Dr. Robert Molt Jr.

We find that the σ bond joining charged carbon centers in oxalic acid consists of a single electron, higher in energy than the π orbitals in the system. The free-energy barrier to bond cleavage is calculated to be 7 kcal/mol. This allows for an understanding of how carbons described as sp^2 in the valence-bond picture may be cleaved easily. This is of particular relevance in understanding the enzymatic mechanism of oxalic acid decarboxylase and organic chemistry mechanisms involving sp^2 carbon-carbon bonds. We show that the structural premise is quite general, existing with various electron-withdrawing and electron-donating groups modifying the oxalic acid structure

Dr. Robert Molt Jr.
r.molt.chemical.physics@gmail.com
Nigel Richards Research Group
Department of Chemistry & Chemical Biology
Indiana University-Purdue University Indianapolis
LD 326
402 N. Blackford St.
Indianapolis, IN 46202