An Interactive Online Teaching Subset of the Cambridge Structural Database

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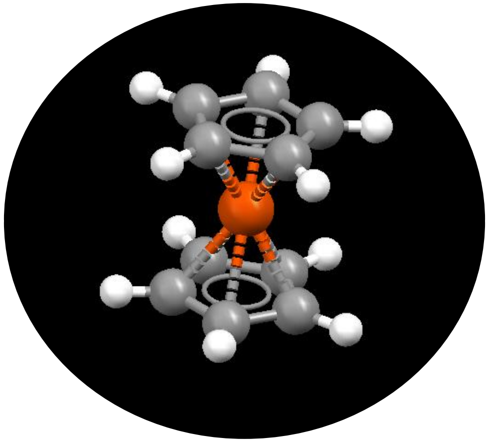
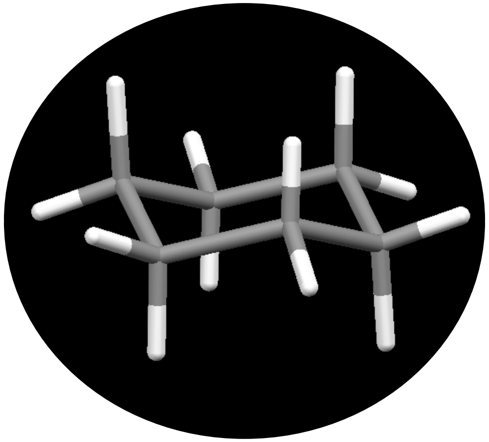




3D Visualisation

- Chemists need 3D visualisation proficiency
- 3D visualisation shown to enhance students conceptual understanding and spatial abilities

Williamson, V. M. *J. Chem. Educ*., **2008**, 85, 718-723
Wu, H. K. *Sci. Educ. Res. Pract*., **2004**, 8, 61-72
Bodner, G. M. *The Chemical Educator*, **1997**, 2

"Because basic 3D spatial relationships in molecules have systematic and profound causal significance, chemistry is an extraordinarily fertile field for visual learning"

2001 NSF Workshop: Molecular Visualisation in Science Education

Experimentally Measured Data

- Use of experimentally measured data is of great pedagogical value
  - Inherent experimental error and statistical variation provides an opportunity to deal with the uncertainties of chemistry
  - Challenges students to think more critically about bonding and molecular structure
  - Encourages method and limitations of data collection to be considered
- Measured data shown to enhance student learning

DeHaan, R. L. *J. Sci. Educ. Technol*., **2005**, 14, 253-269
Handelsman, J. *Science* **2004**, 304, 521-522
Prince, M. *J. Eng. Educ.,* **2004**, 89, 1-9

Encouraging the use of Crystal Structure Data in Teaching

- Free on-line interactive teaching subset of the CSD, and associated example teaching units

These educational materials are designed to demonstrate, to the non-specialist, the utility of crystallographic information across the entire chemistry curriculum

Teaching Subset of the CSD

- 500 structures that have important applications in chemistry and chemical education selected from the full CSD of almost half a million crystal structures
- Key molecules typically used in textbooks to exemplify core concepts and principles, e.g.
  - Bonding and structure: benzene (BENZEN02), diborane (GAFLAA), and ferrocene (FEROCE27)
  - Conformational analysis: half-chair and envelope cyclopentane (LISLOO, IHIPOE), cyclohexane (CYCHEX)
  - Stereochemistry: L-(R)- and D-(S)- alanine (LALNIN23, ALUCAL05), tartaric acid (TARTAC, TARTAL04, TARTAM)
  - Reaction mechanisms: bromonium ion (refcode: DAKVUG)

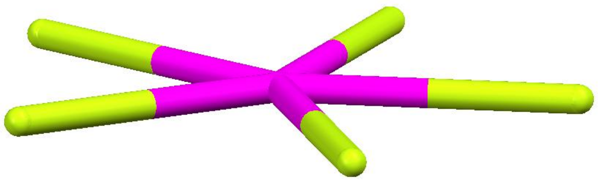
Chemical Diversity

Structure Type	N	%Subset
All structures	500	100.0
Organic	331	66.2
Metal-organic	161	32.2
Organic structures		
Carbohydrates	8	1.6
Nucleosides / nucleotides	6	1.2
Amino-acids and peptides	29	5.8
Porphyrins / corrins	13	2.6
Steroids	12	2.4
Alkaloids	10	2.0
Organic polymers	8	1.6

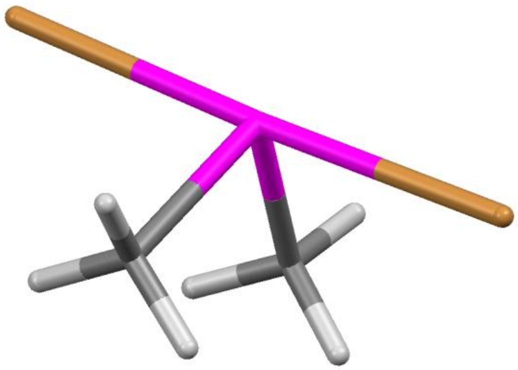
Metal-organic structures		
Any metal: 3-coordinate	9	1.8
Any metal: 4-coordinate	37	7.4
Any metal: 5-coordinate	21	4.2
Any metal: 6-coordinate	52	10.4
Any metal: 7-coordinate	10	2.0
Any metal: 8-coordinate	10	2.0
Any metal: 9-coordinate	6	1.2
Any metal: 10-coordinate	2	0.4
Any metal: 11-coordinate	2	0.4
Any metal: 12-coordinate	3	0.6
π-complexes	33	6.6
Containing keywords		
‘Drug’ or ‘Activity’	42	8.4
‘Polymorph’ or ‘Form’	80	16.0

Diverse Molecular Geometries

- Simple examples (composed entirely of main group elements) of all main VSEPR structure types
- Linear, bent, trigonal planar… square antiprismatic



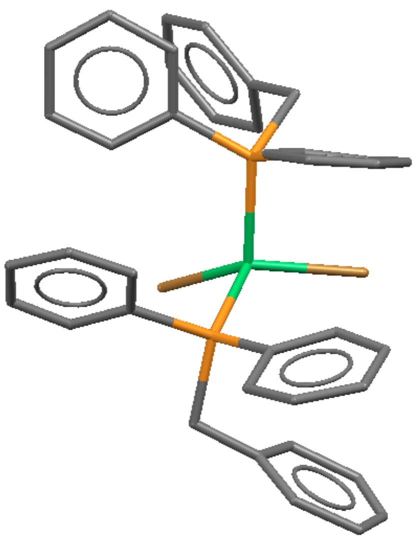
Pentagonal planar
$[XeF_5]^-$ anion
(refcode: SOBWAH)

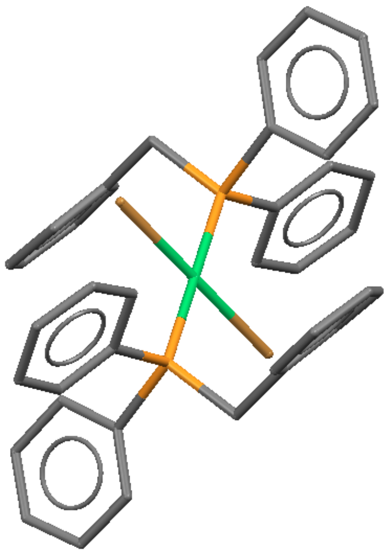


Disphenodial "see-saw"
dibromodimethylselenium
(refcode: RIZMIW)

Diverse Molecular Geometries

- Simple examples (composed entirely of main group elements) of all main VSEPR structure types
- Linear, bent, trigonal planar… square antiprismatic
- Unusual and interesting geometries



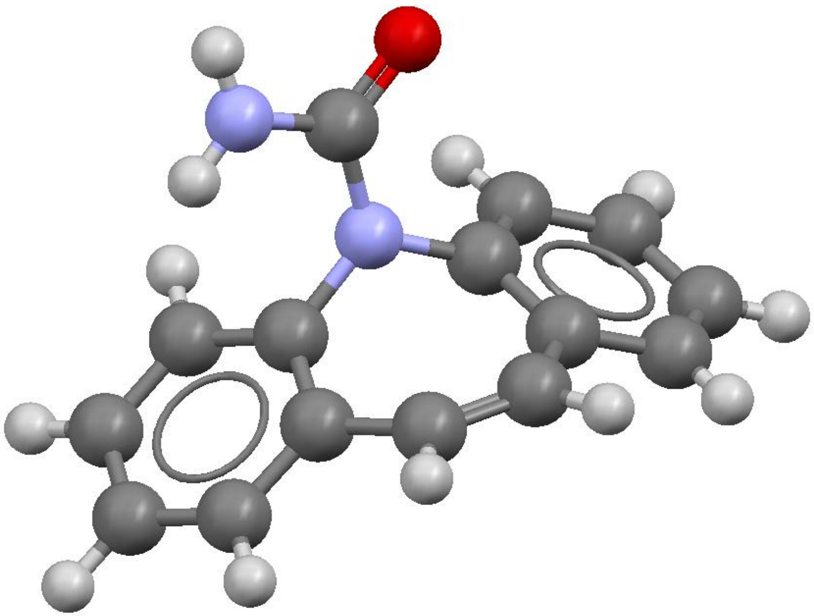


Interallogon compound
(Greek: allos, other, different; gonia, angle)

Dibromo-bis(benzyldiphenyl phosphine) nickel(ii) (refcode: DBBZPN)

Multiple Determinations

- CSD contains multiple determinations of the same crystal structure, e.g. improved model, temperature study etc.
- Such series can be used to study statistical variation and explore different crystal forms (polymorphism).



Carbamazepine, an analgesic and anticonvulsant drug

6 determinations:

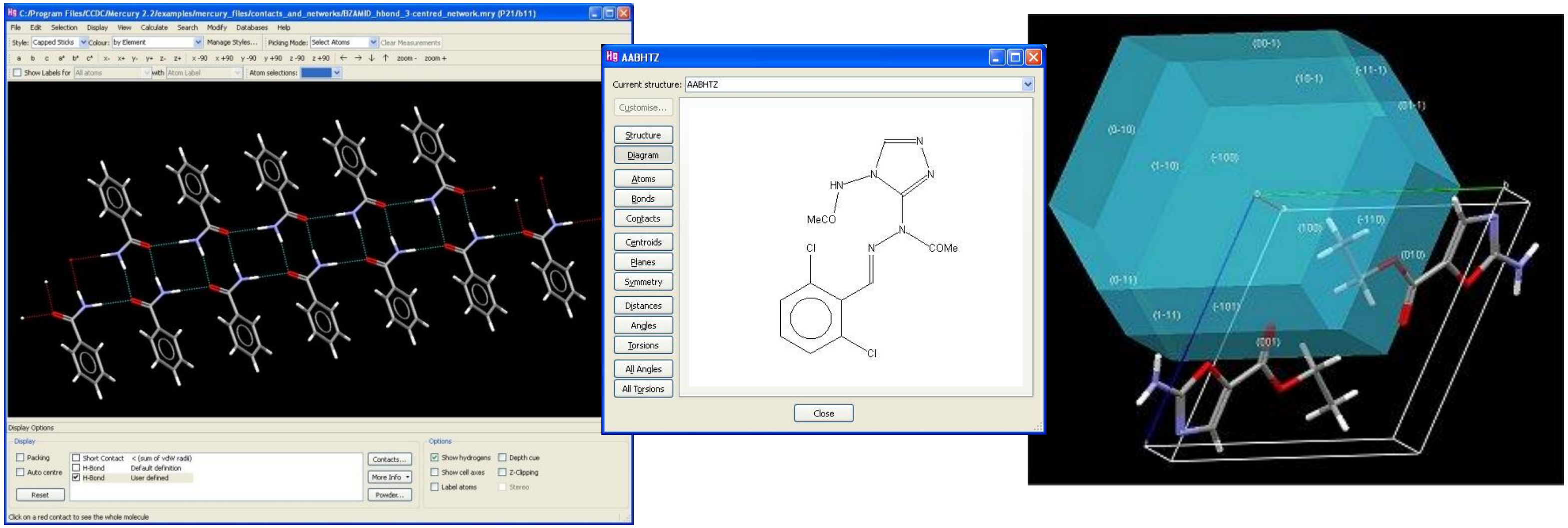
CBMZPN01, CBMZPN02, CBMZPN03, CBMZPN10, CBMZPN11, CBMZPN12,

Structure Quality

Structure Quality	Teaching Subset		CSD V5.30 +Nov & Feb09 Updates	
	N	%Subset	N	%CSD
All structures	500	100.0	472200	100.0
3D Coordinates determined	500	100.0	433866	91.9
Contain unresolved errors	0	0.0	8345	1.8
Contain disorder	29	5.8	99547	21.1
R factor				
< 0.05	301	60.2	251658	53.3
< 0.075	422	84.4	396521	84.0
< 0.1	461	92.2	438989	93.0

How Can I Access the Subset #1

- Mercury visualiser
  - Advanced crystal structure visualisation program by CCDC
  - Freely downloadable desktop application
  - Teaching subset embedded and available via Databases menu

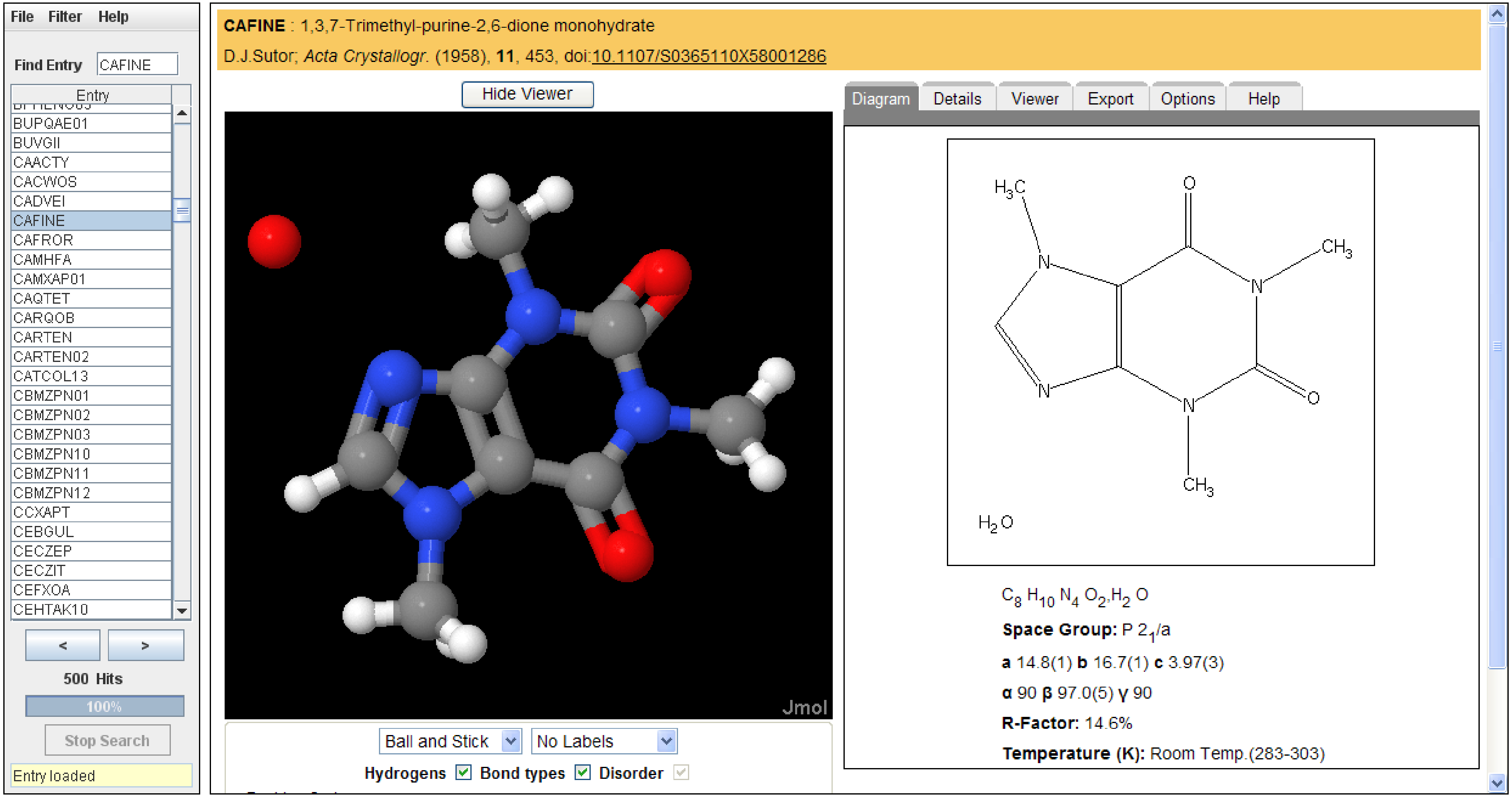


http://www.ccdc.cam.ac.uk/free_services/teaching/

How Can I Access the Subset #2

- Interactive web-based interface
  - Uses WebCSD: new on-line search interface to the CSD
  - Not required to download, install or register any software
  - Browse and visualise teaching subset entries using just a standard web-browser

http://www.ccdc.cam.ac.uk/free_services/teaching/



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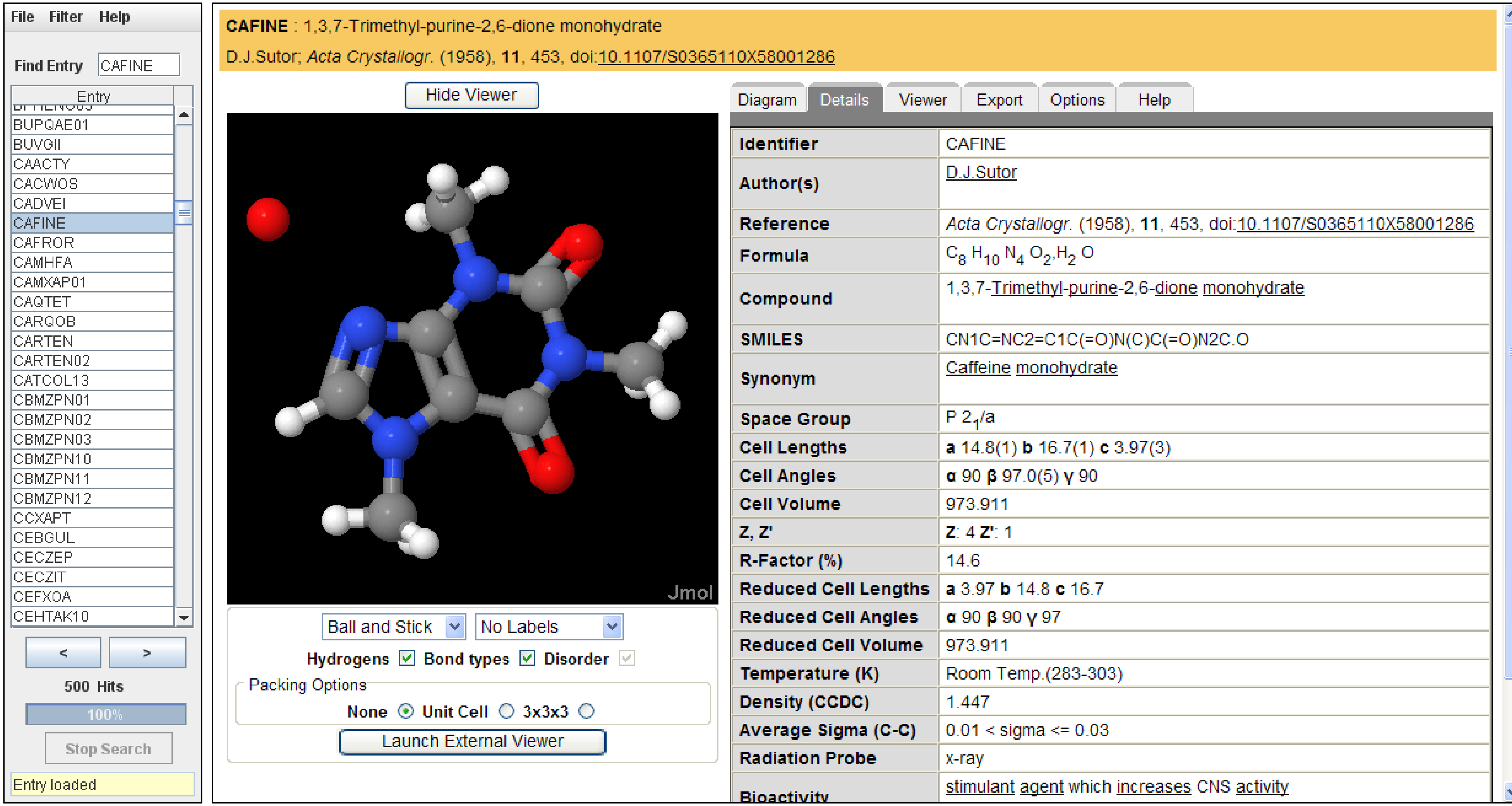

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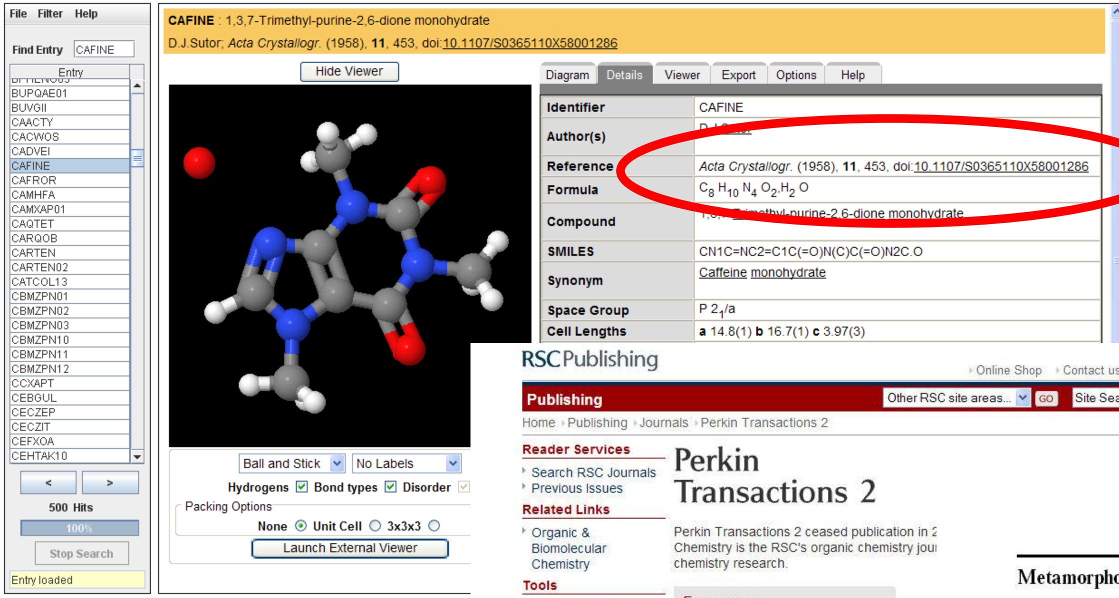

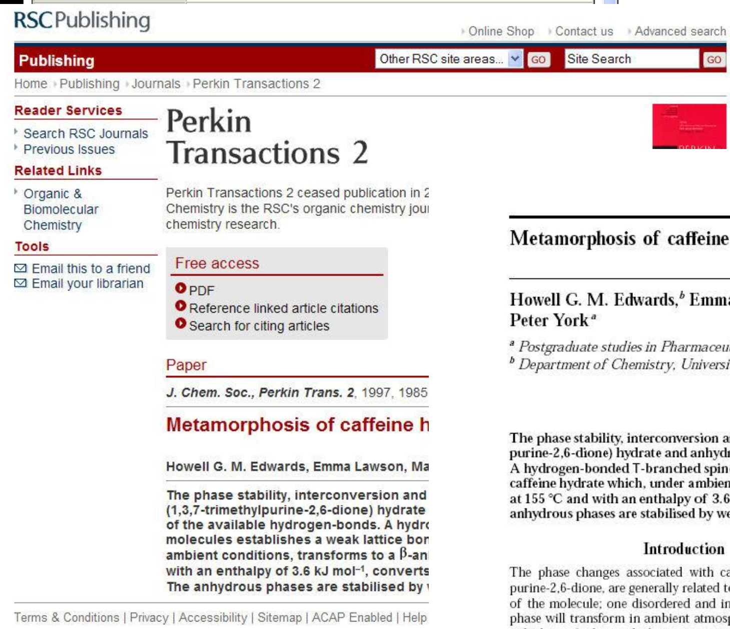

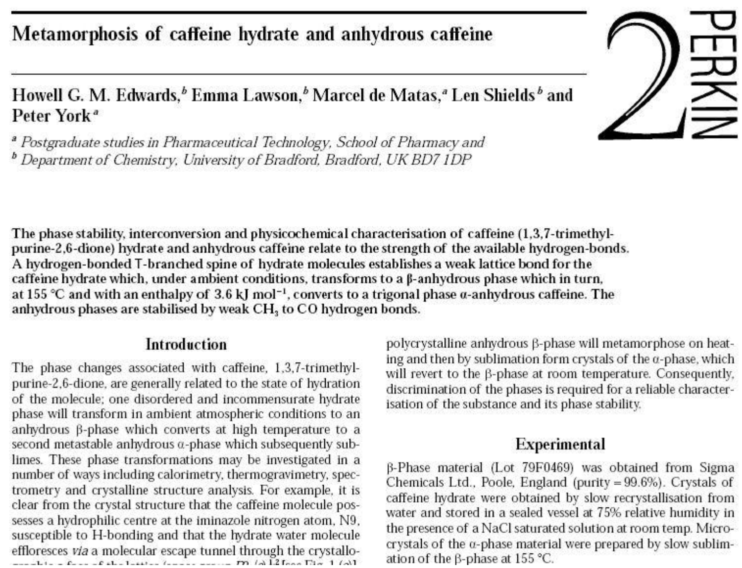

Links to the primary literature

Generating Links to the Teaching Subset

- Easy integration with your own teaching materials, and webpages
- WebCSD interface provides a form that will:
  - Automatically generate a hyperlink that will launch WebCSD and display one or more specified entries
  - **View in WebCSD**

Teaching Units

- Based on structures in the teaching subset
- Provide opportunity to visualise and interact with diverse range of 3D structures
- Illustrate utility of crystal structure data across a broad range of chemical concepts, including:
  - Aromaticity, shapes of molecules (VSEPR)
  - Reaction intermediates, stereochemistry, conformations of rings
  - Metal-carbonyl back-bonding, metal geometry, hapticity
  - Analysing molecular dimensions

http://www.ccdc.cam.ac.uk/free_services/teaching/

WebCSD Teaching Examples

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AROMATICITY

Online Resources

More Teaching Resources

Learn more about the full version of WebCSD

Contact us

For a full CSD evaluation

To share your CSD teaching materials

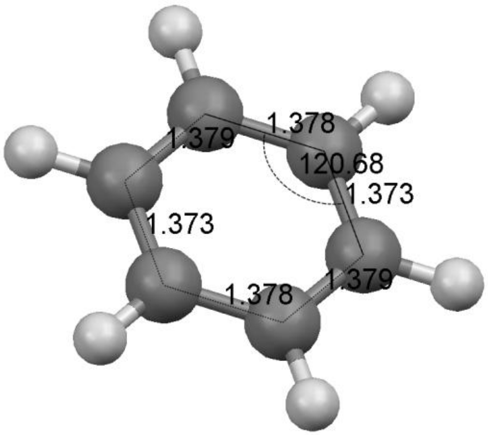
CCDC

News
Events

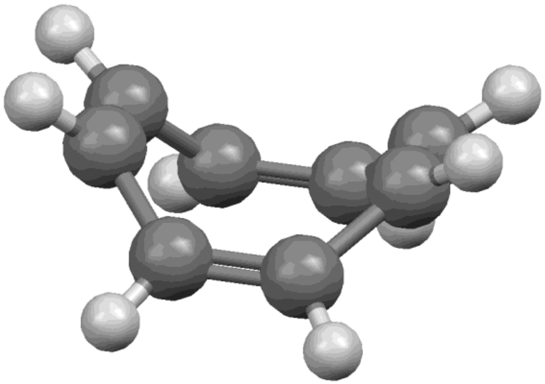
Cambridge Crystallographic Data Centre
Web: http://www.ccdc.cam.ac.uk
Support Email: teaching@ccdc.cam.ac.uk
Support Phone: +44 1223 336022

Teaching Unit: Aromaticity

- Note difference in reactivity of benzene compared to cyclooctatetraene, e.g. addition of Br
- Measure and compare the carbon-carbon bond lengths and planarity of the structures



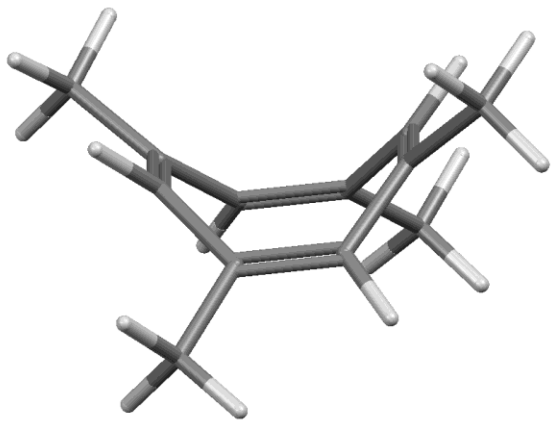
benzene (*BENZEN02*)



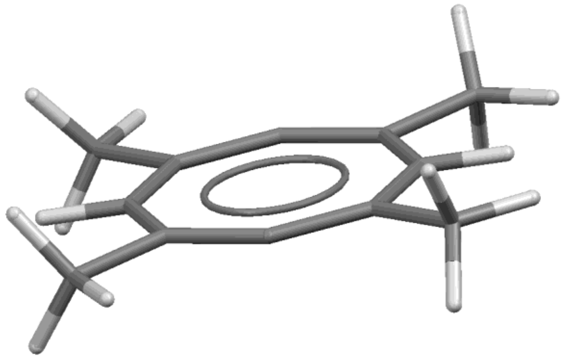
cyclooctatetraene (ZZZSAE01*)*

Teaching Unit: Aromaticity

- Inspect a number of oxidised and reduced benzene and cyclooctatetraene derivatives
- Relate structural characteristics to number of π-electrons
- Arrive at Huckel's rule
- Use findings to predict whether or not certain compounds are aromatic



puckered (*TMCOTT*)



planar dianion (*TMOCKE)*

Further Information

- Battle, G. M.; Allen, F. H.; Ferrence, G. M.
  An interactive web-accessible teaching subset of the Cambridge Structural Database
  J. Chem. Educ., **2009**, submitted
- Battle, G. M.; Allen, F. H.; Ferrence, G. M.
  Example teaching units that utilise an interactive web-accessible subset of the Cambridge Structural Database
  J. Chem. Educ., **2009**, submitted

http://www.ccdc.cam.ac.uk/free_services/teaching/