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Experimental and theoretical studies on the OH-initiated degradation of tert-butylamine

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Amine-based carbon dioxide (CO_2) capture facilities release small amounts of amines into the atmosphere. Once airborne, the amines are photochemically transformed into imines, amides, nitrosamines, nitramines and other breakdown products. As some of these products pose a risk to human health and the environment, we have elucidated photochemical decomposition mechanisms of various types of amines in previous work. Our studies did, however, not include amines in which the primary amino group is attached to a tertiary carbon atom, with 2-amino-2-methyl-1-propanol (AMP, $(CH_3)_2C(NH_2)CH_2OH$) being a prominent candidate used in CO_2 capture. Our initial step in elucidating the degradation mechanism of AMP was to study tert-butylamine (tBA, $(CH_3)_3C(NH_2)$), which is a similar molecule but lacks the OH group. OH-initiated degradation of tBA was studied in chamber experiments at the European Photoreactor (EUPHORE) in Valencia (Spain) using state-of-the-art analytical instrumentation. A Proton-Transfer-Reaction Time-of-Flight Mass Spectrometer (PTR-ToF-MS) was used to measure tBA and tBA degradation products in the gas phase. Propan-2-imine (PI, $(CH3)_2C(=NH)$) and tert-butylnitramine (tBNA, $(CH_3)_3C(NHNO_2)$) were observed as the two major gas-phase products. An Aerosol Mass Spectrometer (AMS) made quantitative measurements of tert-butylaminium nitrate in the particle phase. A PTR-ToF-MS instrument equipped with a "chemical analysis of aerosol online" (CHARON) inlet detected the two major tBA degradation products (PI, tBNA) in the particle phase. Experimental work was supplemented by quantum chemistry calculations. We will present measured product yields and a complete degradation scheme of tBA.
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