Organic "cages" present themselves as highly distorted and yet compact structures. These compounds therefore are viable for external electrophilic and nucleophilic attack. The distorted electron density distributions on the surface of the molecules hamper the directional preferences.

The compound heptacyclo[8.5.0.12.7.0.6.12.5.14.0.11.15]hexadecane-4,7-dione is such an example and high precision data set collected at room temperature data will be presented. The molecular geometry derived from both X-ray analyses showed significant distortions from the expected C3v symmetry. Our recent neutron diffraction refinement of bullvalene, however, based on a 110K measurement revealed only minor deviations from this symmetry (Luger, P., Buschmann, J., McMullan, R.K., Ruble, J.R., Matias, P., Jeffrey, B.A. [1986]. J. Am. Chem. Soc. 108, 7825-7827).

Here we present a charge density study of bullvalene based on the above mentioned neutron data set taken at the High Flux Beam Reactor of the Brookhaven National Laboratory, wavelength 1.0502 Å, 3077 reflections with sin\(\lambda/\lambda<0.78\) and on an X-ray data set taken at 110 K with MoKα radiation, 8600 reflections with sin\(\lambda/\lambda<1.02\).

In the plane of the cyclopropane ring the difference maxima lie clearly outside the three membered ring (Fig. 1), consistent with the description of so called "banana bonds". The non-spherical density distributions derived from both X-ray analyses are indicative of their \(\pi\) character.

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