

Atmospheric Aerosol Sulfur Distribution and Speciation in Mexico City: Sulfate, Organosulfates, and Isoprene-Derived Secondary Organic Aerosol from Low NO Pathways

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Abstract

Poor air quality is a persistent challenge in Mexico City, and addressing this issue requires an understanding of the chemical composition of fine particulate matter, PM_{2.5} (particulate matter less than 2.5 μm in diameter). Sulfate and secondary organic aerosol (SOA) are two of the largest contributors to PM_{2.5} in Mexico City, but uncertainties exist regarding their sources, distribution across individual particles, and ability to form organosulfates. Herein, we show using electron dispersive x-ray spectroscopy that only 41±1% and 25±1% of particles (aerodynamic diameter, 0.32 – 0.56 μm) by number at two sites in Mexico City, respectively, contain sulfur. Vibrational spectroscopy (Optical-Photothermal Infrared + Raman Microspectroscopy) shows that these sulfur-containing particles consist of inorganic sulfate (SO₄²⁻) and organosulfates (ROSO₃). In addition, we unexpectedly measured abundant isoprene-derived SOA from low nitric oxide reaction pathways, specifically organosulfates (methylnol sulfates = avg. 50 ng/m³, max. 150 ng/m³) and polyols (methylnols = avg. 70 ng/m³, max. 190 ng/m³) using hydrophilic interaction liquid chromatography coupled to electrospray ionization high-resolution mass spectrometry. Differences in SO₂ and NO_x concentrations between sites likely contribute to these spatial differences in sulfate, organosulfate, and SOA formation. These findings improve understanding of sulfur distribution and sources of SOA in Mexico City, which can inform efforts to improve air quality.