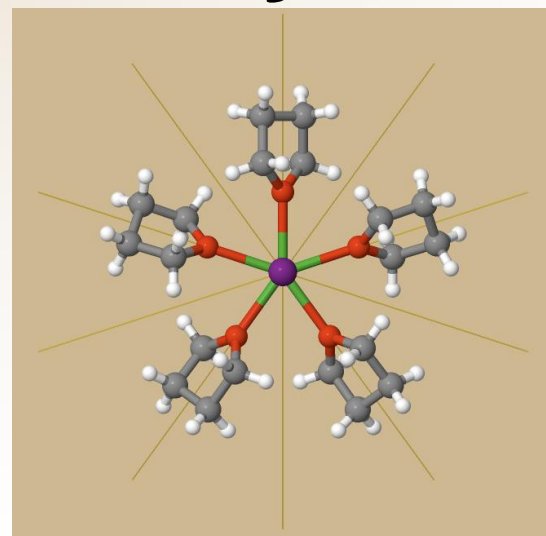
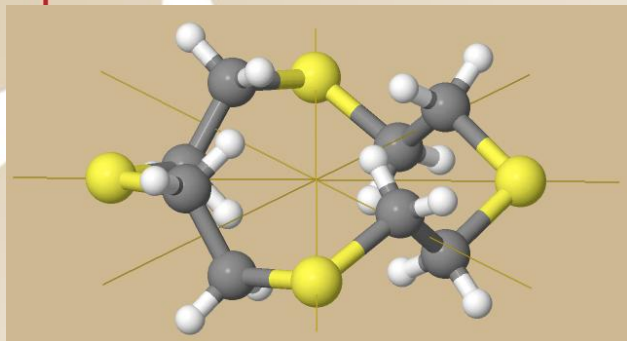


Using the Cambridge Structural Database to Explore Concepts of Symmetry

Dean H. Johnston
Otterbein College

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<http://symmetry.otterbein.edu>



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CSDSymmetry

- Microsoft Access database
- Contains point group and additional symmetry information on each residue for all entries in the CSD
- Some properties include:
 - point group
 - space group
 - number of atoms
 - special positions
 - R factor



How have I used CSDSymmetry?

- CSDSymmetry is an excellent resource to identify molecules with unique point groups
- Some structures have been incorporated into the **Symmetry Gallery**

Symmetry Gallery

- over 60 molecules
- 37 point groups
- interactive (Jmol)
- includes DOI and WebCSD links

Symmetry @ Otterbein

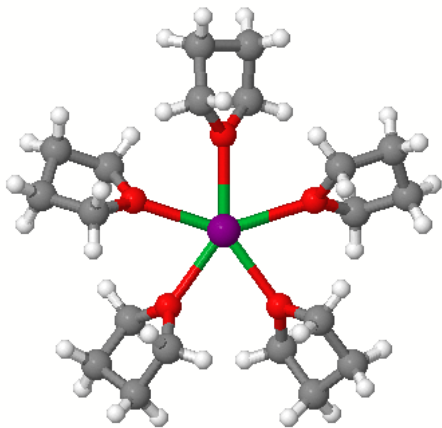
Home Tutorial **Gallery** Challenge Info Feedback

Point Group Type:
All

Select Molecule:

- BH₃
- BrF₅
- Co₄(Cp)₄ cluster
- Cr(CO)₆
- Fe(C₅H₅N)₆²⁺
- Fe(Me₅-Cp)(P₅)
- Mo₆Cl₈Cl₅²⁻
- Os₂Cl₈²⁻
- Re₂Cl₈²⁻
- Si₈O₁₂(CH₃)₈
- Th(NO₃)₆²⁻
- W(CN)₈²⁻
- YbI₂(THF)₅**
- [Ca(THF)₁₂]²⁺

Preferences



Point Group = D₅

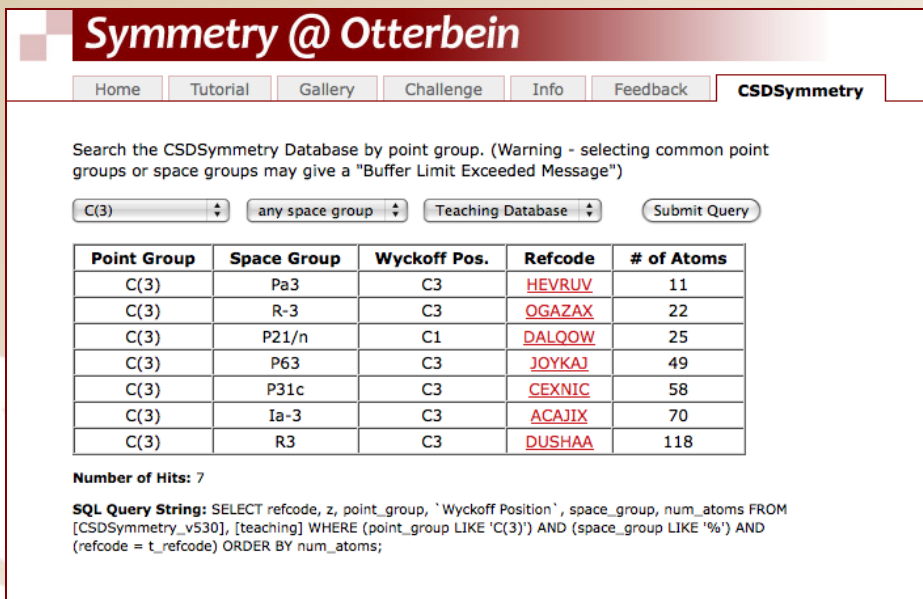
Jmol

Element	Operation
<input type="checkbox"/>	Show All Axes
<input type="checkbox"/>	C ₅ axis Rotate
<input type="checkbox"/>	C ₂ ' axis Rotate
<input type="checkbox"/>	C ₂ ' axis Rotate
<input type="checkbox"/>	C ₂ ' axis Rotate
<input type="checkbox"/>	C ₂ ' axis Rotate
<input type="checkbox"/>	C ₂ ' axis Rotate

Reference: Niemeyer, M. *Acta Crystallogr. Sect. E: Struct. Rep. Online* **2001**, 57, m363. DOI: [10.1107/S1600536801011254](https://doi.org/10.1107/S1600536801011254), WebCSD: [NELMUM](https://www.webcso.org/entry/NELMUM).

How can students use CSDSymmetry?

- With a simple web interface



Symmetry @ Otterbein

Home Tutorial Gallery Challenge Info Feedback **CSDSymmetry**

Search the CSDSymmetry Database by point group. (Warning - selecting common point groups or space groups may give a "Buffer Limit Exceeded Message")

C(3) any space group Teaching Database Submit Query

Point Group	Space Group	Wyckoff Pos.	Refcode	# of Atoms
C(3)	Pa3	C3	HEVRUV	11
C(3)	R-3	C3	OGAZAX	22
C(3)	P21/n	C1	DALQOW	25
C(3)	P63	C3	JOYKAJ	49
C(3)	P31c	C3	CEXNIC	58
C(3)	Ia-3	C3	ACAJIX	70
C(3)	R3	C3	DUSHAA	118

Number of Hits: 7

SQL Query String: SELECT refcode, z, point_group, `Wyckoff Position`, space_group, num_atoms FROM [CSDSymmetry_v530], [teaching] WHERE (point_group LIKE 'C(3)') AND (space_group LIKE '%') AND (refcode = t_refcode) ORDER BY num_atoms;

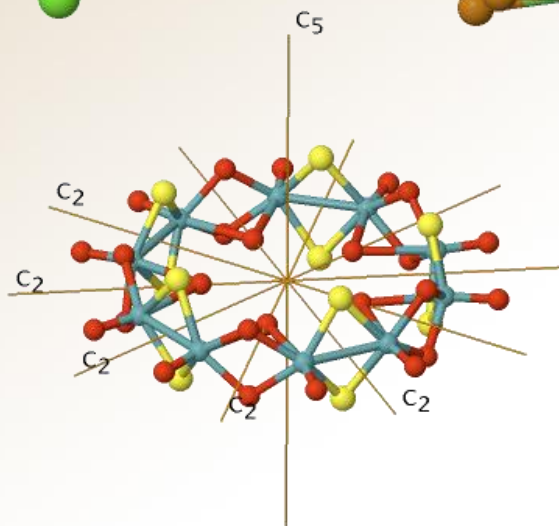
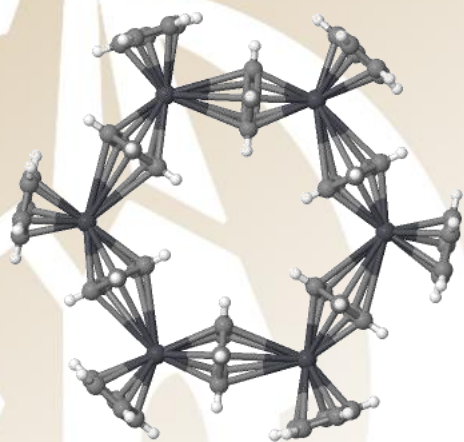
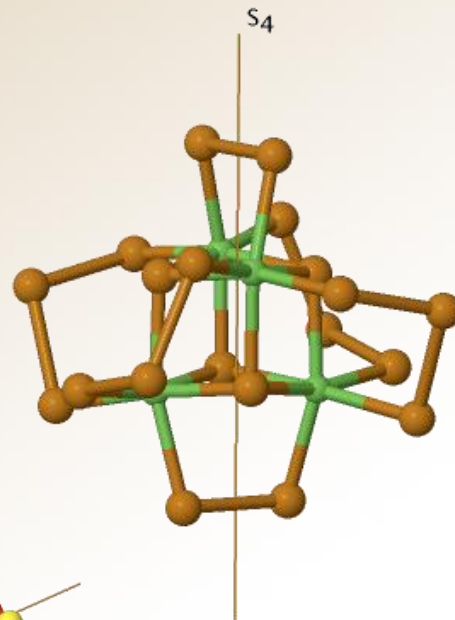
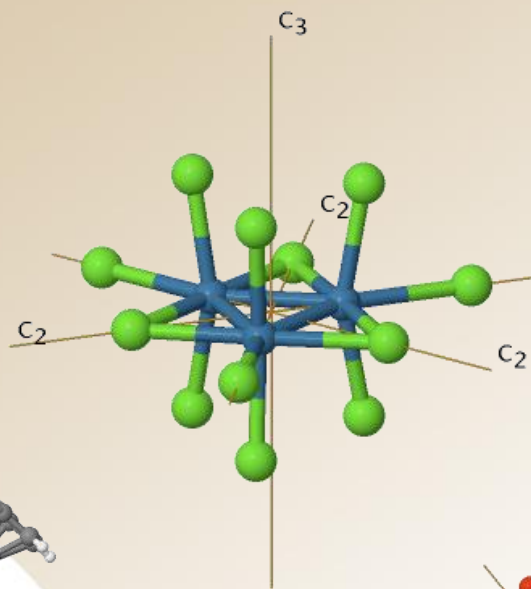
... students can explore the symmetry properties of some very unique molecules

Student Assignment

- Find **three** different molecules with “interesting” (to you) symmetry using the Cambridge Structural Database
- Report the following
 - six-letter reference code
 - point group of the molecule
 - brief description of the structure and why you found it interesting

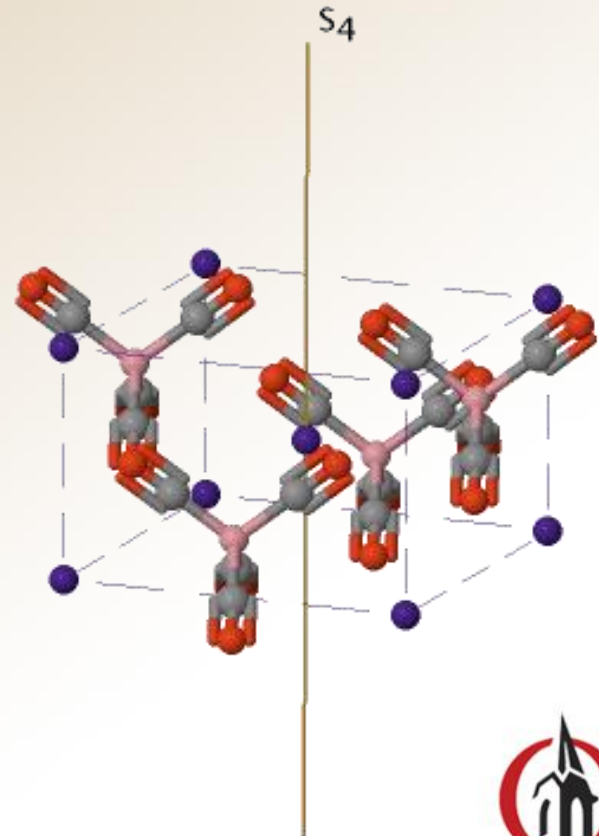


What Did They Find?



Unit Cell Symmetry

- The same concepts can be illustrated for symmetry elements for unit cells



Acknowledgements

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