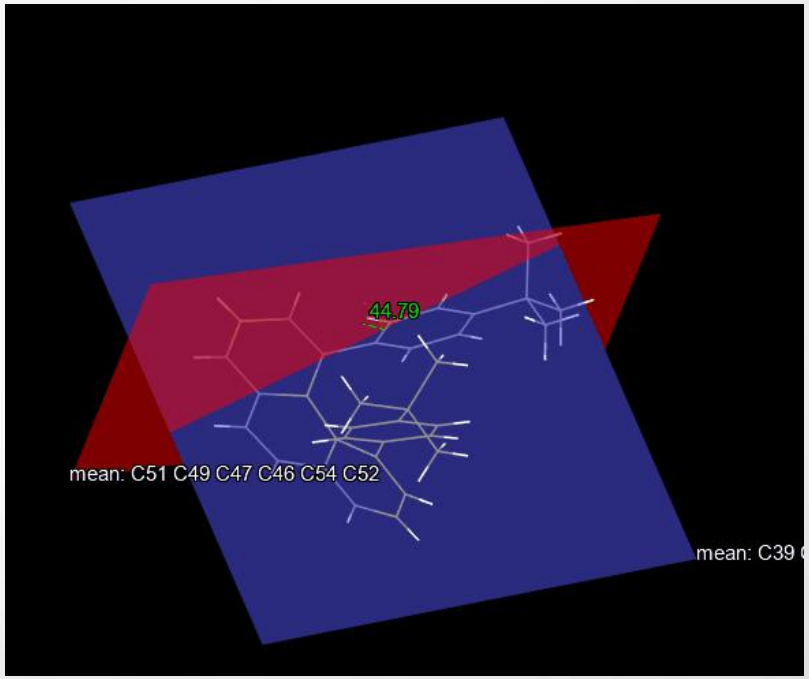
01 基础操作


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
Structure Navigator
Databases
Find
Crystal Structures
Spacegroup
Databases
Structures
Refcode Lists
ConQuest Hits
Mercury Files
Tree View
Multiple Structures
Structures...
Structure Navigator
Searches
Display Options
Display
Packing
Asymmetric Unit
Auto centre
Reset
Short Contact < (sum of vdW radii)
H-Bond Default definition
Contacts...
More Info
Powder...
Options
Show hydrogens
Show cell axes
Label atoms
Depth cue
Z-Clipping
Stereo
Select 'Open' from the File menu to read a structure file or database

1.1原子标签位置设置

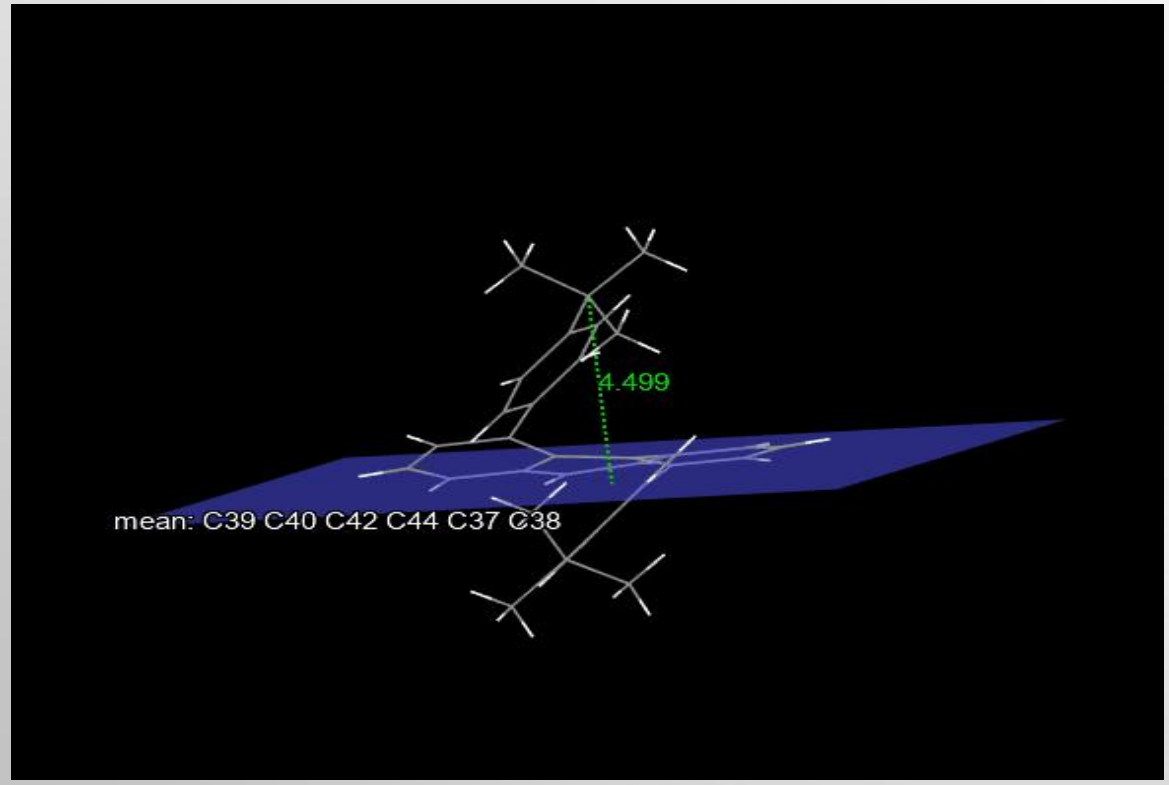


1.2二面角

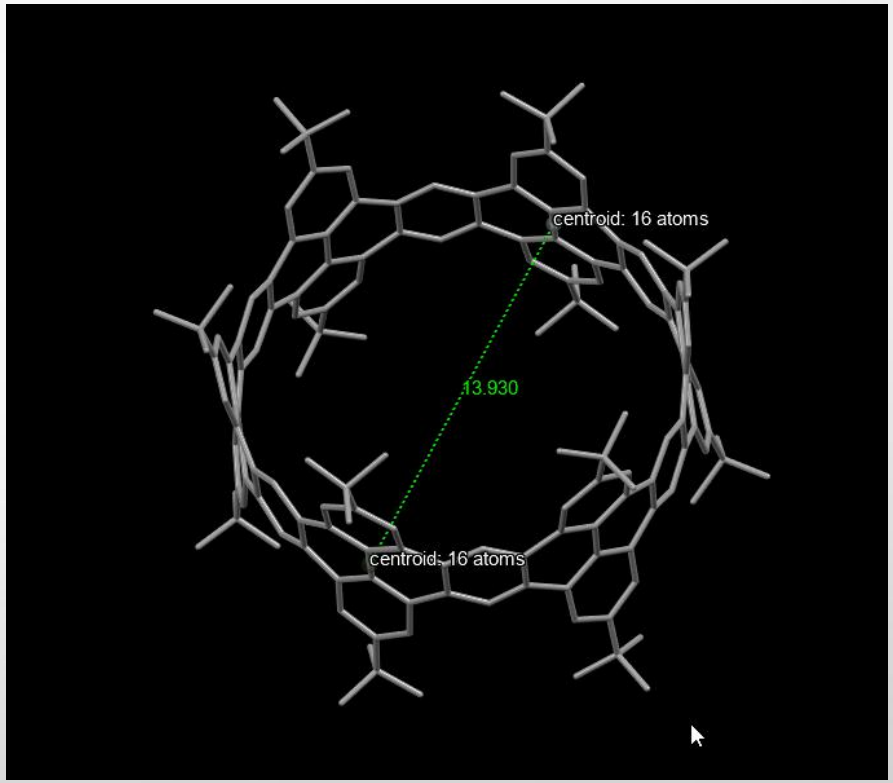


公众号文章链接https://mp.weixin.qq.com/s/li2glrEdSC_IrLdpxb3mfw

1.3点到面的距离

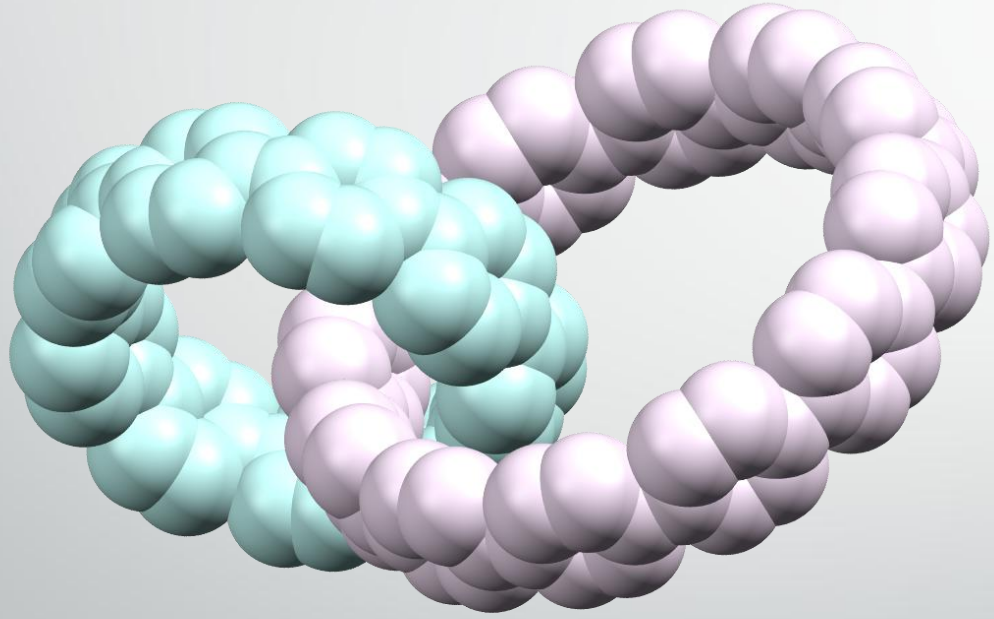


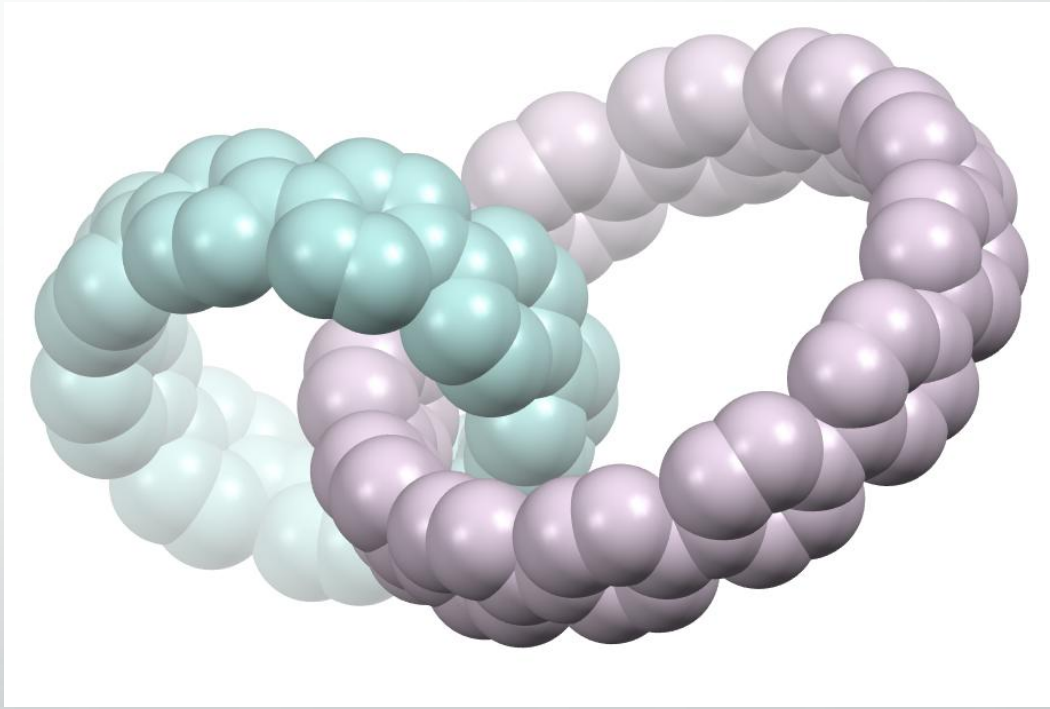
1.4面到面的距离



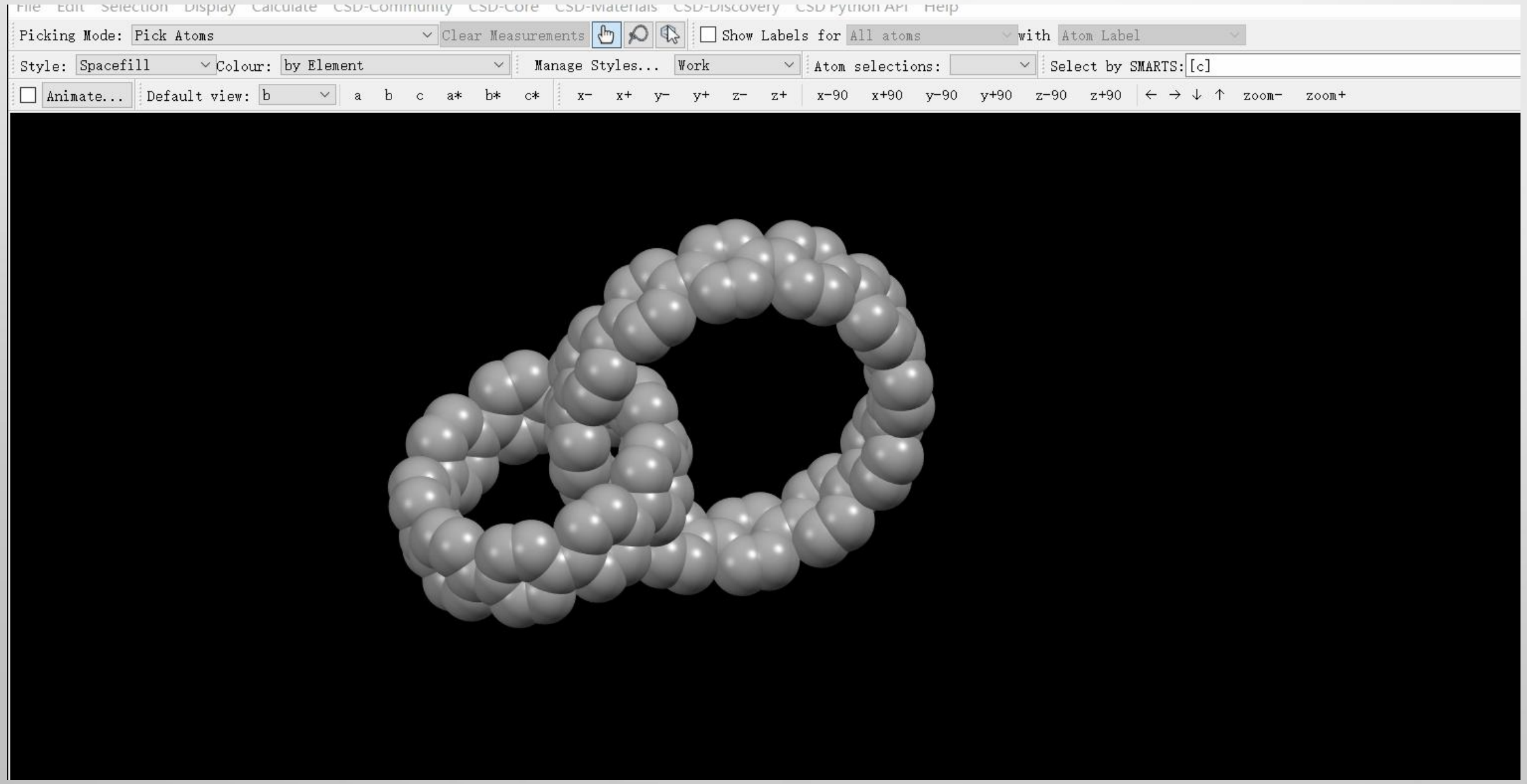
02

画透明背景与景深图

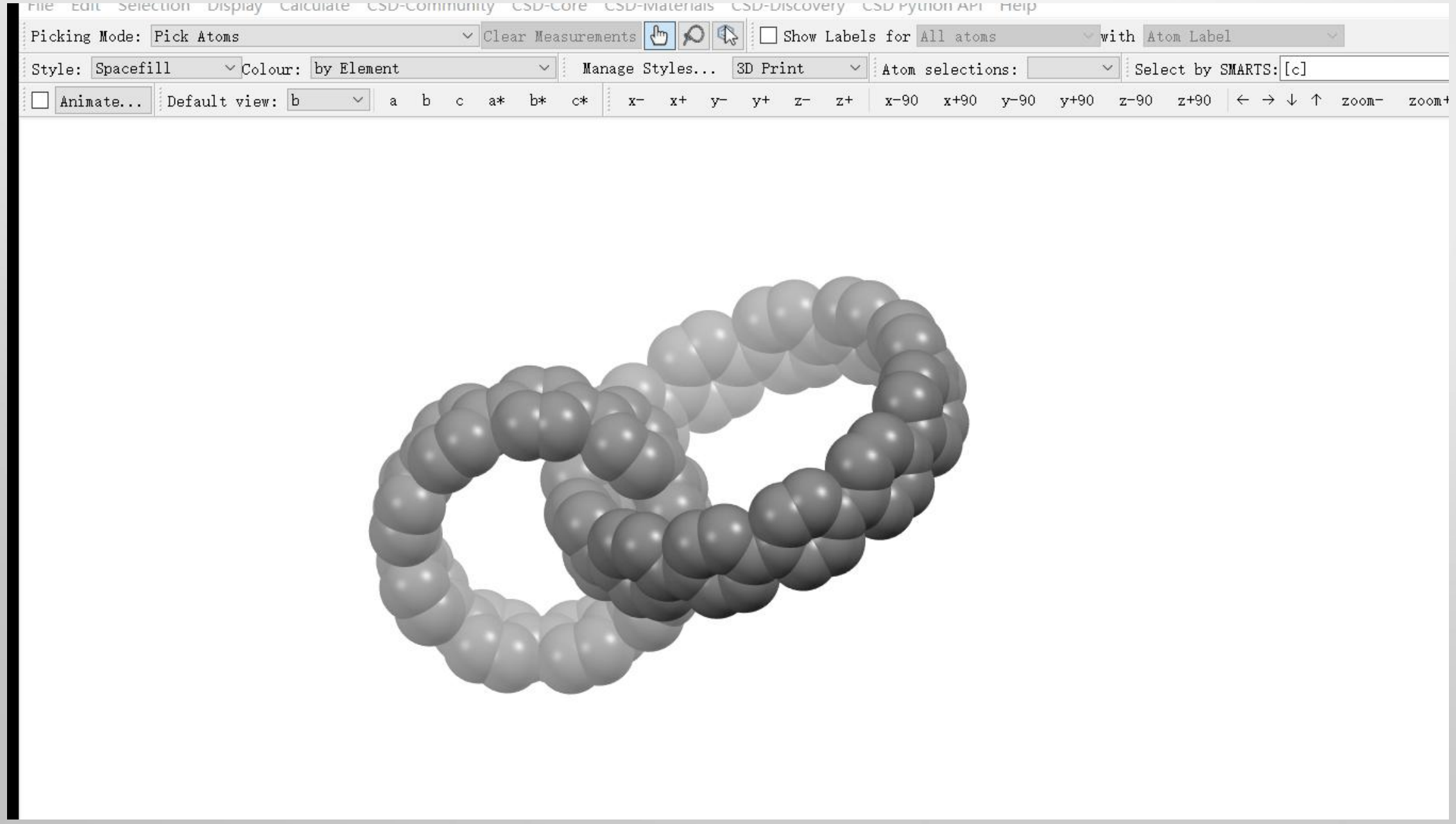




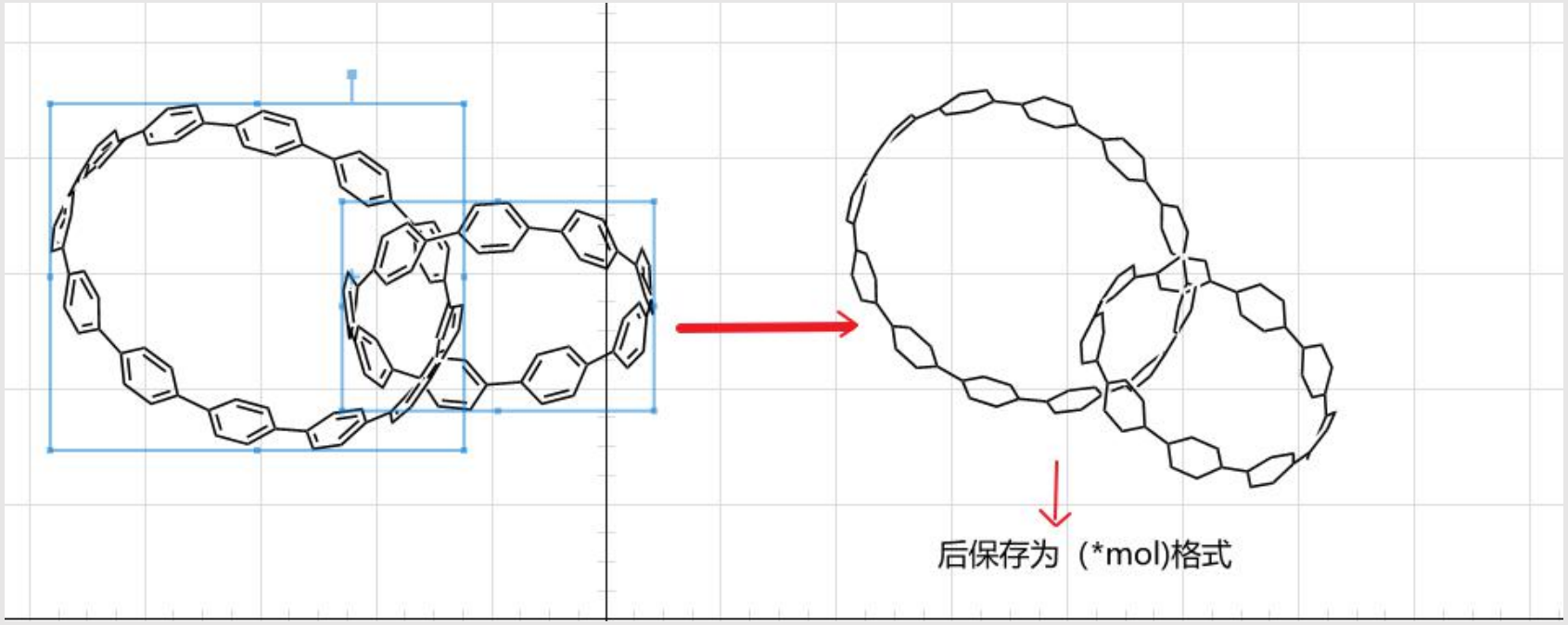
2.1打开File找到POV-Ray Image选项,在这里面可以设置透明背景，同时也能通过material properties变换不同风格



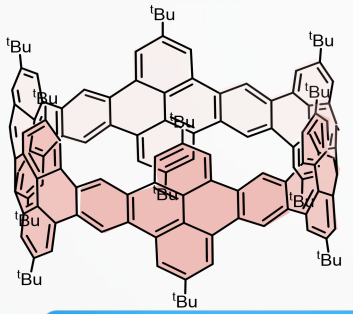
2.2打开Display找到Dispiay Options选项，可以从中获得不同景深的图片



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

Microsoft Bing

Chemistry Reference Resolver

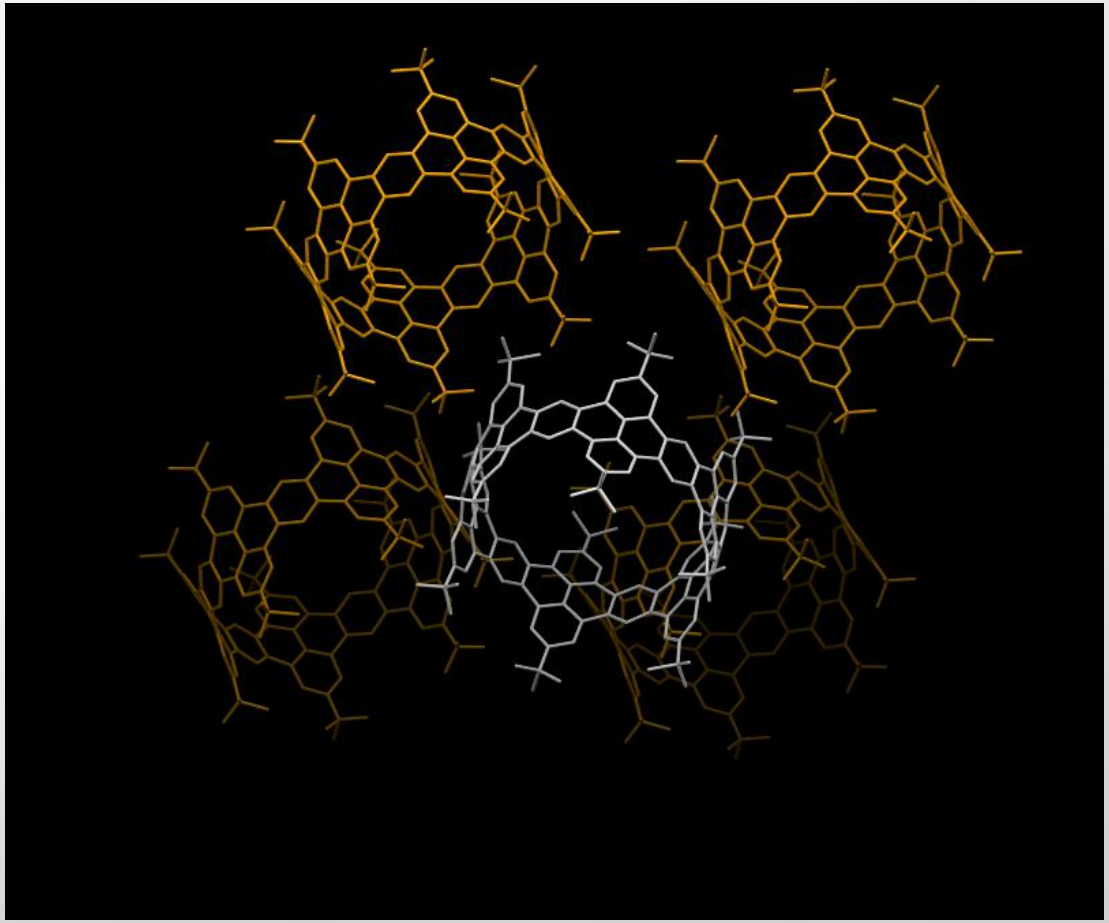
SCI-HUB

下载为cif格式

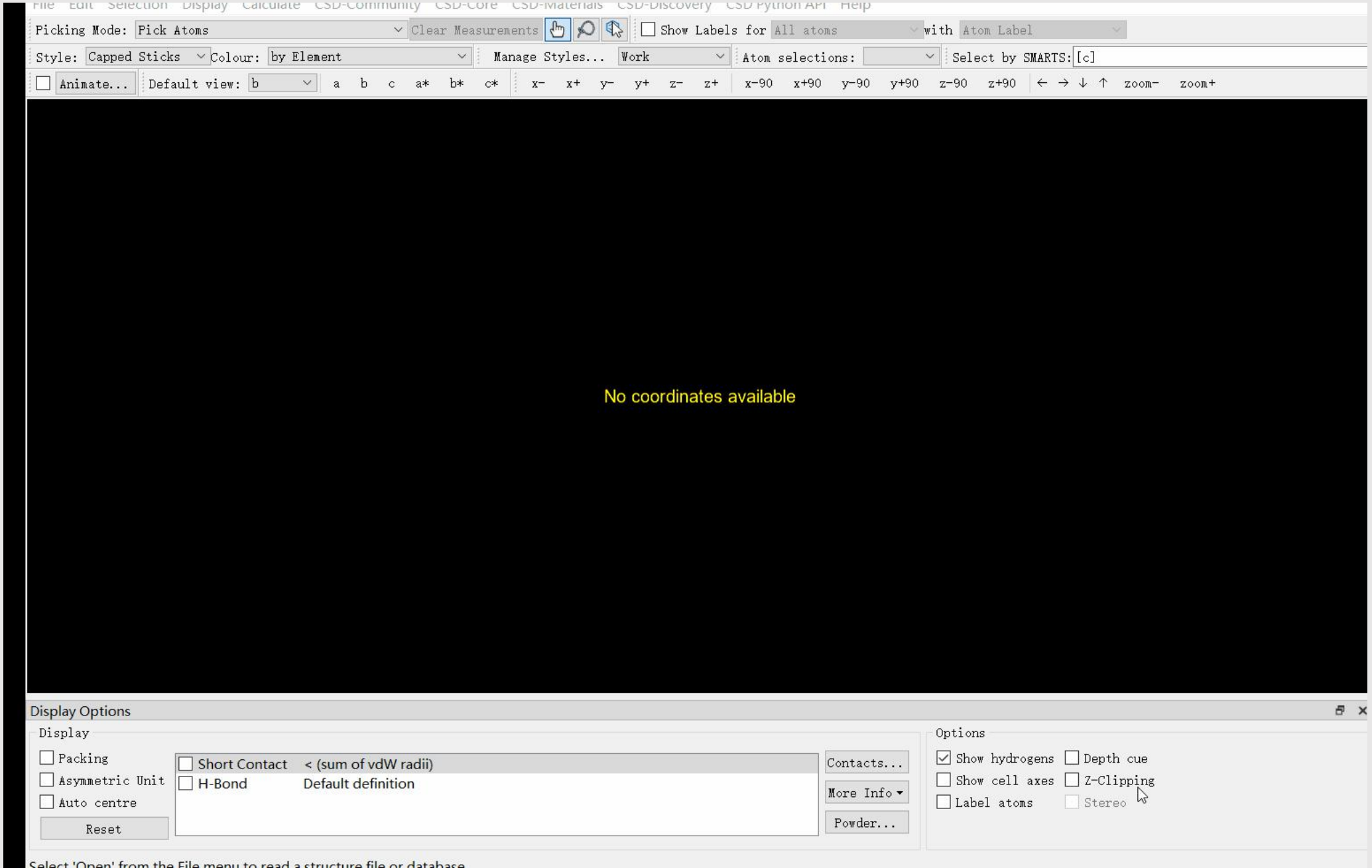
41557_2020_627_MOESM30_ESM.cif

找晶体支撑材料

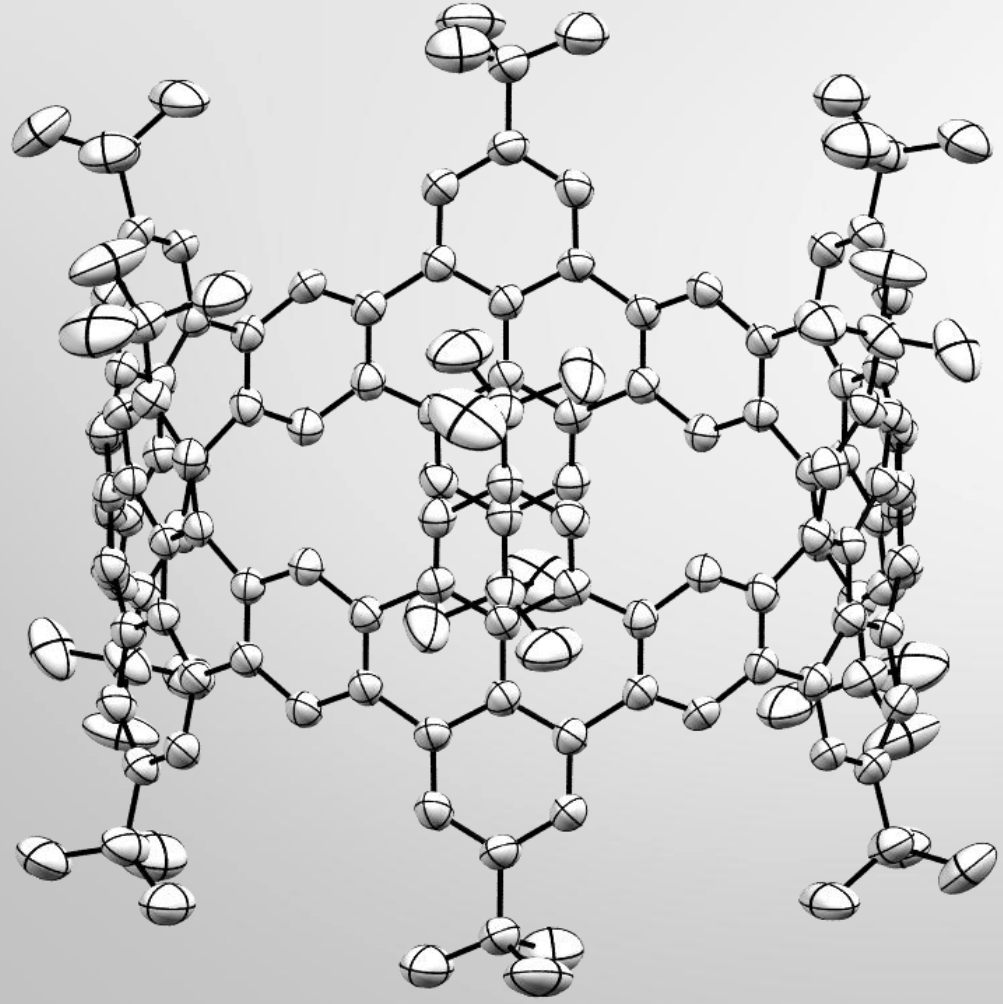
流程：在Mercury中打开cif格式文件,删去多余的溶剂分子，对照文献所示晶体，改变晶体分子的风格及其颜色，选好展示角度，保存图片。

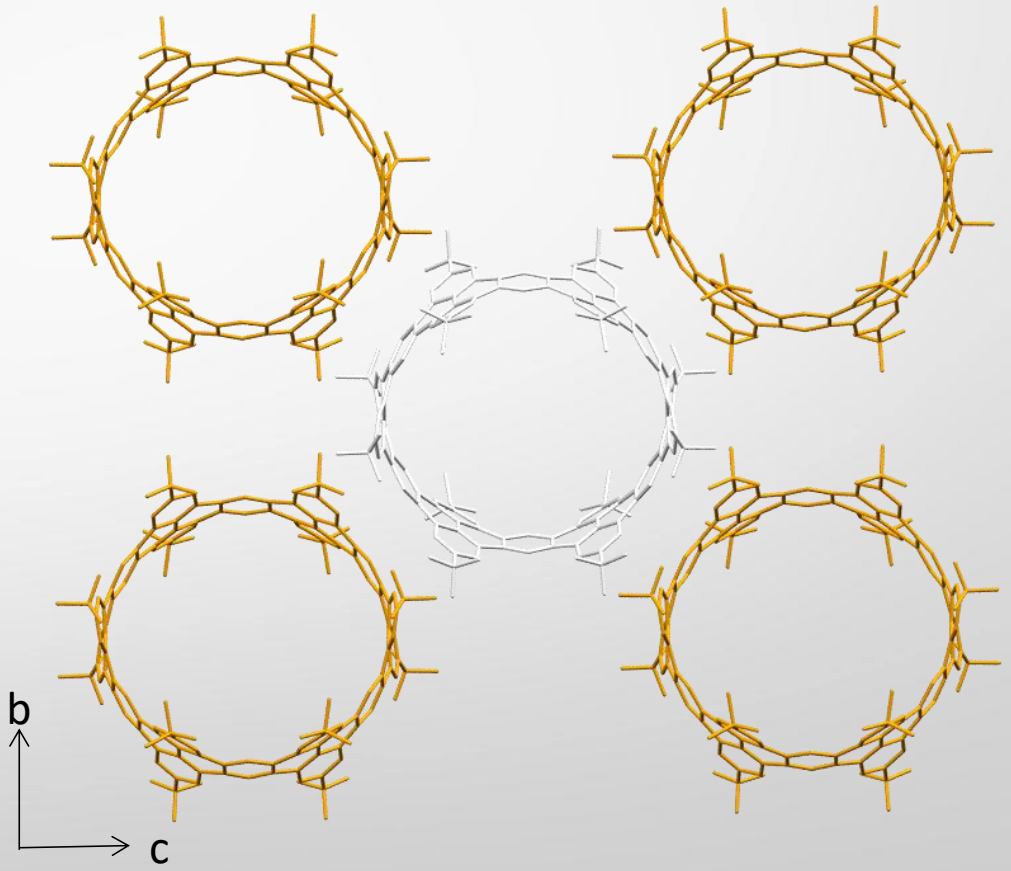


3.1视频


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
Asymmetric Unit
Auto centre
Reset
Short Contact < (sum of vdW radii)
H-Bond Default definition
Contacts...
More Info
Powder...
Options
Show hydrogens
Depth cue
Show cell axes
Z-Clipping
Label atoms
Stereo
Select 'Open' from the File menu to read a structure file or database

3.2例图





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