

2E09: EXPLORING THE OXIDATIVE DECOMPOSITIONS OF METHYL ESTERS: METHYL BUTANOATE AND METHYL PENTANOATE AS MODEL COMPOUNDS FOR BIODIESEL.

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Comment by Katharina Kohse-Hoeinghaus, Bielefeld University, Germany

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Your study is very interesting as it emphasizes the influence of chemical structure. Did you also perform work on similar components that would exhibit a double bond, or do you plan to do that?

Reply by Carrigan Hayes

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Thus far, our work has not explored esters with a double bond in their side chain. However, we hope that by having calibrated an efficient and accurate computational approach (G3MP2B3) against some of the known chemistry of methyl butanoate, we or others can use this method to more quickly explore other esters of interest, in the future. Esters with double bonds in the side chain would be excellent candidates for future work.