Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Solvent effect on the Intermolecular Proton Transfer of the Watson and Crick Guanine-Cytosine and Adenine-Thymine base pairs: A Polarizable Continuum Model study

(Supporting Information)

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(i) Canonical, transition states and rare tautomers coordinates of the AT proton transfer complexes.

Herein the XYZ coordinates of the AT complexes are show. All the structures were calculated without symmetry constrain (C1 symmetry) using PCM and water as solvent, where the theoretical level used was Cam-B3LYP/6-311++G(d,p).

AT

Atom	X	Y	Z
N	0.45007500	-0.18593700	4.97745500
C	-0.89895900	-0.13271200	5.20417500
H	-1.30277100	-0.16723700	6.20457100
N	-1.59903800	-0.03936900	4.10743400
C	-0.65460500	-0.03042800	3.10048100
C	-0.76461200	0.05146000	1.69982500
N	-1.93488600	0.14371900	1.06024600
H	-1.96150600	0.19853800	0.04214000
H	-2.79114200	0.15575100	1.58935500
N	0.37704600	0.03483300	0.98732100
C	1.55211500	-0.05672300	1.62391800
H	2.42446300	-0.06347700	0.97770800
N	1.76965800	-0.13806600	2.92482600
C	0.62668200	-0.12078700	3.62334100
H	1.17390200	-0.25719200	5.67770100
N	0.42465300	0.19556900	-1.90093300
C	-0.80281100	0.28634700	-2.52806900
C	-0.77943300	0.37117500	-3.97868300
C	0.42290600	0.35377800	-4.58054400
C	1.65352500	0.17742300	-2.51103700
O	-1.83443200	0.29204000	-1.85707300
O	2.70206600	0.09437200	-1.89232900
N	1.59785700	0.26075100	-3.87876700
C	-2.07552000	0.47298700	-4.71920500
H	-2.71113200	-0.39154600	-4.51618700
H	-2.63211100	1.36135900	-4.41316000

H	-1.90197000	0.52835800	-5.79385300
H	0.53516000	0.41245600	-5.65492100
H	2.48197400	0.25010100	-4.36668500
H	0.42314400	0.13599300	-0.86173300

AT‡ (First transition state)

Atom	X	Y	Z
N	0.51537600	-0.17873000	4.81101500
C	-0.82697000	-0.13002500	5.07702300
H	-1.20203300	-0.16724600	6.08821400
N	-1.55702000	-0.03702600	3.99982700
C	-0.64231800	-0.02388400	2.97148900
C	-0.80803800	0.06038800	1.57668700
N	-1.97186000	0.14976300	0.95372900
H	-2.01879100	0.20778900	-0.07797000
H	-2.81598700	0.16024500	1.50429400
N	0.34240400	0.04502200	0.86070400
C	1.55626200	-0.04460800	1.44793400
H	2.38528100	-0.04573800	0.74863500
N	1.78670400	-0.12537800	2.73173800
C	0.65322700	-0.11137900	3.45753900
H	1.26033500	-0.24922200	5.48981400
N	0.33762000	0.18896900	-1.73215200
C	-0.82573800	0.28462900	-2.43352800
C	-0.76796200	0.36699200	-3.88794400
C	0.45311900	0.34242400	-4.45094900
C	1.56032400	0.16552500	-2.31664300
O	-1.91768700	0.30034200	-1.82853100
O	2.61182500	0.07795600	-1.67517900

N	1.58879200	0.24519400	-3.69365100
C	-2.03680500	0.47296700	-4.67422100
H	-2.68805700	-0.38351000	-4.48612600
H	-2.59851800	1.36772000	-4.39613600
H	-1.82729100	0.51754100	-5.74366100
H	0.60877500	0.39759500	-5.52060900
H	2.49726400	0.22808600	-4.13278700
H	0.31806500	0.11113800	-0.32123800

AT1

Atom	X	Y	Z
N	0.46181000	-0.17280300	4.82526900
C	-0.88442600	-0.10408300	5.06548300
H	-1.27944700	-0.12952600	6.06934900
N	-1.59223200	-0.00876400	3.97359000
C	-0.65849200	-0.01449700	2.96402600
C	-0.79906800	0.06394600	1.56596600
N	-1.94110600	0.16563600	0.91194500
H	-1.96657200	0.21901300	-0.12549300
H	-2.79805000	0.19155800	1.44260600
N	0.37226400	0.02784200	0.88151900
C	1.57834600	-0.07431700	1.48762000
H	2.41741400	-0.09007700	0.80096600
N	1.77658500	-0.14991100	2.77349800
C	0.62656900	-0.11610700	3.47544500
H	1.19308500	-0.24836600	5.51847500
N	0.35596500	0.17297600	-1.76759000
C	-0.80353400	0.28228500	-2.46544300
C	-0.75526700	0.37124800	-3.92065800

C	0.46311300	0.33867400	-4.48985500
C	1.57171700	0.14250300	-2.35820800
O	-1.89740300	0.30587700	-1.85682000
O	2.62886000	0.04417900	-1.72284800
N	1.60011300	0.22822600	-3.73704100
C	-2.02634800	0.49244000	-4.70131200
H	-2.68582200	-0.35777100	-4.51312200
H	-2.57821500	1.39188600	-4.41838000
H	-1.82133800	0.53822500	-5.77173200
H	0.61460100	0.39747400	-5.56004600
H	2.50697900	0.20552500	-4.17897900
H	0.35707400	0.08678700	-0.22947400

AT‡‡ (Second transition state)

Atom	X	Y	Z
N	4.95539000	0.34654400	0.00098100
C	5.07849000	-1.01534300	0.00108700
H	6.04443200	-1.49604600	0.00154600
N	3.92341800	-1.62561800	0.00051100
C	2.99802700	-0.60937200	0.00006000
C	1.57308200	-0.65581800	-0.00066200
N	0.79387100	-1.69160000	-0.00103100
H	-0.62336900	-1.70598000	-0.00116600
H	1.31325700	-2.56231100	-0.00065200
N	1.01924700	0.61015600	-0.00098000
C	1.73194400	1.76052800	-0.00069600
H	1.13375400	2.66415400	-0.00095100
N	3.02846300	1.84381500	-0.00002500
C	3.62054600	0.62312800	0.00033000
H	5.70897000	1.01913400	0.00136000

N	-1.79103700	0.43046500	-0.00101300
C	-2.41441700	-0.73970500	-0.00058300
C	-3.84944400	-0.85426500	0.00046900
C	-4.52127800	0.31633400	0.00134100
C	-2.48279000	1.60219000	-0.00017700
O	-1.72254100	-1.83411300	-0.00110200
O	-1.93577700	2.70431600	-0.00055700
N	-3.86290400	1.50768700	0.00121000
C	-4.51753500	-2.19411600	0.00062400
H	-4.23277900	-2.77661700	-0.87806000
H	-4.23327700	-2.77622000	0.87974700
H	-5.60198000	-2.08110500	0.00030100
H	-5.60184400	0.37354500	0.00224100
H	-4.37968600	2.37569900	0.00173500
H	-0.02581500	0.65261100	-0.00116700

AT2

Atom	X	Y	Z
N	4.96514600	0.32162000	-0.00047900
C	5.08302200	-1.04061300	-0.00041500
H	6.04703600	-1.52509300	-0.00048700
N	3.92526500	-1.64605900	-0.00029100
C	3.00370900	-0.62621100	-0.00022400
C	1.57703300	-0.66891700	-0.00007900
N	0.79104600	-1.69735900	0.00003800
H	-0.68688600	-1.70741800	-0.00010400
H	1.31042600	-2.56852700	-0.00000200
N	1.03029600	0.60257100	-0.00007500
C	1.74784900	1.74966100	-0.00021900
H	1.15367000	2.65595000	-0.00020500

N	3.04468000	1.82750600	-0.00036200
C	3.63114400	0.60334000	-0.00035600
H	5.72116100	0.99134900	-0.00058800
N	-1.79475600	0.43624200	0.00051500
C	-2.43470000	-0.72185600	-0.00001700
C	-3.86892700	-0.82204100	-0.00020100
C	-4.52615600	0.35742700	0.00020400
C	-2.47167300	1.61767200	0.00102400
O	-1.75642100	-1.82987500	-0.00036700
O	-1.91040400	2.71180200	0.00135200
N	-3.85290800	1.53976400	0.00078100
C	-4.55303100	-2.15382200	-0.00083000
H	-4.27561800	-2.73902800	-0.88001600
H	-4.27595000	-2.73969900	0.87801600
H	-5.63592000	-2.02739800	-0.00098700
H	-5.60581700	0.42812200	0.00009200
H	-4.35907100	2.41413800	0.00105600
H	-0.01197800	0.65005000	-0.00002700

(ii) Canonical, transition states and rare tautomers coordinates of the GC proton transfer complexes.

Herein the XYZ coordinates of the GC complexes are show. All the structures were calculated without symmetry constrains using PCM and water as solvent, where the theoretical level used was M05-2X/6-311++G(d,p).

GC

Atom	X	Y	Z
N	4.66455600	0.52683600	0.01134200
C	4.97707800	-0.81078400	-0.03308000
H	5.99986200	-1.14828000	-0.03796900
N	3.92227400	-1.57314800	-0.06687100
C	2.85799600	-0.69270300	-0.04365200
C	1.45448200	-0.92227300	-0.06049400
O	0.85818500	-2.00234000	-0.10017700
N	0.73562400	0.26974300	-0.02607900
H	-0.29043500	0.16690800	-0.03700300
C	1.28025100	1.52721100	0.02306700
N	0.41395900	2.54928800	0.06392500
H	-0.59264000	2.41045400	-0.00834800
H	0.79536400	3.47793900	0.05641700
N	2.57870100	1.75373100	0.03944500
C	3.30483500	0.62143800	0.00529400
H	5.31557100	1.29477800	0.04207000
O	-2.43318300	2.13427200	-0.11280500
C	-2.93334500	1.00376200	-0.06980600
N	-4.31336400	0.88646600	-0.03940500
N	-2.19767500	-0.12908600	-0.05105900
C	-2.79726000	-1.32081500	-0.00618700
C	-4.22394100	-1.45607100	0.02700600
C	-4.94129800	-0.31406900	0.00850900
N	-2.02227100	-2.40285700	0.00805800
H	-1.00952400	-2.30075100	-0.02830100

H	-2.43077100	-3.31974700	0.03666300
H	-4.84143100	1.74499200	-0.05468100
H	-6.02008100	-0.29115900	0.02991600
H	-4.69890600	-2.42220000	0.06433800

GC‡ (First transition state)

Atom	X	Y	Z
N	4.52852000	0.45948600	0.14857300
C	4.82871500	-0.83634500	-0.19552200
H	5.84748400	-1.18344300	-0.23954500
N	3.76855900	-1.55017900	-0.44842900
C	2.71003000	-0.67800400	-0.26380300
C	1.30117300	-0.85909500	-0.37124200
O	0.73766000	-1.93807700	-0.66811700
N	0.55335500	0.26366300	-0.10851900
H	-0.83426600	0.08250700	-0.19740200
C	1.13383900	1.43912600	0.24499600
N	0.28647300	2.47073700	0.52721600
H	-0.62133500	2.45785800	0.07947600
H	0.73332400	3.36985000	0.58962600
N	2.43439800	1.66689100	0.37450200
C	3.16780800	0.57548800	0.10964700
H	5.18490500	1.18495500	0.38595800
O	-2.30475300	2.09433100	-0.80234300
C	-2.79423200	1.02089100	-0.47653400
N	-4.15722800	0.87446900	-0.34560700
N	-2.03737100	-0.08798200	-0.21888600
C	-2.58456500	-1.27209200	0.13157000
C	-3.99905900	-1.38246300	0.29827400

C	-4.74205100	-0.28688000	0.04202300
N	-1.78093700	-2.30028100	0.30766900
H	-0.79276900	-2.23555400	0.00620500
H	-2.17395400	-3.19371600	0.55017800
H	-4.71381900	1.69421100	-0.53535200
H	-5.81800500	-0.27369100	0.12268300
H	-4.44928600	-2.31512700	0.59283800

GC1

Atom	X	Y	Z
N	4.59340600	0.45302200	0.00972500
C	4.85039900	-0.88484600	-0.16635800
H	5.85879500	-1.25877100	-0.22739500
N	3.76543700	-1.60217000	-0.24555500
C	2.73283900	-0.68786800	-0.11576700
C	1.31544800	-0.83926500	-0.11799300
O	0.73265900	-1.95096700	-0.24910600
N	0.59602700	0.30951900	0.03384300
H	-1.12171700	0.08238200	-0.08037300
C	1.21990800	1.49906000	0.18798600
N	0.40941500	2.58183300	0.38937400
H	-0.55144900	2.50689400	0.08588000
H	0.85123600	3.47637800	0.26527700
N	2.53263100	1.72584300	0.20033900
C	3.23321800	0.59495100	0.04447600
H	5.27548300	1.18837400	0.09582700
O	-2.45186900	2.16442300	-0.41598200
C	-2.94097300	1.06045200	-0.25745100
N	-4.29829300	0.85719600	-0.21607000
N	-2.17836400	-0.07189300	-0.10589000

C	-2.68645600	-1.31859000	0.07045400
C	-4.10494300	-1.47028400	0.12656900
C	-4.86192200	-0.36486500	-0.02420000
N	-1.85092900	-2.31887300	0.17776500
H	-0.81156200	-2.17697300	0.04060000
H	-2.22367100	-3.24583800	0.30276800
H	-4.87428800	1.67784300	-0.32825700
H	-5.94044100	-0.38830800	-0.00469600
H	-4.54582600	-2.44155200	0.27248500

GC‡‡ (Second transition state)

Atom	X	Y	Z
N	-4.62709200	0.44769000	0.06161500
C	-4.87982300	-0.90224300	0.11356500
H	-5.88692000	-1.28090200	0.16582100
N	-3.79667500	-1.62452200	0.09256800
C	-2.76768900	-0.70031600	0.02223900
C	-1.36192300	-0.82791400	-0.02195700
O	-0.78443800	-1.98088800	-0.00010000
N	-0.63829200	0.30287900	-0.08680200
H	1.15656700	0.17295300	-0.00855600
C	-1.25807500	1.50789600	-0.10981200
N	-0.44626100	2.59350900	-0.22483700
H	0.54318100	2.49308100	-0.04449300
H	-0.86576700	3.48855700	-0.04602200
N	-2.57029100	1.73195800	-0.06170400
C	-3.27009800	0.59581500	0.00209800
H	-5.31154400	1.18603500	0.06519800
O	2.56502200	2.22420700	0.15947100
C	3.00001400	1.08451100	0.09911200

N	4.34256600	0.80235900	0.10468500
N	2.18474600	-0.00917300	0.02109100
C	2.59653400	-1.31466600	-0.05272200
C	4.01792100	-1.53819300	-0.04770600
C	4.83313500	-0.47114700	0.03079600
N	1.68409800	-2.23079000	-0.11861400
H	0.40157600	-2.02702700	-0.06402500
H	2.04575600	-3.17232200	-0.17233100
H	4.96704600	1.59164000	0.16203300
H	5.90864400	-0.55757100	0.04139100
H	4.40720900	-2.54081800	-0.10366200

GC2

Atom	X	Y	Z
N	-4.64842200	0.48634000	0.06722200
C	-4.92460600	-0.85972100	0.11308600
H	-5.93842900	-1.22009200	0.16504700
N	-3.85639200	-1.60282500	0.08712900
C	-2.81184900	-0.69650900	0.01971500
C	-1.41567400	-0.83276700	-0.02826100
O	-0.86480500	-2.02096100	-0.01347900
N	-0.66291400	0.26475500	-0.08829000
H	1.21138900	0.15115300	-0.02146900
C	-1.25870000	1.48513600	-0.10284800
N	-0.42876300	2.55266700	-0.20657400
H	0.56487400	2.44063100	-0.05581500
H	-0.83247400	3.45946200	-0.05356600
N	-2.56776000	1.73012800	-0.05209000
C	-3.29012000	0.61131900	0.00646800

H	-5.32038800	1.23623800	0.07573400
O	2.58223200	2.22468600	0.13189800
C	3.03055900	1.08693400	0.08456600
N	4.37522200	0.82071500	0.10436000
N	2.23063100	-0.01370900	0.00816600
C	2.64661900	-1.32957700	-0.05005500
C	4.07850800	-1.52761300	-0.02754100
C	4.88006700	-0.45242100	0.04795700
N	1.73513000	-2.23603100	-0.11656000
H	0.17209200	-2.01812800	-0.06200700
H	2.12839000	-3.16757400	-0.15714500
H	4.99048900	1.61662800	0.16024800
H	5.95648900	-0.52559100	0.06970600
H	4.48218800	-2.52549500	-0.07016300