Supporting Information

In silico kinetics of alkaline hydrolysis of 1,3,5-trinitro-1,3,5-triazinane (RDX): M06-2X investigation

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Table S1

PCM(Pauling)/M06-2X/6-311++G(d,p) calculated relative Gibbs free energies (kcal/mol) and rate constants (min^{-1}, $L \cdot mol^{-1} \cdot min^{-1}$) for kinetic model of alkaline hydrolysis of RDX.

Reaction	ΔG	$k_{scaling}$		Reaction	ΔG	$k_{scaling}$	
$RDX+HO(H_2O)_3^- \rightarrow INT1+NO_2^-$	21.16	k_1	$9.6 \cdot 10^{-1}$	$INT8+HO(H_2O)_3^- \rightarrow INT9$	8.19	k_{10}	$8.4 \cdot 10^{8}$
$INT1+NO_2^- \rightarrow RDX+HO(H_2O)_3^-$	61.52	k_{-1}	$1.4 \cdot 10^{-28}$	$INT9 \rightarrow INT8+HO(H_2O)_3^-$	29.93	k_{-10}	$8.6 \cdot 10^{-7}$
$INT1+HO(H_2O)_3^- \rightarrow INT2$	16.76	k_2	$1.0 \cdot 10^{3}$	$INT9 \rightarrow INT10$	17.36	k_{11}	$4.0 \cdot 10^{2}$
$INT2 \rightarrow INT1+HO(H_2O)_3^-$	7.49	k_{-2}	$2.6 \cdot 10^{9}$	$INT10 \rightarrow INT9$	4.40	k_{-11}	$3.4 \cdot 10^{11}$
$INT2 \rightarrow INT3$	2.29	k_3	$9.8 \cdot 10^{12}$	$INT10 \rightarrow HCOH+NHNO_2^-$	2.68	k_{12}	$5.3 \cdot 10^{12}$
$INT3 \rightarrow INT2$	26.99	k_{-3}	$9.2 \cdot 10^{-5}$	$HCOH+NHNO_2^- \rightarrow INT10$	14.16	k_{-12}	$6.4 \cdot 10^{4}$
$INT3 \rightarrow INT3a$	15.63	k_4	$6.2 \cdot 10^{3}$	$NHNO_2^- \rightarrow N_2O+HO(H_2O)_3^-$	25.37	k_{13}	$1.2 \cdot 10^{-3}$
$INT3a \rightarrow INT3$	20.69	k_{-4}	2.0	$N_2O+HO(H_2O)_3^- \rightarrow NHNO_2^-$	47.33	k_{-13}	$8.7 \cdot 10^{-19}$
$INT3a \rightarrow INT4$	10.47	k_5	$2.2 \cdot 10^{7}$	$INT8+HO(H_2O)_3^- \rightarrow INT11+NO_2^-$	14.35	k_{14}	$4.8 \cdot 10^{4}$
$INT4 \rightarrow INT3a$	30.92	k_{-5}	$1.8 \cdot 10^{-7}$	$INT11+NO_2^- \rightarrow INT8+HO(H_2O)_3^-$	67.75	k_{-14}	$7.3 \cdot 10^{-33}$
$INT2 \rightarrow INT5$	1.65	k_6	$2.7 \cdot 10^{13}$	$INT11+HO(H_2O)_3^- \rightarrow INT13$	19.35	k_{15}	$1.7 \cdot 10^{1}$
$INT5 \rightarrow INT2$	16.86	k_{-6}	$8.9 \cdot 10^{2}$	$INT13 \rightarrow INT11+HO(H_2O)_3^-$	19.97	k_{-15}	6.4
$INT5 \rightarrow INT4$	0.17	k_7	$2.8 \cdot 10^{14}$	$INT13 \rightarrow INT14$	11.05	k_{16}	$9.0 \cdot 10^{6}$
$INT4 \rightarrow INT5$	30.15	k_{-7}	$6.1 \cdot 10^{-7}$	$INT14 \rightarrow INT13$	26.17	k_{-16}	$3.4 \cdot 10^{-4}$
$INT1+HO(H_2O)_3^- \rightarrow INT6+NO_2^-$	18.92	k_8	$3.4 \cdot 10^{1}$	$INT14+HO(H_2O)_3^- \rightarrow INT15$	22.05	k_{17}	$2.3 \cdot 10^{-1}$
$INT6+NO_2^- \rightarrow INT1+HO(H_2O)_3^-$	59.64	k_{-8}	$2.8 \cdot 10^{-27}$	$INT15 \rightarrow INT14+HO(H_2O)_3^-$	4.59	k_{-17}	$2.5 \cdot 10^{11}$
$INT4 \rightarrow INT7+INT8$	21.07	k_9	1.11	$INT15 \rightarrow HCOO^-+NH_3$	10.18	k_{18}	$3.6 \cdot 10^{7}$
$INT7+INT8 \rightarrow INT4$	8.20	k_{-9}	$8.3 \cdot 10^{8}$	$HCOO^-+NH_3 \rightarrow INT15$	42.45	k_{-18}	$2.0 \cdot 10^{-15}$

Scheme S1. System of differential equations for kinetic model of alkaline hydrolysis of RDX.

$$\frac{d}{dt}x_0(t) = -k_1 \cdot x_0(t) \cdot x_1(t) + k_{-1} \cdot x_2(t) \cdot x_3(t)$$

$$\frac{d}{dt}x_1(t) = -k_1 \cdot x_0(t) \cdot x_1(t) + k_{-1} \cdot x_2(t) \cdot x_3(t) - k_2 \cdot x_2(t) \cdot x_1(t) + k_{-2} \cdot x_4(t) - k_8 \cdot x_2(t) \cdot x_1(t) + k_{-8} \cdot x_9(t) \cdot x_3(t) - k_{10} \cdot x_{11}(t) \cdot x_1(t) + k_{-10} \cdot x_{12}(t) - k_{14} \cdot x_{11}(t) \cdot x_1(t) + k_{-14} \cdot x_{17}(t) \cdot x_3(t) - k_{15} \cdot x_{17}(t) \cdot x_1(t) + k_{-15} \cdot x_{18}(t) - k_{17} \cdot x_{19}(t) \cdot x_1(t) - k_{-17} \cdot x_{20}(t)$$

$$\frac{d}{dt}x_2(t) = k_1 \cdot x_0(t) \cdot x_1(t) - k_{-1} \cdot x_2(t) \cdot x_3(t) - k_2 \cdot x_2(t) \cdot x_1(t) + k_{-2} \cdot x_4(t) - k_8 \cdot x_2(t) \cdot x_1(t) + k_{-8} \cdot x_9(t) \cdot x_3(t)$$

$$\frac{d}{dt}x_3(t) = k_1 \cdot x_0(t) \cdot x_1(t) - k_{-1} \cdot x_2(t) \cdot x_3(t) + k_8 \cdot x_2(t) \cdot x_1(t) - k_{-8} \cdot x_9(t) \cdot x_3(t) + k_{14} \cdot x_{11}(t) \cdot x_1(t) - k_{-14} \cdot x_{17}(t) \cdot x_3(t)$$

$$\frac{d}{dt}x_4(t) = k_2 \cdot x_2(t) \cdot x_1(t) - k_{-2} \cdot x_4(t) - k_3 \cdot x_4(t) + k_{-3} \cdot x_5(t) - k_6 \cdot x_4(t) + k_{-6} \cdot x_7(t)$$

$$\frac{d}{dt}x_5(t) = k_3 \cdot x_4(t) - k_{-3} \cdot x_5(t) - k_4 \cdot x_5(t) + k_{-4} \cdot x_6(t)$$

$$\frac{d}{dt}x_6(t) = k_4 \cdot x_5(t) - k_{-4} \cdot x_6(t) - k_5 \cdot x_6(t) + k_{-5} \cdot x_8(t)$$

$$\frac{d}{dt}x_7(t) = k_6 \cdot x_4(t) - k_{-6} \cdot x_7(t) - k_7 \cdot x_7(t) + k_{-7} \cdot x_8(t)$$

$$\frac{d}{dt}x_8(t) = k_5 \cdot x_6(t) - k_{-5} \cdot x_8(t) + k_7 \cdot x_7(t) - k_{-7} \cdot x_8(t) - k_9 \cdot x_8(t) + k_{-9} \cdot x_{10}(t) \cdot x_{11}(t)$$

$$\frac{d}{dt}x_9(t) = k_8 \cdot x_2(t) \cdot x_1(t) - k_{-8} \cdot x_9(t) \cdot x_3(t)$$

$$\frac{d}{dt}x_{10}(t) = k_9 \cdot x_8(t) - k_{-9} \cdot x_{10}(t) \cdot x_{11}(t)$$

$$\frac{d}{dt}x_{11}(t) = k_9 \cdot x_8(t) - k_{-9} \cdot x_{10}(t) \cdot x_{11}(t) - k_{10} \cdot x_{11}(t) \cdot x_1(t) + k_{-10} \cdot x_{12}(t) - k_{14} \cdot x_{11}(t) \cdot x_1(t) + k_{-14} \cdot x_{17}(t) \cdot x_3(t)$$

$$\frac{d}{dt}x_{12}(t) = k_{10} \cdot x_{11}(t) \cdot x_1(t) - k_{-10} \cdot x_{12}(t) - k_{11} \cdot x_{12}(t) + k_{-11} \cdot x_{13}(t)$$

$$\frac{d}{dt}x_{13}(t) = k_{11} \cdot x_{12}(t) - k_{-11} \cdot x_{13}(t) - k_{12} \cdot x_{13}(t) + k_{-12} \cdot x_{14}(t) \cdot x_{15}(t)$$

$$\frac{d}{dt}x_{14}(t) = k_{12} \cdot x_{13}(t) - k_{-12} \cdot x_{14}(t) \cdot x_{15}(t) - k_{13} \cdot x_{14}(t) + k_{-13} \cdot x_{16}(t)$$

$$\frac{d}{dt}x_{15}(t) = k_{12} \cdot x_{13}(t) - k_{-12} \cdot x_{14}(t) \cdot x_{15}(t)$$

$$\frac{d}{dt}x_{16}(t) = k_{13} \cdot x_{14}(t) + k_{-13} \cdot x_{16}(t)$$

$$\frac{d}{dt}x_{17}(t) = k_{14} \cdot x_{11}(t) \cdot x_1(t) - k_{-14} \cdot x_{17}(t) \cdot x_3(t) - k_{15} \cdot x_{17}(t) \cdot x_1(t) + k_{-15} \cdot x_{18}(t)$$

$$\frac{d}{dt}\mathrm{x}_{18}(t) = k_{15}\cdot \mathrm{x}_{17}(t)\cdot \mathrm{x}_{1}(t) - k_{-15}\cdot \mathrm{x}_{18}(t) - k_{16}\cdot \mathrm{x}_{18}(t) + k_{-16}\cdot \mathrm{x}_{19}(t)$$

$$\frac{d}{dt}\mathrm{x}_{19}(t) = k_{16}\cdot \mathrm{x}_{18}(t) - k_{-16}\cdot \mathrm{x}_{19}(t) - k_{17}\cdot \mathrm{x}_{19}(t)\cdot \mathrm{x}_{1}(t) + k_{-17}\cdot \mathrm{x}_{20}(t)$$

$$\frac{d}{dt}\mathrm{x}_{20}(t) = k_{17}\cdot \mathrm{x}_{19}(t)\cdot \mathrm{x}_{1}(t) - k_{-17}\cdot \mathrm{x}_{20}(t) - k_{18}\cdot \mathrm{x}_{20}(t) + k_{-18}\cdot \mathrm{x}_{21}(t)\cdot \mathrm{x}_{22}(t)$$

$$\frac{d}{dt}\mathrm{x}_{21}(t) = k_{18}\cdot \mathrm{x}_{20}(t) - k_{-18}\cdot \mathrm{x}_{21}(t)\cdot \mathrm{x}_{22}(t)$$

$$\frac{d}{dt}\mathrm{x}_{22}(t) = k_{18}\cdot \mathrm{x}_{20}(t) - k_{-18}\cdot \mathrm{x}_{21}(t)\cdot \mathrm{x}_{22}(t)$$

x	structure	x	structure	x	structure	x	structure
x_0	RDX	x_6	INT3a	x_{12}	INT9	x_{18}	INT13
x_1	$OH(H_2O)_3$	x_7	INT5	x_{13}	INT10	x_{19}	INT14
x_2	INT1	x_8	INT4	x_{14}	$NHNO_2^-$	x_{20}	INT15
x_3	NO_2^-	x_9	INT6	x_{15}	HCOH	x_{21}	$HCOO^-$
x_4	INT2	x_{10}	INT7	x_{16}	N_2O	x_{22}	NH_3
x_5	INT3	x_{11}	INT8	x_{17}	INT11		

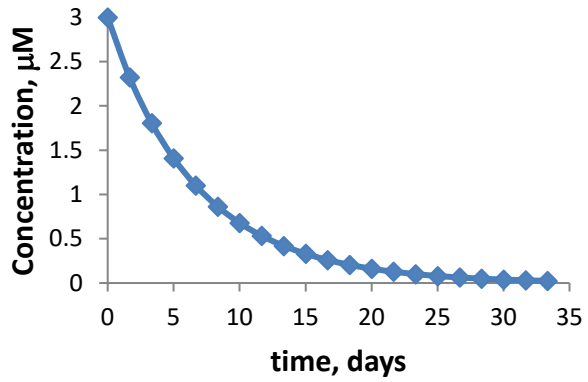


Figure S1. Plots of the concentration *vs*. time for alkaline (pH 10) hydrolysis of RDX calculated at 298.3 K at the PCM(Pauling)/M06-2X/6-311++G(d,p) level using fitted rate constants.

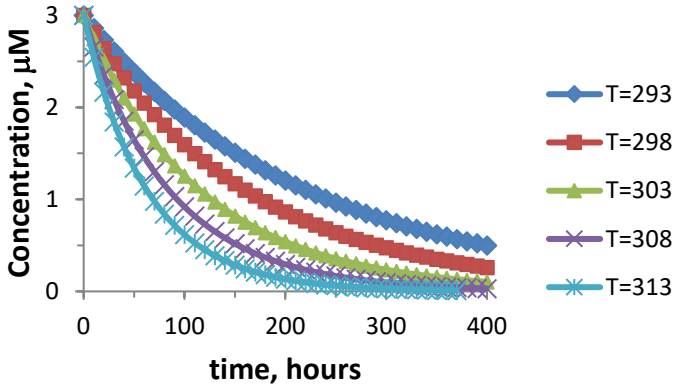


Figure S2. Plots of the concentration *vs*. time for alkaline (pH 10) hydrolysis of RDX calculated at different temperatures at the PCM(Pauling)/M06-2X/6-311++G(d,p) level using fitted rate constants.

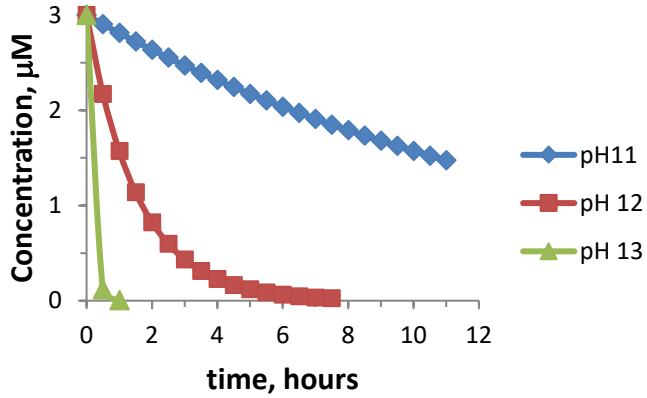
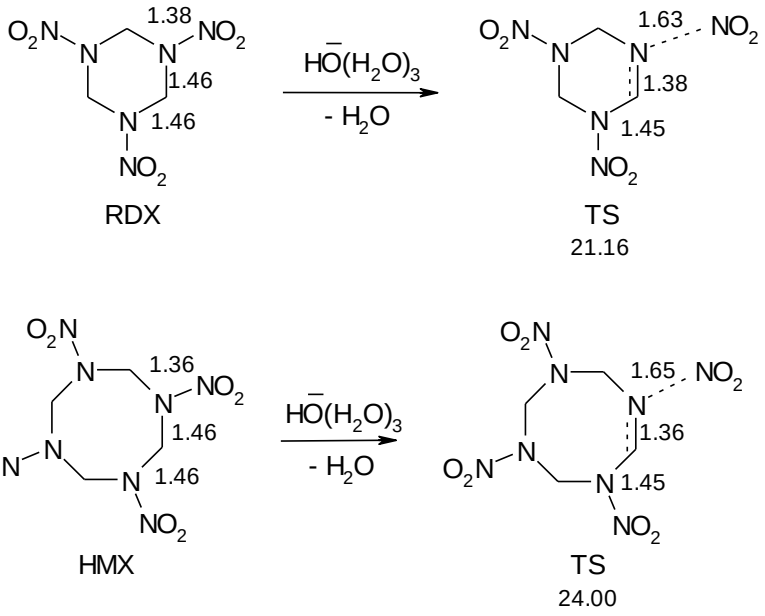


Figure S3. Plots of the concentration *vs*. time for alkaline hydrolysis of RDX at different pH calculated at 298.3 K at the PCM(Pauling)/M06-2X/6-311++G(d,p) level using fitted rate constants.

Scheme S2. Comparison of RDX and HMX.



Analysis of N-N bond in RDX and HMX

Compound	Electron density, $e \cdot Å^{-3}$	Laplacian of electron density, $e \cdot Å^{-5}$	Energy density, au	Energy of homolytic bond cleavage, kcal/mol
RDX	0.3525	0.1581	-0.3370	55.81
HMX	0.3661	0.1708	-0.3607	57.08

Table S2

PCM(Pauling)/M06-2X/6-311++G(d,p) calculated relative Gibbs free energies (kcal/mol) and rate constants (min^{-1}, $L \cdot mol^{-1} \cdot min^{-1}$) for kinetic model of alkaline hydrolysis of INT7.

Reaction	ΔG	k		Reaction	ΔG	k	
INT7+HO$(H_2O)_3^-$→INT16	21.40	k_1	$7.52 \cdot 10^{-2}$	INT25→INT26	15.33	k_8	$2.13 \cdot 10^{3}$
INT16→INT7+HO$(H_2O)_3^-$	2.02	k_{-1}	$1.23 \cdot 10^{13}$	INT26→INT25	4.59	k_{-8}	$1.60 \cdot 10^{11}$
INT16→INT17+$HCOO^-$	9.82	k_2	$2.34 \cdot 10^{7}$	INT26→HCOH+NH_3	1.72	k_9	$2.04 \cdot 10^{13}$
INT17+$HCOO^-$→INT16	43.49	k_{-2}	$4.73 \cdot 10^{-18}$	HCOH+NH_3→INT26	11.71	k_{-9}	$9.61 \cdot 10^{5}$
INT17→INT18+$NHNO_2^-$	30.11	k_3	$3.08 \cdot 10^{-8}$	INT21→INT27	4.08	k_{10}	$3.79 \cdot 10^{11}$
INT18+$NHNO_2^-$→INT17	23.63	k_{-3}	$1.74 \cdot 10^{-3}$	INT27→INT21	3.89	k_{-10}	$5.23 \cdot 10^{11}$
INT7→INT19	22.25	k_4	$1.79 \cdot 10^{-2}$	INT27→INT14+HCOH	12.28	k_{11}	$3.67 \cdot 10^{5}$
INT19→INT7	5.70	k_{-4}	$2.46 \cdot 10^{10}$	INT14+HCOH→INT27	9.56	k_{-11}	$1.06 \cdot 10^{4}$
INT19→INT20+$NHNO_2^-$	16.25	k_5	$4.50 \cdot 10^{2}$	INT14+HO$(H_2O)_3^-$→INT15	22.05	k_{12}	$2.51 \cdot 10^{-2}$
INT20+$NHNO_2^-$→INT19	13.25	k_{-5}	$7.13 \cdot 10^{4}$	INT15→INT14+HO$(H_2O)_3^-$	4.60	k_{-12}	$1.58 \cdot 10^{11}$
INT20+HO$(H_2O)_3^-$→INT21	7.69	k_6	$8.54 \cdot 10^{8}$	INT15→$HCOO^-$+NH_3	10.18	k_{13}	$1.27 \cdot 10^{7}$
INT21→INT20+HO$(H_2O)_3^-$	24.89	k_{-6}	$2.07 \cdot 10^{-4}$	$HCOO^-$+NH_3→INT15	42.45	k_{-13}	$2.74 \cdot 10^{-17}$
INT18→INT25	23.04	k_7	$4.71 \cdot 10^{-3}$	$NHNO_2^-$→N_2O+HO$(H_2O)_3^-$	25.37	k_{14}	$9.21 \cdot 10^{-5}$
INT25→INT18	23.81	k_{-7}	$1.28 \cdot 10^{-3}$	N_2O+HO$(H_2O)_3^-$→ $NHNO_2^-$	47.33	k_{-14}	$7.22 \cdot 10^{-21}$

Scheme S3. System of differential equations for kinetic model of alkaline hydrolysis of INT7.

$$\frac{d}{dt}\mathrm{x}_0(t) = -k_1 \cdot \mathrm{x}_0(t) \cdot \mathrm{x}_1(t) + k_{-1} \cdot \mathrm{x}_2(t) - k_4 \cdot \mathrm{x}_0(t) + k_{-4} \cdot \mathrm{x}_7(t)$$

$$\frac{d}{dt}\mathrm{x}_1(t) = -k_1 \cdot \mathrm{x}_0(t) \cdot \mathrm{x}_1(t) + k_{-1} \cdot \mathrm{x}_2(t) \cdot \mathrm{x}_3(t) - k_6 \cdot \mathrm{x}_8(t) \cdot \mathrm{x}_1(t) + k_{-6} \cdot \mathrm{x}_9(t) - k_{12} \cdot \mathrm{x}_{15}(t) \cdot \mathrm{x}_1(t) + k_{-12} \cdot \mathrm{x}_{16}(t)$$

$$\frac{d}{dt}\mathrm{x}_2(t) = k_1 \cdot \mathrm{x}_0(t) \cdot \mathrm{x}_1(t) - k_{-1} \cdot \mathrm{x}_2(t) - k_2 \cdot \mathrm{x}_2(t) + k_{-2} \cdot \mathrm{x}_3(t) \cdot \mathrm{x}_4(t)$$

$$\frac{d}{dt}\mathrm{x}_3(t) = k_2 \cdot \mathrm{x}_2(t) - k_{-2} \cdot \mathrm{x}_3(t) \cdot \mathrm{x}_4(t) - k_3 \cdot \mathrm{x}_3(t) + k_{-3} \cdot \mathrm{x}_5(t) \cdot \mathrm{x}_6(t)$$

$$\frac{d}{dt}\mathrm{x}_4(t) = k_2 \cdot \mathrm{x}_2(t) - k_{-2} \cdot \mathrm{x}_3(t) \cdot \mathrm{x}_4(t) + k_{13} \cdot \mathrm{x}_{16}(t) - k_{-13} \cdot \mathrm{x}_4(t) \cdot \mathrm{x}_{13}(t)$$

$$\frac{d}{dt}\mathrm{x}_5(t) = k_3 \cdot \mathrm{x}_3(t) - k_{-3} \cdot \mathrm{x}_5(t) \cdot \mathrm{x}_6(t) - k_7 \cdot \mathrm{x}_5(t) \cdot \mathrm{x}_1(t) + k_{-7} \cdot \mathrm{x}_{10}(t)$$

$$\frac{d}{dt}x_6(t) = k_3 \cdot x_3(t) - k_{-3} \cdot x_5(t) \cdot x_6(t) + k_5 \cdot x_7(t) - k_{-5} \cdot x_6(t) \cdot x_8(t) - k_{14} \cdot x_6(t) + k_{-14} \cdot x_{17}(t)$$

$$\frac{d}{dt}x_7(t) = k_4 \cdot x_0(t) - k_{-4} \cdot x_7(t) - k_5 \cdot x_7(t) + k_{-5} \cdot x_6(t) \cdot x_8(t)$$

$$\frac{d}{dt}x_8(t) = k_5 \cdot x_7(t) - k_{-5} \cdot x_6(t) \cdot x_8(t) - k_6 \cdot x_8(t) \cdot x_1(t) + k_{-6} \cdot x_9(t)$$

$$\frac{d}{dt}x_9(t) = k_6 \cdot x_8(t) \cdot x_1(t) - k_{-6} \cdot x_9(t) - k_{10} \cdot x_9(t) + k_{-10} \cdot x_{14}(t)$$

$$\frac{d}{dt}x_{10}(t) = k_7 \cdot x_5(t) \cdot x_1(t) - k_{-7} \cdot x_{10}(t) - k_8 \cdot x_{10}(t) + k_{-8} \cdot x_{11}(t)$$

$$\frac{d}{dt}x_{11}(t) = k_8 \cdot x_{10}(t) - k_{-8} \cdot x_{11}(t) - k_9 \cdot x_{11}(t) + k_{-9} \cdot x_{12}(t) \cdot x_{13}(t)$$

$$\frac{d}{dt}x_{12}(t) = k_9 \cdot x_{11}(t) - k_{-9} \cdot x_{12}(t) \cdot x_{13}(t) + k_{11} \cdot x_{14}(t) - k_{-11} \cdot x_{12}(t) \cdot x_{15}(t)$$

$$\frac{d}{dt}x_{13}(t) = k_9 \cdot x_{11}(t) - k_{-9} \cdot x_{12}(t) \cdot x_{13}(t) + k_{13} \cdot x_{16}(t) - k_{-13} \cdot x_{13}(t) \cdot x_4(t)$$

$$\frac{d}{dt}x_{14}(t) = k_{10} \cdot x_9(t) - k_{-10} \cdot x_{14}(t) - k_{11} \cdot x_{14}(t) + k_{-11} \cdot x_{12}(t) \cdot x_{15}(t)$$

$$\frac{d}{dt}x_{15}(t) = k_{11} \cdot x_{14}(t) - k_{-11} \cdot x_{12}(t) \cdot x_{15}(t) - k_{12} \cdot x_{15}(t) \cdot x_1(t) + k_{-12} \cdot x_{16}(t)$$

$$\frac{d}{dt}x_{16}(t) = k_{12} \cdot x_{15}(t) \cdot x_1(t) - k_{-12} \cdot x_{16}(t) - k_{13} \cdot x_{16}(t) + k_{-13} \cdot x_{13}(t) \cdot x_4(t)$$

$$\frac{d}{dt}x_{17}(t) = k_{14} \cdot x_6(t) - k_{-14} \cdot x_{17}(t)$$

x	structure	x	structure	x	structure	x	structure
x_0	INT7	x_5	INT18	x_{10}	INT25	x_{15}	INT14
x_1	$OH(H_2O)_3$	x_6	$NHNO_2^-$	x_{11}	INT26	x_{16}	INT15
x_2	INT16	x_7	INT19	x_{12}	HCOH	x_{17}	N_2O
x_3	INT17	x_8	INT20	x_{13}	NH_3		
x_4	$HCOO^-$	x_9	INT21	x_{14}	INT27		

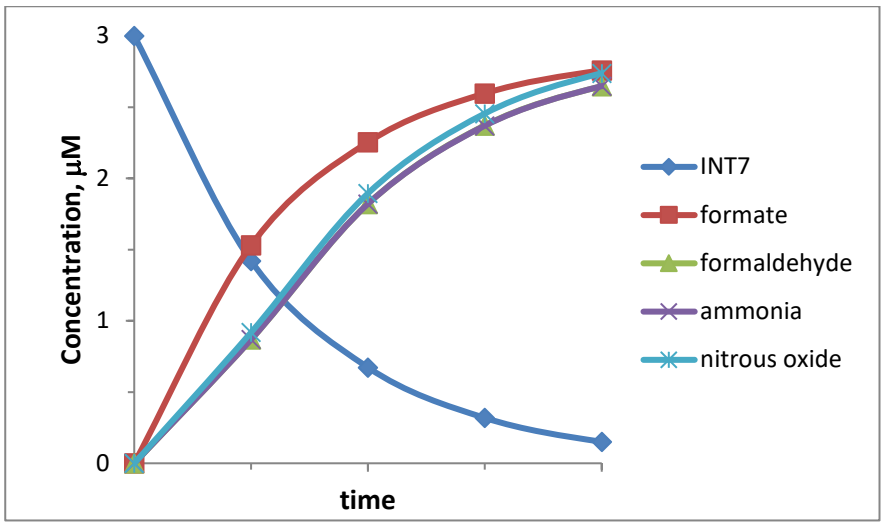


Figure S4. Plots of the concentration *vs*. time for alkaline hydrolysis of INT7 calculated at 298.3 K at the PCM(Pauling)/M06-2X/6-311++G(d,p) level.

Cartesian coordinates for stationary points

RDX

N	-1.469399	-0.032358	0.000436
C	-0.854448	1.209781	0.464226
N	0.584052	1.207694	0.199254
C	1.289681	0.016104	0.670427
N	0.628257	-1.198943	0.198628
C	-0.809243	-1.250394	0.463693
N	-2.031483	-0.042569	-1.254089
O	-2.325656	1.026154	-1.749038
O	-2.272927	-1.120977	-1.755896
N	1.081316	-1.754216	-0.977207
O	2.196960	-1.454779	-1.348973
O	0.370804	-2.570252	-1.526672
N	1.022052	1.793894	-0.965281
O	0.273784	2.570252	-1.523341
O	2.157763	1.558082	-1.322243
H	-0.977935	1.239307	1.544764
H	-1.328658	2.068562	0.010138
H	2.325656	0.035485	0.362464
H	1.220202	0.013132	1.755896
H	-0.927739	-1.287983	1.544421
H	-1.254511	-2.125196	0.011146

INT1

N	-0.605628	2.001533	-0.838138
C	0.535393	1.475939	-0.981026
N	0.912619	0.272382	-0.362634
C	0.011153	-0.342037	0.619930
N	-1.338458	-0.102940	0.154829
C	-1.622736	1.323146	-0.053469
N	-1.769982	-0.959407	-0.845574
O	-1.166906	-2.001533	-0.998003
O	-2.762392	-0.642028	-1.465537
N	2.091356	-0.323130	-0.675095
O	2.762392	0.169585	-1.560831
O	2.398116	-1.310645	-0.036412
H	1.307713	1.938357	-1.582224
H	0.221556	-1.399538	0.708287
H	0.121210	0.153741	1.582224
H	-1.686452	1.783909	0.932608
H	-2.583782	1.420251	-0.545366

INT2

N	-0.354301	1.266617	-0.926623
C	0.939321	0.787626	-0.767838
N	0.960465	-0.667446	-0.331090
C	0.059288	-1.029903	0.777514
N	-1.244484	-0.460826	0.508381
C	-1.149354	1.030320	0.227695
N	-2.016662	-1.168943	-0.363559
O	-1.712367	-2.322209	-0.627025
O	-3.012519	-0.619857	-0.804928
N	2.124867	-1.327043	-0.379941
O	3.012519	-0.887377	-1.099843
O	2.237955	-2.364339	0.264773
H	1.490732	0.821123	-1.705608
H	0.006859	-2.105255	0.882274
H	0.413468	-0.577996	1.705608
H	-0.752458	1.411896	1.178551
H	-2.162447	1.400788	0.104016
O	1.734437	1.420905	0.267124

H 1.546039 2.364339 0.196863

INT3

N	-1.639213	1.292613	-0.515157
C	-0.690477	2.112716	-0.698975
N	0.980979	-0.724578	-0.471676
C	0.233493	-1.157447	0.696981
N	-1.174170	-0.861102	0.487618
C	-1.707345	0.485541	0.695534
N	-1.869142	-1.679628	-0.322975
O	-1.340307	-2.720016	-0.688572
O	-3.008160	-1.356954	-0.628767
N	2.238029	-0.850350	-0.315151
O	3.008159	-0.494785	-1.256893
O	2.747686	-1.314440	0.747202
H	-0.678433	2.720016	-1.599509
H	0.346713	-2.225357	0.887002
H	0.531841	-0.619609	1.599509
H	-1.163119	0.882190	1.554269
H	-2.751515	0.392641	0.981866
O	0.371937	2.396497	0.065764
H	0.435668	1.827600	0.843849

INT3a

N	-1.639225	0.824140	-0.145466
C	-2.865021	0.834025	-0.453018
N	1.591674	0.210522	-0.821090
C	1.231291	-0.755105	0.204184
N	-0.181519	-1.072827	0.079528
C	-1.216905	-0.261945	0.718619
N	-0.554768	-1.863751	-0.938089
O	0.317403	-2.398885	-1.609289
O	-1.752490	-2.029734	-1.128645
N	2.816418	0.550897	-0.751685
O	3.264269	1.391606	-1.587827
O	3.603861	0.082523	0.122439
H	-3.603861	0.102777	-0.125214
H	1.812281	-1.674747	0.124602
H	1.363357	-0.349058	1.208744
H	-0.742594	0.145284	1.609290
H	-2.035680	-0.918015	1.019860
O	-3.403834	1.774900	-1.232111
H	-2.711768	2.398885	-1.498881

INT4

N	1.609666	-1.105622	-0.042053
C	2.838928	-1.240290	-0.569155
N	-1.472598	-0.401987	-0.782602
C	-1.155675	0.649096	0.170566
N	0.274290	0.910057	0.115103
C	1.218219	0.009235	0.781317
N	0.739618	1.609959	-0.939569
O	-0.065327	2.164586	-1.670915
O	1.951114	1.671784	-1.090405
N	-2.704699	-0.724711	-0.754960
O	-3.113675	-1.633766	-1.536314
O	-3.533741	-0.172245	0.025542
H	3.533741	-0.442819	-0.275138
H	-1.696375	1.573042	-0.034531
H	-1.369757	0.346765	1.197927
H	0.698592	-0.337343	1.670915
H	2.102062	0.568559	1.077240
O	3.178040	-2.164586	-1.297634

H 0.905609 -1.793666 -0.284640

INT5
N -0.419338 1.303521 -0.888794
C 1.014966 0.996345 -0.663603
N 0.948728 -0.574841 -0.411610
C 0.085637 -0.982595 0.707611
N -1.236259 -0.428004 0.476811
C -1.225058 1.029522 0.288622
N -2.022635 -1.128560 -0.410164
O -1.750364 -2.294286 -0.624395
O -2.986203 -0.557152 -0.881101
N 2.136412 -1.186002 -0.437746
O 2.986203 -0.767824 -1.217975
O 2.329272 -2.153015 0.296915
H 1.495879 1.062195 -1.647096
H 0.039315 -2.060642 0.782522
H 0.445684 -0.558945 1.647096
H -0.809725 1.431237 1.216355
H -2.237484 1.393879 0.158925
O 1.614506 1.595771 0.326411
H -0.475901 2.294286 -1.109960

INT6
N -1.079832 1.182856 -0.087822
C 0.195285 1.120037 -0.065813
N 0.876629 -0.075653 -0.131238
C 0.176452 -1.380209 -0.075441
N -1.245904 -1.213019 -0.227908
C -1.752025 -0.050837 -0.223464
N 2.237984 -0.084361 -0.167674
O 2.827245 0.974941 -0.246365
O 2.762073 -1.179310 -0.122197
H 0.813540 2.006306 0.006911
H 0.559674 -2.006307 -0.880980
H 0.393926 -1.862357 0.880980
H -2.827245 0.044705 -0.335616

INT7
N 1.094127 0.399733 -0.152055
C 2.164182 -0.169064 -0.721280
N -0.727412 -1.135608 0.350679
C 0.300455 -0.249742 0.878127
N -1.672189 -0.508123 -0.241243
O -2.629555 -1.178340 -0.728034
O -1.692475 0.750355 -0.365196
H 2.614158 0.446915 -1.509701
H 0.963609 -0.871442 1.474463
H -0.132426 0.527985 1.509701
O 2.629555 -1.262681 -0.408026
H 0.748963 1.262681 -0.546175

INT8
N 0.123441 -0.957289 -0.271684
C 1.081490 -0.183143 0.032082
N -1.158327 -0.307939 -0.191233
O -2.040877 -0.999645 0.250074
O -1.280538 0.819754 -0.601481
H 0.942362 0.857159 0.315329
H 2.076774 -0.611013 0.001941

INT9
N -0.054502 -0.855828 -0.472601

C -1.381838 -0.428329 -0.063485
N 0.807186 0.087156 -0.423397
O 2.008894 -0.166498 -0.718185
O 0.504043 1.276131 -0.097282
H -1.349311 -0.015634 0.950824
H -2.008894 -1.316142 -0.077058
O -1.979133 0.502244 -0.950824
H -1.464994 1.316142 -0.869802

INT10
N 0.082011 -0.334965 -0.281012
C -1.143257 0.555794 -0.052737
N 1.302236 0.109995 -0.098821
O 2.229193 -0.699250 0.013449
O 1.473073 1.329600 -0.075166
H -1.105012 1.284339 -0.880786
H -0.904872 1.100075 0.880786
O -2.229193 -0.215522 -0.010622
H -0.013340 -1.329600 -0.101368

INT11
N 0.000000 0.000000 1.108208
C 0.000000 0.000000 -0.036746
H 0.000000 0.000000 -1.108208

INT12
N -1.185482 -0.521578 -0.000364
C -0.171877 0.174485 -0.000196
H -0.059311 1.272901 -0.000102
O 1.185482 -0.307500 -0.000430
H 1.118452 -1.272902 0.000430

INT13
N 1.160756 -0.278967 -0.000137
C -0.056446 0.197745 -0.000056
H -0.114270 1.301035 -0.000016
O -1.160756 -0.431905 -0.000107
H 1.102628 -1.301035 0.000137

INT14
N 0.720890 -0.321668 -0.000911
C -0.494619 0.229925 -0.000426
H -0.482092 1.326545 -0.000374
O -1.547405 -0.403509 -0.000418
H 1.547405 0.255276 0.000911
H 0.827808 -1.326545 0.000572

INT15
N 0.757317 -0.589183 -0.246254
C -0.421503 0.216774 0.148131
H -0.451267 0.168370 1.253873
O -0.479821 1.447852 -0.336521
H 1.577271 -0.152573 0.168946
H 0.868812 -0.475145 -1.253874
O -1.577271 -0.539557 -0.328308
H -1.477246 -1.447853 -0.020665

INT16
N 0.626030 0.119472 -0.514315
C 2.090262 0.015156 -0.448112
N -1.362036 -0.822482 0.524971
C -0.054312 -0.205613 0.735764
N -2.238931 -0.017716 0.075223

O	-3.416662	-0.452690	-0.133567
O	-2.001578	1.202894	-0.176636
H	2.449835	0.468512	-1.390779
H	0.539608	-0.956217	1.254013
H	-0.162822	0.667229	1.390778
O	2.551927	-1.202894	-0.218923
H	0.370250	1.057999	-0.803765
O	2.520003	0.957130	0.613801
H	3.416662	0.687908	0.841676

INT17

N	-2.026742	0.461637	0.405853
N	0.026865	-0.858013	0.002652
C	-1.271868	-0.399156	-0.495550
N	0.911109	0.058138	0.055148
O	2.071937	-0.238683	0.478479
O	0.691153	1.258500	-0.290940
H	-1.848924	-1.306841	-0.666901
H	-1.147780	0.118820	-1.450142
H	-1.491609	1.304655	0.589630
H	-2.154013	-0.008862	1.297243

INT18

N	0.713710	-0.247297	0.000039
C	-0.540040	-0.062134	0.000052
H	-1.205138	-0.924804	-0.000006
H	-1.005492	0.924804	-0.000052
H	1.205139	0.648284	0.000048

INT19

N	0.965183	-0.229136	0.677216
C	2.235843	-0.505542	0.539145
N	-1.037478	0.662111	-0.279840
C	0.374662	0.357577	-0.504050
N	-1.893776	-0.348715	-0.084770
O	-2.969086	-0.085726	0.441537
O	-1.586131	-1.461050	-0.481258
H	2.700705	-0.952355	1.432933
H	0.820018	1.320390	-0.772415
H	0.435894	-0.289511	-1.383207
O	2.969086	-0.318445	-0.480082
H	-1.281780	1.453990	0.304924

INT20

N	0.125726	0.539182	0.421973
C	-1.219308	0.300274	0.158574
C	1.008697	-0.311873	0.107124
H	-1.650051	0.981039	-0.586480
H	2.047238	-0.114513	0.357475
H	0.774033	-1.239905	-0.416166
O	-1.882632	-0.517612	0.753467

INT21

N	-0.013613	-0.894550	-0.299292
C	1.083775	-0.232916	0.361301
C	-1.122602	-0.190379	-0.360985
H	0.777449	0.284631	1.275717
H	1.843855	-0.977467	0.611937
H	-1.955835	-0.714123	-0.859710
O	-1.346882	0.977467	0.070667
O	1.690885	0.790011	-0.447009
H	1.955835	0.375368	-1.275717

INT24

N	-1.333557	-2.117813	0.420922
C	-0.197035	-1.578719	-0.185559
H	-0.110803	-1.894570	-1.232446
H	0.761647	-1.773448	0.322130
H	-1.210220	-2.033892	1.429954
O	-0.246334	-0.064932	-0.260755
H	0.583471	0.240665	-0.669086
H	-1.702741	0.405976	2.442080
O	-0.863226	0.837359	2.254223
H	-0.620597	0.519102	1.359157
H	-1.773929	0.518946	-0.934385
O	-2.635453	0.830645	-1.283275
H	-2.511017	1.768465	-1.456353
H	2.304848	0.245061	-2.380649
O	2.278678	0.531224	-1.460924
H	2.958015	0.008481	-1.020920

INT25

N	-0.784788	-0.506009	-0.080869
C	0.379739	0.355277	-0.005911
H	0.407085	0.979573	0.889708
H	0.386278	0.997145	-0.889708
H	-1.576669	0.005624	-0.455692
O	1.567204	-0.421126	0.053950
H	1.576669	-0.997146	-0.719644
H	-1.049636	-0.832931	0.842887

INT26

N	-0.790262	-0.377656	0.000213
C	0.602914	0.331250	0.000152
H	0.538391	0.973711	0.894074
H	0.538431	0.973286	-0.894073
H	-1.573165	0.277532	0.000012
O	1.573165	-0.571639	0.000359
H	-0.866758	-0.973357	0.824555
H	-0.866628	-0.973711	-0.823887

INT27

C	1.144457	-0.168043	-0.516217
N	-0.050451	0.397645	-0.349615
C	-1.247771	-0.337692	0.153879
H	1.891758	0.491187	-0.978489
H	-1.864399	0.454796	0.611121
H	-0.856761	-0.957509	0.978489
O	1.435281	-1.321348	-0.183027
H	-0.179088	1.321348	-0.740033
O	-1.891758	-1.047834	-0.806148

N_2O

N	-0.001310	1.154677	0.000000
N	0.000087	0.037985	0.000000
O	0.001310	-1.154676	0.000000

HCOH

C	-0.317100	0.000000	-0.000090
H	-0.889648	0.938341	0.000090
H	-0.889648	-0.938341	0.000090
O	0.889648	0.000000	-0.000087

NH_3

N	-0.143863	-0.098602	-0.194729
H	0.773042	-0.295370	0.194729

H	-0.773042	-0.793998	0.194553
H	-0.431911	0.793999	0.194361

$NHNO_2^-$

N	0.688478	-1.009225	-0.000002
N	-0.341190	-0.258003	-0.000019
O	-0.262301	1.009225	-0.000021
O	-1.489293	-0.785476	-0.000044
H	1.489293	-0.379015	0.000044

$HCOO^-$

C	-0.000050	-0.274625	-0.000142
H	0.000009	0.834875	0.000142
O	-1.120429	-0.834875	0.000037
O	1.120428	-0.834866	0.000037

TS(RDX→INT1)

N	1.061964	-1.266007	-0.488517
C	0.142471	-0.958351	0.496924
N	-1.236983	-1.082306	0.069936
C	-1.566223	-0.381328	-1.161465
N	-0.623228	-0.801992	-2.194193
C	0.793981	-0.683427	-1.800683
N	1.284880	-2.862410	-0.749321
O	0.763640	-3.611326	0.035468
O	2.105598	-3.177051	-1.579919
N	-0.974020	-1.926649	-2.906044
O	-2.130996	-2.296901	-2.860569
O	-0.117979	-2.449774	-3.592563
N	-2.123038	-1.883093	0.640246
O	-1.767555	-2.532029	1.626816
O	-3.288746	-1.894939	0.221048
H	0.490787	0.942271	0.640374
H	0.330498	-1.393344	1.466044
H	-2.584421	-0.573496	-1.466595
H	-1.402633	0.683730	-1.004261
H	1.009532	0.381390	-1.733459
H	1.419905	-1.137967	-2.557819
O	0.785770	1.894695	0.581287
H	0.428699	2.347853	1.366190
H	0.040467	3.611326	-2.071471
O	-0.048038	2.662212	-1.941489
H	0.246897	2.497126	-1.024156
H	2.781837	-0.255992	0.046387
O	3.288747	0.540259	0.269790
H	2.593003	1.195536	0.439537
H	0.342833	3.243713	3.592563
O	-0.218104	3.296733	2.811144
H	-1.094652	3.034085	3.113125

TS(INT1→INT2)

N	0.102808	-0.814680	-1.343054
C	0.677332	-0.625057	-0.189476
N	-0.037827	-0.905835	1.030536
C	-1.508390	-0.802224	1.038852
N	-1.978206	-1.325118	-0.224004
C	-1.333141	-0.663053	-1.377594
N	-2.069472	-2.698399	-0.301371
O	-2.126138	-3.332442	0.734667
O	-2.151471	-3.192082	-1.408439
N	0.584090	-0.646714	2.200739
O	1.802364	-0.625923	2.218910
O	-0.119725	-0.472682	3.182399

H	1.738059	-0.809552	-0.096721
H	-1.908784	-1.365795	1.871320
H	-1.812587	0.243041	1.098121
H	-1.636294	0.385888	-1.299407
H	-1.740798	-1.078704	-2.291779
O	0.852486	1.258727	0.157696
H	1.277424	1.557555	-0.654844
H	2.151471	1.667778	2.907187
O	1.833583	2.397778	2.366467
H	1.513174	1.967021	1.532377
H	-1.163344	3.332442	1.108273
O	-1.410401	2.549393	0.607256
H	-0.551686	2.081229	0.415315
H	0.771725	1.670786	-3.182399
O	1.406879	0.955818	-3.075055
H	0.937907	0.279798	-2.532023

TS(INT2→INT3)

N	-0.385993	1.628284	-0.778193
C	0.905807	1.270612	-0.735070
N	0.968172	-0.466567	-0.393877
C	0.125212	-0.817695	0.755192
N	-1.177641	-0.204139	0.553795
C	-1.121891	1.290502	0.401317
N	-2.007941	-0.855963	-0.303572
O	-1.757692	-2.014734	-0.598998
O	-2.999331	-0.262366	-0.696571
N	2.182189	-0.977743	-0.330606
O	2.999331	-0.632110	-1.191282
O	2.475162	-1.780819	0.563307
H	1.435381	1.287467	-1.682271
H	0.031036	-1.893375	0.864177
H	0.524324	-0.398187	1.682271
H	-0.706427	1.615543	1.364785
H	-2.142456	1.653790	0.345231
O	1.781211	1.751295	0.244407
H	1.282709	2.014735	1.027449

TS(INT3→INT3a)

N	0.971113	0.234989	1.086374
C	0.651915	-0.582799	1.948548
N	-0.771278	-0.638710	-1.108260
C	-0.583439	0.790508	-1.331640
N	0.808842	1.146751	-1.098920
C	1.245079	1.351790	0.317616
N	1.707177	0.648650	-1.970274
O	1.293293	0.183385	-3.023427
O	2.897124	0.722312	-1.693426
N	-1.981874	-1.000855	-1.272003
O	-2.277118	-2.220588	-1.092618
O	-2.897123	-0.190837	-1.596118
H	0.846711	-0.530428	3.023427
H	-0.867607	1.083675	-2.342716
H	-1.165919	1.385998	-0.624534
H	0.681431	2.220588	0.661435
H	2.302155	1.602867	0.295664
O	-0.008645	-1.740356	1.651756
H	-0.222657	-1.691399	0.699558

TS(INT3a→INT4)

N	1.594360	-0.383185	0.130131
C	2.778086	-0.460028	-0.388153
N	-1.439015	-0.040732	-0.720722

C	-1.259300	1.095253	0.168488
N	0.129980	1.524217	0.101551
C	1.165015	0.798690	0.838140
N	0.520846	2.177186	-1.013833
O	-0.339222	2.578531	-1.781764
O	1.717775	2.359943	-1.179485
N	-2.614837	-0.524509	-0.655739
O	-2.902250	-1.527336	-1.375374
O	-3.505832	-0.042655	0.103492
H	3.505832	0.343685	-0.283324
H	-1.904490	1.933485	-0.095023
H	-1.446910	0.832046	1.211250
H	0.703903	0.517295	1.781764
H	2.001369	1.467599	1.030309
O	3.138244	-1.512143	-1.047904
H	2.231840	-2.171672	-1.042745
H	0.411435	-2.578531	-1.477023
O	1.000674	-2.569514	-0.714769
H	0.997005	-1.427564	-0.180168

TS(INT2→INT5)

N	-0.070886	0.621823	-0.833896
C	1.165664	-0.070708	-0.703413
N	0.940208	-1.501508	-0.389962
C	-0.021614	-1.817002	0.682513
N	-1.222371	-1.046202	0.443895
C	-0.930292	0.403545	0.303824
N	-2.075098	-1.568702	-0.498770
O	-1.967802	-2.745143	-0.792847
O	-2.934046	-0.832653	-0.944826
N	1.990770	-2.336434	-0.512146
O	2.934046	-1.984534	-1.202599
O	1.927884	-3.422581	0.045290
H	1.704359	-0.033292	-1.648649
H	-0.231387	-2.877527	0.689470
H	0.374851	-1.501543	1.648649
H	-0.488913	0.670434	1.272399
H	-1.866060	0.940435	0.188752
O	2.006332	0.424383	0.343637
H	1.944799	1.394553	0.270324
H	0.395669	3.422581	0.010771
O	0.910693	2.899099	-0.610863
H	0.326423	1.843974	-0.774329

TS(INT5→INT4)

N	-0.438692	1.328750	-0.830064
C	1.003533	1.125018	-0.655451
N	0.952600	-0.658199	-0.442005
C	0.131409	-1.040799	0.709207
N	-1.192207	-0.470531	0.504189
C	-1.194482	0.992378	0.365325
N	-1.993355	-1.146491	-0.381950
O	-1.731719	-2.310497	-0.623272
O	-2.959960	-0.560994	-0.832180
N	2.160018	-1.183918	-0.419226
O	2.959960	-0.836191	-1.296812
O	2.472687	-1.999282	0.459120
H	1.491828	1.135368	-1.635749
H	0.067440	-2.117929	0.814951
H	0.516471	-0.608608	1.635749
H	-0.747340	1.363970	1.289955
H	-2.213495	1.352057	0.285903
O	1.597446	1.620116	0.342376

H	-0.578244	2.310497	-1.058342

TS(INT1→INT6)

N	-0.131921	-0.531572	-2.199526
C	1.110301	-0.218717	-2.070805
N	1.845917	-0.675686	-0.941143
C	1.120777	-1.344725	0.157369
N	-0.005180	-2.067886	-0.391502
C	-0.750692	-1.355797	-1.310320
N	0.631092	-3.411611	-1.040035
O	1.446075	-4.021603	-0.387274
O	0.106105	-3.808529	-2.047611
N	3.084954	-0.288481	-0.733703
O	3.677808	0.307809	-1.642144
O	3.595882	-0.527041	0.368831
H	1.627998	0.461371	-2.727998
H	1.806998	-2.009453	0.670509
H	0.746349	-0.593763	0.854390
H	-1.140874	0.447578	-0.159993
H	-1.731514	-1.730803	-1.557063
O	-0.949772	1.272855	0.317716
H	-1.678974	1.890885	0.115908
H	2.081434	2.239888	-0.801947
O	1.681538	2.221511	0.074454
H	0.775119	1.890555	-0.059999
H	1.346506	1.567868	2.299923
O	0.533471	1.274506	2.727998
H	-0.112404	1.256560	2.001653
H	-2.652597	4.021603	-0.184609
O	-2.958990	3.107415	-0.177360
H	-3.677808	3.080626	0.464028

TS(INT4→INT7+INT8)

N	2.465016	-0.094650	-1.050250
C	2.721339	-1.409302	-1.047321
N	-1.462350	-0.737691	0.650193
C	-0.217950	-0.860825	1.000881
N	0.893326	0.970003	0.500492
C	2.281696	0.703884	0.149382
N	0.265401	1.694032	-0.371090
O	-0.929657	1.983216	-0.139853
O	0.815617	2.104756	-1.423228
N	-1.671854	-0.984102	-0.709172
O	-2.833057	-1.147619	-1.031598
O	-0.745245	-0.988984	-1.499211
H	2.828084	-1.831699	-2.053857
H	-0.015152	-0.721186	2.053857
H	0.515655	-1.367477	0.384607
H	2.705261	0.154807	0.987028
H	2.819942	1.645236	0.024892
O	2.833058	-2.104756	-0.039656
H	2.342696	0.365548	-1.941170

TS(INT8→INT9)

N	1.679406	0.059754	-1.398186
C	0.544980	-0.552520	-1.395398
N	2.714989	-0.693306	-0.801981
O	3.584499	-0.035509	-0.271255
O	2.729557	-1.902830	-0.884295
H	0.426873	-1.579132	-1.068559
H	-0.261481	-0.065106	-1.924930
O	-0.589668	0.038326	0.480625
H	-1.398537	-0.431231	0.243495

H	0.704111	2.268111	-0.858862
O	-0.115810	2.420925	-0.377502
H	-0.363202	1.503792	-0.032767
H	1.936685	-0.432942	1.924930
O	1.274828	-1.121185	1.808299
H	0.515863	-0.680671	1.299741
H	-3.584499	-1.871676	-0.457015
O	-2.736070	-1.597104	-0.820638
H	-2.275369	-2.420925	-1.012584

TS(INT9→INT10)

N	-0.160508	0.162818	-0.664510
C	0.536538	-1.071126	-0.253731
N	-1.440495	0.289026	-0.392100
O	-1.949350	1.408237	-0.479683
O	-2.084074	-0.718106	-0.096476
H	0.140410	-1.916561	-0.816993
H	0.356091	-1.231363	0.816993
O	1.882993	-0.879512	-0.545777
H	2.084074	0.120274	-0.345139
H	2.083732	1.916561	0.659278
O	1.961125	1.604614	-0.242092
H	0.445008	1.026757	-0.535172

TS(INT10→HCOH+$NHNO_2^-$)

N	-0.231817	-0.295267	0.651197
C	1.338471	0.574806	0.009056
N	-1.361753	0.085086	0.138950
O	-2.220794	-0.741787	-0.235832
O	-1.567776	1.308362	0.027438
H	1.412294	1.267685	0.856960
H	0.807777	1.000415	-0.856959
O	2.220794	-0.300155	-0.162357
H	-0.162931	-1.308362	0.558644

TS($NHNO_2^-$→N_2O)

N	1.991749	-0.961170	0.085523
N	0.781613	-0.877404	0.132088
O	0.161515	0.393114	0.207146
O	-0.086079	-1.785730	0.124319
H	2.396285	0.228868	0.123450
H	2.720935	1.785730	0.978369
O	2.386565	1.473534	0.131275
H	0.965787	1.058572	0.213124
H	-2.487887	1.215596	-1.677052
O	-2.309154	0.384928	-1.224646
H	-1.381563	0.441305	-0.943961
H	-2.720935	0.340162	0.779584
O	-2.358719	0.317566	1.677051
H	-1.405643	0.308531	1.510860

TS(INT8→INT11)

N	0.086476	0.575880	-1.516279
C	-0.170960	-0.521648	-0.925563
N	-0.100536	0.526981	-3.023895
O	0.196130	1.556823	-3.580873
O	-0.514730	-0.461274	-3.576752
H	-0.492091	-1.362216	-1.553705
H	-0.027612	-0.533979	0.477363
O	0.140454	-0.509024	1.665303
H	-0.726465	-0.509012	2.097779
H	2.628860	-1.450809	3.180173

O	1.987558	-2.071289	2.821349
H	1.293192	-1.506932	2.400565
H	1.850172	2.071288	1.629215
O	1.772324	1.486006	2.388289
H	1.137735	0.779771	2.108409
H	-2.628860	0.256843	3.524719
O	-2.486506	-0.523103	2.977987
H	-2.593171	-1.266739	3.580873

TS(INT11→INT13)

N	-1.131375	-1.231376	0.284886
C	0.006234	-0.941290	0.186676
H	1.014754	-1.272609	-0.013922
O	0.564430	0.808598	0.445588
H	-0.245903	1.279298	0.682474
H	0.510252	0.852101	-2.607279
O	1.227685	1.237074	-2.095478
H	0.963030	1.112018	-1.146972
H	2.845981	0.813006	2.525395
O	2.024691	0.320654	2.612137
H	1.492864	0.552833	1.806319
H	-2.874196	1.181446	1.765642
O	-2.443511	1.224842	0.906215
H	-2.127735	0.315746	0.730065

TS(INT13→INT14)

N	0.528764	-0.709949	-0.311018
C	1.111980	0.439804	-0.290971
H	2.192182	0.550808	-0.258132
O	0.412156	1.534199	-0.308728
H	-0.623963	1.202455	-0.332047
H	1.113554	-1.534199	-0.293615
H	-2.192183	0.269062	0.405610
O	-1.673923	0.286949	-0.405610
H	-0.677594	-0.518326	-0.332937

TS(INT14→INT15)

N	0.992083	1.393871	0.292363
C	-0.281052	0.855380	-0.017278
H	-1.059992	1.169732	0.686335
O	-0.560672	0.600318	-1.212174
H	0.956621	2.097403	1.020968
H	1.440109	1.759573	-0.540967
O	-0.207219	-0.838278	0.802353
H	0.219159	-0.727062	1.659973
H	1.358692	-1.601790	-1.659973
O	1.387178	-2.097403	-0.835073
H	0.741213	-1.628335	-0.225587
H	-3.048044	-0.680727	-0.105527
O	-2.836838	-1.101447	0.733455
H	-1.846572	-1.040576	0.802780
H	2.375851	0.124646	0.813514
O	3.048044	-0.574360	0.929961
H	2.724809	-1.267445	0.332901

TS(INT15→$HCOO^-$+NH_3)

N	0.782750	-0.212777	0.398644
C	-0.559734	-0.996767	0.415677
H	-0.748113	-1.173235	-0.659382
O	-0.510100	-2.057424	1.168371
H	1.494869	-0.725624	-0.116510
H	1.100426	-0.096283	1.360799
O	-1.494869	-0.021297	0.876302

H	-1.306079	0.806667	0.367405
H	-0.450243	2.057424	-1.360800
O	-0.287532	1.985155	-0.415853
H	0.550213	0.763290	-0.048706

TS(INT7→INT16)

N	0.332483	-0.971824	-0.975405
C	1.667627	-0.934955	-1.395868
N	-1.259957	-1.840617	0.628079
C	0.081995	-1.315673	0.419798
N	-2.177292	-0.962725	0.533735
O	-3.379185	-1.313598	0.718750
O	-1.951103	0.259564	0.258484
H	1.754027	-0.451982	-2.374708
H	0.764692	-2.116833	0.692544
H	0.264497	-0.459987	1.082542
O	2.460039	-1.870323	-1.089769
H	-0.168886	-0.137374	-1.258177
O	2.267742	0.593601	-0.489514
H	3.100956	0.830273	-0.911403
H	3.246400	1.064481	2.374708
O	2.569287	0.434065	2.110299
H	2.479714	0.533321	1.115761
H	-0.517893	1.540194	0.246611
O	0.168092	2.201267	0.071509
H	0.967162	1.678743	-0.170471
H	3.162680	-1.339008	1.871264
O	3.379185	-2.201266	1.478730
H	3.044320	-2.121676	0.561888

TS(INT16→INT17)

N	-0.968635	-0.809726	-0.541734
C	-2.366704	-1.439460	-0.205639
N	1.133155	0.115769	0.251784
C	-0.079953	-0.580116	0.620540
N	1.943091	-0.603555	-0.435057
O	3.047610	-0.100738	-0.780528
O	1.680053	-1.789995	-0.783442
H	-2.152811	-2.207952	0.555333
H	-0.619452	0.063535	1.311705
H	0.122877	-1.544358	1.092541
O	-2.922451	-1.855500	-1.311704
H	-0.504335	-1.419019	-1.213811
O	-3.047610	-0.396151	0.476213
H	-2.921374	0.415539	-0.095921
H	-1.782719	2.207952	-0.780701
O	-2.168179	1.431999	-1.198877
H	-1.235281	0.136074	-0.978789

TS(INT17→INT18)

N	-1.674775	-0.737516	0.199884
N	0.769634	-0.512193	0.060163
C	-0.383627	-1.082439	0.769111
N	1.053259	-1.041860	-1.102615
O	1.963451	-0.521934	-1.770520
O	0.442059	-2.037390	-1.518849
H	-0.319863	-0.657050	1.770521
H	-0.267584	-2.163142	0.842031
H	-1.730545	-1.107955	-0.745014
H	-1.691195	0.475103	0.160380
H	-1.963451	2.069812	-0.676723
O	-1.659095	1.788003	0.191399
H	0.851425	0.674986	0.054971

H	1.035004	2.163142	0.933468
O	0.690606	1.985118	0.052680
H	-0.494047	1.946514	0.131224

TS(INT7→INT19)

N	1.226857	-0.415726	-0.045744
C	2.467324	-0.869043	-0.019315
N	-1.061285	-0.546346	-0.166717
C	0.137966	-1.367028	-0.043390
N	-2.245761	-1.084185	-0.030197
O	-3.227399	-0.337974	-0.016493
O	-2.327614	-2.308824	0.057052
H	3.227400	-0.076660	-0.015166
H	0.199901	-2.063336	-0.884760
H	0.096740	-1.946406	0.884760
O	2.797936	-2.067803	0.000178
H	0.907683	0.697505	-0.025159
H	0.232273	2.308824	0.773598
O	0.178228	1.852171	-0.071230
H	-0.976669	0.489683	-0.097476

TS(INT19→INT20)

N	1.478741	0.113756	-0.202215
C	1.488610	-1.236899	0.061661
N	-1.309736	0.581913	-0.414164
C	0.604272	0.811327	0.474306
N	-1.990246	-0.394163	0.088566
O	-2.432558	-1.330189	-0.624390
O	-2.208267	-0.396039	1.320018
H	2.432558	-1.733444	-0.198250
H	0.173818	0.434083	1.402089
H	0.567302	1.881048	0.307929
O	0.546102	-1.881048	0.498971
H	-1.176979	0.366767	-1.402088

TS(INT20→INT21)

N	-1.425058	-0.985835	-0.758706
C	-0.134821	-1.031191	-0.882597
C	-1.887205	-1.416774	0.476090
H	0.501313	-1.495924	-0.130111
H	0.310377	-0.810082	-1.844343
H	-1.124299	-1.783728	1.185143
O	-3.063202	-1.402589	0.776377
O	0.780757	0.878842	-0.193216
H	0.822728	1.402440	-1.000407
H	3.063202	-1.061935	-0.262047
O	3.036733	-0.289926	0.310739
H	2.169731	0.176133	0.092831
H	-1.384730	1.101903	1.844343
O	-1.147957	1.783728	1.207880
H	-0.359406	1.410142	0.672305
H	-2.314390	1.767384	-0.235206
O	-2.780408	1.559948	-1.066514
H	-2.474010	0.655525	-1.245338

TS(INT18→INT24)

N	-2.117890	-1.178689	0.959296
C	-0.838655	-1.245334	0.623460
H	-0.525942	-2.130121	0.071611
H	-0.067313	-0.832078	1.276047
H	-2.253472	-0.433625	1.640298
O	-0.427660	-0.092886	-0.786930
H	0.538859	-0.107420	-0.835067

H	-2.293169	1.784331	0.565408
O	-1.412830	2.061131	0.293370
H	-1.008601	1.244452	-0.131064
H	-2.885599	-1.047833	-0.726232
O	-2.887389	-0.852434	-1.693321
H	-1.976131	-0.520899	-1.778408
H	2.864777	-1.202023	-0.873268
O	2.542371	-0.338335	-0.594526
H	2.714826	-0.307616	0.352680

TS(INT25→INT26)

N	-0.710546	0.771219	-0.297706
C	-1.134724	-0.585693	0.189068
H	-2.175405	-0.749576	-0.080487
H	-1.024826	-0.554922	1.275844
H	-1.115842	1.526610	0.252832
O	-0.314958	-1.526609	-0.409674
H	0.643912	-1.144157	-0.276216
H	-0.963302	0.908273	-1.275844
H	2.175405	-0.178830	0.712647
O	1.738752	-0.143969	-0.143334
H	0.355988	0.748821	-0.208140

TS(INT26→HCOH+NH_3)

N	1.010381	-0.316610	0.000000
C	-0.979175	0.340469	0.000000
H	-0.783968	0.897221	-0.925265
H	-0.783969	0.897221	0.925265
H	1.150965	-0.897217	-0.821489
O	-1.722741	-0.648505	0.000000
H	1.150968	-0.897221	0.821487
H	1.722741	0.408304	0.000000

TS(INT21→INT27)

N	-0.113122	-0.271773	-0.513129
C	0.184745	1.122077	-0.251496
C	-1.354067	-0.699294	-0.624494
H	-0.543830	1.776644	-0.731948
H	0.176798	1.315791	0.827843
H	-1.433074	-1.776644	-0.827843
O	-2.389212	-0.008034	-0.522938
O	1.462763	1.421560	-0.788580
H	2.016669	0.630416	-0.638583
H	2.389211	-1.683246	0.290524
O	2.148220	-1.284587	-0.550815
H	0.873123	-0.919165	-0.522648

TS(INT27→INT14+HCOH)

C	1.273304	-0.266575	-0.436802
N	0.316874	0.578593	-0.134543
C	-1.673145	-0.284898	0.217400
H	2.042147	0.061876	-1.160815
H	-2.042147	0.747029	0.256972
H	-1.286117	-0.686036	1.160815
O	1.384677	-1.431123	0.036433
H	0.409027	1.431123	-0.681177
O	-1.966827	-1.031379	-0.716349