

EDOT-acid Crystals

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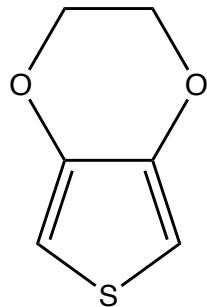
Shrirang Chhatre

David C. Martin

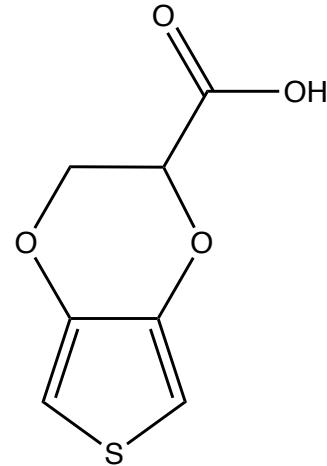
The University of Delaware

EDOT and EDOT-acid

Oily liquid
 $C_6H_6O_2S$
142.18 amu

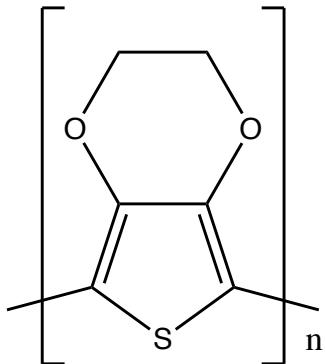


3,4-ethylenedioxythiophene

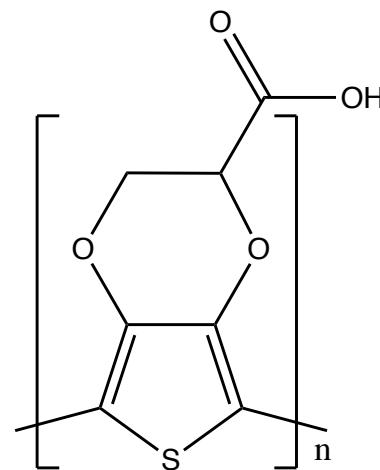


Solid
 $C_7H_6O_4S$
186.18 amu

Electrically and
ionically active
polymers:
dark blue



PEDOT

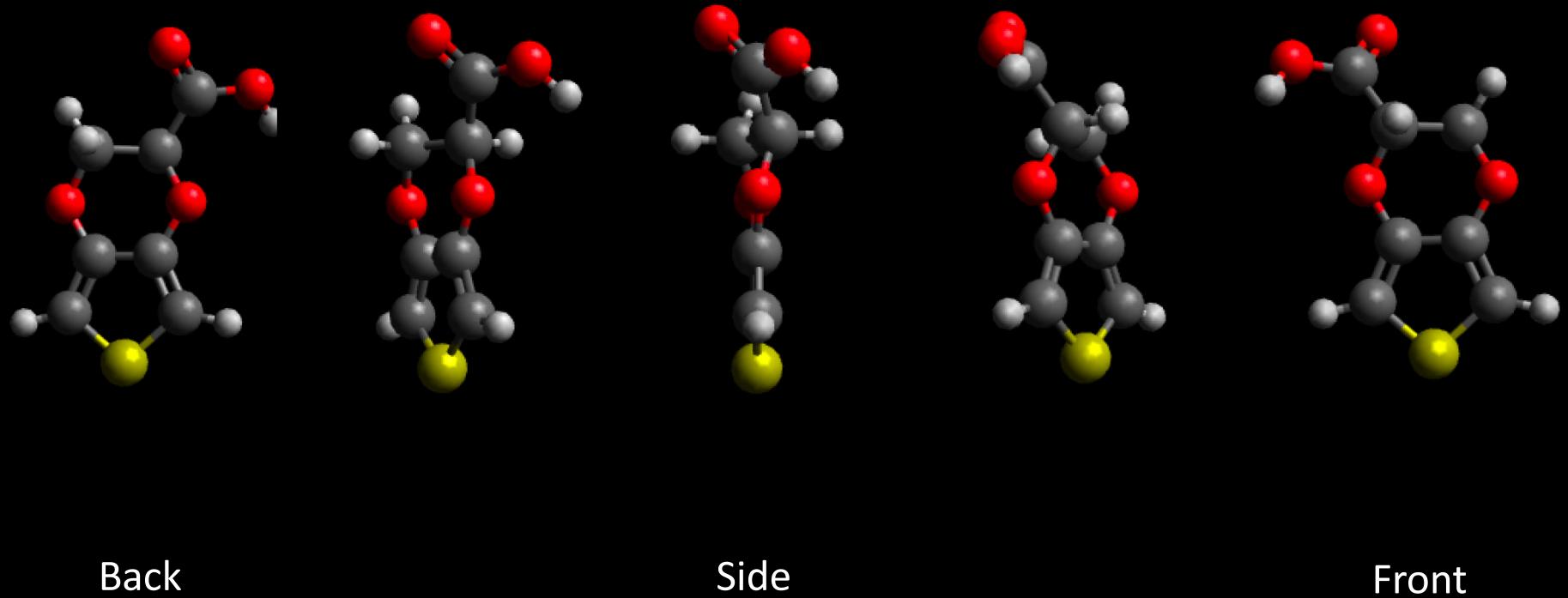


P(EDOT-acid)

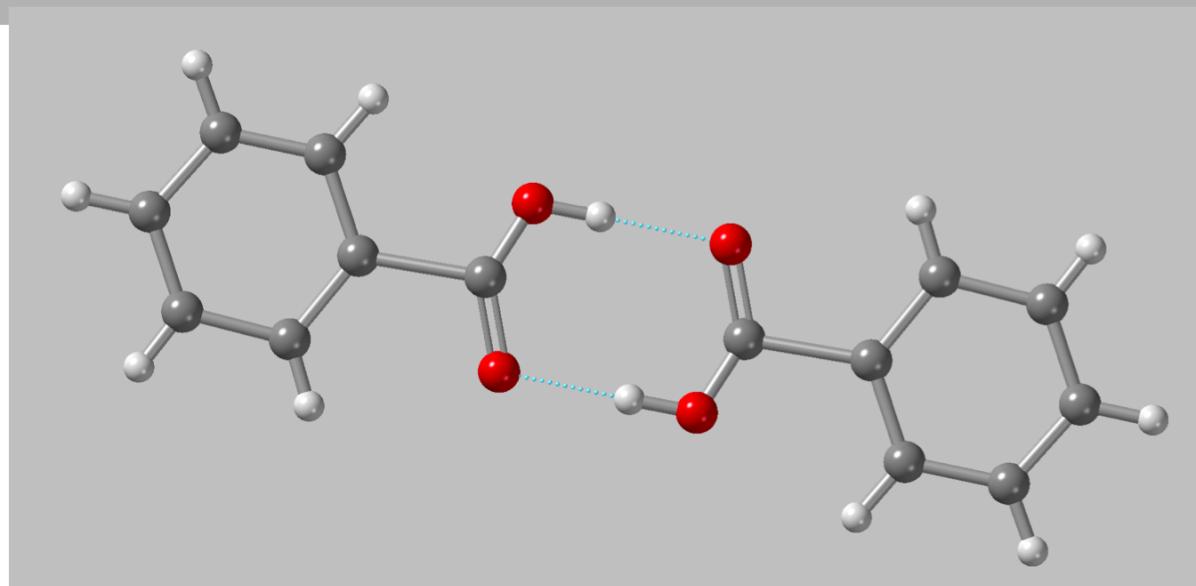
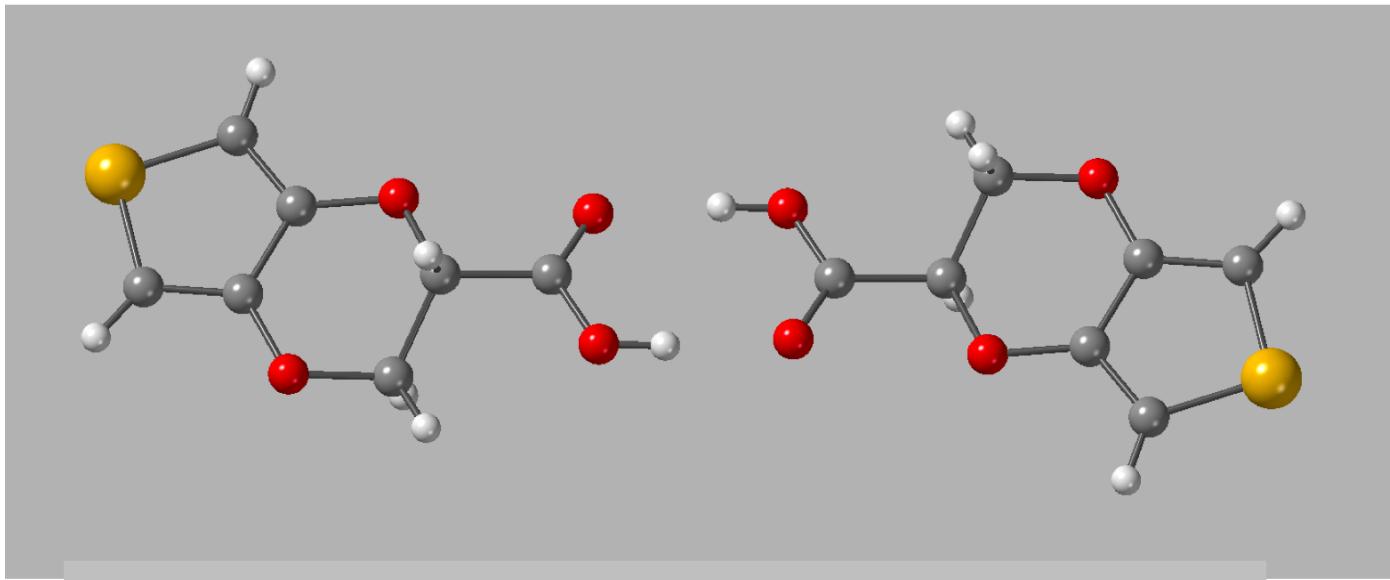
EDOT-acid crystals

- Melt at ~145 C... solid at room temperature
- Dissolve in a variety of common solvents
- Crystallize when evaporated
- Crystal structure was previously unknown
- Molecule has a chiral center... so there are left and right handed versions possible (enantiomers)
- Other molecules with acids form pairs.. dimers
- Other molecules pack in herringbone patterns

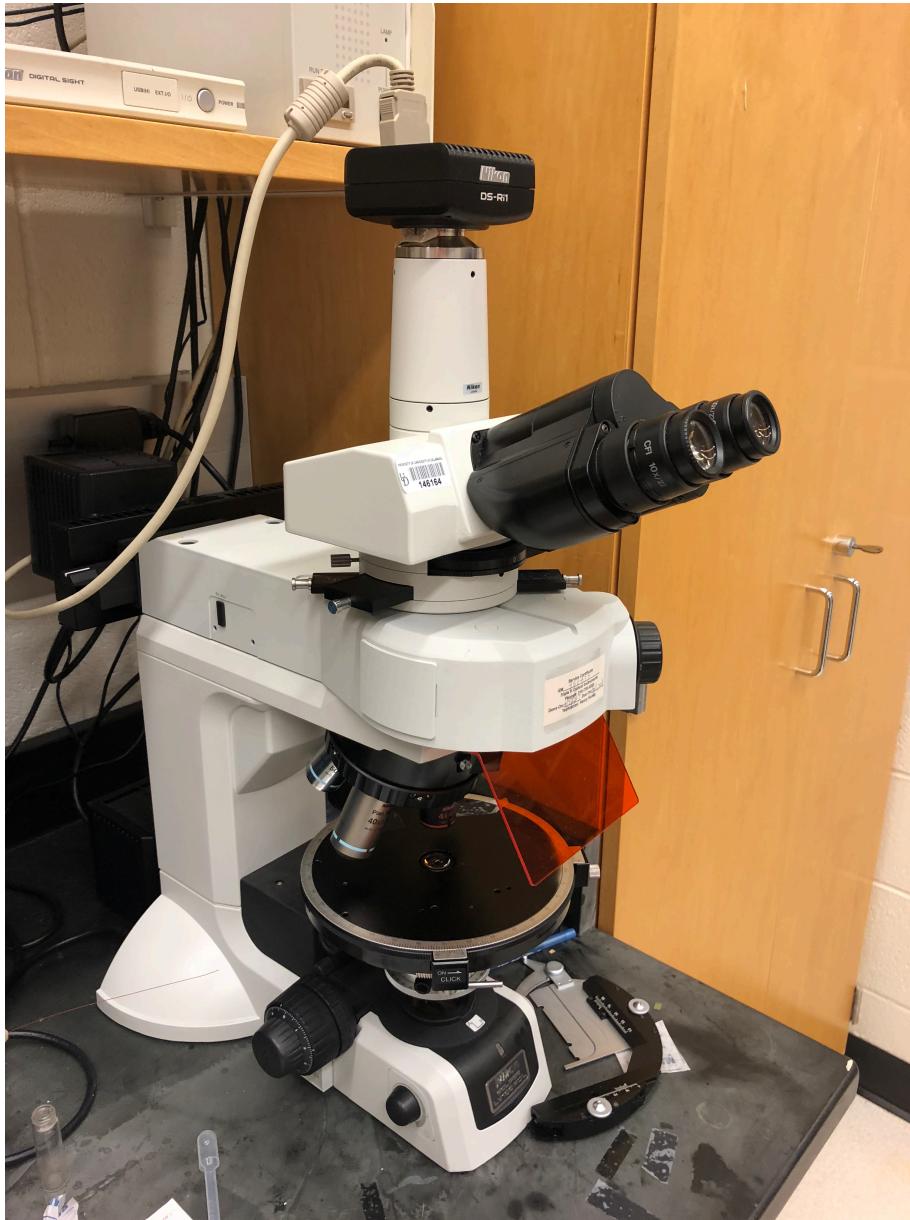
EDOT-acid enantiomers

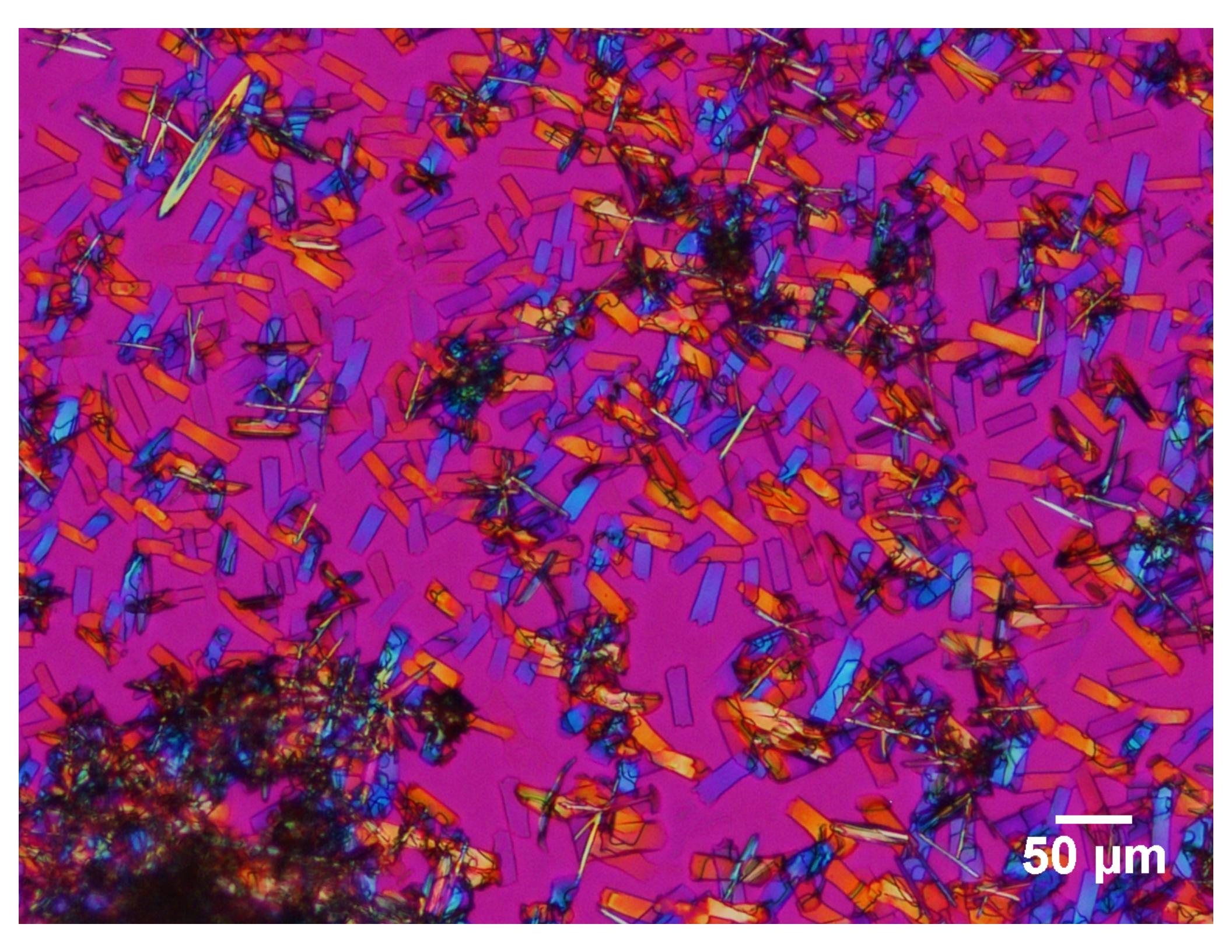


Carboxylic-acid bonded dimers

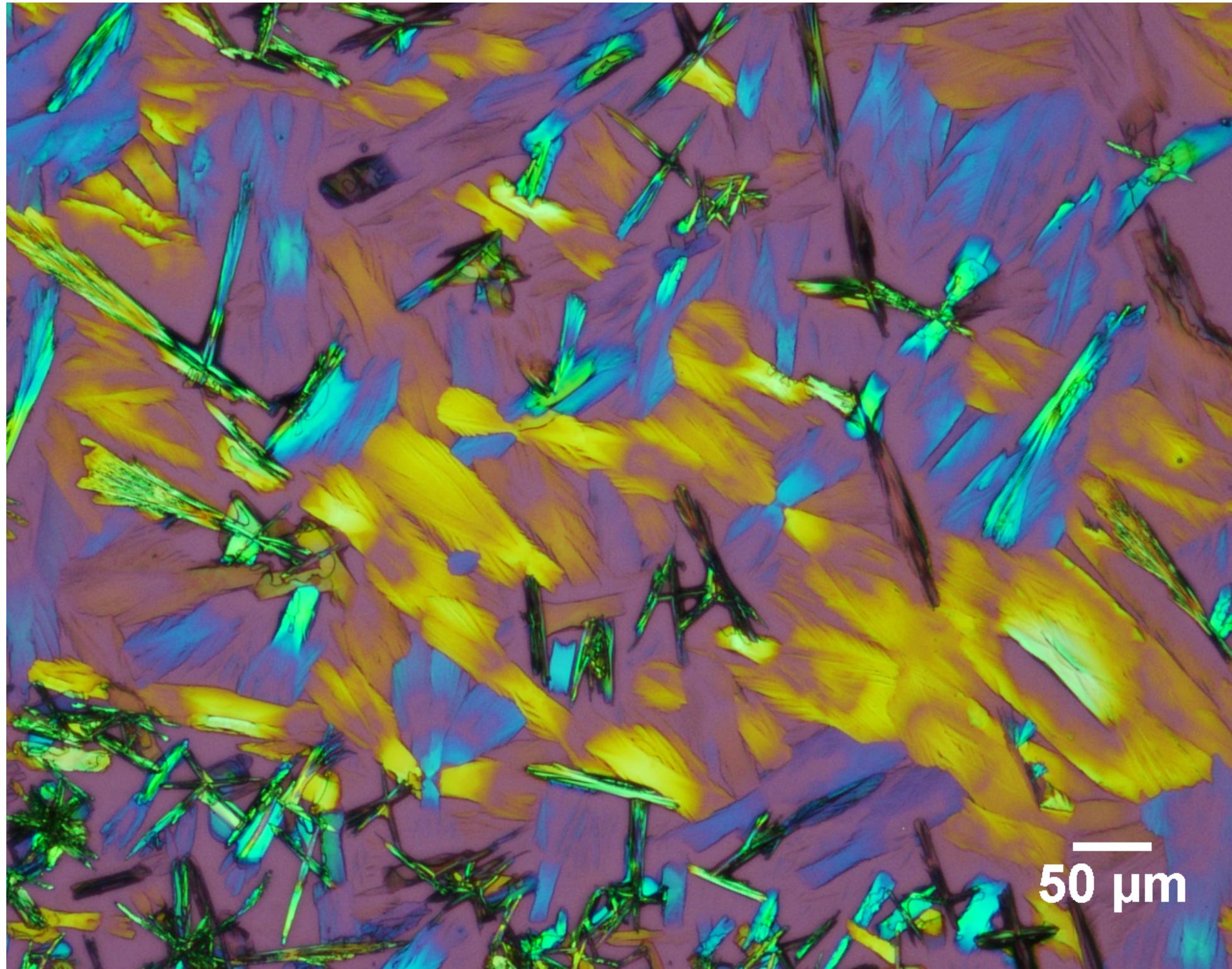


Optical microscopy



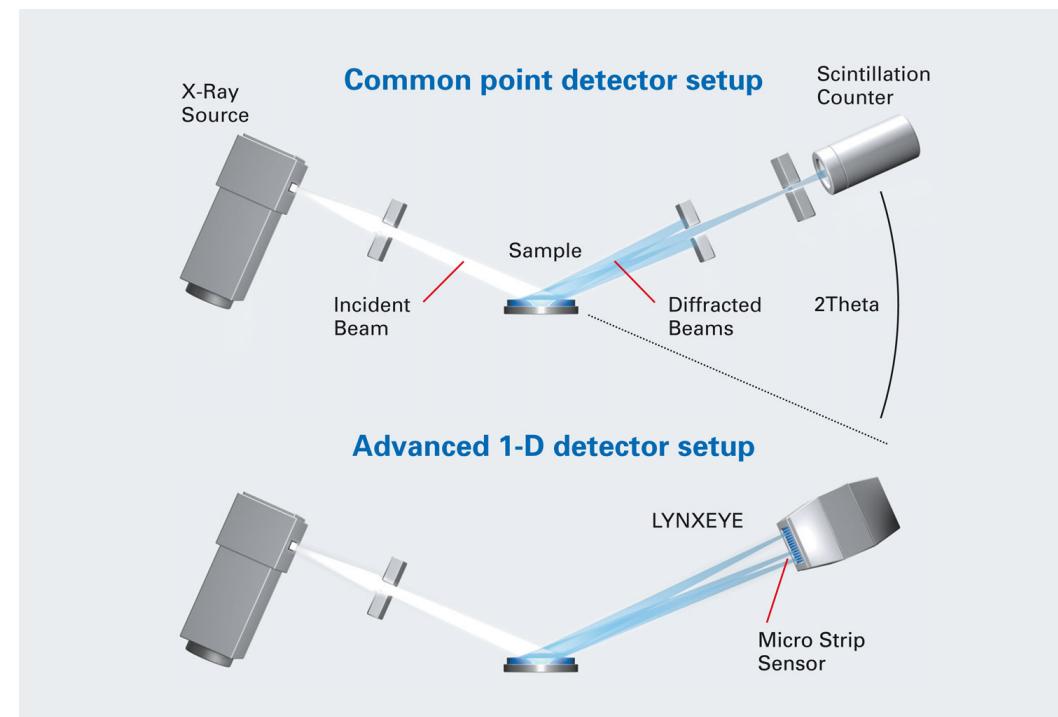


50 μm



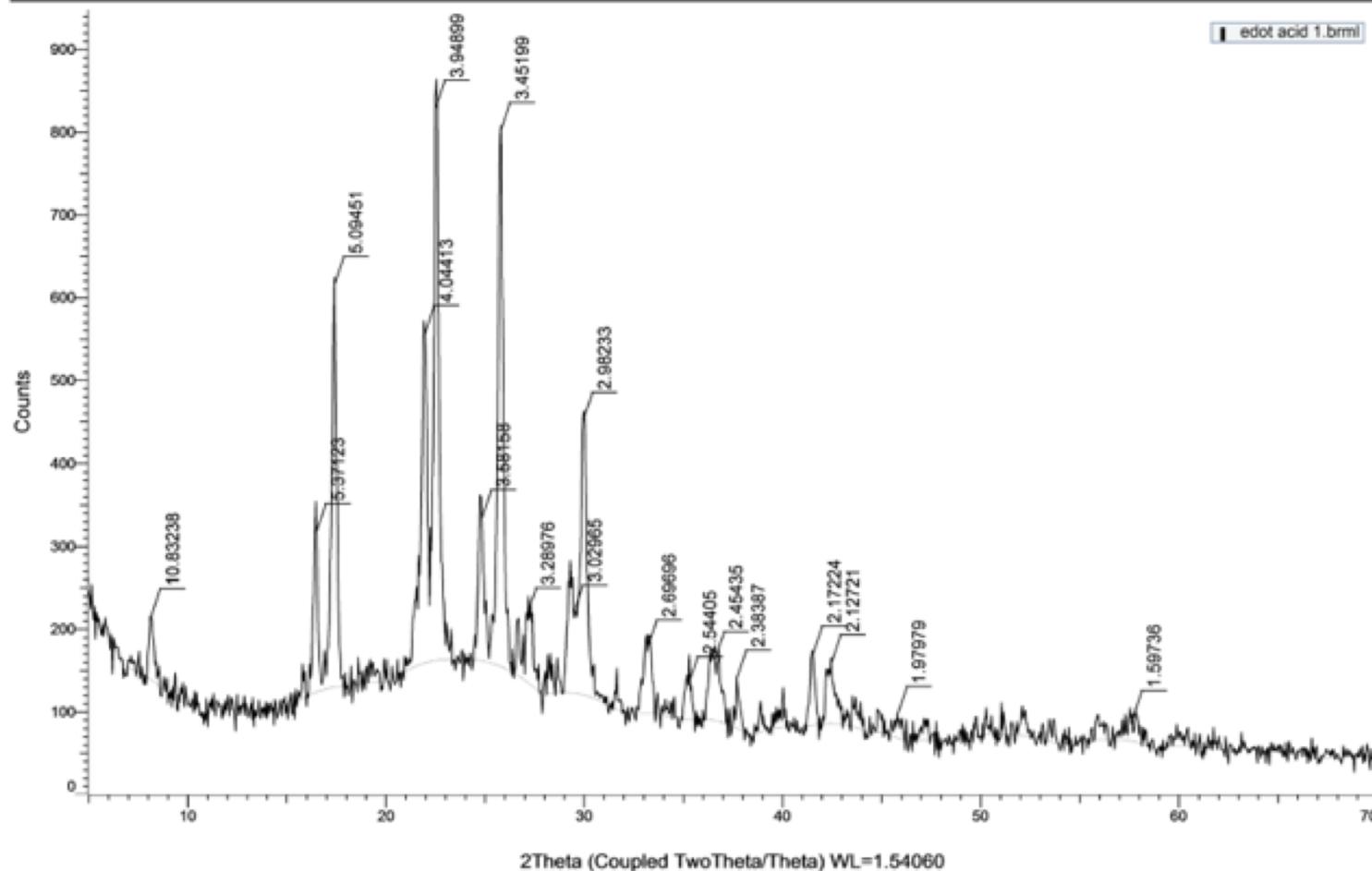
50 μm

Powder X-ray Diffraction

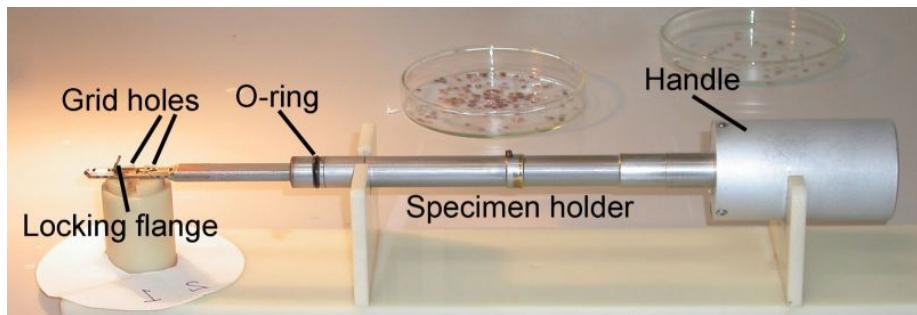


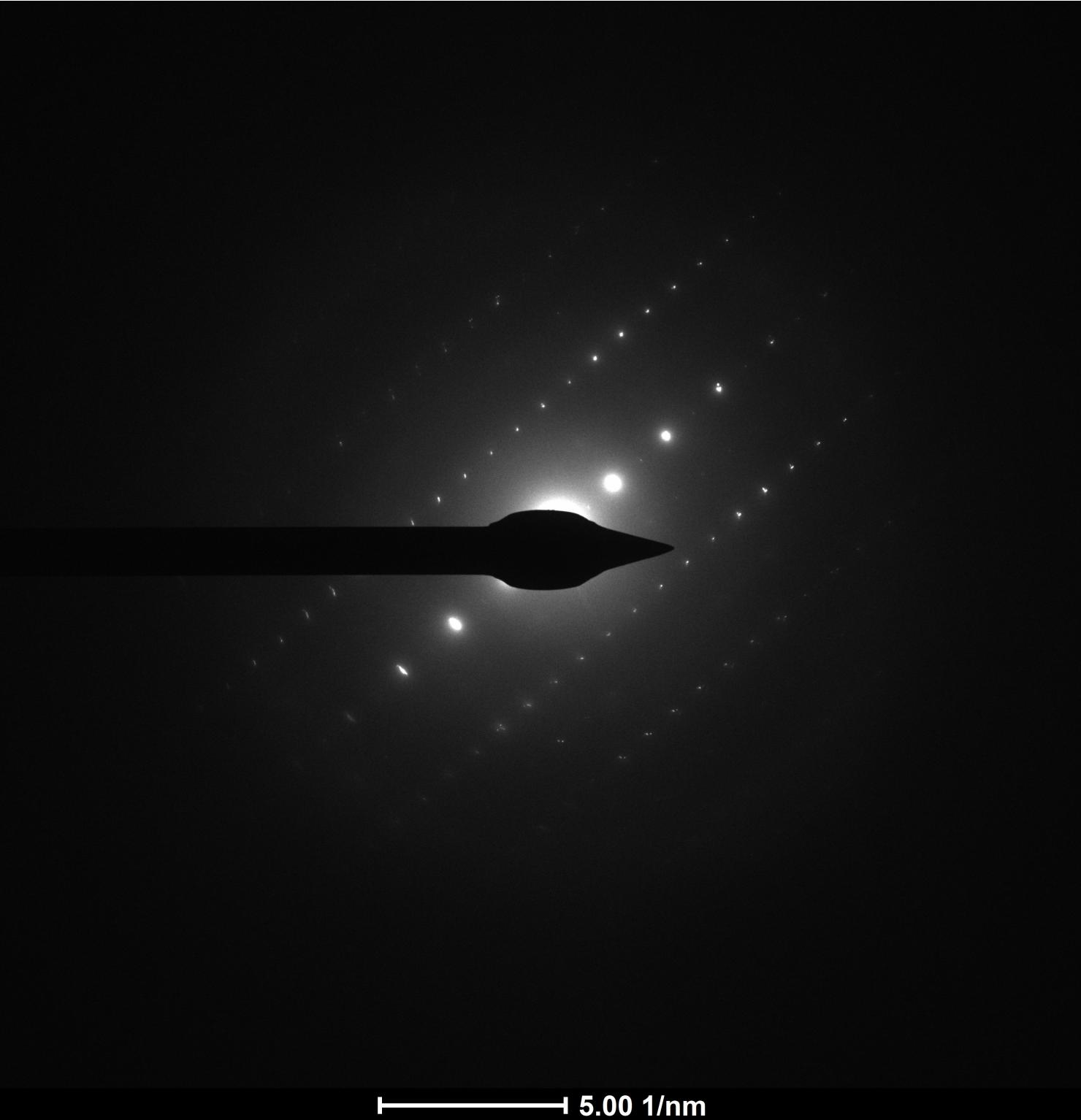
Powder XRD

Commander Sample ID (Coupled TwoTheta/Theta)

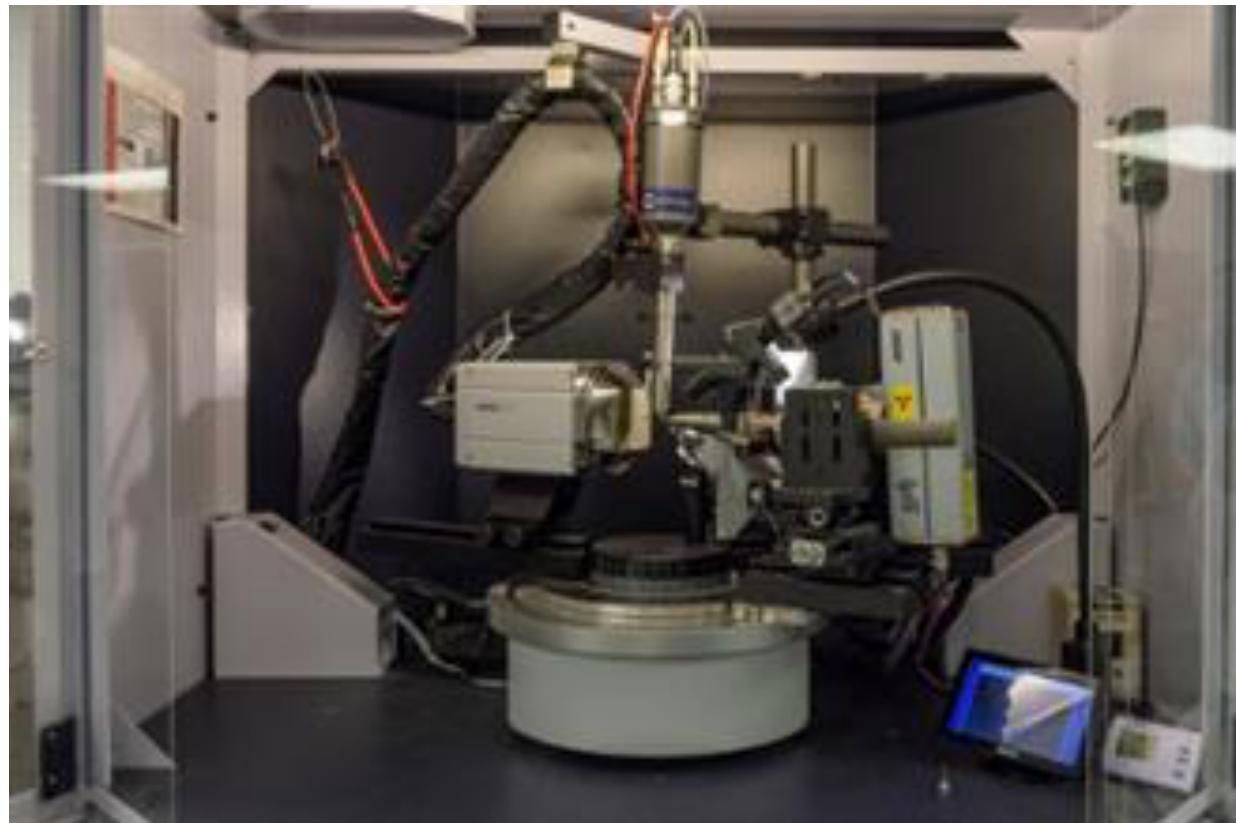


200 kV Talos TEM Electron diffraction





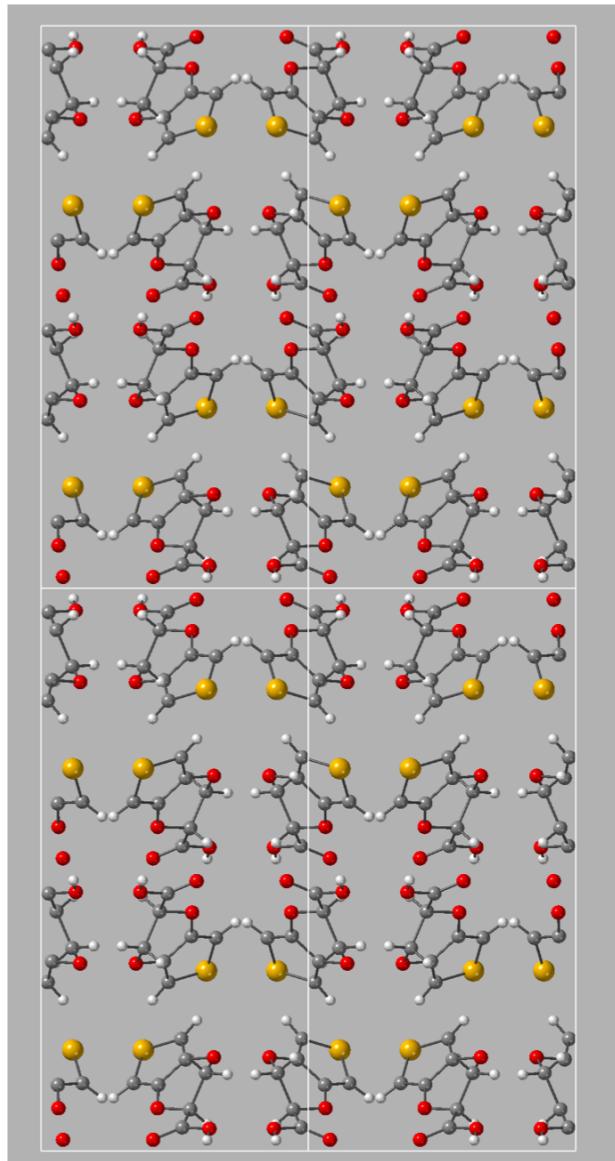
Single Crystal analysis



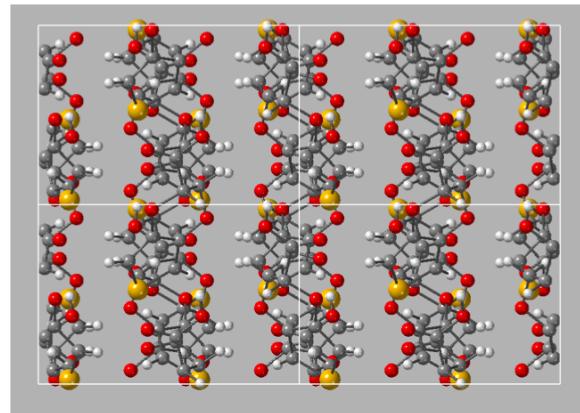
Required slow growth of large (~1 mm) crystals from different solvents

Single Crystal results

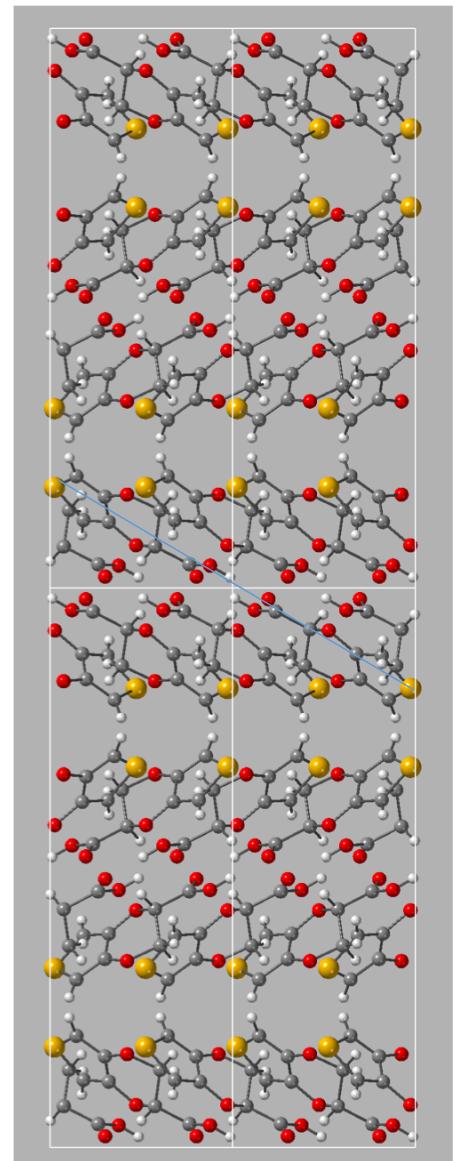
- Space group Pbca, Orthorhombic, No. 61
- 8 monomers / unit cell
- $8 (\text{C}_7\text{H}_6\text{O}_4\text{S} @ 186.18 \text{ amu}) = 1489.44 \text{ amu}$
- $a=1.0142 \text{ nm}, b=0.6992 \text{ nm}, c=2.1392 \text{ nm}$
- $a=10.142 \text{ \AA}, b=6.992 \text{ \AA}, c=21.392 \text{ \AA}$
- EDOT-acid in dimers, in pairs of opposite chirality
- Dimers arrange in layers with herringbone packing
- Density = 1.630 g/cm^3



[010]

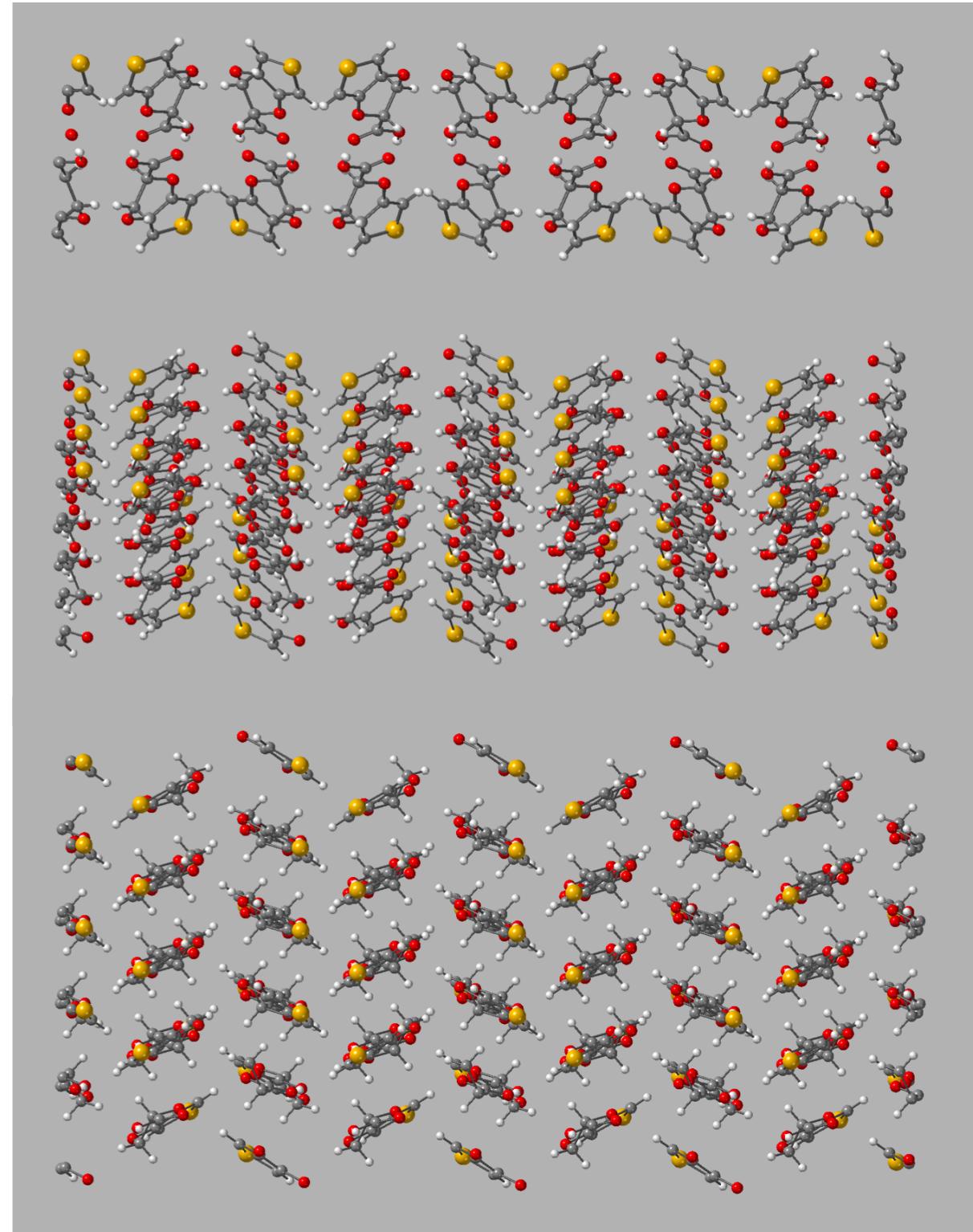


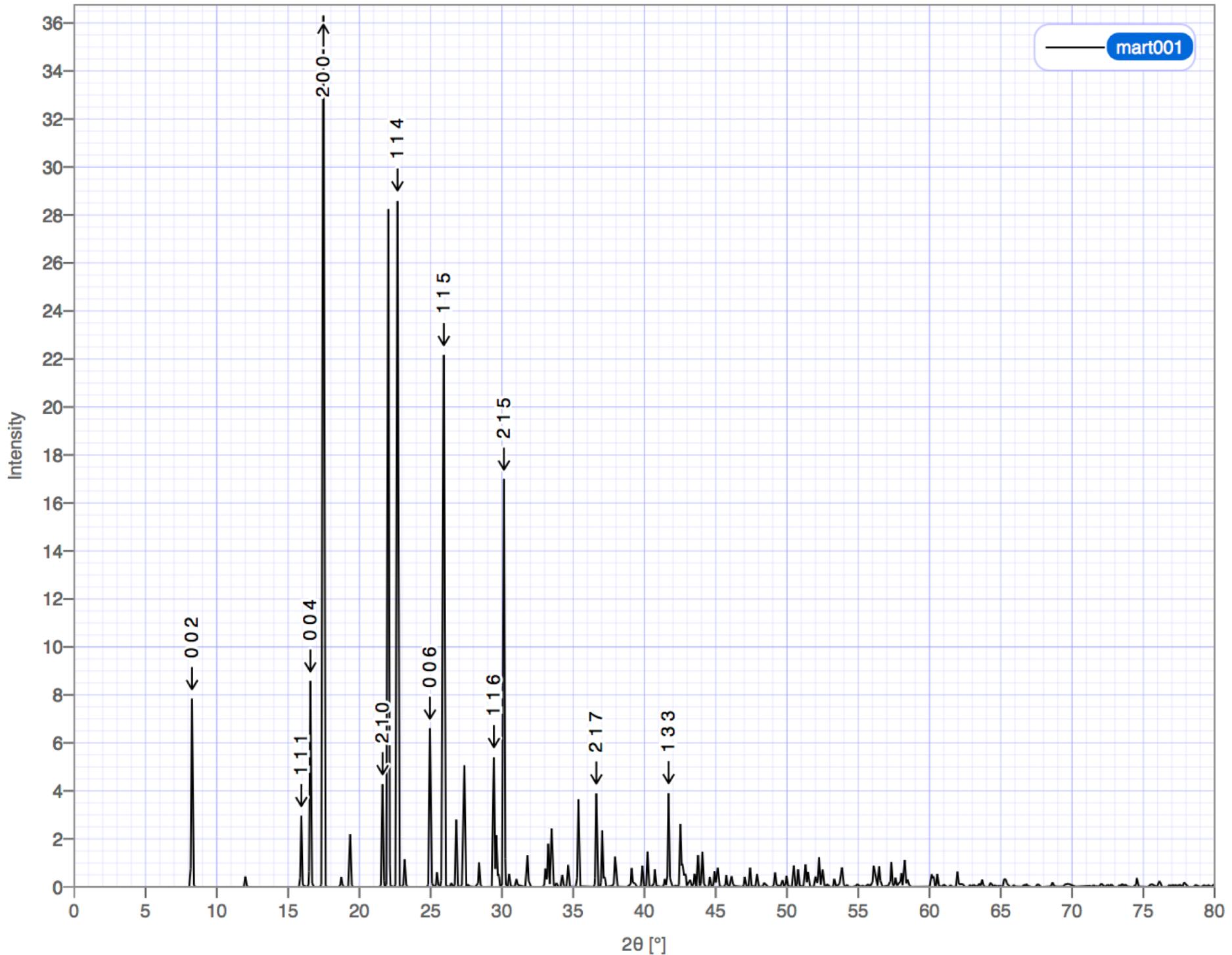
[001]

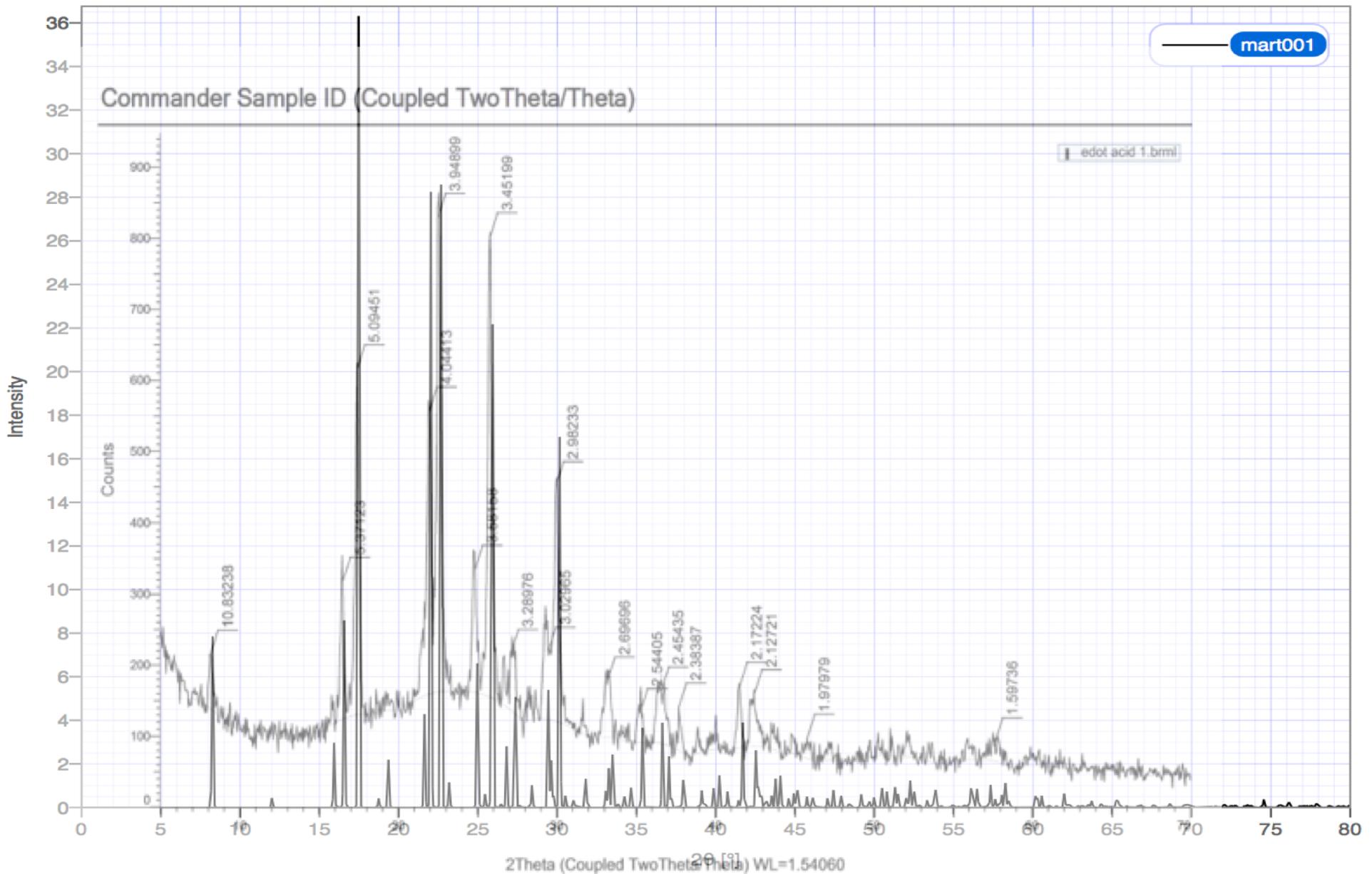


[100]

Herringbone packing of EDOT-acid dimers in (001) slabs







Simulated [001] projection SAED

