Decoding the Reaction Mechanism of the Cyclocondensation of Ethyl acetate 2-oxo-2-(4-oxo-4H-pyrido [1.2-a] pyrimidin-3-yl) polyazaheterocycle and Ethylenediamine using Bond Evolution Theory

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Abstract

The bonding evolution theory has been used to investigate the flow of electron density along the reaction pathways of ethyl acetate 2-oxo-2-(4-oxo-4H-pyrido [1.2-a] pyrimidin-3-yl) polyazaheterocycle (1) and ethylenediamine (2). This reaction has three channels (1-3) and each one takes place via three or four steps. DFT results reveal that channel 2, which goes through imine intermediate is by far the most favorable one, and the main product 3 is more stable than 4 and 5, showing that this reaction is under kinetic and thermodynamic control, in clear agreement with the experimental outcomes. The BET analysis allows identifying unambiguously the main chemical events happening along channel 2. For this reaction channel, the mechanism along the first step (TS2-a) is described by a series of four structural stability domains (SSDs), while five SSDs are required for the second (TS2-b) and the third (TS2-c) one. The first step can be summarized as follow, the appearance of V(N1,C6) basin illustrating the formation of N1-C6 bond (SSD-II), the splitting of N1-H1 bond, followed by the restoration of the nitrogen N1 lone pair (SSD-III), and finally, the formation of the last O1-H1 bond (SSD-IV). For the second step, the formation of hydroxide ion is noted, consequent of the disappearance of V(C6,O7) basin, the transformation of C6-N1 single bond into double one (SSD-IV). Finally, the appearance of V(O7,H2) basin leading to the elimination of water molecule within the last domain. Overall, for the three reaction steps, the formation of the N-C bond appears always before the O-H one.

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