Rapid charge density data collection

Damon A. Parrish¹, J.R. Deschamps¹, A. Coop², L.N. Thatcher², H. Wu², J. Ferrara³, L. Daniels³, ¹Laboratory for the Structure of Matter, Naval Research Laboratory, Washington, DC 2037. ²Department of Pharmaceutical Sciences, University of Maryland School of Pharmacy, Baltimore, MD 21201. ³Rigaku / MSC, Inc., 9009 New Trails Dr. The West of The Trails Dr. The West of Trails Dr. T Trails Dr., The Woodlands, Texas 77381-5209. E-mail: damon.parrish@nrl.navy.mil

A charge density study has been completed on 17-Cyclopropylmethyl-4,14-dihydroxy-3-methoxymorphinan-6-ethylene member of an important class of opioid compounds. The two methoxy groups of this compound exhibit unexpected chemical reactivity. Addition reactions strongly favor the more sterically hindered O5 position rather than the O3 position.

Data were collected on an R-Axis Rapid Curved Image Plate. The statistical analysis of the data set as well as the complete results of the multipole refinement will be presented. This will include topological analysis as well as an analysis of the electrostatic potential.

Keywords: electron density distribution, charge density, chemical reactivity and structure