

Electron Interaction with the DNA Duplex: dCpdC:dGpdG

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Supporting Information

Coordinates of the optimized structure of dC^{□-}pdC:dGpdG and dCpdC^{□-}:dGpdG are attached as following.

dC^{□-}pdC:dGpdG

8	8.000000	-16.806801	-7.480046	1.324906
6	6.000000	-17.846141	-5.481309	2.749049
1	1.000000	-19.762146	-5.160202	2.038125
1	1.000000	-17.972825	-5.983605	4.758937
6	6.000000	-16.290660	-3.076830	2.497588
1	1.000000	-17.109087	-1.591842	3.693729
8	8.000000	-13.783128	-3.630109	3.303148
6	6.000000	-12.009993	-2.744904	1.449918
1	1.000000	-11.474277	-0.782977	1.854059

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7	7.000000	-9.734883	-4.169573	1.625942
6	6.000000	-9.330126	-6.731991	1.233321
1	1.000000	-10.837009	-7.973606	0.625394
7	7.000000	-7.011124	-7.416459	1.656190
6	6.000000	-5.786193	-5.212697	2.331065
6	6.000000	-3.199783	-4.719314	2.964569
8	8.000000	-1.444603	-6.232614	3.152822
7	7.000000	-2.792184	-2.133975	3.417958
1	1.000000	-0.933816	-1.618061	3.763269
6	6.000000	-4.598216	-0.275826	3.327716
7	7.000000	-3.851331	2.104057	3.861896
1	1.000000	-1.970364	2.550373	3.874821
1	1.000000	-5.089672	3.451644	3.304507
7	7.000000	-7.002913	-0.726913	2.820397
6	6.000000	-7.439861	-3.181100	2.323317
6	6.000000	-16.063924	-2.063103	-0.222376
1	1.000000	-17.582978	-2.692936	-1.470812
6	6.000000	-13.455986	-2.949425	-1.031122
1	1.000000	-13.584534	-4.927409	-1.620935
1	1.000000	-12.624573	-1.869546	-2.576877
8	8.000000	-16.225577	0.665044	0.027768
15	15.000000	-15.446795	2.545385	-2.207664
8	8.000000	-17.192813	4.959974	-1.613354
8	8.000000	-15.594697	1.481815	-4.769189

8	8.000000	-12.739154	3.623062	-1.489565
6	6.000000	-12.249422	4.930929	0.854182
1	1.000000	-13.881059	6.114355	1.321714
1	1.000000	-11.920676	3.530043	2.339792
6	6.000000	-9.906804	6.561029	0.538038
1	1.000000	-9.833872	7.885903	2.129922
8	8.000000	-7.685019	5.069313	0.583514
6	6.000000	-6.486735	4.962493	-1.839250
1	1.000000	-4.653291	5.908225	-1.702410
7	7.000000	-5.950411	2.389557	-2.495268
6	6.000000	-7.646641	0.463530	-3.028881
1	1.000000	-9.643854	0.854213	-3.196375
7	7.000000	-6.570054	-1.732207	-3.280786
6	6.000000	-4.029557	-1.273984	-2.867836
6	6.000000	-1.869134	-2.934344	-2.889790
8	8.000000	-1.818881	-5.224583	-3.235655
7	7.000000	0.376547	-1.594287	-2.433587
1	1.000000	2.082667	-2.614344	-2.494584
6	6.000000	0.555686	0.956892	-2.046590
7	7.000000	2.896731	1.890849	-1.727674
1	1.000000	4.482248	0.909713	-2.290670
1	1.000000	3.041254	3.787501	-1.611015
7	7.000000	-1.420681	2.495565	-1.953463
6	6.000000	-3.607238	1.267936	-2.373687

6	6.000000	-9.826826	8.040691	-1.951333
1	1.000000	-11.731611	8.416643	-2.684224
6	6.000000	-8.307939	6.289566	-3.664955
1	1.000000	-9.562016	4.913449	-4.555971
1	1.000000	-7.289950	7.304936	-5.149524
8	8.000000	-8.538241	10.333845	-1.425192
1	1.000000	-15.149374	-7.812128	2.018466
1	1.000000	-8.048015	11.114992	-2.995196
1	1.000000	-18.916986	4.729612	-2.163333
8	8.000000	17.357064	-6.853073	-1.751434
6	6.000000	17.963643	-4.969464	-3.537798
1	1.000000	19.866973	-4.292379	-3.089168
1	1.000000	17.979308	-5.744664	-5.464066
6	6.000000	16.089603	-2.794825	-3.427771
1	1.000000	16.577750	-1.364905	-4.854600
8	8.000000	13.654418	-3.806519	-3.902410
6	6.000000	11.873641	-2.620886	-2.193107
1	1.000000	11.364661	-0.760979	-2.928601
7	7.000000	9.616027	-4.053972	-2.056359
6	6.000000	9.675178	-6.485835	-0.927072
1	1.000000	11.488998	-7.438165	-0.990509
6	6.000000	7.384499	-7.849760	-0.938943
1	1.000000	7.368847	-9.830899	-0.411006
6	6.000000	5.193171	-6.663258	-1.739271

7	7.000000	2.912495	-7.886036	-1.873727
1	1.000000	2.678078	-9.479113	-0.860782
1	1.000000	1.307017	-6.889531	-2.244166
7	7.000000	5.141379	-4.156917	-2.452246
6	6.000000	7.304903	-2.856764	-2.639284
8	8.000000	7.369360	-0.566172	-3.250679
6	6.000000	15.952476	-1.490437	-0.818590
1	1.000000	17.571855	-1.903659	0.394297
6	6.000000	13.440090	-2.394256	0.228756
1	1.000000	13.688229	-4.256362	1.090996
1	1.000000	12.619985	-1.131354	1.640974
8	8.000000	15.937247	1.214899	-1.327228
15	15.000000	15.325464	3.153556	0.905403
8	8.000000	16.439932	5.743115	-0.232205
8	8.000000	16.219524	2.391641	3.424435
8	8.000000	12.377672	3.716765	0.819033
6	6.000000	11.099929	4.812275	-1.339248
1	1.000000	12.470001	5.876200	-2.463942
1	1.000000	10.251903	3.276334	-2.442352
6	6.000000	9.006880	6.550009	-0.392159
1	1.000000	8.581442	7.931571	-1.875452
8	8.000000	6.773668	5.149250	0.096046
6	6.000000	6.193549	5.035223	2.727235
1	1.000000	4.458903	6.085850	3.089934

7	7.000000	5.647436	2.430362	3.394976
6	6.000000	7.452677	0.627186	2.946325
1	1.000000	9.309163	1.330656	2.439474
6	6.000000	6.926971	-1.857163	3.095151
1	1.000000	8.339209	-3.298916	2.727400
6	6.000000	4.333447	-2.531335	3.573032
7	7.000000	3.693153	-4.966729	3.654203
1	1.000000	4.940364	-6.214847	2.908313
1	1.000000	1.810467	-5.444457	3.600854
7	7.000000	2.559855	-0.786512	3.978429
6	6.000000	3.113151	1.713040	3.848220
8	8.000000	1.503807	3.378070	4.137253
6	6.000000	9.622191	7.937335	2.075762
1	1.000000	11.662530	8.211737	2.318882
6	6.000000	8.489862	6.184917	4.075400
1	1.000000	9.861413	4.730583	4.594535
1	1.000000	7.931388	7.195771	5.789424
8	8.000000	8.349266	10.298763	1.957698
1	1.000000	15.626433	-7.340611	-2.087899
1	1.000000	8.403704	11.081929	3.600421
1	1.000000	18.264227	5.768902	-0.246350

dCpdC^{•-}:dGpdG

8	8.000000	-16.899819	-7.514538	1.370951
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6	6.000000	-17.686059	-5.542353	3.001353
1	1.000000	-19.638140	-5.082673	2.503864
1	1.000000	-17.644279	-6.150338	4.981173
6	6.000000	-16.057594	-3.199126	2.704194
1	1.000000	-16.780172	-1.693766	3.930472
8	8.000000	-13.517278	-3.818061	3.418141
6	6.000000	-11.829598	-2.863258	1.544084
1	1.000000	-11.362532	-0.881017	1.939614
7	7.000000	-9.476774	-4.193836	1.648930
6	6.000000	-8.950980	-6.687847	1.077148
1	1.000000	-10.422539	-7.997064	0.530417
7	7.000000	-6.554457	-7.240140	1.294858
6	6.000000	-5.412275	-4.996711	2.030258
6	6.000000	-2.826842	-4.320043	2.491224
8	8.000000	-1.010135	-5.855181	2.310872
7	7.000000	-2.419425	-1.846257	3.141187
1	1.000000	0.961417	-0.965321	3.752359
6	6.000000	-4.360408	-0.192631	3.248260
7	7.000000	-3.771861	2.259024	3.887898
1	1.000000	-1.946761	2.771710	3.555049
1	1.000000	-5.095846	3.516521	3.302423
7	7.000000	-6.814320	-0.674972	2.866895
6	6.000000	-7.196601	-3.096041	2.256014
6	6.000000	-15.904780	-2.206257	-0.031096

1	1.000000	-17.467377	-2.844583	-1.216614
6	6.000000	-13.320757	-3.106854	-0.903265
1	1.000000	-13.461992	-5.093130	-1.460526
1	1.000000	-12.539825	-2.026604	-2.473579
8	8.000000	-16.013107	0.524287	0.173297
15	15.000000	-15.526036	2.373032	-2.164888
8	8.000000	-17.512603	4.588895	-1.709254
8	8.000000	-15.485632	1.133972	-4.664159
8	8.000000	-12.940466	3.790458	-1.572006
6	6.000000	-12.580321	5.248382	0.704734
1	1.000000	-14.182164	6.531266	0.955315
1	1.000000	-12.453447	3.956842	2.314767
6	6.000000	-10.156866	6.756425	0.458354
1	1.000000	-10.054137	8.043513	2.076127
8	8.000000	-8.006371	5.126851	0.527504
6	6.000000	-6.710480	5.116204	-1.832252
1	1.000000	-4.894755	6.080058	-1.614775
7	7.000000	-6.106918	2.542899	-2.520380
6	6.000000	-7.771759	0.633033	-3.146073
1	1.000000	-9.776372	1.006837	-3.290156
7	7.000000	-6.662469	-1.539815	-3.515482
6	6.000000	-4.129352	-1.060596	-3.091211
6	6.000000	-1.960395	-2.678596	-3.208403
8	8.000000	-1.856504	-4.960016	-3.698598

7	7.000000	0.261516	-1.347604	-2.697040
1	1.000000	1.895505	-2.425062	-2.651974
6	6.000000	0.425453	1.183513	-2.151373
7	7.000000	2.765880	2.112551	-1.809324
1	1.000000	4.338929	1.111629	-2.303348
1	1.000000	2.946479	3.968841	-1.413885
7	7.000000	-1.565248	2.684092	-1.990033
6	6.000000	-3.751033	1.462972	-2.463893
6	6.000000	-9.929689	8.262693	-2.003142
1	1.000000	-11.783859	8.756309	-2.782218
6	6.000000	-8.450036	6.467552	-3.706192
1	1.000000	-9.736622	5.123956	-4.600139
1	1.000000	-7.387265	7.456356	-5.172732
8	8.000000	-8.515423	10.466364	-1.414082
1	1.000000	-15.340743	-8.198067	2.027492
1	1.000000	-8.247435	11.425704	-2.942582
1	1.000000	-19.270139	4.076461	-1.752118
8	8.000000	15.834224	-7.277606	-0.954168
6	6.000000	17.028348	-5.954342	-2.960194
1	1.000000	19.053348	-5.705733	-2.589704
1	1.000000	16.795364	-6.962171	-4.754930
6	6.000000	15.805822	-3.374778	-3.208228
1	1.000000	16.815786	-2.290644	-4.652577
8	8.000000	13.222424	-3.663957	-3.967552

6	6.000000	11.582152	-2.593449	-2.129402
1	1.000000	10.979638	-0.709832	-2.714954
7	7.000000	9.291956	-4.100191	-1.984737
6	6.000000	9.415925	-6.560112	-1.210233
1	1.000000	11.308646	-7.293902	-0.890622
6	6.000000	7.297835	-7.962834	-0.912714
1	1.000000	7.385247	-9.913635	-0.306633
6	6.000000	4.928059	-6.732113	-1.426608
7	7.000000	2.745906	-7.952247	-1.083056
1	1.000000	2.739683	-9.646454	-0.208134
1	1.000000	1.087377	-6.968584	-1.120868
7	7.000000	4.835342	-4.370843	-2.296214
6	6.000000	6.973030	-3.010773	-2.662581
8	8.000000	6.928022	-0.851878	-3.569633
6	6.000000	15.726209	-1.874745	-0.730241
1	1.000000	17.281153	-2.321864	0.549317
6	6.000000	13.125407	-2.501723	0.306689
1	1.000000	13.202593	-4.350724	1.219801
1	1.000000	12.424604	-1.109324	1.653845
8	8.000000	15.869738	0.773374	-1.421533
15	15.000000	15.610129	2.887659	0.733159
8	8.000000	17.051901	5.231297	-0.478108
8	8.000000	16.370063	2.015731	3.272301
8	8.000000	12.764894	3.859752	0.708980

6	6.000000	11.643829	5.187146	-1.398372
1	1.000000	13.060950	6.426495	-2.248795
1	1.000000	10.987669	3.799076	-2.784799
6	6.000000	9.425113	6.752341	-0.464684
1	1.000000	8.965206	8.118460	-1.951868
8	8.000000	7.259102	5.212529	-0.028191
6	6.000000	6.559325	5.203282	2.592907
1	1.000000	4.849347	6.326738	2.835739
7	7.000000	5.931480	2.648727	3.320051
6	6.000000	7.827693	0.771196	3.107259
1	1.000000	9.702259	1.452302	2.697946
6	6.000000	7.179051	-1.756245	3.466514
1	1.000000	8.618405	-3.215850	3.420646
6	6.000000	4.695798	-2.413787	3.852267
7	7.000000	3.788208	-4.801453	4.404259
1	1.000000	5.066907	-6.179310	4.039526
1	1.000000	2.043432	-5.200909	3.627140
7	7.000000	2.870815	-0.497318	3.871415
6	6.000000	3.409977	2.013588	3.588082
8	8.000000	1.717174	3.622152	3.634547
6	6.000000	9.926342	8.155399	2.020687
1	1.000000	11.945947	8.505228	2.315044
6	6.000000	8.804098	6.373743	3.994045
1	1.000000	10.188009	4.936557	4.522487

1	1.000000	8.201522	7.373816	5.696465
8	8.000000	8.569286	10.469159	1.877823
1	1.000000	16.556162	-8.945955	-0.825911
1	1.000000	8.762549	11.363357	3.456281
1	1.000000	18.825697	4.953619	-0.838073