ADDITIONS AND CORRECTIONS

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Juha Vaara,* Jaakko Kaski, Jukka Jokisaari, and Peter Diehl: NMR Properties of Formamide: A First Principles and Experimental Study

Page 5076. Left column, line 10 from the top, the sentence should read "For ^{17}O, both the in-plane σ_{ii} components *increase* markedly due to hydrogen bonding."

Page 5078. Left column, line 19 from the bottom, the sentence should read "Table 9 reveals that the out-of-plane F_{cc} decreases for *N and D2 and increases for O* in the trimer."

The experimental results for the nitrogen shielding constant in Table 4 are erroneous due to the use of $\sigma_N = 264.54$ ppm for the NH_3 reference molecule. This value is appropriate to the gas phase, whereas in a liquid $\sigma_N = 245.07$ ppm should be used.[1] This causes for the nitromethane reference molecule the value of $\sigma_N = -135.06$ ppm, and the entries in the σ_N column of Table 4 should read exp/LC NMR (sample 4) *131.6* ppm, exp/LC NMR (sample 3) *131.4* ppm, and exp/liquid NMR (ref 8e of the original article) *133.0* ppm. These changes have the consequence that the calculated change in σ_N induced by the formation of one N−H···O hydrogen bond, −7.4 ppm, is not adequately large in magnitude to explain the deviation of the best monomer calculation from the experimental results. This is likely due to the use of Hartree−Fock-level geometry for the trimer, as a larger change of −17.7 ppm per hydrogen bond was obtained in a calculation[2] for the cyclic dimer where a correlated geometry was used. The latter change, multiplied by 2 due to the additivity of the effects of two simultaneous hydrogen bonds, corrects our RAS−V calculation ($\sigma_N = 167.7$ ppm) by −35.4 ppm and brings it down to 132.3 ppm, in good agreement with the experimental results. Thus, the conclusions of the paper remain unaffected.

References and Notes

(1) Jameson C. J. *Encyclopedia of NMR Spectroscopy*; John Wiley & Sons: New York, 1996; Vol. 2, p 1273.

(2) Unpublished results from the calculations described in ref 16 of the original article.