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Understandings of Formation of N-Ntrosoamine in Smoke.[1] YI-LEI ZHAO[2], CARLOS GONZALEZ[3], NIST, MANUEL MARQUEZ[4], PMUSA Research Center, 4201 Commerce Rd., Richmond, VA 23234, INEST TEAM[5], CTCN TEAM[6] — Formation of N-nitrosoamine compounds is highly concerned in combustion and past-combustion. In chemical laboratory, nitrosylation of amine toward N-nitrosoamine generally requires nitrosonium donor and acidic condition. Recently, an unexpected reaction was observed to be relevant to nitrogen dioxide, a common component of past-combustion gas; an alternative non-ionic pathway must lead to the rapid nitrosylation. Here, we proposed a radical mechanism, by which amino-radical is formed by H-abstraction of nitrogen dioxide, followed by radical scavenging with nitric oxide. Relatively low activation energy of 10-11 kcal/mol (ca., CBS-QB3) of the radical mechanism rationalized the feasibility of N-nitrosoamine formation in colloids after combustion of bio-materials. Acid-catalyzed nitrosylation in aqueous solution was also computed.

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