Triplet (π,π^*) Reactivity of the Guanine-Cytosine DNA Base Pair: Benign Deactivation *versus* Double Tautomerization via Intermolecular Hydrogen Transfer.

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Supporting Information.

Computational Details. The CASSCF calculations (and additional DFT ones) described here were carried out with the Gaussian03 package of programs,[1] while the CAS-PT2 energetics were recalculated with MOLCAS.[2] The CASSCF and B3LYP calculations use the 6-31G* basis set. For the CAS-PT2 calculations (frozen core orbitals), the 6-31G* basis set (305 basis functions) was reduced to 300 basis functions by using a minimal basis set for the cytosine ring hydrogens and the ones attached to the imidazole guanine moiety. The basis set reduction had a small effect (less than 1 kcal mol^{-1}) on the relative CASSCF energies. The CASSCF energies with the reduced basis set (CASSCF reference function for the CAS-PT2 calculation) are shown in the sixth column of Table S1.

Due to the size of the system and the active space, it was not possible to carry out analytical frequency calculations of the optimized structures. However, the transition structures (TS) optimized at the CASSCF level have one negative Hessian eigenvalue as shown by the numerical differentiation algorithm used in the TS optimization procedure of Gaussian03. The ground-state decay path from $\mathbf{CI_{Bir/CS}}$ (intrinsic reaction coordinate, IRC)[3] and the optimized $\mathbf{ISC_1}$[4] were calculated with the algorithms implemented in Gaussian03, and the spin-orbit coupling (SOC) at $\mathbf{ISC_1}$ and $\mathbf{ISC_2}$ was calculated with Gaussian03, using a one-electron approximation for the SOC operator with effective nuclear charges.[5]

Active space choice. The size of the active space for the CASSCF optimizations is limited to (10,10) (with the exception of the search of $\mathbf{CI_{Bir/CS}}$ and $\mathbf{^3Can_{Exc.Tr.}}$, see Table S1 and below). This size limitation is imposed by our computational resources. The composition of the active spaces (guanine and cytosine orbitals) is listed in Table S1 together with the energies of the CASSCF structures. The selection of the active-space orbitals was based on chemical criteria as explained below, and therefore the structures were optimized using different active spaces. The energetics were corrected with CAS-PT2 single-point calculations to account for the different active spaces and include dynamic correlation.

For structures $\mathbf{^3Can_{Cy}}$ and $\mathbf{ISC_1}$, where the excitation is localized on the cytosine base, we use 4 guanine orbitals and 6 cytosine ones. For structure $\mathbf{^3Can_{Gu}}$, where the excitation is localized on guanine, we use 6 guanine orbitals and 4 cytosine orbitals. For structure $\mathbf{^3ST_{Bir}}$, the best (10,10) active space to treat the delocalized radical on guanine and the allyl-type radical on cytosine is made of 7 guanine and 3 cytosine orbitals. The transition structure $\mathbf{^3TS_{H1}}$ connects the two structures $\mathbf{^3Can_{Cy}}$ and $\mathbf{^3ST_{Bir}}$. The optimal active spaces for the two structures are different (see above), and an active space of 6 guanine and 4 cytosine orbitals is chosen as the best possible compromise. Exploratory calculations showed that the CAS-PT2//CASSCF barrier for hydrogen transfer changes only by 1-2 kcal mol^{-1} after optimization of $\mathbf{^3TS_{H1}}$ with larger active spaces (12,12). Structure $\mathbf{^3TS'_{H1}}$ (TS for hydrogen transfer starting from $\mathbf{^3Can_{Gu}}$, see Table S1) was also optimized with an active space of 6 guanine and 4 cytosine orbitals. For the study of the hydrogen transfer on the ground-state surface (closed-shell structures $\mathbf{^1ST_{CS}}$,

Table S1. Energies and active spaces of optimized structures.

Structure	Description	Active space	Active space orbitals (Gu, Cy)	CASSCF/6-31G* Energies [hartree]	CASSCF Energies, reduced 6-31G* basis[a] [hartree]	CAS-PT2[a] Energies [hartree]
^{3}**Can$_{Cy}$**	Canonical base pair T_1 minimum (cytosine localized excitation)	(10,10)	4,6	-932.0326	-932.0020	-934.6300
^{3}**Can$_{Gu}$**	Canonical base pair T_1 minimum (guanine-localized excitation)	(10,10)	6,4	-932.0241	-931.9938	-934.6306
ISC$_1$	Canonical base pair, T_1/S_0 intersystem crossing	(10,10)	4,6	-932.0291 -932.0291	-931.9991 (S_0) -931.9988 (T_1)	-934.6285(S_0) -934.6258 (T_1)
^{3}**TS$_{H1}$**	T_1 transition structure for transfer of H_1 (cytosine-localized excitation)	(10,10)	6,4	-931.9851	-931.9555	-934.6023
^{3}**TS'$_{H1}$**	T_1 transition structure for transfer of H_1 (guanine-localized excitation)	(10,10)	6,4	-931.9756	-931.9452	-934.5997
^{3}**Can$_{Exc.Tr.}$**	Canonical base pair, T_1/T_2 crossing for triplet excitation transfer	(12,12)	6,6	-932.0109 -932.0108	-931.9810 -931.9809	-934.6088 -934.6078
^{3}**ST$_{Bir}$**	H_1 tautomer T_1 minimum	(10,10)	7,3	-932.0408	-932.0107	-934.6469
^{1}**ST$_{Bir}$**	H_1 tautomer S_1 minimum (biradical state)	(12,11)	5,6	-932.0132 (zw.) -932.0003 (bir.)	-932.9825(zw.) -932.9704 (bir.)	-934.6497 (zw.) -934.6453 (bir.)
CI$_{Bir/CS}$	S_1/S_0 conical intersection for H_1 tautomer (biradical and closed shell states)	(12,11)	5,6	-932.0002 (bir.) -932.9998 (zw.)	-931.9700 (bir.) -931.9691 (zw.)	-934.6425 (bir.) -934.6380 (zw.)
^{3}**TS$_{H2}$**	T_1 transition structure for transfer of H_2			-931.9885	-931.9580	-934.6074
^{1}**ST$_{CS}$**	H_1 tautomer S_0 minimum (closed shell state)	(10,10)	6,4	-932.1156	-932.0854	-934.7246
^{1}**TS$_{conc}$**	S_0 transition structure[b] for concerted transfer of H_1 and H_2	(10,10)	6,4	-932.0953	-932.0659	-934.7362
^{1}**TS$_{H1}$**	S_0 transition structure for transfer of H_1	(10,10)	6,4	-932.1132	-	-
^{1}**TS$_{H2}$**	S_0 transition structure for transfer of H_2 (after transfer of H_1)	(10,10)	6,4	-932.1156[c]	-	-

[a]Reduced 6-31G* basis set, see computational details of CAS-PT2 calculations. [b]Structure optimized at the B3LYP/6-31G* level. [c]Energy relative to ^{1}**ST$_{CS}$** 0.03 kcal mol^{-1}.

^{1}**TS$_{H1}$**, ^{1}**TS$_{H2}$**, and ^{1}**TS$_{conc}$**), we chose an active space of 6 guanine and 4 cytosine orbitals to obtain a balanced treatment of the two bases. The search of **CI$_{Bir/CS}$** and the optimization of ^{3}**Can$_{Exc.Tr.}$** was carried out with (12,11) and (12,12) active spaces, respectively (see Table S1 and below), to obtain a balanced treatment of the two states involved in the two crossings.

Barrier for H_1 transfer on the triplet surface – DFT calculations. To confirm the CAS-PT2//CASSCF value obtained for the barrier corresponding to H_1 transfer, structures ^{3}**Can$_{Cy}$** and ^{3}**TS$_{H1}$** were optimized at the B3LYP/6-31G* level of theory and the energetics recalculated using several DFT methods (single-point calculations on the B3LYP geometry, see Table S2). The energetics are very dependent on the method, with the BHLYP value being closest to the CAS-PT2//CASSCF barrier. In contrast to this, all methods agree on the calculated reaction energy of approximately 10 kcal mol^{-1}. The DFT results will be discussed in a future publication.

Table S2. Energetics for H_1 transfer on the triplet surface (6-31G* basis set).

Method	E_{act} [kcal mol^{-1}]	ΔE_r [kcal mol^{-1}]
CAS-PT2//CASSCF	17.4	-10.6
B3LYP	5.2	-9.3
BLYP//B3LYP	-0.9	-9.0
BHLYP//B3LYP	15.5	-8.6

*State Ordering at ^{1}**ST$_{Bir}$**.* The topology of the ET reaction between ^{1}**ST$_{Bir}$** and ^{1}**ST$_{CS}$** depends on the relative energies of the two singlet states at ^{1}**ST$_{Bir}$**. Thus we assume that the ^{1}**ST$_{CS}$** structure lies on the ground-state energy surface (S_0), in agreement with previous HF and MP2 results.[6] Then, if the biradical state is S_1 at ^{1}**ST$_{Bir}$**, the ET will be associated to a sloped conical intersection and an inverted Marcus region. However, if the biradical is S_0 at that point, the intersection will be peaked and correspond to a normal Marcus region[7] (Figure S1).

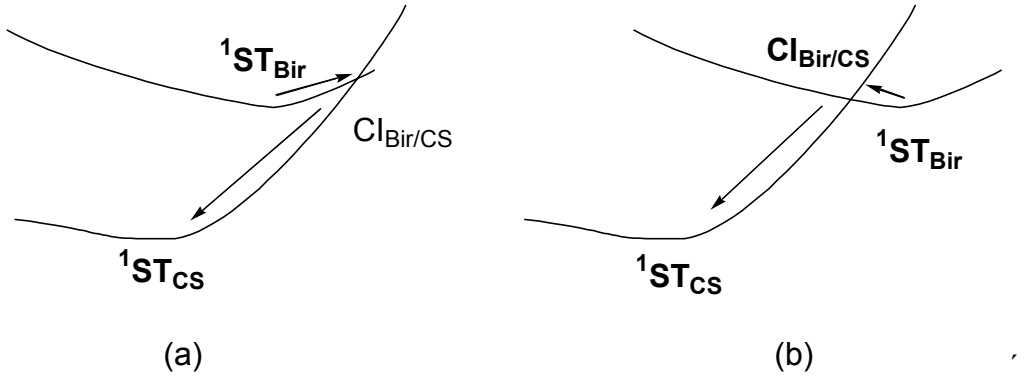


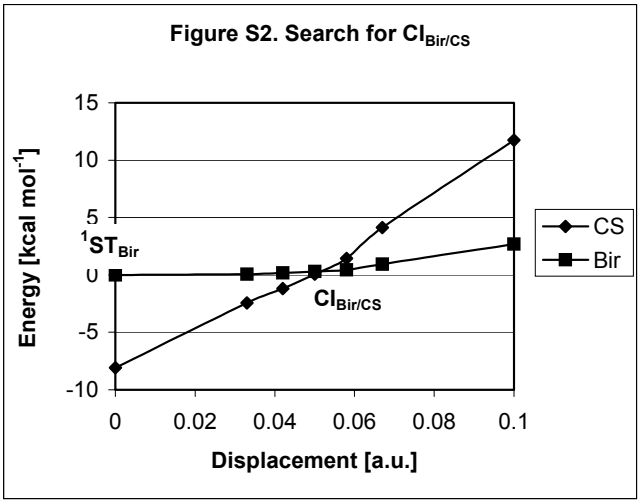
Figure S1. Alternative topologies associated to the ET between ^{1}**ST$_{Bir}$** and ^{1}**ST$_{CS}$**. (a) ^{1}**ST$_{Bir}$** on S_1, ET in the inverted Marcus region (sloped conical intersection). (b) ^{1}**ST$_{Bir}$** on S_0, ET in the normal Marcus region (peaked conical intersection).

To evaluate this alternative, the state ordering at ^{1}**ST$_{Bir}$** was studied at the CASSCF and CAS-PT2 levels with (10,10) and (12,11) active spaces. The results (Table S3) show that the ordering depends on the size of the active space, also at the CAS-PT2 level. The definitive order of the states, and the topology of the ET reaction, can only be assigned with a larger active space calculation (see below).

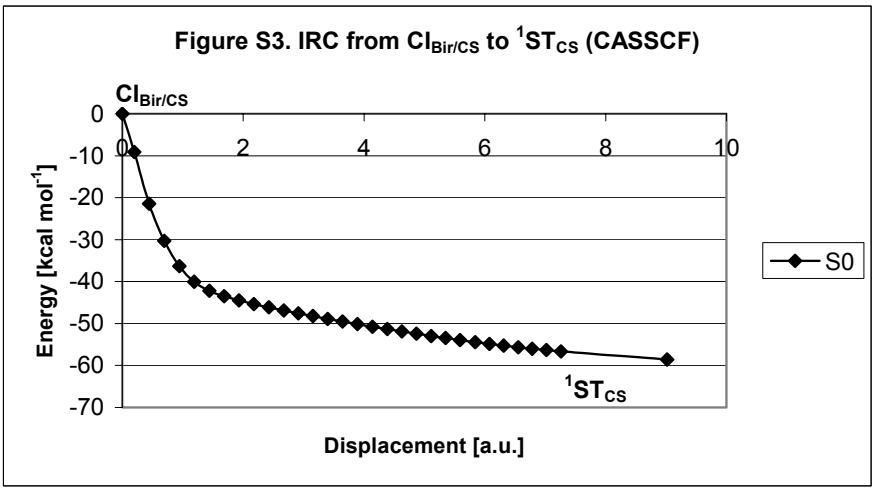
Table S3. Ordering of the states at ^{1}**ST$_{Bir}$**, CASSCF and CAS-PT2 levels.

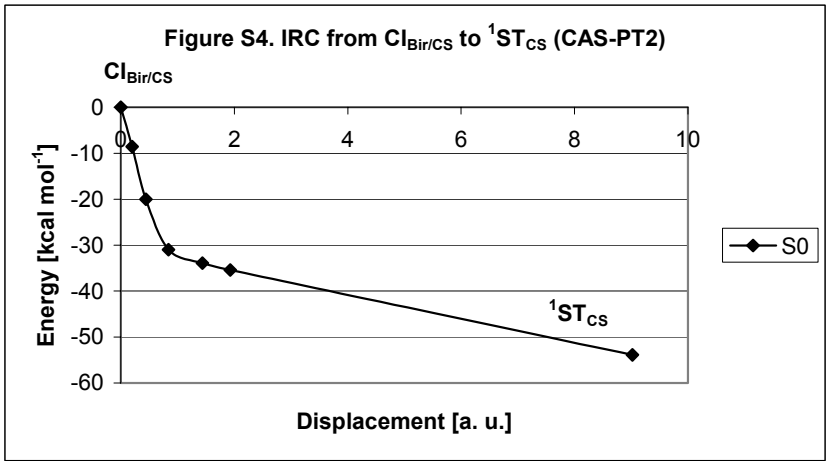
Active Space	E_{Bir}-E_{CS} CASSCF	CAS-PT2	Topology (Figure S2)
(10,10)	-6.9	-6.6	(b)
(12,11)	+7.6	+2.7	(a)

Search for ***CI$_{Bir/CS}$***. The optimization of **CI$_{Bir/CS}$** requires the solution of the coupled MCSCF equations,[4] which is not possible at present for a system the size of **GuCy** with the required (12,11) active space. Therefore, **CI$_{Bir/CS}$** was not optimized using the algorithm implemented in Gaussian. Instead it was located starting from ^{1}**ST$_{Bir}$**, following the gradient difference coordinate between the biradical and zwitterionic states at that point (S_1 and S_0, respectively). The linear coordinate is presented in Figure S1 and shows that, at the CAS(12,11) level of theory, **CI$_{Bir/CS}$** has a sloped topology and can be accessed from ^{1}**ST$_{Bir}$** with a barrier of 0.2 kcal mol^{-1}. CAS-PT2 calculations on the **CI$_{Bir/CS}$** structure confirm the presence of CI because the order of the states is inverted with respect to ^{1}**ST$_{Bir}$**. CAS-PT2 and CASSCF calculations with a larger active space are in progress to confirm the topology of the intersection and the barrier.



Decay from ***CI$_{Bir/CS}$***. The initial part of the ground-state decay route from **CI$_{Bir/CS}$** was studied with an IRC calculation at the CASSCF level (see Figure S3). The IRC leads to the ground-state minimum ^{1}**ST$_{CS}$**. The energetics were recalculated at the CAS-PT2 level (Figure S4). A continous descent of the energy along the path is also obtained at that level.





Ground-state hydrogen transfer process (Figure 2). At the CASSCF level, the tautomer formed after transfer of H_1, $^1\mathbf{ST_{CS}}$, is a ground-state minimum. The CASSCF barriers for back transfer of H_1 to yield the original ^{1}**Can** pair and for transfer of H_2 to give the double tautomer ^{1}**DT** are 1.1 kcal mol^{-1} and 0.03 kcal mol^{-1}, respectively. In contrast to this, no transition structure for the concerted double hydrogen transfer could be optimized at the CASSCF level. However, the concerted transfer structure $^1\mathbf{TS_{conc}}$ was optimized as a transition structure at the B3LYP/6-31G* level.[8] These results are analogous to the Hartree-Fock (HF) calculations reported for the ^{1}**Can** pair.[6] At the HF level the concerted transfer structure is a second-order saddle point, but MP2 calculations on the HF structures strongly favor the concerted transfer structure as the TS of the reaction. Thus the stepwise path and the $^1\mathbf{ST_{CS}}$ minimum appear to be spurious.[6] CAS-PT2 calculations on the CASSCF structures show the same behavior as that described for MP2 with respect to HF. The H_1-transfer tautomer $^1\mathbf{ST_{CS}}$ is more stable than $^1\mathbf{TS_{conc}}$ by 12.2 kcal mol^{-1} at the CASSCF level, but at the CAS-PT2 level the concerted transfer structure is more stable by 7.0 kcal mol^{-1}.

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Cartesian coordinates of structures.

$^3Can_{Cy}$

1	6	0	3.073505	1.006262	-0.152702
2	7	0	2.288788	-0.135747	0.000690
3	6	0	2.830504	-1.311439	-0.033283
4	6	0	4.280242	-1.485092	-0.133280
5	6	0	5.101420	-0.295693	0.189779
6	7	0	4.449967	0.886725	-0.171641
7	7	0	2.057120	-2.408118	-0.045019
8	8	0	2.559845	2.090075	-0.267907
9	8	0	-0.918762	-1.984180	0.103739
10	6	0	-1.509740	-0.929291	0.080231
11	6	0	-2.928234	-0.688853	0.023559
12	6	0	-3.363664	0.603648	0.000826
13	7	0	-2.635121	1.752305	0.024935
14	6	0	-1.360710	1.526180	0.088711
15	7	0	-0.804778	0.275912	0.109151
16	7	0	-4.714856	0.524888	-0.055095
17	6	0	-5.026999	-0.810718	-0.062809
18	7	0	-3.992532	-1.562658	-0.017428
19	7	0	-0.488677	2.558212	0.184715
20	1	0	-6.042249	-1.147801	-0.103572
21	1	0	-5.342171	1.295609	-0.081040
22	1	0	-0.868609	3.455471	-0.013330
23	1	0	0.477200	2.421218	-0.031983
24	1	0	0.196707	0.193781	0.136301
25	1	0	1.060099	-2.314328	0.023286
26	1	0	2.454706	-3.298338	0.142564
27	1	0	4.668758	-2.279044	-0.743845
28	1	0	5.682161	-0.281157	1.100522
29	1	0	4.934557	1.754687	-0.105280

$^3Can_{Gu}$

1	6	0	0.604304	3.143758	0.062557
2	7	0	1.241585	1.925870	0.067723
3	6	0	2.539488	1.848824	0.026898
4	6	0	3.390471	3.033059	-0.020417
5	6	0	2.765917	4.221642	-0.018556
6	7	0	1.394039	4.269444	0.025729
7	7	0	3.117468	0.643380	0.039378
8	8	0	-0.593931	3.249577	0.087691
9	8	0	1.262974	-1.745726	-0.026445
10	6	0	0.061662	-1.678102	0.054481
11	6	0	-0.839245	-2.845229	0.020575
12	6	0	-2.260873	-2.630184	0.109626
13	7	0	-2.883078	-1.524416	0.262151
14	6	0	-2.038413	-0.361741	0.346205
15	7	0	-0.623910	-0.526225	0.184180
16	7	0	-2.777192	-3.908686	0.014586
17	6	0	-1.707749	-4.765899	-0.101563
18	7	0	-0.548554	-4.159011	-0.105475
19	7	0	-2.548619	0.700279	-0.408327
20	1	0	-1.835267	-5.824841	-0.177122
21	1	0	-3.738460	-4.152169	0.062019
22	1	0	-3.505291	0.872184	-0.175784
23	1	0	-2.013093	1.543676	-0.313055
24	1	0	-0.069162	0.311763	0.201480
25	1	0	2.550831	-0.185787	0.027501
26	1	0	4.099684	0.548172	-0.064139
27	1	0	4.458683	2.951044	-0.051067
28	1	0	3.275625	5.164038	-0.049413
29	1	0	0.909440	5.138590	0.018579

ISC_1

1	6	0	3.091364	0.996704	-0.197533
2	7	0	2.295169	-0.128249	0.041233
3	6	0	2.812753	-1.314940	0.011405
4	6	0	4.268134	-1.493630	-0.212630
5	6	0	5.059831	-0.329241	0.237548
6	7	0	4.473192	0.850982	-0.251215
7	7	0	2.051612	-2.402439	0.143285
8	8	0	2.590322	2.081434	-0.344687
9	8	0	-0.903705	-1.989440	0.147905
10	6	0	-1.492310	-0.933544	0.109120
11	6	0	-2.909525	-0.692800	0.030043
12	6	0	-3.345705	0.599601	-0.010062
13	7	0	-2.616549	1.747793	0.018027
14	6	0	-1.343039	1.521620	0.103424
15	7	0	-0.787671	0.271490	0.139748
16	7	0	-4.695212	0.517940	-0.091277
17	6	0	-5.005772	-0.818124	-0.095496
18	7	0	-3.971473	-1.568458	-0.026337
19	7	0	-0.472278	2.553634	0.210255
20	1	0	-6.019787	-1.156541	-0.152826
21	1	0	-5.323436	1.287255	-0.133319
22	1	0	-0.848933	3.449504	-0.000650
23	1	0	0.495319	2.415184	0.001717
24	1	0	0.213861	0.192685	0.181845
25	1	0	1.051829	-2.323959	0.193615
26	1	0	2.462586	-3.305805	0.149045
27	1	0	4.560058	-2.013438	-1.108532
28	1	0	5.463658	-0.314576	1.235930
29	1	0	4.964182	1.711876	-0.138780

$^3TS_{H1}$

1	6	0	2.870959	1.035648	-0.366804
2	7	0	2.054081	-0.074274	-0.136906
3	6	0	2.543863	-1.256343	0.195225
4	6	0	4.004596	-1.415392	0.331262
5	6	0	4.768491	-0.453506	-0.514620
6	7	0	4.236551	0.826731	-0.367803
7	7	0	1.760743	-2.268350	0.410196
8	8	0	2.410632	2.125495	-0.548596
9	8	0	-0.717111	-1.932635	-0.508334
10	6	0	-1.275793	-0.860095	-0.268602
11	6	0	-2.704510	-0.677727	-0.266986
12	6	0	-3.179209	0.553143	0.079687
13	7	0	-2.461235	1.650074	0.413130
14	6	0	-1.177392	1.421284	0.372711
15	7	0	-0.555889	0.258619	0.040653
16	7	0	-4.542952	0.443546	0.030145
17	6	0	-4.803154	-0.847073	-0.340422
18	7	0	-3.751677	-1.551104	-0.525368
19	7	0	-0.346726	2.456337	0.750922
20	1	0	-5.808710	-1.199479	-0.455828
21	1	0	-5.199631	1.160699	0.231699
22	1	0	-0.825447	3.330146	0.773924
23	1	0	0.525888	2.502263	0.271943
24	1	0	0.904658	0.109610	-0.085192
25	1	0	0.760158	-2.205427	0.163147
26	1	0	2.158354	-3.159375	0.607646
27	1	0	4.355793	-1.680176	1.316086
28	1	0	5.835563	-0.519865	-0.585807
29	1	0	4.761806	1.624635	-0.653279

^{3}TS'$_{H1}$

1	6	0	0.462547	3.087294	0.010851
2	7	0	1.068710	1.844060	-0.036983
3	6	0	2.388915	1.656698	0.022097
4	6	0	3.259298	2.815582	0.145813
5	6	0	2.682700	4.026799	0.193402
6	7	0	1.318734	4.153977	0.125643
7	7	0	2.875764	0.454630	-0.032172
8	8	0	-0.718740	3.234611	-0.047407
9	8	0	1.313487	-1.627118	-0.425562
10	6	0	0.102855	-1.487913	-0.199879
11	6	0	-0.769959	-2.683735	-0.142089
12	6	0	-2.128593	-2.508844	0.269905
13	7	0	-2.710164	-1.405008	0.558471
14	6	0	-1.881540	-0.237595	0.294808
15	7	0	-0.488070	-0.340495	0.034822
16	7	0	-2.617847	-3.801895	0.335181
17	6	0	-1.584912	-4.633327	-0.029407
18	7	0	-0.475347	-3.996658	-0.306564
19	7	0	-2.564138	0.611098	-0.604805
20	1	0	-1.699072	-5.696145	-0.068734
21	1	0	-3.547402	-4.063905	0.562697
22	1	0	-3.488521	0.800161	-0.271890
23	1	0	-2.075821	1.475378	-0.725000
24	1	0	0.395303	0.964568	-0.029323
25	1	0	2.266390	-0.384951	-0.179207
26	1	0	3.861621	0.326556	0.015575
27	1	0	4.321447	2.686927	0.193021
28	1	0	3.239522	4.938053	0.281402
29	1	0	0.882155	5.048456	0.155331

^{3}Can$_{Exc.Tr.}$

1	6	0	3.043811	1.067798	-0.141591
2	7	0	2.296581	-0.096814	-0.052644
3	6	0	2.883855	-1.255509	0.023524
4	6	0	4.321711	-1.395397	0.055235
5	6	0	5.094409	-0.223025	-0.010363
6	7	0	4.418538	0.972221	-0.115782
7	7	0	2.127345	-2.369604	0.053765
8	8	0	2.515944	2.147209	-0.242280
9	8	0	-0.910094	-2.006716	0.044294
10	6	0	-1.488888	-0.944362	0.067353
11	6	0	-2.925530	-0.738910	-0.018917
12	6	0	-3.420425	0.599539	-0.003634
13	7	0	-2.728670	1.709054	0.095068
14	6	0	-1.408838	1.521489	0.160907
15	7	0	-0.817818	0.252803	0.193431
16	7	0	-4.792384	0.441094	-0.142547
17	6	0	-5.015065	-0.901506	-0.211547
18	7	0	-3.961693	-1.631898	-0.150762
19	7	0	-0.575329	2.574441	0.488416
20	1	0	-6.010052	-1.288927	-0.313435
21	1	0	-5.473404	1.163562	-0.141636
22	1	0	-0.987318	3.455375	0.269397
23	1	0	0.360074	2.502269	0.138976
24	1	0	0.183880	0.204180	0.176135
25	1	0	1.128903	-2.293257	0.079102
26	1	0	2.535332	-3.253179	0.246198
27	1	0	4.785383	-2.358587	0.119677
28	1	0	6.163729	-0.201933	-0.005550
29	1	0	4.910356	1.834889	-0.175874

$^1ST_{Bir}$, $^3ST_{Bir}$

1	6	0	2.981160	1.086378	-0.060979
2	7	0	2.345577	-0.087765	0.164268
3	6	0	2.981165	-1.341194	0.151086
4	6	0	4.332452	-1.392908	-0.061743
5	6	0	5.051779	-0.202514	-0.237474
6	7	0	4.319647	1.000465	-0.276621
7	7	0	2.152571	-2.402172	0.518584
8	8	0	2.403616	2.153589	-0.070778
9	8	0	-1.028145	-2.033319	-0.224772
10	6	0	-1.517657	-0.928980	-0.110478
11	6	0	-2.962543	-0.706417	-0.116806
12	6	0	-3.416025	0.660003	0.013794
13	7	0	-2.678822	1.687610	0.129647
14	6	0	-1.311919	1.387724	0.127528
15	7	0	-0.755465	0.211708	0.032479
16	7	0	-4.771161	0.558159	-0.023841
17	6	0	-5.070561	-0.786448	-0.167710
18	7	0	-4.015914	-1.552599	-0.225772
19	7	0	-0.543012	2.467925	0.245198
20	1	0	-6.080119	-1.134114	-0.223214
21	1	0	-5.414215	1.313673	0.041486
22	1	0	-0.976951	3.360158	0.266112
23	1	0	0.456038	2.397380	0.172859
24	1	0	1.346361	-0.038104	0.236628
25	1	0	1.235723	-2.360117	0.116548
26	1	0	2.565686	-3.292781	0.339885
27	1	0	4.847133	-2.334943	-0.064751
28	1	0	6.065454	-0.153184	-0.573680
29	1	0	4.783841	1.873431	-0.375260

$CI_{Bir/CS}$

1	6	0	2.984471	1.083413	-0.060701
2	7	0	2.343875	-0.083980	0.164513
3	6	0	2.989718	-1.344606	0.148000
4	6	0	4.322931	-1.395270	-0.062265
5	6	0	5.059667	-0.201612	-0.234375
6	7	0	4.314222	1.004799	-0.278633
7	7	0	2.149872	-2.403729	0.519382
8	8	0	2.403904	2.152952	-0.071114
9	8	0	-1.027943	-2.034258	-0.224817
10	6	0	-1.513872	-0.930118	-0.110471
11	6	0	-2.964073	-0.713132	-0.117615
12	6	0	-3.417804	0.669421	0.014735
13	7	0	-2.683756	1.685829	0.129409
14	6	0	-1.309815	1.387794	0.127385
15	7	0	-0.753608	0.211905	0.033023
16	7	0	-4.770875	0.561002	-0.023548
17	6	0	-5.073657	-0.786347	-0.167757
18	7	0	-4.011895	-1.555665	-0.226044
19	7	0	-0.543865	2.466977	0.244913
20	1	0	-6.082813	-1.134960	-0.223351
21	1	0	-5.415987	1.315527	0.041646
22	1	0	-0.975964	3.361339	0.266313
23	1	0	0.458500	2.397064	0.172721
24	1	0	1.350405	-0.038501	0.236247
25	1	0	1.239597	-2.359720	0.117184
26	1	0	2.566584	-3.290023	0.339497
27	1	0	4.844925	-2.331453	-0.064624
28	1	0	6.060474	-0.153671	-0.572677
29	1	0	4.782478	1.869666	-0.374753

$^{3}TS_{H2}$

1	6	0	3.044995	1.016466	-0.322492
2	7	0	2.204376	-0.050347	-0.077752
3	6	0	2.596236	-1.351199	0.022904
4	6	0	4.026594	-1.605944	0.138889
5	6	0	4.915650	-0.417275	0.314710
6	7	0	4.383994	0.739027	-0.275582
7	7	0	1.709189	-2.286639	-0.006719
8	8	0	2.620157	2.109970	-0.560122
9	8	0	-0.783433	-1.902468	-0.323630
10	6	0	-1.371538	-0.813849	-0.165056
11	6	0	-2.767959	-0.664061	-0.089518
12	6	0	-3.256090	0.613768	0.102841
13	7	0	-2.566503	1.722887	0.224045
14	6	0	-1.252215	1.504981	0.140106
15	7	0	-0.640786	0.338081	-0.049044
16	7	0	-4.612608	0.480658	0.138241
17	6	0	-4.877335	-0.865294	-0.032327
18	7	0	-3.816473	-1.579663	-0.171933
19	7	0	-0.459975	2.594368	0.307335
20	1	0	-5.874460	-1.237545	-0.046040
21	1	0	-5.261081	1.217644	0.263932
22	1	0	-0.934587	3.463019	0.239340
23	1	0	0.467124	2.561047	-0.047438
24	1	0	1.193095	0.168211	-0.097645
25	1	0	0.626443	-2.081548	-0.142620
26	1	0	1.992730	-3.250064	0.111052
27	1	0	4.425797	-2.579784	-0.120732
28	1	0	5.477052	-0.288200	1.231461
29	1	0	4.952764	1.558190	-0.345420

$^{1}ST_{CS}$

1	6	0	3.000593	1.136528	-0.308760
2	7	0	2.198731	0.019048	-0.139533
3	6	0	2.655354	-1.227702	0.042775
4	6	0	4.094531	-1.426407	0.116755
5	6	0	4.885771	-0.352033	-0.034148
6	7	0	4.354924	0.893974	-0.248605
7	7	0	1.821063	-2.204993	0.144056
8	8	0	2.556955	2.230082	-0.496690
9	8	0	-0.687691	-1.911265	-0.296113
10	6	0	-1.284821	-0.830341	-0.136783
11	6	0	-2.716236	-0.725663	-0.110649
12	6	0	-3.251469	0.517350	0.087789
13	7	0	-2.579674	1.672822	0.261472
14	6	0	-1.284068	1.487828	0.225336
15	7	0	-0.615243	0.327012	0.028689
16	7	0	-4.606795	0.345028	0.075139
17	6	0	-4.817474	-1.001309	-0.128458
18	7	0	-3.722914	-1.677248	-0.244453
19	7	0	-0.493825	2.595690	0.452246
20	1	0	-5.804883	-1.412003	-0.180797
21	1	0	-5.290189	1.053542	0.201510
22	1	0	-0.984772	3.454776	0.338265
23	1	0	0.403704	2.585396	0.020487
24	1	0	1.165369	0.184729	-0.116240
25	1	0	0.767712	-2.070279	-0.002624
26	1	0	2.173559	-3.126781	0.280203
27	1	0	4.490541	-2.408374	0.276302
28	1	0	5.955359	-0.408630	-0.001520
29	1	0	4.941579	1.689877	-0.363432

$^1TS_{conc}$

1	6	0	2.847837	1.058731	-0.163635
2	7	0	2.043020	-0.029948	-0.019250
3	6	0	2.534855	-1.310562	0.116346
4	6	0	3.975998	-1.498225	0.139070
5	6	0	4.773581	-0.418194	-0.004968
6	7	0	4.229578	0.827172	-0.161494
7	7	0	1.671914	-2.284550	0.212964
8	8	0	2.447013	2.219790	-0.293277
9	8	0	-0.795474	-2.055465	-0.123193
10	6	0	-1.324995	-0.881304	-0.048089
11	6	0	-2.725384	-0.694363	-0.067603
12	6	0	-3.180129	0.625863	0.033901
13	7	0	-2.448497	1.738803	0.144535
14	6	0	-1.134317	1.489125	0.152685
15	7	0	-0.553020	0.244049	0.054489
16	7	0	-4.548830	0.526389	-0.001774
17	6	0	-4.845609	-0.825832	-0.119687
18	7	0	-3.785232	-1.585416	-0.161123
19	7	0	-0.300455	2.545392	0.297891
20	1	0	-5.868935	-1.173589	-0.169629
21	1	0	-5.195603	1.298345	0.053139
22	1	0	-0.744634	3.447759	0.239600
23	1	0	0.695036	2.472407	0.074463
24	1	0	0.762538	0.129382	0.016571
25	1	0	0.300685	-2.121677	0.030695
26	1	0	2.098982	-3.199434	0.309894
27	1	0	4.390700	-2.490950	0.257536
28	1	0	5.856619	-0.473902	-0.007806
29	1	0	4.801937	1.652394	-0.264477

$^1TS_{H1}$

1	6	0	2.825397	1.096700	-0.473693
2	7	0	2.055983	-0.020083	-0.197935
3	6	0	2.586301	-1.200857	0.101393
4	6	0	4.028457	-1.336857	0.231042
5	6	0	4.778633	-0.253205	-0.023657
6	7	0	4.191518	0.929781	-0.381012
7	7	0	1.813335	-2.233741	0.276228
8	8	0	2.353605	2.154737	-0.779297
9	8	0	-0.713468	-1.934366	-0.565303
10	6	0	-1.282744	-0.874868	-0.307390
11	6	0	-2.708518	-0.713405	-0.232124
12	6	0	-3.184330	0.515421	0.127635
13	7	0	-2.468076	1.624423	0.399780
14	6	0	-1.183802	1.415675	0.290992
15	7	0	-0.560721	0.265127	-0.045250
16	7	0	-4.542329	0.390017	0.160715
17	6	0	-4.816127	-0.918221	-0.178864
18	7	0	-3.754057	-1.612904	-0.417565
19	7	0	-0.364573	2.474914	0.586318
20	1	0	-5.820282	-1.285779	-0.230882
21	1	0	-5.190202	1.105672	0.391451
22	1	0	-0.858923	3.338661	0.627738
23	1	0	0.494294	2.522592	0.083636
24	1	0	0.899454	0.129866	-0.160479
25	1	0	0.815431	-2.183223	0.031504
26	1	0	2.213871	-3.119373	0.487646
27	1	0	4.458655	-2.280433	0.498466
28	1	0	5.849046	-0.256119	0.028475
29	1	0	4.738174	1.738712	-0.574863

$^{1}TS_{H2}$

1	6	0	2.991129	1.141795	-0.262842
2	7	0	2.185340	0.024875	-0.111947
3	6	0	2.636389	-1.230749	0.025060
4	6	0	4.075567	-1.439982	0.065217
5	6	0	4.870922	-0.366682	-0.070596
6	7	0	4.344495	0.888658	-0.238105
7	7	0	1.795790	-2.202779	0.113007
8	8	0	2.551433	2.243742	-0.406264
9	8	0	-0.716754	-1.914707	-0.230359
10	6	0	-1.310899	-0.828446	-0.091017
11	6	0	-2.741884	-0.720688	-0.082180
12	6	0	-3.276356	0.527661	0.081449
13	7	0	-2.603580	1.683715	0.244938
14	6	0	-1.307948	1.494210	0.234680
15	7	0	-0.639307	0.328580	0.064909
16	7	0	-4.631791	0.359234	0.047451
17	6	0	-4.843252	-0.990322	-0.133150
18	7	0	-3.749093	-1.671681	-0.216390
19	7	0	-0.519747	2.602193	0.463514
20	1	0	-5.830920	-1.399087	-0.194803
21	1	0	-5.315018	1.072058	0.147837
22	1	0	-1.003156	3.462122	0.327042
23	1	0	0.391580	2.582787	0.062520
24	1	0	1.154351	0.193025	-0.076624
25	1	0	0.735220	-2.054656	-0.008107
26	1	0	2.142850	-3.131360	0.212972
27	1	0	4.467951	-2.428643	0.188218
28	1	0	5.940540	-0.430855	-0.061706
29	1	0	4.934297	1.683952	-0.340194