

## Structural Investigation of 4,4,8,8-Tetrahalotricyclo[5.1.0.0<sup>3</sup>,5]octanes

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As a means of introducing carbene chemistry into the undergraduate organic chemistry laboratory, our laboratory has been synthesizing dihalocyclopropanes for 25 years. The simplest of these compounds are liquids and volatile solids, so for structural studies the synthesis of 4,4,8,8-tetrahalotricyclo[5.1.0.0]octanes was explored. Now, six tetrahalotricyclooctanes containing chlorine and bromine have been synthesized and a number of been examined by x-ray crystallography. The structure of tetrabromotricyclooctane is very similar to the other halogenated tricyclo[5.1.0.0<sup>3</sup>,5]octanes, exhibiting a nearly planar cyclohexane ring. Also, the orientation of the two cyclopropane rings as determined are anti, although the synthesis possibly yielded a small amount of the syn substituted isomer.

While those results were expected, what has been fascinating is that in compounds containing both bromine and chlorine in the same compound, there is little preference for bromine or chlorine in any position. This leads to mixed site occupancy. For example, in 4,8-dibromo-4,8-dichlorotricyclo[5.1.0.0]octane, the refinement converged with the occupancy of bromine in the equatorial-like positions at 52%. The chlorine had an occupancy in the axial-like position of 52%.