Supplemental Information

Non-covalent interactions in paired DNA nucleobases investigated by terahertz spectroscopy and solid-state density functional theory

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Table 1. Bond lengths and RMSDs for calculated and experimental structures of 1-methylthymine.

bonds	exp.	PBE	PBE-D
C_1-C_2	1.4325	1.4439	1.4460
C_1-C_4	1.3491	1.3678	1.3684
C_1-C_5	1.4988	1.4967	1.4984
C_2-N_1	1.3765	1.3913	1.3926
C_2-O_2	1.2406	1.2538	1.2533
C_3-N_1	1.3764	1.3816	1.3826
C_3-N_2	1.3777	1.3906	1.3924
C_3-O_1	1.2241	1.2354	1.2352
C_4-N_2	1.3793	1.3732	1.3741
C_6-N_2	1.4686	1.4685	1.4697
	RMSD	0.0084	0.0085

Table 2. Bond lengths and RMSDs for calculated and experimental structures of 9-methyladenine.

bonds	exp.	PBE	PBE-D
C_1-N_1	1.3190	1.3299	1.3293
C_1-N_2	1.3672	1.3719	1.3719
C_2-C_3	1.3899	1.4045	1.4048
C_2-C_4	1.4173	1.4241	1.4237
C_2-N_1	1.3853	1.3867	1.3864
C_3-N_2	1.3669	1.3771	1.3777
C_3-N_3	1.3448	1.3455	1.3459
C_4-N_4	1.3513	1.3661	1.3662
C_4-N_5	1.3355	1.3392	1.3402
C_5-N_3	1.3269	1.3353	1.3361
C_5-N_4	1.3429	1.3457	1.3459
C_6-N_2	1.4623	1.4567	1.4573
	RMSD	0.3805	0.3571

Table 3. Bond lengths and RMSDs for calculated and experimental structures of 1-methylthymine and 9-methyladenine in the 1:1 AT co-crystal.

	1-methylthymine				**9-methyladenine**		
bonds	exp.	PBE	PBE-D	bonds	exp.	PBE	PBE-D
C_1-C_2	1.4339	1.4449	1.4463	C_1-N_1	1.3190	1.3272	1.3267
C_1-C_4	1.3550	1.3649	1.3658	C_1-N_2	1.3711	1.3752	1.3755
C_1-C_5	1.4934	1.4938	1.4958	C_2-C_3	1.3883	1.4012	1.4023
C_2-N_1	1.3779	1.3888	1.3894	C_2-C_4	1.4104	1.4218	1.4225
C_2-O_2	1.2364	1.2479	1.2482	C_2-N_1	1.3838	1.3853	1.3849
C_3-N_1	1.3716	1.3762	1.3771	C_3-N_2	1.3738	1.3808	1.3821
C_3-N_2	1.3790	1.3883	1.3899	C_3-N_3	1.3440	1.3461	1.3461
C_3-O_1	1.2313	1.2396	1.2403	C_4-N_4	1.3542	1.3643	1.3643
C_4-N_2	1.3727	1.3755	1.3768	C_4-N_5	1.3325	1.3355	1.3374
C_6-N_2	1.4691	1.4654	1.4672	C_5-N_3	1.3335	1.3392	1.3396
				C_5-N_4	1.3433	1.3441	1.3447
				C_6-N_2	1.4524	1.4535	1.4556
	RMSD	0.0070	0.0075		**RMSD**	0.2475	0.2374

Table 4. Bond angles and RMSDs for calculated and experimental structures of 1-methylthymine.

bond angles	exp.	PBE	PBE-D
C_1-C_2-N_1	115.909	115.579	115.538
C_1-C_2-O_2	123.867	124.256	124.372
C_1-C_4-N_2	123.430	123.536	123.640
C_2-C_1-C_4	118.12	117.825	117.740
C_2-C_1-C_5	119.112	119.384	119.528
C_2-N_1-C_3	126.510	126.954	127.057
C_3-N_2-C_4	120.752	121.349	121.347
C_3-N_2-C_6	117.716	117.495	117.623
C_4-C_1-C_5	122.766	122.792	122.731
C_4-N_2-C_6	121.531	121.156	121.029
N_1-C_3-O_1	121.642	122.788	122.798
N_1-C_2-O_2	120.224	120.164	120.087
N_2-C_3-O_1	123.117	122.505	122.591
	RMSD	0.470	0.504

Table 5. Bond angles and RMSDs for calculated and experimental structures of 9-methyladenine.

bond angles	exp.	PBE	PBE-D
C_1-N_1-C_2	103.577	104.136	104.141
C_1-N_2-C_3	106.241	106.074	106.066
C_1-N_2-C_6	128.258	128.847	128.777
C_2-C_3-N_2	105.681	105.940	105.891
C_2-C_3-N_3	127.608	127.546	127.508
C_2-C_4-N_4	117.498	116.954	116.943
C_2-C_4-N_5	124.168	124.628	124.552
C_3-C_2-N_1	110.735	110.195	110.221
C_3-C_2-C_4	116.123	116.234	116.282
C_3-N_2-C_6	125.487	125.057	125.114
C_3-N_3-C_5	110.464	110.790	110.772
C_4-C_2-N_1	133.133	133.546	133.482
C_4-N_4-C_5	119.119	119.625	119.608
N_1-C_1-N_2	113.760	113.647	113.672
N_2-C_3-N_3	126.707	126.499	126.589
N_3-C_5-N_4	129.146	128.812	128.821
N_4-C_4-N_5	118.333	118.412	118.501
	RMSD	0.380502	0.357077

Table 6. Bond angles and RMSDs for calculated and experimental structures of 1-methylthymine and 9-methyladenine in the 1:1 AT co-crystal.

1-methylthymine				**9-methyladenine**			
bond angles	exp.	PBE	PBE-D	bond angles	exp.	PBE	PBE-D
C_1-C_2-N_1	115.763	115.877	115.820	C_1-N_1-C_2	104.471	104.556	104.578
C_1-C_2-O_2	123.856	123.580	123.697	C_1-N_2-C_3	106.236	106.524	106.442
C_1-C_4-N_2	123.248	122.856	123.054	C_1-N_2-C_6	127.525	127.596	127.494
C_2-C_1-C_4	118.255	118.200	118.061	C_2-C_3-N_2	105.881	105.464	105.461
C_2-C_1-C_5	117.281	117.316	117.440	C_2-C_3-N_3	126.972	127.063	127.037
C_2-N_1-C_3	126.355	126.256	126.475	C_2-C_4-N_4	117.842	117.628	117.555
C_3-N_2-C_4	120.714	121.401	121.322	C_2-C_4-N_5	122.814	123.044	123.077
C_3-N_2-C_6	118.481	117.561	117.719	C_3-C_2-N_1	110.315	110.452	110.438
C_4-C_1-C_5	124.464	124.484	124.499	C_3-C_2-C_4	116.980	116.625	116.672
C_4-N_2-C_6	120.804	121.038	120.958	C_3-N_2-C_6	126.239	125.879	126.062
N_1-C_3-O_1	121.004	122.050	122.064	C_3-N_3-C_5	110.153	110.414	110.412
N_1-C_2-O_2	120.381	120.543	120.484	C_4-C_2-N_1	132.705	132.923	132.889
N_2-C_3-O_1	123.331	122.539	122.669	C_4-N_4-C_5	117.900	118.270	118.323
				N_1-C_1-N_2	113.097	113.004	113.081
				N_2-C_3-N_3	127.148	127.472	127.503
				N_3-C_5-N_4	130.153	129.998	130.001
				N_4-C_4-N_5	119.344	119.327	119.368
	RMSD	0.510	0.455		**RMSD**	0.247	0.237