Table 1: Results for Stacking and Hydrogen Bonding Interactions in Nucleobase Pairs (kcal/mol)

Methods	Stacking								Hydrogen Bonding				AMUE [b]
	A···T S	G···C S	C···C AP [a]	C···C D [a]	C···C S [a]	U···U S	MSE	MUE	A···T WC	G···C WC	MSE	MUE	
Best estimate [c]	11.60	16.90	9.90	9.43	-2.45	10.30			15.40	28.80			
M05-2X	10.28	16.25	10.52	10.02	-5.08	8.76	-0.82	1.22	14.56	28.58	-0.53	0.53	**0.87**
PWB6K	9.50	14.86	10.88	9.66	-5.93	7.94	-1.46	1.86	14.22	28.39	-0.79	0.79	**1.33**
MPWB1K	8.19	13.68	9.63	8.63	-7.02	6.51	-2.68	2.68	13.42	27.45	-1.67	1.67	**2.17**
PW6B95	7.68	13.10	9.48	8.46	-6.56	6.45	-2.84	2.84	13.26	26.68	-2.13	2.13	**2.49**
MPW1B95	7.47	12.83	8.98	8.08	-7.10	6.01	-3.24	3.24	13.18	26.80	-2.11	2.11	**2.67**
M05	5.77	11.95	7.86	7.66	-6.40	5.79	-3.84	3.84	13.68	27.07	-1.72	1.72	2.78
PBE1PBE	3.54	10.44	5.30	5.81	-8.40	3.97	-5.84	5.84	14.42	28.43	-0.67	0.67	3.25
B97-1	3.54	10.26	5.64	6.31	-8.01	4.05	-5.65	5.65	14.08	27.44	-1.34	1.34	3.50
BMK	5.42	11.54	6.37	6.17	-9.14	4.42	-5.15	5.15	12.49	26.30	-2.71	2.71	3.93
τ-HCTHh	2.39	9.38	4.54	5.14	-8.87	3.05	-6.68	6.68	13.79	27.42	-1.49	1.49	4.08
TPSSh	1.42	8.47	3.75	4.46	-9.64	2.29	-7.49	7.49	13.37	26.80	-2.02	2.02	4.75
SPWL	12.59	18.90	11.62	10.70	-2.33	10.64	1.07	1.07	22.30	39.44	8.77	8.77	4.92
B3LYP	-0.10	7.39	2.87	3.64	-10.70	1.47	-8.52	8.52	12.73	26.17	-2.65	2.65	5.59
B97-3	0.71	7.60	3.45	4.24	-10.21	1.90	-8.00	8.00	11.78	24.78	-3.82	3.82	5.91
Average								4.58				2.32	3.45

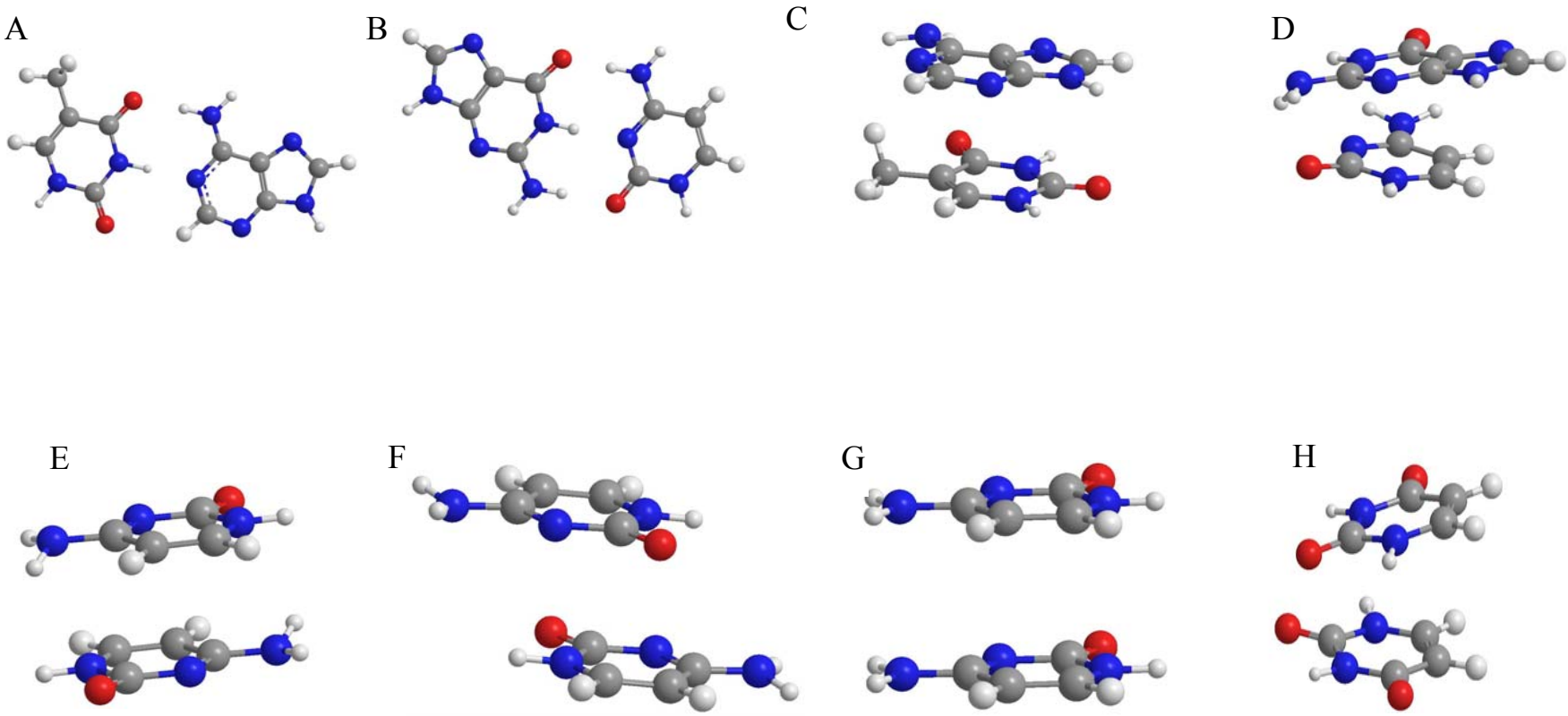
[a] 6-31+G(d,p) is used for all calculations in this table.

[b] AP denotes antiparallel, D denotes displaced, and S denotes sandwich. The structures for all base pairs in this table can be found in Ref. [1] and Supporting Information.

[c] See Ref. [1] and references therein for the sources of these best estimate.

[d] AMUE=0.5 MUE (Stacking) + 0.5 MUE(Hydrogen Bonding)

Figure 1: Structures of the nucleobase pairs. (A) A···T WC, (B) G···C WC, (C) A···T stacking, (D) G···C stacking, (E) C···C antiparallel, (F) C···C displaced, (G) C···C parallel, (H) U···U stacking.



(1) Zhao, Y.; Truhlar, D. G. *Phys. Chem. Chem. Phys.* **2005**, *7*, 2701.