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Department of Chemistry

Seminar

4 p.m. Monday, October 21, 2013 • 331 Smith Hall



Professor

Weston Borden

Department of Chemistry
University of North Texas

Why Does Cyclobutane-1,2,3,4-Tetraone Have a Triplet Ground State?

Research interests: electronic structure calculations to understand and predict the reactions of organic and organometallic compounds, including the contributions of quantum mechanical tunneling to the reaction rates.

Website: <http://chemistry.unt.edu/people-node/weston-t-borden/>

Abstract

Xiaoguang Bao,^{a,b} Xin Zhou,^a Charity Flener,^a Amruth Venkatraman,^a Sebastian Kozuch,^a David A. Hrovat,^a Rolf Gleiter,^c Roald Hoffmann,^d Xue-Bin Wang,^e and Weston Thatcher Borden^a

As predicted,¹ cyclobutane-1,2,3,4-tetraone, (CO)₄, has been found by negative ion photo-electron spectroscopy (NIPES) to have a triplet ground state.² Why does this apparently unexceptional organic molecule have a ground state with two unpaired electrons? Which, if any, other members of the (CO)_n series are calculated to have a triplet ground state? Is (CS)₄ or (SiO)₄ predicted to have a triplet ground state? What are the factors that control the spin of the ground state of these molecules? All of these questions have been addressed by a combination of qualitative MO theory and quantitative electronic structure calculations;^{3,4} and the predictions, made by the calculations, have been tested by NIPES.^{5,6}

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⁶ X. Bao, D. A. Hrovat, W. T., Borden, and X.-B. Wang, *J. Phys. Chem A*, in press.

Host: Laura Gagliardi