

Table 1. Calculated hydrogen bond energies (kcalmol⁻¹) in some gas-phase dimers.^[a]

Dimer	Energy	Ref.
[F-H-F] ⁻	39	[27a]
[H ₂ O-H-OH ₂] ⁺	33	[27b]
[H ₃ N-H-NH ₃] ⁺	24	[27b]
[HO-H-OH] ⁻	23	[27a]
NH ₄ ⁺ ...OH ₂	19	[27c]
NH ₄ ⁺ ...Bz	17	[27d]
HOH...Cl ⁻	13.5	[27c]
O=C-OH...O=C-OH	7.4	[27e]
HOH...OH ₂	4.7; 5.0	[27f,g]
N≡C-H...OH ₂	3.8	[27h]
HOH...Bz	3.2	[27i]
F ₃ C-H...OH ₂	3.1	[27j]
Me-OH...Bz	2.8	[27k]
F ₂ HC-H...OH ₂	2.1; 2.5	[27f,j]
NH ₃ ...Bz	2.2	[27i]
HC≡CH...OH ₂	2.2	[27h]
CH ₄ ...Bz	1.4	[27i]
FH ₂ C-H...OH ₂	1.3	[27f,j]
HC≡CH...C≡CH ⁻	1.2	[27l]
HSH...SH ₂	1.1	[27m]
H ₂ C=CH ₂ ...OH ₂	1.0	[27l]
CH ₄ ...OH ₂	0.3; 0.5; 0.6; 0.8	[27f,n-p]
C=CH ₂ ...C=C	0.5	[27l]
CH ₄ ...F-CH ₃	0.2	[27q]

[a] For computational details, see the original literature. Bz = benzyl.

- [27] a) S. Gronert, *J. Am. Chem. Soc.* **1993**, *115*, 10258–10266; b) J. E. Del Bene, M. J. Frisch, J. A. Pople, *J. Phys. Chem.* **1988**, *89*, 3669–3674; c) J. E. Del Bene, *J. Phys. Chem.* **1988**, *92*, 2874–2880; d) W.-L. Zhu, X.-J. Tan, C. M. Pua, J.-D. Gu, H.-L. Jiang, K.-X. Chen, C. E. Felder, I. Silman, J. L. Sussman, *J. Phys. Chem. A* **2000**, *104*, 9573–9580; e) T. Neuheuser, B. A. Hess, C. Reutel, E. Weber, *J. Phys. Chem.* **1994**, *98*, 6459–6467; f) Y. Gu, T. Kar, S. Scheiner, *J. Am. Chem. Soc.* **1999**, *121*, 9411–9422; g) M. W. Feyereisen, D. Feller, D. A. Dixon, *J. Phys. Chem.* **1996**, *100*, 2993–2997; h) L. Turi, J. J. Dannenberg, *J. Phys. Chem.* **1993**, *97*, 7899–7909; i) S. Tsuzuki, K. Honda, T. Uchimaru, M. Mikami, K. Tanabe, *J. Am. Chem. Soc.* **2000**, *122*, 11450–11458; j) I. Alkorta, S. Maluendes, *J. Phys. Chem.* **1995**, *99*, 6457–6460; k) J. F. Malone, C. M. Murray, M. H. Charlton, R. Docherty, A. J. Lavery, *J. Chem. Soc. Faraday Trans.* **1997**, *93*, 3429–3436; l) J. J. Novoa, F. Mota, *Chem. Phys. Lett.* **2000**, *318*, 345–354; m) E. L. Woodbridge, T.-L. Tso, M. P. McGrath, W. J. Hehre, E. K. C. Lee, *J. Chem. Phys.* **1986**, *85*, 6991–6994; n) T. van Mourik, F. B. van Duijneveldt, *J. Mol. Struct.* **1995**, *341*, 63–73; o) J. J. Novoa, B. Tarron, M. H. Whangbo, J. M. Williams, *J. Chem. Phys.* **1991**, *95*, 5179–5186; p) M. M. Szczesniak, G. Chalasinski, S. M. Cybulski, P. Cieplak, *J. Chem. Phys.* **1993**, *98*, 3078–3089; q) J. A. K. Howard, V. J. Hoy, D. O'Hagan, G. T. Smith, *Tetrahedron* **1996**, *52*, 12613–12622.