

Supporting Information

**Nitrosative Adenine Deamination: Facile Pyrimidine Ring-Opening in the
Deamination of Adenine**

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The Cartesian Coordinate data for the optimized structures at
MP2(full)/6-31G**. Frequency output files available on request.

1

C	0.000000	0.000000	0.000000
N	-1.070724	-0.740067	-0.213500
C	-0.839127	-2.065506	-0.376083
N	0.354019	-2.682663	-0.340851
C	1.378067	-1.864410	-0.121155
C	1.314041	-0.454712	0.070419
N	2.534332	0.102310	0.273468
C	3.349091	-0.947495	0.209229
N	2.712600	-2.137497	-0.023117
N	-0.262466	1.391479	0.168762
N	-0.448959	2.500549	0.305527
H	-1.709305	-2.679077	-0.551254
H	4.419006	-0.891327	0.326492
H	3.141815	-3.049637	-0.107422

2

C	0.000000	0.000000	0.000000
N	0.000000	0.000000	1.206985
C	1.155991	0.000000	2.009995
N	2.266998	0.000000	1.329987
C	2.246994	0.000000	0.002000
C	1.062988	0.000000	-0.878998
N	1.406998	0.000000	-2.168991
C	2.734985	0.000000	-2.153000
N	3.268997	0.000000	-0.892990
H	1.067993	0.000000	3.082993
H	3.355988	0.000000	-3.033997
H	4.253998	0.000000	-0.651993

TS

C	0.000000	0.000000	0.000000
N	0.031693	-1.200562	0.003540
C	0.852905	1.112885	-0.006958
C	2.220337	0.697800	-0.011368
N	0.773438	2.456253	-0.010727
N	2.577759	-0.602203	-0.008881
C	2.036865	2.873703	-0.017258
N	2.942245	1.847244	-0.017883
C	1.959839	-1.636856	-0.003143
H	2.345749	3.905212	-0.021698
H	3.952438	1.928909	-0.022339
H	1.938217	-2.711792	0.000229

3

N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.183990
C	0.127000	0.000000	2.597992
C	1.338989	0.000000	3.299988
N	-0.898987	0.000000	3.483994
N	1.021988	0.000000	4.630997
C	-0.337997	0.000000	4.688995
N	2.600998	0.000000	2.806000
C	3.641998	0.000000	2.283997
H	1.659988	0.000000	5.416992
H	-0.869995	0.000000	5.625000
H	4.605988	0.000000	1.808990

4

N	1.055069	2.768539	0.297791
C	1.093400	1.592957	0.181213
C	1.105500	0.177383	0.042297
C	-0.000870	-0.659790	0.009644
N	0.503235	-1.924850	-0.136398
C	1.861130	-1.812378	-0.185715
N	2.259995	-0.555054	-0.080566
N	-1.336563	-0.409973	0.093400
C	-2.505737	-0.178955	0.167892
H	-0.047119	-2.768524	-0.194412
H	2.505737	-2.666031	-0.297791

5

N	1.144333	2.772171	-0.104004
C	1.162018	1.590012	-0.062912
C	1.151306	0.168564	-0.013931
C	0.023560	-0.651459	-0.000961
N	0.525681	-1.928085	0.050018
C	1.884338	-1.836166	0.065323
N	2.298553	-0.581375	0.027603
C	-1.359818	-0.361938	-0.029800
N	-2.519363	-0.124969	-0.053757
H	-0.026703	-2.772186	0.071655
H	2.519363	-2.704926	0.104004