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Abstract for an Invited Paper for the MAS20 Meeting of the American Physical Society

Is direct molecular analysis of atmospheric oxidized mercury possible?¹ ALEXEI KHALIZOV, New Jersey Inst of Tech

Mercury is a persistent environmental pollutant, entering the atmosphere mostly in elemental form and leaving in various oxidized forms, commonly named gaseous oxidized mercury (GOM). Little is known about the molecular identity of GOM and this hinders the ability to evaluate the fate of mercury in the environment. All current detection methods pre-concentrate GOM before analysis, producing various artifacts. A direct method capable of molecular analysis of GOM is needed. This presentation will cover our recent work on the development of an analytical technique for direct molecular analysis of GOM, based on the ion drift - chemical ionization mass spectrometry (ID-CIMS). In this method, gaseous molecules react in a drift tube with an appropriate reagent ion to form well-defined product ions, which are detected by a mass spectrometer. Using quantum chemical calculations and ID-CIMS experiments, we show that surrogate GOM molecules, such as HgX_2 and HgXY (where X and Y are halides) can be analyzed quantitatively via ion-molecule reactions with several negatively charged reagent ions. I will discuss challenges associated with detecting mercury-containing molecules, ways to overcome those challenges, and prospective of using ID-CIMS for direct detection of GOM in the atmosphere.

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