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DFT STUDIES ON THE MECHANISM OF RING-OPENING POLYMERIZATION OF LACTIDE WITH ADENINE ^EP18

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- 110 The use of organic molecules as catalysts for the ring-opening polymerization (ROP) of cyclic esters has gained much interest last years.[1] The use of a molecule of biological interest, able to initiate ROP of cyclic esters without any cocatalyst is even more interesting, as the resulting material will not contain any catalytic residue. Nucleobase-polymer conjugates development is thus an emerging area envisaging biomedical applications.[2] However, they are usually synthesized by tedious multistep procedures. Recently, adenine was used as organoinitiator for the ROP of L-lactide.[3] Reaction conditions involving short reaction times and relatively low temperatures enable the access to adenine-poly(lactide) (Adn-PLA) conjugates in a simple one-step procedure, without additional catalyst and in the absence of solvent. In this study, computational investigations with density functional theory (DFT) were performed in order to clarify the reaction mechanism leading to the desired Adn-PLA. The results show that a hydrogen bond catalytic mechanism, involving a nucleophilic attack of the activated amine group of adenine onto the carbonyl group of lactide, seem to be plausible.

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