

The excited states of π -stacked 9-methyl adenine oligomers: a TD-DFT study in aqueous solution

SUPPORTING INFORMATION

Table 1. (9-MA)₂ S_{CT} state minimum. PCM/TD-PBE0/6-31G(d) partial geometry optimizations in solution

Atomic number	Cartesian coordinates (in Å)		
7	-2.623552	1.040201	-0.025989
6	-3.181240	0.229373	-0.969545
7	-2.750677	-1.059612	-0.853407
6	-1.866055	-1.035699	0.135861
6	-1.722042	0.271910	0.688905
6	-1.024899	-2.052462	0.761345
7	-0.266095	-1.696626	1.808344
6	-0.212504	-0.443709	2.198731
7	-0.930886	0.649601	1.657679
6	-2.759335	2.475340	0.107448
1	-1.869434	2.975292	-0.279601
1	-2.880439	2.726909	1.160308
1	-3.634301	2.797521	-0.453512
1	-3.910652	0.584480	-1.685019
7	-0.902176	-3.283442	0.191200
1	-1.257148	-3.395867	-0.756397
1	-0.052552	-3.805816	0.402891
1	0.406234	-0.206728	3.055643
7	1.479743	2.176504	-0.259229
6	0.674817	2.127067	-1.368862
7	0.562924	0.932315	-1.895186
6	1.328142	0.140303	-1.067869
6	1.905546	0.893089	-0.046802
6	1.631852	-1.236795	-1.073208
7	2.447730	-1.716511	-0.117522
6	2.920210	-0.868028	0.804472
7	2.716151	0.442024	0.919796
6	1.679226	3.301128	0.636667
1	2.697352	3.270595	1.018933
1	1.523260	4.224366	0.082068
1	0.973498	3.238563	1.465580
1	0.218168	3.028826	-1.762028
7	1.152165	-2.071912	-2.006500
1	1.324658	-3.065540	-1.914497
1	0.451558	-1.754970	-2.664954
1	3.570193	-1.314534	1.553429

Table 2. (9-MA)₂ S_B state minimum. PCM/TD-PBE0/6-31G(d)
partial geometry optimizations in solution

Atomic number	Cartesian coordinates (in Å)		
7	1.674598	2.048235	-0.197628
6	0.874640	2.087889	-1.316930
7	0.673310	0.877968	-1.854314
6	1.454225	0.048867	-1.146567
6	2.110512	0.736313	-0.076433
6	1.513972	-1.396869	-1.054073
7	2.290680	-1.983533	-0.151307
6	3.044297	-1.195661	0.651125
7	2.811069	0.184356	0.868746
6	1.983823	3.117103	0.713349
1	0.470757	3.020751	-1.699584
7	0.804872	-2.134160	-1.924893
1	0.866075	-3.150418	-1.902548
1	0.241804	-1.688757	-2.646310
1	3.717240	-1.680961	1.351508
1	1.666828	2.839273	1.724920
1	3.059085	3.326732	0.722618
1	1.446686	4.015454	0.401752
7	-2.486999	1.271670	-0.058205
6	-3.125852	0.500321	-0.991452
7	-2.836073	-0.777644	-0.915760
6	-1.942683	-0.848824	0.129842
6	-1.710114	0.414458	0.675612
6	-1.244925	-1.918382	0.726238
7	-0.436211	-1.653984	1.768209
6	-0.299325	-0.384496	2.166744
7	-0.877249	0.712073	1.678495
6	-2.565015	2.706764	0.104216
1	-3.813393	0.944603	-1.707450
7	-1.381285	-3.195365	0.318140
1	-1.822367	-3.383801	-0.576285
1	-0.704437	-3.874362	0.654503
1	0.388022	-0.229949	2.999360
1	-2.106269	3.217278	-0.747880
1	-2.021116	2.969598	1.013117
1	-3.607217	3.022345	0.201875

Table 3. (9-MA)₅ S₀ state minimum. PCM/TD-PBE0/6-31G(d) partial geometry optimizations in solution

Atomic number	Cartesian coordinates (in Å)		
7	7.90728	-0.2627	1.21412
6	8.03589	-1.60758	1.43661
7	7.61712	-2.35494	0.44263
6	7.17187	-1.44227	-0.48832
6	7.34384	-0.13597	-0.0278
6	6.61862	-1.57494	-1.77714
7	6.29283	-0.45917	-2.45302
6	6.48788	0.72683	-1.86405
7	6.99644	0.98826	-0.66217
6	8.2665	0.81875	2.10514
1	7.67572	0.77314	3.02458
1	8.05704	1.75762	1.58958
1	9.33057	0.77382	2.35339
1	8.46463	-1.98183	2.36335
7	6.44793	-2.77225	-2.38136
1	6.42822	-3.60014	-1.79311
1	5.82043	-2.7873	-3.18104
1	6.18282	1.59357	-2.45228
7	4.15107	1.69266	1.13361
6	4.47204	0.75034	2.07357
7	4.29544	-0.48664	1.67421
6	3.77823	-0.34607	0.40586
6	3.68174	0.99842	0.04941
6	3.36599	-1.279	-0.56853
7	2.87713	-0.81542	-1.7335
6	2.81151	0.5084	-1.91358
7	3.183	1.48832	-1.09222
6	4.28832	3.12668	1.2373
1	3.83023	3.5705	0.35155
1	3.78018	3.49756	2.13168
1	5.34447	3.41069	1.27014
1	4.86309	1.04376	3.04516
7	3.45031	-2.60414	-0.37997
1	3.1192	-3.23936	-1.09734
1	3.8013	-2.98156	0.4917
1	2.38935	0.82493	-2.86861
7	0.13671	2.5231	0.1211
6	0.55425	2.34706	1.4131
7	0.63196	1.09125	1.78437
6	0.19569	0.39858	0.67589
6	-0.11766	1.26863	-0.36764
6	0.02789	-0.97615	0.41007
7	-0.45349	-1.34372	-0.79153
6	-0.74364	-0.38746	-1.6802
7	-0.61254	0.93193	-1.56494
6	0.00252	3.766	-0.60213
1	-0.47398	3.54459	-1.55883
1	-0.61921	4.46992	-0.04212
1	0.9847	4.21049	-0.78911
1	0.81261	3.20027	2.03619
7	0.30984	-1.92595	1.31643
1	0.26305	-2.90091	1.04353
1	0.76711	-1.68475	2.18782
1	-1.14769	-0.74326	-2.6295
7	-3.87691	1.85965	-1.01218
6	-3.52967	2.51783	0.13697
7	-3.25139	1.72783	1.14594
6	-3.47425	0.46681	0.63961
6	-3.86565	0.52529	-0.69834
6	-3.37618	-0.82023	1.20428
7	-3.6909	-1.88163	0.44107
6	-4.08624	-1.66438	-0.81809
7	-4.21035	-0.51083	-1.47156
6	-4.16619	2.43209	-2.30639
1	-4.49807	1.62445	-2.9613
1	-4.95735	3.18282	-2.22714
1	-3.26789	2.88796	-2.73326
1	-3.47607	3.60365	0.16068
7	-3.01425	-1.02489	2.48608
1	-2.78539	-1.97154	2.77181
1	-2.59735	-0.26412	3.01149
1	-4.34734	-2.56044	-1.38332
7	-7.61673	-0.05382	-1.39554
6	-7.47133	1.18806	-0.83613
7	-7.12603	1.17073	0.42867
6	-7.07657	-0.17139	0.73241
6	-7.38076	-0.94939	-0.38569
6	-6.78767	-0.87327	1.91866
7	-6.85645	-2.21573	1.90099
6	-7.17289	-2.82383	0.75139
7	-7.44117	-2.28509	-0.43607
6	-7.90995	-0.37488	-2.77458
1	-7.02564	-0.22015	-3.40002
1	-8.20058	-1.42581	-2.82277
1	-8.73263	0.24544	-3.13896
1	-7.62503	2.08612	-1.42979
7	-6.48888	-0.2491	3.07952
1	-6.18337	0.71815	3.03122
1	-6.04165	-0.81586	3.79475
1	-7.20589	-3.91409	0.79709