

Teaching Chemical Crystallography Without a Diffractometer

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Most of what we know about molecular geometry comes from crystallography. Because crystallography is becoming increasingly important in all branches of chemistry, it needs to be a part of the undergraduate chemistry curriculum. However, most chemistry departments do not own a single-crystal X-ray diffractometer because they are still relatively expensive. This is especially true at a Primarily Undergraduate Institutions (PUIs). Nevertheless, it is possible to teach the basics of chemical crystallography using the Cambridge Structural Database (CSD). We demonstrate how this can be done with two free software tools available from the Cambridge Crystallographic Data Centre: WebCSD and Mercury. Particular attention will be paid to the free teaching subset of the CSD, showing how the basics of crystallography can be taught to undergraduate chemistry, physics, biology and environmental science majors, using only an internet-enabled computer classroom. Our approach, a three-hour “dry lab” exercise involving these tools, has been implemented and used successfully at the University of West Florida, a PUI, for several years.