

TABLE 1: Thermodynamic Parameters (kJ/mol) for Hydrogen Bonds in the Hydronium Solvation Shells from MS-EVB2 Simulations of Protonated Water at 300 K (Extracted from the Linear Fits in Figure 4)

HB type	ΔG^0	$T\Delta S^0$	ΔH^0
D0	13.8	4.5	18.3
D1	4.6	4.5	9.1
D2	2.9	5.2	8.1
water	2.7	5.2	7.9
A2	1.9	3.5	5.4
A1	-3.3	3.9	0.6