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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Estimating the NH_3:H_2SO_4ratio of nucleating clusters in atmospheric conditions using quantum chemical methods" *by* T. Kurtén et al.

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Thank you for your constructive comments. The typing error will be corrected in the revised version of the manuscript. The main reason for the differences between the results of Ianni and Bandy (1999) and Kurten et al (2007) is the different density functional used in the studies; the B3LYP functional used by Ianni and Bandy tends to underpredict binding energies for sulfuric acid - water clusters while the PW91 functional used by Kurten et al. tends to somewhat overpredict them. This has been extensively discussed both by us (Kurtén et al., 2006, reference given in manuscript) and for example Nadykto and Yu in their recent paper (Chem. Phys. Lett. 435, 14-18, 2007). A short discussion on this will be added to the revised version of the manuscript along with a reference to the Nadykto and Yu paper.

Interactive comment on Atmos. Chem. Phys. Discuss., 7, 2937, 2007.

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Interactive Comment

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