

## W0135

**Charge Density Studies of Urotropine-*N*-Oxide·Formic Acid.** Cara L. Nygren<sup>1</sup>, Chick C. Wilson<sup>2</sup>, John F.C. Turner<sup>1</sup>, <sup>1</sup>Dept. of Chemistry, Univ. of Tennessee, Knoxville, TN 37996, USA, <sup>2</sup>Dept. of Chemistry, Univ. of Glasgow, Glasgow G128QQ.

The variable temperature single crystal X-ray diffraction data for urotropine-*N*-oxide·formic have been collected using a Bruker AXS 1000 diffractometer. It crystallizes in the space group  $P2_1/n$ .

Initial spherical atom refinements were performed using the SHELXTL suite of programs (Sheldrick, 1997). Difference Fourier maps were used to examine the electron density associated with the proton position associated with the hydrogen bond between urotropine-*N*-oxide and the formate segment using WinGX (Farrugia, 1999). Further spherical atom refinements were performed using GSAS (Larson, 2000) employing anisotropic refinements on the hydrogen bonded proton position. Aspherical atom refinements were performed using the XD suite of programs (Koritsanszky et al, 2003). Charge density and deformation density analysis has given a considerable amount of insight into the nature of the bonds present urotropine-*N*-oxide·formic acid.

