

Angewandte Addendum

Anti-Electrostatic Hydrogen Bonds

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Following recent coverage in *Chemical & Engineering News* (September 22, **2014**, p. 10) the authors of this Communication were kindly informed by Prof. Ibon Alkorta (Madrid, Spain) and Prof. Steven R. Kass (Minneapolis) of earlier experimental^[1,2] and theoretical^[3,4] works pertaining to doubly-ionic H-bonded species in the gas phase that are peripherally related to this Communication. Their studies involve somewhat different species (such as large peptide clusters) and different theoretical focus than the central “What is H-bonding?” question of the present work, but should be recognized (along with crystallographic evidence on bicarbonate dimers^[5] previously noted) as relevant to the attempted experimental and theoretical detection and characterization of paradoxical “anti-electrostatic” (or “electrostatics-defying”^[3]) H-bond species that challenge current empirical modeling and pedagogy.

[1] S. W. Lee, J. L. Beauchamp, *J. Am. Soc. Mass Spectrom.* **1999**, 10, 347–351.

[2] L. Feketeova, R. A. J. O’Hair, *Chem. Commun.* **2008**, 4942–4944.

[3] S. R. Kass, *J. Am. Chem. Soc.* **2005**, 127, 13098–13099; A. Shokri, M. Ramezani, A. Fattahi, S. R. Kass, *J. Phys. Chem. A*, **2013**, 117, 9252–9258.

[4] I. Mata, I. Alkorta, E. Molins, E. Espinosa, *ChemPhysChem* **2012**, 13, 1421–1424.

[5] D. Braga, F. Grepioni, J. J. Novoa, *Chem. Commun.* **1998**, 1959–1960. See also ensuing discussions: T. Steiner, *Chem. Commun.* **1999**, 2299–2300; M. Mascal, C. E. Marjo, A. J. Blake, *Chem. Commun.* **2000**, 1591–1592; P. Macchi, B. B. Iversen, A. Sironi, B. C. Chakoumakos, F. K. Larsen, *Angew. Chem. Int. Ed.* **2000**, 39, 2719–2722; *Angew. Chem.* **2000**, 112, 2831–2834.