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University of Toronto

Atmospheric sources and sinks of amines, amides and isocyanic acid (HNCO)

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There has been a growing interest in the use of amines as efficient solvents for carbon capture and storage (CCS) technology to minimize CO2 emissions from large industrial processes. Monoethanolamine (MEA) is the current benchmark solvent and so understanding its atmospheric fate is instrumental in implementing CCS. To address this gap, we investigated the reaction of MEA with oxidants like OH radicals and ozone within a smog chamber experimental setup, using online proton-transfer-reaction mass spectrometry. Since, MEA has a lifetime of a few hours in the atmosphere, we focused on characterizing its gas-phase products to further assess the fate of this amine. Formamide is the major oxidation product detected and we provide the first report of its rate coefficient with OH radicals, (4.44 ± 0.46) ´ 10-12 cm3 molec-1 s-1 at room temperature and atmospheric pressure, translating to a lifetime of ~ 1 day. Other alkylated amides were studied to gain a better understanding of their reactivity trends. A detailed mechanistic study of these amides involving ab initio calculations identified production of isocyanates, including isocyanic acid (HNCO) and methyl isocyanate, two toxic substances, as a major pathway. Current work is now focused on studying the sources and sinks of isocyanic acid. In particular, recent experiments on the formation of HNCO from cigarette smoke as well as from nicotine oxidation will be presented.

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