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***Interactive comment on “ISORROPIA II: a computationally efficient thermodynamic equilibrium model for  $\text{K}^+$ - $\text{Ca}^{2+}$ - $\text{Mg}^{2+}$ - $\text{NH}_4^+$ - $\text{Na}^+$ - $\text{SO}_4^{2-}$ - $\text{NO}_3^-$ - $\text{Cl}^-$ - $\text{H}_2\text{O}$  aerosols” by C. Fountoukis and A. Nenes***

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Incorporating mineral cations ( $\text{Ca}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{K}^+$ ) into the thermodynamic equilibrium model ISORROPIA is an important advancement. However, the model neglects hydrated forms of calcium and magnesium salts [e.g.,  $\text{Ca}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$ ,  $\text{Mg}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ ,  $\text{CaCl}_2 \cdot 6\text{H}_2\text{O}$ , etc.], which are known to be stable for some atmospheric conditions. Previous work [Kelly and Wexler, 2005; JGR, 110, D11201, doi:10.1029/2004JD005583] has shown that neglecting these hydrates results in incorrect predictions of the temperature dependence of DRH and alters the thermodynamically preferred behavior

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of some dust reactions.

Measurements of Tang and Fung [1997; J. Chem. Phys., 106(5):1653-1660] indicate that the stable hydrate,  $\text{Ca}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$ , does not form in levitated microparticles in the laboratory. Instead of transforming into the stable tetrahydrate at 11.4 %RH, anhydrous calcium nitrate particles deliquesce at 18 %RH when exposed to increasing RH in an electrodynamic balance. If neglecting hydrates in ISORROPIA is an attempt to capture such non-equilibrium behavior, then the DRH value for  $\text{Ca}(\text{NO}_3)_2$  should be modified to Tang's value. As it stands, the DRH used for calcium nitrate (i.e., 49%) corresponds to the tetrahydrate, whereas the temperature variation of DRH is calculated using properties of anhydrous calcium nitrate. This approach—basing DRH on measurements of solutions saturated with respect to hydrates, but calculating DRH(T) with anhydrous properties—is used for other salts as well (e.g.,  $\text{CaCl}_2$ ,  $\text{MgCl}_2$ , etc.) without explanation.

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Interactive comment on Atmos. Chem. Phys. Discuss., 7, 1893, 2007.

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