

## Characterization of didehydro cyclooctatetraene dianion

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Didehydro cyclooctatetraene dianion (COT) is an aromatic 8 membered carbon ring diradical. Aromatic diradicals are studied because of their presence in oil shale and because of their potential as antitumor drugs. Gaussian 09 was used to get preliminary structures and visualize molecular orbitals. Using the generated images, each orbital was assigned an irreducible representation under the  $C_{2v}$  point group. Using COLUMBUS, singlet ( $^1B_2$ ) and triplet ( $^3B_2$ ) states will be characterized with MCSCF, MR-CISD, and AQCC levels of theory. Data was collected on adiabatic gaps, vertical excitations, and geometries. Interesting resulting geometries were found in which the ring was distorted from the normal octagonal shape. The singlet and triplet shapes are significantly different from each other, which may suggest there is some interaction between the two radicals.

