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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.

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

(a) B3LYP/CBSB7/RI-CC2/aug-cc-pVT+dZ (Ortega et al., 2012)
(b) RI-MP2/aug-cc-pV(D+d)Z/RI-CC2/aug-cc-pVT+dZ (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)

References
Clusters, Entropy, 13, 554-569, 2011.