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Electronic supplementary material

Elucidating the Mechanism and Kinetics of the Water-assisted Reaction of Nitrous Acid with Hydroxyl Radical

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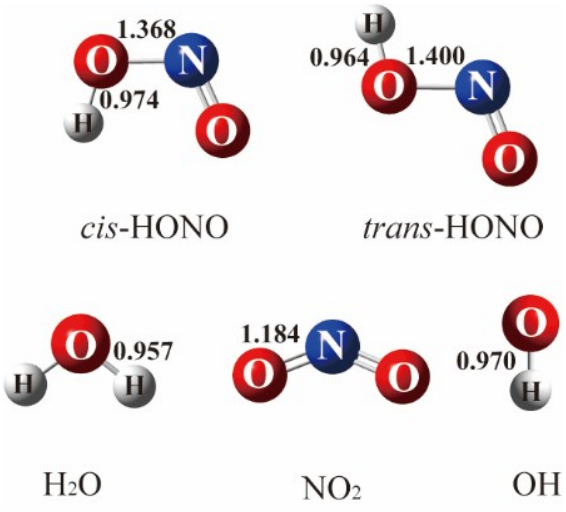

Figure S1. Optimized geometries of reactants and products in the HONO + OH reaction at the UωB97X-D/cc-pVTZ level of theory (bond distances in angstroms are indicated for selected bonds).

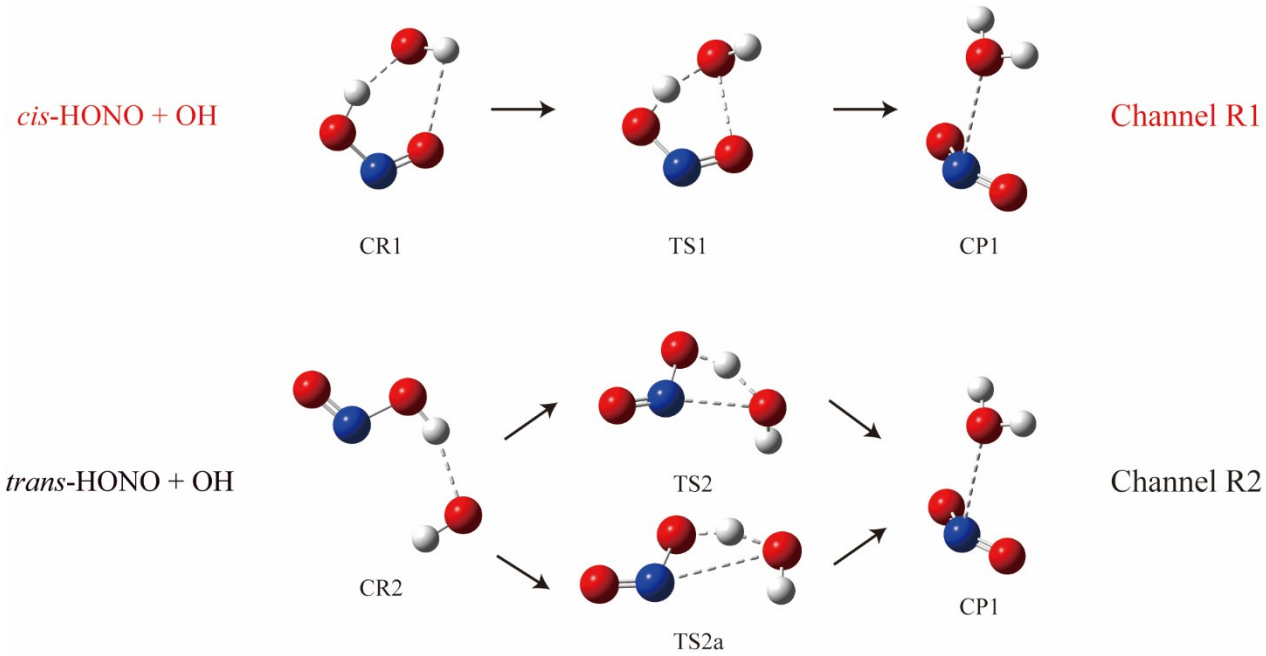

Figure S2. Optimized geometries of the intermediates in the water-free HONO + HO reaction calculated at the UωB97X-D/aug-cc-pVTZ level of theory.

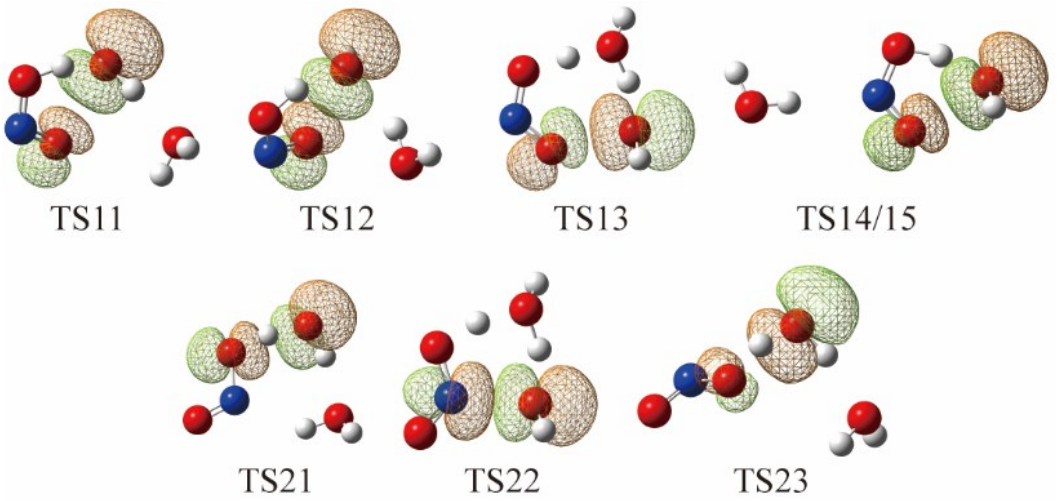

Figure S3. Electronic features of the transition states in the oxidation of HONO by OH radicals in the presence of water.

Table S1. Value of relative energies (ΔE with and without ZPE), enthalpies (ΔH (298 K)), and Gibbs free energies (ΔG (298 K)) of intermediates in the HONO + OH reaction at the CCSD(T)/aug-cc-pVTZ//UωB97X-D /aug-cc-pVTZ level of theory. All energy values (in kcal mol^{-1}) are relative to the energy of *trans*-HONO + OH.

System	Δ*E*	Δ*H*	Δ*G*	Δ(*E*+ZPE)
cis-HONO + OH	0.47	0.33	0.38	0.42
CR1	-3.82	-0.76	7.88	-1.90
TS1	-1.06	-1.76	7.86	-0.78
TS3	16.00	14.38	24.94	16.09
CP1	-41.02	-37.26	-33.36	-39.45
trans-HONO + OH	0.00	0.00	0.00	0.00
CR2	-5.15	-2.54	4.33	-3.73
TS2	9.63	9.18	18.65	10.00
TS2a	-4.62	-9.87	-1.19	-6.85
CP2	-41.02	-37.26	-33.36	-39.45
NO_2 + H_2O	-38.69	-36.94	-37.14	-37.89

Table S2. Value of relative energies (ΔE with and without ZPE), enthalpies (ΔH (298 K)), and Gibbs free energies (ΔG (298 K)) of intermediates in the HONO + OH reaction at the CCSD(T)/aug-cc-pVTZ//UM06-2X/aug-cc-pVTZ level of theory. All energy values (in kcal mol^{-1}) are relative to the energy of *trans*-HONO + OH.

System	Δ*E*	Δ*H*	Δ*G*	Δ(*E*+ZPE)
cis-HONO' + OH'	0.43	0.36	0.41	0.41
CR1'	-4.77	-3.57	4.33	-3.07
TS1'	-0.93	-2.29	7.33	-1.04
CP1'	-41.02	-39.47	-33.35	-39.46
trans-HONO' + OH'	0.00	0.00	0.00	0.00
CR2'	-4.40	-3.17	3.73	-2.95
TS2'	9.42	8.63	18.18	9.86
CP2'	-41.02	-39.47	-33.35	-39.46
NO_2' + H_2O'	-38.69	-37.82	-38.01	-37.95

Table S3. Calculated equilibrium constants (in cm^3 $molecule^{-1}$) for the formation of the hydrogen bonded complexes shown in Fig. 2 in the main article.[a]

T (K)	K_{eq} ($OH\cdots H_2O$)	K_{eq} ($H_2O\cdots OH$)	K_{eq} (HB1)	K_{eq} (HB2)	K_{eq} (HB3)	K_{eq} (HB4)	K_{eq} (HB5)	K_{eq} (HB6)	K_{eq} (HB7)	K_{eq} (HB8)
216	1.81×10^{-22}	7.78×10^{-23}	2.18×10^{-22}	1.91×10^{-24}	1.53×10^{-24}	2.10×10^{-24}	2.43×10^{-24}	1.94×10^{-21}	1.71×10^{-24}	6.81×10^{-23}
223	1.58×10^{-22}	7.39×10^{-23}	1.72×10^{-22}	2.01×10^{-24}	1.60×10^{-24}	2.19×10^{-24}	2.53×10^{-24}	1.51×10^{-21}	1.78×10^{-24}	6.54×10^{-23}
236	1.24×10^{-22}	6.74×10^{-23}	1.11×10^{-22}	2.20×10^{-24}	1.76×10^{-24}	2.36×10^{-24}	2.74×10^{-24}	9.62×10^{-22}	1.92×10^{-24}	6.08×10^{-23}
249	1.00×10^{-22}	6.23×10^{-23}	7.59×10^{-23}	2.39×10^{-24}	1.91×10^{-24}	2.53×10^{-24}	2.94×10^{-24}	6.43×10^{-22}	2.05×10^{-24}	5.72×10^{-23}
262	8.33×10^{-23}	5.82×10^{-23}	5.39×10^{-23}	2.58×10^{-24}	2.07×10^{-24}	2.71×10^{-24}	3.15×10^{-24}	4.50×10^{-22}	2.18×10^{-24}	5.43×10^{-23}
275	7.04×10^{-23}	5.48×10^{-23}	3.96×10^{-23}	2.77×10^{-24}	2.23×10^{-24}	2.88×10^{-24}	3.36×10^{-24}	3.25×10^{-22}	2.32×10^{-24}	5.18×10^{-23}
288	6.05×10^{-23}	5.20×10^{-23}	3.00×10^{-23}	2.97×10^{-24}	2.39×10^{-24}	3.06×10^{-24}	3.57×10^{-24}	2.43×10^{-22}	2.45×10^{-24}	4.98×10^{-23}
298	5.44×10^{-23}	5.02×10^{-23}	2.46×10^{-23}	3.12×10^{-24}	2.51×10^{-24}	3.19×10^{-24}	3.73×10^{-24}	1.98×10^{-22}	2.56×10^{-24}	4.85×10^{-23}

[a] Hydrogen bonded complexes, *cis*-$HONO\cdots H_2O$, $H_2O\cdots$*cis*-HONO (a), $H_2O\cdots$*cis*-HONO (b), $H_2O\cdots$*cis*-HONO (c), $H_2O\cdots$*cis*-HONO (d), *trans*-$HONO\cdots H_2O$, $H_2O\cdots$*trans*-HONO (a) and $H_2O\cdots$*trans*-HONO (b) are named as HB1, HB2, HB3, HB4, HB5, HB6, HB7 and HB8, respectively.

Table S4. Fractions of hydrated HONO (or OH) (%) formed upon complexation with water, assuming thermal equilibrium. [a]

T (K)	x (OH···H_2O)	x (H_2O···OH)	x (HB1)	x (HB2)	x (HB3)	x (HB4)	x (HB5)	x (HB6)	x (HB7)	x (HB8)
216	1.83×10^{-5}	7.86×10^{-6}	2.20×10^{-5}	1.93×10^{-7}	1.55×10^{-7}	2.12×10^{-7}	2.45×10^{-7}	1.96×10^{-4}	1.73×10^{-7}	6.88×10^{-6}
223	3.40×10^{-5}	1.59×10^{-5}	3.70×10^{-5}	4.32×10^{-7}	3.44×10^{-7}	4.71×10^{-7}	5.44×10^{-7}	3.25×10^{-4}	3.83×10^{-7}	1.41×10^{-5}
236	1.01×10^{-4}	5.49×10^{-5}	9.05×10^{-5}	1.79×10^{-6}	1.43×10^{-6}	1.92×10^{-6}	2.23×10^{-6}	7.84×10^{-4}	1.56×10^{-6}	4.96×10^{-5}
249	2.64×10^{-4}	1.64×10^{-4}	2.00×10^{-4}	6.31×10^{-6}	5.04×10^{-6}	6.68×10^{-6}	7.76×10^{-6}	1.70×10^{-3}	5.41×10^{-6}	1.51×10^{-4}
262	6.19×10^{-4}	4.32×10^{-4}	4.00×10^{-4}	1.92×10^{-5}	1.54×10^{-5}	2.01×10^{-5}	2.34×10^{-5}	3.34×10^{-3}	1.62×10^{-5}	4.03×10^{-4}
275	1.33×10^{-3}	1.04×10^{-3}	7.48×10^{-4}	5.24×10^{-5}	4.21×10^{-5}	5.44×10^{-5}	6.35×10^{-5}	6.14×10^{-3}	4.38×10^{-5}	9.79×10^{-4}
288	2.63×10^{-3}	2.26×10^{-3}	1.30×10^{-3}	1.29×10^{-4}	1.04×10^{-4}	1.33×10^{-4}	1.55×10^{-4}	1.05×10^{-2}	1.06×10^{-4}	2.16×10^{-3}
298	4.24×10^{-3}	3.91×10^{-3}	1.92×10^{-3}	2.43×10^{-4}	1.96×10^{-4}	2.49×10^{-4}	2.91×10^{-4}	1.54×10^{-2}	1.99×10^{-4}	3.78×10^{-3}

[a] Hydrogen bonded complexes, *cis*-HONO···H_2O, H_2O···*cis*-HONO (a), H_2O···*cis*-HONO (b), H_2O···*cis*-HONO (c), H_2O···*cis*-HONO (d), *trans*-HONO···H_2O, H_2O···*trans*-HONO (a) and H_2O···*trans*-HONO (b) are named as HB1, HB2, HB3, HB4, HB5, HB6, HB7 and HB8, respectively.

Table S5. The <S**2> values of the stationary points optimized with the UωB97X-D/aug-cc-pVTZ method.

Geometries	S**2
CR1	0.7555
TS1	0.7573
CP1	0.7540
CR2	0.7530
TS2	0.7599
TS2a	0.7574
CP2	0.7540
CR11	0.7541
TS11	0.7568
CP11	0.7540
CR12	0.7568
TS12	0.7576
CP12	0.7540
CR13	0.7530
TS13	0.7591
CP13	0.7540
CR14	0.7550
TS14	0.7572
CP14	0.7540
CR15	0.7551
TS15	0.7572
CP15	0.7540
CR21	0.7530
TS21	0.7573
CP21	0.7540
CR22	0.7530
TS22	0.7682
CP22	0.7540
CR23	0.7530
TS23	0.7594
CP23	0.7540
CR24	0.7530
TS24	0.7573
CP24	0.7540

Table S6. Cartesian coordinates (in Å) of the stationary points optimized.

Geometries optimized with the UωB97X-D/aug-cc-pVTZ method

cis-HONO

O	-1.00498600	-0.38639000	0.00000000
N	0.00000000	0.54112800	0.00000000
O	1.07631900	0.07020700	0.00000000
H	-0.57066400	-1.25842500	0.00000000

trans-HONO

O	0.88591100	-0.57507600	0.00000000
N	0.00000000	0.50946700	0.00000000
O	-1.10483900	0.14816300	0.00000000
H	1.75141900	-0.15096700	0.00000000

OH

O	0.00000000	0.00000000	0.10779500
H	0.00000000	0.00000000	-0.86236300

NO_2

N	0.00000000	0.00000000	0.31840800
O	0.00000000	1.09187200	-0.13930300
O	0.00000000	-1.09187200	-0.13930300

H_2O

O	0.00000000	0.00000000	0.11644300
H	0.00000000	0.76000500	-0.46577200
H	0.00000000	-0.76000500	-0.46577200

CR1

O	-0.68384200	1.03211800	0.02866800
N	-1.15433500	-0.19795600	-0.01603800
O	-0.32836000	-1.05381600	-0.01122600
H	0.31750400	0.94354400	0.05289700
O	1.74163400	0.13976800	-0.08659800
H	1.92738400	-0.50241100	0.61261700

TS1

O	0.57316000	-1.03819000	0.02718300
N	1.12218700	0.12124000	-0.00929200
O	0.37884500	1.05777000	-0.01464300
H	-0.48157100	-0.83090300	0.03985100
O	-1.64662500	-0.08437700	-0.09151800
H	-1.81677700	0.50059500	0.65701700

CP1

O	-0.95972600	-1.09110200	-0.13808300
N	-0.87329100	0.00000000	0.31215600

O	-0.95972700	1.09110200	-0.13808400
H	2.44065900	-0.76137000	-0.35726000
O	2.07341700	0.00000100	0.09234500
H	2.44066900	0.76136800	-0.35725800

TS3

O	-0.60978800	1.03988800	0.00013200
N	-1.10886000	-0.15071400	-0.00038500
O	-0.28863500	-1.06332700	0.00023000
H	0.43676400	0.96065200	0.00089100
O	1.70974200	0.11326600	-0.00018400
H	0.83471000	-0.62426700	0.00038400

CR2

O	-0.22312100	0.92624700	-0.00000500
N	-0.72824700	-0.35514700	0.00000000
O	-1.89669300	-0.36566600	0.00000000
H	0.73883200	0.77449400	-0.00000200
O	2.40883000	-0.20778900	0.00000400
H	2.04677000	-1.11080400	0.00000700

TS2

O	0.09114000	1.01105800	0.02363000
N	0.50011100	-0.20981000	0.01003000
O	1.64160700	-0.45949200	-0.01288100
H	-0.96742300	0.69278600	0.00628800
O	-1.79682100	-0.36103500	-0.11298200
H	-2.02076200	-0.74836000	0.74136700

TS2a

O	0.03186100	0.73830500	-0.02102000
N	-0.73092200	-0.39562100	0.03983400
O	-1.87349600	-0.14253400	-0.01980500
H	1.10646400	0.41208500	0.21416500
O	2.11112900	-0.16453100	-0.00783700
H	1.85403600	-1.09266100	-0.10370700

CR11

O	0.51675800	1.50052400	-0.38588000
H	1.26366400	0.91727400	-0.11841300
O	2.45697700	-0.40773700	0.23207700
H	2.00153300	-1.17981800	-0.11072500
H	2.69399500	-0.62379700	1.13461300
O	-1.73042400	0.45794800	0.53014600
N	-1.54526400	-0.75735800	0.03278300
O	-0.52111800	-0.90233200	-0.55537200
H	-0.91989900	1.00063200	0.29727700

TS11

O	0.30452400	1.33596600	-0.46941500
H	1.09709200	0.83725300	-0.18111800
O	2.49745100	-0.27071200	0.24937800
H	2.25113300	-1.12437200	-0.11138700
H	2.73827400	-0.43159600	1.16226500
O	-1.64459000	0.42626600	0.60298700
N	-1.48773500	-0.73811500	0.09032200
O	-0.51859100	-0.88165300	-0.60182900
H	-0.78271000	1.00658400	0.24902100

CP11

O	-0.83713900	1.68607900	0.02051100
H	-1.51242800	0.99464700	-0.02736900
O	-2.33359300	-0.73244600	-0.01729900
H	-1.50320600	-1.21656100	-0.03956500
H	-2.76607600	-0.99649200	0.79511600
O	2.24609500	0.31808000	0.01512900
N	1.25794500	-0.27066200	0.26415600
O	0.67851100	-1.17133400	-0.25663700
H	-1.05490000	2.31001300	-0.67091400

CR12

O	-0.35718000	1.52438800	-0.05008600
H	-0.04062300	1.98844900	0.73520600
O	-2.24949300	-0.71544800	-0.04448800
H	-2.96931300	-0.57655400	-0.65913200
H	-1.81321800	0.13961000	0.03584000
O	1.23883000	-0.20721800	-1.00540600
N	1.31811100	-0.76350500	0.17154500
O	0.73536300	-0.20401900	1.04523400
H	0.65622500	0.61140400	-0.87475700

TS12

O	-0.31091200	1.49383100	0.04889500
H	0.02219700	1.89654000	0.85940300
O	-2.26816600	-0.66848000	-0.09661700
H	-2.98816300	-0.45875400	-0.69054000
H	-1.79844200	0.16196000	0.03950300
O	1.24158100	-0.09714500	-0.99574700
N	1.30339200	-0.77991600	0.09419500
O	0.71279400	-0.33609500	1.02940800
H	0.63829100	0.72277500	-0.75524700

CR13

O	-1.16607900	1.49613200	-0.10423400

H	-1.73998600	0.71712700	-0.02946600
H	-1.52836100	2.17113300	0.46933700
N	1.74077500	-0.43196200	0.01814000
O	1.45094400	0.86100200	0.03778200
H	0.46207600	1.00693800	-0.00439100
O	0.79967000	-1.16204300	-0.04310100
O	-2.11245200	-1.13724900	0.04250200
H	-1.15581400	-1.33420500	-0.02605300

TS13

O	-1.31977900	-1.18534000	0.21703000
H	-1.50328000	-0.15150100	0.06689100
H	-1.77813500	-1.69134400	-0.45658700
N	1.56050800	0.11145300	-0.01331600
O	1.05980800	-1.03923400	-0.15294700
H	-0.14303300	-1.13626900	0.01294200
O	0.83641800	1.06374300	0.16873300
O	-1.34962000	1.21222300	-0.24042600
H	-1.31372400	1.78782000	0.53085000

CR14

O	0.38833300	1.09411900	0.01704700
N	-0.17111700	-0.09918400	-0.05635000
O	0.58111000	-1.01709100	-0.04266700
H	1.37711800	0.93591800	0.06711500
O	2.76576500	0.02701600	-0.04694400
H	2.89095400	-0.63316500	0.65022700
O	-3.36216700	-0.13444700	0.05667200
H	-2.40607500	-0.11757200	-0.03453700
H	-3.64850100	0.75232800	-0.16122600

TS14

O	0.45279700	1.05926700	-0.01018100
N	-0.12334100	-0.07963000	-0.09716000
O	0.58518100	-1.04278400	-0.07262600
H	1.51209300	0.81294200	0.06544800
O	2.63045100	0.04228900	-0.00396900
H	2.74353600	-0.53366400	0.76275500
O	-3.33718900	-0.10692300	0.09818700
H	-2.38949800	-0.08766100	-0.05389600
H	-3.65266500	0.75099500	-0.18547600

CR15

O	0.45862500	1.13555100	-0.01486900
N	-0.17293000	-0.01855800	-0.07072900
O	0.51977500	-0.98341600	-0.03167200
H	1.43545700	0.91656900	0.04812200

O	2.76304700	-0.07980700	-0.03227100
H	2.84049800	-0.72351500	0.68686500
O	-3.36312000	0.00946800	0.10345000
H	-2.41113700	0.01386100	-0.02474500
H	-3.68092400	-0.73137600	-0.41224400

CR21

O	1.81793300	-1.31304800	0.02650900
H	1.99850200	-0.33990500	-0.00152600
O	1.66768500	1.38892300	-0.08713200
H	1.97553700	2.08865700	0.48853500
H	0.70398500	1.36305800	-0.01226100
O	-0.94276200	-1.10783400	-0.01604500
N	-1.07286900	0.24079100	0.00578400
O	-2.19271500	0.58993700	0.01446300
H	0.03093500	-1.26117500	-0.01759000

TS21

O	0.66282100	1.22097600	-0.53879800
H	1.38169300	0.62973200	-0.23792700
O	2.65493000	-0.61174600	0.25650900
H	2.35517500	-1.50993100	0.10896700
H	3.49411700	-0.53958300	-0.20001200
O	-1.26571000	0.71323700	0.68181300
N	-1.12532700	-0.23722700	-0.17385100
O	-1.93177800	-1.08875700	-0.24699200
H	-0.31579800	1.21068800	0.32568000

CP21

O	-0.83710200	1.68607300	0.02053500
H	-1.51239900	0.99465100	-0.02737600
O	-2.33361900	-0.73241300	-0.01732700
H	-1.50325100	-1.21656300	-0.03954500
H	-2.76615000	-0.99642300	0.79507400
O	2.24609200	0.31806900	0.01509100
N	1.25796400	-0.27068700	0.26417600
O	0.67848700	-1.17133600	-0.25660800
H	-1.05481400	2.31000400	-0.67090900

CR22

O	-1.85683300	-1.03212100	0.10480200
H	-2.29064000	-0.78487000	-0.72393500
O	-1.63722600	1.30300200	-0.10428500
H	-0.67577800	1.22822600	-0.01365600
H	-1.97064700	1.43998700	0.78421300
O	0.87630100	-1.08386400	-0.02412500
N	1.12218900	0.24819000	0.01313900

O	2.26651300	0.50348500	0.00737700
H	-0.10830400	-1.14469200	-0.00875000

TS22

O	-1.80384500	-0.73890100	0.09853800
H	-2.15453600	-0.70737300	-0.79797800
O	-1.22339900	1.28436300	-0.09958000
H	-0.14407700	0.90755800	-0.01878300
H	-1.56992600	1.42511200	0.78927700
O	0.62207100	-1.11262400	0.00335400
N	0.97236300	0.10729500	-0.00271900
O	2.13276900	0.39761800	-0.00053700
H	-0.75876100	-1.02001600	0.03232300

CP22

O	2.03688400	-0.79644100	-0.11519500
H	2.40046400	-0.82277700	0.77142100
O	1.31879000	1.43686600	0.10553900
H	-0.32640300	0.73629700	-0.01913800
H	1.86110800	1.38052600	-0.69356900
O	-0.76848500	-1.13487100	0.03307300
N	-1.11394200	0.03718400	-0.00368400
O	-2.24560900	0.44199500	-0.02295600
H	1.12978200	-1.13473100	-0.03662200

CR23

O	1.88018100	-1.03983400	-0.08291800
H	2.05537400	-0.08702300	-0.03372000
H	2.45354200	-1.46336600	0.55570300
N	-1.08258400	0.18655000	-0.00614100
O	-0.81004500	-1.13544600	0.00541200
H	0.17849700	-1.18352700	-0.01126900
O	-2.23294900	0.42051000	0.01046600
O	1.45926600	1.74970700	0.01262500
H	0.51904600	1.46857200	-0.03240600

TS23

O	-1.93199600	-0.47198800	0.16904200
H	-1.51951700	0.50753500	0.05575900
H	-2.52142500	-0.65065300	-0.56553300
N	0.87869700	-0.06766900	0.15725800
O	0.33347700	-1.18246600	-0.13912200
H	-0.82416500	-0.98423400	0.00894900
O	2.02708800	0.11040100	0.00322800
O	-0.55221000	1.49465800	-0.18280200
H	-0.29663900	1.99619300	0.59724700

CP23

O	2.31516200	-0.71200900	-0.20140900
H	1.48748000	0.99972000	0.01608800
H	2.88679200	-0.98864600	0.51529800
N	-1.23359900	-0.27147100	-0.25640600
O	-0.66116200	-1.16703200	0.28027100
H	1.49482300	-1.19913800	-0.08021100
O	-2.24205400	0.29773600	-0.04512500
O	0.81129200	1.67035100	0.18855100
H	0.98020300	2.37600000	-0.43464600

Geometries optimized with the UM06-2X/aug-cc-pVTZ method

cis-HONO

O	-1.00151200	-0.38342200	0.00000000
N	0.00000000	0.54033500	0.00000000
O	1.07289600	0.06806000	0.00000000
H	-0.57107200	-1.25945100	0.00000000

trans-HONO

O	0.88254600	-0.56722300	0.00000000
N	0.00000000	0.50787200	0.00000000
O	-1.10170600	0.14150900	0.00000000
H	1.75328100	-0.14939700	0.00000000

OH

O	0.00000000	0.00000000	0.10799200
H	0.00000000	0.00000000	-0.86393700

NO_2

N	0.00000000	0.00000000	0.31444000
O	0.00000000	1.09026200	-0.13756800
O	0.00000000	-1.09026200	-0.13756800

H_2O

O	0.00000000	0.00000000	0.11639000
H	0.00000000	0.76257800	-0.46556100
H	0.00000000	-0.76257800	-0.46556100

CR1

O	-0.73250000	1.04130300	0.02974800
N	-1.20508100	-0.21054300	-0.02477200
O	-0.37276900	-1.04840900	-0.00714700
H	0.25218700	0.98388000	0.06833500
O	1.87763500	0.14256200	-0.07749600
H	2.00445600	-0.59372300	0.54422800

TS1

O	0.58150900	-1.03102400	0.02730100
N	1.11073700	0.13171600	-0.00870800
O	0.35338000	1.05494200	-0.01528200
H	-0.49598300	-0.82696600	0.03696300
O	-1.62054700	-0.09661400	-0.09171500
H	-1.79390900	0.48652200	0.66156500

CP1

O	0.90733700	1.08945900	-0.13718700
N	0.82938500	0.00000000	0.30875100
O	0.90733800	-1.08945900	-0.13718700
H	-2.37489500	0.76471800	-0.30911500
O	-1.94666200	-0.00000100	0.08149600
H	-2.37490400	-0.76471400	-0.30911600

CR2

O	-0.30469100	1.04637900	0.02408600
N	-0.55746300	-0.30071900	0.02298700
O	-1.69849000	-0.53082000	-0.03465000
H	0.66604300	1.08026000	0.05955700
O	2.15393400	-0.26484300	-0.08694200
H	2.03017000	-0.98095600	0.55958500

TS2

O	0.09172400	1.02421000	0.02409600
N	0.48153900	-0.20075200	0.01104600
O	1.61489000	-0.47206500	-0.01386700
H	-0.97388500	0.71088600	0.00472900
O	-1.75935200	-0.36886200	-0.11294000
H	-1.97499100	-0.77188300	0.73963300

CP2

O	0.90727300	1.08947600	-0.13718500
N	0.82938600	0.00001100	0.30875100
O	0.90740000	-1.08944200	-0.13718900
H	-2.37480700	0.76472200	-0.30911800
O	-1.94666300	-0.00004400	0.08149800
H	-2.37497400	-0.76471100	-0.30913000

Geometries optimized with the UB3LYP-D3/aug-cc-pVTZ method

trans-HONO

O	0.89019600	-0.60534400	0.00000000
N	0.00000000	0.51933900	0.00000000
O	-1.11061200	0.17419800	0.00000000
H	1.76332900	-0.18620100	0.00000000

OH

O	0.00000000	0.00000000	0.10836800
H	0.00000000	0.00000000	-0.86694100

NO_2

N	0.00000000	0.00000000	0.32059900
O	0.00000000	1.09857700	-0.14026200
O	0.00000000	-1.09857700	-0.14026200

H_2O

O	0.00000000	0.00000000	0.11698300
H	0.00000000	0.76357100	-0.46793300
H	0.00000000	-0.76357100	-0.46793300

CR2

O	-0.31995200	1.10714800	-0.02099100
N	-0.47643500	-0.26588300	-0.03008600
O	-1.59130100	-0.61035200	0.03278200
H	0.65597200	1.16918400	-0.05393300
O	1.98948600	-0.29336600	0.09972900
H	2.05320800	-0.93543900	-0.62762600

TS2

O	0.09164600	0.98323000	0.02542600
N	0.54555800	-0.23824300	0.00485800
O	1.70571700	-0.42817900	-0.01097100
H	-0.95786200	0.67075500	0.00705600
O	-1.89030500	-0.33961700	-0.11284400
H	-2.11750600	-0.72653000	0.74604800

CP2

O	0.93618900	1.09762300	-0.14008600
N	0.86313300	0.00000900	0.31524100
O	0.93630500	-1.09759300	-0.14009300
H	-2.46137400	0.76508700	-0.29372300
O	-2.01237300	-0.00003800	0.07777000
H	-2.46153000	-0.76508800	-0.29368800