

## Supplementary material:

# Mechanism of Nitric Oxide Induced Deamination of Cytosine

Vanessa Labet,<sup>a</sup> André Grand,<sup>a</sup> Christophe Morell,<sup>a</sup> Jean Cadet<sup>a</sup> and Leif A. Eriksson<sup>b\*</sup>

**Table S1.** Absolute energies (in Hartrees) of the molecular systems involved in the NO<sup>•</sup>-induced deamination of cytosine, calculated at the (PCM)/B3LYP/6-311G(d,p) level of theory. (E<sub>0,vac</sub>: Electronic energy in vacuum at 0K with no zero-point correction; E<sub>0+ZPE,vac</sub>: electronic energy in vacuum with the zero-point correction calculated at 298.15K and 1 atm; E<sub>vac</sub>: electronic energy in vacuum with the thermal corrections calculated at 298.15K and 1 atm; H<sub>vac</sub>: enthalpy in vacuum at 298.15K and 1 atm; G<sub>vac</sub>: Gibbs free energy in vacuum at 298.15K and 1 atm; G<sub>aq</sub>: Gibbs free energy in aqueous solution at 298.15K and 1 atm).

	E <sub>0,vac</sub>	E <sub>0+ZPE,vac</sub>	E <sub>vac</sub>	H <sub>vac</sub>	G <sub>vac</sub>	G <sub>aq</sub>
Cytosine	-395.041052	-394.942845	-394.936108	-394.935163	-394.973621	-394.991877
Cytosine-H <sub>2</sub> O	-471.511715	-471.387927	-471.378587	-471.377642	-471.422311	-471.436957
TS0	-471.484062	-471.366534	-471.358692	-471.357748	-471.399043	-471.412323
Cytosine_tautomer-H <sub>2</sub> O	-471.508597	-471.384100	-471.375055	-471.374111	-471.418183	-471.429410
R	-547.962691	-547.814888	-547.801552	-547.800608	-547.855816	-547.868860
I1	-677.678870	-677.522258	-677.507303	-677.506359	-677.564785	-677.636145
TS1	-677.653457	-677.498528	-677.485535	-677.484591	-677.538629	-677.617438
I2_1	-677.670902	-677.514322	-677.499393	-677.498449	-677.557996	-677.629348
I2_2	-677.666059	-677.509559	-677.494890	-677.493945	-677.553794	-677.625056
TS2	-677.623313	-677.471076	-677.457059	-677.456115	-677.513215	-677.589795
I3_1	-677.652720	-677.498389	-677.483090	-677.482146	-677.542221	-677.617100
I3_2	-677.652780	-677.499498	-677.483311	-677.482367	-677.544224	-677.620321
TS3	-677.650628	-677.499287	-677.482880	-677.481936	-677.544730	-677.616471
P	-677.790551	-677.636071	-677.621251	-677.620307	-677.680931	-677.747082
Uracil (enol form)	-414.902330	-414.816200	-414.809944	-414.809000	-414.846647	-414.867911
Uracil	-414.934611	-414.847616	-414.841449	-414.840505	-414.878037	-414.890114
H <sub>2</sub> O	-76.447448	-76.426123	-76.423288	-76.422343	-76.443769	-76.448316
NO <sup>+</sup>	-129.571276	-129.565594	-129.563233	-129.562289	-129.584776	-129.713184
N2	-109.555930	-109.550354	-109.547994	-109.547050	-109.568787	-109.564620

Cartesian coordinates corresponding to the B3LYP/6-311G(d,p) optimized geometries of the stationary points involved in the NO<sup>•</sup>-induced deamination of cytosine.

### Cytosine

C	-1.04930300	1.18521500	-0.00081100
C	0.20005300	1.71222900	0.00164200
C	1.18732900	-0.53179900	-0.00003900
C	-1.12910800	-0.25285900	-0.00281300
H	-1.92832600	1.81331900	-0.01007900
H	0.39106800	2.77873700	0.00246400
O	2.21636700	-1.17430000	0.00125500
N	-2.35412300	-0.84332900	-0.03576700
H	-2.37960100	-1.84428800	0.07741100
H	-3.18805100	-0.31513400	0.15253100
N	-0.08171100	-1.04934100	0.00297500
N	1.27891200	0.89564300	0.00096600
H	2.21860000	1.26423300	0.00254200

### Cytosine-H<sub>2</sub>O

C	0.88252700	-1.68779600	-0.00006300
C	2.03802100	-0.98042900	-0.01059400
C	0.80091000	1.13109800	0.00509600
C	-0.33963100	-0.92471500	0.01118400
H	0.88158200	-2.76812100	0.00092400
H	3.01497900	-1.44852400	-0.02143100
O	0.87176000	2.34281100	0.01078200
N	-1.52630100	-1.56313700	0.03398900
H	-2.37512000	-0.99621900	-0.00331800
H	-1.57340700	-2.56389900	-0.03712600
N	-0.35919000	0.40287700	0.00900400
N	2.00866100	0.37372300	-0.00709300
H	2.85739900	0.91981800	-0.01468900
O	-3.15771100	0.77764700	-0.10896100
H	-2.20469600	1.00710800	-0.14098000
H	-3.46628300	1.16297600	0.71701500

### TS0

C	0.61384000	-1.76718500	0.00814500
C	1.84000000	-1.19599100	0.00389100
C	0.89381300	1.06061600	-0.00139700
C	-0.53316300	-0.89204700	0.00332200
H	0.49246500	-2.84038300	0.01161900
H	2.75445700	-1.77674400	0.00373000
O	1.09492000	2.25588300	0.00180200
N	-1.78962200	-1.28447000	0.00500600
H	-2.53849800	-0.27239700	-0.02803700
H	-1.95726900	-2.27970700	-0.01193200
N	-0.33550500	0.46043400	-0.00441200
N	1.98547100	0.15676500	0.00000100
H	2.89706200	0.58877900	-0.00258800
O	-2.71909000	0.95750600	-0.09429500
H	-1.46238900	1.00959400	-0.04004500
H	-3.10182300	1.30227900	0.71926900

### Cytosine\_tautomer-H<sub>2</sub>O

C	0.85195300	-1.71589900	0.00606600
C	2.00359600	-1.01804400	0.01310200
C	0.84792600	1.13152100	-0.00490700
C	-0.41915800	-1.00755500	-0.00543600
H	0.85688300	-2.79608400	0.00913600
H	2.97556700	-1.49516800	0.02203300
O	0.88715300	2.34138500	-0.00625500
N	-1.60138500	-1.51820900	-0.00606500
H	-2.91552500	-0.13447200	-0.09934100
H	-1.56272800	-2.53317200	-0.00680600
N	-0.30993600	0.38663700	-0.01550700
N	2.01228800	0.35352500	0.01019700
H	2.87415500	0.87603300	0.01591300
O	-3.13083200	0.82272300	-0.07788500
H	-1.19604400	0.90594800	-0.04156700
H	-3.49554700	0.97024000	0.80042900

### R

C	-0.72298000	-0.40744200	0.00016700
C	-1.31697200	0.92876700	0.01581800
C	-0.52707200	2.01435400	0.02111500
C	1.51077300	0.68406100	-0.01161400
H	-2.39459600	1.00858300	0.02444400
H	-0.91250700	3.02583200	0.03359600
N	0.85095300	1.90395000	0.01209700
H	1.44677300	2.71617600	0.01146600
N	0.68773700	-0.40676900	-0.01974000
H	1.16562700	-1.31101700	-0.04896800
N	-1.32315400	-1.53436900	0.00418100
H	-2.32960800	-1.36965200	0.01491200
O	2.73591100	0.62645100	-0.02343600
O	-4.39456300	-0.61000100	-0.00703600
H	-4.70812100	-1.13815100	0.73441400
H	-4.65974900	-1.10592400	-0.78863200
O	2.99916500	-2.16843100	-0.07102300
H	3.25280900	-1.22899800	-0.11724000
H	3.24402500	-2.43912100	0.81929200

### I1

C	-0.30556300	-0.38895800	-0.00895600
C	-0.34547200	-1.80402300	0.01137100
C	0.84691400	-2.46670300	0.00882400
C	2.12464800	-0.40061800	-0.03060400
H	-1.29382900	-2.31953800	0.02741300
H	0.90820000	-3.54767400	0.02329900
N	2.02112200	-1.79799700	-0.01355600
H	2.90570600	-2.29247200	-0.01356700
N	0.87911000	0.24683100	-0.02826100
H	0.96967500	1.29615300	-0.01277800
N	-1.45653400	0.31886800	-0.00914900
H	-2.37637300	-0.16861600	0.01936000
O	3.17123300	0.18485200	-0.04494100
N	-1.41728000	1.72418500	-0.07593000
O	-2.50114100	2.20953600	-0.07221000
O	-3.66127500	-1.38389900	0.06315800
H	-4.25465800	-1.48445900	-0.69049800

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H	-4.22042900	-1.46301600	0.84503100
O	1.65436500	2.79420000	0.15937300
H	2.61480500	2.80134500	0.07591300
H	1.33336700	3.65936200	-0.11274800

**TS1**

C	0.10520600	-0.64239600	-0.00164600
C	-0.29994300	-1.99677200	0.01423300
C	-1.63849600	-2.26873900	0.00833300
C	-2.22049700	0.08882800	-0.02197000
H	0.43243400	-2.78804100	0.01928800
H	-2.02595800	-3.27983500	0.01549000
N	-2.55125700	-1.27487700	-0.00975200
H	-3.54486900	-1.47450100	-0.01301000
N	-0.83891200	0.32001900	-0.01625300
H	-0.59828500	1.34306700	-0.00328600
N	1.43899900	-0.35237200	-0.00142200
H	2.79101200	-1.16185700	0.06487500
O	-3.04169400	0.96374300	-0.03511900
N	1.70011100	0.95075000	-0.09159300
O	2.90464700	1.23523500	-0.10393700
O	3.83797400	-1.04960000	-0.00314200
H	4.31650300	-1.37056300	0.77704400
H	3.78588700	-0.00006200	-0.03739700
O	-0.83045600	2.99614700	0.15869000
H	-1.75248000	3.26085900	0.06140700
H	-0.28820800	3.71656400	-0.17691300

**I2\_1**

C	-2.34967100	0.10049000	-0.00407900
C	-0.04134700	-0.66187800	-0.01324900
C	-0.44645700	-2.00635700	-0.00572100
C	-1.79223400	-2.26827800	-0.00354500
H	0.29366100	-2.79046900	-0.00599600
H	-2.19130200	-3.27508300	-0.00137900
N	-0.96489100	0.31436100	-0.00918200
N	-2.69006800	-1.26486700	-0.00389900
H	-3.68642800	-1.45421700	0.00269800
O	-3.16348800	0.98073200	0.00094700
N	1.32354600	-0.40804000	-0.00581400
N	1.58967600	0.81460600	-0.19462400
O	2.85681400	1.08788000	-0.17018400
H	3.43786500	0.26198000	-0.01587300
H	-0.70567100	1.33574000	0.00767400
O	4.59084300	-0.83919400	0.12403500
H	4.83265100	-1.19832200	0.98465500
H	5.41445300	-0.72100600	-0.36276600
O	-0.83770100	2.98192700	0.18324900
H	-0.25721500	3.65595300	-0.18394300
H	-1.73934900	3.31837100	0.12475000

**I2\_2**

C	-1.61778600	-1.26563700	-0.00295200
C	-0.76175900	0.99235300	-0.04028800
C	-2.04228400	1.53738800	0.13115500
C	-3.09029700	0.65862200	0.24933900

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H	-2.17895100	2.60638100	0.16912000
H	-4.11347700	0.98424700	0.39142100
N	-0.57863500	-0.32980800	-0.10433500
N	-2.88098100	-0.66779500	0.18879400
H	-3.65245700	-1.32239700	0.26400100
O	-1.46023700	-2.45104300	-0.07412500
N	0.29941900	1.89334600	-0.18007100
N	1.42217400	1.38936900	0.04828800
O	2.41077300	2.23972300	-0.13633000
H	2.03263700	3.09836400	-0.43271700
H	0.39501900	-0.79443200	-0.28677500
H	2.44611000	-1.53376500	-0.19471400
O	1.58830800	-1.61663100	-0.67003200
H	1.41003200	-2.55439700	-0.79804400
H	4.75147900	-1.14185200	0.08769800
O	3.95058700	-1.31076100	0.59457700
H	4.23308300	-1.76459400	1.39503500

### TS2

C	2.07543600	1.04196700	0.01570800
C	0.71497900	-0.82488900	-0.09620200
C	1.73486000	-1.78642400	-0.07313700
C	2.98930400	-1.23406200	0.01664800
H	1.56158900	-2.84948900	-0.12285300
H	3.89047300	-1.83397700	0.05036400
N	0.80195800	0.45584500	-0.06113800
N	3.14260800	0.10129600	0.05810700
H	4.06863200	0.51120100	0.11654700
O	2.27248100	2.22240300	0.05429000
N	-0.68979800	-1.31039300	-0.25978100
N	-1.47489900	-1.12338800	0.56871400
O	-3.10123300	-1.54793800	-0.03042400
H	-3.00611000	-1.82404900	-0.95858500
H	-0.77420500	1.78596500	-0.16740400
H	-3.06301300	1.38435900	0.02335700
O	-1.65349800	2.20112400	-0.18151700
H	-1.54001400	3.08565900	0.18130100
H	-3.52941700	-0.52795200	0.01299700
O	-3.83441100	0.76095800	0.13523300
H	-4.62120500	1.13284800	-0.27579500

### I3\_1

C	-1.19877300	1.26212100	0.01492600
C	-0.87742500	-0.98431200	-0.27899000
C	-2.20283400	-1.39763700	-0.08435000
C	-3.04241300	-0.34356800	0.18881600
H	-2.53613200	-2.42207000	-0.13807200
H	-4.10259000	-0.46920600	0.36995700
N	-0.36038800	0.18310100	-0.26073400
N	-2.55735800	0.91083300	0.23238800
H	-3.17540600	1.69254600	0.42660500
O	-0.83936100	2.41000900	0.07327300
N	0.11433700	-2.04171200	-0.57647900
N	1.09742500	-2.55061400	-0.44417300
O	2.05165100	-1.54909700	1.22643800
H	2.72519200	-2.15839100	1.55305300
H	2.37066900	3.29769800	0.55281300

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H	2.68880200	1.12122900	-0.31281700
O	2.06107300	2.69459100	-0.12949100
H	1.09498600	2.77198700	-0.13999100
H	2.53271400	-0.84803100	0.68881800
O	3.01987000	0.19684600	-0.41644400
H	3.92646400	0.26456700	-0.72998700

### I3\_2

C	-0.11007500	-1.67781700	-0.32932100
C	1.20177000	0.18540200	-0.32296800
C	2.22014300	-0.27236600	0.52194800
C	2.00936200	-1.57570000	0.90156200
H	3.06206600	0.31652600	0.84828700
H	2.69430800	-2.11503400	1.54387800
N	0.16366000	-0.38339000	-0.78247700
N	0.91292500	-2.23673400	0.48193300
H	0.75031900	-3.19473200	0.77546000
O	-1.11051500	-2.29201000	-0.58507500
N	1.39797300	1.55438600	-0.92413800
N	1.52651600	2.47739000	-1.50021200
O	0.21463400	2.20308100	1.08064200
H	0.37725900	2.41140000	2.00604900
H	-4.15847700	-0.93080300	-0.05482600
H	-2.74832600	0.92195300	0.45938300
O	-3.39279400	-0.45948100	-0.39743600
H	-2.79639800	-1.13865300	-0.74175200
H	-0.76585600	2.05141700	1.00872500
O	-2.38222500	1.72320400	0.89320800
H	-2.98241600	2.44090500	0.67102200

### TS3

C	-0.44253900	-1.60891300	-0.39819000
C	1.20596000	-0.07210700	-0.25231200
C	2.12690900	-0.71735400	0.56297800
C	1.63414500	-1.96305500	0.86927800
H	3.05486100	-0.31413400	0.93123400
H	2.17639500	-2.65671400	1.50016900
N	0.13027100	-0.36765300	-0.76393500
N	0.43272500	-2.37924900	0.40453800
H	0.08419400	-3.29855100	0.65498900
O	-1.52893300	-1.98920200	-0.72103400
N	1.83490600	1.45093500	-0.92592600
N	2.09567100	2.36072300	-1.47631900
O	0.58347500	1.85625800	1.22470000
H	0.76563400	2.10247900	2.13703500
H	-4.34256000	-0.14600800	-0.05291800
H	-2.58215900	1.40735300	0.47371500
O	-3.50024300	0.18150600	-0.38283600
H	-3.06223300	-0.57393500	-0.79560700
H	-0.39321600	1.98451500	1.10133900
O	-2.03891600	2.10972600	0.88944800
H	-2.42583700	2.94396400	0.60879400

### P

C	1.44738300	0.99882700	-0.00322700
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C	-0.69906000	0.13298300	-0.01336100
C	-1.29604800	1.42512000	0.00044300
C	-0.44251800	2.48392900	0.01111900
H	-2.36677200	1.56614500	0.00121100
H	-0.77150200	3.51473300	0.02094600
N	0.61078600	-0.06192700	-0.01399800
N	0.89617800	2.27127600	0.00907900
H	1.55095000	3.04436600	0.01377200
O	2.69290000	0.91755100	-0.00443800
N	-4.44021100	-0.80252900	0.00450200
N	-5.52350800	-0.95891800	0.01349200
O	-1.41603600	-0.97764600	-0.02768500
H	-2.37277600	-0.80819900	-0.01844000
H	4.48482500	-1.34282300	0.60921200
H	3.08295400	-1.96168900	-0.02768700
O	3.83151400	-1.23629600	-0.09426000
H	3.33748800	-0.26088000	-0.05193800
H	1.15617600	-1.96458300	0.06852500
O	1.82480800	-2.67920700	0.10711200
H	1.57190900	-3.36274500	-0.52279000

### Uracil (enol form)

N	-0.03430900	0.03819900	0.03352000
C	-0.02122300	-0.01995400	1.38212500
H	0.94621700	0.01038800	1.86846000
C	-1.19284800	-0.11189700	2.06479900
H	-1.21349300	-0.15979400	3.14458300
N	-2.40523100	-0.08496300	-0.03584500
C	-1.23239200	0.00848400	-0.74958400
O	-1.13869700	0.06597700	-1.95411700
H	0.82195000	0.10720000	-0.49775200
C	-2.38157200	-0.14001700	1.26018600
O	-3.58678400	-0.22978800	1.86016600
H	-3.47271500	-0.26353200	2.81596900

### Uracil

N	-0.02736700	0.00043100	0.00126400
C	-0.01274800	0.00021500	1.37499400
H	0.97052500	-0.00015100	1.82835100
C	-1.14724600	0.00036400	2.10048000
H	-1.13583900	0.00018500	3.17941300
N	-2.34061300	0.00065500	0.01849700
C	-1.19645200	0.00133200	-0.76015200
O	-1.19062900	0.00009700	-1.96991400
H	0.82860200	0.00004500	-0.53178200
C	-2.44280100	0.00035700	1.42830600
O	-3.52975400	0.00035000	1.96562500
H	-3.21497300	0.00032700	-0.49115000