Supporting Information for

DFT studies on the oxidation of 5′-dGMP and 5′-dAMP by a Pt^{IV} complex

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Table S1. Cartesian coordinates and total energies for all of the calculated structures

1

E (B3LYP/BS1, Solvent = water) = -2306.691272 au
H (B3LYP/BS1, Solvent = water) = -2306.456888 au
G(B3LYP/BS1, Solvent = water) = -2306.517752 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -2307.198458 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -2306.764307 au

Pt	-0.79434400	-0.00012700	-0.00008300
N	0.75959300	-0.76048500	1.15432000
N	0.75946900	0.76039100	-1.15442500
Cl	-2.42861900	-0.96080000	1.44051400
Cl	-2.42915600	0.96046300	-1.44020900
Cl	-0.72520800	-1.99299400	-1.31913100
C	2.04336900	0.66712500	-0.37711200
C	2.04353300	-0.66685000	0.37725900
C	3.28787800	0.80571500	-1.25969700
H	2.00358100	1.48826100	0.34512000
C	3.28790300	-0.80525600	1.25992800
H	2.00392900	-1.48787600	-0.34507900
C	4.55643600	0.65704400	-0.39803300
C	4.55656100	-0.65622500	0.39848600
H	3.27600800	-1.77706800	1.76481700
H	3.27091600	-0.02966300	2.03725000
H	5.43680500	0.70431700	-1.04790700
H	4.62619800	1.50795900	0.29252600
H	5.43687300	-0.70326400	1.04846200
H	4.62663800	-1.50710500	-0.29207400
H	0.80062800	-0.21040100	2.01857800
H	0.55391100	-1.72731000	1.41967100
H	0.80094200	0.21034200	-2.01860400
H	0.55357300	1.72730700	-1.41937400
H	3.27120500	0.02996600	-2.03689400
H	3.27588900	1.77741000	-1.76477700
Cl	-0.72677100	1.99323600	1.31885400

2

E (B3LYP/BS1, Solvent = water) = -1846.259234 au
H (B3LYP/BS1, Solvent = water) = -1846.02765 au
G(B3LYP/BS1, Solvent = water) = -1846.084215 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -1846.730132 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -1846.321389 au

Pt	0.84474600	0.01000400	-0.20863400
N	-0.71714600	1.38240300	-0.01399300
N	-0.72950700	-1.38506400	-0.14833700
Cl	2.48566700	1.73275300	-0.24016100
Cl	2.46710500	-1.66394500	-0.56683600
C	-2.00231900	-0.68705600	0.24538100
C	-1.99746300	0.69929000	-0.40660900
C	-3.25536200	-1.48392800	-0.13475200

H	-1.95018400	-0.57485700	1.33288300
C	-3.24274800	1.50765000	-0.02391100
H	-1.94882900	0.59112200	-1.49571500
C	-4.51751300	-0.68177300	0.23467100
C	-4.51051900	0.71733700	-0.39866200
H	-3.22288400	2.47394700	-0.53838000
H	-3.23038100	1.70768000	1.05580200
H	-5.40050400	-1.24083100	-0.09255800
H	-4.58512800	-0.59289900	1.32694800
H	-5.38995700	1.28379400	-0.07462000
H	-4.57462200	0.62978400	-1.49131600
H	-0.74722300	1.72237800	0.95320300
H	-0.53047800	2.19656600	-0.60763500
H	-0.80401300	-1.80530400	-1.08101700
H	-0.50017500	-2.14304300	0.50087800
H	-3.24442600	-1.68806600	-1.21381000
H	-3.24569800	-2.44872000	0.38279300
Cl	0.97466600	-0.14541900	2.06320600

2_G

E (B3LYP/BS1, Solvent = water) = -3377.169911 au

H (B3LYP/BS1, Solvent = water) = -3376.648487 au

G(B3LYP/BS1, Solvent = water) = -3376.752187 au

E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -3378.104657 au

E(M06/BS2//B3LYP/BS1, Solvent = water) = -3377.010362 au

Pt	1.90388000	0.15829700	-0.93735400
N	0.11629500	0.93970000	-0.19221700
P	-2.18042200	-2.94798100	0.24932800
O	-2.08300500	-2.72332600	1.72813500
O	-3.53959600	-2.25561100	-0.37725800
C	-4.65576700	-1.92328500	0.45012300
H	-4.40091500	-2.06602200	1.50393900
H	-5.50137000	-2.57532000	0.19708000
C	-5.05369000	-0.47143600	0.22073700
H	-5.95975900	-0.26325000	0.80184600
O	-3.99981900	0.39700900	0.69496200
C	-3.51258900	1.20398900	-0.36388000
H	-3.91117000	2.21781400	-0.27333000
N	-2.05998000	1.35886500	-0.20328100
C	-1.07054700	0.52623300	-0.61587800
C	-0.10409800	2.10269000	0.55932800
C	0.72632700	2.92800800	1.38472500
N	-0.00724200	3.98651300	1.94450100
H	0.54591200	4.60993800	2.52498600
C	-1.36318300	4.18626200	1.82561100
N	-1.89553900	5.27292500	2.41597700
H	-1.38697500	5.80382900	3.10897800
H	-2.90428100	5.33454200	2.43958400
N	-2.14004100	3.36280400	1.13769400
C	-1.47198700	2.36434700	0.54485600
C	-5.30010500	-0.07525600	-1.24697900

H	-5.56970600	-0.93929700	-1.86568100
C	-3.95626000	0.53504700	-1.66555400
H	-3.27338100	-0.26638000	-1.95403600
H	-4.04498200	1.24553000	-2.49123900
O	-6.34719200	0.89354900	-1.23754000
H	-6.49819600	1.17682900	-2.15420300
O	-1.08286000	-2.49256600	-0.70503900
N	1.48245100	-1.78290100	-0.30380900
N	2.76454100	0.31384000	0.94132300
Cl	0.89331600	-0.23641900	-3.07283700
Cl	2.53776700	2.37079400	-1.60854500
Cl	3.96187800	-0.70912400	-1.73831800
C	2.19114100	-0.76081600	1.81162000
C	2.18004300	-2.05581100	0.99691800
C	2.95024300	-0.93275300	3.13071600
H	1.15864800	-0.45930900	2.01851600
C	1.54389900	-3.20770900	1.78408100
H	3.21434100	-2.31048000	0.73958200
C	2.33185700	-2.09135600	3.93622900
C	2.28703600	-3.39261200	3.12082700
H	1.59115600	-4.12709800	1.18949900
H	0.48359700	-2.98872200	1.96287000
H	2.91110800	-2.23907500	4.85425200
H	1.31432400	-1.81478000	4.24367100
H	1.79393800	-4.18193500	3.69903800
H	3.31132100	-3.73749500	2.92417900
H	0.44238300	-1.97627300	-0.27982600
H	1.85050900	-2.40200200	-1.03072000
H	3.77612500	0.20205100	0.82199700
H	2.57574900	1.27376200	1.30827400
H	4.00581200	-1.14800200	2.91703600
O	-2.44074900	-4.55487500	0.01041100
O	1.92673400	2.81890800	1.67097400
H	-1.23297800	-0.38482900	-1.17347400
H	2.91498200	0.00108200	3.70186700
H	-2.30828300	-4.78198100	-0.92547300

5′-dGMP

E (B3LYP/BS1, Solvent = water) = -1530.819287 au

H (B3LYP/BS1, Solvent = water) = -1530.531768 au

G(B3LYP/BS1, Solvent = water) = -1530.605881 au

E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -1531.307065 au

E(M06/BS2//B3LYP/BS1, Solvent = water) = -1530.596042 au

P	-3.50201800	-1.46975100	0.22804100
O	-2.40318300	-2.15974300	-0.53816900
O	-3.55934200	0.12305100	-0.25289100
C	-3.35919000	1.18667400	0.67041700
H	-3.48316800	0.82681100	1.69612300
H	-4.12008300	1.95117500	0.47067700
C	-1.99980100	1.85298600	0.51614800
H	-2.00700100	2.77143000	1.12631500
O	-0.95769400	0.97786300	0.97150700

C	0.27919100	1.38353000	0.39888600
H	0.89279000	1.90589700	1.14008900
N	1.03133100	0.18071600	0.04850200
C	0.54954900	-1.02612500	-0.43884000
C	2.67639500	-1.22849600	-0.35155000
C	4.04146100	-1.66120300	-0.40596700
N	4.90672400	-0.62478500	0.04733300
H	5.89402500	-0.85604300	0.00705500
C	4.52265100	0.62092800	0.48502700
N	5.51687000	1.49703100	0.82229200
H	6.39666300	1.12233100	1.15378700
H	5.19656800	2.31106000	1.33164800
N	3.26436400	1.01116800	0.53451800
C	2.39890100	0.05918000	0.10758700
C	-1.59004000	2.22907400	-0.91112100
H	-1.88866900	1.42204200	-1.58967700
C	-0.05689300	2.30946600	-0.79641300
H	0.46837500	2.00810000	-1.70582400
H	0.22285700	3.34072200	-0.55966900
O	-2.22560000	3.44866200	-1.26596300
H	-2.12253000	3.57194700	-2.22244000
O	-4.90920900	-1.99495900	-0.46831100
H	-5.66909000	-1.63453200	0.01829000
N	1.50804000	-1.89234300	-0.68390300
O	-3.59986400	-1.53826400	1.72966600
O	4.51729100	-2.73567000	-0.77192600
H	-0.51432000	-1.22078100	-0.54452300

1TS_G (Imaginary Frequency = -287.07 i)
E (B3LYP/BS1, Solvent = water) = -3377.140561 au
H (B3LYP/BS1, Solvent = water) = -3376.620622 au
G(B3LYP/BS1, Solvent = water) = -3376.721846 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -3378.067066 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -3376.979738 au

Pt	1.68396700	0.43536500	-0.97749900
N	-0.00790800	0.58670700	0.26865900
P	-1.68926100	-2.68203100	0.46278500
O	-1.51874300	-1.24378700	1.03907900
O	-3.11989200	-2.79674900	-0.29295700
C	-4.37466500	-2.58249800	0.39626500
H	-4.23670200	-2.69179300	1.47536600
H	-5.04682900	-3.37410800	0.05261800
C	-5.00126500	-1.22341000	0.09771300
H	-5.99576900	-1.23004200	0.56082100
O	-4.24390400	-0.15824700	0.69056300
C	-3.64531300	0.67041100	-0.30875100
H	-4.11733400	1.65507200	-0.27037400
N	-2.24296100	0.90831000	-0.00502600
C	-1.19103900	-0.00376400	-0.14679400
C	-0.39257500	1.77405600	0.90935700
C	0.31529500	2.63141200	1.78815200
N	-0.51262800	3.65698000	2.29360200
H	-0.04337400	4.31714400	2.90533200

C	-1.85291800	3.78928000	2.04290700
N	-2.49415600	4.86227000	2.55603700
H	-2.08366500	5.40621500	3.30226000
H	-3.50381800	4.85184800	2.50643000
N	-2.52681900	2.92182900	1.29579400
C	-1.76541400	1.95717000	0.76444400
C	-5.14887300	-0.85922600	-1.38875100
H	-5.20056300	-1.74766700	-2.03017200
C	-3.89093700	-0.02586700	-1.65667200
H	-3.06712700	-0.69220900	-1.92106800
H	-4.02303500	0.69238400	-2.46987500
O	-6.34092300	-0.08334400	-1.49542700
H	-6.42344200	0.20621900	-2.41863900
O	-0.63139200	-3.13799200	-0.49919000
N	1.79351100	-1.62258500	-0.63507500
N	2.77415800	0.54136000	0.78164600
Cl	0.42069000	0.10644600	-2.99332300
Cl	1.73630300	2.79769900	-1.34125200
Cl	3.77457200	0.17223100	-2.20266900
C	2.62609800	-0.75993100	1.50494200
C	2.76756300	-1.88655300	0.47953900
C	3.62705600	-0.91761000	2.65410700
H	1.60301400	-0.76143500	1.89452200
C	2.57728500	-3.26360700	1.12459900
H	3.76243500	-1.82293500	0.02608700
C	3.45523300	-2.29895700	3.31323000
C	3.57152100	-3.43735800	2.28816800
H	2.72187000	-4.04702100	0.37240900
H	1.54743900	-3.35442400	1.49301700
H	4.20901000	-2.41952400	4.09915200
H	2.47426500	-2.34601000	3.80521100
H	3.39210100	-4.40286600	2.77404500
H	4.59477300	-3.46927400	1.88957300
H	0.86499300	-2.05691000	-0.45567100
H	2.13426200	-2.04337900	-1.50318400
H	3.75015800	0.72421000	0.53137200
H	2.40811600	1.34033800	1.35044000
H	4.64896900	-0.81675200	2.26302700
O	-1.81915600	-3.56327000	1.81423900
O	1.51065600	2.59819100	2.14037200
H	-1.15973100	-0.59192600	-1.05177800
H	3.47734800	-0.11612500	3.38580100
H	-1.77232300	-4.51920900	1.63192900

3_G

E (B3LYP/BS1, Solvent = water) = -3377.145187 au

H (B3LYP/BS1, Solvent = water) = -3376.623633 au

G(B3LYP/BS1, Solvent = water) = -3376.725831 au

E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -3378.06697 au

E(M06/BS2//B3LYP/BS1, Solvent = water) = -3376.983202 au

Pt	1.58488900	0.47076700	-0.97559500

N	0.01173700	0.43372600	0.53626800
P	-1.70122400	-2.72642800	0.62808400
O	-1.56473500	-1.20662200	1.11408300
O	-3.07328300	-2.85769000	-0.19592000
C	-4.38849600	-2.66855400	0.39832100
H	-4.32318100	-2.78963200	1.48209900
H	-5.01140700	-3.46920300	-0.00780400
C	-5.00275200	-1.31263800	0.06606100
H	-6.01917700	-1.32785000	0.47918000
O	-4.27686700	-0.25107200	0.69766400
C	-3.63426600	0.59295200	-0.27094200
H	-4.10916800	1.57646100	-0.23994600
N	-2.24958700	0.81649700	0.08715400
C	-1.22133200	-0.19863000	0.09405000
C	-0.41036700	1.64163700	1.07125400
C	0.30017100	2.55999300	1.88881500
N	-0.51849700	3.63198200	2.31041400
H	-0.04899600	4.33094700	2.87701500
C	-1.84186300	3.78173900	1.99530700
N	-2.47950000	4.88194900	2.43346900
H	-2.07478000	5.49335500	3.12845900
H	-3.48017800	4.92449700	2.29900500
N	-2.51389700	2.89416600	1.26149800
C	-1.77482900	1.86984400	0.82808900
C	-5.08337100	-0.94685400	-1.42592600
H	-5.09314500	-1.83463300	-2.07050800
C	-3.82827600	-0.09348100	-1.63415000
H	-2.98134700	-0.73783800	-1.88143900
H	-3.94327300	0.63400200	-2.44177400
O	-6.28166500	-0.18972900	-1.58444500
H	-6.32533400	0.10471100	-2.50875800
O	-0.56631800	-3.21803000	-0.20370900
N	1.83931100	-1.58089500	-0.68981400
N	2.82449200	0.60539700	0.68658300
Cl	0.17922300	0.10198200	-2.89223400
Cl	1.47372500	2.84356300	-1.28261300
Cl	3.67722100	0.33637300	-2.40564100
C	2.85076600	-0.72376500	1.37148700
C	2.94961400	-1.80815000	0.29674600
C	3.98107500	-0.84668700	2.39809900
H	1.87969500	-0.80587500	1.86950300
C	2.92536200	-3.21238900	0.90906300
H	3.87817500	-1.66219200	-0.26507600
C	3.97614400	-2.25497700	3.02170100
C	4.05241700	-3.35194000	1.94829900
H	3.03438300	-3.96290500	0.11795800
H	1.95148300	-3.38313200	1.38596100
H	4.81810700	-2.34587500	3.71696900
H	3.06013900	-2.38474400	3.61403300
H	3.99364400	-4.34177200	2.41451400
H	5.02423100	-3.29954400	1.43865100
H	0.96802300	-2.05405300	-0.39474000

H	2.09064200	-1.98147000	-1.59669500
H	3.75354800	0.87562000	0.35252200
H	2.45598600	1.34492600	1.32059700
H	4.94497700	-0.66379700	1.90333500
O	-1.92396700	-3.39898100	2.06680500
O	1.49271100	2.53858700	2.24148600
H	-1.11737300	-0.68642300	-0.86977900
H	3.86176000	-0.07921500	3.17100200
H	-1.84867500	-4.37040300	2.04480200

TS_G (Imaginary Frequency = 1425.51i)
E (B3LYP/BS1, Solvent = water) = -3606.432028 au
H (B3LYP/BS1, Solvent = water) = -3605.833141 au
G(B3LYP/BS1, Solvent = water) = -3605.959443 au

P	-3.63559400	-2.38455400	0.50169400
O	-3.13515800	-1.07643400	1.32856700
O	-4.74762000	-1.91890900	-0.53216500
C	-6.03316700	-1.33130900	-0.17224800
H	-6.26013800	-1.55063200	0.87265900
H	-6.76939600	-1.82639300	-0.80880700
C	-6.04885100	0.16999700	-0.41150300
H	-7.07152500	0.51503800	-0.22233200
O	-5.17425000	0.82975100	0.52265400
C	-4.10269900	1.46845100	-0.14998000
H	-4.21942200	2.55382100	-0.09050200
N	-2.85851600	1.18628300	0.57188200
C	-2.24424800	-0.11300100	0.83905100
C	-0.92898700	1.39752000	1.65086800
C	0.19976400	2.15645500	2.19527900
N	0.01262600	3.53066800	2.01100800
H	0.76323700	4.11634200	2.36719300
C	-1.06156400	4.12199200	1.36824900
N	-1.06687300	5.44915600	1.27719200
H	-0.33141400	6.03497900	1.64798100
H	-1.84178900	5.89414800	0.80309400
N	-2.08084500	3.43823600	0.84091500
C	-1.99638000	2.12124100	1.00298200
C	-5.61121300	0.63821100	-1.81039700
H	-5.75615100	-0.13868300	-2.57068200
C	-4.12899100	0.97369200	-1.60506500
H	-3.51935900	0.07648600	-1.72725500
H	-3.76359100	1.73186300	-2.30180700
O	-6.38630500	1.79602300	-2.10252700
H	-6.10543000	2.13204900	-2.96937800
O	-2.54240800	-3.13305800	-0.17046700
Pt	3.10550400	0.52152000	-0.50596200
N	-1.13415000	0.10505500	1.64801100
N	2.06911700	-1.26123200	-0.58208200
N	3.33404300	0.01925500	1.47402000
Cl	2.76890800	0.94649600	-2.85095900
Cl	4.38496500	2.53035400	-0.18207200
Cl	4.02851600	-3.36074400	-2.15931600
C	3.04916700	-1.44263800	1.65067500
C	2.85387400	-1.85217600	3.11307200
C	1.80883000	-1.74986300	0.80952800

H	3.90813100	-1.97363300	1.22465200
C	2.47547900	-3.34209500	3.19907000
H	2.05553600	-1.23891200	3.55349000
H	3.76897600	-1.65175800	3.68278500
C	1.42733200	-3.23274300	0.87954700
C	1.23826000	-3.66275900	2.34580200
H	2.29531000	-3.61278000	4.24568700
H	3.32401300	-3.95066500	2.85688900
H	0.50493500	-3.39967000	0.31064600
H	2.21652900	-3.83158200	0.40708500
H	1.01942900	-4.73601900	2.38703400
H	0.36360700	-3.14597400	2.76494900
H	1.17167300	-1.14680900	-1.06659700
H	2.64137200	-1.95080800	-1.11043000
H	4.26937900	0.25542900	1.81229000
H	2.66654800	0.57745900	2.02263100
H	0.97693900	-1.14896900	1.19393100
O	-4.47724000	-3.12927300	1.63255900
O	1.19525300	1.71504200	2.74965300
H	-1.56829800	-0.45031100	-0.31770200
H	-3.94948500	-3.43362800	2.39338600
O	-0.83027200	-0.64056200	-1.33364500
H	-0.71831400	0.21204400	-1.88372300
H	-1.18535600	-1.37944800	-1.94045400
O	-0.37204700	1.49514900	-2.76310400
O	-1.71536600	-2.66853900	-2.72229900
H	-2.11439700	-3.08145100	-1.92192300
H	-2.46988200	-2.43471600	-3.28816300
H	0.60774100	1.43706500	-2.84804200
H	-0.52956000	2.31075600	-2.25912400

2TS_G (Imaginary Frequency = 84.76i)
E (B3LYP/BS1, Solvent = water) = -3377.141292 au
H (B3LYP/BS1, Solvent = water) = -3376.620150 au
G(B3LYP/BS1, Solvent = water) = -3376.724585 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -3378.058807 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -3376.974511 au

Pt	1.59454100	0.41594700	-1.01603000
N	-0.13481600	0.46415000	0.80809400
P	-1.72464500	-2.75951800	0.69519600
O	-1.66915300	-1.23605100	1.23794700
O	-3.04533300	-2.88149300	-0.20327100
C	-4.39833500	-2.77065600	0.32693900
H	-4.38209200	-2.92275000	1.40826900
H	-4.96197300	-3.58408100	-0.13547700
C	-5.05310300	-1.43330700	0.00206200
H	-6.08534000	-1.50003900	0.36610200
O	-4.40358600	-0.36115800	0.70363100
C	-3.76162100	0.53673700	-0.20046700
H	-4.26233900	1.50695800	-0.15816600
N	-2.39746500	0.78581800	0.24759900
C	-1.33090200	-0.21381500	0.29348600
C	-0.55426000	1.66603400	1.16867200
C	0.18568100	2.71004700	1.85212900

N	-0.62171200	3.83205800	2.11241500
H	-0.15201100	4.59935500	2.58488400
C	-1.94180300	3.95602300	1.75454000
N	-2.57344400	5.08696600	2.05110100
H	-2.13433500	5.85994300	2.53246000
H	-3.54740300	5.17354700	1.79130400
N	-2.63632100	2.99136400	1.12638900
C	-1.94184300	1.90214400	0.85040500
C	-5.07817300	-1.01835100	-1.47889400
H	-5.01466800	-1.88125300	-2.15302600
C	-3.85420000	-0.10288100	-1.59695900
H	-2.96593500	-0.69657500	-1.82538000
H	-3.96454100	0.65012400	-2.38114200
O	-6.29969700	-0.30930400	-1.66867400
H	-6.32026100	0.00773300	-2.58634200
O	-0.52888500	-3.18328300	-0.07950400
N	1.95380600	-1.59385500	-0.62358400
N	2.85494600	0.69846000	0.59903500
Cl	0.16639700	-0.15251200	-2.86524100
Cl	1.27862900	2.77121200	-1.37394300
Cl	4.27036400	0.21041900	-2.36568100
C	2.91854900	-0.57230700	1.38515200
C	3.05448700	-1.72665600	0.39147200
C	4.04686300	-0.59194200	2.42126300
H	1.94991400	-0.64758100	1.88979000
C	3.06083800	-3.08321600	1.10264200
H	3.98438700	-1.59198000	-0.17030300
C	4.07044200	-1.94911000	3.14818200
C	4.17997400	-3.12080200	2.16028600
H	3.19707700	-3.88586300	0.36857800
H	2.08682600	-3.24615100	1.58344800
H	4.90854400	-1.97010000	3.85385400
H	3.15296900	-2.05612700	3.74316000
H	4.13968900	-4.07464600	2.69831100
H	5.15529700	-3.08357200	1.65577200
H	1.09688300	-2.08147200	-0.31976700
H	2.24022500	-2.03581500	-1.49947600
H	3.77083800	0.93622100	0.20558500
H	2.52083300	1.47259400	1.18967700
H	5.00816000	-0.42464200	1.91564400
O	-2.00907800	-3.45547100	2.10682700
O	1.36569100	2.69829800	2.18779500
H	-1.14223100	-0.63305900	-0.69254900
H	3.90868300	0.22760400	3.13589300
H	-1.86356000	-4.41915600	2.09320500

4_G

E (B3LYP/BS1, Solvent = water) = -1530.470162 au
H (B3LYP/BS1, Solvent = water) = -1530.180294 au
G(B3LYP/BS1, Solvent = water) = -1530.248530 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -1530.926378 au

E(M06/BS2//B3LYP/BS1, Solvent = water) = -1530.222466 au

P	2.36397600	-1.86569700	-0.20702300
O	0.77993900	-1.55961400	-0.50826000
O	2.99493700	-0.50064500	0.33414000
C	3.51304600	0.49594500	-0.59105800
H	3.60403500	0.05793300	-1.58744300
H	4.50834200	0.76421000	-0.23001100
C	2.60334400	1.71589200	-0.62968300
H	3.00669400	2.40626000	-1.37845900
O	1.28304000	1.31647500	-1.04711600
C	0.34113300	1.52809800	-0.00839500
H	-0.33542100	2.34218100	-0.28122900
N	-0.51958600	0.34479200	0.10709200
C	-0.08687900	-1.03233100	0.45481700
C	-2.27431500	-1.04560100	0.23909200
C	-3.73102000	-1.35287600	0.17927100
N	-4.47560900	-0.19934200	-0.10053400
H	-5.48201900	-0.33933700	-0.14614200
C	-3.95695900	1.06033300	-0.31274900
N	-4.79545800	2.04445700	-0.57797700
H	-5.79928700	1.92394100	-0.63457900
H	-4.41520300	2.97151500	-0.72924100
N	-2.63990500	1.35904600	-0.26861600
C	-1.84620700	0.34824700	-0.00775500
C	2.41837700	2.47189400	0.69703400
H	3.27524100	2.34445300	1.36947900
C	1.13866200	1.84851900	1.26631200
H	1.38203400	0.94002200	1.82205100
H	0.59420200	2.52362700	1.93041100
O	2.23538700	3.84042800	0.34978400
H	2.08344200	4.33882100	1.16943900
O	2.38254500	-2.65497500	1.18721400
H	2.09589000	-3.58325800	1.10563900
N	-1.30742700	-1.84179300	0.48043800
O	2.95461700	-2.48456700	-1.40960800
O	-4.23961200	-2.43679300	0.34774800
H	0.34638500	-1.04621800	1.46007400

8

E (B3LYP/BS1, Solvent = water) = -1386.293881 au

H (B3LYP/BS1, Solvent = water) = -1386.066015 au

G(B3LYP/BS1, Solvent = water) = -1386.119860 au

E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -1386.721569 au

E(M06/BS2//B3LYP/BS1, Solvent = water) = -1386.353332 au

Pt	0.93580500	-0.00003300	-0.00010900
N	-0.61034300	1.37216400	0.06430400
N	-0.61035400	-1.37231000	-0.06441500
Cl	2.55992500	1.74864900	0.04641800
Cl	2.56029700	-1.74839500	-0.04602100
C	-1.89612800	-0.69812200	0.31619300
C	-1.89608900	0.69800400	-0.31606000
C	-3.14506300	-1.48943100	-0.08355700
H	-1.86076600	-0.59109700	1.40635500
C	-3.14496800	1.48941200	0.08366400

H	-1.86089200	0.59073300	-1.40621900
C	-4.41545800	-0.70804300	0.29890200
C	-4.41541000	0.70811200	-0.29874600
H	-3.13305100	2.47013800	-0.40527200
H	-3.12900200	1.66631800	1.16847100
H	-5.29794300	-1.26144000	-0.04079200
H	-4.48458900	-0.64430400	1.39344300
H	-5.29786500	1.26155900	0.04095200
H	-4.48454000	0.64440200	-1.39329000
H	-0.67493300	1.75213200	1.01285200
H	-0.42596900	2.16959300	-0.54813000
H	-0.67502400	-1.75212800	-1.01304700
H	-0.42604000	-2.16979500	0.54788800
H	-3.12915400	-1.66626200	-1.16837900
H	-3.13319400	-2.47017200	0.40533300

Cl^-
E (B3LYP/BS1, Solvent = water) = -460.365922 au
H (B3LYP/BS1, Solvent = water) = -460.363561 au
G(B3LYP/BS1, Solvent = water) = -460.380944 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -460.414794 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -460.373427 au

5_G
E (B3LYP/BS1, Solvent = water) = -1759.755351 au
H (B3LYP/BS1, Solvent = water) = -1759.382340 au
G(B3LYP/BS1, Solvent = water) = -1759.469881 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -1760.346441 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -1759.529586 au

P	2.28404400	-1.03234900	-1.17350800
O	0.69920500	-0.69757300	-1.34195100
O	2.92413300	0.16583200	-0.33382700
C	3.22144600	1.48667200	-0.87114300
H	3.21161100	1.44772600	-1.96191100
H	4.23203800	1.72580500	-0.53277900
C	2.23335200	2.52977300	-0.37430500
H	2.53168600	3.48892700	-0.81246200
O	0.91055600	2.21178300	-0.84694800
C	0.03702900	1.93944000	0.23421500
H	-0.71280700	2.73071300	0.31500300
N	-0.72572300	0.72216700	-0.06806000
C	-0.16110100	-0.63758000	-0.23284400
C	-2.35339400	-0.78713600	-0.36271400
C	-3.78070200	-1.20475700	-0.43443200
N	-4.63149600	-0.10853800	-0.24885800
H	-5.62479700	-0.32531300	-0.27541800
C	-4.22923000	1.19338200	-0.02921800
N	-5.16278400	2.11559800	0.11686100
H	-6.15491100	1.91959200	0.06944400
H	-4.87170400	3.07171100	0.28352500
N	-2.94177000	1.58941400	0.04798100
C	-2.05290700	0.63654300	-0.11543600

C	2.11582200	2.69798700	1.15056300
H	3.02208100	2.36962900	1.67369800
C	0.90199600	1.82846400	1.50155000
H	1.20935400	0.79660500	1.68840200
H	0.36981600	2.18761000	2.38561900
O	1.86726000	4.08228200	1.37470800
H	1.75863700	4.21544400	2.33049100
O	2.59575700	-2.34259600	-0.55002000
N	-1.30748500	-1.51307900	-0.46789300
O	2.66142600	-0.83489800	-2.71248500
O	-4.18502800	-2.32964700	-0.61995700
H	0.30739900	-0.97500800	0.71863400
H	3.19938600	-2.65421400	1.14327000
H	3.46805200	-1.31891900	-2.96763800
O	3.29726100	-2.74610700	2.11633800
H	3.20544800	-3.69934000	2.27618900
H	1.63574900	-2.08836400	2.39731700
O	0.69870400	-1.77757700	2.40143200
H	0.18247200	-2.57307300	2.13527400
O	-0.81217100	-3.88357500	1.27325100
H	-1.65862800	-3.93917700	1.74637300
H	-1.03743100	-3.41415500	0.44764100

3TS_G (Imaginary Frequency = 1318.95i)
E (B3LYP/BS1, Solvent = water) = -1759.741526 au
H (B3LYP/BS1, Solvent = water) = -1759.374850 au
G(B3LYP/BS1, Solvent = water) = -1759.461017 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -1760.329555 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -1759.511381 au

P	2.56724500	-1.29557600	-0.74485700
O	1.10759100	-0.88313700	-1.31358700
O	3.14075400	-0.04220600	0.06454100
C	3.55863000	1.20704300	-0.55706500
H	3.70704100	1.05330000	-1.62770800
H	4.51743600	1.46058300	-0.09912000
C	2.54924200	2.31993100	-0.32162200
H	2.95836700	3.22751300	-0.77976500
O	1.30660500	2.00743100	-0.97835600
C	0.26432800	1.83791500	-0.03237900
H	-0.44781900	2.66355400	-0.11338300
N	-0.50902400	0.64348700	-0.38789600
C	-0.03817100	-0.73493600	-0.51959000
C	-2.17969000	-0.76247500	-0.80142000
C	-3.59512600	-1.12952600	-0.93301000
N	-4.41834200	-0.00979700	-0.71153300
H	-5.41476300	-0.19380300	-0.78515100
C	-3.98731400	1.26195300	-0.38921600
N	-4.91475100	2.20038300	-0.20879000
H	-5.90621600	2.02583100	-0.29743300
H	-4.61133900	3.13465700	0.03188400
N	-2.70168600	1.60051400	-0.25034900
C	-1.84899300	0.60306000	-0.46820600
C	2.19368000	2.61665400	1.14484300
H	2.99709000	2.32385900	1.83177700
C	0.92199200	1.78902000	1.35706000

H	1.17525200	0.76475700	1.63681000
H	0.27026600	2.20444700	2.12981000
O	1.94350400	4.01750900	1.21569600
H	1.67133000	4.22586300	2.12430800
O	2.63032500	-2.52308700	0.08472000
N	-1.11604100	-1.51264900	-0.93027600
O	3.28728600	-1.33843000	-2.17243900
O	-4.05725300	-2.22312400	-1.19604300
H	0.09843600	-1.16972400	0.77085000
H	1.80702600	-3.63145300	1.24696800
H	4.13005600	-1.82736600	-2.15438200
O	1.15992300	-3.91067100	1.93298500
H	0.53174600	-4.48205700	1.46056100
H	0.50110700	-2.43517200	2.05282300
O	0.20440500	-1.46502600	2.00314200
H	-0.70524500	-1.39055500	2.43162800
O	-2.20117400	-1.24716400	3.13306400
H	-2.54145800	-0.34623900	3.00204300
H	-2.83528300	-1.81650400	2.66608200

6_G

E (B3LYP/BS1, Solvent = water) = -1759.803925 au
H (B3LYP/BS1, Solvent = water) = -1759.432755 au
G(B3LYP/BS1, Solvent = water) = -1759.516943 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -1760.390777 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -1759.572850 au

P	-1.88033100	1.98803700	0.10604300
O	-0.87828900	1.17297700	-0.89699400
O	-2.97279200	0.94456700	0.60596100
C	-3.91556100	0.28164800	-0.29184500
H	-3.95485200	0.81675900	-1.24248500
H	-4.88889800	0.35341200	0.19745000
C	-3.53941000	-1.17395100	-0.52141500
H	-4.30911800	-1.60482700	-1.17094500
O	-2.27661700	-1.26053300	-1.21293200
C	-1.29186000	-1.84651400	-0.38878700
H	-0.99422600	-2.81789100	-0.79231000
N	-0.06076600	-1.03032100	-0.42371400
C	0.11513900	0.33430100	-0.53057900
C	2.07196500	-0.46554600	-0.20503500
C	3.47038500	-0.70289300	-0.04387200
N	3.72472800	-2.07847200	0.12902700
H	4.70721000	-2.31384700	0.23215000
C	2.78223900	-3.08329500	0.13070200
N	3.22480000	-4.35412100	0.26650100
H	4.13856600	-4.54272700	0.65525900
H	2.51749200	-5.05864800	0.42738900
N	1.48866100	-2.85427100	-0.03794400
C	1.20261800	-1.55210500	-0.21060700
C	-3.39499000	-2.04559500	0.73672300
H	-3.99539100	-1.66617400	1.57252000
C	-1.89149800	-1.97136700	1.02249000
H	-1.66045900	-1.08352300	1.61676500
H	-1.51456600	-2.84969900	1.55185500

O	-3.80815800	-3.35535000	0.35981200
H	-3.68061700	-3.94000800	1.12472300
O	-1.22162500	2.66592500	1.25033300
N	1.36440700	0.70844700	-0.41150700
O	-2.51974600	2.88760400	-1.04697100
O	4.42110300	0.09155800	-0.04273500
H	1.91024500	2.12580900	0.16972500
H	-0.17754900	4.13068600	0.98721200
H	-3.09814300	3.59656500	-0.70985700
O	0.56218100	4.73778500	0.74489500
H	0.31138500	5.10987300	-0.11738900
H	1.71592200	3.74419400	0.59282700
O	2.35772900	2.93274000	0.62692500
H	3.26969100	3.06221100	0.14879200
O	4.60221300	2.78742300	-0.54432100
H	5.32680500	3.09311100	0.02711100
H	4.60651300	1.79964700	-0.45640500

7_G

E (B3LYP/BS1, Solvent = water) = -1530.058919 au

H (B3LYP/BS1, Solvent = water) = -1529.782039 au

G(B3LYP/BS1, Solvent = water) = -1529.850572 au

E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -1530.523821 au

E(M06/BS2//B3LYP/BS1, Solvent = water) = -1529.826808 au

P	2.33353900	-1.83929100	0.20681600
O	1.12756200	-1.52605900	-0.85868000
O	2.86952300	-0.41199200	0.68574100
C	3.55364300	0.46527700	-0.25154800
H	3.80731100	-0.07980500	-1.16443000
H	4.47963700	0.77610500	0.23738700
C	2.69241900	1.67554900	-0.58297900
H	3.27168000	2.31623100	-1.25672600
O	1.49944400	1.26590200	-1.27857100
C	0.35343000	1.46005100	-0.47297300
H	-0.28855600	2.22128100	-0.92497100
N	-0.46583100	0.23603900	-0.45393300
C	-0.12603500	-1.10936300	-0.53314200
C	-2.22046600	-1.08910300	-0.20705100
C	-3.60248400	-1.40041900	0.00916600
N	-4.35695500	-0.20237800	0.15740100
H	-5.34393200	-0.35160900	0.34001900
C	-3.86636100	1.08071200	0.10514300
N	-4.74699100	2.09741800	0.32509700
H	-5.72921100	1.94906100	0.13205900
H	-4.40240400	3.01756000	0.08295700
N	-2.58931300	1.35509300	-0.09261000
C	-1.82993700	0.24638400	-0.23802600
C	2.21562800	2.50151500	0.62278100
H	2.90159900	2.41964300	1.47505900
C	0.84228500	1.89056200	0.92143800
H	0.94563000	1.02040300	1.57379300
H	0.15631000	2.59894500	1.39267400
O	2.12159500	3.84920600	0.16893700
H	1.76790100	4.38425900	0.89803400
O	1.62762600	-2.26658300	1.57727200

H	1.37510000	-3.20755300	1.59478500
N	-1.13398000	-1.92443700	-0.40437200
O	3.29761600	-2.76065800	-0.42926000
O	-4.16403900	-2.49160300	0.07946100

$(H_2O)_3$
E (B3LYP/BS1, Solvent = water) = -229.274579 au
H (B3LYP/BS1, Solvent = water) = -229.193259 au
G(B3LYP/BS1, Solvent = water) = -229.229146 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -229.413950 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -229.296081 au

O	-0.83962600	-1.35171100	-0.10698100
H	-1.08382500	-0.39413900	-0.14156600
O	-0.74036000	1.40830600	-0.10770100
H	-0.98775500	1.71192000	0.78065000
H	0.20796700	1.14318400	-0.01677600
O	1.58893100	-0.05604200	0.12454900
H	0.88581300	-0.74846800	0.06301100
H	2.02376100	-0.08133800	-0.74314400
H	-1.11751700	-1.63558400	0.77888200

$(H_2O)_2(H_3O)^+$
E (B3LYP/BS1, Solvent = water) = -229.705651 au
H (B3LYP/BS1, Solvent = water) = -229.613561 au
G(B3LYP/BS1, Solvent = water) = -229.652156 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -229.837834 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -229.715523 au

O	2.02282400	-0.53919500	0.00851300
H	0.85765000	0.35424100	0.05235000
O	-0.00092000	0.96652200	0.09086500
H	0.01923600	1.58261600	-0.66705400
H	-0.87682800	0.37946300	0.02523800
O	-2.11901100	-0.39133400	-0.05632000
H	-1.97577000	-1.23517000	-0.51994900
H	-2.42028200	-0.63806200	0.83578900
H	2.53647500	-0.39830600	-0.80618500
H	2.63638300	-0.33272100	0.73534200

2′_G
E (B3LYP/BS1, Solvent = water) = -3377.157366 au
H (B3LYP/BS1, Solvent = water) = -3376.635786 au
G(B3LYP/BS1, Solvent = water) = -3376.741825 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -3378.095702 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -3376.999297 au

Pt	-1.58978800	-0.44889300	0.49262000
N	0.05132600	0.74984300	0.13726600
P	3.60156600	-2.83991200	-0.63188800
O	3.20326900	-2.73704400	-2.07694400
O	5.12477400	-2.21279200	-0.42714400
C	5.64356300	-1.22503000	-1.31303900
H	5.19665100	-1.33124000	-2.30656500
H	6.72234600	-1.40437400	-1.39216000

C	5.44036000	0.19841400	-0.80757500
H	6.11279900	0.86310900	-1.36591300
O	4.07646300	0.62060900	-1.04586000
C	3.63332200	1.32544700	0.10417900
H	3.94438300	2.37396200	0.06326700
N	2.17279000	1.36816300	0.09724600
C	1.30614800	0.32715200	0.23600000
C	0.09161200	2.13126100	-0.08968300
C	-0.90241500	3.12916600	-0.36326000
N	-0.31113000	4.39675700	-0.51812500
H	-0.97646500	5.14071600	-0.70540400
C	1.03402600	4.67897000	-0.48125900
N	1.41238500	5.96546400	-0.61251900
H	0.77457600	6.67562800	-0.94320700
H	2.40066200	6.14569600	-0.72419400
N	1.94783500	3.73951100	-0.29361400
C	1.43015700	2.51592600	-0.11095500
C	5.70448300	0.39993900	0.70478100
H	6.20575400	-0.46751600	1.14651600
C	4.29283700	0.60163100	1.27540800
H	3.81026600	-0.36841100	1.42854000
H	4.28504700	1.18068200	2.20277100
O	6.51023900	1.57310700	0.83191100
H	6.69302000	1.70171200	1.77704400
O	2.71508100	-2.31983900	0.48298100
N	-3.30311600	-1.56813400	0.79762000
N	-2.72463900	0.41029300	-1.02571700
Cl	-0.48676500	-1.61705300	2.26028500
Cl	-2.41653800	1.08565500	2.12972000
Cl	-0.87446200	-2.03426500	-1.14546400
C	-3.99650100	-0.36456900	-1.21227200
C	-4.46626300	-0.86083200	0.15606600
C	-5.09135800	0.44532200	-1.91481000
H	-3.72588400	-1.22977800	-1.82697300
C	-5.71699100	-1.73504900	0.03710200
H	-4.67019400	-0.00014400	0.80010800
C	-6.36722600	-0.40887100	-2.04072800
C	-6.83159300	-0.94829000	-0.67901500
H	-6.04559200	-2.04893000	1.03377000
H	-5.47816200	-2.64361100	-0.53166900
H	-7.15875500	0.19532300	-2.49706100
H	-6.17512900	-1.24762300	-2.72336400
H	-7.70260500	-1.59964200	-0.80812300
H	-7.15196600	-0.11341600	-0.04144700
H	-3.15709000	-2.49800700	0.39107400
H	-3.45560400	-1.69935900	1.80151200
H	-2.84326000	1.41189800	-0.77468900
H	-2.17763700	0.39128300	-1.89033500
H	-5.30321800	1.35216100	-1.33316100
O	3.94594100	-4.41853900	-0.28518600
O	-2.12922200	3.03112100	-0.48901300
H	1.64238600	-0.70192900	0.38772300

H	-4.73932100	0.76322000	-2.90199200
H	3.65947800	-4.60259300	0.62402000

2″_G

E (B3LYP/BS1, Solvent = water) = -3377.160675 au
H (B3LYP/BS1, Solvent = water) = -3376.639343 au
G(B3LYP/BS1, Solvent = water) = -3376.745169 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -3378.097616 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -3377.003574 au

Pt	1.56518500	-0.97541700	0.33337900
N	-0.48555000	-1.21610400	0.10607000
P	-1.02426800	3.51363000	-0.61257000
O	-1.09283000	3.14137300	-2.06085800
O	-2.52391500	3.73124900	0.03118500
C	-3.70939500	3.58567000	-0.75517500
H	-3.45175400	3.48722300	-1.81288700
H	-4.31911000	4.48671200	-0.61908900
C	-4.51899800	2.37495700	-0.31157300
H	-5.48915000	2.40416900	-0.82376900
O	-3.82741900	1.16462700	-0.69385400
C	-3.77119400	0.28370200	0.41997100
H	-4.62755600	-0.39663100	0.41916600
N	-2.59894000	-0.57538600	0.26867200
C	-1.30024200	-0.21821700	0.42168200
C	-1.29238700	-2.29393100	-0.28803600
C	-1.03433100	-3.62648800	-0.78567700
N	-2.26420200	-4.29582500	-1.04490100
H	-2.14024400	-5.24720600	-1.37667600
C	-3.52800300	-3.78805300	-0.89806300
N	-4.57592300	-4.60090700	-1.16688300
H	-4.45273600	-5.42020400	-1.74605100
H	-5.48262900	-4.15557500	-1.21556500
N	-3.74743500	-2.55692800	-0.46765900
C	-2.62062400	-1.88107600	-0.18718000
C	-4.77229000	2.27036400	1.20902500
H	-4.59648200	3.22423900	1.71894300
C	-3.77503500	1.19119500	1.65000000
H	-2.79036100	1.64276700	1.79849800
H	-4.07788600	0.67230700	2.56297800
O	-6.12581300	1.84766900	1.37121400
H	-6.30177900	1.77834800	2.32388500
O	-0.28533700	2.63509500	0.40004800
N	1.59849200	0.93370500	-0.51281400
N	3.59672100	-0.63370700	0.54472100
Cl	1.24323600	-0.00241200	2.49627500
Cl	1.85892000	-3.09627900	1.40807700
Cl	2.01969700	-1.79915500	-1.86370000
C	4.01184700	0.55459200	-0.27856800
C	2.89594300	1.59172700	-0.16005300
C	5.36770900	1.13207800	0.13422900
H	4.05754600	0.19253300	-1.31014300

C	3.18509500	2.82955800	-1.01620400
H	2.79406500	1.89017100	0.88876800
C	5.67661500	2.37869200	-0.71664500
C	4.55316900	3.42336700	-0.62905300
H	2.38636500	3.56483100	-0.87292000
H	3.18789300	2.54770900	-2.07772400
H	6.62466300	2.81400900	-0.38276500
H	5.81786900	2.07591100	-1.76290700
H	4.77487200	4.27185000	-1.28552900
H	4.49921300	3.81949800	0.39392000
H	1.51982100	0.80479800	-1.52647300
H	0.80559000	1.56253200	-0.19499100
H	3.77802500	-0.47617000	1.54140800
H	4.11494000	-1.47446800	0.27575500
H	5.34094400	1.40390800	1.19812500
O	-0.37657700	5.02146400	-0.50237300
O	0.01270400	-4.21578800	-1.00557800
H	-0.99086600	0.77925200	0.71459200
H	6.14924600	0.37483800	0.00899800
H	-0.03834100	5.17589400	0.39552800

1′TS_G (Imaginary Frequency = 264.91i)
E (B3LYP/BS1, Solvent = water) = -3377.124560 au
H (B3LYP/BS1, Solvent = water) = -3376.604881 au
G(B3LYP/BS1, Solvent = water) = -3376.707865 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -3378.055616 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -3376.966303 au

Pt	-1.51923800	-0.40971500	0.57425000
N	0.23924200	0.35328900	-0.24631100
P	2.78908900	-2.34389900	-1.19608800
O	2.17266100	-0.90515600	-1.26401900
O	4.36395200	-2.25191400	-0.79474500
C	5.30259700	-1.31650800	-1.35291500
H	4.96074700	-0.94691700	-2.32455400
H	6.23278100	-1.87401700	-1.50064400
C	5.56012700	-0.13774800	-0.41766600
H	6.48735200	0.34959800	-0.74243700
O	4.50115800	0.82546800	-0.50464000
C	3.75591300	0.88594300	0.71540600
H	3.97049500	1.84372500	1.19556100
N	2.33298200	0.91795200	0.42702600
C	1.47642100	-0.16324100	0.12278200
C	0.42740900	1.74062800	-0.41609200
C	-0.38259100	2.75630600	-0.98553200
N	0.27767200	4.00727700	-0.99412200
H	-0.28092600	4.76832000	-1.36673600
C	1.55234600	4.23858000	-0.55778400
N	2.01924400	5.51198900	-0.58106500
H	1.59022500	6.20134600	-1.18339800
H	3.01462200	5.61604000	-0.43524500
N	2.32054500	3.27073300	-0.07880200

C	1.71698600	2.07353100	-0.02226600
C	5.67009000	-0.50463800	1.07260700
H	6.00584600	-1.53762300	1.22190100
C	4.23667600	-0.28477200	1.58075600
H	3.64462900	-1.18734300	1.41652300
H	4.20489300	-0.04394700	2.64671400
O	6.58891100	0.42053300	1.65183100
H	6.62856600	0.23817500	2.60477700
O	2.18726000	-3.35432700	-0.28293400
N	-3.43052200	-1.06978400	1.18558900
N	-2.55662700	0.20973000	-1.10715900
Cl	-0.49383800	-1.28181100	2.56274200
Cl	-1.98534000	1.61509400	1.76787600
Cl	-1.25219900	-2.49302300	-0.57474500
C	-3.96603100	-0.29980200	-1.07430600
C	-4.45432100	-0.32814000	0.37749700
C	-4.91197900	0.51636600	-1.96240700
H	-3.91462000	-1.33059300	-1.44188100
C	-5.86118300	-0.92508100	0.47704100
H	-4.45442000	0.69103100	0.77550000
C	-6.33953200	-0.05426500	-1.86918400
C	-6.83174900	-0.12889100	-0.41550500
H	-6.19551000	-0.90931100	1.52030600
H	-5.83657500	-1.97584400	0.15742900
H	-7.01579800	0.56825600	-2.46534700
H	-6.35672100	-1.05779400	-2.31563800
H	-7.82296200	-0.59360800	-0.37547300
H	-6.94143400	0.88695600	-0.01246500
H	-3.48977300	-2.08028400	1.02912300
H	-3.55924900	-0.90758900	2.18685100
H	-2.44345400	1.24579300	-1.17712800
H	-2.06386200	-0.17746800	-1.91578600
H	-4.90411600	1.56421900	-1.63401900
O	2.78534900	-2.72381000	-2.77832100
O	-1.54382600	2.71319200	-1.44019600
H	1.47455100	-1.01002200	0.79353300
H	-4.55483200	0.49601200	-2.99784900
H	3.14862100	-3.61509700	-2.92610200

3′_G

E (B3LYP/BS1, Solvent = water) = -3377.128184 au

H (B3LYP/BS1, Solvent = water) = -3376.607423 au

G(B3LYP/BS1, Solvent = water) = -3376.712063 au

E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -3378.055416 au

E(M06/BS2//B3LYP/BS1, Solvent = water) = -3376.970283 au

Pt	-1.45298600	-0.40354700	0.55286700
N	0.19643500	0.23962300	-0.62390400
P	2.92461200	-2.13926000	-1.61439500
O	2.17376300	-0.72773200	-1.46996100
O	4.16783200	-2.16185800	-0.58957900
C	5.42413400	-1.46838700	-0.78633100

H	5.51603200	-1.15691400	-1.82915200
H	6.21048700	-2.19529800	-0.56403000
C	5.54440900	-0.25843200	0.12844900
H	6.53800300	0.17761100	-0.03448700
O	4.55303300	0.71362600	-0.22212400
C	3.58102700	0.86070000	0.82900400
H	3.71859900	1.84866900	1.27536400
N	2.24090900	0.86311100	0.29500200
C	1.50184900	-0.26973000	-0.23219700
C	0.38746100	1.62493500	-0.71362900
C	-0.43843800	2.62739100	-1.28189700
N	0.16688400	3.90694700	-1.21332600
H	-0.39755900	4.66075800	-1.59158400
C	1.38773200	4.17334100	-0.66030300
N	1.80519800	5.45912100	-0.61588700
H	1.38577600	6.16177800	-1.20906800
H	2.77228000	5.60645900	-0.36045000
N	2.15881600	3.22480900	-0.13773400
C	1.62128200	1.99781100	-0.17810000
C	5.36074400	-0.53468700	1.63049900
H	5.63436700	-1.56273700	1.89926100
C	3.86956100	-0.25500200	1.84341700
H	3.29282000	-1.15571800	1.62322900
H	3.63937700	0.05624700	2.86579300
O	6.18789800	0.40589600	2.31391200
H	6.03899800	0.29293200	3.26684900
O	2.11664000	-3.36823100	-1.43189800
N	-3.36536100	-1.00667500	1.38886000
N	-2.63555700	0.06053100	-1.08235300
Cl	-0.22079500	-1.06093200	2.50764000
Cl	-1.86456600	1.73063700	1.58754800
Cl	-1.25064200	-2.60172700	-0.39127900
C	-4.03317600	-0.44926200	-0.90391800
C	-4.43102900	-0.34688800	0.57461400
C	-5.04072100	0.27744800	-1.80257600
H	-3.99349900	-1.50951100	-1.17724300
C	-5.82920700	-0.93190500	0.80463100
H	-4.41665300	0.70630800	0.87237700
C	-6.45572500	-0.28418100	-1.57561100
C	-6.85954400	-0.22483800	-0.09455000
H	-6.10175500	-0.82657500	1.86081800
H	-5.81347900	-2.00725100	0.57815500
H	-7.17032700	0.27878300	-2.18632100
H	-6.49211400	-1.32514500	-1.92469700
H	-7.84333500	-0.68564700	0.04832100
H	-6.95319600	0.82395400	0.21888900
H	-3.43020900	-2.02612700	1.33765200
H	-3.43192700	-0.74174400	2.37263200
H	-2.54738000	1.08129500	-1.25389800
H	-2.19482600	-0.38871900	-1.88843900
H	-5.02392100	1.35066100	-1.56922900
O	3.53513900	-1.88292900	-3.08509300

O	-1.57503500	2.53856300	-1.78418100
H	1.43594300	-1.10111500	0.46116300
H	-4.74542700	0.16746900	-2.85195500
H	3.76116600	-2.72128000	-3.52630100

2′TS_G (Imaginary Frequency = 64.58i)
E (B3LYP/BS1, Solvent = water) = -3377.113303 au
H (B3LYP/BS1, Solvent = water) = -3376.593873 au
G(B3LYP/BS1, Solvent = water) = -3376.702062 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -3378.037005 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -3376.955812 au

P	-3.14878500	-2.15135500	1.57930500
O	-2.53998200	-0.64390300	1.62859800
O	-4.36043800	-2.13183100	0.52936700
C	-5.61769300	-1.43118000	0.72498200
H	-5.73119800	-1.15524300	1.77560700
H	-6.40206300	-2.14410500	0.45930500
C	-5.71269700	-0.19296700	-0.15342500
H	-6.72269700	0.21478900	-0.02983100
O	-4.77267100	0.80131500	0.28608200
C	-3.76584700	1.02542200	-0.69624900
H	-3.88264100	2.03195700	-1.10523100
N	-2.45625900	1.02807600	-0.05188700
C	-1.76520300	-0.13015900	0.55353100
C	-0.57694700	1.68528800	0.97595700
C	0.38302000	2.69912900	1.42243600
N	-0.05078500	3.99640600	1.09713300
H	0.58028200	4.74248200	1.37576800
C	-1.20378000	4.30127700	0.41501300
N	-1.46976100	5.57699400	0.16799900
H	-0.86988700	6.33693900	0.46122200
H	-2.31782800	5.80146700	-0.33683000
N	-2.08612800	3.38007300	-0.01526200
C	-1.76143800	2.13172000	0.25654600
C	-5.43620500	-0.40376800	-1.65148900
H	-5.64571400	-1.43172300	-1.97141300
C	-3.94749700	-0.05316900	-1.77533000
H	-3.33615500	-0.93469600	-1.57094200
H	-3.68408300	0.31799300	-2.76881600
O	-6.26496900	0.52715600	-2.34211400
H	-6.07544000	0.44716700	-3.29112700
O	-2.19261800	-3.22760100	1.24122200
Pt	1.52073700	-0.60194700	-0.62626500
N	-0.51660500	0.39449900	1.12524400
N	4.03357000	-0.97007300	-1.64421500
N	2.84970100	0.13061600	0.77861900
Cl	-0.05274500	-1.45163900	-2.24385100
Cl	1.41023000	1.60669500	-1.57994800
Cl	1.68181500	-2.73538700	0.46530400
C	4.26939600	-0.34772200	0.72433500
C	4.84715800	-0.19875500	-0.69432200

C	5.10561900	0.40537900	1.77275800
H	4.23020700	-1.41319000	0.97540200
C	6.33771800	-0.59680200	-0.70936000
H	4.75823900	0.85556000	-0.98890700
C	6.58170700	-0.01709900	1.73676300
C	7.16876500	0.16652000	0.33157400
H	6.73362400	-0.43309800	-1.71905100
H	6.41001100	-1.67698400	-0.51257700
H	7.14632100	0.56837100	2.47184000
H	6.66859800	-1.07073200	2.03693800
H	8.20936000	-0.17829600	0.30311000
H	7.18330100	1.23605600	0.07784100
H	4.20790000	-1.96925400	-1.54034300
H	4.26596900	-0.72012200	-2.60363100
H	2.82217900	1.15208200	0.71530900
H	2.46095400	-0.08667300	1.69874200
H	5.03342500	1.48522600	1.57652800
O	-3.77992700	-2.11515300	3.05335300
O	1.43747500	2.50970300	2.00433800
H	-1.54138400	-0.89055500	-0.19540900
H	4.68077500	0.23384000	2.76945000
H	-4.01340600	-3.00371900	3.37810300

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E (B3LYP/BS1, Solvent = water) = -1846.640493 au
H (B3LYP/BS1, Solvent = water) = -1846.411712 au
G(B3LYP/BS1, Solvent = water) = -1846.473060 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -1847.114395 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -1846.717826 au

Pt	-1.15028700	0.05483500	-0.12613500
N	1.60223500	-1.38470000	1.66848700
N	0.72791600	-0.34299400	-0.92597300
Cl	-3.34371100	0.46362100	0.74672800
Cl	-1.70407000	-2.21621700	-0.65204800
Cl	-0.55168700	2.33643200	0.26286300
C	2.00733800	0.10963900	-0.26608100
C	2.58558500	-0.97968400	0.65387200
C	3.01893500	0.51860800	-1.35128000
H	1.75193500	0.98804000	0.33266400
C	3.92860100	-0.50044200	1.24770500
H	2.78483800	-1.86849100	0.03574700
C	4.34906400	0.98926100	-0.74624400
C	4.94315300	-0.08448400	0.17374900
H	4.33681400	-1.30323200	1.87487300
H	3.72894700	0.35112100	1.91546700
H	5.04946000	1.24140700	-1.55124900
H	4.18101500	1.91156000	-0.17240200
H	5.86274800	0.28203700	0.64592000
H	5.22458000	-0.96310300	-0.42437500
H	1.44626400	-0.60827700	2.31281100
H	2.00312900	-2.13325800	2.23368100

H	0.75636400	-1.35711100	-1.06242600
H	0.69746800	0.05936100	-1.86556600
H	3.20075800	-0.34001900	-2.01398300
H	2.58187000	1.31411800	-1.96883500

1TS (Imaginary Frequency = 129.08i)
E (B3LYP/BS1, Solvent = water) = -1846.624853 au
H (B3LYP/BS1, Solvent = water) = -1846.396694 au
G(B3LYP/BS1, Solvent = water) = -1846.456411 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -1847.094247 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -1846.697731 au

Pt	0.99041500	0.08238400	0.05013200
N	-0.84241700	-1.06823200	-1.22472800
N	-0.70611300	0.73330500	0.98275600
Cl	2.93467000	-0.75202500	-1.11152900
Cl	0.67160800	-2.12103000	1.55937900
Cl	1.75983300	2.38192300	-0.04608700
C	-1.94038700	0.66612000	0.13268000
C	-2.06841400	-0.74302200	-0.47009700
C	-3.18629900	1.06089100	0.93906700
H	-1.78217200	1.38550000	-0.67946100
C	-3.35444700	-0.85644900	-1.30812200
H	-2.11473500	-1.45790300	0.36039900
C	-4.45993400	0.94805100	0.08576900
C	-4.60552300	-0.45972300	-0.50839300
H	-3.44418000	-1.88234500	-1.68518900
H	-3.25963700	-0.20184600	-2.18732400
H	-5.33347600	1.19838100	0.69894700
H	-4.42134700	1.68779900	-0.72608300
H	-5.49039200	-0.51133400	-1.15386400
H	-4.76397200	-1.18365400	0.30330500
H	-0.88984000	-0.70315800	-2.17515900
H	-0.71093900	-2.07517100	-1.28598600
H	-0.82711400	0.14462100	1.81324900
H	-0.56853100	1.69309900	1.31022700
H	-3.27128800	0.39709500	1.81160900
H	-3.06885800	2.08150300	1.32341500

1″TS_G (Imaginary Frequency = 255.05i)
E (B3LYP/BS1, Solvent = water) = -3377.122699 au
H (B3LYP/BS1, Solvent = water) = -3376.602833 au
G(B3LYP/BS1, Solvent = water) = -3376.704630 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -3378.052912 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -3376.965536 au

Pt	-1.52844900	0.84203300	0.23848700
N	0.43994500	0.83991800	-0.51240700
P	1.31058600	-2.67508100	-1.35373300
O	1.62268400	-1.14026400	-1.42162500
O	2.45221100	-3.44274900	-0.50691500
C	3.86342000	-3.36917000	-0.82108600

H	4.00789600	-3.05019100	-1.85700600
H	4.24703900	-4.38752700	-0.71347100
C	4.61826500	-2.43277900	0.11652800
H	5.68813300	-2.58854400	-0.06945300
O	4.30957100	-1.06295300	-0.17025100
C	3.59358800	-0.45371700	0.91262300
H	4.24624200	0.28871600	1.37725700
N	2.45804500	0.29642700	0.41456300
C	1.24276500	-0.22125700	-0.07027700
C	1.28513200	1.96621200	-0.52089100
C	1.16418700	3.24067200	-1.16002000
N	2.34367000	4.02433600	-0.94814400
H	2.29303300	4.95381000	-1.35190000
C	3.49306100	3.60236800	-0.34875500
N	4.51326900	4.48727200	-0.20965400
H	4.55709000	5.30442600	-0.80363400
H	5.40542800	4.08818600	0.05078600
N	3.62904700	2.37370200	0.13151200
C	2.51992400	1.62490000	0.02410800
C	4.33577800	-2.62696400	1.61652600
H	4.00187000	-3.64622200	1.84694200
C	3.24404700	-1.58526400	1.89070300
H	2.26487400	-2.01861100	1.67567700
H	3.24265600	-1.24021100	2.92800000
O	5.55149300	-2.32284200	2.29792900
H	5.37799100	-2.38395400	3.25143100
O	-0.00800400	-3.05669100	-0.74752500
N	-1.94574800	-1.02917100	-0.58488500
N	-3.55685600	0.67828500	0.88601600
Cl	-0.89377400	-0.15284800	2.33164200
Cl	-1.36266000	2.99765200	1.26348500
Cl	-2.40061000	1.73372900	-1.82401700
C	-4.20797800	-0.48455400	0.20262400
C	-3.16395200	-1.59744400	0.07298200
C	-5.46770800	-0.98508600	0.91774600
H	-4.46801900	-0.12721700	-0.79902400
C	-3.72644700	-2.80670000	-0.68289400
H	-2.84005000	-1.90425000	1.07288900
C	-6.04462300	-2.20757200	0.18051100
C	-4.99751300	-3.31980300	0.01832300
H	-2.96342400	-3.59043900	-0.73665700
H	-3.96548100	-2.51074500	-1.71376200
H	-6.91415000	-2.58361600	0.73072600
H	-6.40639500	-1.89616800	-0.80883300
H	-5.41603700	-4.15242700	-0.55777300
H	-4.73042800	-3.72020100	1.00569800
H	-2.12906000	-0.84833700	-1.57722700
H	-1.16614800	-1.72010500	-0.55227500
H	-3.54177400	0.55190500	1.90145400
H	-4.05751000	1.54848500	0.69563100
H	-5.21224000	-1.26085000	1.95040000
O	1.52749100	-3.09276900	-2.89859000

O	0.25229400	3.73272400	-1.82117700
H	0.76515000	-0.96057700	0.55598500
H	-6.20786300	-0.17884400	0.96912500
H	1.30792400	-4.02797400	-3.06216300

3″_G

E (B3LYP/BS1, Solvent = water) = -3377.124286 au
H (B3LYP/BS1, Solvent = water) = -3376.603522 au
G(B3LYP/BS1, Solvent = water) = -3376.707187 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -3378.051777 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -3376.96784 au

Pt	-1.50826300	0.83535100	0.21981200
N	0.42738100	0.80885900	-0.70395900
P	1.37860400	-2.63174400	-1.47352000
O	1.69129000	-1.06655000	-1.43435800
O	2.45094600	-3.40663000	-0.56520100
C	3.88792300	-3.36556000	-0.77834000
H	4.10586500	-3.05591600	-1.80355800
H	4.23447300	-4.39255800	-0.63905700
C	4.58931700	-2.43675600	0.20595000
H	5.66713300	-2.59583200	0.07627000
O	4.29542400	-1.06785500	-0.09154800
C	3.52076100	-0.45890000	0.95724000
H	4.14750100	0.28666200	1.45158200
N	2.40704000	0.27759100	0.40645800
C	1.24917600	-0.28922300	-0.23248200
C	1.26772600	1.92489400	-0.61806100
C	1.16799600	3.21015500	-1.23990700
N	2.30445900	4.02106300	-0.92168400
H	2.26534400	4.95600400	-1.31377100
C	3.40113600	3.62016200	-0.22061100
N	4.38017200	4.52256200	0.02169100
H	4.44410300	5.37200400	-0.52246500
H	5.25082000	4.15279300	0.37886800
N	3.52818400	2.38581200	0.25637400
C	2.46223800	1.60394900	0.03736600
C	4.23018300	-2.63963900	1.68872700
H	3.88222300	-3.65934600	1.89572900
C	3.13210800	-1.59447000	1.91747300
H	2.15764200	-2.01998400	1.66687000
H	3.09202400	-1.25096000	2.95451900
O	5.41343200	-2.34573400	2.42938000
H	5.19359300	-2.40793800	3.37320400
O	0.01022100	-3.01780000	-1.01808400
N	-1.98991500	-1.01293500	-0.61786700
N	-3.55084500	0.65226800	0.97645000
Cl	-0.78672100	-0.21143500	2.26843400
Cl	-1.26284900	2.97156900	1.27500900
Cl	-2.49327700	1.78112300	-1.78499500
C	-4.21653400	-0.49615000	0.29337900
C	-3.17172600	-1.59984000	0.09037000

C	-5.44264800	-1.02842600	1.04552800
H	-4.52145100	-0.11957000	-0.68881600
C	-3.75970000	-2.79906400	-0.66216000
H	-2.79779800	-1.92163900	1.06791500
C	-6.04251000	-2.23949000	0.30942400
C	-4.99460000	-3.33898300	0.08162200
H	-2.99489100	-3.57646000	-0.76636900
H	-4.04566600	-2.48478100	-1.67566600
H	-6.88593900	-2.63376400	0.88713800
H	-6.44720200	-1.91194900	-0.65797700
H	-5.42946600	-4.16515100	-0.49183400
H	-4.68213200	-3.75491800	1.04919500
H	-2.22928100	-0.80665500	-1.59320500
H	-1.21277300	-1.69851800	-0.65029500
H	-3.48379600	0.49840600	1.98498300
H	-4.06540500	1.52178900	0.83092300
H	-5.14184400	-1.32327500	2.06075800
O	1.75829000	-2.89707400	-3.01025000
O	0.30002900	3.68939000	-1.96680400
H	0.71666300	-0.97543000	0.41536400
H	-6.18570700	-0.22936900	1.14686600
H	1.57231300	-3.81072500	-3.29377300

2″TS_G (Imaginary Frequency = -69.16i)
E (B3LYP/BS1, Solvent = water) = -3377.114890 au
H (B3LYP/BS1, Solvent = water) = -3376.595313 au
G(B3LYP/BS1, Solvent = water) = -3376.700982 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -3378.037106 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -3376.955548 au

Pt	1.50167600	-0.00722800	-1.09075200
N	-0.08846200	0.60513200	0.67784300
P	-1.81869300	-2.60928400	1.24963100
O	-1.53637900	-1.03119000	1.52909800
O	-3.08031700	-2.68015000	0.25611200
C	-4.44029900	-2.63951700	0.77411300
H	-4.42143600	-2.79839000	1.85469900
H	-4.97274000	-3.47030300	0.30516400
C	-5.11801500	-1.31417600	0.45071100
H	-6.11874800	-1.34592000	0.89729000
O	-4.38720100	-0.23313600	1.05070400
C	-3.80436400	0.60725700	0.05451900
H	-4.29285300	1.58427100	0.07901000
N	-2.41280700	0.86765500	0.39016900
C	-1.34349000	-0.12415100	0.43691500
C	-0.46009000	1.89121000	0.79765600
C	0.33532900	3.05073600	1.12456700
N	-0.44763200	4.21167100	1.26261400
H	0.07770800	5.05518500	1.47303900
C	-1.80566800	4.27675800	1.08785300
N	-2.40814800	5.45688000	1.23075500
H	-1.91566000	6.30345700	1.47936100

H	-3.41088000	5.50121400	1.10860700
N	-2.55353000	3.20856700	0.78628100
C	-1.87503700	2.07768100	0.64857900
C	-5.25200600	-0.96372000	-1.04076400
H	-5.27338200	-1.85813600	-1.67573200
C	-4.01411200	-0.09884000	-1.29728800
H	-3.16321100	-0.73390000	-1.55490800
H	-4.16051700	0.61820200	-2.10906300
O	-6.46168600	-0.22007100	-1.16513900
H	-6.54183700	0.06307700	-2.09056900
O	-0.62949500	-3.10239100	0.29021500
H	-0.65213000	-2.78328800	-0.64412700
N	2.09609600	-1.66234700	0.03481700
N	2.89363500	0.96124900	0.08441600
Cl	-0.01340200	-1.40500500	-2.38119400
Cl	0.91295900	1.97600300	-2.28708000
Cl	3.69215300	-0.63302700	-2.65419900
C	3.19186100	0.12408800	1.28746800
C	3.32699400	-1.32510300	0.82562100
C	4.43591000	0.58914600	2.05092100
H	2.30795600	0.21502700	1.92784800
C	3.57591700	-2.27262900	2.00245100
H	4.15322500	-1.38931300	0.11046200
C	4.70948700	-0.35445200	3.23712300
C	4.82213600	-1.81888000	2.78546400
H	3.70163700	-3.29760100	1.63543100
H	2.69970700	-2.26803400	2.66565600
H	5.63004600	-0.04315200	3.74320200
H	3.89705900	-0.25855900	3.97037500
H	4.96149800	-2.47255700	3.65361800
H	5.71140400	-1.94035300	2.15191800
H	1.33119500	-1.96948400	0.64300200
H	2.29278100	-2.43698400	-0.60276700
H	3.72553600	1.08123400	-0.50098900
H	2.54277200	1.88225200	0.39099200
H	5.29975100	0.59172100	1.37184500
O	-1.91001700	-3.34057000	2.52848200
O	1.55843000	3.13263500	1.26228800
H	-1.29782400	-0.66550700	-0.50338300
H	4.29144100	1.61820800	2.39842700

5′-dAMP

E (B3LYP/BS1, Solvent = water) = -1455.578267 au

H (B3LYP/BS1, Solvent = water) = -1455.296490 au

G(B3LYP/BS1, Solvent = water) = -1455.368430 au

E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -1456.033223 au

E(M06/BS2//B3LYP/BS1, Solvent = water) = -1455.351303 au

P	-3.15327200	-1.66250400	0.11811400
O	-2.04315400	-2.55873600	-0.35558000
O	-2.73958900	-0.13281400	-0.38902000
C	-3.04633900	1.01927900	0.38707200

H	-3.37454900	0.72404400	1.38771700
H	-3.85462600	1.58787700	-0.09380400
C	-1.83440300	1.93048100	0.48318900
H	-2.13876700	2.84840100	1.00950400
O	-0.78749500	1.27853500	1.22863200
C	0.48683700	1.65727500	0.74192500
H	1.08013200	2.10298200	1.54586700
N	1.22135400	0.44579300	0.33923500
C	0.72724200	-0.77700900	-0.07633400
C	2.85114800	-0.96197700	-0.14742000
C	4.21041400	-1.31711700	-0.27875600
N	5.15247700	-0.40027400	0.02500000
C	4.75291300	0.81154500	0.44642300
N	3.50956400	1.27328200	0.61130200
C	2.59530100	0.33966000	0.29835900
C	-1.18989100	2.33448400	-0.84704700
H	-1.21292900	1.48102400	-1.53507900
C	0.24965700	2.64632000	-0.41263000
H	0.99330100	2.54719800	-1.20673800
H	0.28209900	3.67161100	-0.02853700
O	-1.90358700	3.43666300	-1.38583900
H	-1.61579300	3.55756000	-2.30422300
O	-4.45073300	-1.98785100	-0.86257200
H	-5.25088800	-1.58509100	-0.48621700
N	1.67132500	-1.64724900	-0.37458800
O	-3.61072500	-1.60784900	1.55297400
H	-0.33441900	-0.98553600	-0.12387000
N	4.60727300	-2.55936900	-0.66271000
H	5.57151100	-2.67033300	-0.94688500
H	3.93019900	-3.15863600	-1.11437000
H	5.55484900	1.50995700	0.67980100

2_A

E (B3LYP/BS1, Solvent = water) = -3301.915778 au

H (B3LYP/BS1, Solvent = water) = -3301.399651 au

G(B3LYP/BS1, Solvent = water) = -3301.500415 au

E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -3302.818076 au

E(M06/BS2//B3LYP/BS1, Solvent = water) = -3301.752469 au

Pt	-1.93490700	-0.17589600	-0.83462000
N	-0.30239300	-1.22248000	-0.05579600
P	2.69924200	2.50353200	-0.24518500
O	2.64285200	2.72428100	1.23642700
O	4.09116300	1.73442500	-0.67934300
C	5.01960400	1.26546000	0.30075100
H	4.75124800	1.64928300	1.28842500
H	6.01500400	1.63936600	0.03276100
C	5.06150500	-0.25547400	0.33554800
H	5.87904100	-0.56405300	0.99885200
O	3.81479500	-0.75962000	0.87009000
C	3.29963400	-1.75398400	-0.00053800
H	3.62908100	-2.74802400	0.31621300
N	1.84030300	-1.77475100	0.13474400
C	0.93192800	-1.00285800	-0.49866600
C	-0.20338300	-2.20325600	0.94694900

C	-1.07193400	-2.86872900	1.84480700
N	-0.53689000	-3.68716600	2.76198300
C	0.78706600	-3.88993100	2.77741900
N	1.69723000	-3.36447200	1.95598700
C	1.15461200	-2.52768700	1.07499000
C	5.25341400	-0.94171600	-1.03393500
H	5.65870800	-0.25286200	-1.78366500
C	3.83225200	-1.40101600	-1.38706000
H	3.28117000	-0.55738300	-1.81012100
H	3.80946800	-2.24235800	-2.08398900
O	6.13555100	-2.04238000	-0.82078800
H	6.26173300	-2.49181400	-1.67251400
O	1.57824000	1.77208000	-0.98176200
N	-1.08561900	1.70063300	-0.50661200
N	-2.68997500	0.13152100	1.09311600
Cl	-0.99247600	-0.27377600	-3.02418600
Cl	-3.06069300	-2.26351700	-1.23837700
Cl	-3.81086700	1.00482100	-1.67438300
C	-1.86726500	1.19463700	1.75943600
C	-1.66265700	2.31260000	0.73756000
C	-2.50679000	1.71513000	3.05007300
H	-0.90152200	0.73076800	1.98693900
C	-0.79835400	3.44639800	1.30228100
H	-2.64510200	2.70474800	0.45349100
C	-1.64863000	2.85516900	3.63045300
C	-1.42821800	3.97653600	2.60447300
H	-0.72271400	4.24905600	0.55999800
H	0.21883500	3.08212700	1.49083800
H	-2.13915200	3.25092200	4.52640300
H	-0.67862800	2.45168300	3.95057700
H	-0.77706600	4.75031400	3.02594800
H	-2.38842600	4.45957300	2.37771500
H	-0.02648400	1.68037700	-0.51777900
H	-1.34774200	2.26290500	-1.32106200
H	-3.66255300	0.43613600	0.97789400
H	-2.70458300	-0.75033300	1.63956400
H	-3.51768100	2.08443900	2.83182500
O	2.89415000	3.96358500	-0.97596400
H	1.19475000	-0.24563100	-1.22162800
H	-2.60511700	0.89606200	3.77058900
H	2.60522900	3.91352800	-1.90245100
N	-2.43850600	-2.67729000	1.88017000
H	-2.89780600	-2.74327600	0.96887900
H	-2.88341400	-3.26916200	2.57708800
H	1.15671700	-4.56605900	3.54377200

1TS_A (Imaginary Frequency = 221.38i)
E (B3LYP/BS1, Solvent = water) = -3301.886461 au
H (B3LYP/BS1, Solvent = water) = -3301.371591 au
G(B3LYP/BS1, Solvent = water) = -3301.468221 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -3302.780387 au

E(M06/BS2//B3LYP/BS1, Solvent = water) = -3301.722445 au

Pt	-1.70308000	-0.58615200	-0.80362500
N	0.01723100	-0.78840200	0.35769800
P	1.91277500	2.40152300	-0.06575300
O	1.55380300	1.10057000	0.73424500
O	3.38751100	2.28433100	-0.70990500
C	4.59856800	2.17929600	0.07882900
H	4.41704600	2.53850500	1.09515400
H	5.32701900	2.83978700	-0.39948000
C	5.14002500	0.75601900	0.12411300
H	6.10557000	0.79934100	0.64318500
O	4.26157700	-0.09272900	0.87455200
C	3.67364200	-1.09705700	0.03939400
H	4.08894400	-2.06640400	0.32597100
N	2.24942400	-1.20943000	0.29098000
C	1.24452300	-0.30924600	-0.10821600
C	0.31259700	-1.79111600	1.29430000
C	-0.38920200	-2.49919100	2.27329000
N	0.28084100	-3.28930000	3.13930700
C	1.60093700	-3.39971100	3.01698300
N	2.38252600	-2.79669600	2.10493200
C	1.70637900	-2.00826600	1.28280900
C	5.33952900	0.06710700	-1.23706800
H	5.48960700	0.78905800	-2.04921200
C	4.04236000	-0.73237900	-1.40617300
H	3.28192900	-0.10115900	-1.87146300
H	4.17348500	-1.62062100	-2.02947400
O	6.47750900	-0.78040600	-1.09241100
H	6.59472700	-1.26351400	-1.92657100
O	0.96011400	2.75263200	-1.16888700
N	-1.55374800	1.49246300	-0.93037600
N	-2.71763600	-0.13821800	0.96227700
Cl	-0.50539200	-0.84645300	-2.86031500
Cl	-2.08169800	-2.95295700	-0.73730300
Cl	-3.77387100	-0.30249100	-2.00746600
C	-2.37802400	1.26399100	1.36376800
C	-2.43903200	2.12848300	0.10472600
C	-3.30028700	1.80409800	2.46210700
H	-1.34404600	1.22396800	1.72258100
C	-2.07081900	3.58729100	0.39889400
H	-3.45433800	2.08109500	-0.30278900
C	-2.95243900	3.27367400	2.76626300
C	-2.99418200	4.14165400	1.49965700
H	-2.15920200	4.18191800	-0.51680500
H	-1.02560400	3.64560400	0.72496600
H	-3.65387300	3.66026400	3.51369100
H	-1.95119800	3.32458500	3.21477100
H	-2.69439300	5.16864800	1.73564200
H	-4.02416900	4.19132400	1.12118600
H	-0.57714300	1.85188500	-0.88576500
H	-1.88945100	1.73262600	-1.86703100

H	-3.71967300	-0.23716700	0.77102800
H	-2.45925700	-0.82429000	1.70665900
H	-4.34381500	1.73255100	2.12630200
O	2.01755200	3.46808100	1.14249400
H	1.26834700	0.02336800	-1.13756000
H	-3.20366200	1.18763300	3.36239200
H	2.08843000	4.38518700	0.82075400
H	2.10407600	-4.04686100	3.73134000
N	-1.78784400	-2.42013100	2.42611800
H	-2.25972200	-2.85803000	1.63040900
H	-2.06222800	-2.90972100	3.27628500

3_A

E (B3LYP/BS1, Solvent = water) = -3301.886681 au

H (B3LYP/BS1, Solvent = water) = -3301.370420 au

G(B3LYP/BS1, Solvent = water) = -3301.469030 au

E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -3302.778893 au

E(M06/BS2//B3LYP/BS1, Solvent = water) = -3301.724961 au

Pt	-1.49577700	-0.69086500	-0.80795300
N	-0.01423500	-0.38216600	0.72359200
P	1.92125800	2.60603500	0.29176000
O	1.68445900	1.21407900	1.04537600
O	3.31804800	2.50383700	-0.49286400
C	4.59888400	2.31516300	0.17385100
H	4.51619400	2.61246700	1.22193300
H	5.29266000	2.99321400	-0.32923900
C	5.11717700	0.88291900	0.08376000
H	6.12685700	0.89954500	0.51311700
O	4.31462600	-0.01059100	0.86373400
C	3.61448100	-0.95119700	0.03188400
H	4.00659100	-1.94972300	0.24041400
N	2.21335500	-1.00649500	0.38814300
C	1.26986900	0.06983200	0.20698000
C	0.32693200	-1.48008400	1.52347800
C	-0.34307900	-2.14394500	2.54935500
N	0.22156000	-3.22606300	3.12629100
C	1.45470600	-3.56109100	2.74592200
N	2.25878200	-2.90939300	1.88533800
C	1.66089600	-1.87582300	1.30241700
C	5.19220700	0.26983700	-1.32476800
H	5.27188500	1.03477900	-2.10719800
C	3.88432400	-0.52252800	-1.42138500
H	3.08958400	0.12095100	-1.80547000
H	3.96629300	-1.38438000	-2.08874300
O	6.33807600	-0.57995700	-1.32638100
H	6.37113500	-1.02982600	-2.18631900
O	0.83835100	2.98871400	-0.65909800
N	-1.60994200	1.38347400	-1.02591100
N	-2.90723100	-0.36910400	0.67789500
Cl	0.05021000	-0.90265700	-2.62665900
Cl	-1.56745200	-3.06209400	-0.52807700

Cl	-3.38011900	-0.81311400	-2.40282700
C	-2.90436600	1.08566500	1.04056100
C	-2.79913600	1.88973700	-0.25868400
C	-4.13368800	1.50350300	1.85396100
H	-1.99095800	1.24050800	1.62349000
C	-2.72978900	3.39518200	0.01690700
H	-3.67083700	1.66322400	-0.88100000
C	-4.08892000	3.01705400	2.13700800
C	-3.95186600	3.83492800	0.84345400
H	-2.68887300	3.94114500	-0.93219400
H	-1.80431500	3.62136900	0.56217900
H	-4.99780600	3.30868200	2.67464300
H	-3.24309000	3.23583100	2.80274100
H	-3.86339700	4.90133400	1.07831000
H	-4.86067500	3.71837600	0.23764900
H	-0.74015900	1.86509100	-0.73712200
H	-1.72650700	1.58036200	-2.02316100
H	-3.80992000	-0.65421900	0.28667500
H	-2.69780100	-0.97618100	1.49060700
H	-5.04273400	1.25776700	1.28811400
O	2.14688400	3.52685300	1.58500700
H	1.21111500	0.39578400	-0.82548100
H	-4.17074200	0.93649900	2.79053000
H	2.18433300	4.47713000	1.37144400
H	1.87465700	-4.45142600	3.20859500
N	-1.60543500	-1.73760500	2.99802400
H	-1.93631600	-2.34810200	3.74212500
H	-1.59358100	-0.77648000	3.33789500

2TS_A (Imaginary Frequency = 75.88i)
E (B3LYP/BS1, Solvent = water) = -3301.874660 au
H (B3LYP/BS1, Solvent = water) = -3301.359193 au
G(B3LYP/BS1, Solvent = water) = -3301.461189 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -3302.762794 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -3301.706711 au

Pt	-1.58409900	-0.67540700	-0.76929700
N	0.26273400	-0.54381500	1.16411000
P	1.90918000	2.62918600	0.58678800
O	1.85183300	1.16308000	1.27588100
O	3.19491500	2.65633300	-0.36380300
C	4.56705000	2.53007100	0.10903000
H	4.60830500	2.72728400	1.18251300
H	5.13096700	3.30484200	-0.41522400
C	5.15472300	1.15768000	-0.19225300
H	6.21288000	1.20030800	0.09136700
O	4.52011000	0.14750700	0.60804200
C	3.77883300	-0.76460000	-0.20075400
H	4.24805500	-1.75027100	-0.15251900
N	2.45246400	-0.94842400	0.37692600
C	1.40644800	0.07372000	0.46737100
C	0.70982400	-1.72166700	1.55980700

C	0.14582300	-2.70435000	2.45586400
N	0.80121800	-3.86979900	2.63916000
C	1.98322900	-4.02580100	2.04486100
N	2.69080900	-3.15471100	1.29112700
C	2.03793500	-2.02511500	1.06996000
C	5.04753800	0.67476500	-1.64887800
H	4.96346200	1.50792200	-2.35735100
C	3.78265600	-0.19280100	-1.62834600
H	2.90122000	0.42325200	-1.81811600
H	3.80416900	-0.98465500	-2.38083800
O	6.22200500	-0.09253700	-1.89818600
H	6.16128400	-0.44456200	-2.80125400
O	0.69481700	2.98864100	-0.19132400
N	-1.69044700	1.40061100	-0.91248500
N	-3.09547100	-0.39114400	0.60947100
Cl	0.05770600	-0.79678000	-2.51359600
Cl	-1.62635200	-3.04947200	-0.47655100
Cl	-4.05691900	-0.53325100	-2.48011600
C	-3.06589200	1.02782600	1.08760500
C	-2.88730600	1.90425000	-0.15499400
C	-4.31392600	1.42903000	1.87927700
H	-2.17519000	1.11502300	1.71990100
C	-2.79069800	3.38684700	0.21765100
H	-3.74268700	1.73762000	-0.81743100
C	-4.24337700	2.92003200	2.25813000
C	-4.03220200	3.81066000	1.02337100
H	-2.69820700	3.99043100	-0.69250900
H	-1.88180000	3.55376900	0.80985900
H	-5.16442600	3.20570500	2.77835100
H	-3.41878400	3.07405300	2.96772500
H	-3.92760600	4.85818500	1.32755500
H	-4.91927000	3.75642000	0.37733300
H	-0.83259400	1.87072400	-0.58443500
H	-1.78734300	1.64011000	-1.90151500
H	-3.94777300	-0.56889900	0.06279000
H	-3.08487000	-1.05965800	1.38109500
H	-5.20595800	1.24310900	1.26524500
O	2.24553000	3.44660600	1.91805800
H	1.11810800	0.40691600	-0.52594900
H	-4.40071200	0.80456800	2.77593600
H	2.21567200	4.41363200	1.79631800
H	2.46137600	-4.98915200	2.20682200
N	-0.97565900	-2.48437900	3.13170500
H	-1.30627900	-3.18631800	3.78354800
H	-1.41250100	-1.57356200	3.14298000

4_A

E (B3LYP/BS1, Solvent = water) = -1455.206658 au
H (B3LYP/BS1, Solvent = water) = -1454.922916 au
G(B3LYP/BS1, Solvent = water) = -1454.988909 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -1455.631198 au

E(M06/BS2//B3LYP/BS1, Solvent = water) = -1454.955193 au

P	1.80930100	-2.08658400	-0.14187300
O	0.30748300	-1.54547300	-0.49398500
O	2.63733300	-0.83698700	0.42610700
C	3.38022200	0.03292000	-0.47489800
H	3.47452300	-0.45050200	-1.44942300
H	4.37469100	0.15361700	-0.04026800
C	2.68140200	1.37909200	-0.61327800
H	3.22057200	1.95721600	-1.37116600
O	1.33114500	1.17336800	-1.08020400
C	0.39544100	1.59534000	-0.10577200
H	-0.12473800	2.49364800	-0.44867800
N	-0.66012900	0.57879400	0.01732800
C	-0.48469900	-0.84674800	0.41510500
C	-2.63256300	-0.47388300	0.15226300
C	-4.10480400	-0.45030400	0.05276200
N	-4.70015000	0.70699800	-0.26067400
C	-3.93135300	1.78485200	-0.47111900
N	-2.58975600	1.93438100	-0.41703700
C	-1.96047200	0.81188400	-0.11584100
C	2.56288900	2.22413900	0.66635600
H	3.35570900	1.99475900	1.38834300
C	1.17433400	1.84537100	1.19578300
H	1.24101900	0.93870500	1.80183400
H	0.71734200	2.63205400	1.80022300
O	2.62300500	3.58318600	0.24868100
H	2.51887600	4.14364300	1.03499100
O	1.49864900	-2.90127000	1.19962800
H	2.29401400	-3.14289200	1.70928000
N	-1.82852200	-1.42906700	0.42434000
O	2.36717100	-2.77842300	-1.31945700
H	-0.09979000	-0.89344900	1.43932400
H	-4.47889300	2.68835000	-0.72754400
N	-4.80236000	-1.54141200	0.26912600
H	-4.35173900	-2.41845900	0.50835600
H	-5.81535800	-1.51695900	0.19692800

7_A

E (B3LYP/BS1, Solvent = water) = -1454.817773 au

H (B3LYP/BS1, Solvent = water) = -1454.546597 au

G(B3LYP/BS1, Solvent = water) = -1454.612179 au

E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -1455.249918 au

E(M06/BS2//B3LYP/BS1, Solvent = water) = -1454.580483 au

P	1.66979100	-2.01205200	0.34645200
O	0.61051300	-1.47319600	-0.77753800
O	2.65555100	-0.78403900	0.62909500
C	3.34422100	-0.05235200	-0.42360500
H	3.34013000	-0.63043600	-1.35061300
H	4.37602200	0.05970200	-0.08268600
C	2.71713400	1.31617800	-0.65216900
H	3.36676600	1.85797000	-1.34818700
O	1.42220100	1.19308200	-1.27103900
C	0.39326900	1.56452800	-0.37444700
H	-0.11912900	2.45515400	-0.74902200
N	-0.64465100	0.52082800	-0.34710200

C	-0.55882700	-0.85725300	-0.46526000
C	-2.61725600	-0.47284000	-0.16344200
C	-4.01524500	-0.47228900	0.02858700
N	-4.63842100	0.71121000	0.20997900
C	-3.90249200	1.83318600	0.19507600
N	-2.58153300	1.96575600	0.02841400
C	-1.99179500	0.77596200	-0.14833500
C	2.49924300	2.16265900	0.61197700
H	3.20796300	1.90409400	1.40820900
C	1.05213400	1.82502900	0.99231300
H	1.01953400	0.92606600	1.61225900
H	0.55877400	2.63582900	1.53435400
O	2.64916500	3.52229700	0.21302000
H	2.45981800	4.08077100	0.98459300
O	1.08786300	-2.53331300	1.59899400
N	-1.69794300	-1.48747800	-0.37294100
O	2.42582700	-3.01904900	-0.64554900
H	3.12298600	-3.53361100	-0.19948800
N	-4.75889900	-1.60557500	0.00218700
H	-5.71034400	-1.55041600	0.33994500
H	-4.29263400	-2.49795600	0.08681600
H	-4.45789600	2.75732700	0.34324600

4TS_G (Imaginary Frequency = 224.83i)
E (B3LYP/BS1, Solvent = water) = -1759.800698 au
H (B3LYP/BS1, Solvent = water) = -1759.432614 au
G(B3LYP/BS1, Solvent = water) = -1759.516556 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -1760.389633 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -1759.570805 au

P	-1.93343100	1.96759500	0.21481700
O	-0.85960100	1.22228900	-0.79040100
O	-2.98845900	0.85727100	0.63740800
C	-3.91317600	0.22708500	-0.30340000
H	-3.95510700	0.81368800	-1.22278400
H	-4.89127600	0.25252700	0.18066300
C	-3.49957100	-1.20367600	-0.60733200
H	-4.23608200	-1.60974300	-1.30879700
O	-2.21189900	-1.21752400	-1.25978200
C	-1.24457300	-1.83748400	-0.44562600
H	-0.90324500	-2.76808000	-0.90611300
N	-0.02977500	-0.98915600	-0.37857300
C	0.11161900	0.37234400	-0.43666200
C	2.09861300	-0.41993200	-0.07693300
C	3.49840300	-0.64325200	0.10119000
N	3.75820400	-2.02225600	0.23621500
H	4.73945400	-2.25314000	0.36054300
C	2.82515800	-3.03479200	0.16999800
N	3.26796200	-4.30230500	0.27162700
H	4.19880500	-4.51730200	0.59954100
H	2.57133200	-5.03074300	0.34626300
N	1.53157500	-2.80818800	-0.02407400
C	1.23796100	-1.50581200	-0.14801700
C	-3.37560600	-2.15154800	0.59668100
H	-4.00628300	-1.83546500	1.43634900
C	-1.88234200	-2.07342500	0.93433400

H	-1.68471700	-1.22879900	1.59939200
H	-1.50605100	-2.98234000	1.40941000
O	-3.75425500	-3.43966000	0.12386600
H	-3.65204400	-4.06893800	0.85641600
O	-1.32109400	2.62842600	1.39078800
N	1.36638600	0.74202600	-0.26243400
O	-2.56616200	2.87176300	-0.93555800
O	4.42946000	0.16722200	0.14044900
H	1.78435100	1.85691500	-0.01035100
H	-0.25128000	4.13626100	1.04837800
H	-3.14018800	3.58489900	-0.59918000
O	0.42794600	4.76545200	0.72036600
H	0.05741500	5.11650100	-0.10559900
H	1.69117100	3.70602000	0.41324100
O	2.32533300	2.92989600	0.42029100
H	3.14120400	3.10547800	-0.13243400
O	4.60609400	2.77150500	-0.91748200
H	5.31271800	3.20444400	-0.41088500
H	4.63300000	1.83290600	-0.62059300

10_G

E (B3LYP/BS1, Solvent = water) = -1759.801021 au
H (B3LYP/BS1, Solvent = water) = -1759.429700 au
G(B3LYP/BS1, Solvent = water) = -1759.515122 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -1760.391308 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -1759.571811 au

P	-1.92859600	1.97329900	0.22718400
O	-0.85276900	1.22617500	-0.78457700
O	-2.98020800	0.85817500	0.64183900
C	-3.91086000	0.23840600	-0.30096100
H	-3.95214600	0.83148000	-1.21610100
H	-4.88745500	0.26501400	0.18587600
C	-3.50330800	-1.19173200	-0.61483200
H	-4.23957200	-1.58892300	-1.32143600
O	-2.21380900	-1.20591800	-1.26516100
C	-1.25204500	-1.83712700	-0.45547200
H	-0.90885700	-2.76225500	-0.92524800
N	-0.03405600	-0.99002300	-0.37503000
C	0.10472300	0.36729900	-0.43531100
C	2.10105100	-0.43500900	-0.06660100
C	3.50032300	-0.66309600	0.11328400
N	3.75034100	-2.04375300	0.24957000
H	4.72974800	-2.28104900	0.37704100
C	2.81082900	-3.05067100	0.18201700
N	3.24216000	-4.31868900	0.29278500
H	4.18092200	-4.54568700	0.58769400
H	2.54486900	-5.04832500	0.34300400
N	1.51801600	-2.81563400	-0.01613700
C	1.23279000	-1.51308900	-0.13999400
C	-3.38564400	-2.15081800	0.58089200
H	-4.01486200	-1.83827700	1.42291400
C	-1.89209500	-2.08449800	0.92128500
H	-1.69064200	-1.24825300	1.59568700
H	-1.52141000	-3.00055400	1.38672600
O	-3.77113800	-3.43218800	0.09638400

H	-3.67778300	-4.06789700	0.82456600
O	-1.30820100	2.62608400	1.40205100
N	1.36690600	0.72446600	-0.25639400
O	-2.55765500	2.87903600	-0.92249900
O	4.43172600	0.14455000	0.15221300
H	1.74516300	1.75777400	-0.06529100
H	-0.24701900	4.16829900	1.05358600
H	-3.11571500	3.60506600	-0.58655000
O	0.40381000	4.82177500	0.71998300
H	0.01278200	5.15188500	-0.10488900
H	1.73349600	3.75109800	0.39391000
O	2.35569300	2.97729700	0.41434700
H	3.15101500	3.15051700	-0.15228500
O	4.65858900	2.74713700	-0.96472200
H	5.36970400	3.17101700	-0.45728300
H	4.65024300	1.82004000	-0.63793500

11_G

E (B3LYP/BS1, Solvent = water) = -1530.499947 au
H (B3LYP/BS1, Solvent = water) = -1530.210147 au
G(B3LYP/BS1, Solvent = water) = -1530.280052 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -1530.958256 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -1530.256443 au

P	2.28237100	-1.80455100	0.40834900
O	1.12362500	-1.51207800	-0.76838100
O	2.91620600	-0.37637400	0.69766000
C	3.54798800	0.45967700	-0.31875400
H	3.73117300	-0.12461000	-1.22264400
H	4.50496600	0.77197200	0.10341900
C	2.68071700	1.66746900	-0.63244000
H	3.23232500	2.29176200	-1.34234900
O	1.45737300	1.24974200	-1.27910500
C	0.34785100	1.47822900	-0.44998500
H	-0.32454200	2.20777800	-0.90756900
N	-0.47282500	0.23486200	-0.37289200
C	-0.08981000	-1.06207700	-0.49171800
C	-2.28077200	-1.06562600	-0.19691500
C	-3.66795900	-1.38466500	-0.02780600
N	-4.40426800	-0.18529000	0.13570600
H	-5.40370500	-0.32324700	0.25135100
C	-3.89193100	1.09353200	0.13485700
N	-4.75094500	2.11537900	0.27795100
H	-5.71930800	1.97960800	0.53076200
H	-4.36663200	3.04594300	0.36403900
N	-2.59547300	1.35194000	-0.02120200
C	-1.85571000	0.24932300	-0.18453900
C	2.24635600	2.52149000	0.57040300
H	2.94987700	2.44165100	1.40767600
C	0.86913600	1.93942200	0.92095600
H	0.97260800	1.09143300	1.60164900
H	0.20611000	2.67460700	1.38218200
O	2.15970500	3.85894100	0.09368500
H	1.86715000	4.42109900	0.82960800
O	1.75087400	-2.45004400	1.62026500
N	-1.15863300	-1.85454300	-0.39231400

O	3.24318800	-2.59963800	-0.58328200
O	-4.21055700	-2.48072200	-0.01492000
H	-1.12923300	-2.86674800	-0.45907600
H	3.96015300	-3.07867300	-0.12677200

12_G

E (B3LYP/BS1, Solvent = water) = -1759.782983 au
H (B3LYP/BS1, Solvent = water) = -1759.409576 au
G(B3LYP/BS1, Solvent = water) = -1759.500601 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -1760.378217 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -1759.562024 au

P	-1.86972400	-0.84430900	-0.48904400
O	-0.45573200	-0.70014500	-1.39798600
O	-2.54132000	0.57312700	-0.63657200
C	-2.68525000	1.51483600	0.47506200
H	-2.96184800	0.95174500	1.36682400
H	-3.52340400	2.15237900	0.19081800
C	-1.41928700	2.33358300	0.65898100
H	-1.55575700	2.95916200	1.54823000
O	-0.31949800	1.42592800	0.88715300
C	0.74059000	1.70118900	-0.01490500
H	1.52798600	2.28101200	0.47249500
N	1.37288000	0.41498000	-0.34527500
C	0.76790700	-0.66681900	-0.89915100
C	2.84600200	-1.25774500	-0.44444000
C	4.09899600	-1.93013400	-0.26550400
N	5.01882700	-1.04344100	0.34687900
H	5.93964600	-1.44160000	0.50501100
C	4.76972600	0.25798100	0.72322000
N	5.77361300	0.95643200	1.27552000
H	6.65043600	0.53218200	1.54185400
H	5.57019300	1.88317600	1.62294100
N	3.59035800	0.84911600	0.54259700
C	2.68629400	0.05383700	-0.03593700
C	-0.99734600	3.24486200	-0.51422200
H	-1.83123800	3.45193400	-1.19509400
C	0.11934900	2.44671100	-1.20143900
H	-0.30172700	1.74829700	-1.92811500
H	0.84292200	3.08641000	-1.71143000
O	-0.50932400	4.44349700	0.07877700
H	-0.23585500	5.04109100	-0.63634900
O	-2.76114300	-1.64833500	-1.54278000
N	1.63229900	-1.67549900	-0.97317600
O	-1.58736500	-1.44746400	0.83016900
O	4.40792900	-3.07551000	-0.56288200
H	1.42113700	-2.58698900	-1.36745800
O	-4.86327700	-0.47286800	1.74496100
H	-5.18559900	-0.68524700	0.84359900
H	-4.46101100	-1.31011200	2.06153100
O	-3.43708000	-2.80385000	2.49383800
H	-3.78058500	-3.51194600	1.92552400
H	-2.68880400	-2.43483900	1.98216600
O	-5.63545400	-1.04978700	-0.94399700
H	-4.78829900	-1.35653700	-1.31288600
H	-5.75556100	-0.17154000	-1.34038700

H	-2.49637300	-2.58161400	-1.65486500

13_G

E (B3LYP/BS1, Solvent = water) = -1759.829288 au
H (B3LYP/BS1, Solvent = water) = -1759.460002 au
G(B3LYP/BS1, Solvent = water) = -1759.548936 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -1760.422207 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -1759.602235 au

P	-3.06048900	-0.69528500	0.25625900
O	-0.18268600	-0.71622900	-1.85708100
O	-2.74399600	0.84710300	0.13752600
C	-2.37675800	1.71672700	1.24883300
H	-2.34007000	1.13461600	2.17024700
H	-3.15306300	2.48072600	1.32553800
C	-1.02603800	2.34669800	0.96420600
H	-0.80180900	3.02222800	1.80093000
O	-0.03907800	1.30838700	0.89422600
C	0.85222800	1.59669900	-0.18745800
H	1.65771300	2.25012700	0.16173900
N	1.50537400	0.36918100	-0.59612800
C	0.94394800	-0.68548300	-1.32665200
C	3.04271700	-1.25007200	-0.70006300
C	4.29208900	-1.88888500	-0.46643100
N	5.12763200	-1.03488600	0.30541400
H	6.04921800	-1.41368000	0.49995000
C	4.79495800	0.21442900	0.76624200
N	5.74164300	0.90916500	1.44726000
H	6.50232500	0.41596200	1.89505100
H	5.41296300	1.73413000	1.93164300
N	3.61811400	0.77724200	0.53285700
C	2.79184200	0.01060400	-0.20067300
C	-0.91808800	3.16966900	-0.34541400
H	-1.89921900	3.33912000	-0.80488100
C	-0.01279800	2.30518400	-1.23265200
H	-0.60208300	1.57425300	-1.78732700
H	0.57827100	2.90016100	-1.93402800
O	-0.31146400	4.40966900	0.01496800
H	-0.24343000	4.95065700	-0.78870900
O	-2.52254100	-1.35589000	-1.05340500
N	1.89720200	-1.65720400	-1.38371000
O	-2.39929500	-1.20146900	1.57224800
O	4.68455500	-2.99646100	-0.83027800
H	1.76597400	-2.53151700	-1.87325000
O	-4.58735200	-1.00161000	0.33743700
H	-5.15203900	-0.82556700	-0.50697000
H	-4.10555300	-3.52240200	2.54565300
O	-3.13528200	-3.45789900	2.51628900
H	-2.85159900	-4.18501100	1.93548300
H	-2.71226000	-2.11791900	1.93583800
O	-6.06106500	-0.56458100	-1.71376500
H	-5.69895300	-0.98555200	-2.51245500
H	-6.07827600	0.38647900	-1.91741700
H	-1.56950500	-1.10359700	-1.32574300

$(H_2O)(OH^-)$

E (B3LYP/BS1, Solvent = water) = -228.761526 au
H (B3LYP/BS1, Solvent = water) = -228.695840 au
G(B3LYP/BS1, Solvent = water) = -228.730606 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -228.926337 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -228.804665 au

O	-0.01728000	1.42249800	-0.11909600
H	1.07885700	0.21236400	-0.09926800
O	1.49805100	-0.71124600	-0.00140400
H	0.66527900	-1.19327400	0.15737600
O	-1.40837800	-0.70167600	0.11017800
H	-0.90373400	0.22561500	0.01960500
H	-1.48594800	-0.99094200	-0.81266000
H	0.06640400	1.66962700	0.81752100

2TS_G(dep) (Imaginary Frequency = 277.78i)
E (B3LYP/BS1, Solvent = water) = -3376.622901 au
H (B3LYP/BS1, Solvent = water) = -3376.117170 au
G(B3LYP/BS1, Solvent = water) = -3376.219973 au
E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -3377.553168 au
E(M06/BS2//B3LYP/BS1, Solvent = water) = -3376.469575 au

Pt	1.69208400	0.37554500	-0.98100600
N	-0.13527000	0.62438200	0.35950000
P	-1.67819800	-2.75019200	0.40106100
O	-1.49605600	-1.45387200	1.20501900
O	-3.09499500	-2.74273100	-0.41254600
C	-4.35454300	-2.62405300	0.27473600
H	-4.22768300	-2.79965200	1.34682100
H	-5.00352800	-3.41146500	-0.12423000
C	-5.02999300	-1.27270300	0.06276200
H	-6.04194500	-1.35580200	0.47934500
O	-4.34943700	-0.22729500	0.77171700
C	-3.72146500	0.68587000	-0.13053600
H	-4.20618500	1.65996800	-0.02427900
N	-2.33159400	0.89394100	0.24483200
C	-1.25769400	0.05952300	-0.06337000
C	-0.44309600	1.88701000	0.86367700
C	0.31922700	2.83542800	1.60100700
N	-0.48017800	3.92794800	2.01134300
H	0.02489700	4.65793900	2.50319400
C	-1.83366600	4.04398900	1.81923800
N	-2.43085000	5.19606600	2.21539200
H	-1.98362800	5.78963200	2.90099100
H	-3.44168100	5.17874800	2.24339800
N	-2.55738900	3.09608200	1.24392100
C	-1.83378000	2.04802400	0.81297400
C	-5.12691200	-0.80005300	-1.39613500
H	-5.11264000	-1.63898100	-2.10357100
C	-3.89644900	0.09747500	-1.53790000
H	-3.01831300	-0.49999700	-1.79100300
H	-4.02493400	0.87572000	-2.29601400
O	-6.34969400	-0.06834300	-1.50537700
H	-6.38429300	0.31170000	-2.39822200
O	-0.61604400	-3.17550100	-0.57617600
N	1.77518700	-1.65060900	-0.52046500

N	2.74373400	0.56841700	0.79149900
Cl	0.52420800	-0.06720300	-3.05500000
Cl	1.80369100	2.72780700	-1.50937400
Cl	4.11808600	-0.11732600	-2.10608500
C	2.53101700	-0.67043900	1.59935700
C	2.67920000	-1.86732300	0.65769600
C	3.47813100	-0.77976200	2.79842300
H	1.49297300	-0.62115300	1.94364000
C	2.42216700	-3.19094000	1.38540500
H	3.69733800	-1.86079900	0.25298200
C	3.24047600	-2.10785700	3.54054000
C	3.36263900	-3.31598800	2.59873000
H	2.56931000	-4.02858000	0.69391800
H	1.37669900	-3.22672900	1.71735400
H	3.95626100	-2.19774700	4.36556000
H	2.23848900	-2.09543800	3.99121400
H	3.13718500	-4.24156000	3.14071900
H	4.40000500	-3.40135000	2.24622100
H	0.83058800	-2.06680300	-0.38904900
H	2.17355600	-2.11267600	-1.34043500
H	3.73032200	0.68409600	0.54323600
H	2.41078100	1.41796700	1.29114600
H	4.51832000	-0.73275800	2.44621800
O	-1.90328000	-3.86636400	1.58009600
O	1.52190900	2.83046200	1.91624200
H	3.32481100	0.07280900	3.46996500
H	-1.82429500	-4.76612800	1.21768800

2_G(dep)

E (B3LYP/BS1, Solvent = water) = -3376.658522 au

H (B3LYP/BS1, Solvent = water) = -3376.151324 au

G(B3LYP/BS1, Solvent = water) = -3376.254595 au

E(B3LYP/BS2//B3LYP/BS1, Solvent = water) = -3377.601139 au

E(M06/BS2//B3LYP/BS1, Solvent = water) = -3376.513991 au

Pt	1.91806100	0.19756700	-0.91905200
N	0.14822700	0.99568300	-0.23295600
P	-2.29443500	-2.94542900	0.28642100
O	-2.12543000	-2.45956000	1.69845000
O	-3.51375900	-2.12996900	-0.47521900
C	-4.67107100	-1.72707300	0.25720300
H	-4.49990600	-1.83925500	1.33229800
H	-5.52104300	-2.36084300	-0.03021900
C	-5.01665100	-0.27110500	-0.03274700
H	-5.97179000	-0.05157100	0.46257300
O	-4.00856000	0.59583900	0.51691200
C	-3.40032600	1.38491100	-0.50896800
H	-3.78302700	2.40757700	-0.43615200
N	-1.96526000	1.46665800	-0.26724200
C	-1.00369600	0.61447300	-0.79654300
C	-0.04168300	2.07949600	0.65449900
C	0.75598000	2.78596700	1.59853100
N	0.02271100	3.80112100	2.24428800
H	0.56523200	4.34540700	2.90730000
C	-1.31741500	4.04828000	2.08741000
N	-1.84824200	5.10663000	2.75593100

H	-1.38739500	5.45658700	3.58547200
H	-2.85918200	5.13620000	2.78087100
N	-2.07663300	3.32438400	1.28702700
C	-1.40540800	2.36979600	0.61147100
C	-5.13901300	0.10151800	-1.52097800
H	-5.34950600	-0.77409500	-2.14783800
C	-3.77580800	0.72126500	-1.83343000
H	-3.04401300	-0.05453000	-2.06077800
H	-3.81378500	1.43401900	-2.66289100
O	-6.20244800	1.05422000	-1.61680300
H	-6.23922700	1.35817600	-2.53830000
O	-1.14859400	-2.95034400	-0.70392700
N	1.31787700	-1.73971600	-0.44684300
N	2.65368300	0.17775400	1.01113100
Cl	1.14895900	0.00408600	-3.19455400
Cl	2.74715600	2.40890800	-1.36392500
Cl	4.03747800	-0.78841400	-1.61596400
C	2.00480800	-0.93782200	1.76449200
C	1.97419000	-2.15761300	0.84118000
C	2.71689000	-1.24427300	3.08589800
H	0.97649500	-0.61385200	1.96011900
C	1.29874700	-3.35542900	1.51698400
H	3.00645000	-2.41436500	0.57868200
C	2.06254300	-2.45752600	3.77166000
C	2.01938300	-3.67796600	2.83927900
H	1.32260400	-4.21826900	0.84226100
H	0.24645600	-3.11897200	1.70788700
H	2.61543500	-2.69563100	4.68730400
H	1.04090400	-2.19355800	4.07706400
H	1.50736400	-4.51117500	3.33420200
H	3.04395900	-4.01650700	2.63048600
H	0.27712000	-1.87817500	-0.43277900
H	1.64833100	-2.33893000	-1.20715200
H	3.66394700	0.02761300	0.92990000
H	2.48725700	1.11681800	1.44762700
H	3.77515200	-1.46033400	2.88376000
O	-2.91127400	-4.47810300	0.39250400
O	1.94612300	2.62901700	1.93727100
H	2.68334800	-0.36262500	3.73548400
H	-2.87834100	-4.90419600	-0.48037700

Oxidation of guanine starting from the stereoisomer 2″_G. The redox reaction from **2″_G** is computed to be energetically more demanding than that from **2_G** (Figure S1). The rate of the redox reaction at 298 K from **2″_G** is computed to be nearly 5.1×10^8 times lesser than that from **2_G**. In fact, the disruption of the intramolecular NH-C6O hydrogen bonding interaction causes all the stationary points on the PES to be considerably destabilized. In contrast, all the stationary points of the energy profiles given in Figures 1 profit from both the NH-C6O and NH-PO hydrogen bonding interactions. This result confirms the contribution of the intramolecular hydrogen bonding to the stability of both the transition structures and the intermediates on the potential energy surfaces.

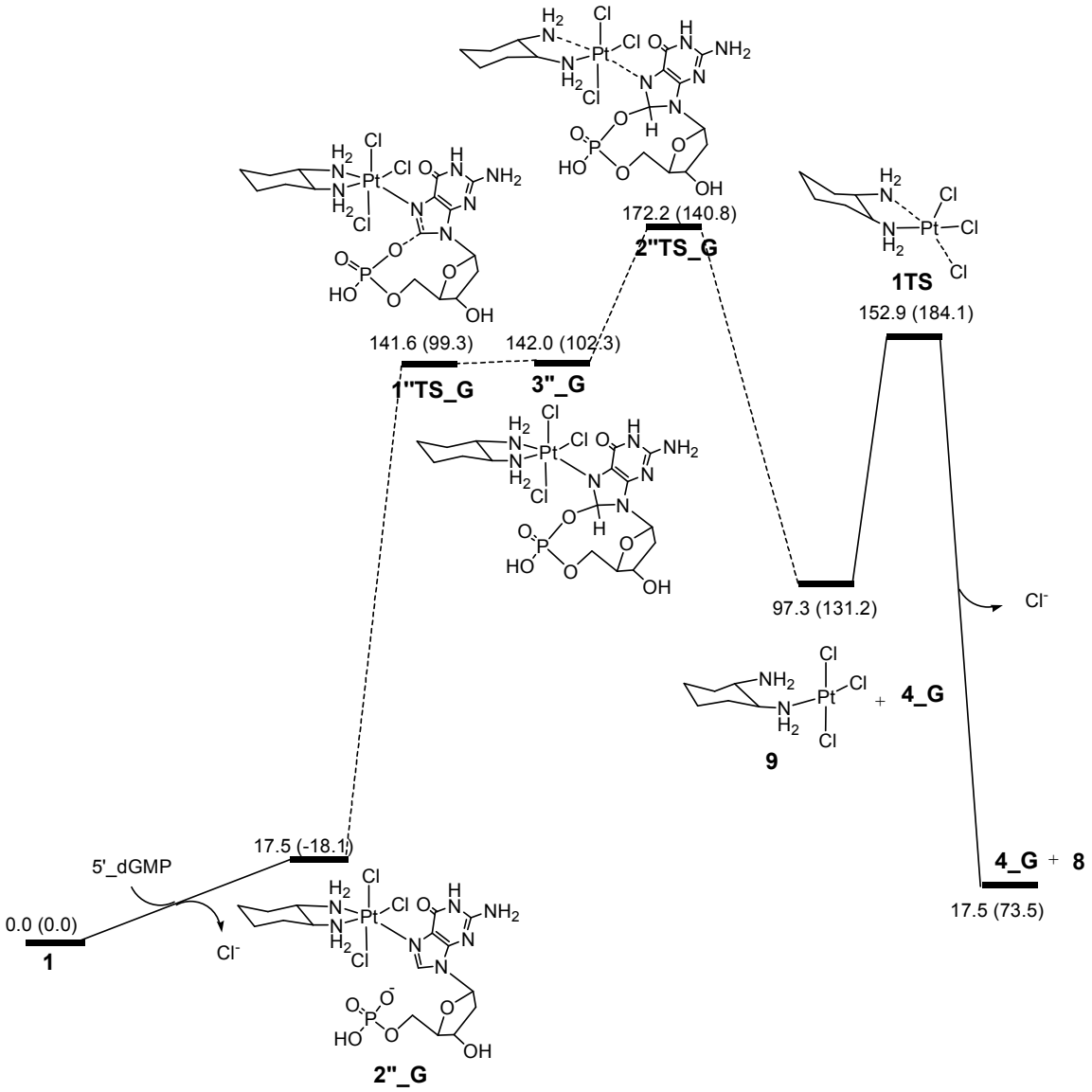
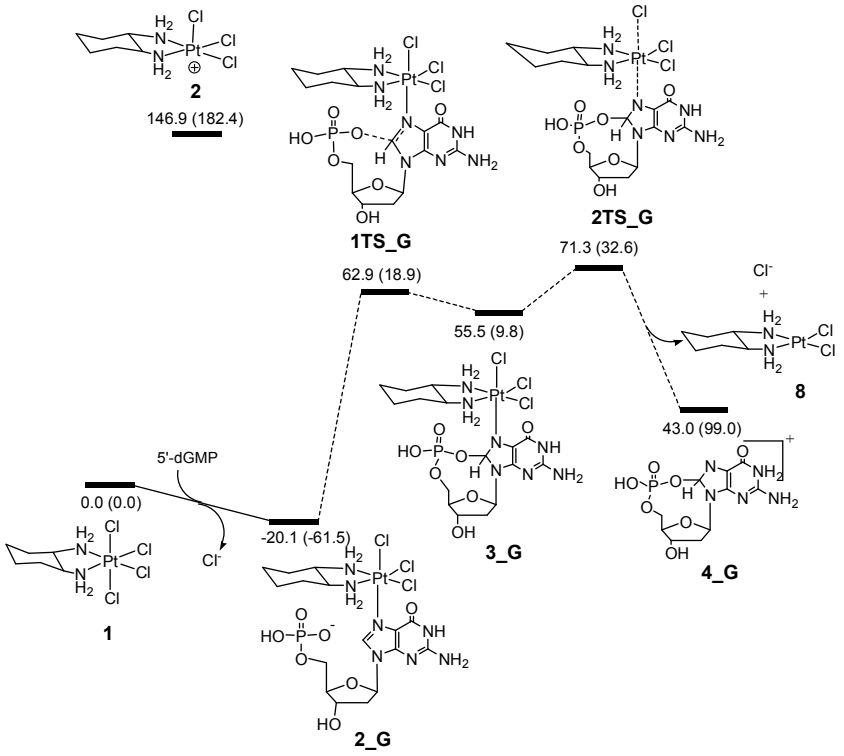
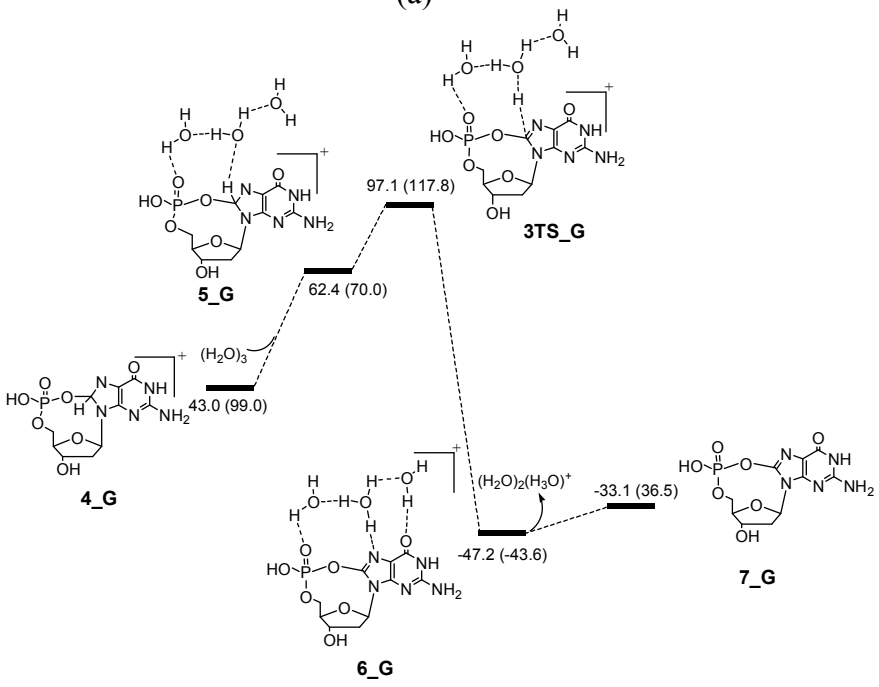


Figure S1. Energy profile calculated for the oxidation of 5′-dGMP by Pt^{IV} starting from the stereoisomer **2′′_G**. The relative free energies and electronic energies (in parentheses) obtained from the B3LYP/BS2//B3LYP/BS1 calculations are given in kJ mol^{-1}.



(a)



(b)

Figure S2. Energy profile calculated for the oxidation of 5′-dGMP by [$Pt^{IV}Cl4$(dach)] leading to (a) the formation of the cationic intermediate **4_G** and subsequently to (b) **7_G** through deprotonation of **4_G** by water. The relative free energies and electronic energies (in parenthesis) obtained from the M06/BS2//B3LYP/BS1 calculations are given in kJ mol^{-1}.

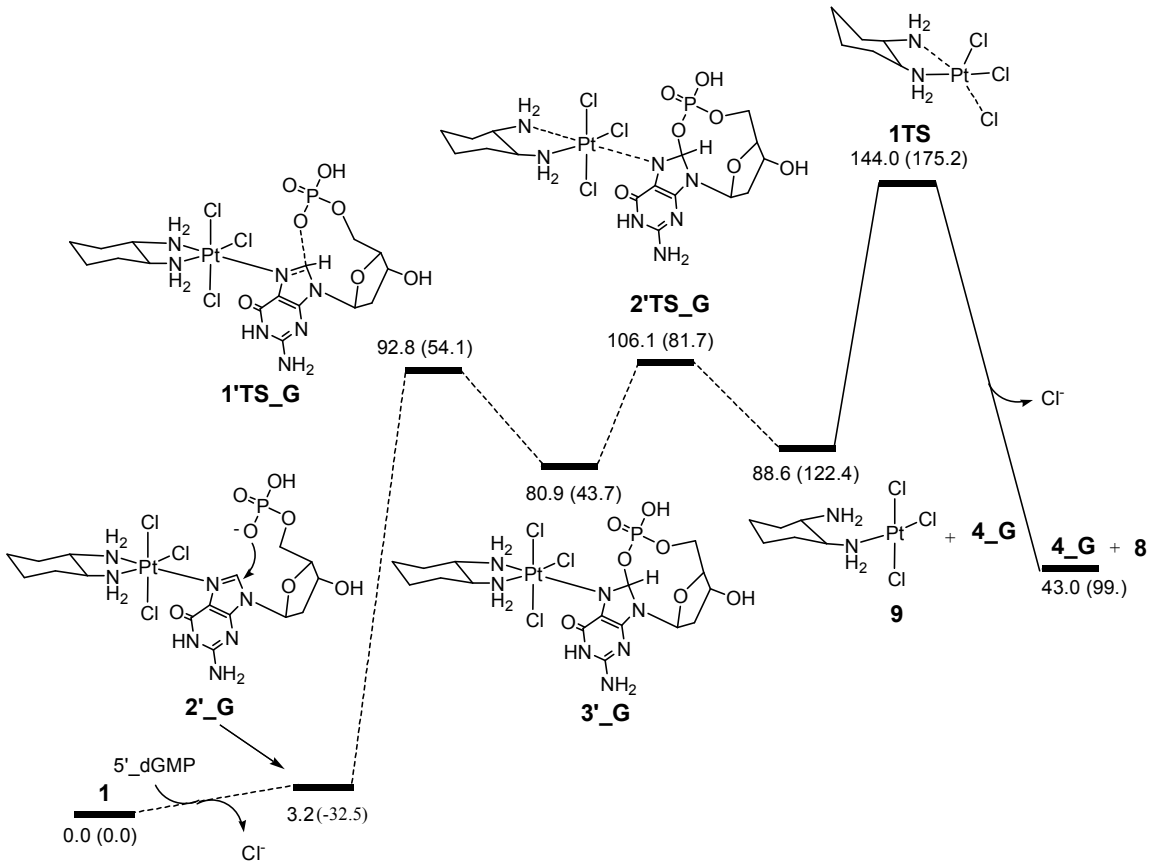


Figure S3. Energy profile calculated for the oxidation of 5′-dGMP by Pt^{IV} starting from the stereoisomer **2′_G**. The relative free energies and electronic energies (in parenthesis) obtained from the M06/BS2//B3LYP/BS1 calculations are given in kJ mol^{-1}.

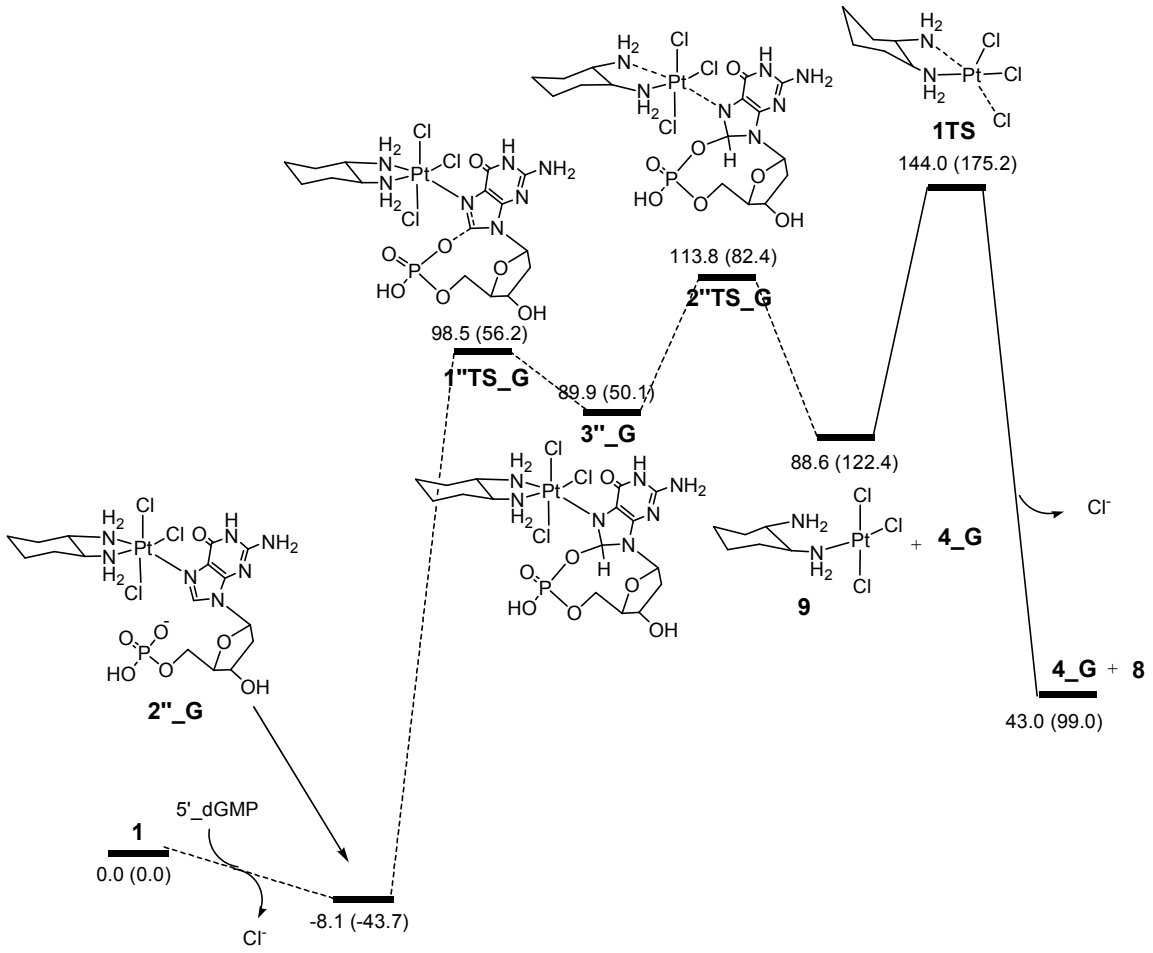


Figure S4. Energy profile calculated for the oxidation of 5′-dGMP by Pt^{IV} starting from the stereoisomer **2′′_G**. The relative free energies and electronic energies (in parenthesis) obtained from the M06/BS2//B3LYP/BS1 calculations are given in kJ mol^{-1}.

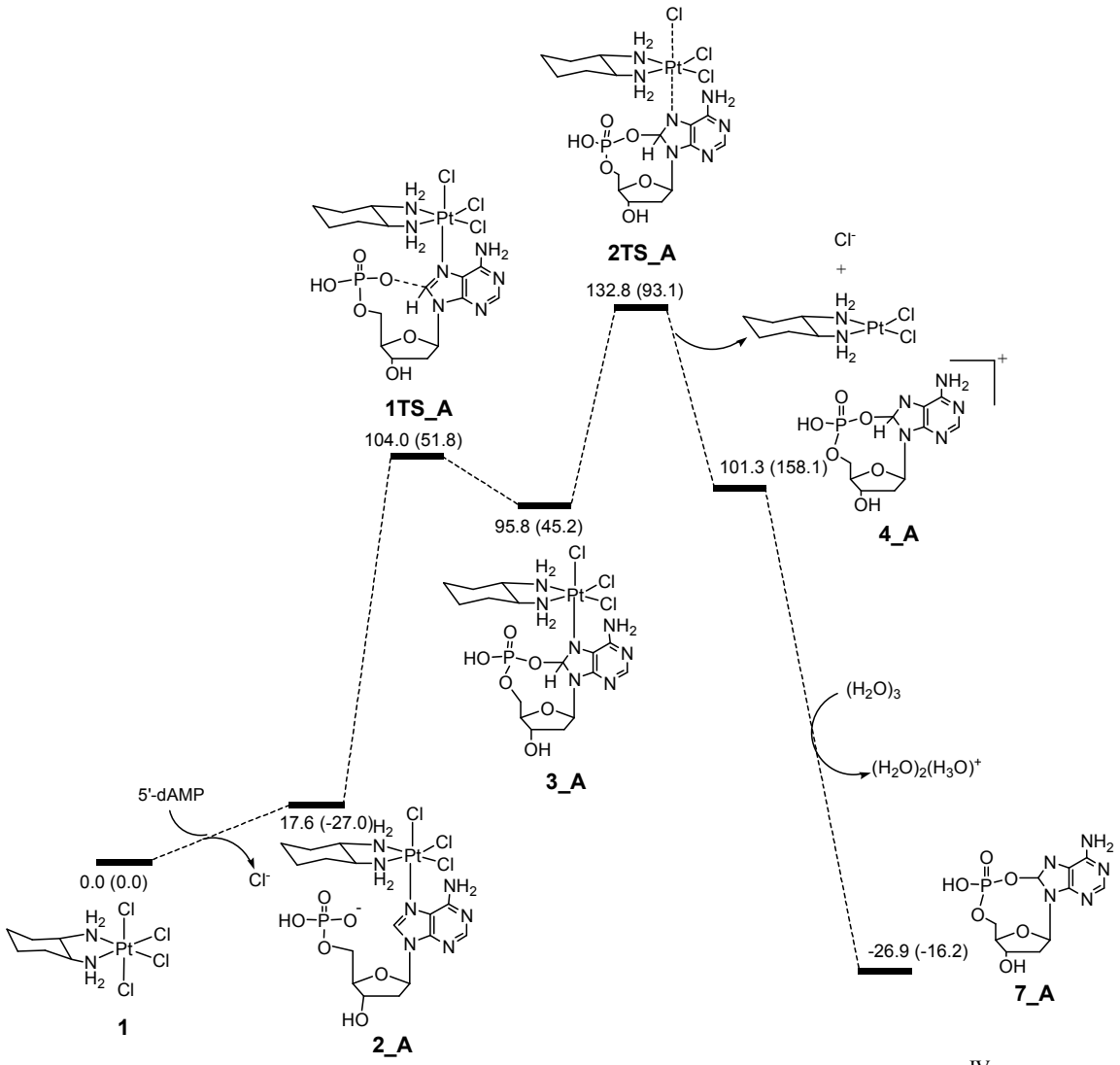


Figure S5. Energy profile calculated for the oxidation of 5′-dAMP by [$Pt^{IV}Cl_4$(dach)] leading to the formation of **7_A**. The relative free energies and electronic energies (in parenthesis) obtained from the M06/BS2//B3LYP/BS1 calculations are given in kJ mol^{-1}.

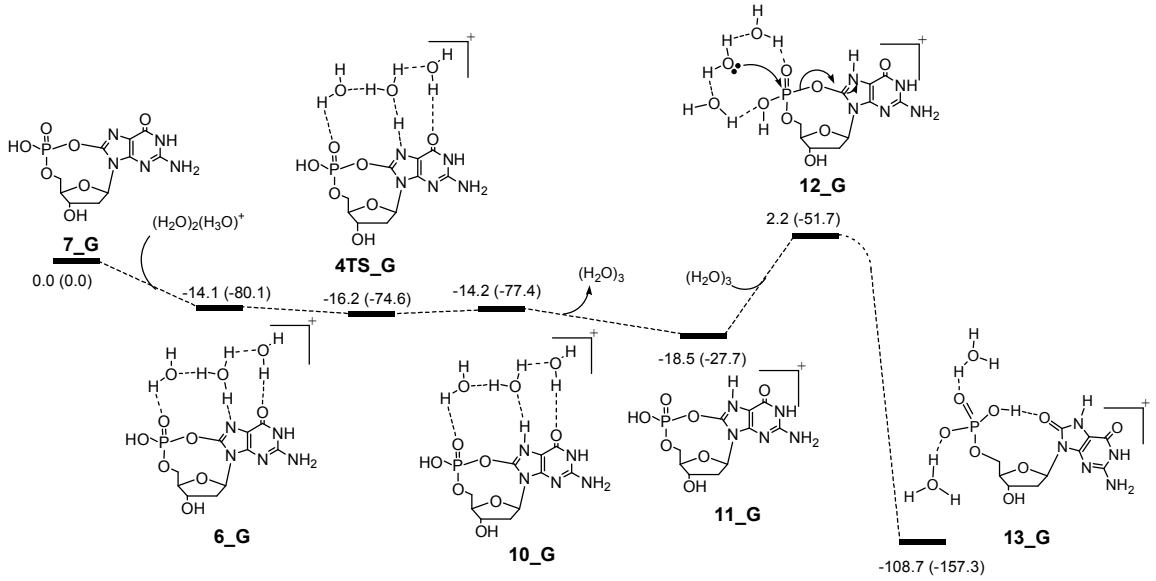


Figure S6. Energy profile calculated for the hydrolysis of the cyclic phosphodiester to 8-oxo-dGMP in the presence of $H3O^{+}$. The relative free energies and electronic energies (in parenthesis) obtained from the M06/BS2//B3LYP/BS1 calculations are given in kJ mol^{-1}.

An alternative mechanism for oxidation of 5′-dGMP. We also explored an alternative reaction mechanism (pathway 2) for the oxidation of 5′-dGMP in which the cyclic phosphodiester intermediate **7_G** is formed via the initial C8-H deprotonation of **2_G** by a base such as (H_2O or OH^-), followed by simultaneous the phosphate nucleophilic attack at C8 and redox reaction. Regardless of the nature of the base (H_2O or OH^-), pathway 2 is calculated to be more energy demanding than the pathway presented in Figure 1 (pathway 1); **2TS_G(dep)** lies much higher in energy than **2TS_G** at both B3LYP and M06 levels of theory (Figures S7-S10). Our calculations show that the overall activation barrier for pathway 2 depends on the basicity of the base; the stronger the base, the lower the overall activation barrier. This is because the deprotonation reaction (**2_G** → **2_G(dep)**) is far less endothermic in the presence of a stronger base (Figures S7-S10).

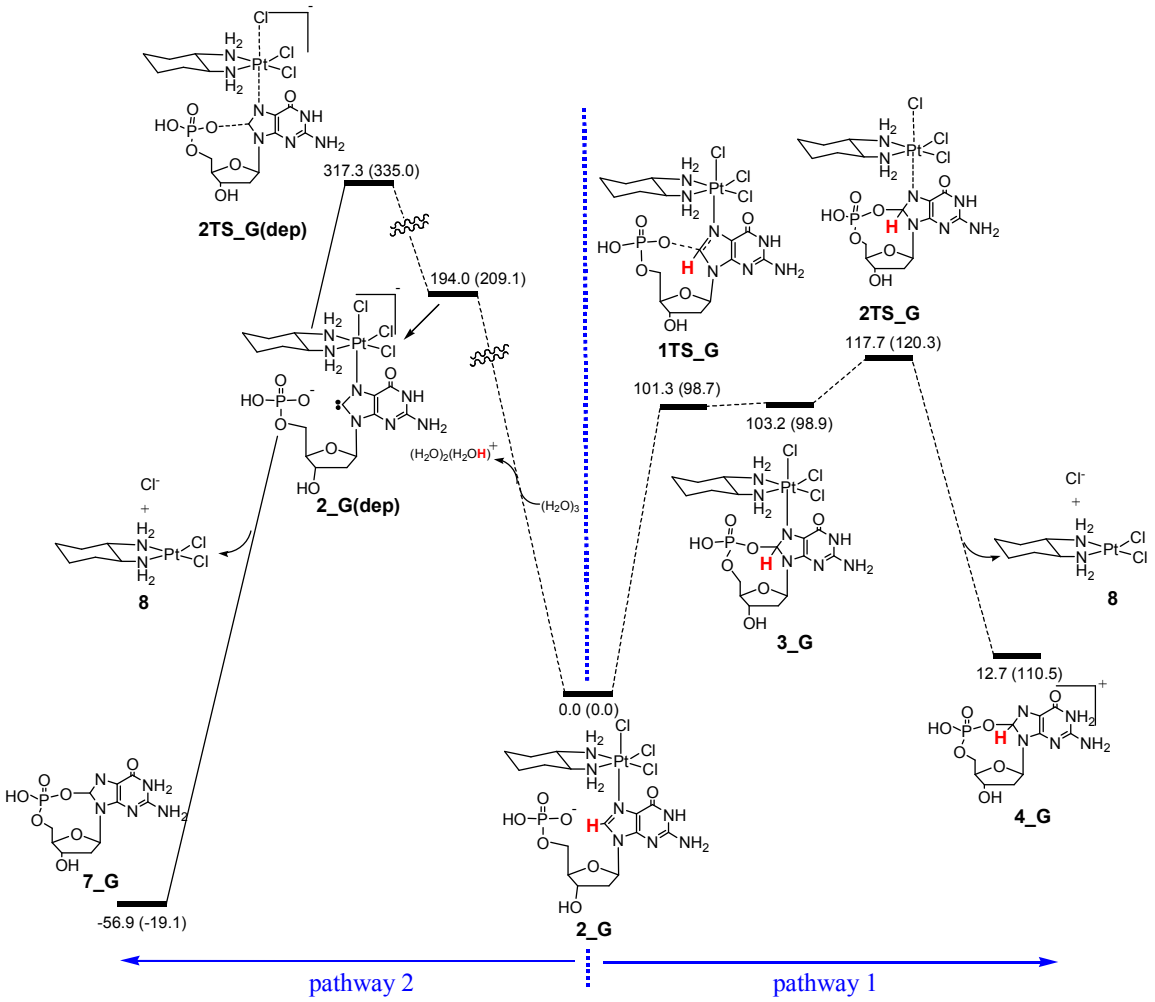


Figure S7. Comparison of energy profiles calculated for the oxidation of 5′-dGMP by [Pt^{IV}Cl4(dach)] via pathways 1 and 2. In pathway 2, H_2O is considered as the base. The relative free energies and electronic energies (in parenthesis) obtained from the B3LYP/BS2//B3LYP/BS1 calculations are given in kJ mol^{-1}.

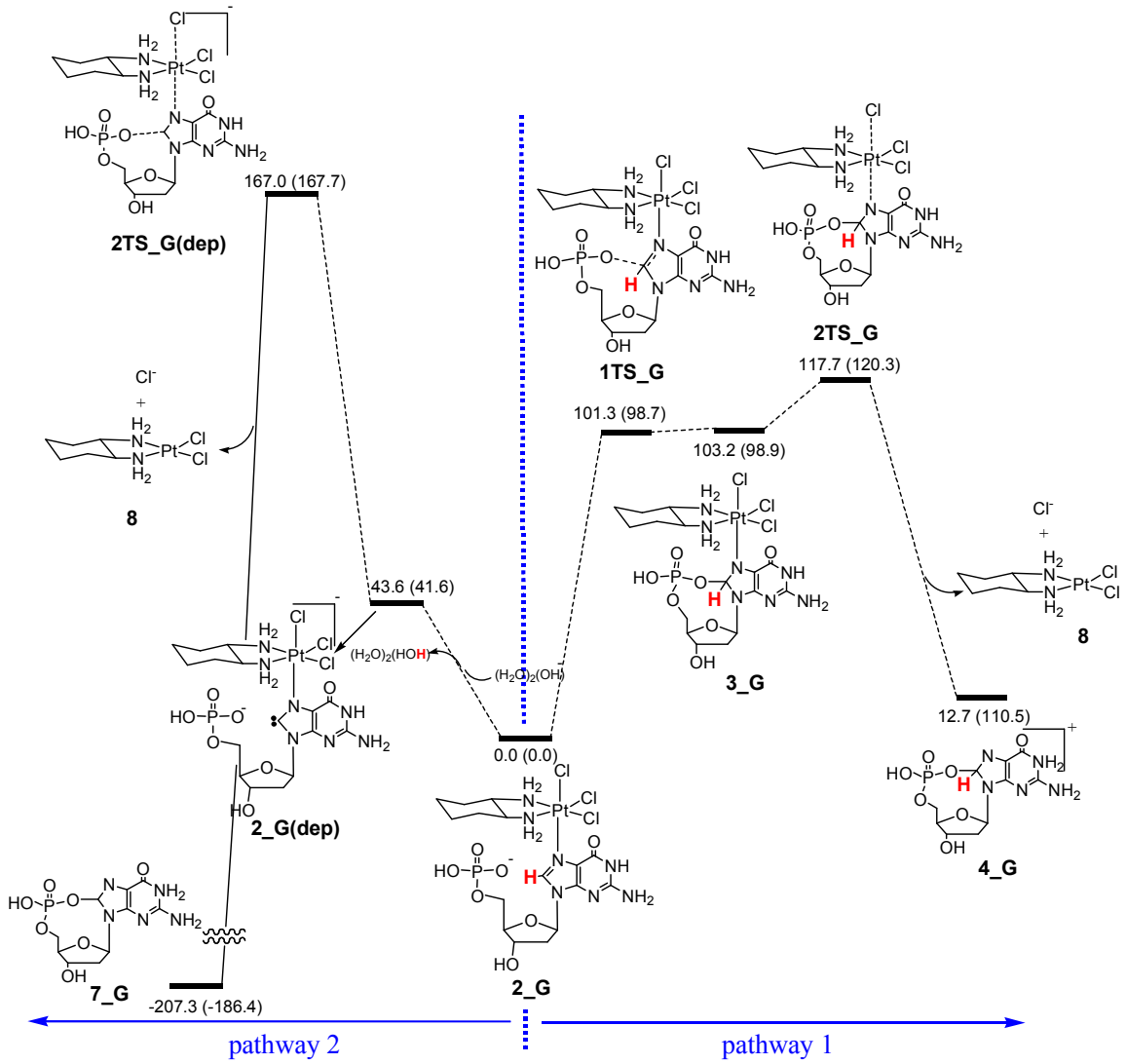


Figure S8. Comparison of energy profiles calculated for the oxidation of 5′-dGMP by [Pt^{IV}Cl4(dach)] via pathways 1 and 2. In pathway 2, OH^- is considered as the base. The relative free energies and electronic energies (in parenthesis) obtained from the B3LYP/BS2//B3LYP/BS1 calculations are given in kJ mol^{-1}.

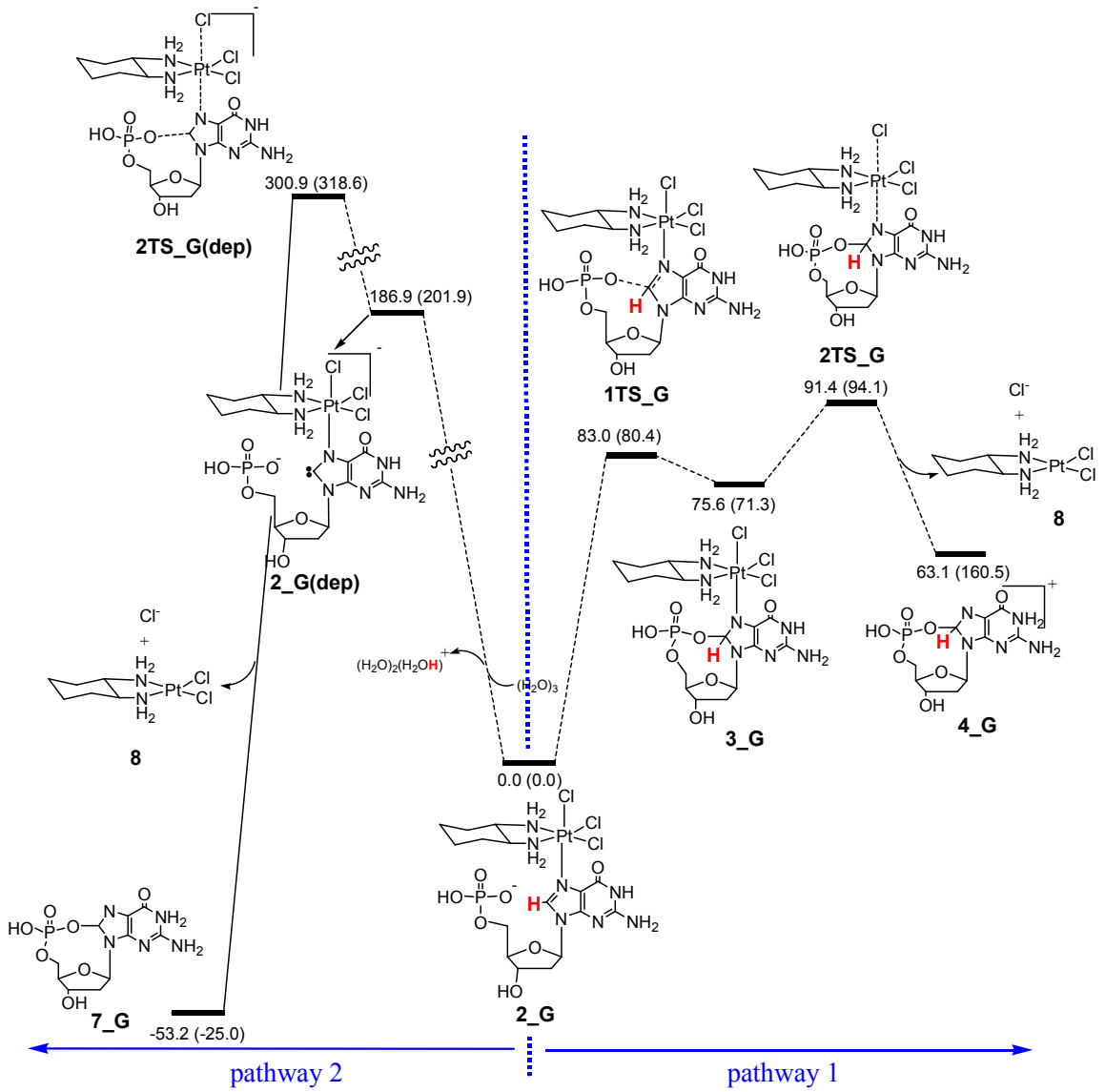


Figure S9. Comparison of energy profiles calculated for the oxidation of 5′-dGMP by [Pt^{IV}Cl4(dach)] via pathways 1 and 2. In pathway 2, H_2O is considered as the base. The relative free energies and electronic energies (in parenthesis) obtained from the M06/BS2//B3LYP/BS1 calculations are given in kJ mol^{-1}.

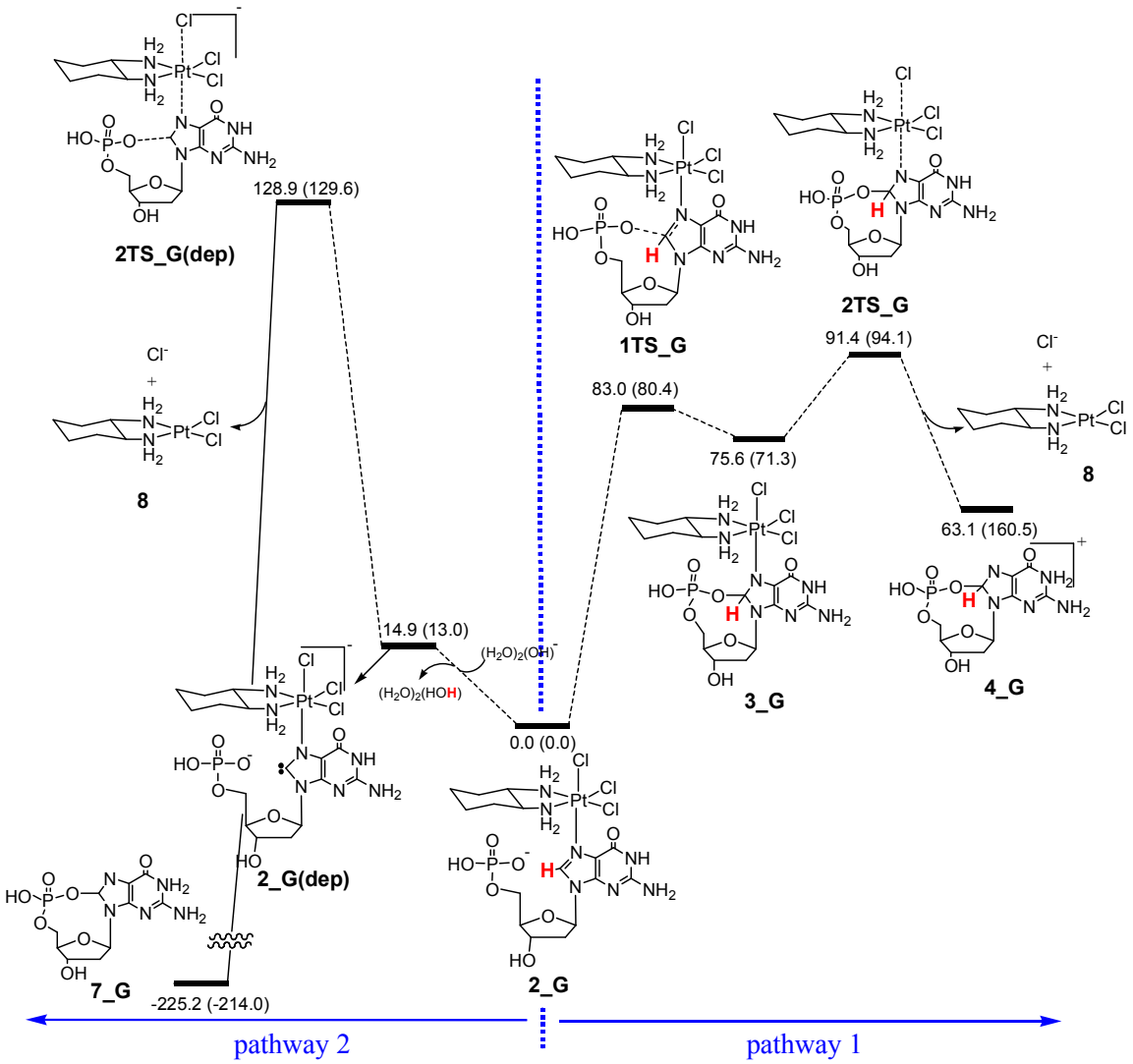


Figure S10. Comparison of energy profiles calculated for the oxidation of 5′-dGMP by [Pt^{IV}Cl4(dach)] via pathways 1 and 2. In pathway 2, OH^- is considered as the base. The relative free energies and electronic energies (in parenthesis) obtained from the M06/BS2//B3LYP/BS1 calculations are given in kJ mol^{-1}.