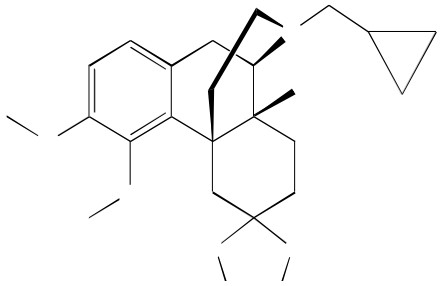
W0273

Rapid Charge Density Data Collection. D.A. Parrish[1], J.R. Deschamps[1], A. Coop[2], L.N. Thatcher[2], H. Wu[2], J. Ferrara[3], and L. Daniels[3], [1]Laboratory for the Structure of Matter, Naval Research Laboratory, Washington, DC 20375, [2]Dept. of Pharmaceutical Sciences, Univ. of Maryland School of Pharmacy, Baltimore, MD 21201, [3]Rigaku/MSC, Inc., 9009 New Trails Dr., The Woodlands, Texas 77381-5209.



A charge density study has been initiated on 17-Cyclopropylmethyl-4,14-dihydroxy-3-methoxymorphinan-6-ethylene ketal, a 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. The goal of this study is to determine the cause for this reactivity while testing the data quality obtained by a new Rigaku/MSC curved image plate. Preliminary results have suggested that the increase in data collection speed did not come at the cost of data quality. The statistical analysis of the data set as well as the preliminary results of the multipole refinement will be presented.

Data were collected on an R-Axis Rapid Curved Image Plate. A rotating molybdenum anode equipped with VariMax Mo optics were used for the data collection. The data collection took less than two days and yielded data that was complete to 0.40Å with an average redundancy of 6.4.