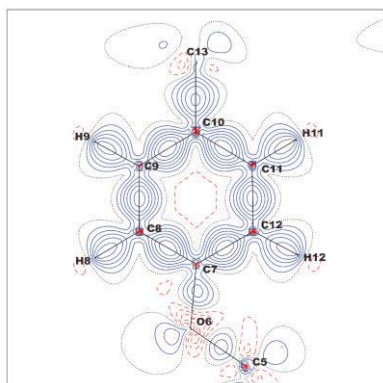


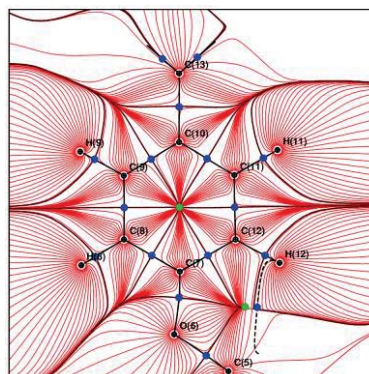
## Experimental Electron Density Distribution of Tamoxifen Citrate

Edwin Stevens & Skyler Hornback  
Western Kentucky University

The experimental electron density distribution of tamoxifen citrate has been determined from high resolution single crystal x-ray intensity measurements collected at a reduced temperature. Tamoxifen is a drug with mixed estrogenic antagonist and agonist properties. It has been proven to produce survival advantages in both node-positive and node-negative breast cancer, reduce the likelihood of cancer cells spreading to both breasts, and in low doses can be used as a preventative for breast cancer and other post-menopausal diseases such as osteoporosis. A total of 123477 intensity measurements were collected with Mo K $\alpha$  radiation from a small needle-shaped crystal cooled to 120 K in a stream of cold N<sub>2</sub> gas, yielding 13634 independent x-ray structure factor. The electron density distribution was determined by multipole refinement of density distortion parameters using *XD2006*. Topological analysis of the density distribution using the Quantum Theory of Atoms in Molecules shows evidence for bond paths corresponding to C-H  $\cdots$  O hydrogen bonds in addition to stronger N-H  $\cdots$  O and O-H  $\cdots$  O hydrogen bonds. Of particular interest are plots of the molecular electrostatic potentials of the separate tamoxifen cation and citrate anion that show distinct regions of positive and negative potential at opposite ends of each ion.



Static experimental deformation density of the central aromatic ring of tamoxifen. Contours are plotted at 0.1 eÅ<sup>-3</sup>.



Gradient trajectory plot of the total electron density in the central aromatic ring of tamoxifen.