

## Supplementary Information

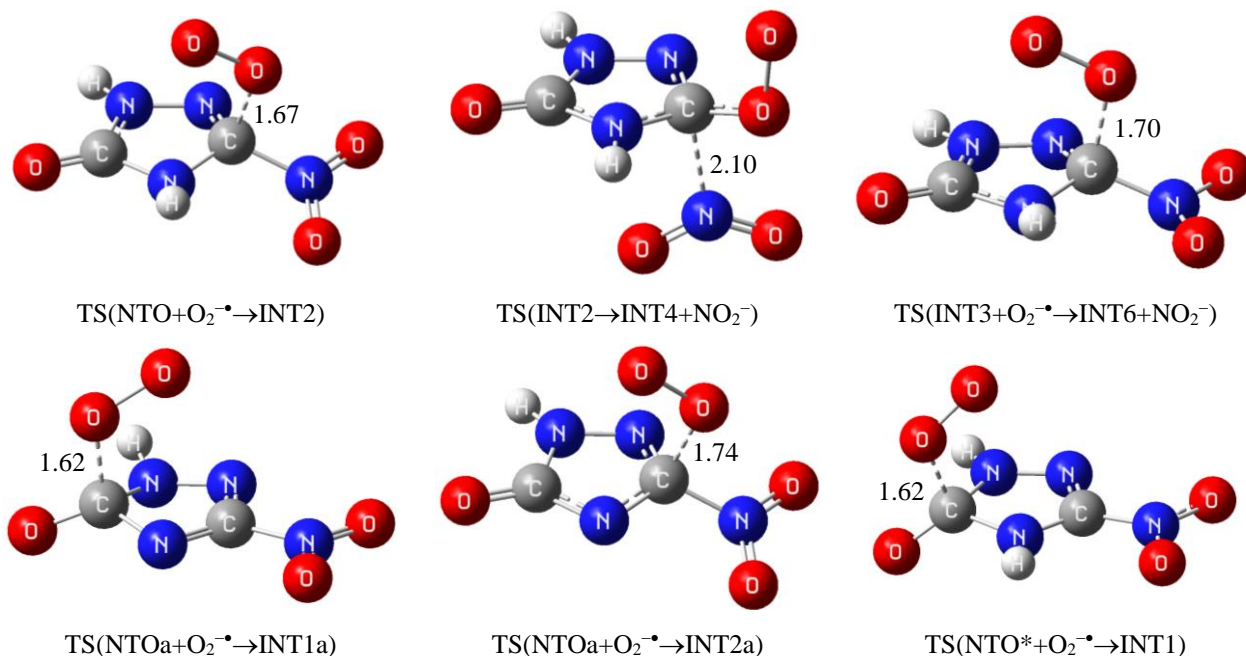
### Degradation of NTO induced by superoxide and hydroperoxyl radical: Comprehensive DFT study

Liudmyla K. Sviatenko,<sup>a</sup> Leonid Gorb,<sup>b,c</sup> and Jerzy Leszczynski<sup>\*,a</sup>

<sup>a</sup>Interdisciplinary Center for Nanotoxicity, Department of Chemistry, Physics & Atmospheric Sciences, Jackson State University, Jackson, Mississippi, 39217, USA

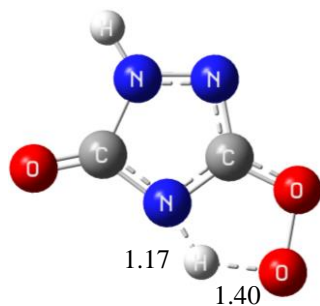
<sup>b</sup>Institute of Molecular Biology and Genetics, NAS of Ukraine, 150 Zabolotny Str., Kyiv, 03143, Ukraine

<sup>c</sup>QSAR Lab Sp. z o.o. Trzy Lipy 3, B, Gdańsk, 80-172, Poland

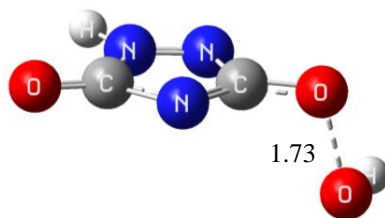
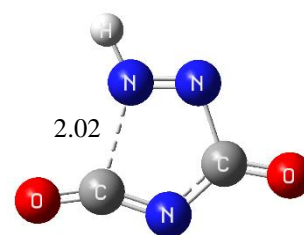


**Figure S1.** PCM(Pauling)/M06-2X/6-311++G(d,p) optimized structures of transition states for NTO and NTOa decomposition in water under action of superoxide (O<sub>2</sub><sup>•-</sup>) with selected interatomic distances in Å. Color for atoms: grey – carbon, light grey – hydrogen, blue – nitrogen, red – oxygen.

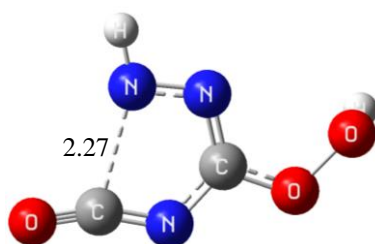
Continue Figure S1



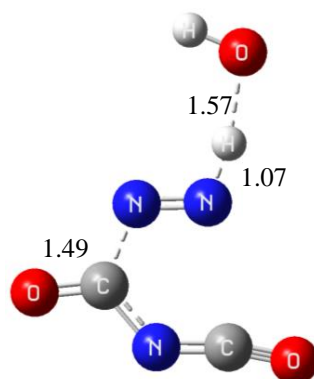
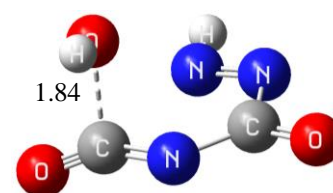
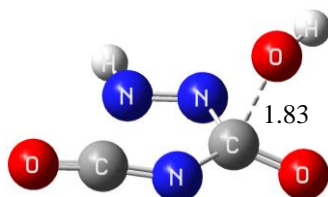
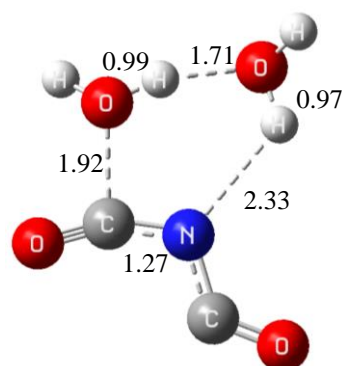
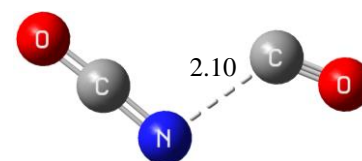
TS(INT4→INT7)

TS(INT7→INT8+OH<sup>\*</sup>)

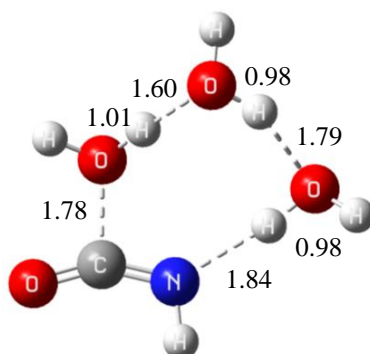
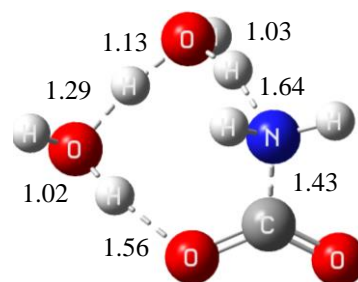
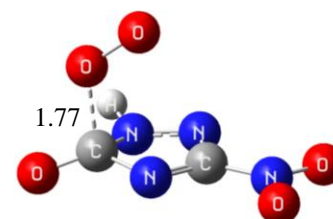
TS(INT8→INT9)



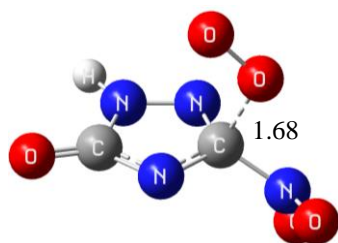
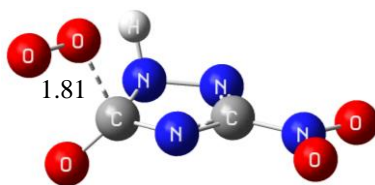
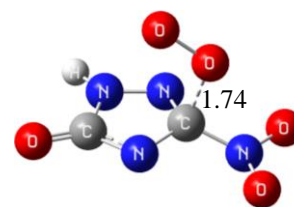
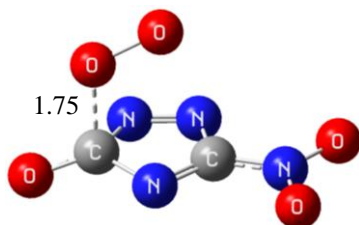
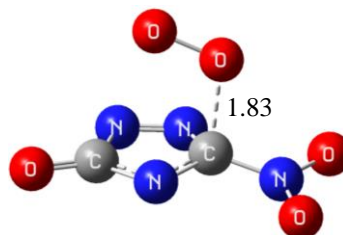
TS(INT7→INT10)

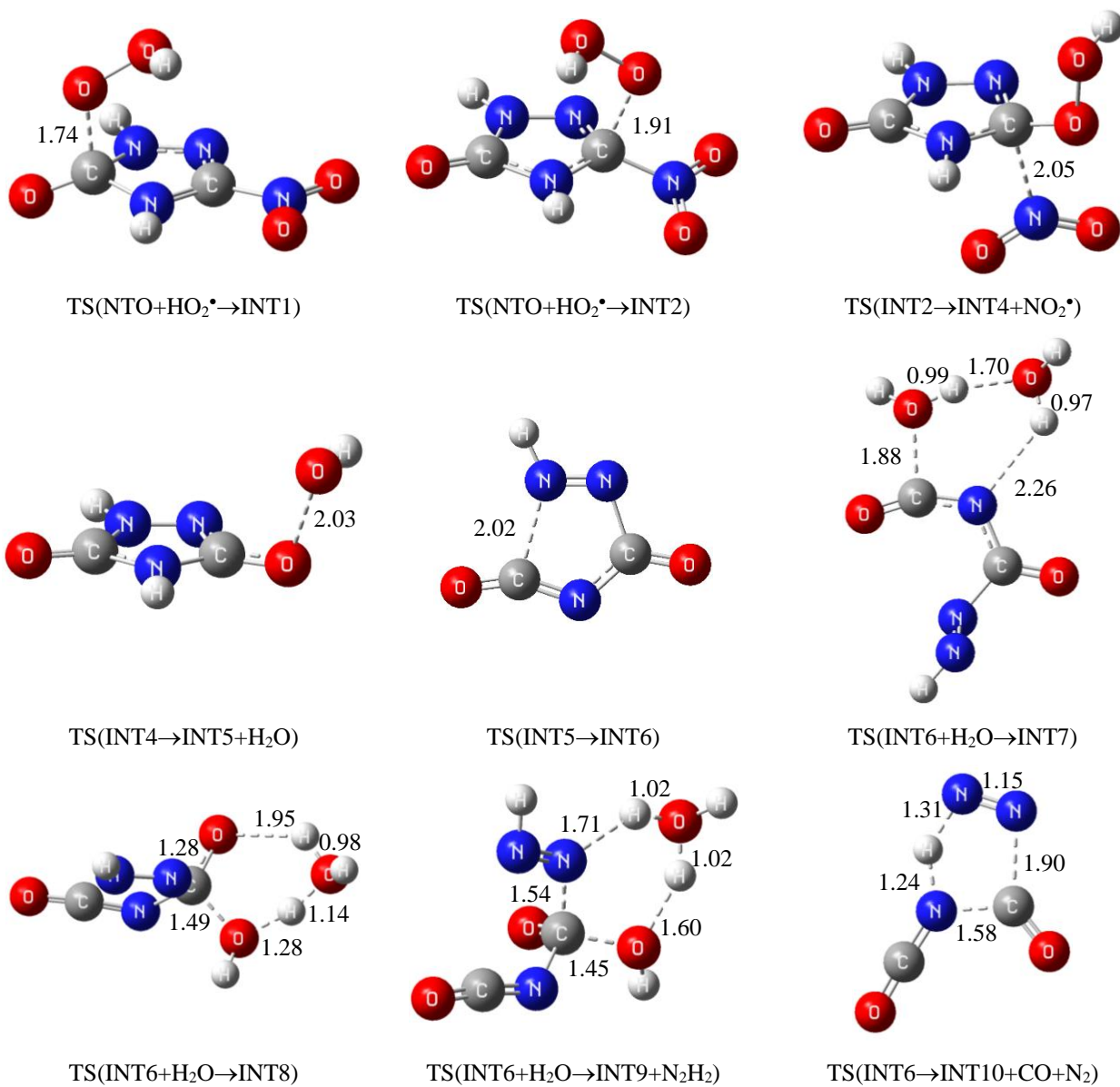
TS(INT9+OH<sup>\*</sup>→INT11+N<sub>2</sub>+H<sub>2</sub>O)TS(INT9+OH<sup>\*</sup>→INT12)TS(INT9+OH<sup>\*</sup>→INT13)TS(INT11+H<sub>2</sub>O→INT14)

TS(INT11→INT15+CO)

TS(INT16+H<sub>2</sub>O→INT17)TS(INT17→NH<sub>3</sub>+CO<sub>2</sub>)TS(NTOa<sup>\*</sup>+O<sub>2</sub><sup>-\*</sup>→INT1a)

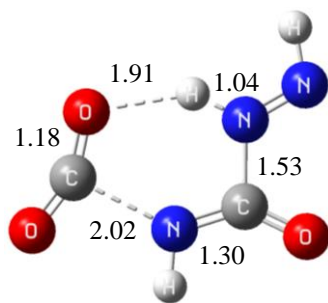
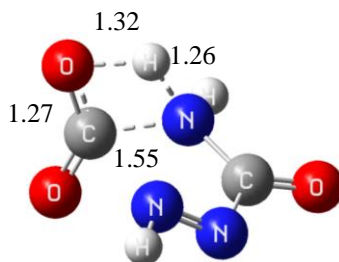
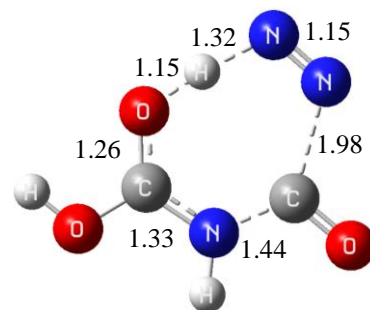
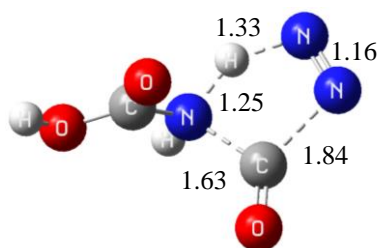
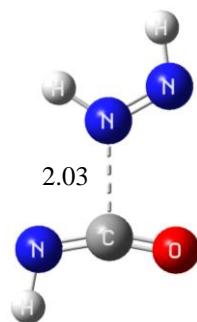
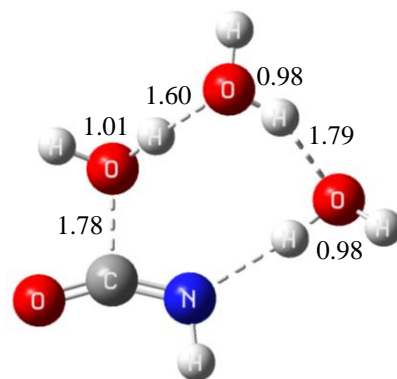
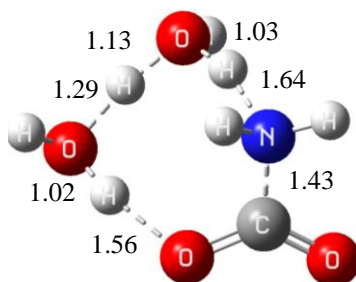
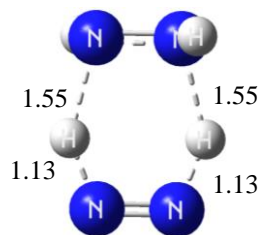
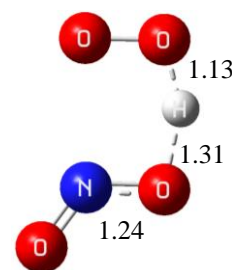
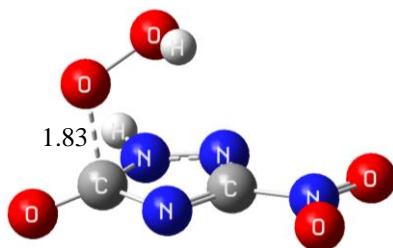
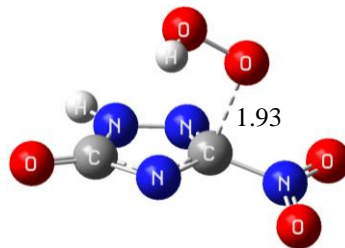
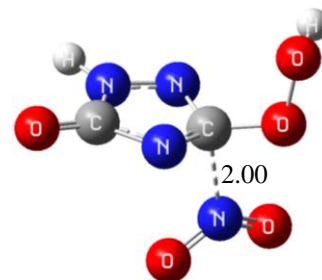
Continue Figure S1

 $\text{TS}(\text{INT0a}^* + \text{O}_2^{\bullet-} \rightarrow \text{INT2a})$  $\text{TS}(\text{INT3a} + \text{O}_2^{\bullet-} \rightarrow \text{INT5a})$  $\text{TS}(\text{INT3a} + \text{O}_2^{\bullet-} \rightarrow \text{INT6a} + \text{NO}_2^-)$  $\text{TS}(\text{INT4a} + \text{O}_2^{\bullet-} \rightarrow \text{INT7a})$  $\text{TS}(\text{INT4a} + \text{O}_2^{\bullet-} \rightarrow \text{INT8a})$

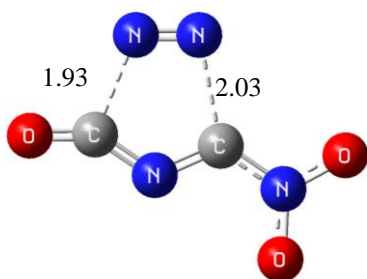
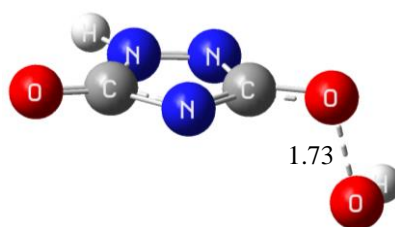
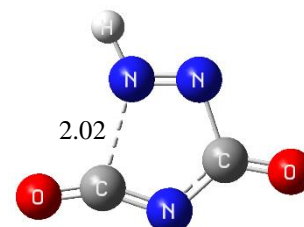


**Figure S2.** PCM(Pauling)/M06-2X/6-311++G(d,p) optimized structures of transition states for NTO and NTOa decomposition in water under action of hydroperoxyl radical ( $\text{HO}_2^\bullet$ ) with selected interatomic distances in Å. Color for atoms: grey – carbon, light grey – hydrogen, blue – nitrogen, red – oxygen.

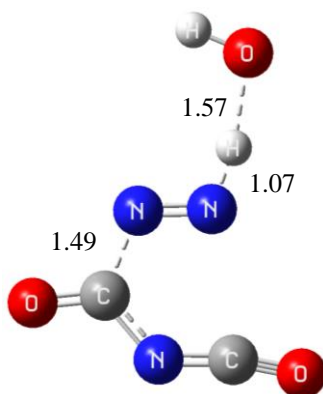
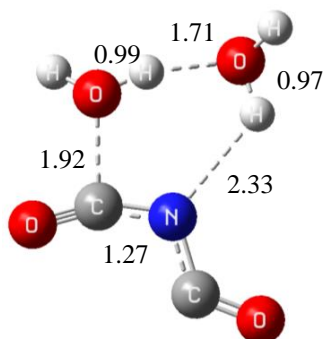
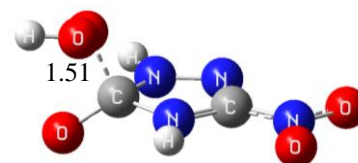
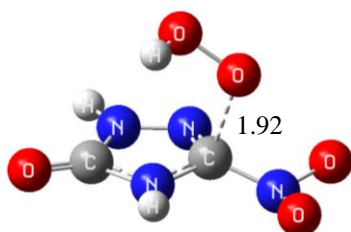
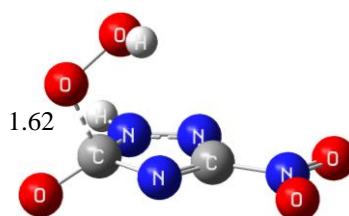
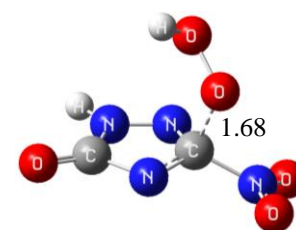
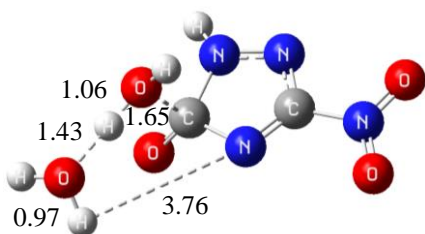
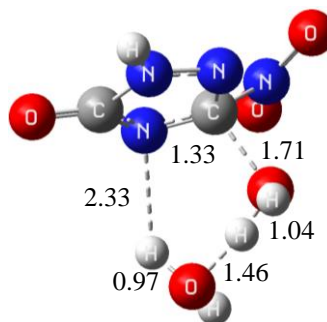
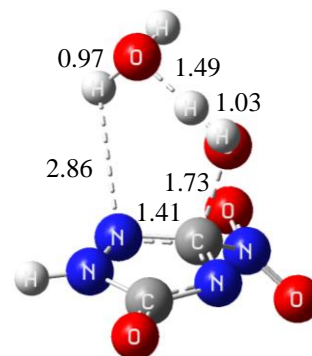
Continue Figure S2

TS(INT7→INT11+CO<sub>2</sub>)TS(INT7→INT12+CO<sub>2</sub>)TS(INT7→INT13+CO+N<sub>2</sub>)TS(INT7→INT14+CO+N<sub>2</sub>)TS(INT11→INT10+N<sub>2</sub>H<sub>2</sub>)TS(INT10+H<sub>2</sub>O→INT14)TS(INT14→NH<sub>3</sub>+CO<sub>2</sub>)TS(N<sub>2</sub>H<sub>2</sub>→N<sub>2</sub>H<sub>4</sub>+N<sub>2</sub>)TS(NO<sub>2</sub><sup>\*</sup>+HO<sub>2</sub><sup>\*</sup>→HNO<sub>2</sub>+O<sub>2</sub>)TS(NTOa+HO<sub>2</sub><sup>\*</sup>→INT1a)TS(NTOa+HO<sub>2</sub><sup>\*</sup>→INT2a)TS(INT2a→INT4a+NO<sub>2</sub><sup>-</sup>)

Continue Figure S2

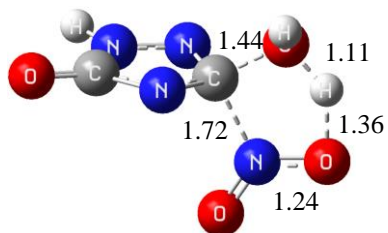
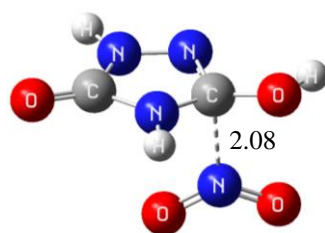
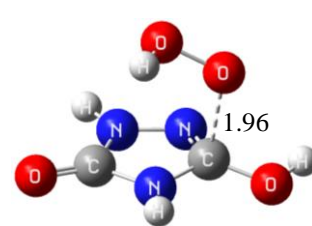
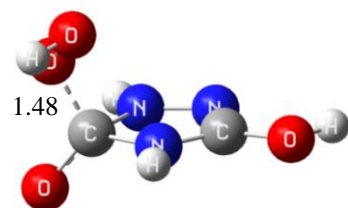
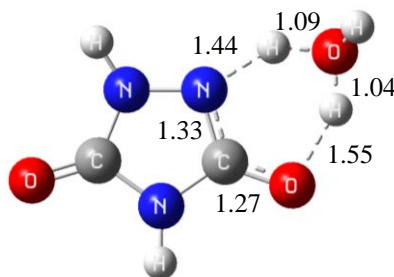
TS(INT3a→INT5a+N<sub>2</sub>)TS(INT4a→INT5+OH<sup>\*</sup>)

TS(INT5→INT6)

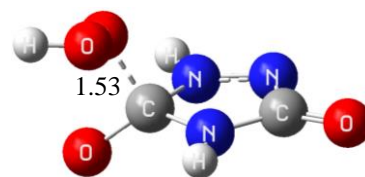
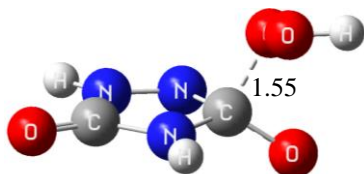
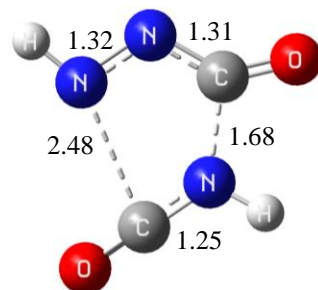
TS(INT6+OH<sup>\*</sup>→INT6a+N<sub>2</sub>+H<sub>2</sub>O)TS(INT6a+H<sub>2</sub>O→INT7a)TS(NTO<sup>\*</sup>+HO<sub>2</sub><sup>\*</sup>→INT1)TS(NTO<sup>\*</sup>+HO<sub>2</sub><sup>\*</sup>→INT2)TS(NTOr+HO<sub>2</sub><sup>\*</sup>→INT15)TS(NTOr+HO<sub>2</sub><sup>\*</sup>→INT16)TS(NTOr+H<sub>2</sub>O→INT17)TS(NTOr+H<sub>2</sub>O→INT18)TS(NTOr+H<sub>2</sub>O→INT19)



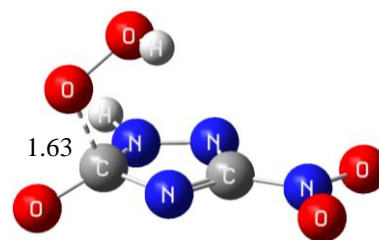
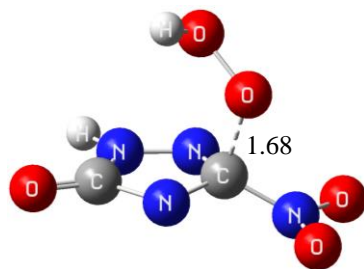
Continue Figure S2

TS(NTOr+H<sub>2</sub>O→INT20+HNO<sub>2</sub>)TS(INT18→INT21+NO<sub>2</sub><sup>\*</sup>)TS(INT21+HO<sub>2</sub><sup>\*</sup>→INT23)TS(INT21+HO<sub>2</sub><sup>\*</sup>→INT24)

TS(INT21→INT25)

TS(INT22+HO<sub>2</sub><sup>\*</sup>→INT26)TS(INT22+HO<sub>2</sub><sup>\*</sup>→INT27)

TS(INT22→INT10+INT28)

TS(NTOa<sup>\*</sup>+HO<sub>2</sub><sup>\*</sup>→INT1a)TS(NTOa<sup>\*</sup>+HO<sub>2</sub><sup>\*</sup>→INT2a)

## Cartesian coordinates for optimized local minima and transition states species

### Superoxide induced degradation of NTO and NTOa

#### NTO

N	-0.12666700	1.32311000	-0.00010500
C	0.36226000	0.13534300	-0.00006400
N	-1.45970700	1.10938500	0.00015700
C	-1.80641500	-0.22101300	-0.00023200
N	-0.57239800	-0.84500400	-0.00001900
H	-0.41365700	-1.84430400	0.00016100
H	-2.10256000	1.88985600	0.00045900
O	-2.91770500	-0.72084900	0.00004300
N	1.78328300	-0.13448200	0.00003200
O	2.53711800	0.81007700	-0.00002600
O	2.10678200	-1.30205200	0.00007100

#### O<sub>2</sub><sup>-•</sup>

O	0.00000000	0.00000000	0.65872000
O	0.00000000	0.00000000	-0.65872000

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

H	0.00000000	0.76115400	-0.47140900
O	0.00000000	0.00000000	0.11785200
H	0.00000000	-0.76115400	-0.47140900

#### dimer H<sub>2</sub>O

H	1.80326700	0.77067100	0.22496900
O	1.48240400	-0.10266100	-0.01842500
H	0.51258200	-0.02675700	-0.01326300
H	-1.73867200	0.83042600	0.14811000
O	-1.33458800	-0.01171600	-0.08722600
H	-1.75969700	-0.65932800	0.48539400

#### INT1

N	0.34645100	1.38381500	0.02062500
C	0.78340300	0.12193300	-0.07603500
N	-0.92978900	1.30543700	-0.12077100
C	-1.51137900	-0.10575100	-0.48381700
N	-0.11119500	-0.78830100	-0.28917100
H	0.07198800	-1.77504900	-0.43473700
H	-1.47479100	2.16377200	-0.14365000
O	-1.97036600	-0.18513300	-1.65335600
N	2.21162000	-0.15933600	0.02767500
O	2.94844300	0.76430500	0.27996100
O	2.54392400	-1.30994500	-0.14687400
O	-2.35733400	-0.51086900	0.50818900
O	-1.77078600	-0.34299700	1.82070400

#### TS(NTO+O<sub>2</sub><sup>-•</sup>→INT2)

N	0.10251000	-0.18868100	1.38856300
C	-0.35549800	-0.05198100	0.12428500
N	1.44660500	-0.29764800	1.19768300
C	1.79824900	-0.52527200	-0.11179000
N	0.58691700	-0.51188200	-0.78124500
H	0.54152900	-0.30040400	-1.76986700



H	2.06415200	-0.41925200	1.98839100
O	2.91056200	-0.71380700	-0.57021700
N	-1.77133800	-0.47205600	-0.08403800
O	-2.56157800	-0.16069100	0.77644500
O	-2.03933500	-1.05371500	-1.10938900
O	0.56172700	2.15615500	-0.49592900
O	-0.59825500	1.58143900	-0.14344000

## INT2

N	0.13285200	0.31628500	1.30909200
C	-0.38226800	0.31449000	-0.04626900
N	1.38239000	-0.10120300	1.18627700
C	1.81624400	-0.28268900	-0.13454300
N	0.71825000	0.01957500	-0.87522800
H	0.67732300	-0.04505800	-1.88236900
H	1.98368400	-0.18963500	1.99658000
O	2.92399700	-0.62230800	-0.48191200
N	-1.41727800	-0.92026200	-0.07477000
O	-2.53304900	-0.71785000	0.33741600
O	-0.99014000	-1.98781300	-0.43863700
O	-0.35810100	2.56985800	-0.27336100
O	-1.16500100	1.36350200	-0.37437300

## INT3

N	0.12953800	1.35371100	0.00014500
C	-0.38814400	0.15584400	0.00011900
N	1.48259700	1.10652500	-0.00031600
C	1.79955100	-0.21528500	0.00044400
N	0.56367100	-0.82607700	-0.00001000
H	0.39196900	-1.82138500	-0.00030500
H	2.14020200	1.87169900	-0.00079400
O	2.90877300	-0.74343800	-0.00003700
N	-1.73313800	-0.13082400	0.00002300
O	-2.58049200	0.83444100	0.00005700
O	-2.09069300	-1.36813100	-0.00016700

O<sub>2</sub>

O	0.00000000	0.00000000	0.59379900
O	0.00000000	0.00000000	-0.59379900

## NTOa

N	-0.13372800	1.30609700	-0.00001200
C	0.31491900	0.08067200	0.00000800
N	-1.46473900	1.08068800	0.00010000
C	-1.75975000	-0.27043600	-0.00036100
N	-0.56606200	-0.92463300	0.00010200
H	-2.11815400	1.85145000	0.00039500
O	-2.91269800	-0.74723500	0.00005000
N	1.75143100	-0.15063100	0.00004900
O	2.49071300	0.81351300	-0.00008400
O	2.13183800	-1.30296700	0.00003900

HO<sub>2</sub>•

H	-0.87849200	-0.88366200	0.00000000
O	0.05490600	-0.59537500	0.00000000
O	0.05490600	0.70583300	0.00000000

## NTOa'

N	-0.16677700	1.33693100	-0.00012700
C	0.34517200	0.14105100	-0.00002900
N	-1.50614700	1.20048800	-0.00004200
C	-1.81300900	-0.13371200	-0.00004000
N	-0.61253100	-0.81969000	0.00002500
H	-0.48263000	-1.82142500	0.00010300
O	-2.94453800	-0.65030200	0.00004100
N	1.73421900	-0.13492900	0.00001500
O	2.51923800	0.79881200	-0.00000700
O	2.06883700	-1.31128600	0.00011800

TS(INT2→INT4+NO<sub>2</sub><sup>-</sup>)

N	0.13626900	0.40321000	1.28935500
C	-0.29181900	0.59729700	0.01681400
N	1.37370300	-0.05352000	1.15525900
C	1.83281900	-0.06900400	-0.16043700
N	0.75338100	0.41719300	-0.85387300
H	0.70082600	0.49625200	-1.86065200
H	1.91346300	-0.34532800	1.96115500
O	2.92113500	-0.42451200	-0.55705100
N	-1.24287200	-1.27039500	-0.11468900
O	-2.42478300	-1.35032500	0.10436400
O	-0.49185200	-2.19445200	-0.30414500
O	-1.00416400	2.70921000	-0.16172700
O	-1.37579300	1.28556700	-0.27783200

## INT4

N	0.34400600	1.12127100	-0.00049600
C	0.62482500	-0.12991600	-0.00052000
N	-1.02539400	1.12355800	0.00005100
C	-1.57540600	-0.12423100	0.00029900
N	-0.45790700	-0.94398500	0.00027500
H	-0.46585400	-1.95517700	-0.00115400
H	-1.53268900	1.99639500	0.00015800
O	-2.75357900	-0.44998600	0.00013200
O	2.83979400	0.18413700	0.00067700
O	1.87342100	-0.68693200	-0.00037000

NO<sub>2</sub><sup>-</sup>

N	0.00000000	0.45926700	0.00000000
O	1.05332200	-0.20083000	0.00000000
O	-1.05332200	-0.20102900	0.00000000

## INT5

N	0.44945100	1.29833600	0.45188000
C	0.83035600	0.14000200	0.05689400
N	-0.91110800	1.27218700	0.37851600
C	-1.38076800	0.11003200	-0.48231200
N	-0.13640100	-0.74967700	-0.31924000
H	0.07200400	-1.30543100	-1.14310900
H	-1.29486700	2.17274300	0.10746300
O	-1.68189900	0.41602600	-1.70509900
N	2.22964300	-0.20308900	0.03879800
O	3.04185400	0.59345400	0.47044000

O	2.51796400	-1.29043500	-0.43026700
O	-2.48371600	-0.51337400	0.13086700
O	-2.25617300	-0.91714900	1.50136900

TS(INT3+O<sub>2</sub><sup>-•</sup>→INT6+NO<sub>2</sub><sup>-</sup>)

N	0.10953700	-0.23624400	1.39930500
C	-0.40862100	-0.11841200	0.13170400
N	1.43814400	-0.34003400	1.16932300
C	1.76192200	-0.54869400	-0.15491400
N	0.54296200	-0.58488700	-0.78550100
H	0.46220900	-0.39997500	-1.77609900
H	2.09164100	-0.39638600	1.93802200
O	2.87579700	-0.70473800	-0.63078500
N	-1.75755600	-0.50422400	-0.07018200
O	-2.59995900	-0.25759800	0.87997400
O	-2.14549900	-0.63102800	-1.29961000
O	0.74474100	2.08714300	-0.33054300
O	-0.50073700	1.56331000	-0.12069600

INT6

N	-0.05576600	1.49497600	0.00000100
C	0.66935500	0.41554800	0.00007200
N	-1.35300400	0.99769500	-0.00062300
C	-1.41496800	-0.35090600	-0.00001600
N	-0.08251900	-0.72077900	-0.00025900
H	0.29226700	-1.65844900	0.00051900
H	-2.14096900	1.62640600	0.00180800
O	-2.40318200	-1.08782800	0.00025100
O	2.51366500	-0.92822500	-0.00021200
O	1.98469300	0.42117200	0.00039900

HO<sub>2</sub><sup>-</sup>

H	-0.88184500	-0.89906000	0.00000000
O	0.05511500	-0.67615800	0.00000000
O	0.05511500	0.78854000	0.00000000

NTOa

N	-0.13372800	1.30609700	-0.00001200
C	0.31491900	0.08067200	0.00000800
N	-1.46473900	1.08068800	0.00010000
C	-1.75975000	-0.27043600	-0.00036100
N	-0.56606200	-0.92463300	0.00010200
H	-2.11815400	1.85145000	0.00039500
O	-2.91269800	-0.74723500	0.00005000
N	1.75143100	-0.15063100	0.00004900
O	2.49071300	0.81351300	-0.00008400
O	2.13183800	-1.30296700	0.00003900

TS(NTOa+O<sub>2</sub><sup>-•</sup>→INT1a)

N	0.20042000	0.52593000	-1.25629800
C	0.63892700	-0.20208400	-0.21503800
N	-1.07391500	0.15934200	-1.30992600
C	-1.46748100	-0.54582800	-0.07912500
N	-0.18354300	-0.94458500	0.45072100
H	-1.71402600	0.76028300	-1.81732900
O	-2.46821500	-1.32746900	-0.08909300

N	2.07395800	-0.15142300	0.09788100
O	2.78685500	0.53843500	-0.60025000
O	2.46151100	-0.80606000	1.04095100
O	-1.87413400	0.68861100	0.88757300
O	-0.96015300	1.73177500	0.97402700

## INT1a

N	-0.34587000	1.29608700	-0.51418100
C	-0.73208100	0.12947500	0.07156000
N	0.94358600	1.27149700	-0.34356700
C	1.43646300	0.06295200	0.48962300
N	0.11561000	-0.64546100	0.62912500
H	1.49610300	2.08307800	-0.59820200
O	1.98735200	0.40463500	1.60427300
N	-2.17492100	-0.17554400	0.04968200
O	-2.90752800	0.57786200	-0.55552100
O	-2.54214000	-1.16881100	0.63741700
O	2.30803700	-0.69028900	-0.30193200
O	1.71787500	-1.05635800	-1.57377600

TS(NTOa+O<sub>2</sub>\*→INT2a)

N	0.15676600	-0.06314100	1.37375100
C	-0.29987100	-0.09386500	0.07719700
N	1.47484500	-0.18388500	1.16782700
C	1.76214100	-0.54308300	-0.16618700
N	0.59943100	-0.55411700	-0.83537500
H	2.11437600	-0.24093900	1.94906600
O	2.91065900	-0.79837400	-0.56151900
N	-1.72020100	-0.52561000	-0.05945200
O	-2.48998900	-0.19452900	0.81863900
O	-2.04084400	-1.13868700	-1.05422600
O	0.48449600	2.22708400	-0.56660300
O	-0.67230700	1.57324200	-0.25408900

## INT2a

N	0.14754000	0.30233800	1.30472900
C	-0.31099600	0.33867400	-0.07671300
N	1.38412500	-0.13418900	1.16567100
C	1.77777000	-0.23870100	-0.20686200
N	0.72991900	0.08731300	-0.95582300
H	1.99841700	-0.23911900	1.96344500
O	2.92382300	-0.57463600	-0.51987100
N	-1.36896500	-0.95567200	-0.10452100
O	-2.50097600	-0.79341100	0.29725400
O	-0.91788600	-2.02708700	-0.43852100
O	-0.45479200	2.60982100	-0.25003900
O	-1.18109300	1.35290600	-0.35537100

## INT3a

N	-0.13894300	1.32130400	-0.00003700
N	-1.48895400	1.07775400	0.00001400
C	-1.76138000	-0.26482100	-0.00013600
O	-2.91707100	-0.76011100	0.00003300
N	-0.57071900	-0.91481700	0.00003200
C	0.33730900	0.08929800	-0.00001300
N	1.71193600	-0.14761100	0.00001300

O	2.52997300	0.85481900	-0.00001800
O	2.15002200	-1.36231300	0.00006200
H	-2.15219100	1.83756300	0.00011800

## INT4a

N	0.17489900	1.31796900	-0.00007200
C	-0.30145200	0.08272600	-0.00000400
N	1.50588600	1.17190100	0.00008700
C	1.76855800	-0.18656400	-0.00003500
N	0.61261800	-0.90362400	-0.00001800
O	2.94785100	-0.67132000	0.00006500
N	-1.69916400	-0.15062800	-0.00002700
O	-2.47203600	0.80590100	0.00001000
O	-2.09610500	-1.31286800	-0.00001900

## NTO\*

N	-0.17797500	1.36792100	0.00006600
C	0.38720300	0.09633300	0.00008900
N	-1.46881800	1.11554800	-0.00024000
C	-1.79411500	-0.24046700	0.00022900
N	-0.52730800	-0.85373000	-0.00008000
H	-0.35644100	-1.85528500	-0.00022300
H	-2.14676100	1.87234200	-0.00052500
O	-2.87194500	-0.75314100	0.00007000
N	1.72835400	-0.12817900	0.00011700
O	2.49736900	0.88237200	0.00006300
O	2.13268900	-1.33712700	-0.00015800

TS(NTO\*+O<sub>2</sub>\*→INT1)

N	0.28263300	1.40355800	0.35275100
C	0.77523800	0.21408600	-0.14771900
N	-1.00799900	1.31860100	0.12346900
C	-1.46169400	0.09199300	-0.53999900
N	-0.13618300	-0.53874000	-0.69992900
H	0.02144800	-1.47079200	-1.06439400
H	-1.61169900	2.10934600	0.31236200
O	-2.28976300	0.12394600	-1.45989600
N	2.12035100	-0.13935700	-0.05855300
O	2.92538800	0.68233400	0.49584700
O	2.48062200	-1.26500700	-0.56179400
O	-2.11233500	-0.77699100	0.66223300
O	-1.39174000	-0.86221500	1.72038100

## TS(INT4→INT7)

N	0.17347100	1.55109900	-0.00009600
C	-0.64010200	0.45779600	-0.00025000
N	1.35665800	0.98811800	0.00041400
C	1.32194000	-0.43890500	-0.00017700
N	-0.02919100	-0.70891900	-0.00092800
H	2.20293200	1.55012800	-0.00171200
O	2.27784600	-1.16312100	0.00056100
O	-2.32251200	-0.92732000	0.00025600
O	-1.93079800	0.45251000	0.00043400
H	-0.99682000	-1.37211000	-0.00145300

## INT7

N	0.28026500	1.09225300	-0.00231800
C	0.51760700	-0.26920700	-0.00042800
N	-1.02083400	1.12275500	-0.00238300
C	-1.58390200	-0.18445400	-0.00193200
N	-0.51563100	-1.05678700	0.00088700
H	-1.52980300	2.00118200	-0.00367500
O	-2.77075700	-0.41340800	-0.00248500
O	2.72643600	0.23348600	0.11044100
O	1.74607800	-0.77452900	-0.00450200
H	3.10691200	0.24884200	-0.78310000

## TS(INT7→INT8+OH\*)

N	-0.06734000	1.29173000	-0.10288700
C	-0.55700700	-0.02546600	-0.40090300
N	1.13290900	1.10134700	0.14750200
C	1.50247300	-0.34430300	0.05419100
N	0.35971700	-0.97048800	-0.28866600
H	1.76587400	1.87010800	0.38090400
O	2.62559300	-0.71655400	0.26674200
O	-2.64359600	-0.40427400	0.77002300
O	-1.77959400	-0.14094500	-0.71097200
H	-3.03489900	0.48456400	0.80137800

## INT8

N	-0.64526400	1.24483900	0.00031000
C	-1.10068500	-0.26089100	-0.00004900
N	0.55716600	1.16891900	-0.00016300
C	1.07708300	-0.33687600	0.00008900
N	-0.02790200	-1.05764500	0.00040500
H	1.15984200	2.00234100	-0.00010800
O	2.25136800	-0.52500500	-0.00021400
O	-2.27714600	-0.46356000	-0.00028500

## OH\*

O	0.00000000	0.00000000	0.10827300
H	0.00000000	0.00000000	-0.86618500

## TS(INT8→INT9)

N	0.82793400	1.20317500	0.00009100
C	1.06292300	-0.29124100	-0.00006100
N	-0.36565200	1.39473600	0.00016300
C	-1.19384900	-0.45195200	-0.00000800
N	-0.07364600	-1.03722100	-0.00015400
H	-0.64169400	2.38566600	0.00027000
O	-2.35517900	-0.42948300	0.00004100
O	2.19352800	-0.67693500	-0.00011000

## INT9

N	1.05936100	1.10864800	0.00065600
C	1.00334700	-0.37287400	-0.00008600
N	-0.05299600	1.61174800	-0.00033600
C	-1.34650400	-0.48448800	0.00000800
N	-0.22684800	-0.98561400	-0.00054500
H	0.04019400	2.63692100	0.00030400
O	-2.47209600	-0.24135800	0.00035500



O 2.04236200 -0.96316900 -0.00013700

TS(INT7→INT10)

N -0.44867800 1.14999600 0.00428300  
 C -0.48876100 -0.16691200 0.00164900  
 N 0.79538200 1.55520100 -0.00406400  
 C 1.74866800 -0.50351700 0.00102100  
 N 0.59518100 -0.97525300 0.00023900  
 H 0.80477500 2.57679000 0.00779800  
 O 2.90100700 -0.43837300 0.00129700  
 O -2.75991400 -0.03886000 -0.11849600  
 O -1.62935500 -0.86478700 0.01362100  
 H -3.05131900 0.07233500 0.80159400

INT10

N -0.50790000 1.15987600 0.00625600  
 C -0.47374400 -0.15033800 -0.00014500  
 N 0.69632700 1.68610600 -0.00982600  
 C 1.79604400 -0.55706700 0.00103600  
 N 0.62814700 -0.94314800 -0.00538100  
 H 0.57146600 2.70043400 0.01116700  
 O 2.94085400 -0.43699000 0.00566100  
 O -2.75534700 -0.13539000 -0.11731900  
 O -1.58570800 -0.90227200 0.01685200  
 H -3.01967600 0.02137700 0.80458600

TS(INT9+OH\*→INT11+N<sub>2</sub>+H<sub>2</sub>O)

N -0.67680700 -0.84576100 -0.00335300  
 C 0.79174000 -1.12159300 -0.00022500  
 N -0.93114900 0.33730000 -0.00180200  
 C 1.42725100 1.14864100 0.00081700  
 N 1.65435400 -0.05583100 0.00119300  
 H -1.98385900 0.50192700 -0.00474500  
 O 1.43594000 2.29919700 0.00077100  
 O 1.13076700 -2.26480400 0.00058200  
 O -3.55434600 0.44046400 -0.00186900  
 H -3.75375600 -0.51302000 0.03304700

INT11

C 1.14779300 -0.35107100 -0.00005500  
 C -1.15452000 0.06329100 -0.00029800  
 N 0.01469600 0.42554200 0.00006200  
 O -2.28138600 -0.15530200 0.00015100  
 O 2.27357200 -0.00121200 0.00005900

TS(INT9+OH\*→INT12)

N 1.31607100 1.08409200 0.15645900  
 C 1.18817600 -0.35784400 -0.15054200  
 N 0.24635300 1.66589700 0.07163800  
 C -1.17147900 -0.25035000 -0.41470500  
 N -0.06368400 -0.88382800 -0.41636800  
 H 0.38406200 2.66443300 0.28176700  
 O -2.16960500 0.10344400 -0.88135400  
 O 2.18669900 -1.01478900 -0.17535000  
 O -1.21474400 -0.42702600 1.41305700  
 H -1.39423000 -1.37142700 1.57680100

## INT12

N	1.91434500	0.33866000	-0.01228700
C	0.91174800	-0.73876900	0.07226700
N	1.40842700	1.45691100	-0.00038000
C	-1.40206700	0.05523000	0.06628700
N	-0.25594500	-0.41434900	0.76061300
H	2.15276800	2.16087800	-0.09320000
O	-2.33143800	-0.67951900	-0.11930200
O	1.17677800	-1.82141000	-0.34883200
O	-1.37187600	1.32388700	-0.26414500
H	-0.46634900	1.68813900	-0.11551700

TS(INT9+OH<sup>•</sup>→INT13)

N	-0.67817400	1.30196600	0.10193900
C	-0.74659600	-0.16510200	0.35132500
N	0.46720600	1.69699300	-0.03292900
C	1.56289700	-0.54640300	0.05167500
N	0.43142900	-0.89291700	0.35735400
H	0.45188300	2.71346400	-0.19413800
O	2.68570700	-0.43413300	-0.18944300
O	-1.75275400	-0.57044000	0.94579900
O	-1.50792600	-0.63607300	-1.24127800
H	-2.29313100	-0.06156200	-1.32903300

## INT13

N	-0.81642500	1.24591900	0.07727500
C	-0.81562800	-0.25039800	0.02359500
N	0.29502700	1.73376300	-0.02846500
C	1.54668000	-0.48151100	-0.13152800
N	0.40823900	-0.87425900	-0.32777900
H	0.21473100	2.75775000	0.03598600
O	2.68210800	-0.29890200	-0.02276600
O	-1.05858300	-0.69728100	1.31061200
O	-1.77932000	-0.63209600	-0.87409200
H	-2.56257400	-0.07802800	-0.74563100

TS(INT11+H<sub>2</sub>O→INT14)

C	1.89040300	0.11734400	-0.01293600
C	0.01273600	-1.07989900	-0.02318000
N	0.52212800	0.07717600	0.12242400
O	0.00929600	-2.22017200	-0.22620600
O	2.60133600	1.06390300	0.05941600
O	-1.82343900	-0.63440500	0.32978700
H	-2.40429100	-1.16528200	-0.23168900
H	-0.80200800	1.98428300	-0.12507400
O	-1.75953900	1.97759600	-0.25944100
H	-1.97331500	0.31664900	0.10712500
H	-2.11534100	2.60407100	0.38091600

## INT14

C	1.45322100	0.26147200	0.00000800
C	-0.92469100	0.10818500	-0.00008600
N	0.32959000	-0.48787100	-0.00016600
O	-1.11264200	1.29764600	-0.00000100
O	2.58738900	-0.08674000	0.00010400

O	-1.86697800	-0.82402400	0.00016300
H	-2.73508400	-0.39409900	-0.00009500
H	0.39463400	-1.50380000	-0.00039900

## TS(INT11→INT15+CO)

C	-1.34614600	-0.44264600	0.00058700
C	1.26919600	0.17014900	0.00020900
N	0.27686900	0.89561400	0.00004000
O	2.23237400	-0.47876800	-0.00023600
O	-2.41692200	-0.10052200	-0.00039500

## INT15

C	0.00000000	-0.04294000	0.00000000
N	-0.70453000	-1.02643300	0.00000000
O	0.61646400	0.93033300	0.00000000

## CO

C	0.00000000	0.00000000	-0.64144300
O	0.00000000	0.00000000	0.48108200

## INT16

C	0.04265800	0.01519000	-0.00004100
N	-1.15647800	-0.12520800	0.00001300
O	1.20550500	0.01659900	0.00001600
H	-1.80464700	0.65252400	0.00002100

HOO<sup>-</sup>

H	-0.88184500	-0.89906000	0.00000000
O	0.05511500	-0.67615800	0.00000000
O	0.05511500	0.78854000	0.00000000

CO<sub>2</sub>

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.15522600
O	0.00000000	0.00000000	-1.15522600

TS(INT16+H<sub>2</sub>O →INT17)

C	-1.46611500	-0.32693100	0.07115500
N	-0.57152200	-1.20824800	0.16767900
O	-2.59468400	0.02518200	0.18602900
H	-0.98845200	-2.06477600	0.53063000
H	-1.11565200	1.86043000	-0.45424500
O	-0.58002600	1.06792900	-0.59843300
H	0.31824700	1.21604000	-0.16637900
H	2.29907000	2.04576100	0.10916600
O	1.76073900	1.35110500	0.50402700
H	2.17746700	0.50104400	0.25393600
O	2.19665600	-1.19339900	-0.33143100
H	2.61558500	-1.85422100	0.22934000
H	1.22961000	-1.29149100	-0.18467400

## INT17

C	-0.03079300	0.11038000	-0.00000100
N	1.26130000	-0.24168700	0.00005100
H	1.53920400	-1.21003800	-0.00014100
O	-0.45112300	1.25795900	-0.00000500

H	1.96568300	0.47785400	-0.00013800
O	-0.84759700	-0.95814300	-0.00000400
H	-1.75946800	-0.63681700	0.00000500

TS(INT17→NH<sub>3</sub>+CO<sub>2</sub>)

C	1.24025700	-0.16438900	0.02411400
N	0.64598600	0.89774500	0.77524100
O	2.24848300	0.09986300	-0.64615400
H	1.28932400	1.66813000	0.91868100
H	-0.92080800	-1.28168500	0.08650800
O	0.64225100	-1.27942200	0.07806500
H	0.27027400	0.57318500	1.66155900
H	-1.72241400	1.56558000	-1.25111900
O	-1.70978400	1.28238300	-0.32602000
H	-0.74516900	1.32846100	0.02950300
O	-1.91021800	-1.09917000	-0.04838400
H	-2.37595800	-1.35767300	0.75630900
H	-1.92455900	0.17688800	-0.23285700

NH<sub>3</sub>

N	-0.00000100	0.00000700	-0.11707800
H	-0.85705800	0.38028400	0.27318900
H	0.75789800	0.55203300	0.27318800
H	0.09916600	-0.93236700	0.27316700

## NTOa\*

N	-0.19016300	1.33225400	0.00004800
C	0.33730600	0.03396800	0.00011000
N	-1.48067900	1.08853600	-0.00001300
C	-1.75856900	-0.28843600	-0.00003900
N	-0.53036000	-0.94102100	0.00007400
H	-2.16014600	1.84063400	-0.00004300
O	-2.86717900	-0.77496300	-0.00006900
N	1.70546200	-0.14273400	0.00015600
O	2.45339400	0.89795300	-0.00013400
O	2.18352200	-1.33212400	-0.00007700

TS(NTOa\*+O<sub>2</sub><sup>•-</sup>→INT1a)

N	0.23099100	-0.89037400	-1.10469100
C	0.70470100	-0.26006500	0.06535700
N	-1.01243800	-1.16641400	-0.77732200
C	-1.40789200	-0.45388900	0.45352400
N	-0.15147000	-0.03164800	1.00200100
H	-1.66861400	-1.41180400	-1.51093100
O	-2.36335200	-0.83300600	1.12947500
N	2.05318000	0.04655200	0.15377300
O	2.82497400	-0.28776700	-0.81440900
O	2.49232300	0.65710400	1.19420100
O	-2.01117300	1.03699700	-0.29012300
O	-1.18703200	1.92526200	-0.78398000

TS(NTOa\*+O<sub>2</sub><sup>•-</sup>→INT2a)

N	0.25076100	-0.32237600	1.33866900
C	-0.33867200	0.00621800	0.08544300
N	1.50380300	-0.54975100	0.99303700
C	1.69590000	-0.49343300	-0.41942400

N	0.51595800	-0.19765800	-0.97239100
H	2.20225900	-0.79553500	1.68291900
O	2.79229800	-0.71630000	-0.93648300
N	-1.71921300	-0.40631900	-0.05473900
O	-2.07155900	-1.51501300	0.51747700
O	-2.34080000	0.02931300	-1.10449200
O	0.46816100	2.30751700	0.19505100
O	-0.62370200	1.65092700	0.22706500

TS(INT3a+O<sub>2</sub><sup>-</sup>→INT5a)

N	-0.69788000	1.42170400	-0.31736000
C	-0.92751800	0.15205700	0.00781900
N	0.72728800	1.54239900	-0.12851600
C	1.16379500	0.25667600	0.46630000
N	0.08773100	-0.63321700	0.37908900
H	1.11146100	1.61530300	-1.06943400
O	1.91232000	0.28085100	1.49136900
N	-2.24768900	-0.34165100	-0.02844900
O	-3.22862100	0.45555700	-0.31014300
O	-2.46954500	-1.59764400	0.18062600
O	2.21065600	-0.26671100	-0.90833300
O	3.12328100	-1.12109600	-0.59209700

## INT5a

N	-0.59583500	1.37622700	-0.43619300
C	-0.80813300	0.19799000	0.08458400
N	0.76130100	1.59210700	-0.05124500
C	1.34380100	0.26051200	0.35747300
N	0.11706400	-0.52209100	0.66203900
H	1.27674400	1.98071200	-0.83785200
O	2.24317500	0.32177700	1.30852100
N	-2.21031700	-0.30774400	0.01830700
O	-3.07309100	0.41370700	-0.44204500
O	-2.42429700	-1.42995300	0.42731800
O	1.89581700	-0.22349900	-0.91407000
O	2.48386700	-1.54468400	-0.77532800

TS(INT3a+O<sub>2</sub><sup>-</sup>→INT6a+NO<sub>2</sub><sup>-</sup>)

N	0.17014000	-0.09538800	1.37573700
C	-0.33985200	-0.13872600	0.07791800
N	1.48185800	-0.21667000	1.14299000
C	1.74769100	-0.56634800	-0.19807200
N	0.58554800	-0.59475000	-0.84624400
H	2.14601600	-0.22712700	1.90476500
O	2.90259400	-0.80737100	-0.60639400
N	-1.69322200	-0.58446400	-0.03738000
O	-2.50829300	-0.30613500	0.93504600
O	-2.15965400	-0.80422000	-1.22734300
O	0.58099400	2.22979300	-0.42119100
O	-0.61605600	1.54999100	-0.25881200

## INT6a

N	-0.03385000	1.44352800	0.05985500
C	0.62707000	0.30967300	-0.05569300
N	-1.34114000	0.98737200	0.05962100
C	-1.39057300	-0.37166200	-0.00917400

N	-0.10831100	-0.82120200	-0.09704200
H	-2.11364900	1.62339700	0.18154900
O	-2.44663200	-1.05818900	0.00101800
O	2.62044300	-0.87348300	0.18075100
O	1.96091000	0.36675400	-0.17544200

TS(INT4a+O<sub>2</sub><sup>-•</sup>→INT7a)

N	0.06117400	0.42047400	-1.31423300
C	0.60604200	-0.26569000	-0.18361300
N	-1.16449300	0.15685700	-1.32340100
C	-1.48453200	-0.57566400	-0.08635500
N	-0.25276500	-0.97261600	0.48547700
O	-2.55590200	-1.23717000	0.01392700
N	1.95435400	-0.18699700	0.06159300
O	2.70650300	0.52322800	-0.69166800
O	2.44020700	-0.82576700	1.05685700
O	-1.77446300	0.92933100	0.76336900
O	-0.68096300	1.75089100	0.88923500

## INT7a

N	-0.24999700	-1.12577900	0.85111600
C	-0.75195500	-0.09327400	-0.06627800
N	0.96669200	-1.17893900	0.69518900
C	1.41301100	-0.21453100	-0.44367400
N	0.13198200	0.47264500	-0.78795400
O	1.94525000	-0.88216400	-1.42286300
N	-2.10798000	0.14754100	-0.07670700
O	-2.88319100	-0.50922000	0.70097200
O	-2.57108600	1.03509100	-0.87298900
O	2.33145300	0.68651800	0.11266900
O	1.78367300	1.37459300	1.26823600

TS(INT4a+O<sub>2</sub><sup>-•</sup>→INT8a)

N	0.16054000	0.25949400	1.33321100
C	-0.38426200	-0.16691900	0.08178900
N	1.39705100	0.07180400	1.25837400
C	1.66230300	-0.66529400	0.00148300
N	0.51353800	-0.89058400	-0.63560500
O	2.81494300	-1.02296000	-0.27727300
N	-1.74950600	-0.42241500	0.02819300
O	-2.53856500	0.22130300	0.82365900
O	-2.22760000	-1.10043100	-0.96046100
O	1.00632900	1.84382900	-0.80811700
O	-0.29505800	1.54140700	-0.57641300

## INT8a

N	0.29390900	-0.27843700	-1.33209300
C	-0.30965200	-0.16772900	0.07439900
N	1.44944100	0.11001200	-1.28988000
C	1.75622500	0.54590000	0.14948200
N	0.70062200	0.37334400	0.89448500
O	2.88847100	0.97706200	0.38522800
N	-1.49094700	0.72454100	-0.04826700
O	-2.33993200	0.42826600	-0.98651200
O	-1.91344200	1.28240900	1.04475300
O	0.25908700	-2.38113900	0.49595000



O           -0.81301200 -1.40350400 0.44645600

### Hydroperoxyl radical induced degradation of NTO and NTOa

#### NTO

N           -0.12666700 1.32311000 -0.00010500  
 C           0.36226000 0.13534300 -0.00006400  
 N           -1.45970700 1.10938500 0.00015700  
 C           -1.80641500 -0.22101300 -0.00023200  
 N           -0.57239800 -0.84500400 -0.00001900  
 H           -0.41365700 -1.84430400 0.00016100  
 H           -2.10256000 1.88985600 0.00045900  
 O           -2.91770500 -0.72084900 0.00004300  
 N           1.78328300 -0.13448200 0.00003200  
 O           2.53711800 0.81007700 -0.00002600  
 O           2.10678200 -1.30205200 0.00007100

#### HO<sub>2</sub><sup>•</sup>

H           -0.87849200 -0.88366200 0.00000000  
 O           0.05490600 -0.59537500 0.00000000  
 O           0.05490600 0.70583300 0.00000000

#### NTO<sub>r</sub>

N           -0.19126100 1.31077600 0.00010300  
 C           0.30404400 0.04038500 0.00006600  
 N           -1.46449200 1.09343000 0.00008500  
 C           -1.76488100 -0.29229600 -0.00002700  
 N           -0.52927300 -0.94195100 0.00002100  
 H           -2.13298800 1.86027500 0.00012600  
 O           -2.87370900 -0.76614400 -0.00006000  
 N           1.76120500 -0.14532400 0.00009300  
 O           2.44225900 0.85234200 -0.00003500  
 O           2.16454500 -1.28211400 -0.00021500

#### NTO<sub>r</sub>'

N           -0.20876600 1.34429100 -0.00017700  
 C           0.32086000 0.11081700 -0.00009800  
 N           -1.49859900 1.21344700 0.00067100  
 C           -1.81736300 -0.16428100 -0.00086400  
 N           -0.58466000 -0.84138800 0.00010900  
 H           -0.43937100 -1.84622100 0.00053000  
 O           -2.91812300 -0.65442600 0.00005700  
 N           1.74992900 -0.13382000 -0.00004700  
 O           2.47266800 0.83322600 -0.00001800  
 O           2.09708800 -1.29263800 0.00013000

#### HOOH

H           -0.94925600 -0.89789800 0.00000000  
 O           0.00002200 -0.71540800 0.00000000  
 O           0.00002200 0.71526400 0.00000000  
 H           0.94889900 0.89904900 0.00000000

#### TS(NTO+HO<sub>2</sub><sup>•</sup>→INT1)

N           -0.21256300 -0.20453700 1.37770400  
 C           -0.69600900 -0.31051100 0.15028600

N	1.05340400	-0.47773400	1.24367500
C	1.49604800	-0.60626200	-0.13842400
N	0.18756700	-0.63220600	-0.76750700
H	1.68363200	-0.37411400	2.03434600
O	2.47663400	-1.23850100	-0.50665200
N	-2.10731800	-0.09111300	-0.13568800
O	-2.82970700	0.15208700	0.79875600
O	-2.43088100	-0.17100200	-1.29729300
O	1.91763200	1.06385300	-0.39396100
O	0.93939600	1.97648200	-0.03879900
H	0.45581200	2.15217600	-0.86159000
H	0.02809300	-0.70164100	-1.76762400

## INT1

N	-0.36407800	1.23062500	-0.66114300
C	-0.80039700	0.17394300	0.03477400
N	0.90887000	1.24779000	-0.47223100
C	1.46462200	0.19449100	0.50931700
N	0.10076800	-0.50064500	0.67858100
H	1.46181000	2.01217900	-0.85428600
O	2.01490500	0.62906100	1.53987300
N	-2.22466600	-0.15343900	0.05818700
O	-2.96804300	0.56189900	-0.56674200
O	-2.53575900	-1.12547000	0.70536900
O	2.32012200	-0.67578800	-0.22138900
O	1.70413300	-1.10407900	-1.42399500
H	1.39146600	-1.99424100	-1.20128900
H	-0.06773600	-1.28383600	1.30233800

TS(NTO+HO<sub>2</sub>\*→INT2)

N	0.14173500	-0.25079300	1.37424900
C	-0.35023900	-0.20839500	0.13440000
N	1.44835900	-0.37026800	1.18827700
C	1.81576300	-0.56042300	-0.14601000
N	0.59699600	-0.52224400	-0.79230700
H	2.08193900	-0.39858200	1.97873600
O	2.92423400	-0.72385400	-0.59507200
N	-1.76416200	-0.53867700	-0.08765700
O	-2.52971700	-0.29697900	0.81294600
O	-2.05063600	-0.99191300	-1.17026000
O	0.49239400	2.25218800	-0.28202400
O	-0.71142800	1.65622100	-0.09823000
H	0.69138000	2.15486500	-1.22879000
H	0.47426300	-0.53480300	-1.79709700

## INT2

N	0.14798900	0.25279900	1.31996000
C	-0.36326400	0.23871600	-0.02488100
N	1.40854900	-0.12070900	1.19071500
C	1.83742700	-0.30082800	-0.13273000
N	0.72073200	-0.01464300	-0.86746200
H	2.01289600	-0.19507700	2.00088800
O	2.94090900	-0.62214600	-0.49367600
N	-1.42819500	-0.94644200	-0.07830800
O	-2.53322000	-0.71835300	0.34339100
O	-1.02073200	-2.00917300	-0.46848800

O	-0.38607900	2.49650000	-0.17471000
O	-1.16649000	1.32851300	-0.33829200
H	-0.13136600	2.71014400	-1.08695400
H	0.65486900	-0.14216400	-1.86841200

## INT3

N	0.12953800	1.35371100	0.00014500
C	-0.38814400	0.15584400	0.00011900
N	1.48259700	1.10652500	-0.00031600
C	1.79955100	-0.21528500	0.00044400
N	0.56367100	-0.82607700	-0.00001000
H	0.39196900	-1.82138500	-0.00030500
H	2.14020200	1.87169900	-0.00079400
O	2.90877300	-0.74343800	-0.00003700
N	-1.73313800	-0.13082400	0.00002300
O	-2.58049200	0.83444100	0.00005700
O	-2.09069300	-1.36813100	-0.00016700

O<sub>2</sub>

O	0.00000000	0.00000000	0.59379900
O	0.00000000	0.00000000	-0.59379900

TS(INT2→INT4+NO<sub>2</sub>•)

N	0.14883200	0.40561500	1.27991600
C	-0.28822000	0.48747000	0.00690300
N	1.42022200	0.05230100	1.16374600
C	1.88263200	0.02370100	-0.15356900
N	0.76173300	0.38457500	-0.86386000
H	1.98626500	-0.13529300	1.98294100
O	2.99542800	-0.24767300	-0.53948500
N	-1.16700400	-1.35756800	-0.10688000
O	-2.32494700	-1.47262300	0.18163200
O	-0.37289400	-2.22773100	-0.32843100
O	-1.21045000	2.52498100	-0.26779100
O	-1.44084700	1.11417800	-0.31415500
H	-1.56440900	2.75808800	0.60593100
H	0.69487400	0.38665700	-1.87350400

## INT4

N	0.03898000	1.38276000	0.03022400
C	0.61162100	0.26070400	-0.23131000
N	-1.27881600	1.04376500	0.17584700
C	-1.51663900	-0.28960600	0.02248800
N	-0.25786800	-0.78946200	-0.25016500
H	-1.97305200	1.75231800	0.36248300
O	-2.57777200	-0.89730000	0.10205900
O	2.53711700	-0.66610600	0.48056100
O	1.92107200	0.15425100	-0.51786100
H	2.88015100	-0.00436900	1.10313200
H	-0.03639300	-1.76073900	-0.42210300

NO<sub>2</sub>•

N	0.00000000	0.31564900	0.00000000
O	1.08972200	-0.13834700	0.00000000
O	-1.08972200	-0.13784600	0.00000000

TS(INT4→INT5+H<sub>2</sub>O)

N	0.02049700	1.34297600	-0.01636200
C	0.58844200	0.15636300	-0.45162900
N	-1.18442200	1.06994800	0.25297000
C	-1.54028100	-0.32190100	0.06968600
N	-0.36668400	-0.84486100	-0.35008500
H	-1.83488800	1.78770800	0.57297100
O	-2.62870200	-0.78616900	0.26533700
O	2.79638000	-0.56332000	0.81453200
O	1.75255200	0.06265900	-0.80565500
H	3.13176500	0.32955900	0.95661200
H	-0.23341600	-1.80584200	-0.63730500

## INT5

N	0.64577000	1.24457800	-0.00010900
C	1.10070200	-0.25981100	-0.00032700
N	-0.55673900	1.16909800	0.00005300
C	-1.07711400	-0.33755500	0.00054400
N	0.02773700	-1.05740100	0.00003400
H	-1.15889000	2.00288300	0.00028200
O	-2.25174300	-0.52462200	-0.00027500
O	2.27674200	-0.46445500	0.00009600

H<sub>2</sub>O

H	0.00000000	0.76115400	-0.47140900
O	0.00000000	0.00000000	0.11785200
H	0.00000000	-0.76115400	-0.47140900

## TS(INT5→INT6)

N	0.82793400	1.20317500	0.00009100
C	1.06292300	-0.29124100	-0.00006100
N	-0.36565200	1.39473600	0.00016300
C	-1.19384900	-0.45195200	-0.00000800
N	-0.07364600	-1.03722100	-0.00015400
H	-0.64169400	2.38566600	0.00027000
O	-2.35517900	-0.42948300	0.00004100
O	2.19352800	-0.67693500	-0.00011000

## INT6

N	1.05936100	1.10864800	0.00065600
C	1.00334700	-0.37287400	-0.00008600
N	-0.05299600	1.61174800	-0.00033600
C	-1.34650400	-0.48448800	0.00000800
N	-0.22684800	-0.98561400	-0.00054500
H	0.04019400	2.63692100	0.00030400
O	-2.47209600	-0.24135800	0.00035500
O	2.04236200	-0.96316900	-0.00013700

TS(INT6+H<sub>2</sub>O→INT7)

N	2.12618700	-0.14262300	-0.38354400
C	1.05068800	0.79015500	-0.09658700
N	2.94207600	-0.23098500	0.53100200
C	-0.37614500	-0.99856600	-0.07890700
N	-0.20744100	0.25488200	0.04348500
H	3.67828000	-0.88484700	0.22822100
O	-0.05124900	-2.09447500	-0.29552600

O	1.27419300	1.97351300	-0.06139800
O	-2.20046600	-1.11060600	0.36004300
H	-2.63538200	-0.23935500	0.18082100
H	-2.63154500	-1.78182800	-0.18629600
O	-2.91198000	1.40978000	-0.13049700
H	-3.38706300	1.90468800	0.54638000
H	-1.98128600	1.65719700	-0.03373800

## INT7

N	-1.37105400	0.66132100	-0.45150300
C	-0.91477900	-0.65978300	-0.07478400
N	-2.11747000	1.16036300	0.38677700
C	1.40367800	0.17648500	0.00815000
N	0.44054600	-0.81932900	0.01304200
H	-2.45238000	2.05669800	0.00622100
O	1.18810000	1.36056600	-0.03701200
O	-1.69556700	-1.57069600	0.03775500
O	2.60955500	-0.38002500	0.06687100
H	0.76078100	-1.77387000	0.13484400
H	3.27734600	0.32171400	0.07961100

TS(INT6+H<sub>2</sub>O→INT8)

N	0.12738900	1.32470700	0.08110500
C	0.26399800	-0.17819900	-0.08164700
N	-1.02247100	1.73087600	0.03028300
C	-2.12490800	-0.59297200	0.02362300
N	-0.97587000	-0.88730600	0.23977500
H	-1.00937400	2.75971700	0.06434700
O	-3.27632100	-0.47569200	-0.13374500
O	0.80435600	-0.45310800	-1.20683800
O	1.18535900	-0.55561000	1.02614300
H	2.35914300	-0.31541500	0.57583500
H	0.94564500	-0.15560600	1.87564100
O	3.23162900	-0.18474900	-0.13943500
H	3.68770600	0.66153700	-0.01577600
H	2.71880900	-0.14788200	-0.97905100

## INT8

N	-0.73172500	1.25649000	-0.00116400
C	-0.79670800	-0.24128900	-0.00195600
N	0.40048300	1.70478100	-0.01385900
C	1.59011800	-0.50941600	-0.01636800
N	0.45092700	-0.91370800	-0.05917900
H	0.35082000	2.73275600	-0.00516600
O	2.73870500	-0.33235100	0.01110900
O	-1.41150800	-0.60855500	1.18396900
O	-1.50585600	-0.61002500	-1.13236800
H	-2.19889700	-0.06265000	1.32121400
H	-2.32090700	-0.09136900	-1.18838300

TS(INT6+H<sub>2</sub>O→INT9+N<sub>2</sub>H<sub>2</sub>)

N	-0.55359500	0.94572300	0.12984500
C	-0.16478200	-0.53819500	0.22873500
N	0.37631600	1.73232100	0.15156900
C	2.19788800	-0.18805100	-0.27139000
N	1.14800900	-0.75329200	-0.43273900

H	-0.00145500	2.68930400	0.18977300
O	3.27602400	0.25956900	-0.20020600
O	-0.25215000	-0.93800100	1.43367500
O	-1.13368400	-1.12267500	-0.68424500
H	-2.55414600	-0.40843900	-0.49394600
H	-3.60545200	0.78113300	-0.89460000
O	-3.06712900	0.41179900	-0.17549400
H	-2.26382900	1.00789400	0.01974600
H	-1.15334600	-2.07121900	-0.49561200

## INT9

C	-0.88062000	0.09952100	0.00008200
C	1.43148300	-0.20698000	-0.00019900
N	0.29466400	-0.64893500	0.00039000
O	2.54087400	0.09347000	-0.00011900
O	-0.94957700	1.30145100	0.00008800
O	-1.92047600	-0.72200700	-0.00007100
H	-2.73439800	-0.19601100	-0.00121600

N<sub>2</sub>H<sub>2</sub>

N	-0.61614600	-0.11960700	0.00008200
N	0.61632700	-0.11947700	-0.00008200
H	-1.00925700	0.83646700	-0.00035300
H	1.00798600	0.83711900	0.00035200

TS(INT6→INT10+CO+N<sub>2</sub>)

N	-2.18863200	-0.16937200	-0.00020700
C	-0.56557100	0.81950200	0.00061600
N	-1.87192400	-1.27609300	-0.00023100
C	1.58421900	-0.44711300	0.00002800
N	0.37311300	-0.44542500	0.00039800
H	-0.55847100	-1.25829200	0.00056500
O	2.74176200	-0.39208800	-0.00025300
O	-0.20942600	1.92461200	-0.00026600

## INT10

C	0.04265800	0.01519000	-0.00004100
N	-1.15647800	-0.12520800	0.00001300
O	1.20550500	0.01659900	0.00001600
H	-1.80464700	0.65252400	0.00002100

## CO

C	0.00000000	0.00000000	-0.64144300
O	0.00000000	0.00000000	0.48108200

N<sub>2</sub>

N	0.00000000	0.00000000	0.54480100
N	0.00000000	0.00000000	-0.54480100

TS(INT7→INT11+CO<sub>2</sub>)

N	-1.22340000	0.74288100	0.00001000
C	-0.96050300	-0.76489300	0.00000500
N	-2.36103100	1.16754700	-0.00001000
C	1.94843800	0.25064100	-0.00000300
N	0.32460100	-0.94406200	0.00002300
H	-2.35525200	2.19857300	-0.00000300



O	2.81140800	-0.54492500	-0.00001300
O	-1.95312400	-1.47184000	-0.00001300
O	1.52403400	1.35486500	0.00000000
H	0.57033000	-1.93104300	0.00001900
H	-0.38242500	1.34862000	0.00002900

## INT11

N	0.78758100	-0.52380800	0.00000700
C	-0.62668000	0.09646400	-0.00000800
N	1.78427300	0.16851400	-0.00000600
N	-1.45731100	-0.88548700	0.00003500
H	2.62736500	-0.42277400	0.00000300
O	-0.63570400	1.32476200	-0.00003400
H	-2.40655500	-0.51506600	0.00004300
H	0.82309700	-1.55357700	0.00002200

CO<sub>2</sub>

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.15522600
O	0.00000000	0.00000000	-1.15522600

TS(INT7→INT12+CO<sub>2</sub>)

N	1.47622200	-0.07714700	0.83388800
C	0.99775000	-0.47481800	-0.48598600
N	2.58814400	0.44101700	0.78593000
C	-1.04034300	1.00863600	-0.23198600
N	-0.37693700	-0.30050900	-0.63015400
H	2.88037600	0.63591900	1.75383100
O	-0.28699000	1.91165900	0.12046200
O	1.70071200	-1.03686700	-1.27745000
O	-2.26991400	0.93656200	-0.31921500
H	-0.67992500	-0.58192200	-1.56264400
H	-2.69060600	-1.13358400	0.83464800
O	-1.92808800	-1.73848900	0.78218100
H	-1.16472800	-1.21540800	0.22106300
H	-1.62731800	-1.93435800	1.68546500

## INT12

N	-0.79526300	-0.66952600	-0.00048600
C	0.45283100	0.14030500	-0.00007500
N	-1.79389200	0.04157100	0.00040800
N	1.50172800	-0.67492100	0.00007000
H	-2.61535400	-0.57891400	0.00007300
O	0.46303500	1.35396000	-0.00009300
H	2.43858600	-0.29962200	0.00074600
H	1.36749800	-1.67484800	0.00043500

TS(INT7→INT13+CO+N<sub>2</sub>)

N	2.02928400	0.82593400	0.00010100
C	0.96701000	-0.84303400	-0.00002400
N	1.44174400	1.81375600	0.00001000
C	-1.29752800	0.04507000	-0.00002100
N	-0.46031400	-0.99201800	0.00000300
H	0.14169500	1.58911400	-0.00022000
O	-0.95764400	1.25618500	-0.00007800
O	1.61690300	-1.85874200	-0.00004600

H	-0.86627700	-1.92781200	0.00012800
O	-2.56659400	-0.26571200	0.00006300
H	-3.10863900	0.53893600	0.00004100

## INT13

C	-0.10194000	-0.02580000	-0.00019600
N	-1.30381700	-0.42189000	-0.00003500
H	0.62267400	-1.76844400	0.00090900
O	0.94556300	-0.85683300	-0.00006900
H	-1.93184600	0.37826200	0.00039300
O	0.27975800	1.25449200	0.00007200
H	1.24496200	1.31694400	0.00009600

TS(INT7→INT14+CO+N<sub>2</sub>)

N	-2.32401900	-0.38386700	0.15929900
C	-0.96180700	0.84203000	-0.04567200
N	-1.88359800	-1.40011600	-0.19108600
C	1.30595500	-0.26543400	0.09610600
N	0.16446800	-0.13893500	-0.68773100
H	-0.64824600	-1.08366100	-0.57070000
O	1.25826700	-0.53279300	1.27338200
O	-0.75259400	1.96011500	0.19645900
H	0.34376100	0.10998800	-1.65882600
O	2.41463100	-0.03750900	-0.59790200
H	3.17919400	-0.14398300	-0.01197100

## INT14

C	-0.03079300	0.11038000	-0.00000100
N	1.26130000	-0.24168700	0.00005100
H	1.53920400	-1.21003800	-0.00014100
O	-0.45112300	1.25795900	-0.00000500
H	1.96568300	0.47785400	-0.00013800
O	-0.84759700	-0.95814300	-0.00000400
H	-1.75946800	-0.63681700	0.00000500

TS(INT11→INT10+N<sub>2</sub>H<sub>2</sub>)

N	0.99130900	-0.56251700	0.00001600
C	-0.90907300	0.15068100	0.00000200
N	1.91763400	0.22933400	-0.00002200
N	-1.52412200	-0.93125800	0.00002600
H	2.83474200	-0.24525600	-0.00001800
O	-0.72162300	1.31516400	-0.00002500
H	-2.53048900	-0.76130500	0.00002200
H	1.22943100	-1.56775000	0.00004600

TS(INT10+H<sub>2</sub>O→INT14)

C	-1.46611500	-0.32693100	0.07115500
N	-0.57152200	-1.20824800	0.16767900
O	-2.59468400	0.02518200	0.18602900
H	-0.98845200	-2.06477600	0.53063000
H	-1.11565200	1.86043000	-0.45424500
O	-0.58002600	1.06792900	-0.59843300
H	0.31824700	1.21604000	-0.16637900
H	2.29907000	2.04576100	0.10916600
O	1.76073900	1.35110500	0.50402700
H	2.17746700	0.50104400	0.25393600

O	2.19665600	-1.19339900	-0.33143100
H	2.61558500	-1.85422100	0.22934000
H	1.22961000	-1.29149100	-0.18467400

## INT14

C	-0.03079300	0.11038000	-0.00000100
N	1.26130000	-0.24168700	0.00005100
H	1.53920400	-1.21003800	-0.00014100
O	-0.45112300	1.25795900	-0.00000500
H	1.96568300	0.47785400	-0.00013800
O	-0.84759700	-0.95814300	-0.00000400
H	-1.75946800	-0.63681700	0.00000500

TS(INT14→NH<sub>3</sub>+CO<sub>2</sub>)

C	1.24025700	-0.16438900	0.02411400
N	0.64598600	0.89774500	0.77524100
O	2.24848300	0.09986300	-0.64615400
H	1.28932400	1.66813000	0.91868100
H	-0.92080800	-1.28168500	0.08650800
O	0.64225100	-1.27942200	0.07806500
H	0.27027400	0.57318500	1.66155900
H	-1.72241400	1.56558000	-1.25111900
O	-1.70978400	1.28238300	-0.32602000
H	-0.74516900	1.32846100	0.02950300
O	-1.91021800	-1.09917000	-0.04838400
H	-2.37595800	-1.35767300	0.75630900
H	-1.92455900	0.17688800	-0.23285700

NH<sub>3</sub>

N	-0.00000100	0.00000700	-0.11707800
H	-0.85705800	0.38028400	0.27318900
H	0.75789800	0.55203300	0.27318800
H	0.09916600	-0.93236700	0.27316700

TS(NO<sub>2</sub><sup>\*</sup>+HO<sub>2</sub><sup>\*</sup>→HNO<sub>2</sub>+O<sub>2</sub>)

N	0.86019300	-0.12942200	0.00003500
O	1.97822100	-0.50650400	-0.00001600
O	0.51113800	1.05764200	-0.00000900
O	-1.75306300	0.32474900	-0.00000100
H	-0.79150600	0.90888300	0.00000500
O	-1.39002800	-0.87625300	-0.00000500

HNO<sub>2</sub>

N	0.14458700	0.47875800	-0.00009600
O	-1.00216900	-0.25587100	-0.00008200
O	1.09072900	-0.21254300	0.00007700
H	-1.72058300	0.39600200	0.00071600

O<sub>2</sub>

O	0.00000000	0.00000000	0.59379900
O	0.00000000	0.00000000	-0.59379900

## NTOa

N	-0.13372800	1.30609700	-0.00001200
C	0.31491900	0.08067200	0.00000800
N	-1.46473900	1.08068800	0.00010000

C	-1.75975000	-0.27043600	-0.00036100
N	-0.56606200	-0.92463300	0.00010200
H	-2.11815400	1.85145000	0.00039500
O	-2.91269800	-0.74723500	0.00005000
N	1.75143100	-0.15063100	0.00004900
O	2.49071300	0.81351300	-0.00008400
O	2.13183800	-1.30296700	0.00003900

HO<sub>2</sub><sup>•</sup>

H	-0.87849200	-0.88366200	0.00000000
O	0.05490600	-0.59537500	0.00000000
O	0.05490600	0.70583300	0.00000000

TS(NTOa+HO<sub>2</sub><sup>•</sup>→INT1a)

N	-0.21473500	-0.32238800	1.34695200
C	-0.65951400	-0.32428300	0.07413000
N	1.04942100	-0.61516200	1.18236500
C	1.42532900	-0.65495500	-0.21633400
N	0.17184900	-0.55569300	-0.88901600
H	1.69059800	-0.58625700	1.96720800
O	2.42745100	-1.25163900	-0.63116900
N	-2.08629000	-0.07607300	-0.16147800
O	-2.79779900	0.08304000	0.80579100
O	-2.45963200	-0.04665700	-1.31187700
O	1.93236800	1.09903100	-0.35342700
O	1.00116800	2.01867300	0.13603900
H	0.44435100	2.22731600	-0.62859800

## INT1a

N	0.36035100	-1.09452600	-0.88448500
C	0.74594600	-0.17191700	0.03834600
N	-0.92670000	-1.14273400	-0.69873500
C	-1.40082200	-0.28099300	0.46653600
N	-0.10629600	0.36654600	0.82464900
H	-1.48196100	-1.84425500	-1.17673100
O	-2.02490300	-0.89775200	1.38801000
N	2.18519900	0.14456300	0.10943000
O	2.92262100	-0.39496200	-0.68574400
O	2.53741900	0.92813800	0.96116400
O	-2.27912000	0.73924000	-0.08561800
O	-1.65116200	1.43395600	-1.15302900
H	-1.21549500	2.17580500	-0.70683400

TS(NTOa+HO<sub>2</sub><sup>•</sup>→INT2a)

N	0.15243300	-0.30288100	1.36473900
C	-0.30658900	-0.24336600	0.08124800
N	1.44942700	-0.41357700	1.15880500
C	1.76050300	-0.55986600	-0.21674800
N	0.57979700	-0.50317500	-0.88208800
H	2.09841700	-0.46341500	1.93504000
O	2.90186600	-0.71431300	-0.64139600
N	-1.74503800	-0.51871300	-0.11988200
O	-2.48774700	-0.31654800	0.81547900
O	-2.09386500	-0.89478400	-1.21492000
O	0.54283500	2.20780400	-0.26723500
O	-0.68803700	1.64873800	-0.01362400

H	0.72135000	2.00404900	-1.19949200
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## INT2a

N	0.16307000	0.26302700	1.29657700
C	-0.29312100	0.23578300	-0.07800400
N	1.41121500	-0.13739800	1.16761700
C	1.79443700	-0.31141900	-0.20315900
N	0.72584100	-0.05080200	-0.95607000
H	2.02746200	-0.20294600	1.96855000
O	2.93840600	-0.63773200	-0.51327200
N	-1.42420100	-0.93465800	-0.08470300
O	-2.53324400	-0.67122600	0.32152300
O	-1.05352300	-2.03405700	-0.41365800
O	-0.31624500	2.49310100	-0.35258400
O	-1.12336300	1.33114600	-0.39104400
H	-0.46307900	2.82571700	0.54676600

## INT3a

N	-0.22652900	1.32743400	0.00002000
C	0.27762800	0.05485500	-0.00003500
N	-1.51117000	1.18402100	-0.00028400
C	-1.77570700	-0.21092400	0.00058300
N	-0.57546400	-0.92040700	-0.00014400
O	-2.90458100	-0.69076200	-0.00017200
N	1.71701800	-0.14835500	-0.00007800
O	2.42684900	0.83704000	0.00016500
O	2.12291700	-1.29158200	0.00002200

TS(INT2a→INT4a+NO<sub>2</sub><sup>-</sup>)

N	0.18893700	0.37461200	1.27578000
C	-0.18942600	0.47080900	-0.06962000
N	1.41860400	-0.06604700	1.16680400
C	1.84708000	-0.12404500	-0.18991500
N	0.79469700	0.28617700	-0.94431800
H	1.98264800	-0.27023700	1.98383600
O	2.96925900	-0.47482000	-0.52066800
N	-1.29322900	-1.19245200	-0.11608200
O	-2.42520600	-1.24857400	0.33111900
O	-0.68114700	-2.17752700	-0.47819600
O	-0.88361400	2.60228000	-0.30632600
O	-1.29195700	1.23590400	-0.36024100
H	-1.19032000	2.87552400	0.57258000

## INT4a

N	0.28026500	1.09225300	-0.00231800
C	0.51760700	-0.26920700	-0.00042800
N	-1.02083400	1.12275500	-0.00238300
C	-1.58390200	-0.18445400	-0.00193200
N	-0.51563100	-1.05678700	0.00088700
H	-1.52980300	2.00118200	-0.00367500
O	-2.77075700	-0.41340800	-0.00248500
O	2.72643600	0.23348600	0.11044100
O	1.74607800	-0.77452900	-0.00450200
H	3.10691200	0.24884200	-0.78310000

NO<sub>2</sub><sup>-</sup>

N	0.00000000	0.45926700	0.00000000
O	1.05332200	-0.20083000	0.00000000
O	-1.05332200	-0.20102900	0.00000000

TS(INT3a→INT5a+N<sub>2</sub>)

N	-0.72109500	1.79252800	0.00030700
C	0.42928200	0.12177300	0.00020600
N	-1.76370200	1.33804400	0.00025500
C	-1.71886800	-0.59379800	-0.00013100
N	-0.44668300	-0.83363000	-0.00056900
O	-2.78556700	-1.08087300	-0.00008500
N	1.76782500	-0.13652900	-0.00001500
O	2.54719300	0.86141500	-0.00059800
O	2.22376100	-1.31688500	0.00064600

## INT5a

C	-0.27510800	-0.80914000	-0.00015900
C	2.01737500	-0.04622200	0.00002800
N	0.81562300	0.02861200	0.00017600
O	3.18012000	0.01285900	-0.00004300
N	-1.43054400	-0.01217000	-0.00005200
O	-2.52797300	-0.63151200	0.00007500
O	-1.42079200	1.24578800	-0.00004200

N<sub>2</sub>

N	0.00000000	0.00000000	0.54480100
N	0.00000000	0.00000000	-0.54480100

TS(INT4a→INT5+OH<sup>•</sup>)

N	-0.06734000	1.29173000	-0.10288700
C	-0.55700700	-0.02546600	-0.40090300
N	1.13290900	1.10134700	0.14750200
C	1.50247300	-0.34430300	0.05419100
N	0.35971700	-0.97048800	-0.28866600
H	1.76587400	1.87010800	0.38090400
O	2.62559300	-0.71655400	0.26674200
O	-2.64359600	-0.40427400	0.77002300
O	-1.77959400	-0.14094500	-0.71097200
H	-3.03489900	0.48456400	0.80137800

## INT5

N	-0.64526400	1.24483900	0.00031000
C	-1.10068500	-0.26089100	-0.00004900
N	0.55716600	1.16891900	-0.00016300
C	1.07708300	-0.33687600	0.00008900
N	-0.02790200	-1.05764500	0.00040500
H	1.15984200	2.00234100	-0.00010800
O	2.25136800	-0.52500500	-0.00021400
O	-2.27714600	-0.46356000	-0.00028500

OH<sup>•</sup>

O	0.00000000	0.00000000	0.10827300
H	0.00000000	0.00000000	-0.86618500

## TS(INT5→INT6)

N	0.82793400	1.20317500	0.00009100
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C	1.06292300	-0.29124100	-0.00006100
N	-0.36565200	1.39473600	0.00016300
C	-1.19384900	-0.45195200	-0.00000800
N	-0.07364600	-1.03722100	-0.00015400
H	-0.64169400	2.38566600	0.00027000
O	-2.35517900	-0.42948300	0.00004100
O	2.19352800	-0.67693500	-0.00011000

## INT6

N	1.05936100	1.10864800	0.00065600
C	1.00334700	-0.37287400	-0.00008600
N	-0.05299600	1.61174800	-0.00033600
C	-1.34650400	-0.48448800	0.00000800
N	-0.22684800	-0.98561400	-0.00054500
H	0.04019400	2.63692100	0.00030400
O	-2.47209600	-0.24135800	0.00035500
O	2.04236200	-0.96316900	-0.00013700

TS(INT6+OH<sup>\*</sup>→INT6a+N<sub>2</sub>+H<sub>2</sub>O)

N	-0.67680700	-0.84576100	-0.00335300
C	0.79174000	-1.12159300	-0.00022500
N	-0.93114900	0.33730000	-0.00180200
C	1.42725100	1.14864100	0.00081700
N	1.65435400	-0.05583100	0.00119300
H	-1.98385900	0.50192700	-0.00474500
O	1.43594000	2.29919700	0.00077100
O	1.13076700	-2.26480400	0.00058200
O	-3.55434600	0.44046400	-0.00186900
H	-3.75375600	-0.51302000	0.03304700

## INT6a

C	1.14779300	-0.35107100	-0.00005500
C	-1.15452000	0.06329100	-0.00029800
N	0.01469600	0.42554200	0.00006200
O	-2.28138600	-0.15530200	0.00015100
O	2.27357200	-0.00121200	0.00005900

TS(INT6a+H<sub>2</sub>O→INT7a)

C	1.89040300	0.11734400	-0.01293600
C	0.01273600	-1.07989900	-0.02318000
N	0.52212800	0.07717600	0.12242400
O	0.00929600	-2.22017200	-0.22620600
O	2.60133600	1.06390300	0.05941600
O	-1.82343900	-0.63440500	0.32978700
H	-2.40429100	-1.16528200	-0.23168900
H	-0.80200800	1.98428300	-0.12507400
O	-1.75953900	1.97759600	-0.25944100
H	-1.97331500	0.31664900	0.10712500
H	-2.11534100	2.60407100	0.38091600

## INT7a

C	1.45322100	0.26147200	0.00000800
C	-0.92469100	0.10818500	-0.00008600
N	0.32959000	-0.48787100	-0.00016600
O	-1.11264200	1.29764600	-0.00000100
O	2.58738900	-0.08674000	0.00010400

O	-1.86697800	-0.82402400	0.00016300
H	-2.73508400	-0.39409900	-0.00009500
H	0.39463400	-1.50380000	-0.00039900

## INT10

C	0.04265800	0.01519000	-0.00004100
N	-1.15647800	-0.12520800	0.00001300
O	1.20550500	0.01659900	0.00001600
H	-1.80464700	0.65252400	0.00002100

## HOOH

H	-0.94925600	-0.89789800	0.00000000
O	0.00002200	-0.71540800	0.00000000
O	0.00002200	0.71526400	0.00000000
H	0.94889900	0.89904900	0.00000000

CO<sub>2</sub>

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.15522600
O	0.00000000	0.00000000	-1.15522600

TS(INT10+H<sub>2</sub>O→INT14)

C	-1.46611500	-0.32693100	0.07115500
N	-0.57152200	-1.20824800	0.16767900
O	-2.59468400	0.02518200	0.18602900
H	-0.98845200	-2.06477600	0.53063000
H	-1.11565200	1.86043000	-0.45424500
O	-0.58002600	1.06792900	-0.59843300
H	0.31824700	1.21604000	-0.16637900
H	2.29907000	2.04576100	0.10916600
O	1.76073900	1.35110500	0.50402700
H	2.17746700	0.50104400	0.25393600
O	2.19665600	-1.19339900	-0.33143100
H	2.61558500	-1.85422100	0.22934000
H	1.22961000	-1.29149100	-0.18467400

## INT14

C	-0.03079300	0.11038000	-0.00000100
N	1.26130000	-0.24168700	0.00005100
H	1.53920400	-1.21003800	-0.00014100
O	-0.45112300	1.25795900	-0.00000500
H	1.96568300	0.47785400	-0.00013800
O	-0.84759700	-0.95814300	-0.00000400
H	-1.75946800	-0.63681700	0.00000500

TS(INT14→NH<sub>3</sub>+CO<sub>2</sub>)

C	1.24025700	-0.16438900	0.02411400
N	0.64598600	0.89774500	0.77524100
O	2.24848300	0.09986300	-0.64615400
H	1.28932400	1.66813000	0.91868100
H	-0.92080800	-1.28168500	0.08650800
O	0.64225100	-1.27942200	0.07806500
H	0.27027400	0.57318500	1.66155900
H	-1.72241400	1.56558000	-1.25111900
O	-1.70978400	1.28238300	-0.32602000
H	-0.74516900	1.32846100	0.02950300



O	-1.91021800	-1.09917000	-0.04838400
H	-2.37595800	-1.35767300	0.75630900
H	-1.92455900	0.17688800	-0.23285700

NH<sub>3</sub>

N	-0.00000100	0.00000700	-0.11707800
H	-0.85705800	0.38028400	0.27318900
H	0.75789800	0.55203300	0.27318800
H	0.09916600	-0.93236700	0.27316700

TS(NTO\*+HO<sub>2</sub>\*→INT1)

N	-0.63779100	1.48310800	-0.37825100
C	-0.94648100	0.20122700	0.03687300
N	0.65307100	1.58051200	-0.11822300
C	1.26299600	0.36331900	0.34075800
N	0.09885600	-0.46378500	0.48439000
H	1.17173000	2.41976500	-0.35642200
O	2.16912600	0.39542800	1.26770300
N	-2.20550500	-0.31821500	0.00510600
O	-3.14552900	0.41901000	-0.42783800
O	-2.36829900	-1.51727800	0.41187600
O	2.13188200	-0.13230500	-0.79336800
O	2.24768200	-1.50534400	-0.72578300
H	3.19745100	-1.64225700	-0.56848200
H	0.09241200	-1.41222000	0.84724700

TS(NTO\*+HO<sub>2</sub>\*→INT2)

N	0.18791600	-0.35148400	1.35142400
C	-0.33537300	-0.30256500	0.11488700
N	1.50111300	-0.39539700	1.13600300
C	1.85090400	-0.52058700	-0.20500600
N	0.62336100	-0.53151500	-0.83416200
H	2.15136700	-0.39906200	1.91241300
O	2.95965200	-0.60081300	-0.68090800
N	-1.67352900	-0.72506000	-0.08920300
O	-2.53686500	-0.45407000	0.85732700
O	-2.19262200	-0.57965100	-1.26351900
O	0.40435400	2.27020600	-0.04056300
O	-0.75637700	1.56671900	-0.06495500
H	0.76181000	2.21336500	-0.94261800
H	0.49647000	-0.47032300	-1.83657600

TS(NTO<sub>r</sub>+HO<sub>2</sub>\*→INT15)

N	-0.32506700	-1.01489200	0.97690100
C	-0.74151200	-0.23320500	-0.04991800
N	0.94320400	-1.14445300	0.71716400
C	1.33381200	-0.36617300	-0.42939800
N	0.11577800	0.15971600	-0.92887000
H	1.56384200	-1.66321800	1.33120200
O	2.22020300	-0.86350800	-1.25229900
N	-2.16795800	0.11365700	-0.13735300
O	-2.89114300	-0.30047900	0.73733000
O	-2.50825700	0.78582300	-1.08025700
O	2.21924400	0.86759700	0.12610900
O	1.44990300	1.53936100	1.04653700
H	1.00104500	2.23092900	0.53043800

## INT15

N	0.70283500	1.59033400	0.01177900
C	0.68761300	0.17132200	-0.15782000
N	-0.34222800	1.99192500	0.52068300
C	-1.55885400	-0.20022500	-0.62635600
N	-0.23564500	-0.61136500	-0.42364500
H	-0.29560500	3.01954300	0.55954000
O	-1.97866600	0.25211400	-1.64845600
N	2.07641000	-0.41590700	-0.05737700
O	2.90897800	0.27823600	0.47208700
O	2.24002500	-1.52859300	-0.48322300
O	-2.41489700	-0.48848600	0.37522100
O	-1.75350600	-0.87526200	1.56045000
H	-1.90202800	-1.83512000	1.57679500

TS(NTOr+HO<sub>2</sub><sup>•</sup>→INT16)

N	0.22706000	0.06238300	1.32561600
C	-0.30318500	-0.11400000	0.04866500
N	1.50759500	-0.16932600	1.12149300
C	1.78321800	-0.62066000	-0.17371700
N	0.54276300	-0.68424800	-0.83979500
H	2.18009500	-0.08409100	1.87722600
O	2.85746800	-0.92704900	-0.62180800
N	-1.74763800	-0.53777600	0.00051700
O	-2.36128700	-0.51604800	1.03554200
O	-2.17632700	-0.83990800	-1.08387300
O	0.26208700	2.31010600	-0.10158000
O	-0.54441700	1.38428400	-0.67838300
H	0.93105400	2.50373200	-0.78091400

## INT16

N	0.17690400	0.09776200	1.37538800
C	-0.33455900	0.23210500	-0.07439600
N	1.32502000	-0.24201200	1.24549000
C	1.76639500	-0.37421200	-0.33578300
N	0.67581200	-0.03586900	-0.95407100
H	1.91905400	-0.39931600	2.07061300
O	2.88512000	-0.71096600	-0.56537700
N	-1.48144700	-0.84790400	-0.12013300
O	-1.12836700	-1.97060200	-0.36088600
O	-2.60251400	-0.48170200	0.11321200
O	-0.08029100	2.47536100	-0.14774000
O	-1.02111200	1.42205500	-0.20931500
H	0.19321900	2.57494900	-1.07540300

TS(NTOr+H<sub>2</sub>O→INT17)

N	-1.10814000	1.43010900	-0.19550800
C	-1.11937400	0.08925600	0.04178000
N	0.16618600	1.70680600	-0.13220200
C	0.96246200	0.54412400	0.35751700
N	-0.03157500	-0.53180800	0.30686400
H	0.47029800	2.67285400	-0.05915600
O	1.71038100	0.68448800	1.33038000
N	-2.42038200	-0.60490700	-0.01893200
O	-3.37422400	0.03183800	-0.40314200

O	-2.44079900	-1.76457800	0.31881800
H	2.67068100	-0.43626100	-0.67850800
O	1.90754100	0.24424800	-0.96293100
H	1.41146400	-0.09910900	-1.72136600
H	4.53651300	-0.89508200	-0.04583800
O	3.71503300	-1.33922100	-0.29164100
H	3.46644000	-1.89828300	0.45565500

## INT17

N	0.17594200	1.37001300	0.00932400
C	0.62415200	0.10899700	0.01209500
N	-1.10796500	1.26624200	0.00727900
C	-1.68981900	-0.18118900	-0.11668800
N	-0.27113200	-0.82621100	-0.00346400
H	-1.67232800	2.10925700	-0.07096900
O	-2.29589400	-0.40151200	-1.18817200
N	2.06272400	-0.15249200	0.00362200
O	2.39171000	-1.31543400	-0.02536400
O	2.80246700	0.80077300	0.02758100
O	-2.39799600	-0.47618000	1.03828900
H	-1.86241600	-0.31706800	1.82816300
H	-0.09053100	-1.82308300	-0.06563400

TS(NTOr+H<sub>2</sub>O→INT18)

N	0.49830100	-1.34247000	0.87885900
C	-0.15629400	-0.34011500	0.13171700
N	1.75101500	-1.09235000	0.58647900
C	1.88864800	-0.04545400	-0.37696600
N	0.63058700	0.37173700	-0.67697600
H	2.50238600	-1.64960900	0.97805700
O	2.96378700	0.32431100	-0.80603500
N	-1.50117200	-0.78172400	-0.45068300
O	-1.93188500	-1.85537800	-0.11258700
O	-2.03421300	-0.01283400	-1.21162700
H	-0.42501600	0.54231300	2.14504200
O	-0.91442300	0.64204300	1.31246100
H	-0.81219200	1.62049400	0.96521100
H	-1.35905400	3.34071200	-0.02282200
O	-0.56307300	2.87677800	0.26536100
H	-0.11291300	2.57379100	-0.53834000

## INT18

N	0.13229300	-0.76084300	-1.18232000
C	-0.38712100	-0.57876100	0.15557200
N	1.36156500	-0.27490200	-1.11654400
C	1.77548200	0.10664600	0.16662100
N	0.69171800	-0.17321500	0.95121400
H	1.96678100	-0.28425900	-1.92921000
O	2.85164900	0.55824200	0.46980800
N	-1.42918400	0.65815100	-0.00808800
O	-0.96704500	1.77045800	-0.04278500
O	-2.59308300	0.37193800	-0.14985000
H	-1.82225300	-1.84325300	0.06990700
O	-1.08831300	-1.61535200	0.66102400
H	0.60489000	0.13357600	1.91074000

TS(NTOr+H<sub>2</sub>O→INT19)

N	-0.16768800	-0.65715600	0.96290300
C	-0.09083300	0.27528800	-0.09660300
N	-1.43044300	-0.99561200	0.90231300
C	-2.14811400	-0.24133800	-0.07812200
N	-1.24869300	0.60293600	-0.65233400
H	-1.82437100	-1.66944500	1.54986800
O	-3.33764900	-0.38055100	-0.28108400
N	0.91154300	1.38950100	0.20167400
O	1.97192000	1.05278200	0.67197200
O	0.56656000	2.51868500	-0.02901400
H	0.35203000	-0.93789000	-1.87037000
O	0.94851800	-0.45979900	-1.27262400
H	1.58921700	-1.13821900	-0.82707200
H	2.31143800	-2.08259200	0.82138000
O	2.49166800	-2.09263200	-0.12757700
H	3.42419100	-1.86110500	-0.22072600

## INT19

N	-0.31611600	-0.31894500	1.30091400
C	0.35635800	-0.59056700	0.03701300
N	-1.49877800	0.14109700	1.02259300
C	-1.69569600	0.06899300	-0.43529400
N	-0.57727900	-0.39507000	-0.96993000
H	-2.16425500	0.39997900	1.74695100
O	-2.76307000	0.40298300	-0.91228300
N	1.47307500	0.58625900	-0.09928000
O	2.51130100	0.29609800	-0.63501600
O	1.15757400	1.69134500	0.27295700
H	0.98357900	-2.17159600	-0.79380000
O	1.03990600	-1.75252000	0.07695300
H	0.08469300	-0.29558400	2.23556400

TS(NTOr+H<sub>2</sub>O→INT20+HNO<sub>2</sub>)

N	0.30144400	0.44358700	1.31232300
C	-0.20604000	0.51095100	-0.01368600
N	1.52211200	0.00653100	1.08956900
C	1.82225500	-0.08398900	-0.30694600
N	0.70343900	0.27775100	-0.97638500
H	2.17634300	-0.12903900	1.85176100
O	2.91506600	-0.42447800	-0.72319200
N	-1.47115100	-0.65559200	-0.05285800
O	-1.24087900	-1.81297900	0.02275400
O	-2.60110400	-0.15319100	-0.16040700
H	-0.90194700	2.10296300	-1.00252100
O	-1.10767300	1.62202200	-0.17797200
H	-2.08588200	1.10737300	-0.22346100

## INT20

N	0.59122600	1.21786800	0.00038300
C	0.99252000	-0.11205600	0.00006000
N	-0.70551300	1.10147100	-0.00052100
C	-1.11513200	-0.26036600	-0.00005800
N	0.04295200	-1.00588800	0.00012700
H	-1.31320400	1.91417100	0.00061300
O	-2.27080500	-0.62103400	0.00007700

H	2.46123500	-1.28059500	-0.00045000
O	2.28167800	-0.32811800	-0.00008900

TS(INT18→INT21+NO<sub>2</sub>\*)

N	0.15726700	0.74516600	1.22472700
C	-0.21834800	0.91950000	-0.07614000
N	1.28315500	0.05064600	1.13698800
C	1.73766000	-0.13571500	-0.16939200
N	0.77245300	0.50651000	-0.91493700
H	1.75813100	-0.27947100	1.96893200
O	2.73470900	-0.71174000	-0.52964500
N	-1.44483100	-0.76525800	-0.06337000
O	-0.90977400	-1.85150200	-0.08175100
O	-2.63964100	-0.58762700	0.01515500
H	-1.67489400	2.06128500	0.26886200
O	-1.09874900	1.80641300	-0.46907400
H	0.73222600	0.51167100	-1.92593600

## INT21

N	-0.67493800	1.18652600	-0.00006200
C	-1.03914700	-0.05301200	0.00025700
N	0.70824500	1.11156800	0.00097500
C	1.17712000	-0.15761500	-0.00002100
N	0.01636200	-0.91291800	-0.00047800
H	1.26629500	1.95140800	-0.00285300
O	2.33821000	-0.55988700	-0.00030300
H	-2.90481100	0.21296000	-0.00162200
O	-2.27710900	-0.52441600	-0.00007300
H	-0.02580800	-1.92241800	0.00302600

## INT22

N	-0.68952400	1.21002300	0.00001000
C	-1.14048200	-0.12072000	-0.00006200
N	0.61854000	1.12158300	0.00002000
C	1.11224900	-0.19459400	0.00006300
N	-0.03046200	-0.94455500	-0.00057200
H	1.20401800	1.94985500	-0.00037000
O	2.27193300	-0.52463200	0.00019500
O	-2.30557900	-0.45188900	0.00021900
H	-0.05532900	-1.95516400	0.00084800

TS(INT21+HO<sub>2</sub>\*→INT23)

N	-0.35581600	-0.64718300	1.21300300
C	-0.76833100	-0.65461800	-0.06889300
N	0.94121900	-0.32621200	1.13010000
C	1.42115300	-0.25981500	-0.16698700
N	0.30397200	-0.55595100	-0.91612500
H	1.49348500	-0.17835300	1.96460100
O	2.55142900	-0.01186400	-0.53432900
O	-0.39059300	2.05530200	0.06569300
O	-1.44416000	1.18625600	-0.04792900
H	-0.02682900	2.13350900	-0.83088300
H	0.25608500	-0.50004100	-1.92465800
O	-1.88492900	-1.22694700	-0.48672700
H	-2.51928700	-1.28508200	0.24370500

## INT23

N	-0.17202600	-0.42808200	1.27282400
C	-0.70384000	-0.44440600	-0.08773200
N	1.11345900	-0.14624300	1.12833000
C	1.53433400	0.03935200	-0.19369300
N	0.40569800	-0.14021600	-0.92343700
H	1.72787000	-0.08335100	1.93061600
O	2.66192500	0.30060000	-0.55222400
O	-1.30463800	1.77283000	0.16377000
O	-1.77023300	0.49196400	-0.21090800
H	-1.09857800	2.18563200	-0.68916100
H	0.36695100	-0.10374800	-1.93195600
O	-1.27098600	-1.65051100	-0.42579500
H	-1.93766300	-1.88548600	0.23628400

TS(INT21+HO<sub>2</sub><sup>•</sup>→INT24)

N	-1.35006200	0.85167100	-0.78442600
C	-1.42437600	-0.18368600	0.08753200
N	-0.10448100	1.25135400	-0.70563900
C	0.76523100	0.50186000	0.28750600
N	-0.30683300	-0.43567200	0.72173600
H	0.19065800	2.09051700	-1.19413900
O	1.34843400	1.20857300	1.14997700
O	1.72696700	-0.23080100	-0.57460100
O	1.60142900	-1.63738500	-0.49394600
H	2.24618800	-1.87348200	0.18950700
H	-0.17635600	-1.16824400	1.40656400
O	-2.51914600	-0.85564700	0.29185600
H	-3.23745200	-0.50723300	-0.26013800

## INT24

N	1.10850300	-0.26759700	-1.18077500
C	1.40142300	-0.01087200	0.12108000
N	-0.17260200	-0.53675900	-1.17990500
C	-0.84895100	-0.53859000	0.17836600
N	0.37939100	-0.11661300	0.93023900
H	-0.62455200	-0.84929300	-2.03307800
O	-1.43234300	-1.59985800	0.52812500
O	-1.79437800	0.55589900	0.19471500
O	-1.19718700	1.76292600	-0.24811400
H	-0.93755000	2.19605000	0.57899300
H	0.41982800	-0.03669700	1.93818800
O	2.59962000	0.29661800	0.52061200
H	3.21470500	0.30880600	-0.23039100

## TS(INT21→INT25)

N	-0.47007200	-0.71650800	0.05954200
C	-0.42802700	0.60920000	0.03253300
N	0.84646400	-1.14349300	-0.02516400
C	1.71158400	-0.10199700	-0.01344800
N	0.89052000	1.00861800	-0.01480900
H	1.21772900	1.96360400	-0.03476100
H	1.08825700	-2.10083100	0.18183900
O	2.94129800	-0.12769000	-0.01263100
H	-2.58349700	0.33081200	-0.04236400
O	-1.43749100	1.37507900	0.03054000

H	-1.86626800	-1.06363800	-0.05872600
O	-2.88062300	-0.65951000	-0.13441600
H	-3.41142100	-0.91652400	0.63457100

## INT25

N	0.69099100	1.10485500	-0.00029200
C	1.14717600	-0.16717800	0.00030600
N	-0.69081600	1.10471400	-0.00172500
C	-1.14728600	-0.16700600	-0.00019900
N	0.00001000	-0.94114600	-0.00024400
H	-0.00023400	-1.95095500	-0.00163600
H	-1.22556300	1.96025200	0.00481200
O	-2.30910200	-0.55263800	0.00044800
H	1.22603600	1.96024400	0.00217900
O	2.30899300	-0.55278700	0.00078000

TS(INT22+HO<sub>2</sub>\*→INT26)

N	-1.53832200	0.91927700	-0.59416600
C	-1.60182200	-0.33258700	0.03979300
N	-0.31700100	1.35514400	-0.37040300
C	0.53520800	0.41427200	0.30079800
N	-0.37790300	-0.59976200	0.60352100
H	0.00476600	2.24005100	-0.74491100
O	1.40408600	0.84587300	1.17785300
O	1.57716200	-0.00795900	-0.74374800
O	2.01401100	-1.28871300	-0.45826900
H	2.96740300	-1.16983600	-0.31644800
H	-0.14827300	-1.42552200	1.13772900
O	-2.59421300	-1.03137800	0.07509300

## INT26

N	-1.52373000	1.02848000	-0.44841000
C	-1.60833100	-0.41386200	0.01241200
N	-0.36860200	1.36465500	-0.32027500
C	0.64981200	0.24724700	0.35613300
N	-0.39884800	-0.77440500	0.42173900
H	-0.08884600	2.32688000	-0.55512200
O	1.22431700	0.59939400	1.39120300
O	1.45158800	0.05655800	-0.82502500
O	2.36613500	-0.98357100	-0.53687700
H	3.07785500	-0.52733600	-0.06106800
H	-0.22916600	-1.65845800	0.88369500
O	-2.66334800	-0.98144300	-0.03557000

TS(INT22+HO<sub>2</sub>\*→INT27)

N	1.42708200	0.87669300	-0.55094900
C	1.56747400	-0.36980500	0.07664600
N	0.24620100	1.44857500	-0.39303500
C	-0.53806400	0.45556700	0.29170700
N	0.34462700	-0.58639400	0.63443100
H	2.18723300	1.36677500	-1.00762000
O	-1.42890100	0.87167300	1.15989200
O	-1.57015500	0.00728800	-0.77167400
O	-2.01857900	-1.26752800	-0.47186800
H	-2.96597200	-1.13657700	-0.30475400
H	0.08443600	-1.41425600	1.15129600

O	2.56669400	-1.04926300	0.09837900
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## INT27

N	1.39260300	0.96589500	-0.44241400
C	1.56282500	-0.46689300	0.04894500
N	0.27224000	1.42419400	-0.39277300
C	-0.64025400	0.33821900	0.30145000
N	0.33719600	-0.77388200	0.41627200
H	2.19189300	1.51406900	-0.78782800
O	-1.17512100	0.74896800	1.35491700
O	-1.50283400	0.06826200	-0.82434100
O	-2.30467800	-1.04171700	-0.46935300
H	-3.04930000	-0.63562300	0.00075100
H	0.11530300	-1.62917200	0.90875800
O	2.63168400	-0.99934900	0.02732100

## TS(INT22→INT10+INT28)

N	1.05859500	1.15355600	-0.02057700
C	1.21368400	-0.14862300	-0.02120600
N	-0.18167100	1.58981900	0.07506300
C	-1.41998100	-0.55433500	0.02747300
N	-0.24581300	-0.96145300	0.16540400
H	-0.13303600	2.60970800	0.07378300
O	-2.48994500	-0.19588200	-0.14191500
O	2.12300100	-0.91813000	-0.10928100
H	-0.11140800	-1.95331700	0.35895600

## INT28

N	-0.54379800	0.37174600	0.00001700
C	0.62815500	0.02656200	-0.00001200
N	-1.68180300	-0.32443400	0.00000600
H	-2.41647300	0.38907600	-0.00008100
O	1.77834300	-0.10995300	-0.00000100

TS(NTOa\*+HO<sub>2</sub>\*→INT1a)

N	-0.31054100	-1.14450800	0.84115600
C	-0.76650100	-0.22226400	-0.09864900
N	0.96744300	-1.24782700	0.52011700
C	1.33416900	-0.29883600	-0.47990900
N	0.12232600	0.27146700	-0.91865000
H	1.61573100	-1.75045300	1.11454700
O	2.25794900	-0.63375900	-1.35300100
N	-2.10523100	0.11264500	-0.12963200
O	-2.89919300	-0.45814000	0.69984500
O	-2.51684700	0.97938300	-0.98159800
O	2.18616900	0.87437400	0.26099100
O	1.39644700	1.34851300	1.28509600
H	0.86407900	2.05164600	0.87520100

TS(NTOa\*+HO<sub>2</sub>\*→INT2a)

N	0.18689400	0.10930300	1.35251300
C	-0.37358900	-0.12928400	0.07144400
N	1.47095300	-0.14841300	1.15274000
C	1.74805000	-0.65693800	-0.11002400
N	0.51692000	-0.74618800	-0.78961400
H	2.15072100	-0.00841000	1.89184700



O	2.82596600	-0.98407100	-0.54477300
N	-1.72427700	-0.55431800	0.04392500
O	-2.48198900	-0.16619700	1.01006400
O	-2.20284500	-0.94372900	-1.08793000
O	0.52424900	2.21622100	-0.31146000
O	-0.49890200	1.36353700	-0.67805600
H	1.11725600	2.21698200	-1.08007900