

Coupled-cluster and density functional theory studies of the electronic 0–0 transitions of the DNA bases

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1 Adenine

1.1 Cartesian coordinates of the adenine ground state tautomers optimized at the B3LYP/def2-TZVPPD level.

				H	2.0141235	-2.5622085	-0.0217971
				H	-1.2647223	2.2936672	-0.1270719
				H	-3.3556002	0.9019485	0.0599459
				(A3)			
(A1)				C	1.2010748	0.6828748	-0.0424906
C	1.2017051	0.5658856	-0.0383836	C	-0.2193593	0.4254081	-0.0076234
C	-0.1960253	0.4146295	-0.0061683	C	-0.6715640	-0.8816188	0.0199747
C	-0.6701850	-0.8958114	0.0184301	N	0.0661926	-2.0270719	0.0197103
N	0.0657966	-2.0073865	0.0160883	N	-1.2715720	1.3070532	0.0034160
N	-1.2385411	1.3221402	0.0070219	N	-2.0369853	-0.7868151	0.0480575
N	-2.0380399	-0.7688963	0.0457829	C	-2.3402285	0.5528217	0.0366412
C	-2.3114941	0.5798205	0.0375315	C	1.3403944	-1.7856230	-0.0111974
C	1.3674598	-1.7328008	-0.0127029	N	1.9016162	-0.5492555	-0.0403850
N	1.9637425	-0.5349505	-0.0390425	N	1.8804451	1.7604399	-0.0728657
N	1.7978768	1.7765526	-0.0785904	H	2.0389786	-2.6135483	-0.0151143
H	2.7999134	1.8288640	-0.0410014	H	-2.6803878	-1.5601135	0.0722536
H	1.2469797	2.6131237	-0.0171800	H	-3.3578364	0.9071337	0.0538955
H	2.0356847	-2.5860751	-0.0144247	H	1.2640051	2.5676200	-0.0711995
H	-2.7008644	-1.5252413	0.0673968	H	2.9073965	-0.4623146	-0.0632630
H	-3.3240095	0.9501495	0.0552423	(A4)			
(A2)				C	1.2675899	0.6878695	-0.0438696
C	1.2260926	0.5952030	-0.0791807	C	-0.1387981	0.4319180	-0.0085495
C	-0.1632816	0.4469880	-0.0260146	C	-0.6860371	-0.8403771	0.0210195
C	-0.7003221	-0.8474921	0.0476782	N	0.0648029	-1.9903137	0.0197930
N	0.0567634	-1.9515564	0.0546884	N	-1.2012262	1.2931142	0.0031725
N	-1.2554449	1.2947051	-0.0209739	N	-2.0530406	-0.7692565	0.0502436
N	-2.0780275	-0.7864653	0.0971549	C	-2.3224744	0.5163057	0.0384631
C	-2.3598656	0.4864334	0.0481744	C	1.3345011	-1.7836393	-0.0114686
C	1.3536798	-1.7026428	-0.0168594	N	1.9446403	-0.5498836	-0.0419869
N	1.9684936	-0.5085698	-0.0769310	N	1.7918599	1.8568990	-0.0720736
N	1.8659163	1.8075428	-0.1847998	H	2.0188636	-2.6244864	-0.0153204
H	2.8638160	1.7597682	-0.0475032	H	-1.1419496	2.2978140	-0.0120733
H	1.4257984	2.6181175	0.2166697	H	-3.3116319	0.9443727	0.0542161
				H	2.9522149	-0.5238277	-0.0649331
				H	2.8081142	1.8410808	-0.0948727
				(A5)			
				C	1.2438559	0.6902447	-0.0493942

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C	-0.1670011	0.4351816	-0.0115245
C	-0.6993247	-0.8469893	0.0229143
N	0.0558763	-1.9904521	0.0243282
N	-1.2513497	1.2790144	-0.0001048
N	-2.0682374	-0.7961738	0.0544729
C	-2.3594865	0.4815405	0.0397061
C	1.3269984	-1.7722638	-0.0095843
N	1.9198529	-0.5413434	-0.0445358
N	1.9409309	1.7662369	-0.0842908
H	2.0163161	-2.6086638	-0.0118501
H	-1.2406871	2.2843627	-0.0175801
H	-3.3548610	0.8954390	0.0563769
H	2.9268931	-0.4741703	-0.0694962
H	1.3618633	2.5988260	-0.0852176

(A6)

C	1.2300627	0.6983776	-0.0437013
C	-0.1942887	0.4472541	-0.0084730
C	-0.6517567	-0.8601831	0.0193168
N	0.0745788	-2.0143632	0.0192133
N	-1.2483115	1.3269947	0.0025402
N	-2.0159731	-0.7662864	0.0476702
C	-2.3162039	0.5740454	0.0359447
C	1.3474406	-1.7893838	-0.0115815
N	1.9207523	-0.5520763	-0.0412234
N	1.7958793	1.8394915	-0.0727225
H	2.0399463	-2.6229129	-0.0149821
H	-2.6579478	-1.5405458	0.0720796
H	-3.3334467	0.9299665	0.0530945
H	2.9278350	-0.5057881	-0.0639644
H	2.8114227	1.7775606	-0.0946412

1.2 Cartesian coordinates of the adenine first excited state tautomers optimized at the B3LYP/def2-TZVPPD level.

(A1)

C	1.2136384	0.5661857	-0.1042607
C	-0.2258330	0.4445716	-0.0493864
C	-0.6938498	-0.8859559	0.0155879
N	0.0853273	-1.9510773	0.0190388
N	-1.2361909	1.3186343	-0.0332504
N	-2.0484803	-0.7665164	0.0651047
C	-2.3520450	0.6086032	0.0372008
C	1.4569200	-1.8025567	-0.0067108
N	1.8988928	-0.5538530	-0.0803088
N	1.8244999	1.7993788	-0.2261121
H	2.7773045	1.8508039	0.0995118
H	1.2484678	2.5705474	0.0768930
H	2.1137212	-2.6506965	0.0049862
H	-2.7031457	-1.5271651	0.1214581
H	-3.3592278	0.9791001	0.0602479

(A2)

C	1.1914815	0.5991339	-0.1088967
C	-0.1841798	0.4591643	-0.0503860
C	-0.7650906	-0.8346693	0.0702078
N	0.1281155	-1.8643568	0.0291439
N	-1.2643924	1.3159358	-0.0240172
N	-2.0839251	-0.7865262	0.1374219
C	-2.4156224	0.5143492	0.0433855
C	1.4409331	-1.7252188	-0.0189261
N	1.9803464	-0.5305072	-0.1145481
N	1.8464306	1.8268957	-0.1871473
H	2.8442587	1.7389959	-0.0589521
H	1.4640930	2.5524960	0.4054814
H	2.0642604	-2.6080672	-0.0085604
H	-1.2472851	2.2664336	-0.3508682
H	-3.4020042	0.9213801	0.1598417

(A3)

C	1.1754866	0.6070643	-0.0146098
C	-0.1862231	0.4095841	0.1975919
C	-0.6755219	-0.9447833	0.0610010
N	0.0316847	-2.0303653	-0.0146774
N	-1.2342622	1.3138511	0.1745710
N	-2.0379441	-0.7812150	-0.0353568
C	-2.2988102	0.5862777	0.0550373
C	1.3845684	-1.8011000	0.1613604
N	1.9207050	-0.5279451	-0.0938356
N	1.8268480	1.7688847	-0.1954400
H	2.0733450	-2.6258725	0.0973307
H	-2.7109663	-1.5217032	-0.1345038
H	-3.3097916	0.9620191	0.0309093
H	1.1591830	2.5308881	-0.0748806
H	2.9038688	-0.4085940	-0.2846876

(A4)

C	1.2363327	0.6264870	0.0228961
C	-0.1171405	0.4003874	0.3018047
C	-0.6936346	-0.8953741	-0.0200270
N	0.0455362	-1.9646676	-0.1617548
N	-1.1823435	1.2846964	0.2293251
N	-2.0420917	-0.7387108	-0.2544431
C	-2.2790026	0.5374682	-0.0757232
C	1.3619786	-1.7628744	0.1912016
N	1.9682871	-0.5363117	-0.0898313
N	1.7392567	1.8413998	-0.1341914
H	2.0143040	-2.6078896	0.3363394
H	-1.1370186	2.2822696	0.3443829
H	-3.2580159	0.9875362	-0.1453013
H	2.9436048	-0.4724286	-0.3416899
H	2.7273763	1.8056022	-0.3812277

(A5)

C	1.2153334	0.6229335	-0.0587487	H	1.3843015	2.3442409	-0.6982108
C	-0.1457557	0.4207349	-0.2875213	H	1.8854395	-1.1239116	-0.2327583
C	-0.6995388	-0.8916049	0.0430472	H	0.1837839	-2.7480913	-0.3194147
N	0.0332262	-1.9606972	0.1462397	H	-2.7384142	-0.0088945	0.1559242
N	-1.2264016	1.2984867	-0.1407831				
N	-2.0479166	-0.7519673	0.3205188				
C	-2.3081398	0.5135365	0.1579422				
C	1.3479956	-1.7729107	-0.2147631				
N	1.9464131	-0.5302177	0.0063421				
N	1.8985663	1.7576787	0.1350148				
H	2.0080669	-2.6207344	-0.2864245				
H	-1.2891337	2.2392155	-0.4893402				
H	-3.2939212	0.9468554	0.2448934				
H	2.9324815	-0.4317431	0.1948374				
H	1.2803637	2.5612238	0.0429654				

(A6)

C	1.1978457	0.6255187	0.0297915
C	-0.1690879	0.4226831	0.2342178
C	-0.6604487	-0.9269099	0.0405382
N	0.0426081	-2.0180118	-0.0546960
N	-1.2218865	1.3218216	0.2347997
N	-2.0152105	-0.7633191	-0.0823025
C	-2.2813373	0.5999019	0.0673266
C	1.3856342	-1.7918191	0.1756419
N	1.9345413	-0.5274698	-0.0801906
N	1.7575048	1.8368463	-0.0714141
H	2.0746398	-2.6190561	0.1710992
H	-2.6829252	-1.5044684	-0.2093460
H	-3.2934799	0.9731003	0.0478000
H	2.9203621	-0.4432120	-0.2737482
H	2.7412294	1.7565451	-0.3309475

2 Thymine

2.1 Cartesian coordinates of the thymine ground state tautomers optimized at the B3LYP/def2-TZVPPD level.

(T1)

C	-0.8714621	0.8617913	0.1463649
C	0.5453437	0.5096761	0.0269296
C	0.8615384	-0.7888973	-0.1367105
N	-0.0846891	-1.7860572	-0.1954467
N	-1.7547210	-0.2257840	0.0760708
C	-1.4461932	-1.5607540	-0.0929151
C	1.5563160	1.6117253	0.0921675
O	-1.3011160	1.9893197	0.2958990
O	-2.2718836	-2.4472670	-0.1468407
H	1.4831244	2.1517778	1.0375858
H	2.5686539	1.2211238	-0.0086500

(T2)

C	-0.8707202	0.8761612	0.1471514
C	0.5293718	0.5090939	0.0266186
C	0.8381044	-0.8055455	-0.1387102
N	-0.0663428	-1.8353783	-0.2027636
N	-1.7412558	-0.2330037	0.0730627
C	-1.3078876	-1.5003996	-0.0939312
C	1.5483937	1.6031951	0.0921100
O	-1.3280071	1.9948538	0.2981717
O	-2.2880412	-2.4146914	-0.1398961
H	1.4820947	2.1426037	1.0388657
H	2.5563979	1.2031914	-0.0123611
H	1.3804868	2.3402478	-0.6954550
H	1.8745320	-1.1091203	-0.2320023
H	-1.8636137	-3.2749354	-0.2605345
H	-2.7308425	-0.0423226	0.1508338

(T3)

C	-0.8710670	0.7286230	0.1143125
C	0.5427280	0.5092744	0.0215903
C	0.8795256	-0.7965820	-0.1339670
N	-0.0690974	-1.7624649	-0.1900449
N	-1.7944992	-0.1848477	0.0637103
C	-1.4556540	-1.5087892	-0.0935224
C	1.5368397	1.6295478	0.0918646
O	-1.2613652	2.0050504	0.2677054
O	-2.2395583	-2.4328176	-0.1520868
H	1.4606351	2.1714221	1.0361869
H	2.5534720	1.2469819	0.0008483
H	1.3741246	2.3569080	-0.7053761
H	-2.2288543	1.9962142	0.3143115
H	0.1838258	-2.7313858	-0.3059007
H	1.9070544	-1.1241153	-0.2198917

(T4)

C	-0.8667015	0.7479928	0.1151637
C	0.5142863	0.5094739	0.0229927
C	0.8377224	-0.8258695	-0.1343657
N	-0.0621541	-1.8153706	-0.1944435
N	-1.7834746	-0.2026507	0.0599646
C	-1.3294511	-1.4421904	-0.0925081
C	1.5287312	1.6112513	0.0912270
O	-1.2958400	2.0127957	0.2685905
O	-2.2694385	-2.4003552	-0.1465015
H	1.4655059	2.1541294	1.0361050
H	2.5371942	1.2092060	-0.0033936

H	1.3770238	2.3426743	-0.7047083	H	1.4076488	2.3354934	-0.7193263
H	-1.8038939	-3.2393845	-0.2571359	H	-1.7956709	-3.2327414	-0.2578347
H	-2.2618386	1.9822599	0.3125426	H	-0.6555949	2.6401331	0.3157430
H	1.8781488	-1.1230330	-0.2174495	H	1.8801461	-1.1162748	-0.2233178

(T5)

C	-0.8721620	0.7531680	0.1133289
C	0.5057114	0.5110974	0.0236575
C	0.8259290	-0.8272935	-0.1345961
N	-0.0670532	-1.8208976	-0.1991539
N	-1.7846922	-0.2035534	0.0542274
C	-1.3292359	-1.4495223	-0.1000633
C	1.5243090	1.6095870	0.0933582
O	-1.3029382	2.0184148	0.2672751
O	-2.2475106	-2.4292825	-0.1612415
H	1.4624532	2.1531659	1.0380868
H	2.5310931	1.2027851	0.0007561
H	1.3779207	2.3411801	-0.7036190
H	-3.1161749	-2.0178812	-0.0761599
H	-2.2684537	1.9930309	0.3097690
H	1.8675951	-1.1219195	-0.2152553

(T6)

C	-0.8904065	0.8446680	0.1297845
C	0.5459423	0.4943064	0.0217179
C	0.8829074	-0.7964149	-0.1423192
N	-0.0910090	-1.7766561	-0.2077406
N	-1.8125219	-0.2098891	0.0560304
C	-1.3912994	-1.4104462	-0.1013005
C	1.5503145	1.5988550	0.1004192
O	-1.2583115	1.9955114	0.2765142
O	-2.2401093	-2.4509123	-0.1764128
H	1.4543526	2.1356184	1.0456408
H	2.5691043	1.2214955	0.0092811
H	1.3722452	2.3334242	-0.6866300
H	1.9017841	-1.1453466	-0.2319364
H	0.1429010	-2.7476128	-0.3291559
H	-3.1308836	-2.0840603	-0.0915528

(T7)

C	-0.8757328	0.7539913	0.1249859
C	0.5084721	0.5105696	0.0248333
C	0.8384519	-0.8234370	-0.1362263
N	-0.0575524	-1.8115307	-0.1952052
N	-1.7849661	-0.1994490	0.0708448
C	-1.3272095	-1.4338364	-0.0871617
C	1.5347403	1.6056815	0.0863160
O	-1.3720552	1.9978777	0.2851369
O	-2.2628396	-2.3953849	-0.1424042
H	1.5021836	2.1492696	1.0356646
H	2.5388287	1.1940174	-0.0113083

(T8)

C	-0.8777683	0.7617896	0.1244701
C	0.5026294	0.5135934	0.0252165
C	0.8277753	-0.8239506	-0.1363507
N	-0.0622463	-1.8157724	-0.1968188
N	-1.7834397	-0.1967040	0.0690139
C	-1.3258121	-1.4379746	-0.0892755
C	1.5325780	1.6052982	0.0875118
O	-1.3779556	2.0045710	0.2841597
O	-2.2434245	-2.4168737	-0.1465012
H	1.5019740	2.1488694	1.0369902
H	2.5349141	1.1893668	-0.0095509
H	1.4092925	2.3357162	-0.7182484
H	-3.1099132	-2.0005609	-0.0555369
H	-0.6624624	2.6480568	0.3153656
H	1.8703791	-1.1150663	-0.2229554

(T9)

C	-0.8946976	0.7422882	0.1327033
C	0.5259849	0.5218381	0.0284139
C	0.8736974	-0.7801545	-0.1360026
N	-0.0670399	-1.7481252	-0.1911093
N	-1.8051118	-0.1775718	0.0820383
C	-1.4573163	-1.4955695	-0.0840058
C	1.5312748	1.6355458	0.0960661
O	-1.3560713	1.9993498	0.2982642
O	-2.2316998	-2.4268218	-0.1433806
H	1.4917088	2.1695534	1.0504900
H	2.5435317	1.2458246	-0.0082083
H	1.3882754	2.3691572	-0.7033195
H	-0.6266532	2.6270884	0.3261092
H	0.1879006	-2.7158071	-0.3137268
H	1.9037158	-1.0984266	-0.2300121

2.2 Cartesian coordinates of the thymine first excited state tautomers optimized at the B3LYP/def2-TZVPPD level.

(T1)

C	-0.8109291	0.7971114	0.1527611
C	0.5278791	0.5304962	0.0339246
C	0.8981715	-0.8093655	-0.1519580
N	-0.0961201	-1.7929032	-0.2108214
N	-1.7589648	-0.2184828	0.0926440
C	-1.4327202	-1.5637556	-0.0966056
C	1.5485822	1.6348190	0.0922281

O	-1.3725529	1.9852611	0.3292000	O	-1.3289037	2.0321767	0.0159065
O	-2.2946909	-2.4189775	-0.1477398	O	-2.3133917	-2.4436361	-0.1814648
H	1.4477389	2.2304195	1.0012828	H	2.1529496	1.5703616	1.0287407
H	2.5549053	1.2188382	0.0795439	H	2.2282873	1.5853884	-0.7317441
H	1.4595081	2.3149264	-0.7576851	H	1.0660432	2.6158869	0.1077144
H	1.9158932	-1.1414162	-0.2508898	H	-1.8831783	-3.3070703	-0.1890188
H	0.1529316	-2.7585068	-0.3469159	H	-2.2898056	1.9664020	-0.0273921
H	-2.7396097	-0.0084662	0.1810261	H	1.9291137	-1.1849871	-0.0096912

(T2)

C	-0.8145174	0.7872911	0.2347754
C	0.5011894	0.5431942	0.0118103
C	0.8534529	-0.8029962	-0.3281631
N	-0.0772805	-1.7985929	-0.3689768
N	-1.7627028	-0.2178458	0.0925464
C	-1.2994055	-1.5026378	-0.1447548
C	1.5400250	1.6254982	0.1009665
O	-1.3790388	1.9484547	0.5757872
O	-2.2981341	-2.4095163	-0.1317731
H	1.1312076	2.5502875	0.5048195
H	2.3655846	1.3166224	0.7459282
H	1.9627857	1.8507456	-0.8818122
H	1.8809862	-1.0809347	-0.5034277
H	-1.8946960	-3.2701102	-0.3035741
H	-2.6967857	-0.0855096	0.4470084

(T3)

C	-0.8224955	0.7733120	0.0814276
C	0.5210340	0.5269963	0.0199150
C	0.9252309	-0.8058534	-0.1050002
N	-0.0931321	-1.7907495	-0.1433729
N	-1.8089494	-0.2137475	-0.0113386
C	-1.3822530	-1.4174278	-0.1029557
C	1.5369399	1.6316246	0.1031798
O	-1.3095267	2.0250590	0.2358764
O	-2.2524914	-2.4255872	-0.1678250
H	1.6402528	1.9945877	1.1278573
H	2.5137924	1.2819677	-0.2303046
H	1.2453235	2.4812256	-0.5135867
H	-2.2719059	1.9548655	0.2290775
H	0.1420225	-2.7673277	-0.1696658
H	1.9342680	-1.1459258	-0.2435443

(T4)

C	-0.8267792	0.7724122	0.0103534
C	0.5290382	0.5450454	0.0698274
C	0.9193897	-0.8292830	0.0989996
N	-0.1125677	-1.7304657	-0.0338270
N	-1.7721735	-0.2203733	-0.0378646
C	-1.3784797	-1.4903882	-0.0860935
C	1.5462780	1.6394601	0.1216338

(T5)

C	-0.8331088	0.7597830	0.1179078
C	0.5217224	0.5278899	0.0409171
C	0.9163546	-0.8354886	-0.0707412
N	-0.1346636	-1.7154213	-0.1710036
N	-1.8043169	-0.2163277	0.0782695
C	-1.3975042	-1.4796858	-0.0953322
C	1.5338531	1.6323073	0.0916124
O	-1.2984231	2.0255916	0.2624982
O	-2.2833929	-2.4747850	-0.1815936
H	1.4733825	2.1822241	1.0333240
H	2.5437517	1.2337777	0.0006316
H	1.3784755	2.3517441	-0.7146403
H	-3.1601051	-2.0764364	-0.1077425
H	-2.2605517	1.9825096	0.3044212
H	1.9113173	-1.1856032	-0.2781583

(T6)

C	-0.8279546	0.7717185	0.0478693
C	0.5261340	0.5187561	0.0272199
C	0.9266414	-0.8291040	-0.0448392
N	-0.0982706	-1.7920712	-0.1414494
N	-1.8086068	-0.1989708	-0.0201366
C	-1.3814761	-1.4198356	-0.1106089
C	1.5393362	1.6252449	0.1130957
O	-1.3426178	1.9926917	0.1461551
O	-2.2567944	-2.4323910	-0.1809895
H	1.7063800	1.9410205	1.1464850
H	2.4986943	1.3008123	-0.2909385
H	1.2199136	2.5029067	-0.4496959
H	1.9299284	-1.1620370	-0.2418857
H	0.1139257	-2.7751408	-0.1805262
H	-3.1402232	-2.0410599	-0.1474150

(T7)

C	-0.8195277	0.7675826	0.1770543
C	0.5319929	0.5399077	0.0261497
C	0.9107819	-0.8102259	-0.1942761
N	-0.1130158	-1.7374354	-0.2428416
N	-1.7463068	-0.2446839	0.1259012
C	-1.3736554	-1.4961883	-0.0857990
C	1.5534010	1.6380475	0.0689043

O	-1.3880706	1.9804966	0.3876619
O	-2.3153181	-2.4434761	-0.1322996
H	1.3415533	2.3710262	0.8531131
H	2.5391133	1.2280732	0.2904339
H	1.6278815	2.1728196	-0.8824473
H	-1.8869957	-3.2931662	-0.2937741
H	-0.7030979	2.6558534	0.4053820
H	1.9201140	-1.1542518	-0.3324226

(T8)

C	-0.8327101	0.7670958	0.1739596
C	0.5207059	0.5367810	0.0355830
C	0.9083542	-0.8206441	-0.1542002
N	-0.1344836	-1.7110045	-0.2437807
N	-1.7831249	-0.2217445	0.1350967
C	-1.3917519	-1.4764428	-0.0976995
C	1.5502014	1.6278888	0.0736012
O	-1.3798591	1.9917244	0.3785562
O	-2.2862901	-2.4634423	-0.1764457
H	1.3382368	2.3684057	0.8510939
H	2.5319772	1.2146316	0.3057673
H	1.6336160	2.1554907	-0.8810606
H	-3.1565786	-2.0639038	-0.0476003
H	-0.6837874	2.6556404	0.3996335
H	1.9020145	-1.1601173	-0.3850143

(T9)

C	-0.8373985	0.7750243	0.1289990
C	0.5075922	0.5309860	0.0299556
C	0.9210112	-0.7957878	-0.1338234
N	-0.0899725	-1.7817533	-0.1890833
N	-1.8107293	-0.2176361	0.0648486
C	-1.3801787	-1.4103296	-0.0839702
C	1.5290933	1.6351138	0.0961922
O	-1.3874051	2.0014647	0.2997207
O	-2.2458439	-2.4234034	-0.1484321
H	1.4960536	2.1615622	1.0540489
H	2.5357562	1.2351934	-0.0160221
H	1.3830670	2.3712517	-0.6989250
H	-0.6944204	2.6675731	0.3439434
H	0.1460216	-2.7534007	-0.2883522
H	1.9348527	-1.1276890	-0.2547801

3 Cytosine

3.1 Cartesian coordinates of the cytosine ground state tautomers optimized at the B3LYP/def2-TZVPPD level.

(C1)

C	-0.6120987	0.7028198	0.1135464
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C	0.7018500	0.7633955	-0.4640331
C	1.3821988	-0.4052891	-0.5235058
N	-1.1579975	-0.4023308	0.5713628
N	0.8201526	-1.5399087	-0.0555943
C	-0.4824276	-1.5886661	0.5151856
N	-1.3529521	1.8353513	0.1888270
O	-0.8995554	-2.6597985	0.9092223
H	-0.9698703	2.7308864	-0.0474841
H	-2.2435521	1.7880824	0.6529092
H	1.1278345	1.6825938	-0.8343452
H	2.3785022	-0.4860847	-0.9364153
H	1.3079225	-2.4210442	-0.0896792

(C2)

C	-0.6038170	0.7215837	0.0888625
C	0.6901857	0.7550341	-0.4669156
C	1.3681313	-0.4423770	-0.5046103
N	-1.1311073	-0.4147814	0.5531331
N	0.8549325	-1.5913573	-0.0478643
C	-0.3737333	-1.4964750	0.4548308
N	-1.3898599	1.8285367	0.1591664
O	-0.9243782	-2.6282737	0.9271900
H	-1.0000442	2.7392776	0.0026292
H	-2.2440273	1.7599227	0.6850880
H	1.1268626	1.6671056	-0.8472008
H	2.3692232	-0.4965211	-0.9176745
H	-0.2706376	-3.3270546	0.7954453

(C3)

C	-0.6102873	0.7255665	0.0885214
C	0.6811252	0.7497028	-0.4675280
C	1.3555421	-0.4519733	-0.4973171
N	-1.1322830	-0.4115371	0.5579516
N	0.8484837	-1.6010366	-0.0362645
C	-0.3734386	-1.5019723	0.4639908
N	-1.3971065	1.8348177	0.1510050
O	-0.9061575	-2.6428804	0.9356003
H	-0.9946066	2.7425830	0.0073474
H	-2.2392833	1.7772174	0.6971026
H	1.1199883	1.6580042	-0.8543473
H	2.3565072	-0.5071492	-0.9113007
H	-1.7889228	-2.4283226	1.2621882

(C4)

C	-0.6345276	0.8167382	0.0972808
C	0.7044807	0.7664348	-0.4714880
C	1.3695279	-0.3987012	-0.5217898
N	0.8202936	-1.5649545	-0.0462816
C	-0.4490665	-1.6345081	0.5171525
N	-1.4141204	1.8196739	0.2290317
O	-0.9193121	-2.6731017	0.9317493

H	1.1490293	1.6737720	-0.8482561
H	2.3646149	-0.4854259	-0.9346100
H	1.3207887	-2.4366544	-0.0863961
N	-1.1004876	-0.4258955	0.5536920
H	-2.0263591	-0.4372390	0.9567237
H	-0.9856418	2.6669420	-0.1298984

(C5)

C	-0.6257803	0.8545763	0.1159609
C	0.7019095	0.7838729	-0.4716196
C	1.3564112	-0.3846341	-0.5258649
N	0.8050316	-1.5489182	-0.0337746
C	-0.4497620	-1.6063029	0.5469186
N	-1.2767072	1.9508897	0.1837922
O	-0.9312678	-2.6334894	0.9781798
H	1.1320689	1.6937794	-0.8554308
H	2.3437458	-0.4826657	-0.9533606
H	1.2998936	-2.4236049	-0.0776274
N	-1.0969498	-0.3876341	0.5876600
H	-2.0121551	-0.4256637	1.0108355
H	-2.1900683	1.8423655	0.6201506

(C6)

C	-0.6177618	0.7898172	0.0700696
C	0.6571359	0.7828880	-0.4594594
C	1.3238570	-0.4529289	-0.4776932
N	0.8572728	-1.5978439	-0.0380105
C	-0.4044979	-1.6305942	0.4954460
N	-1.4257066	1.8871533	0.1255958
O	-0.9726039	-2.6068909	0.9386652
H	-1.0022120	2.7833134	-0.0407046
H	-2.2078586	1.8924769	0.7581968
N	-1.1076173	-0.3846565	0.5260461
H	-2.0427115	-0.4487213	0.9020860
H	2.3293057	-0.4834481	-0.8907223
H	1.1135191	1.6832345	-0.8397859

(C7)

C	-0.6329557	0.8283215	0.0934931
C	0.6996384	0.7602814	-0.4707149
C	1.3639919	-0.4184698	-0.5055771
N	0.8638823	-1.6095761	-0.0316292
C	-0.3256890	-1.5447774	0.4723625
N	-1.4392042	1.8111790	0.2309881
O	-0.9242201	-2.6361350	0.9686723
H	1.1443779	1.6648267	-0.8585482
H	2.3602122	-0.4774678	-0.9259180
N	-1.0734152	-0.4277162	0.5571017
H	-1.9960645	-0.4658253	0.9670347
H	-1.0343314	2.6684198	-0.1308195
H	-0.3032922	-3.3688198	0.8571841

(C8)

C	-0.6486315	0.7815552	0.1208638
C	0.6961637	0.7564024	-0.4576666
C	1.3811876	-0.3912471	-0.5260360
N	0.8142592	-1.5635923	-0.0463698
C	-0.4378399	-1.5040277	0.4849267
N	-1.3047587	1.8768755	0.1877003
O	-0.8763898	-2.7019402	0.9138339
H	1.1153025	1.6805187	-0.8234166
H	2.3744533	-0.4828360	-0.9386466
H	1.2976357	-2.4442917	-0.0804325
N	-1.1555305	-0.4508868	0.5861128
H	-2.2138023	1.7093477	0.6156894
H	-1.7642092	-2.5598662	1.2691511

3.2 Cartesian coordinates of the cytosine first excited state tautomers optimized at the B3LYP/def2-TZVPPD level.

(C1)

C	-0.5720904	0.7506660	0.0566803
C	0.6899877	0.7685068	-0.4735541
C	1.4312665	-0.4131752	-0.5528427
N	-1.1311637	-0.4189776	0.6046597
N	0.7990078	-1.5786844	-0.0502428
C	-0.4292757	-1.4813921	0.4920051
N	-1.4371738	1.8168141	0.0865453
O	-0.9234275	-2.6339416	0.9464329
H	-1.0511693	2.7378255	-0.0325658
H	-2.1778352	1.7445297	0.7653144
H	1.1174382	1.6878369	-0.8500093
H	2.4690850	-0.4961062	-0.8148700
H	1.2153574	-2.4838949	-0.1775568

(C2)

C	-0.5751112	0.7495267	0.0399126
C	0.7022930	0.8030924	-0.4754522
C	1.4648743	-0.3941498	-0.4753045
N	-1.0911178	-0.4261722	0.5417232
N	0.7926059	-1.5165264	-0.0322855
C	-0.3926008	-1.5563077	0.4744463
N	-1.4496677	1.8173592	0.0759207
O	-0.9629575	-2.6768139	0.9343162
H	-1.0332420	2.7313073	0.0132748
H	-2.1770622	1.7483461	0.7706615
H	1.1127103	1.7257069	-0.8615086
H	2.4183145	-0.5265202	-0.9547902
H	-0.3373084	-3.4042281	0.8311654

(C3)

C	-0.5838673	0.7430663	0.0537146	O	-0.9720096	-2.6149005	0.9971937
C	0.6919158	0.7863437	-0.4701428	H	-1.1556008	2.6992528	-0.2670787
C	1.4648613	-0.4084518	-0.4501136	H	-1.8573818	2.0505372	1.0904614
N	-1.1270309	-0.4104770	0.5797473	N	-1.1545228	-0.4315798	0.5315378
N	0.7624979	-1.5064593	-0.0170880	H	-2.1564621	-0.5404921	0.5833196
C	-0.4150388	-1.5443733	0.4979448	H	2.3540975	-0.4806230	-0.8981547
N	-1.4363027	1.8275149	0.0781450	H	1.0963876	1.6880350	-0.7969820
O	-0.9296197	-2.6931572	0.9459791				
H	-1.0099658	2.7360543	0.0075589	(C7)			
H	-2.1770111	1.7711323	0.7592354	C	-0.5860091	0.7813592	0.1211593
H	1.1059505	1.6977627	-0.8775142	C	0.7511053	0.7966933	-0.2535395
H	2.3961101	-0.5616571	-0.9657525	C	1.3353929	-0.4832415	-0.5716499
H	-1.8229385	-2.4942784	1.2552357	N	0.8408653	-1.6084536	-0.1671900
(C4)				C	-0.2422351	-1.4761567	0.7010072
C	-0.4249383	0.8551687	0.1568779	N	-1.4704768	1.7988731	0.1497561
C	0.8299858	0.8010838	-0.3748149	O	-0.8389317	-2.6035789	1.1453611
C	1.4656236	-0.4347077	-0.5171570	H	1.2192642	1.7209915	-0.5537720
N	0.7795535	-1.5792657	-0.1145132	H	2.1815151	-0.5269063	-1.2511298
C	-0.4740388	-1.5863987	0.4433719	N	-1.1110380	-0.4214482	0.5023367
N	-1.1988009	2.0225084	0.4246420	H	-2.1075093	-0.5007731	0.6547979
O	-1.0446052	-2.5893528	0.8197491	H	-1.0061791	2.6497667	-0.1645908
H	1.3281062	1.7079251	-0.6764988	H	-0.2628333	-3.3428845	0.9110833
H	2.4662184	-0.5687059	-0.8859344	(C8)			
H	1.2053188	-2.4879747	-0.1927602	C	-0.5895831	0.7126430	0.2786721
N	-1.0486673	-0.3232858	0.5439559	C	0.6064604	0.7698335	-0.3916082
H	-1.9226092	-0.2904406	1.0432684	C	1.3433839	-0.3964381	-0.6038220
H	-1.7619266	2.1605267	-0.4232768	N	0.7854510	-1.5843943	-0.0961007
(C5)				C	-0.4013577	-1.5463349	0.5397701
C	-0.5672684	0.7884425	0.2667690	N	-1.3832213	1.8504606	0.6144214
C	0.6407418	0.8184152	-0.3658482	O	-0.8293442	-2.7458592	0.9607281
C	1.3428458	-0.3722236	-0.5676395	H	0.9926752	1.7154671	-0.7406215
N	0.7687393	-1.5602115	-0.1183745	H	2.3211111	-0.4578209	-1.0427594
C	-0.4313212	-1.6510119	0.5406442	H	1.2464407	-2.4719755	-0.2040771
N	-1.3922060	1.9015936	0.6037794	N	-1.1032315	-0.4855726	0.7546192
O	-0.9009621	-2.6900904	0.9562641	H	-2.0374817	1.9424073	-0.1717542
H	1.0513321	1.7568013	-0.7010388	H	-1.6734626	-2.5964043	1.4082418
H	2.3166168	-0.4394036	-1.0175096				
H	1.2449900	-2.4388638	-0.2376951	4 Guanine			
N	-1.0780030	-0.4290702	0.6960391	4.1 Cartesian coordinates of the guanine ground state tautomers optimized at the B3LYP/def2-TZVPPD level.			
H	-1.9085496	-0.4545919	1.2650426				
H	-2.0305853	2.0027849	-0.1946129	(G1)			
(C6)				C	0.8603259	1.5171163	0.0003127
C	-0.6270109	0.7869051	0.0711781	C	-0.5092664	1.1349543	0.0177967
C	0.6530765	0.7682182	-0.4384653	C	-0.9181391	-0.1944639	-0.0110093
C	1.3612442	-0.4156133	-0.4848793	N	-1.6655846	1.8790158	0.0488984
N	0.8302362	-1.6041691	0.0414967	N	-0.0660254	-1.2562686	-0.0374470
C	-0.3567712	-1.5473958	0.4868057	N	1.6640799	0.3538385	-0.0424029
N	-1.5151618	1.8556248	0.1532968				

C	1.1934267	-0.9398757	-0.0598477	N	-1.6721949	1.8926685	0.0223655
C	-2.6894842	0.9851678	0.0385491	N	-0.0828840	-1.3089713	-0.0308694
N	-2.2854065	-0.2663634	0.0036779	N	1.6796549	0.3397996	-0.0211961
H	2.6546252	0.5320269	-0.1233041	C	1.2010797	-0.9252407	-0.0411503
N	2.1470363	-1.9268475	-0.1579583	C	-2.6771663	1.0635517	0.0210636
O	1.3592957	2.6317873	0.0102387	N	-2.2855862	-0.2623144	0.0013309
H	3.0369363	-1.7697117	0.2865848	H	-3.7183177	1.3427556	0.0334942
H	1.7729228	-2.8523669	-0.0194756	H	-2.8829715	-1.0713672	-0.0060906
H	-1.7255890	2.8829199	0.0721755	N	2.1421738	-1.9089134	-0.1041660
H	-3.7201542	1.3011286	0.0579813	O	1.3138174	2.5820093	0.0216789
(G2)				H	3.0947218	-1.6533992	0.0829387
C	0.8233548	1.5121386	0.0029142	H	1.8485866	-2.8518317	0.0754377
C	-0.5620697	1.1344789	0.0161459	H	0.5735680	3.2030552	0.0360332
C	-0.8850080	-0.2176737	-0.0126945	(G5)			
N	-1.7032194	1.9074247	0.0460982	C	0.8667419	1.3583253	-0.0016552
N	-0.0591928	-1.2897213	-0.0379912	C	-0.5009022	1.1237868	0.0042571
N	1.6415636	0.3351203	-0.0376938	C	-0.9305245	-0.2136323	-0.0092647
C	1.2042134	-0.9587780	-0.0576717	N	-1.6528777	1.8854639	0.0324607
C	-2.6857994	1.0537135	0.0367930	N	-0.0900167	-1.2514333	-0.0338816
N	-2.2501532	-0.2567137	0.0018070	N	1.7066725	0.3463803	-0.0281458
H	-3.7348377	1.3010571	0.0539062	C	1.1946463	-0.9117839	-0.0500782
H	-2.8131388	-1.0903202	-0.0129097	C	-2.6859642	0.9947324	0.0338463
H	2.6293535	0.5344020	-0.1036303	N	-2.3073243	-0.2591524	0.0106229
N	2.1594255	-1.9384252	-0.1500863	N	2.1145815	-1.9209334	-0.1276326
O	1.3552390	2.6016576	0.0149152	O	1.3491084	2.6170455	0.0224704
H	3.0709777	-1.7584607	0.2362451	H	3.0653155	-1.7003922	0.1082776
H	1.8093059	-2.8698989	0.0038523	H	1.7828937	-2.8483027	0.0711995
(G3)				H	-1.7179408	2.8880324	0.0470149
C	0.8314355	1.3442132	0.0056237	H	-3.7121324	1.3273982	0.0523393
C	-0.5468874	1.1058239	0.0082289	H	2.3141026	2.5512217	0.0084593
C	-0.8997369	-0.2503456	-0.0123293	(G6)			
N	-1.6736894	1.9095358	0.0325987	C	0.8703983	1.4773431	-0.0068545
N	-0.0773602	-1.2942045	-0.0363329	C	-0.5153017	1.1193280	0.0089334
N	1.6862766	0.3355783	-0.0205281	C	-0.9517136	-0.1861582	-0.0151697
C	1.2070123	-0.9277390	-0.0461095	N	-1.6694636	1.8749398	0.0480228
C	-2.6687428	1.0729016	0.0269563	N	-0.0735015	-1.2303636	-0.0566252
N	-2.2692015	-0.2517470	0.0010353	N	1.6761167	0.3256617	-0.0497458
H	-3.7122617	1.3441804	0.0405123	C	1.2979041	-1.0240761	-0.0758342
H	-2.8572818	-1.0673409	-0.0113513	C	-2.7020493	1.0019854	0.0451366
N	2.1419555	-1.9200550	-0.1186741	N	-2.3065368	-0.2614440	0.0072237
O	1.3177989	2.5903405	0.0325474	H	2.6669373	0.5145047	-0.0631078
H	3.0921165	-1.6778425	0.0968026	N	2.0786118	-2.0310035	-0.1140307
H	1.8349908	-2.8567485	0.0733808	O	1.3553032	2.5953043	0.0122620
H	2.2822055	2.5171488	0.0211991	H	-1.7138471	2.8798016	0.0735766
(G4)				H	-3.7301969	1.3229524	0.0713335
C	0.8192263	1.3345626	-0.0007731	H	3.0583414	-1.7713307	-0.1250474
C	-0.5563398	1.0760188	0.0010743	H	-0.3908519	-2.1859361	-0.0738432
C	-0.9128774	-0.2727940	-0.0124814	(G7)			

C	0.8670687	1.4761696	-0.0045841	O	1.3707515	2.6499762	0.0174827
C	-0.5232378	1.1167326	0.0098239	H	3.0680098	-1.7927037	0.1759897
C	-0.9594815	-0.1856251	-0.0146128	H	1.7321823	-2.8500023	-0.1312410
N	-1.6766512	1.8713486	0.0475374	H	-1.7003454	2.8836315	-0.0122957
N	-0.0759519	-1.2333253	-0.0552257	H	-3.7449667	1.2827683	0.0163361
N	1.6687519	0.3315553	-0.0468461				
C	1.2983784	-1.0157375	-0.0755609				
C	-2.7104902	0.9993342	0.0436308				
N	-2.3134497	-0.2642108	0.0062235				
H	2.6665390	0.4859698	-0.0612983				
N	2.2164796	-1.8991827	-0.1161350				
O	1.3393600	2.5994351	0.0158074				
H	-1.7197550	2.8764309	0.0728448				
H	-3.7384060	1.3204846	0.0686367				
H	1.8514714	-2.8450660	-0.1337748				
H	-0.4210148	-2.1779145	-0.0748867				

(G8)

C	0.8886994	1.4338532	0.0147170
C	-0.5205853	1.0985568	0.0267617
C	-0.9845165	-0.1906154	-0.0068523
N	-1.6637866	1.8657691	0.0527817
N	-0.0860912	-1.2308280	-0.0393649
N	1.7184465	0.3095783	-0.0057948
C	1.2486720	-0.9004300	-0.0450332
C	-2.7155471	1.0104871	0.0320284
N	-2.3392003	-0.2585369	-0.0041899
N	2.1210379	-1.9581083	-0.1398992
O	1.3155563	2.5777177	0.0292257
H	3.0822357	-1.6946580	0.0068711
H	1.8550969	-2.8370893	0.2730783
H	-1.6867763	2.8717299	0.0804930
H	-3.7383193	1.3485076	0.0447808
H	-0.4056810	-2.1746749	-0.1840232

4.2 Cartesian coordinates of the guanine first excited state tautomers optimized at the B3LYP/def2-TZVPPD level.

(G1)

C	0.8625848	1.5252445	0.0706532
C	-0.4958570	1.1483672	0.0397569
C	-0.9455889	-0.2228958	0.0333423
N	-1.6432625	1.8799988	0.0251314
N	-0.0781548	-1.2397078	0.0100898
N	1.7425947	0.3643241	0.1554201
C	1.2143236	-0.9043988	0.0305248
C	-2.7202207	0.9548173	0.0129886
N	-2.3016796	-0.2867708	0.0175981
H	2.6444823	0.5353486	-0.2950327
N	2.1041462	-1.9159394	-0.0819742

(G2)

C	0.8497475	1.4910773	0.0038080
C	-0.5668937	1.1339701	0.0064210
C	-0.9042833	-0.2571050	0.0017357
N	-1.6666385	1.8987496	0.0126270
N	-0.1132754	-1.2879155	-0.0052534
N	1.6560872	0.3353686	-0.0034484
C	1.2245172	-0.9528190	-0.0081090
C	-2.6813914	1.0403314	0.0122242
N	-2.2834310	-0.2623086	0.0059102
H	-3.7209271	1.3240332	0.0164234
H	-2.8679792	-1.0826879	0.0042351
H	2.6873141	0.4564152	-0.0051789
N	2.1124972	-1.9066462	-0.0151855
O	1.3168169	2.6010016	0.0073125
H	3.1535340	-1.6540538	-0.0159523
H	1.8043199	-2.8774101	-0.0175702

(G3)

C	0.8714340	1.4020916	-0.2724426
C	-0.5479280	1.1202418	-0.0807582
C	-0.8939283	-0.2372482	0.1206977
N	-1.6595877	1.8666294	-0.2081465
N	-0.0770969	-1.2877220	0.0572397
N	1.7183905	0.3417376	-0.2055867
C	1.2214328	-0.8876756	-0.0588058
C	-2.6900712	1.0291586	-0.0581200
N	-2.2772924	-0.2534289	0.0971819
H	-3.7259812	1.3207834	-0.0258840
H	-2.8558065	-1.0695998	0.2106786
N	2.1128608	-1.9023742	-0.0323803
O	1.3402887	2.6000153	0.1813464
H	3.0942403	-1.6996085	-0.1098134
H	1.7817568	-2.8450787	0.0749762
H	2.2759185	2.4757776	0.4033771

(G4)

C	0.8524710	1.3926227	-0.2087045
C	-0.5622586	1.0850050	-0.0600679
C	-0.9146652	-0.2774082	0.0567438
N	-1.6643394	1.8596495	-0.1091167
N	-0.0877851	-1.3190805	-0.0143266
N	1.7056018	0.3461929	-0.0857086
C	1.2131573	-0.8857037	-0.0305127
C	-2.7008214	1.0176161	-0.0277865

N	-2.2948411	-0.2787482	0.0411448
H	-3.7372053	1.3070781	0.0045809
H	-2.8827239	-1.0934932	0.1070223
N	2.1115195	-1.8969753	0.0058972
O	1.3343378	2.5964209	0.2295714
H	3.0942458	-1.6824043	0.0139227
H	1.7814539	-2.8464187	0.0280028
H	0.6363436	3.2552362	0.1280275

(G5)

C	0.8741641	1.3796216	0.0093924
C	-0.4921694	1.1253407	0.0146130
C	-0.9586562	-0.2331344	0.0112773
N	-1.6250093	1.8767868	0.0222565
N	-0.0799074	-1.2623833	0.0025645
N	1.7624845	0.3512326	0.0020216
C	1.2082945	-0.8675694	-0.0007746
C	-2.7262977	0.9703951	0.0202526
N	-2.3021275	-0.2868876	0.0153195
N	2.0851962	-1.9097351	-0.0084086
O	1.3547720	2.6463323	0.0134960
H	3.0758838	-1.7313298	-0.0112810
H	1.7181157	-2.8476859	-0.0107949
H	-1.6720849	2.8803482	0.0199361
H	-3.7451841	1.3100077	0.0295154
H	2.3189053	2.5854170	0.0109042

(G6)

C	0.8358017	1.5389785	-0.0047821
C	-0.5037011	1.1611565	0.0095083
C	-0.9713209	-0.1664199	-0.0145968
N	-1.6788605	1.8919250	0.0483204
N	-0.0423873	-1.2241338	-0.0568142
N	1.6917853	0.2805047	-0.0510751
C	1.2646959	-0.9710657	-0.0738585
C	-2.7426653	0.9811674	0.0454253
N	-2.2901812	-0.2731375	0.0065923
H	2.6833425	0.4649640	-0.0641925
N	2.0690823	-2.0746770	-0.1146360
O	1.4371066	2.6153619	0.0111522
H	-1.7360015	2.8937293	0.0745923
H	-3.7727631	1.2816043	0.0712030
H	3.0473066	-1.7912534	-0.1258238
H	-0.3410896	-2.1871957	-0.0747849

(G7)

C	0.8286049	1.5501354	-0.0012639
C	-0.5058855	1.1654460	0.0108493
C	-0.9659698	-0.1652424	-0.0156603
N	-1.6897606	1.8885701	0.0483204
N	-0.0357927	-1.2241516	-0.0577074

N	1.6906811	0.2869914	-0.0495747
C	1.2735553	-0.9615048	-0.0747569
C	-2.7450631	0.9696398	0.0431535
N	-2.2846198	-0.2811619	0.0033453
H	2.6880060	0.4424060	-0.0651130
N	2.2193300	-1.9509293	-0.1195063
O	1.4260728	2.6260306	0.0162902
H	-1.7550148	2.8896423	0.0778779
H	-3.7779186	1.2612825	0.0677098
H	1.7697870	-2.8654005	-0.1259587
H	-0.3664015	-2.1753543	-0.0764250

(G8)

C	0.8479036	1.3534510	0.0230713
C	-0.5160412	1.1258113	0.0350780
C	-0.9994551	-0.1906391	0.0082880
N	-1.6696827	1.8932759	0.0546708
N	-0.0836792	-1.2366418	-0.0182603
N	1.7136210	0.3021043	0.0062262
C	1.2555871	-0.9135160	-0.0410581
C	-2.7429766	1.0165800	0.0333508
N	-2.3266635	-0.2542937	0.0074409
N	2.1269101	-1.9736270	-0.1540320
O	1.3829547	2.5828481	0.0306976
H	3.0911592	-1.6990317	-0.0486088
H	1.8884050	-2.8113179	0.3561068
H	-1.7190176	2.8951291	0.0654300
H	-3.7658096	1.3440080	0.0416442
H	-0.3939741	-2.1628814	-0.2644651