Preliminary report on the 1,2-dioxethane dissociation at the MS-CASPT2 level of theory

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Abstract. In this poster we present some preliminary results from our investigation of the 1,2-dioxethane dissociation at the MS-CASPT2 level of theory. This dissociation is of fundamental importance of the understanding of chemical initiated electron-exchange luminescence (CIEEL). Previous investigations has failed to demonstrate in a convincing way the nature of the interaction between the S_0 and T_1 states as well as to compute an activation barrier in agreement with experiment. In this multi-state CASPT2 investigation we will share results of the first half of the title reaction. Results reproduce the experimental activation energy and demonstrate that the interaction after the first TS do not only require the S_0 and T_1 state but that actually four singlet and four triplet states are crowded all along the reaction path from the TS to the intermediate product. All these eight states are crowded with in an energy gap of 6 kcal/mol. This explains the existence of several possible reactions channels being populated for the second half of the title reaction. One of them being the channel which will produce formaldehyde in an excited state, a path which is of fundamental importance in the luminescence.