How Crystallography in Synergy with Spectroscopy and Computation Catalyzed a Career in Chemical Crystallography

Joel Bernstein

Ben-Gurion University & NYU Abu Dhabi/Shanghai
yoel@bgu.ac.il

As a graduate student in the 1960's my thesis research dealt with using the technique of polarized specular reflection spectroscopy on single crystals to determine the polarization of the electronic transitions in two classic molecular crystals, *trans*-stilbene and *trans*-azobenzene, both planar in the solid state. This spectroscopic method required having available the crystal structures of the materials and knowing how the molecules in those structures projected onto each of the observed crystal faces.

Thus the technique was limited to solids with known crystal structures, so in order to expand the possibilities for systems to investigate I sought a postdoctoral in a crystallography laboratory – actually successive postdoctorals in the laboratories of Ken Trueblood and Gerhardt Schmidt. In that period I also became interested in benzylideneaniline, the molecular "hybrid" of the two above compounds, which though isoelectronic with them exhibits a very different solution absorption spectrum, presumably due to a non-planar conformation. A serendipitous discovery of a crystal structure of a substituted benzylideneaniline with a planar conformation – as one of a pair of polymorphic structures in which the second structure was non-planar – led to a combination of collaborative crystallographic and spectroscopic studies. The computational investigation of the two polymorphs resulted in our first study of conformational polymorphism.

This talk will recount these decade-long developments.