

## Introduction to Mercury (Instructions for iPad)

The Cambridge Crystallographic Data Centre (CCDC) curates the Cambridge Crystallographic Database (CSD), which contains over 950,000 structures. A teaching subset of the database is freely available and this can be accessed using a web browser at the link found below.

<https://www.ccdc.cam.ac.uk/structures/search?compound=Teaching%20Subset>

We will be using this resource regularly over the course of the semester and this exercise will provide an introduction to finding structures in the database and how visualize and analyze these structures on an iPad. (Note that these instructions will also be valid for accessing the structures using a web browser on a laptop or desktop computer.)

### Accessing Structures

You can access and search the structures in the teaching subset using the CCDC's Access Structures page (<https://www.ccdc.cam.ac.uk/structures/>).



## Access Structures

Sign In

Entry search

Welcome to Access Structures, the CCDC's and FIZ Karlsruhe's free service to view and retrieve structures. Please use one or more of the boxes to find entries. If you enter details in more than one field the search will try to find records containing all the terms entered. More information and search help

More advanced search functionality and additional curated data for the Cambridge Structural Database (CSD) and the Inorganic Crystal Structure Database (ICSD) is available through the CSD-System and ICSD, respectively. Click here for more information.

Identifier(s)	CCDC Number(s), CSD Number(s), CSD Refcode(s) or ICSD Number(s) ?		
Compound name	e.g. sulfadiazine ?		
DOI	A single publication DOI, CSD DOI or ICSD DOI ?		
Authors	e.g. F.H.Allen ?		
Journal	e.g. Journal of the American Chemical Society ?		
Publication details	Year ?	Volume ?	Page ?
Database to search	<input checked="" type="radio"/> Entire published collection <input type="radio"/> CSD <input type="radio"/> ICSD <input type="radio"/> Teaching subset		

In the *Identifiers* box, enter the accession code for the structure of interest (in this case, BAZSUR) and hit the **Search** button. The following page will appear.

The Cambridge Crystallographic Data Centre **FIZ Karlsruhe** Leibniz Institute for Information Infrastructure **CSD Entry: BAZSUR** [Sign In](#)

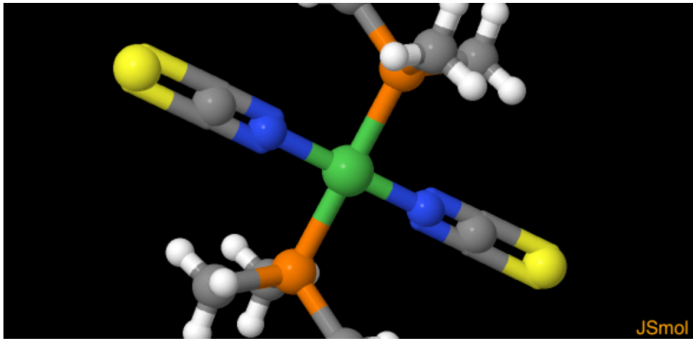
Your query was: Identifier(s): Bazsur and the search returned 1 record. [New Search](#)

Database Identifier	Deposition Number
<input checked="" type="checkbox"/> BAZSUR	210413

[Download](#)

BAZSUR : trans-bis(isothiocyanato)-bis(trimethylphosphine)-nickel(ii)  
**Space Group:** P 2<sub>1</sub>/n (14), **Cell:** a 6.1832(13)Å b 7.2920(11)Å c 16.744(3)Å,  $\alpha$  90°  $\beta$  91.906(16)°  $\gamma$  90°

3D viewer



[H](#) [Disorder](#) [Menu](#) [Open](#)

**Style** **Labels** **Packing** **Measure**  
Ball and Stick No Labels None None

### Structural Information

From this window, you are able to get all of the background information about this structure.

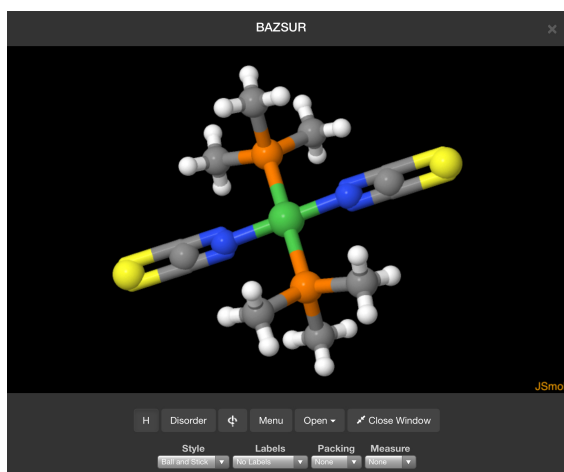
Please enter or write the name and formula of the complex below.

Please enter or write the literature reference for the structure below.

Please draw the diagram of the complex below. (You can also take a screenshot of the diagram provided on the page and inserting it below.)

## Visualizing Structures


Choose the **Expand** button (the blue button with the diagonal arrow) so that you can view a larger structure.



The molecule can be manipulated using several common gestures:

- A *one-finger hold and drag* will rotate the structure.
- A *two-finger hold and drag* will translate the structure.
- A *pinch/unpinch* will zoom out from/in towards the structure.

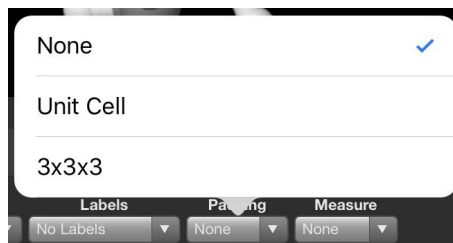
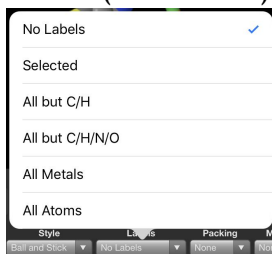
The buttons at the bottom of the window allow you to perform several common functions. (These buttons are also available on the original web page.) From left to right the buttons have the following functions:

- **H**: This button toggles between showing/hiding the hydrogen atoms in the structure.
- **Disorder**: This allows the visualization of any disorder present in the structure.
- : This button switches the view from a static to a rotating structure.
- **Menu**: This menu provides access to many advanced JSmol commands. (This will not routinely be used in this class.)
- **Open**: This allows you to open the structure in an external viewer. (This is not used on the iPad, only on desktop or laptop computers.)

- **Close Window:** This button closes the expanded window and returns to the original web page.

The representation of the structure can be changed by choosing options from the **Style** menu found at the bottom of the window. (In the figures included in this document, the “Ball and Stick” style is used.) Take a few moments and look at the different representations (wireframe, capped sticks, ball and stick, and spacefill) that could be used.

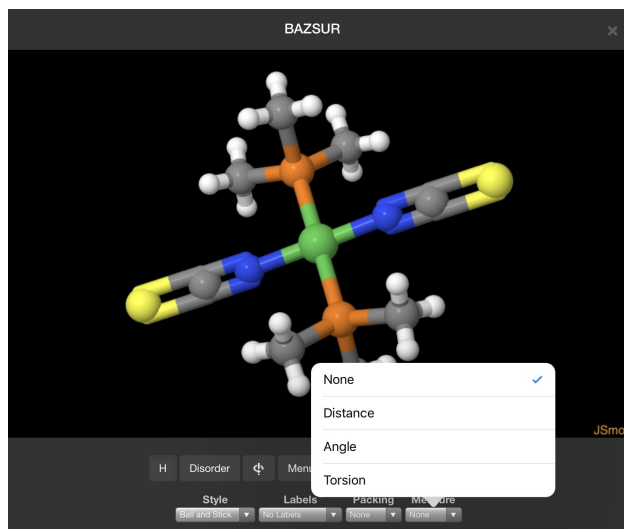
Some (or all) of the atoms in the structure can be labeled by choosing an option from the **Labels** menu (below left) found at the bottom of the window.



The **Packing** menu (above right) provides several options for changing how the structure is displayed: None, where one molecule/complex is shown; Unit Cell, where all molecules fully or partially contained in a single unit cell are shown; and 3x3x3, where an array of unit cells are displayed.

## Analyzing Structures

Bond lengths and angles can be measured using the the **Measurement** drop-down menu. From the menu you must first choose the appropriate measurement. To begin a measurement, tap twice on the first atom and then tap twice on the final atom to end the measurement. If there are any atoms that need to be chosen in between, tap them once. (To clear the measurement, you can either repeat the taps you made to create the measurement or choose *None* from the **Measurement** menu.)



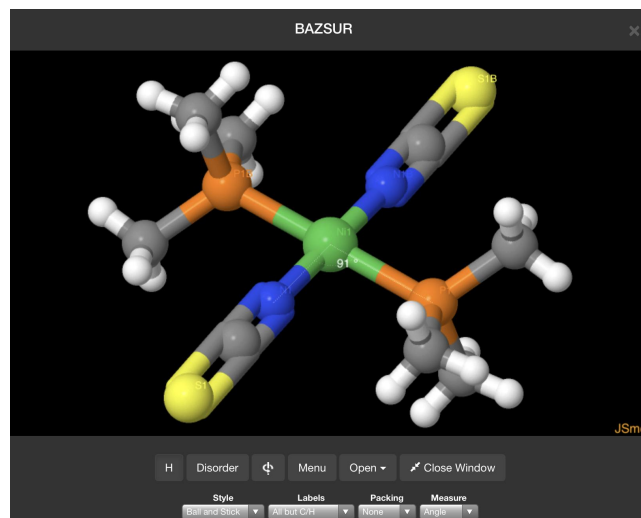
For example, to measure the Ni-N bond length, you would choose *Distance* from the **Measurement** menu, then tap twice on the nickel (green) and then twice on one of the nitrogens (blue). (Note that there is no visual clue when you have tapped or double-tapped on an atom.) The measurement will then appear on the screen.

Please measure the distances between the nickel and the 4 attached atoms and enter them in the table below. The numbering indicated in the table can be seen when the atoms in the structure are labeled. The atom numbers may be hard to see because they may overlap with the atoms.

Bond	Bond length (Å)
Ni <sub>1</sub> -N <sub>1</sub>	
Ni <sub>1</sub> -N <sub>1B</sub>	
Ni <sub>1</sub> -P <sub>1</sub>	
Ni <sub>1</sub> -P <sub>1B</sub>	

To measure the bond angles in the structure, choose *Angle* and then choose the three atoms that define the angle in succession, starting with one of the “terminal” atoms. For example, to measure the P<sub>1</sub>-Ni<sub>1</sub>-N<sub>1</sub> angle, double tap on N<sub>1</sub> first, then single tap on Ni<sub>1</sub>, then double tap on P<sub>1</sub> to get the angle defined by those three atoms (as shown in the figure below). Measure the angles listed and enter them in the table below.

Angle	Bond Angle (°)
P <sub>1</sub> -Ni <sub>1</sub> -N <sub>1</sub>	
N <sub>1</sub> -Ni <sub>1</sub> -P <sub>1B</sub>	
P <sub>1B</sub> -Ni <sub>1</sub> -N <sub>1B</sub>	
N <sub>1B</sub> -Ni <sub>1</sub> -P <sub>1</sub>	
N <sub>1</sub> -Ni <sub>1</sub> -N <sub>1B</sub>	
P <sub>1</sub> -Ni <sub>1</sub> -P <sub>1B</sub>	



Given the bond angle measurements that you just made, what is the geometry of the complex?

Geometry =

### Further work

Once you have finished this exercise, please call up the structure with the code **BILMIS**. Please go through the same steps that we followed above and provide the requested information below.

*Please enter the name and formula of the complex below.*

*Please enter the literature reference for the structure below.*

*Please draw the diagram of the complex below.*

*Please determine the bond lengths of the following bonds.*

Bond	Bond length (Å)
Mo <sub>1</sub> -C <sub>1</sub>	
Mo <sub>1</sub> -C <sub>2</sub>	
Mo <sub>1</sub> -C <sub>3</sub>	
Mo <sub>1</sub> -C <sub>4</sub>	
Mo <sub>1</sub> -P <sub>1</sub>	
Mo <sub>1</sub> -P <sub>2</sub>	

*Please determine the bond angles listed in the table below.*

Angle	Bond Angle (°)
C <sub>1</sub> -Mo <sub>1</sub> -C <sub>2</sub>	
C <sub>1</sub> -Mo <sub>1</sub> -C <sub>3</sub>	
C <sub>1</sub> -Mo <sub>1</sub> -C <sub>4</sub>	
C <sub>2</sub> -Mo <sub>1</sub> -C <sub>3</sub>	
C <sub>2</sub> -Mo <sub>1</sub> -C <sub>4</sub>	
C <sub>3</sub> -Mo <sub>1</sub> -C <sub>4</sub>	
C <sub>1</sub> -Mo <sub>1</sub> -P <sub>2</sub>	
P <sub>1</sub> -Mo <sub>1</sub> -P <sub>2</sub>	
P <sub>1</sub> -Mo <sub>1</sub> -C <sub>1</sub>	
P <sub>1</sub> -Mo <sub>1</sub> -C <sub>2</sub>	
P <sub>1</sub> -Mo <sub>1</sub> -C <sub>3</sub>	
P <sub>1</sub> -Mo <sub>1</sub> -C <sub>4</sub>	
P <sub>2</sub> -Mo <sub>1</sub> -C <sub>1</sub>	
P <sub>2</sub> -Mo <sub>1</sub> -C <sub>2</sub>	
P <sub>2</sub> -Mo <sub>1</sub> -C <sub>3</sub>	
P <sub>2</sub> -Mo <sub>1</sub> -C <sub>4</sub>	

Given the bond angle measurements that you just made, what is the geometry of the complex?