Home
Online Library ACP
- Recent Final Revised Papers
- Volumes and Issues
- Special Issues
- Library Search
- Title and Author Search

Online Library ACPD
Alerts & RSS Feeds
General Information
Submission
Review
Production
Subscription
Comment on a Paper

Volumes and Issues | Contents of Issue 14 | Special Issue

Atmos. Chem. Phys., 8, 4095-4103, 2008
www.atmos-chem-phys.net/8/4095/2008/

Amines are likely to enhance neutral and ion-induced sulfuric acid-water nucleation in the atmosphere more effectively than ammonia

T. Kurtén, V. Loukonen, H. Vehkamäki, and M. Kulmala
Division of Atmospheric Sciences and Geophysics, Dept. of Physics, P.O.Box 64, 00014 University of Helsinki, Finland

Abstract. We have studied the structure and formation thermodynamics of dimer clusters containing H_2SO_4 or HSO_4^- together with ammonia and seven different amines possibly present in the atmosphere, using the high-level ab initio methods RI-MP2 and RI-CC2. As expected from e.g. proton affinity data, the binding of all studied amine-H_2SO_4 complexes is significantly stronger than that of $NH_3 \cdot H_2SO_4$, while most amine-HSO_4^- complexes are only somewhat more strongly bound than $NH_3 \cdot HSO_4^-$. Further calculations on larger cluster structures containing dimethylamine or ammonia together with two H_2SO_4 molecules or one H_2SO_4 molecule and one HSO_4^- ion demonstrate that amines, unlike ammonia, significantly assist the growth of not only neutral but also ionic clusters along the H_2SO_4 co-ordinate. A sensitivity analysis indicates that the difference in complexation free energies for amine- and ammonia-containing clusters is large enough to overcome the mass-balance effect caused by the fact that the concentration of amines in the atmosphere is probably 2 or 3 orders of magnitude lower than that of ammonia. This implies that amines might be more important than ammonia in enhancing neutral and especially ion-induced sulfuric acid-water nucleation in the atmosphere.

Final Revised Paper (PDF, 464 KB) | Supplement (50 KB) | Discussion Paper (ACPD)

Citation: Kurtén, T., Loukonen, V., Vehkamäki, H., and Kulmala, M.: Amines are likely to enhance neutral and ion-induced sulfuric acid-water nucleation in the atmosphere more effectively than ammonia, Atmos. Chem. Phys., 8, 4095-4103, 2008. Bibtex | EndNote | Reference Manager

Search ACP
Library Search
Author Search

News
- Sister Journals AMT & GMD
- Financial Support for Authors
- Journal Impact Factor
- Public Relations & Background Information

Recent Papers
01 | ACPD, 14 Nov 2008: SCIAMACHY formaldehyde observations: constraint for isoprene emissions over Europe?
02 | ACPD, 14 Nov 2008: Observation of nitrate coatings on atmospheric mineral dust particles
03 | ACP, 14 Nov 2008: FRESCO+: an improved O_2 A-band cloud retrieval algorithm for tropospheric trace gas retrievals
04 | ACPD, 14 Nov 2008: