SINGLE CRYSTAL X-RAY DIFFRACTION

APEX5: The central hub of your crystallography programs

Link all your favorite programs for enhanced productivity

Introduction

APEX5 is the most widely used software suite for single crystal structure determination. It covers the entire process from crystal mounting to CIF report. World-class algorithms ensure reliable and best-in-class results.

Apart from APEX5, there are several other scientific programs developed by the crystallographic community that are specialized in addressing crystallographic problems. These programs, such as ShelXle, PLATON, Mercury, DIAMOND, VESTA, EVAL, JANA2020, or Olex2, offer alternative approaches to crystallography. However, switching between these software packages can be challenging. The poor integration between them requires scientists to repeatedly process the same data and meticulously verify the results for any inconsistencies and errors. These tasks are tedious, error-prone, and redundant, making them time-consuming and unproductive.
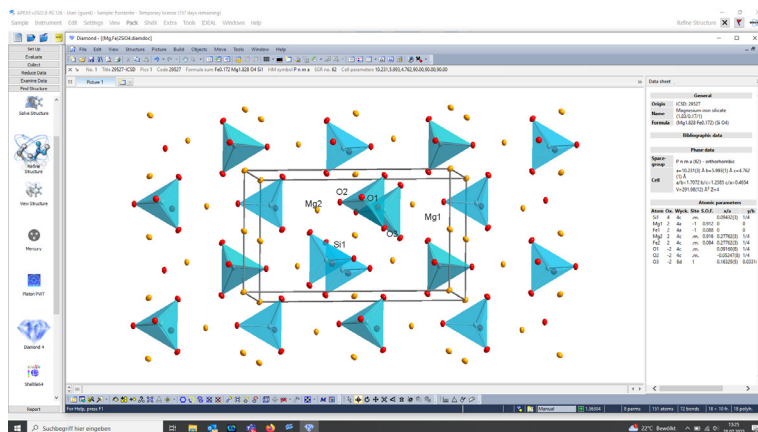
To enhance productivity, it is important to be flexible and agile.

As a flexible and agile crystallographic software suite, APEX5 is designed to meet the requirements of modern scientific research while catering to individual preferences. One of its key strengths is its ability to interface with a range of external crystallographic software packages. The software has been meticulously tested to ensure that data integrity is maintained during the import and export process. This feature significantly boosts productivity, making APEX5 an indispensable tool for scientific research.

How does interfacing with external programs work?

The integration of third-party crystallographic software is extremely simple:
You can set up your APEX5 installation as our crystallographic software hub by linking it directly to your preferred programs. Simply drag and drop the third-party program's startup file to the APEX5 task menu. The APEX5 software integration dialog will then open, automatically loading all the information needed to configure the link. You can also specify advanced program settings if desired. Once linked, your external program will appear in the APEX5 tools box for easy access.

APEX5 simplifies linking external programs. It eliminates search and reloading of data files, saving time and effort. With a single click, continue working with the external program.

APEX5 unlimited - simply drag and drop the third-party program's startup file to the APEX5 task menu. This will create icons in the APEX5 taskbar for the new programs. With a single click, the linked external program will open, loading your most recent files.

PLATON

Platon is a comprehensive collection of powerful crystallographic programs that has been developed over several decades. It includes features such as geometry evaluation, void calculations, solvent removal (SQUEEZE), symmetry and twinning checks, and many others that are popular among users. By clicking on the program link in APEX5, users can access a plethora of highly specialized programs, which provide detailed data and structure analysis.
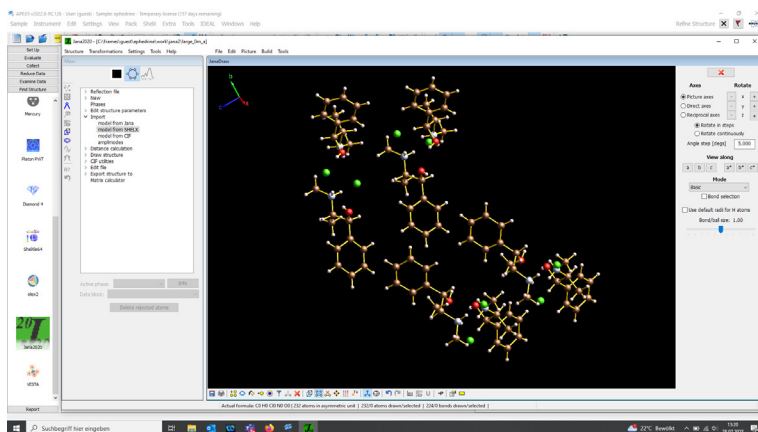
DIAMOND/VESTA

In order to comprehend the arrangement of solid-state compounds, it is essential to conduct a thorough examination of their coordination spheres. Displaying coordination polyhedra serves as a useful method to visualize the coordination environments. DIAMOND and VESTA offer exceptional capabilities in this regard. Simply click on the program link in APEX5 and benefit from these excellent tools for solid-state chemistry.
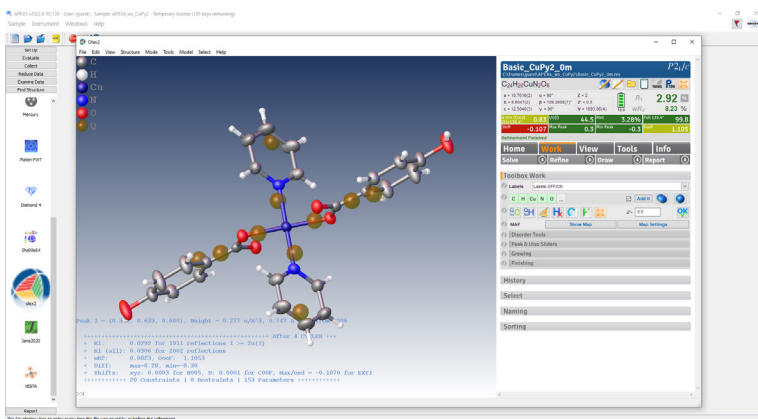

JANA2020

Modulated and Quasi-crystals pose an ongoing challenge to most crystallographers. JANA2020 is the gold standard if the periodicity of the crystal under investigation expands to "higher" dimensions. Just click the program link in APEX5 and the multidimensional journey seamlessly continues.

Olex2

Olex2 and NoSphereA2 can be utilized for building and refining structures. Simply click on the program link icon in APEX5 to continue your work.
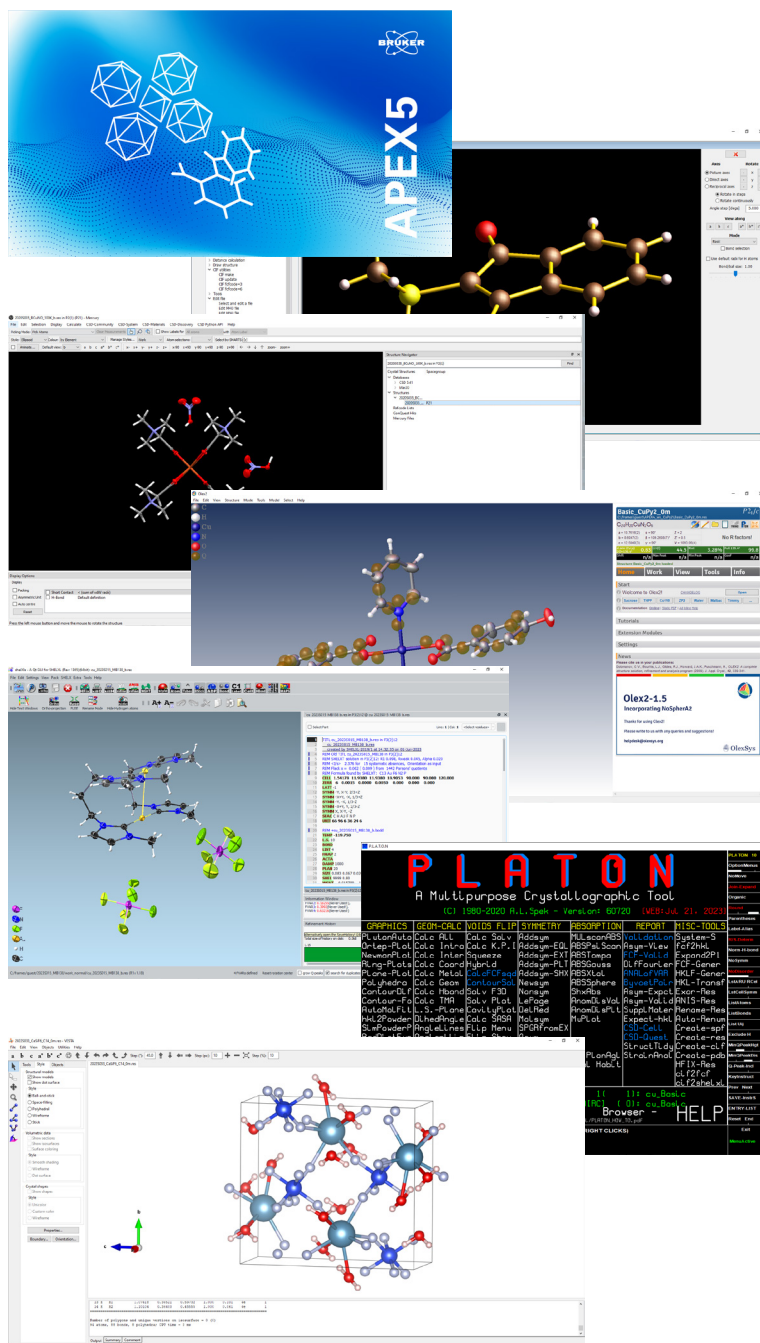
Conclusion

APEX5 serves as the central hub of your crystallographic workflow, providing a direct link to any external software. It allows you to access frequently used programs with a single click, and fully integrates them into the APEX5 interface. This ensures that your latest data is automatically transferred to the third-party program, eliminating the need for manual switching between programs and time-consuming reloading of data. With APEX5 in the center for all your crystallography software needs, you can significantly increase your productivity and streamline your workflow.

Designed for the Future

APEX5 continues to evolve, driven by invaluable user suggestions and the collective experience of the scientific community. This forward-thinking approach ensures that APEX5 remains at the forefront of cutting-edge crystallography software.

Empowering the Crystallographic Community

By being a part of the Bruker Users' Group, APEX5 users gain access to a vibrant global family in crystallography. Exchange insights, receive timely responses, and stay informed on the latest developments within the community.