Supporting Information: CASSCF/CAS-PT2 Study of hole transfer in stacked DNA nucleobases

Authors: Lluís Blancafort, Alexander A. Voityuk

Complete References 26 and 27:

(26) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; J. A. Montgomery, J.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A.; Gaussian03 Revision B.02 ed.; Gaussian, Inc.: Pittsburgh, PA, 2003.

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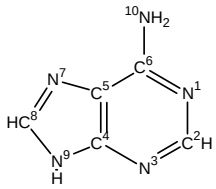
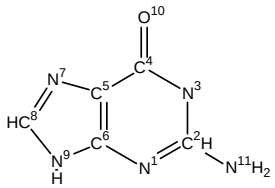
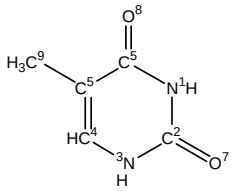
Tables SI1a-c. CASSCF/6-31G* Mulliken charges on heavy atoms (including charges on attached hydrogens) calculated for the radical cations with different active spaces.



	ADENINE		
	(11,10)	(5,6)	(3,4)
N_1	-0.532	-0.542	-0.607
C_2	0.531	0.565	0.614
N_3	-0.451	-0.454	-0.478
C_4	0.631	0.659	0.680
C_5	0.170	0.194	0.183
C_6	0.623	0.675	0.706
N_7	-0.516	-0.547	-0.539
C_8	0.625	0.711	0.722
N_9	-0.333	-0.362	-0.361
N_{10}	0.253	0.101	0.079



	GUANINE		
	(11,10)	(5,6)	(3,4)
N_1	-0.588	-0.650	-0.650
C_2	0.965	1.009	1.011
N_3	-0.458	-0.483	-0.474
C_4	0.809	0.822	0.872
C_5	0.115	0.124	0.117
C_6	0.671	0.738	0.743
N_7	-0.449	-0.446	-0.434
C_8	0.636	0.658	0.670
N_9	-0.340	-0.365	-0.362
O_{10}	-0.401	-0.394	-0.490
N_{11}	0.039	-0.013	-0.002



	THYMINE		
	(9,8)	(5,6)	(3,4)
N_1	-0.442	-0.458	-0.448
C_2	1.010	1.029	1.069
N_3	-0.202	-0.308	-0.311
C_4	0.525	0.596	0.613
C_5	-0.059	-0.039	-0.040
C_6	0.782	0.787	0.786
O_7	-0.408	-0.433	-0.514
O_8	-0.420	-0.407	-0.398
C_9	0.214	0.235	0.242

Table SI2. CASSCF, CAS-PT2, and MS-PT2 absolute energies (6-31G* basis set)for the base dimers (ground and excited state) and trimers (ground and two lowest excited states).

	CASSCF(11,12)	CASSCF(7,8)	CAS-PT2[a,b]	MS-PT2[b]
AA	-928.8646	-928.8040	-931.6039 (0.56)	-931.6040
	-928.8629	-928.7987	-931.6001 (0.56)	-931.6005
GG	-1078.6391	-1078.5787	-1081.7009 (0.54)	-1081.7009
	-1078.6255	-1078.5635	-1081.6865 (0.54)	-1081.6865
AG	-1003.7644	-1003.7122	-1006.6616 (0.55)	-1006.6616
	-1003.7474	-1003.6904	-1006.6491 (0.55)	-1006.6491
GA	-1003.7632	-1003.7112	-1006.6639 (0.55)	-1006.6641
	-1003.7369	-1003.6784	-1006.6437 (0.55)	-1006.6435
GT	-990.7416	-990.6842	-993.4996 (0.57)	-993.4997
	-990.6896	-990.6181	-993.4565 (0.57)	-993.4565
TG	-990.7473	-990.6915	-993.5008 (0.57)	-993.5008
	-990.7070	-990.6462	-993.4716 (0.57)	-993.4715
GvacG	-1078.6343	-1078.5740	-1081.6817 (0.54)	-1081.6817
	-1078.6282	-1078.5677	-1081.6756 (0.54)	-1081.6756
GAG	-1543.1199	-	-	-
	-1543.1156			
	-1543.1074			
GTG	-1530.1093	-	-	-
	-1530.1028			
	-1530.0638			

[a]Reference weight in parentheses. [b]CASSCF(11,12) reference.

Table SI 3. CASSCF/6-31G* Dipole moment differences ($\Delta\mu$) and transition dipole moments (μ_{ij}) for the dimers and trimers.

			$\Delta\mu^a$			μ_{ij}^a		
	Active space	States	x	y	z	x	y	z
AA	(11,12)	1->2	1.828	1.195	-6.197	-0.113	-0.045	0.256
	(7,8)	1->2	0.538	0.659	-2.439	-0.632	-0.573	2.810
GG	(11,12)	1->2	-2.450	-1.451	6.019	0.349	0.159	-0.819
	(7,8)	1->2	-2.290	-1.427	5.903	0.429	0.219	-1.015
AG	(11,12)	1->2	2.433	0.391	-6.027	-0.330	-0.065	0.817
	(7,8)	1->2	2.642	1.536	-6.182	-0.213	-0.150	0.475
GA	(11,12)	1->2	-1.845	-2.310	6.197	-0.181	-0.095	0.410
	(7,8)	1->2	-2.300	-1.351	6.165	-0.189	-0.058	0.374
GT	(11,12)	1->2	-2.640	1.041	6.123	-0.216	0.143	0.424
	(7,8)	1->2	-2.588	1.373	6.220	-0.177	0.141	0.340
TG	(11,12)	1->2	0.969	5.3206	-6.244	0.071	0.386	-0.484
	(7,8)	1->2	1.449	5.420	-6.274	0.103	0.360	-0.445
GTG	(11,12)	1->2	-3.769	-4.404	12.593	-0.028	-0.009	0.068
		1->3	-2.354	1.396	6.248	-0.198	0.141	0.398
		2->3	1.414	5.801	-6345	-0.121	-0.421	0.496
GAG	(11,12)	1->2	-3.507	-3.995	11.852	-0.430	-0.455	1.376
		1->3	-1.892	-2.008	6.103	0.356	0.257	-0.916
		2->3	1.615	1.987	-5.749	0.422	0.530	-1.523

[a]Z-axis oriented along stacking direction in all cases.

Cartesian coordinates of dimers and trimers.
The AG, GA, GT, TG, and GvacG dimers were extracted from the corresponding trimers.

AA

1	7	0	-1.334000	4.521000	0.000000
2	6	0	0.000000	4.846000	0.000000
3	7	0	0.797000	3.806000	0.000000
4	6	0	-0.070000	2.721000	0.000000
5	6	0	0.152000	1.333000	0.000000
6	7	0	1.365000	0.777000	0.000000
7	7	0	-0.932000	0.526000	0.000000
8	6	0	-2.147000	1.085000	0.000000
9	7	0	-2.484000	2.372000	0.000000
10	6	0	-1.386000	3.147000	0.000000
11	1	0	-2.108000	5.154000	0.000000
12	1	0	0.392000	5.852000	0.000000
13	1	0	2.189000	1.362000	0.000000
14	1	0	1.460000	-0.229000	0.000000
15	1	0	-2.915000	0.326000	0.000000
16	7	0	-3.737000	2.873000	3.380000
17	6	0	-2.848000	3.920000	3.380000
18	7	0	-1.592000	3.548000	3.380000
19	6	0	-1.656000	2.160000	3.380000
20	6	0	-0.660000	1.168000	3.380000
21	7	0	0.648000	1.431000	3.380000
22	7	0	-1.063000	-0.122000	3.380000
23	6	0	-2.374000	-0.384000	3.380000
24	7	0	-3.404000	0.459000	3.380000
25	6	0	-2.971000	1.731000	3.380000
26	1	0	-4.735000	2.931000	3.380000
27	1	0	-3.121000	4.965000	3.380000
28	1	0	0.971000	2.388000	3.380000
29	1	0	1.316000	0.673000	3.380000
30	1	0	-2.549000	-1.450000	3.380000

GG

1	7	0	-1.330000	4.518000	0.000000
2	6	0	0.000000	4.862000	0.000000
3	7	0	0.798000	3.830000	0.000000
4	6	0	-0.056000	2.734000	0.000000
5	6	0	0.230000	1.346000	0.000000
6	8	0	1.333000	0.786000	0.000000
7	7	0	-0.934000	0.583000	0.000000
8	6	0	-2.210000	1.093000	0.000000
9	7	0	-3.204000	0.193000	0.000000
10	7	0	-2.490000	2.384000	0.000000
11	6	0	-1.373000	3.144000	0.000000
12	1	0	-2.113000	5.140000	0.000000
13	1	0	0.378000	5.874000	0.000000
14	1	0	-0.877000	-0.415000	0.000000
15	1	0	-4.156000	0.499000	0.000000
16	1	0	-2.993000	-0.785000	0.000000
17	7	0	-3.731000	2.873000	3.380000
18	6	0	-2.858000	3.934000	3.380000
19	7	0	-1.605000	3.567000	3.380000
20	6	0	-1.653000	2.179000	3.380000
21	6	0	-0.605000	1.224000	3.380000
22	8	0	0.617000	1.420000	3.380000
23	7	0	-1.098000	-0.077000	3.380000
24	6	0	-2.430000	-0.415000	3.380000
25	7	0	-2.705000	-1.727000	3.380000
26	7	0	-3.416000	0.465000	3.380000
27	6	0	-2.959000	1.736000	3.380000
28	1	0	-4.730000	2.916000	3.380000
29	1	0	-3.148000	4.974000	3.380000
30	1	0	-0.465000	-0.851000	3.380000
31	1	0	-3.655000	-2.039000	3.380000
32	1	0	-1.960000	-2.394000	3.380000

GTG

1	7	0	-1.330000	4.518000	-0.001000
2	6	0	0.000000	4.862000	0.000000
3	7	0	0.798000	3.830000	-0.001000
4	6	0	-0.056000	2.734000	-0.001000
5	6	0	0.230000	1.346000	0.000000
6	8	0	1.333000	0.786000	-0.001000
7	7	0	-0.934000	0.583000	-0.001000
8	6	0	-2.210000	1.093000	-0.001000
9	7	0	-3.204000	0.193000	-0.001000
10	7	0	-2.490000	2.384000	0.000000
11	6	0	-1.373000	3.144000	-0.001000
12	1	0	-2.113000	5.140000	-0.001000
13	1	0	0.378000	5.874000	-0.001000
14	1	0	-0.877000	-0.415000	0.000000
15	1	0	-4.156000	0.499000	-0.001000
16	1	0	-2.993000	-0.785000	-0.001000
17	7	0	-3.622000	2.780000	3.380000
18	6	0	-3.047000	1.529000	3.380000
19	8	0	-3.699000	0.497000	3.380000
20	7	0	-1.674000	1.529000	3.380000
21	6	0	-0.839000	2.630000	3.380000
22	8	0	0.379000	2.476000	3.380000
23	6	0	-1.509000	3.911000	3.380000
24	6	0	-0.687000	5.161000	3.381000
25	6	0	-2.848000	3.920000	3.380000
26	1	0	-4.618000	2.873000	3.380000
27	1	0	-1.174000	0.663000	3.380000
28	1	0	-3.284000	4.820000	3.380000
29	1	0	0.381000	4.898000	3.382000
30	1	0	-0.918000	5.753000	2.483000
31	1	0	-0.919000	5.752000	4.279000
32	7	0	-4.708000	0.131000	6.759000
33	6	0	-4.624000	1.503000	6.760000
34	7	0	-3.395000	1.942000	6.759000
35	6	0	-2.618000	0.792000	6.759000
36	6	0	-1.209000	0.634000	6.760000
37	8	0	-0.336000	1.511000	6.759000
38	7	0	-0.843000	-0.708000	6.759000
39	6	0	-1.722000	-1.764000	6.759000
40	7	0	-1.173000	-2.987000	6.759000
41	7	0	-3.037000	-1.631000	6.760000
42	6	0	-3.414000	-0.335000	6.759000
43	1	0	-5.542000	-0.421000	6.759000
44	1	0	-5.469000	2.175000	6.759000
45	1	0	0.124000	-0.963000	6.760000
46	1	0	-1.758000	-3.798000	6.759000
47	1	0	-0.178000	-3.088000	6.759000

GAG

1	7	0	-1.330000	4.518000	-0.001000
2	6	0	0.000000	4.862000	0.000000
3	7	0	0.798000	3.830000	-0.001000
4	6	0	-0.056000	2.734000	-0.001000
5	6	0	0.230000	1.346000	0.000000
6	8	0	1.333000	0.786000	-0.001000
7	7	0	-0.934000	0.583000	-0.001000
8	6	0	-2.210000	1.093000	-0.001000
9	7	0	-3.204000	0.193000	-0.001000
10	7	0	-2.490000	2.384000	0.000000
11	6	0	-1.373000	3.144000	-0.001000
12	1	0	-2.113000	5.140000	-0.001000
13	1	0	0.378000	5.874000	-0.001000
14	1	0	-0.877000	-0.415000	0.000000
15	1	0	-4.156000	0.499000	-0.001000
16	1	0	-2.993000	-0.785000	-0.001000
17	7	0	-3.622000	2.780000	3.380000
18	6	0	-3.047000	1.529000	3.380000
19	8	0	-3.699000	0.497000	3.380000
20	7	0	-1.674000	1.529000	3.380000
21	6	0	-0.839000	2.630000	3.380000
22	8	0	0.379000	2.476000	3.380000
23	6	0	-1.509000	3.911000	3.380000
24	6	0	-0.687000	5.161000	3.381000
25	6	0	-2.848000	3.920000	3.380000
26	1	0	-4.618000	2.873000	3.380000
27	1	0	-1.174000	0.663000	3.380000
28	1	0	-3.284000	4.820000	3.380000
29	1	0	0.381000	4.898000	3.382000
30	1	0	-0.918000	5.753000	2.483000
31	1	0	-0.919000	5.752000	4.279000
32	7	0	-4.708000	0.131000	6.759000
33	6	0	-4.624000	1.503000	6.760000
34	7	0	-3.395000	1.942000	6.759000
35	6	0	-2.618000	0.792000	6.759000
36	6	0	-1.209000	0.634000	6.760000
37	8	0	-0.336000	1.511000	6.759000
38	7	0	-0.843000	-0.708000	6.759000
39	6	0	-1.722000	-1.764000	6.759000
40	7	0	-1.173000	-2.987000	6.759000
41	7	0	-3.037000	-1.631000	6.760000
42	6	0	-3.414000	-0.335000	6.759000
43	1	0	-5.542000	-0.421000	6.759000
44	1	0	-5.469000	2.175000	6.759000
45	1	0	0.124000	-0.963000	6.760000
46	1	0	-1.758000	-3.798000	6.759000
47	1	0	-0.178000	-3.088000	6.759000