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Mechanism of addition-fragmentation reaction of thiocarbonyls compounds in free radical polymerization. A DFT study

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In the present study we analyze the reaction mechanisms involved by Xanthates (SA(C@S)AO) and Thiocarbonates
(OA(C@S)AO) compounds in a reversible addition fragmentation chain transfer (RAFT) polymerization. For the purpose, theoretical calculations have been performed by means of density functional theory (DFT), using the B3LYP, M06, CAM-B3LYP, LC-xPBE exchange correlation functionals and 6-31G′ basis sets. Thanks to the transition state theory, the rates of addition and fragmentation reactions were obtained. It is shown that, for these systems, the fragmentation step is more selective than the addition step, and that the range-separated functionals give results close to the experimental trends.

Primary author: Dr LATELLI, nadjia (chemistry)

Presenter: Dr LATELLI, nadjia (chemistry)

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