

2019 Research Week Abstract Instructions and Template
Posters and Presentations

Title – Theoretical Studies on the Transition Dipole Moments of Bromoethanol

Program of Study – Chemistry

Presentation Type – **Choose one of the following:** Physical Poster

Subtype –Basic

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Abstract: Presented herein are the preliminary results on the theoretical investigation of various excited state transitions of bromoethanol. Using the *Gaussian 16* software package, the direction of the transition dipole moments from the ground to these various excited states were determined at the TD-B3LYP and EOMCCSD levels of theory. Prior experimental results suggest the accessed excited states are repulsive in the Franck-Condon region, leading to carbon-bromine bond dissociation which occurs rapidly compared to the rotational period of the bromoethanol molecule. As such, the relationship between the transition dipole moment vector and the vector along the carbon-bromine bond may be used to predict the distribution of the recoiling bromine atoms' velocity vectors resulting from the photodissociation process. This poster presents the transition dipole moment vectors as a function of various molecular configurations of bromoethanol in its ground electronic state. The aim of this investigation is to better understand and possibly predict aspects of the photodissociation dynamics of bromoethanol upon 193 nm photoexcitation as previously reported in prior velocity map imaging studies.