

Division of Academic Affairs
Technology Fee – Project Proposal
2015

Proposal Deadline: Wednesday, January 21, 2015

Project Proposal Type

Instructional Technology Enhancement Project (ITEP)

Focused projects proposed by an individual or small team with the intention of exploring new applications of instructional technology. ITEPs will typically be led by a faculty “principal investigator.” ITEPs are time-limited projects (up to two years in length) and allocations of Technology Fee funds to these projects are non-recurring.

Project Title

Crystallography Training Across the Sciences

Total Amount of Funding Requested

\$9,100

Primary Project Coordinator

Tim Royappa, Department of Chemistry

Crystallography Training Across the Sciences

Tim Royappa
Department of Chemistry

I. Project Description

a. Introduction

Crystallography has become an indispensable technique in the physical and life sciences. Its importance is demonstrated in Table 1, which outlines the chief developments in crystallography since its inception in the early 20th century. In fact, 2014 was designated as the International Year of Crystallography, and the key contributions of crystallography to a wide variety of science disciplines were celebrated across the globe. The reason that crystallography is so important is that it is the best way to elucidate the atomic structure of matter, leading to a better understanding of its physical, chemical and biological properties.

Era	Discovery/Advance in Crystallography	Major Awards
1910s	Diffraction of X-rays by crystals discovered by Paul Ewald and Max von Laue; von Laue formulates the basics of crystallography; William L. Bragg works out the fundamental equation of crystallography	Nobel Prize in Physics (1914) to von Laue; Nobel Prize in Physics (1915) to Bragg and his father, William H. Bragg
1920s-1930s	Other forms of crystallography developed by Clinton Davisson and George Thompson	Nobel Prize in Physics (1937) to Davisson and Thompson
1940s-1960s	James Watson and Francis Crick discover the structure of DNA, and Dorothy Hodgkin elucidates the structures of several important small biomolecules, all done by X-ray crystallography	Nobel Prize in Physiology or Medicine (1962) to Watson and Crick; Nobel Prize in Chemistry (1964) to Hodgkin
1970s-1980s	Herbert Hauptman and Jerome Karle greatly simplify crystal structure calculations	Nobel Prize in Chemistry (1985)
1990s-present	Structures of large molecules now routinely solved by crystallography, mostly made possible by prodigious improvements in technology	Several Nobel Prizes in Physics and Chemistry

Table 1. Timeline of some major developments in crystallography.

A prior ITEP project piloted by the PI successfully trained Chemistry students in the basics of crystallography through the use of the Cambridge Scientific Database (CSD), a repository of crystal structures of small molecules. In this proposal, the PI will expand this training to other sciences, namely Biology, Environmental Studies and Physics, while continuing to train Chemistry students in crystallography as before.

b. Project details

The PI will deliver annual training sessions in crystallography, using the appropriate crystallography database(s), to students and interested faculty in Biology, Environmental Studies, Physics and of course, Chemistry. Each training session will be tailored to the needs of the department, and will last one to three hours, depending on the complexity of the training, and the depth to which the database will be explored. The training sessions will be assessed using appropriate quantitative evaluation methods (see sections III. and V. below).

The most relevant crystallography database for Environmental Studies and Physics is the Inorganic Crystal Structure Database (ICSD), which contains crystal structures of important minerals and other inorganic compounds. It requires a paid subscription. For Biology, the key database is the Protein Data Bank (PDB), which contains crystal structures of proteins and peptides. Access to the PDB is free. However, many molecules of biological interest are also found in the CSD, which is a pay-for-access database.

The PI requests funds to purchase a site license for full access to the Inorganic Crystal Structure Database (currently \$2,200 per year) and to the Cambridge Structural Database (currently \$2,200 per year also) for two years in order to train students in the Biology, Environmental Studies, Physics and Chemistry departments. These paid subscriptions will start in 2016, since it is uneconomical to pay a full annual price for a part-year subscription. In the meantime, the PI will be able to use the existing subscription to the CSD and the freely accessible PDB, to provide training for the Chemistry and Biology departments.

II. Alignment of project with UWF Strategic Plan

This project aligns best with the UWF Strategic Plan Values of Quality and Innovation, as well as the Priority area of Teaching and Research. Subscription to these crystallography databases will allow the PI to deliver annual crystallography training sessions to undergraduates and faculty in four different departments (Biology, Environmental Studies, Physics and Chemistry). The training sessions will improve the quality of education at UWF, since the first three of these departments have little education in this important field of science. In addition, the training will acquaint STEM students with modern crystallography, preparing them for greater success, no matter whether they enter the workforce directly or attend graduate/professional schools. Since these databases will be used directly to enhance teaching and research in a wide variety of STEM fields, it is clear that the project is aligned with the stated priorities of the UWF Strategic Plan.

III. Benefits provided

The databases requested in this proposal can be accessed directly through the internet, based on the IP addresses of UWF computers. With a site license, anyone physically at UWF (or logged in through a proxy, e.g., at the UWF library) will be able to access all database features without restriction. This is the main way in which student access to technology will be enhanced. The project will also enhance the student experience by (a) allowing the PI to provide higher quality crystallography instruction and (b) allowing any interested student to view or download any crystal structures that they need for their research or class work. Students and faculty in each department desiring to develop crystallography skills will be trained by the PI in crystallography basics using the appropriate database. The PI has customarily used the library classroom for crystallography instruction, as the necessary software has already been installed on the computers in the room by Fred Barry, UWF Pace Library IT staff. This room can easily accommodate all students and faculty needing training in a single session. Since I have already worked closely with Fred to optimize this room for crystallography instruction, and have his approval for this project (see his support letter in Appendix A), I have no doubts that it will be implemented smoothly.

Assessment will be conducted by a simple pre-post survey method, similar to the PI's previous ITEP proposal that was funded in 2013. This survey instrument is given in Appendix B. It will be given to students participating in this project before and after they complete the crystallography training sessions delivered by the PI.

The estimated number of students impacted by this project is shown in Table 2, below, broken down by department. These estimates were obtained from the average annual enrollment in the courses affected by this project in each department.

Department	Annual number of students affected
Biology	100
Environmental Studies	50
Physics	30
Chemistry	30
TOTAL	210

Table 2. Estimated number of students to be impacted by the project, by department.

It is not known how many students with special needs or disabilities would be affected by this project.

IV. Scope of project

The PI has successfully used the crystallography exercise developed for a previous ITEP-funded pilot project (see Appendix C) to train Chemistry students in the basics of this important

technique. This proposal, which represents an elaboration of that project, will expand crystallography training to allied STEM fields (Biology, Environmental Studies and Physics) by offering annual training sessions tailored for each individual department's needs, while continuing training of Chemistry students.

V. Measurement of success

An identical survey will be administered to students both before and after receiving crystallography instruction in each of the two years of the project. A simple Student's *t*-test will be used to determine whether there is a statistically significant difference between students' crystallography skills before and after instruction, namely in the average score on the seven areas assessed by the survey. A statistically significant increase at the 95% confidence level will indicate that the project was successful. This simple method has yielded very satisfactory results when used by the PI to demonstrate the effectiveness of the PI's two previously funded ITEP projects.

VI. Resources required for the project

Software requirements:

Unlimited Site License to Inorganic Crystal Structure Database, Year 1	\$2,200
Unlimited Site License to Cambridge Structural Database, Year 1	\$2,200
Unlimited Site License to Inorganic Crystal Structure Database, Year 2 (est.)*	\$2,350
<u>Unlimited Site License to Cambridge Structural Database, Year 2 (est.)*</u>	<u>\$2,350</u>
<u>TOTAL REQUESTED</u>	<u>\$9,100</u>

* The prices for the site licenses in Year 2 of the project are estimated based on the recent pricing trends of the CSD.

Hardware requirements:

None

Personnel costs:

None

VII. Project timeline

Date	Project Milestone
<i>2015</i>	
May 1, 2015	Start development of crystallography training exercise for Biology
Aug. 1, 2015	Finish development of crystallography training exercise for Biology
Oct. 1, 2015	Conduct crystallography training session for Biology
Dec. 1, 2015	Purchase site licenses to CSD and ICSD, register UWF IP addresses with vendors

2016

Jan. 1, 2016	PI starts crystallography sabbatical at Northwestern University
Jan. 5, 2016	Testing of full access to CSD and ICSD via internet
Jan. 15, 2016	Start development of crystallography training exercises for Physics, Environ. Studies
Feb. 1, 2016	Start revising crystallography training materials for Biology based on 2015 experience
Mar. 30, 2016	PI completes crystallography sabbatical
Apr. 15, 2016	Conduct crystallography training for Chemistry
May 1, 2016	Finish revising crystallography training materials for Biology
Jul. 15, 2016	Finish development of crystallography training exercises for Physics, Environ. Studies
Sep. 15, 2016	Conduct crystallography training for Environmental Studies
Oct. 1, 2016	Conduct crystallography training session for Biology
Oct. 15, 2016	Conduct crystallography training for Physics

2017

Jan. 1, 2017	Start revising crystallography training materials for Physics, Environ. Studies
Apr. 1, 2017	Finish revising crystallography training materials for Physics, Environ. Studies
Apr. 15, 2017	Conduct crystallography training for Chemistry
Sep. 15, 2017	Conduct crystallography training for Environmental Studies
Oct. 1, 2017	Conduct crystallography training session for Biology
Oct. 15, 2017	Conduct crystallography training for Physics
Nov. 1, 2017	Analysis of survey and usage data
Dec. 5, 2017	Submission of final report on ITEP project

VIII. Sustainability plan

The Pace Library maintains active subscriptions to a number of databases, so if there are sufficient users of these crystallography databases, the Library may have funds available to renew the licenses in future years. Because of the importance of keeping track of the number of users of the database for future sustainability, the PI will maintain usage statistics of the databases. The Chemistry department chair fully supports this project (see Appendix A). However, three years from now is too far in the future to be able to commit department funds for renewal of the database licenses, due to budget uncertainties. Nevertheless, at that time, it may be possible to renew the database subscriptions by pooling funds from Chemistry as well as a collection of interested departments such as Biology, Environmental Studies and Physics, if a sufficient number of faculty are trained by the PI and make use of the databases. It may also be possible to obtain resources for this purpose from the CSEH Dean. Lastly, the PI will be submitting an NSF-IUSE proposal in 2016 for acquisition of a single-crystal X-ray diffractometer, and if funded, this grant may also be able to pick up the subscription costs for the databases. Thus, it appears that many promising avenues exist for sustaining the project in the long term.

IX. Resource matching

None

X. Project implementation

The PI will implement the project. The WebCSD interface that the PI has used successfully in the past allowed IP-based access to the CSD over the internet (no installation required), and the

ICSD is expected to operate similarly. Thus, any computer on the UWF network will be able to access the databases directly, so no IT-related work will be required to implement this project.

XI. Lead person

The PI is Tim Royappa, Department of Chemistry.

XII. Notification of concerned authorities

The Chemistry department chairs, Dr. Matt Schwartz and Dr. Alan Schrock, and the CSEH Dean, Dr. Mike Huggins, have each been given a copy of this proposal.

Appendix A – Support letters



John C. Pace Library
11000 University Parkway
Pensacola, FL 32514-5750

January 14, 2015

To whom it may concern:

I'm happy to have this opportunity to lend my support to Dr. Tim Royappa and this Instructional Technology Enhancement Project proposal, "Crystallography Training Across the Sciences."

The UWF Libraries maintains some of the largest collections of student use computer workstations at our locations on both campuses, and, at the request of Dr. Royappa, for more than the past six years, we've deployed CCDC's *Mercury* software on all of our general student-use workstations and laptops (>300 machines as of this writing). Dr. Royappa has also used this software in our library classroom (currently 30 workstations) for multiple face-to-face instruction sessions using the full Cambridge Structural Database (~600,000 structures). We have already made this database available through the library website for authorized off-campus users, and we anticipate being able to do the same with the Inorganic Crystal Structure Database proposed for acquisition in Dr. Royappa's new ITEP project. Approval of this proposal would greatly expand our collection of databases available and would open up new avenues for instruction and independent exploration by faculty and students in several departments.

I support the instruction work of Dr. Royappa and assisting UWF students by providing access to the software tools that can help them learn most effectively. This proposal does both which is why I'm happy to support it. Please contact me if you have any questions.

A handwritten signature in black ink, appearing to read "Frederic Barry".

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RE: ITEP proposal "Crystallography Across the Sciences" letter of support

Dear Tim,

I am writing this letter to express my support and willingness to participate in the development of laboratory curriculum that involves the use of crystal structure databases that would be acquired through the ITEP proposal titled "Crystallography Training Across the Sciences." As we have discussed, I am charged with the task of developing new laboratory curriculum for Cell Biology that will be changed to a 3000 level course starting in Spring of 2015. While thinking about laboratory exercises to focus on, I have found that my students struggle understanding the structures of macromolecules and other bioinorganic molecules. Because of this, the use of crystallography databases such as the Protein Data Bank to expose students to the fundamentals of crystallographic structure would be a wonderful asset to have. The newly designed Cell Biology course will be required of all of the pre-professional biology majors. We predict that roughly 100 students will pass through this course every year. Because of this, this the equipment gathered through the ITEP proposal would have a high impact on our pre-professional students. In closing, I look forward to working with you further in implementing this project that will provide high impact learning practices for our undergraduates.

Sincerely,



Peter Cavnar, Ph.D.
Assistant Professor, Biology



Department of Environmental Studies
11000 University Parkway
Pensacola, FL 32514-5750

January 16, 2015

Letter of support for Dr. Royappa's ITEP proposal

I am writing in support of Dr. Tim Royappa of the Department of Chemistry, who is submitting a proposal for an ITEP project entitled "Crystallography Training Across the Sciences." Crystallography is important not only in chemistry, but also in a broad range of sciences. This includes environmental science and geology, in which crystallography is valuable in the analysis of mineral samples. The Inorganic Structural Database is known to contain an excellent collection of important mineral crystal structures, and knowing how to use this database will be important for students in my department.

My colleague Dr. Matthew Schwartz and I are willing to participate in this project. Dr. Royappa will work with us to develop a simple and student-accessible training exercise using this database that will be relevant for the crystallographic study of selected minerals. We plan to incorporate versions of this exercise into the Physical Geology course (GLY 2010/L), Environmental Soil Science (EVS4192C), and Sampling and Analysis in Environmental Science (EVS6196C). I estimate that approximately 50 students in my department will be affected per year by this project.

In summary, I strongly recommend that this proposal be funded, as it will have a significant impact on the professional development and career preparedness of students in Chemistry, Environmental Studies and other departments.

Thank you.

Sincerely,

A handwritten signature in blue ink that reads "Liebens".

Johan Liebens
Professor

To the ITEP committee:

I am writing in support of Dr. Tim Royappa, who is submitting a proposal for an ITEP project, titled "Crystallography Across the Sciences." Crystallography is important not only in Chemistry, but also in Biology, Materials Science and other STEM fields. However, the principles underlying this important technology are entirely grounded in Physics. Therefore, it is important that our Physics majors have an understanding of X-ray diffraction as applied to crystallography. My colleagues who teach PHY3106L (Modern Physics Laboratory) and I are quite interested in taking part in this project, particularly in view of the fact that one of our experiments in that course is x-ray diffraction. Dr. Royappa has offered to collaborate with us on developing a suitable exercise for this course using the Inorganic Crystal Structure Database, and this exercise will provide an excellent departure and further study following the existing basic experiment. I also envision that this training will play an important role in enhancing PHY4990L (Undergraduate Research), which is a required course for all Physics majors. Approximately 30 Physics undergraduates per year (15 per semester) can be expected to be affected by our participation in this project.

Dr. Royappa and I have collaborated successfully on several research efforts, and I know that he will be able to implement this project. This proposal has the full support of the Physics faculty, and I wholeheartedly recommend that it be funded through the ITEP program.

Sincerely,

Chandra Prayaga
Chair, Department of Physics.

January 20, 2015

Tim,

The Chemistry department is in full support of your ITEP proposal entitled "Crystallography Training Across The Sciences". The Chemistry department has seen the value of your efforts in teaching our students the important methods for solving crystal structures of organic molecules. Your proposed expansion of the crystallography databases to include inorganic and biological molecules will be very valuable for chemistry students interested in biochemistry and environmental chemistry specializations.

The opportunity to expand the proven success of your approach to teaching crystallography across STEM fields is clearly valued as shown by the support letters from biology, physics, and environmental science. It just makes sense to expand this successful training to other STEM arenas.

Our chemistry students are entering graduate school or the workplace with enhanced skills as a result of your training. Expanding the training to include the Physics, Biology, and Environmental Science departments will make our student population that much more valuable.

Your ITEP proposal is an excellent opportunity to expand collaborative High Impact Practices using a known and successful model. I strongly support this proposal.



Dr. Alan Schrock
Associate Chair, Chemistry

Appendix B – Sample survey instrument for assessing project

SURVEY OF KEY CRYSTALLOGRAPHY SKILLS

Name _____

For each skill listed in the table below, select one of the five options that best describes your comfort level with the application of the skill, at this point in your learning, using this scale:

- A. I am very confident of my understanding of the required skill, and I am certain I could explain it so others could understand it and apply the necessary skill.
- B. I am reasonably confident of my understanding of the required skill. I can apply the skill and I might be able to explain it so others could understand it.
- C. I have some understanding of the required skill. I can apply the skill but I could not explain it to others.
- D. I have heard of the skill, but I do not understand it. I cannot apply the required skill.
- E. I have not heard of the required skill.

Please mark one of the five options at right to represent your comfort level with the application of each of these skills:	A	B	C	D	E
Accessing the Cambridge Structural Database to look up a crystal structure					
Knowing what types of chemical entities are represented in the Cambridge Structural Database					
Finding a crystal structure that has been deposited with the Cambridge Crystallographic Data Centre					
Searching for crystal structures by researcher name, molecular features, etc.					
Obtaining molecular parameters (bond lengths, bond angles, etc.) from a crystal structure file					
Identifying non-covalent bonding interactions (e.g., hydrogen bonding) in the crystal structure of a molecule					
Recognizing the presence of disorder (e.g., disordered solvent molecules) in crystal structures					

Appendix C – Sample crystallography exercise used in training sessions

X-ray Crystallography
Tim Royappa
Department of Chemistry
University of West Florida

Introduction

When X-rays strike a crystal, they are diffracted by the ordered atoms in the crystal, via elastic scattering from the electrons. Measurements of the angles and intensities of these diffracted rays are used to obtain the three-dimensional arrangement of the atoms. This is called X-ray crystallography, and this technique is widely used to determine the structure of a variety of organic, inorganic and biological substances. A timeline of major discoveries and advances in X-ray crystallography is shown in Table 1 below.

Year(s)	Discovery/Advance	Notes
1895	X-rays discovered by Wilhelm Röntgen	First Nobel Prize in Physics (1901)
1912	Diffraction of X-rays by crystals discovered by Paul Ewald and Max von Laue	Nobel Prize in Physics (1914) to von Laue for working out the relationship between diffraction angles and unit cell parameters
1912-1913	William Lawrence Bragg develops an equation for determining spacings between crystal planes by X-ray diffraction	Nobel Prize in Physics (1915) to Bragg and his father, William Henry Bragg, for their contributions to X-ray crystallography
1940s-1960s	Dorothy Crowfoot Hodgkin obtains the crystal structures of several important small biomolecules by X-ray crystallography	Nobel Prize in Chemistry (1964)
2000s	Structures of large molecules ($\sim 10^5$ g/mol) routinely solved by X-ray crystallography	Mostly made possible by prodigious improvements in computer technology

Table 1. Timeline of developments in X-ray crystallography.

Single-crystal X-ray diffraction patterns are obtained using a diffractometer. A schematic diagram of one is shown in Fig. 1(a) below. The diffraction pattern (angles and positions) of spots on the detector screen obtained by rotating the single crystal mounted on a goniometer is analyzed by computer to provide the arrangements of atoms in the crystal, called “solving the

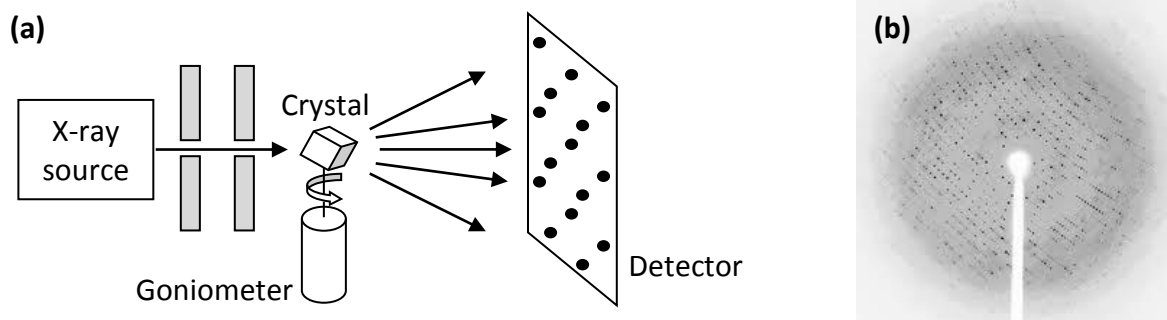


Figure 1. (a) Schematic diagram of a single crystal X-ray diffractometer. (b) A sample diffraction pattern (adapted from <http://departments.colgate.edu/chemistry>).

crystal structure.” Hundreds of thousands of crystal structures of elements, metals, alloys, organic molecules, inorganic complexes, biological molecules and other chemical entities have been solved by X-ray crystallography. Besides providing fundamental physical data such as bond lengths, bond angles and atomic radii, these structures have yielded insights into the very nature of chemical bonding and the relationship between chemical structure and function.

The number of solved structures increases every year, and there exist journals devoted to nothing but crystal structure reports. These structural data are often freely available for research and study, commonly as a standard Crystallographic Information File (CIF), from the major international crystal structure databases shown in Table 2 below.

<i>Crystallography Database</i>	<i>Scope and Content</i>
Cambridge Structural Database, CSD http://www.ccdc.cam.ac.uk/products/csd/	Small organics and organometallics
Protein Data Bank, PDB http://www.rcsb.org/pdb/	Proteins, polypeptides and polysaccharides
Nucleic Acid Database, NDB http://ndbserver.rutgers.edu/	Oligonucleotides
Inorganic Crystal Structure Database, ICSD http://www.fiz-karlsruhe.de/icsd.html	Purely inorganic compounds
CRYSTMET® http://www.tothcanada.com/databases.htm	Metals, alloys and minerals

Table 2. Major international crystal structure databases.

In this exercise, you will be exploring some aspects of the CSD (top entry in Table 2 above) using a small teaching version of the complete database. After learning the basics of how to access and manipulate crystal structure data through the WebCSD interface, you will extract actual chemical information from selected structures stored in the teaching database.

Exercises

You can access the main CSD page from <http://www.ccdc.cam.ac.uk/products/csd/>. Read the introductory material and answer the following questions.

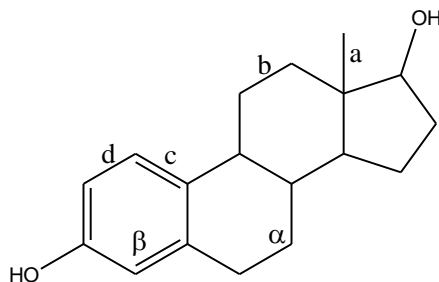
1. Which of the following would you expect to find structures for in the CSD?

Copper	Propane	Sodium chloride	Acetanilide	Aspirin	Heroin
Ferrocene	Glucose	Hemoglobin	Serine	DNA	Steel

2. Approximately how many crystal structures does the CSD contain?

- a. 6,000
- b. 60,000
- c. 600,000
- d. 6,000,000

The demo version, http://webcsd.ccdc.cam.ac.uk/teaching_database_demo.php, is a restricted set of 650 structures selected from the full CSD for teaching purposes. Go to this page, then type the refcode "ESTDOL10" into the "Find Entry" box in the upper left to examine the crystal structure of estradiol hemihydrate. You can check its chemical formula by clicking on the Diagram tab (upper right). Explore different views of the crystal by selecting different packing options. Manipulate the structure on the screen with the mouse and the Shift and Control keys. Right click the display for more options and features.



3. (i) What are the carbon-carbon bond lengths marked a, b, c and d in estradiol?

a _____ b _____ c _____ d _____

Measure the bond angles α and β : α _____ β _____

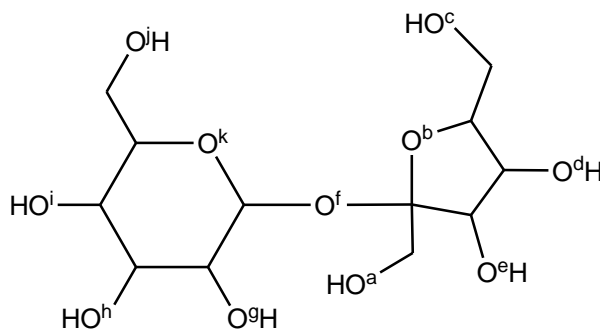
(ii) Are these bond lengths and angles what you would expect? Explain.

Display the unit cell for the crystal structure of citric acid monohydrate, refcode CITARC.

4. (i) How many citric acid molecules are there in the unit cell? _____
How many water molecules? _____
- (ii) What is the total mass of these molecules, in grams? _____
- (iii) Find the unit cell volume, in cm^3 . _____
- (iv) Calculate the density of this crystal in g/cm^3 . _____

Hydrogen bonds are ca. 20 kJ/mol non-bonding interactions between a hydrogen bond donor X–H and a hydrogen bond acceptor Y, where X and Y are strongly electronegative atoms and Y bears a lone pair of electrons [1]. Generally, in such interactions, denoted X–H---Y, the H---Y distance is about 1.2 – 2.2 Å and the X–Y distance is about 2.5 – 3.2 Å [2]. Enter refcode SUCROS01 to display the crystal structure of sucrose.

5. Using the labeling scheme shown below, identify two O–H---O *intramolecular* hydrogen bonding interactions, and one OH group involved in *intermolecular* hydrogen bonding.



Intramolecular H-bonds _____

Intermolecular H-bonding OH group _____

The crystal structure of a compound may sometimes have been determined repeatedly, for a variety of reasons. Open all structures corresponding to refcodes beginning with QAXMEH.

6. What is a crystal polymorph? How many polymorphs of 5-methyl-2-((2-nitrophenyl)amino)-3-thiophenecarbonitrile are there in the teaching database?

Solvent molecules are often incorporated into crystals during crystallization, the most common example being waters of hydration in simple inorganic salts. Dichloromethane is found as a solvate in the structures given by refcodes BEJKUW, (η^2 -C₇₀ fullerene) bis(triphenylphosphine) palladium; DAMROY, (μ_2 -chloro) bis(pentafluorophenyl) xenon(II) hexafluoroarsenate; and NOCHUI, 2,2'-bis(adamant-2-ylidene) chloronium hexachloroantimonate.

7. Explain why the dichloromethane solvate looks so unusual in the NOCHUI structure.

Open refcodes TPASTB, tetraphenylarsonium tribromide; CLPYSB, 2-chloropyridinium pentabromoantimonate(III); and SOBWAH, tetramethylammonium pentafluoroxenate(IV).

8. Draw the Lewis dot structure of Br₃⁻ to explain its geometry using VSEPR theory.

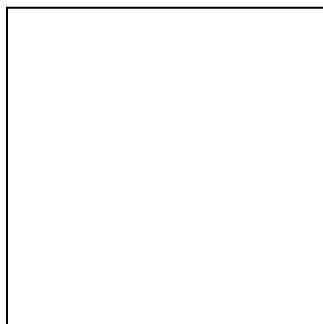


9. (i) How many lone pairs does Sb have in the SbBr₅²⁻ anion?

- a. 0
- b. 1
- c. 2
- d. 3

(ii) What is the geometry of this ion? _____

(iii) Draw the 3-D structure of this ion (including any lone pairs) using wedge bonds.



10. (i) What is the geometry of the XeF_5^- ion? _____

(ii) Draw its Lewis dot structure and use it to explain its shape by VSEPR theory.



The molecule 1,3,5,7-tetramethylcyclooctatetraene (refcode TMCOTT) is tub-shaped, but the corresponding dianion (refcode TMOCKE) is planar.

11. Explain this difference in shape.

References

1. P. W. Atkins and J. De Paula, *Physical Chemistry*, 9th ed., p. 637 (W. H. Freeman & Co., 2010).
2. G. A. Jeffrey, *An Introduction to Hydrogen Bonding*, p. 12 (Oxford University Press, 1997).