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Experimental and Theoretical Charge Density Study of Estrone. E.A. Zhurova, C.F. Matta, N. Wu, V.V. Zhurov, A.A. Pinkerton, Dept. of Chem., Univ. of Toledo, Toledo, OH 43606; Dept. of Chem., Dalhousie Univ., Halifax, Nova Scotia, Canada B3H 4J3; Dept. of Biochem., Case Western Reserve Univ., Cleveland, OH 44106.

The electron density and the electrostatic potential (ESP) distributions of estrone have been determined using X-ray diffraction analysis and compared with theoretical calculations in the solid and gas phases. X-ray diffraction measurements were performed with a Rigaku Rapid rotating anode diffractometer at 20 K. The electron density in the estrone crystal (orthorhombic phase II) has been described with the Hansen-Coppens multipole model, which allowed extensive topological analysis and calculation of the ESP. An interesting locally stabilizing hydrogen-hydrogen bond path is found in the experimental and all three calculated densities and represents the first characterization of such bonding in a steroid molecule. It is estimated that this interaction contributes between 8 and 11 kcal/mol of *local* stabilization to estrone. The aromaticity of ring A is discussed and quantified since it is crucial to biological activity. Chemical bonding, the O(1)...O(2) distance necessary for estrogenic activity, and the electrostatic potential (ESP) features are also discussed.