

## ***Interactive comment on “Amine substitution into sulfuric acid – ammonia clusters” by O. Kupiainen et al.***

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There were errors in Table 1 of our earlier response to the comments by Referee Nadykto. Most of the values on the second row corresponded to the reaction  $(\text{H}_2\text{SO}_4)_2 + \text{H}_2\text{SO}_4 \rightarrow (\text{H}_2\text{SO}_4)_3$  instead of  $\text{NH}_3 + \text{H}_2\text{SO}_4 \rightarrow \text{H}_2\text{SO}_4 \cdot \text{NH}_3$ . Here is a corrected version of the table. We apologize for the inconvenience.

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**Table 1.** Gibbs free energies (at 298 K and 1 atm reference pressure) for the addition of sulfuric acid to form ammonia and dimethylamine containing clusters. All values in kcal/mol.

	B3RICC2 <sup>a</sup>	RI-CC2 <sup>b</sup>	CBS-QB3 <sup>c</sup>	B3LYP <sup>d</sup>	PW91 <sup>e</sup>
$\text{H}_2\text{SO}_4 + \text{H}_2\text{SO}_4 \rightarrow (\text{H}_2\text{SO}_4)_2$	-7.89	-6.93	-8.66	-5.86	-5.59
$(\text{H}_2\text{SO}_4)_2 + \text{H}_2\text{SO}_4 \rightarrow (\text{H}_2\text{SO}_4)_3$	-6.41		-7.19	-2.42	-3.31
$\text{NH}_3 + \text{H}_2\text{SO}_4 \rightarrow \text{H}_2\text{SO}_4 \cdot \text{NH}_3$	-7.61	-6.64	-7.34	-9.45	-7.77
$(\text{CH}_3)_2\text{NH} + \text{H}_2\text{SO}_4 \rightarrow \text{H}_2\text{SO}_4 \cdot (\text{CH}_3)_2\text{NH}$	-15.40	-13.66	-14.37	-11.07	-11.38
$\text{H}_2\text{SO}_4 \cdot \text{NH}_3 + \text{H}_2\text{SO}_4 \rightarrow (\text{H}_2\text{SO}_4)_2 \cdot \text{NH}_3$	-16.21	-14.43	-17.13	-10.96	-11.65
$\text{H}_2\text{SO}_4 \cdot (\text{CH}_3)_2\text{NH} + \text{H}_2\text{SO}_4$ $\rightarrow (\text{H}_2\text{SO}_4)_2 \cdot (\text{CH}_3)_2\text{NH}$	-19.48	-19.29	-20.71	-15.78	-14.30

(a) B3LYP/CBSB7//RI-CC2/aug-cc-pV(T+d)Z (Ortega et al., 2012)

(b) RI-MP2/aug-cc-pV(D+d)Z//RI-CC2/aug-cc-pV(T+d)Z (Kurtén et al., 2008)

(c) (Ortega et al., 2012)

(d) B3LYP/CBSB7

(e) PW91/6-311++G(3df,3pd) (Nadykto et al., 2007, Nadykto et al., 2011 and Herb et al., 2011)

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