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Atmos. Chem. Phys., 6, 5649-5666, 2006

www.atmos-chem-phys.net/6/5649/2006/

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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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Abstract. We applied hierarchical cluster analysis to an Aerodyne aerosol mass spectrometer (AMS) bulk mass spectral dataset collected aboard the NOAA research vessel R. H. Brown during the 2002 New England Air Quality Study off the east coast of the United States. Emphasizing the organic peaks, the cluster analysis 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 and represents oxidized organic matter probably originating from both anthropogenic as well as biogenic sources. On the basis of spectral and trace gas correlations, the second most common category with strong signals at m/z 29, 43, and 44 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. Taken together, the second through the fifth most common categories represent on average 17% of the total organic mass that stems likely from biogenic sources during the ship's cruise. These numbers have to be viewed as lower limits since the most common category was attributed to anthropogenic sources for this calculation. The cluster analysis was also very effective in identifying a few contaminated mass spectra that were not removed during pre-processing. 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.

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Citation: Marcolli, C., Canagaratna, M. R., Worsnop, D. R., Bahreini, R., de Gouw, J. A., Warneke, C., Goldan, P. D., Kuster, W. C., Williams, E. J., Lerner, B. M., Roberts, J. M., Meagher, J. F., Fehsenfeld, F. C., Marchewka, M., Bertman, S. B., and Middlebrook, A. M.: 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, *Atmos. Chem. Phys.*, 6, 5649-5666, 2006. [Bibtex](#) [EndNote](#) [Reference Manager](#)