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Cluster analysis of the organic peaks in bulk mass spectra obtained during the 2002 New England Air Quality Study with an Aerodyne aerosol mass spectrometer

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We applied hierarchical cluster analysis to an Aerodyne aerosol mass spectrometer (AMS) bulk mass spectral dataset collected aboard the NOAA research vessel Ronald H. Brown during the 2002 New England Air Quality Study off the east coast of the United States. A cluster analysis emphasizing the organic peaks yielded a series of categories that are distinguishable with respect to their mass spectra and their occurrence as a function of time. The differences between the categories mainly arise from relative intensity changes rather than from the presence or absence of specific peaks. The most frequent category exhibits a strong signal at m/z 44, a signature fragment of oxidized organic species in AMS spectra. This category correlates with ozone and contributes to the aerosol mass for any wind direction, but particularly at times when winds are from the east or south. Moreover, its occurrence shows a diurnal cycle, with higher concentrations during daytime than at night. The second most common category has strong signals at m/z 29, 43, and 44, indicative of less oxidized, less aged particles than in the most common category. On the basis of spectral and trace gas correlations, this category contains contributions from isoprene oxidation products. The third through the fifth most common categories have peak patterns characteristic of

monoterpene oxidation products and were most frequently observed when air masses from monoterpene rich regions were sampled. The average signals of the high mass peaks in nearly all of the categories are consistent with the organic material being from biogenic precursors that reacted with oxidants from anthropogenic processes. This study demonstrates that hierarchical clustering is a useful tool to analyze the complex patterns of the organic peaks in bulk aerosol mass spectra from a field study.