

MS25-P05 | CONTINUOUS ROTATIONAL ELECTRON DIFFRACTION METHOD FOR STRUCTURE DETERMINATION OF SMALL ORGANIC MOLECULES

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The properties of a material are well related to their structures. X-ray diffraction method is the most commonly used technique for structure determination of crystalline materials. Compared with X-ray, electrons have much shorter wavelength and much stronger interaction with atoms in the crystal. Therefore, electron crystallography can effectively determine the structures of nano- and micron-sized crystals. In recent years, 3D electron diffraction techniques are used for structure determination of various types of complex structures such as zeolites and metal-organic frameworks (MOFs). However, some materials are sensitive to the high energy of electrons which will lead to structural distortion. Here we use the continuous rotation electron diffraction (cRED) method developed in our group to investigate the crystal structure of a small molecule. During the cRED data acquisition, the goniometer is continuously rotated at a constant speed. The typical collection time of cRED data is less than 5 mins which makes it possible to study electron beam sensitive materials. We demonstrate that by using cRED we could determine the structure of a small organic molecule, which is nano-crystal and highly beam sensitive. The unit cell parameters and space group were determined from 3D reciprocal space, and the structure was solved by using Shelx. All the atoms were found directly.