Experimental Electron Density Distribution of Dimethoxygossypol, a Derivative of the Disesquiterpene Gossypol Isolated from Cotton Plants

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Gossypol is a natural product isolated from the cotton plant that is of interest because of its wide sphere of bioactivity. We have isolated and synthesized a number of derivatives of gossypol to explore their anticancer and antifungal activity. Crystals of the 6,6'-dimethoxy derivative were found to be suitable for a high-resolution study of the electron density distribution. A highly redundant set of x-ray diffraction intensity measurements was collected to $(\sin \theta / \lambda)_{\text{max}}$ of 1.19 Å\(^{-1}\) at 120 K. The experimental electron density distribution was obtained by least-squares refinement of the x-ray data using the Hansen-Coppens aspherical atom multipole model.

In addition to maps of the molecular deformation density, the topology of the electron distribution of dimethoxygossypol has been analyzed using the \textit{Atoms in Molecules} approach. The locations of the critical points of the electron distribution, and the values of the density, $\rho(r_b)$, Laplacian $\nabla^2 \rho(r_b)$, and bond ellipticity, $\epsilon$, at the bond critical points have been determined for the wide variety of different covalent bonds and hydrogen bonds present in the structure.