Signatures of diradicals in X-ray absorption spectroscopy

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In the past decade, core-electron spectroscopies, have seen significantly improvements in temporal resolution. These advances, driven by evolution in synchrotron technology, have enabled the use of X-rays to probe short-lived transient species, including diradicals. Theoretical simulations are crucial for analyzing and interpreting core-electron spectroscopies of transient open-shell species. In this poster, we discuss a simplified model that accounts for many-body interactions in core-excited states of symmetric diradicals. Using this model, we analyze the carbon K-edge transitions of *o*-, *m*-, and *p*-benzyne, three organic diradicals with unusual electronic structures. To assess the accuracy of our model, we compare its predictions with high-level multireference computations of the benzynes' K-edge spectrum obtained using the driven similarity renormalization group truncated to third order in perturbation theory. Our model highlights the significance of the many-body nature of core-excited states of open-shell species and establishes a theoretical framework for understanding what features of the ground state of these diradicals are discernible from their X-ray absorption spectra.

[1] K. Marin, M. Huang, and F. A. Evangelista, Signatures of diradicals in x-ray absorption spectroscopy, *J. Chem. Phys*. **158** (2023)