

Impact of water dimer on the atmospheric reactivity of carbonyl oxides.

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(supplementary information)

Table S1 Relative energies ($\Delta(E+ZPE)$, in kcal·mol⁻¹) for the stationary points of reaction 2 between carbonyl oxides with water and with water dimer. **a**, **b**, **c**, **A**, **B**, and **C** are as defined in Figure 2.^{a,b}

		R1R2COO + H₂O			R1R2COO + (H₂O)₂		
Entry	Path	a	b	c	A	B	C
		HHCOO + H₂O			HHCOO + (H₂O)₂		
1	TS1a	-6.14 (-6.88)	1.50	-42.69	-10.53 (-11.78)	-8.31	-45.73
		[-6.66]	[2.22]	[-42.64]	[-11.23]	[-7.30]	[-45.42]
	TS1b	-6.14 (-6.88)	2.33	-42.52	-10.70 (-11.94)	-8.49	-46.24
		[-6.66]	[3.08]	[-42.50]	[-11.38]	[-7.50]	[-45.95]
	TS1c	--	--	--	-10.34 (-11.55)	-7.35	-46.30
		--	--	--	[-11.08]	[-6.28]	[-46.05]
	TS1d	--	--	--	-10.79 (-12.04)	-8.49	-47.00
		--	--	--	[-11.47]	[-7.42]	[-46.74]
2		CH₃HCOO + H₂O			CH₃HCOO + (H₂O)₂		
	TS1a	-6.58 (-7.46)	5.34	-36.67	-11.86 (-13.08)	-5.87	-39.66
		{-7.29}	{5.98}	{-35.97}	--	--	--
	TS1b	-6.58 (-7.46)	6.74	-36.31	-11.55 (-12.74)	-5.56	-40.09

		{-7.29}	{7.34}	{-35.56}	--	--	--
	TS1c	--	--	--	-11.55 (-12.74)	-3.95	-40.20
	TS1d	--	--	--	-11.86 (-13.08)	-5.51	-41.02
3		HCH₃COO + H₂O			HCH₃COO + (H₂O)₂		
	TS1a	-7.70 (-8.54)	-1.20	-41.20	-13.87 (-15.11)	-9.44	-44.14
	TS1b	-7.70 (-8.54)	-0.58	-41.31	-13.47 (-14.68)	-9.66	-44.65
	TS1c	--	--	--	-13.47 (-14.68)	-8.75	-45.22
	TS1d	--	--	--	-13.87 (-15.11)	-9.94	-45.84
4		CH₃CH₃COO + H₂O			CH₃CH₃COO + (H₂O)₂		
	TS1a	-7.63 (-8.58)	3.57	-34.93	-13.89 (-15.23)	-6.05	-37.72
	TS1b	-7.63 (-8.58)	4.64	-34.81	-13.49 (-14.80)	-5.76	-38.20
	TS1c	--	--	--	-13.49 (-14.80)	-4.37	-39.02
	TS1d	--	--	--	-13.89 (-15.23)	-5.93	-39.62
5		(CH₃)(<i>t</i>-CH=CH₂)COO + H₂O			(CH₃)(<i>t</i>-CH=CH₂)COO + (H₂O)₂		
	TS1a	-6.45 (-7.36)	6.82	-30.46	-10.85 (-12.07)	-3.59	-34.65
	TS1b	-6.45 (-7.36)	8.35	-28.95	-10.64 (-11.82)	-1.39	-32.38
	TS1c	--	--	--	-10.64 (-11.82)	0.36	-31.86
	TS1d	--	--	--	10.85 (-12.07)	-3.51	-34.98
6		(CH₃)(<i>c</i>-CH=CH₂)COO + H₂O			(CH₃)(<i>c</i>-CH=CH₂)COO + (H₂O)₂		
	TS1a	-6.62 (-7.54)	5.24	-31.50	-10.49 (-11.73)	-4.01	-34.70
	TS1b	-6.62 (-7.54)	6.68	-30.59	-10.49 (-11.73)	-3.69	-35.07
	TS1c	--	--	--	-11.11 (-12.33)	-1.15	-34.94
	TS1d	--	--	--	-11.11 (-12.33)	-2.81	-35.66
7		(<i>c</i>-CH=CH₂)(CH₃)COO + H₂O			(<i>c</i>-CH=CH₂)(CH₃)COO + (H₂O)₂		
	TS1a	-5.19 (-5.96)	5.84	-32.04	-11.69 (-12.98)	-2.38	-37.60
	TS1b	-5.19 (-5.96)	6.02	-32.90	-11.17 (-12.44)	-1.06	-37.03
	TS1c	--	--	--	-11.17 (-12.44)	-2.07	-35.14
	TS1d	--	--	--	-11.69 (-12.98)	-1.79	-34.13
8		(<i>t</i>-CH=CH₂)(CH₃)COO + H₂O			(<i>t</i>-CH=CH₂)(CH₃)COO + (H₂O)₂		
	TS1a	-6.50 (-7.40)	4.70	-31.40	-12.44 (-13.74)	-4.33	-36.54
	TS1b	-6.50 (-7.40)	4.31	-31.69	-12.27 (-13.61)	-2.92	-35.89
	TS1c	--	--	--	-12.27 (-13.61)	-3.22	-36.26
	TS1d	--	--	--	12.44 (-13.74)	-2.93	-35.58

9		$\text{H}(t\text{-C}(\text{CH}_3)=\text{CH}_2)\text{COO} + \text{H}_2\text{O}$			$\text{H}(t\text{-C}(\text{CH}_3)=\text{CH}_2)\text{COO} + (\text{H}_2\text{O})_2$		
	TS1a	-6.89 (-7.73)	1.85	-34.15	-12.54 (-13.82)	-5.03	-37.62
	TS1b	-6.89 (-7.73)	2.24	-34.55	-12.54 (-13.82)	-5.52	-37.69
	TS1c	--	--	--	-12.54 (-13.82)	-5.16	-37.15
	TS1d	--	--	--	-11.70 (-12.95)	-6.24	-39.05
10		$(t\text{-C}(\text{CH}_3)=\text{CH}_2)\text{HCOO} + \text{H}_2\text{O}$			$(t\text{-C}(\text{CH}_3)=\text{CH}_2)\text{HCOO} + (\text{H}_2\text{O})_2$		
	TS1a	-6.17 (-7.12)	4.69	-34.91	-11.17 (-12.46)	-3.95	-38.00
	TS1b	-6.17 (-7.12)	4.94	-34.32	-11.17 (-12.46)	-3.16	-38.23
	TS1c	--	--	--	-10.73 (-11.98)	-3.55	-38.41
	TS1d	--	--	--	-10.73 (-11.98)	-4.91	-39.02
11		$(c\text{-C}(\text{CH}_3)=\text{CH}_2)\text{HCOO} + \text{H}_2\text{O}$			$(c\text{-C}(\text{CH}_3)=\text{CH}_2)\text{HCOO} + (\text{H}_2\text{O})_2$		
	TS1a	-4.54 (-5.19)	6.82	-33.12	-10.35 (-11.67)	-2.00	-36.20
	TS1b	-4.54 (-5.19)	7.93	-33.45	-10.35 (-11.67)	-0.50	-37.45
	TS1c	--	--	--	-10.41 (-11.69)	-1.80	-38.05
	TS1d	--	--	--	-10.60 (-11.93)	-1.86	-35.35
12		$\text{H}(c\text{-C}(\text{CH}_3)=\text{CH}_2)\text{COO} + \text{H}_2\text{O}$			$\text{H}(c\text{-C}(\text{CH}_3)=\text{CH}_2)\text{COO} + (\text{H}_2\text{O})_2$		
	TS1a	-6.58 (-7.42)	0.16	-37.30	-12.21 (-13.46)	-7.27	-41.49
	TS1b	6.58 (-7.42)	1.45	-36.55	-12.06 (-13.37)	-5.96	-40.78
	TS1c	--	--	--	-12.06 (-13.37)	-7.95	-40.84
	TS1d	--	--	--	-11.96 (-13.28)	-7.79	-40.47

- a) **R1** stands for the substituent in *syn* and **R2** stands for the substituent in *anti*.
- b) Plain numbers correspond to CCSD(T)/aug-cc-pVTZ// B3LYP/6-311+G(2df,2p) relative energies. Values in parenthesis are without considering the BSSE correction, values in brackets correspond to CCSD(T)/CBS//B3LYP/6-311+G(2df,2p) relative energies, and values in braces correspond to CCSD(T)/aug-cc-pVTZ//QCISD/6-311+G(2df,2p) relative energies.

Table S2 Relative energies ($\Delta(\text{E}+\text{ZPE})$, in $\text{kcal}\cdot\text{mol}^{-1}$) for the stationary points of reaction 3 between carbonyl oxides with water and with water dimer. **a**, **b**, **c**, **A**, **B**, and **C** are as defined in Figure 3.^{a,b}

		R1R2COO + H₂O ^a			R1R2COO + (H₂O)₂ ^a		
Entry	Path	a^b	b	c	A^b	B	C
2		CH₃HCOO + H₂O			CH₃HCOO + (H₂O)₂		
	TS2a	-6.58 (-7.46)	8.31	-24.46	-11.86 (-13.08)	2.06	-29.66
		{-7.29}	{8.50}	{-24.06}	--	--	--
	TS2b	-6.58 (-7.46)	8.17	-24.82	-11.86 (-13.08)	3.49	-29.32
		{-7.29}	{8.35}	{-24.39}	--	--	--
	TS2c	--	--	--	-11.55 (-12.74)	3.00	-29.21
	TS2d	--	--	--	-11.55 (-12.74)	3.16	-28.88
4		CH₃ CH₃COO + H₂O			CH₃ CH₃COO + (H₂O)₂		
	TS2a	-7.63 (-8.58)	7.52	-22.39	-13.89 (-15.23)	1.38	-27.72
	TS2b	-7.63 (-8.58)	7.56	-22.64	-13.89 (-15.23)	3.06	-27.27
	TS2c	--	--	--	-13.49 (-14.80)	2.41	-27.19
	TS2d	--	--	--	-13.49 (-14.80)	2.43	-27.01
5		(CH₃)(<i>t</i>-CH=CH₂)COO + H₂O			(CH₃)(<i>t</i>-CH=CH₂)COO + (H₂O)₂		
	TS2a	-6.45 (-7.36)	10.27	-18.81	-10.85 (-12.07)	4.42	-24.17
	TS2b	-6.45 (-7.36)	10.10	-19.14	-10.64 (-11.82)	5.53	-23.49
	TS2c	--	--	--	-10.64 (-11.82)	5.12	-23.83
	TS2d	--	--	--	-10.85 (-12.07)	5.67	-23.84
6		(CH₃)(<i>c</i>-CH=CH₂)COO + H₂O			(CH₃)(<i>c</i>-CH=CH₂)COO + (H₂O)₂		
	TS2a	-6.62 (-7.54)	8.88	-22.32	10.49 (-11.73)	2.69	-27.60
	TS2b	-6.62 (-7.54)	8.70	-22.80	-11.11 (-12.33)	3.71	-26.86
	TS2c	--	--	--	-11.11 (-12.33)	3.49	-27.44
	TS2d	--	--	--	10.49 (-11.73)	4.07	-27.39

- a) **R1** stands for the substituent in *syn* and **R2** stands for the substituent in *anti*.
- b) Plain numbers correspond to CCSD(T)/aug-cc-pVTZ// B3LYP/6-311+G(2df,2p) relative energies. Values in parenthesis are without considering the BSSE correction, values in brackets correspond to CCSD(T)/CBS//B3LYP/6-311+G(2df,2p) relative energies, and values in braces correspond to CCSD(T)/aug-cc-pVTZ//QCISD/6-311+G(2df,2p) relative energies.

Table S3: Calculated values at different temperatures (T in K) of equilibrium constants (K_{eq} in $\text{cm}^3 \text{ molecule}^{-1}$), tunneling parameters, κ , unimolecular rate constants (k_2 in s^{-1}), rate constants (k_T in $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) for all elementary reactions between the different carbonyl oxides investigated and water monomer.

T	K_{eq}	κ	k_2	k_T
1 + H₂O TS1a ctst				
225.00	5.97e-19	1.48	1.76e+03	1.56e-15
230.00	4.41e-19	1.45	2.58e+03	1.65e-15
240.00	2.51e-19	1.40	5.24e+03	1.85e-15
250.00	1.50e-19	1.37	1.00e+04	2.06e-15
260.00	9.33e-20	1.34	1.82e+04	2.27e-15
270.00	6.03e-20	1.30	3.16e+04	2.48e-15
275.00	4.91e-20	1.29	4.10e+04	2.59e-15
280.00	4.03e-20	1.28	5.26e+04	2.70e-15
290.00	2.78e-20	1.26	8.43e+04	2.95e-15
298.00	2.10e-20	1.24	1.20e+05	3.13e-15
300.00	1.96e-20	1.24	1.31e+05	3.18e-15
310.00	1.42e-20	1.22	1.97e+05	3.41e-15
325.00	9.16e-21	1.19	3.46e+05	3.78e-15
1 + H₂O TS1b ctst				
225.00	5.97e-19	1.54	1.38e+02	1.27e-16
230.00	4.41e-19	1.51	2.10e+02	1.40e-16
240.00	2.51e-19	1.46	4.61e+02	1.68e-16
250.00	1.50e-19	1.41	9.47e+02	2.01e-16
260.00	9.33e-20	1.37	1.84e+03	2.35e-16
270.00	6.03e-20	1.34	3.38e+03	2.73e-16
275.00	4.91e-20	1.32	4.51e+03	2.93e-16
280.00	4.03e-20	1.31	5.95e+03	3.14e-16
290.00	2.78e-20	1.29	1.00e+04	3.59e-16
298.00	2.10e-20	1.26	1.49e+04	3.95e-16
300.00	1.96e-20	1.26	1.63e+04	4.04e-16
310.00	1.42e-20	1.25	2.57e+04	4.54e-16
325.00	9.16e-21	1.22	4.81e+04	5.37e-16
1 + H₂O TS1a ctst cbs				
225.00	1.91e-18	1.48	5.76e+02	1.63e-15
230.00	1.38e-18	1.45	8.63e+02	1.73e-15
240.00	7.48e-19	1.40	1.84e+03	1.93e-15
250.00	4.27e-19	1.36	3.67e+03	2.14e-15
260.00	2.55e-19	1.33	6.93e+03	2.35e-15
270.00	1.59e-19	1.30	1.25e+04	2.58e-15
275.00	1.27e-19	1.29	1.64e+04	2.69e-15
280.00	1.03e-19	1.28	2.14e+04	2.81e-15
290.00	6.85e-20	1.25	3.54e+04	3.04e-15
298.00	5.06e-20	1.24	5.16e+04	3.23e-15
300.00	4.70e-20	1.24	5.65e+04	3.28e-15
310.00	3.31e-20	1.21	8.74e+04	3.51e-15
325.00	2.05e-20	1.20	1.59e+05	3.92e-15
1 + H₂O TS1b ctst cbs				
225.00	1.91e-18	1.55	4.21e+01	1.25e-16

230.00	1.38e-18	1.52	6.58e+01	1.38e-16
240.00	7.48e-19	1.45	1.52e+02	1.65e-16
250.00	4.27e-19	1.41	3.26e+02	1.96e-16
260.00	2.55e-19	1.37	6.58e+02	2.30e-16
270.00	1.59e-19	1.34	1.26e+03	2.69e-16
275.00	1.27e-19	1.32	1.71e+03	2.87e-16
280.00	1.03e-19	1.31	2.29e+03	3.09e-16
290.00	6.85e-20	1.28	4.00e+03	3.52e-16
298.00	5.06e-20	1.27	6.07e+03	3.90e-16
300.00	4.70e-20	1.26	6.72e+03	3.99e-16
310.00	3.31e-20	1.24	1.09e+04	4.47e-16
325.00	2.05e-20	1.22	2.12e+04	5.29e-16

1 + H₂O TS1a vtst

225.00	5.97e-19	1.87	1.19e+03	1.33e-15
230.00	4.41e-19	1.82	1.75e+03	1.40e-15
240.00	2.51e-19	1.72	3.64e+03	1.57e-15
250.00	1.50e-19	1.64	7.12e+03	1.75e-15
260.00	9.33e-20	1.58	1.32e+04	1.94e-15
270.00	6.03e-20	1.53	2.32e+04	2.13e-15
275.00	4.91e-20	1.50	3.04e+04	2.23e-15
280.00	4.03e-20	1.48	3.93e+04	2.34e-15
290.00	2.78e-20	1.43	6.40e+04	2.55e-15
298.00	2.10e-20	1.41	9.22e+04	2.73e-15
300.00	1.96e-20	1.40	1.01e+05	2.76e-15
310.00	1.42e-20	1.36	1.54e+05	2.98e-15
325.00	9.16e-21	1.33	2.75e+05	3.34e-15

1 + H₂O TS1b vtst

225.00	5.97e-19	1.99	8.39e+01	9.97e-17
230.00	4.41e-19	1.94	1.29e+02	1.10e-16
240.00	2.51e-19	1.82	2.91e+02	1.33e-16
250.00	1.50e-19	1.73	6.13e+02	1.59e-16
260.00	9.33e-20	1.66	1.21e+03	1.88e-16
270.00	6.03e-20	1.59	2.28e+03	2.19e-16
275.00	4.91e-20	1.56	3.07e+03	2.36e-16
280.00	4.03e-20	1.54	4.09e+03	2.53e-16
290.00	2.78e-20	1.49	7.03e+03	2.92e-16
298.00	2.10e-20	1.47	1.05e+04	3.23e-16
300.00	1.96e-20	1.46	1.16e+04	3.31e-16
310.00	1.42e-20	1.41	1.86e+04	3.73e-16
325.00	9.16e-21	1.37	3.56e+04	4.46e-16

2 + H₂O TS1a ctst

225.00	5.98e-19	1.93	9.72e-02	1.12e-19
230.00	4.33e-19	1.85	1.77e-01	1.42e-19
240.00	2.37e-19	1.72	5.45e-01	2.22e-19
250.00	1.36e-19	1.63	1.53e+00	3.39e-19
260.00	8.19e-20	1.57	3.94e+00	5.05e-19
270.00	5.13e-20	1.51	9.47e+00	7.34e-19
275.00	4.11e-20	1.49	1.43e+01	8.75e-19
280.00	3.33e-20	1.46	2.13e+01	1.04e-18
290.00	2.23e-20	1.42	4.54e+01	1.44e-18

298.00	1.65e-20	1.40	8.00e+01	1.85e-18
300.00	1.54e-20	1.38	9.17e+01	1.96e-18
310.00	1.09e-20	1.36	1.77e+02	2.62e-18
325.00	6.78e-21	1.32	4.37e+02	3.91e-18
2 + H₂O TS1b ctst				
225.00	5.98e-19	2.13	5.30e-03	6.76e-21
230.00	4.33e-19	1.95	1.03e-02	8.70e-21
240.00	2.37e-19	1.76	3.57e-02	1.49e-20
250.00	1.36e-19	1.65	1.12e-01	2.52e-20
260.00	8.19e-20	1.58	3.21e-01	4.15e-20
270.00	5.13e-20	1.52	8.47e-01	6.62e-20
275.00	4.11e-20	1.50	1.34e+00	8.26e-20
280.00	3.33e-20	1.47	2.09e+00	1.02e-19
290.00	2.23e-20	1.43	4.82e+00	1.54e-19
298.00	1.65e-20	1.41	9.02e+00	2.10e-19
300.00	1.54e-20	1.40	1.05e+01	2.26e-19
310.00	1.09e-20	1.36	2.18e+01	3.24e-19
325.00	6.78e-21	1.32	5.95e+01	5.34e-19
2 + H₂O TS2a ctst				
225.00	5.98e-19	8560.61	1.32e-04	6.76e-19
230.00	4.33e-19	4404.33	2.77e-04	5.28e-19
240.00	2.37e-19	1354.55	1.10e-03	3.53e-19
250.00	1.36e-19	494.90	3.92e-03	2.64e-19
260.00	8.19e-20	214.29	1.26e-02	2.21e-19
270.00	5.13e-20	107.28	3.71e-02	2.04e-19
275.00	4.11e-20	79.74	6.17e-02	2.02e-19
280.00	3.33e-20	60.69	1.01e-01	2.04e-19
290.00	2.23e-20	38.24	2.55e-01	2.17e-19
298.00	1.65e-20	27.88	5.13e-01	2.36e-19
300.00	1.54e-20	25.99	6.08e-01	2.43e-19
310.00	1.09e-20	18.69	1.37e+00	2.79e-19
325.00	6.78e-21	12.66	4.18e+00	3.59e-19
2 + H₂O TS2b ctst				
225.00	5.98e-19	6649.75	1.97e-04	7.83e-19
230.00	4.33e-19	3480.39	4.08e-04	6.15e-19
240.00	2.37e-19	1087.50	1.60e-03	4.12e-19
250.00	1.36e-19	407.47	5.62e-03	3.11e-19
260.00	8.19e-20	180.34	1.78e-02	2.63e-19
270.00	5.13e-20	92.10	5.19e-02	2.45e-19
275.00	4.11e-20	68.95	8.60e-02	2.44e-19
280.00	3.33e-20	53.07	1.40e-01	2.47e-19
290.00	2.23e-20	33.90	3.51e-01	2.65e-19
298.00	1.65e-20	25.00	7.00e-01	2.89e-19
300.00	1.54e-20	23.34	8.27e-01	2.97e-19
310.00	1.09e-20	17.12	1.84e+00	3.43e-19
325.00	6.78e-21	11.72	5.57e+00	4.43e-19
2 + H₂O TS1a vtst				
225.00	5.98e-19	2.39	4.85e-02	6.94e-20
230.00	4.33e-19	2.29	9.00e-02	8.92e-20
240.00	2.37e-19	2.11	2.86e-01	1.43e-19

250.00	1.36e-19	1.98	8.25e-01	2.22e-19
260.00	8.19e-20	1.87	2.19e+00	3.35e-19
270.00	5.13e-20	1.77	5.41e+00	4.91e-19
275.00	4.11e-20	1.73	8.28e+00	5.88e-19
280.00	3.33e-20	1.69	1.25e+01	7.03e-19
290.00	2.23e-20	1.63	2.71e+01	9.86e-19
298.00	1.65e-20	1.58	4.86e+01	1.27e-18
300.00	1.54e-20	1.57	5.60e+01	1.36e-18
310.00	1.09e-20	1.53	1.10e+02	1.83e-18
325.00	6.78e-21	1.46	2.80e+02	2.78e-18

2 + H₂O TS1b vtst

225.00	5.98e-19	2.57	2.60e-03	3.99e-21
230.00	4.33e-19	2.45	5.14e-03	5.46e-21
240.00	2.37e-19	2.26	1.84e-02	9.84e-21
250.00	1.36e-19	2.10	5.95e-02	1.70e-20
260.00	8.19e-20	1.97	1.75e-01	2.83e-20
270.00	5.13e-20	1.87	4.75e-01	4.55e-20
275.00	4.11e-20	1.82	7.62e-01	5.71e-20
280.00	3.33e-20	1.77	1.20e+00	7.09e-20
290.00	2.23e-20	1.71	2.83e+00	1.08e-19
298.00	1.65e-20	1.65	5.40e+00	1.47e-19
300.00	1.54e-20	1.65	6.31e+00	1.60e-19
310.00	1.09e-20	1.59	1.33e+01	2.31e-19
325.00	6.78e-21	1.52	3.75e+01	3.86e-19

2 + H₂O TS2a vtst

225.00	5.98e-19	8089.43	1.23e-04	5.95e-19
230.00	4.33e-19	5155.04	2.58e-04	5.76e-19
240.00	2.37e-19	2320.39	1.03e-03	5.66e-19
250.00	1.36e-19	1149.46	3.68e-03	5.75e-19
260.00	8.19e-20	621.01	1.19e-02	6.05e-19
270.00	5.13e-20	361.82	3.51e-02	6.52e-19
275.00	4.11e-20	282.05	5.85e-02	6.78e-19
280.00	3.33e-20	223.62	9.57e-02	7.13e-19
290.00	2.23e-20	146.50	2.43e-01	7.94e-19
298.00	1.65e-20	107.55	4.90e-01	8.70e-19
300.00	1.54e-20	99.83	5.81e-01	8.93e-19
310.00	1.09e-20	70.99	1.31e+00	1.01e-18
325.00	6.78e-21	45.52	4.02e+00	1.24e-18

2 + H₂O TS2b vtst

225.00	5.98e-19	2886.36	1.76e-04	3.04e-19
230.00	4.33e-19	1899.18	3.67e-04	3.02e-19
240.00	2.37e-19	903.45	1.45e-03	3.10e-19
250.00	1.36e-19	473.58	5.11e-03	3.29e-19
260.00	8.19e-20	269.94	1.63e-02	3.60e-19
270.00	5.13e-20	165.20	4.77e-02	4.04e-19
275.00	4.11e-20	132.58	7.92e-02	4.32e-19
280.00	3.33e-20	106.98	1.29e-01	4.60e-19
290.00	2.23e-20	73.54	3.25e-01	5.33e-19
298.00	1.65e-20	55.91	6.51e-01	6.01e-19
300.00	1.54e-20	52.34	7.70e-01	6.21e-19

310.00	1.09e-20	38.84	1.72e+00	7.28e-19
325.00	6.78e-21	26.39	5.23e+00	9.36e-19
3 + H₂O TS1a ctst				
225.00	8.67e-18	1.96	2.24e+04	3.81e-13
230.00	5.92e-18	1.90	3.13e+04	3.52e-13
240.00	2.91e-18	1.78	5.85e+04	3.03e-13
250.00	1.51e-18	1.69	1.04e+05	2.66e-13
260.00	8.29e-19	1.63	1.75e+05	2.36e-13
270.00	4.77e-19	1.56	2.85e+05	2.12e-13
275.00	3.67e-19	1.53	3.58e+05	2.01e-13
280.00	2.86e-19	1.51	4.45e+05	1.92e-13
290.00	1.78e-19	1.47	6.75e+05	1.76e-13
298.00	1.25e-19	1.43	9.21e+05	1.65e-13
300.00	1.14e-19	1.43	9.93e+05	1.62e-13
310.00	7.59e-20	1.39	1.42e+06	1.50e-13
325.00	4.31e-20	1.35	2.34e+06	1.36e-13
3 + H₂O TS1b ctst				
225.00	8.67e-18	2.09	6.54e+03	1.19e-13
230.00	5.92e-18	2.02	9.42e+03	1.12e-13
240.00	2.91e-18	1.89	1.86e+04	1.02e-13
250.00	1.51e-18	1.78	3.48e+04	9.36e-14
260.00	8.29e-19	1.70	6.19e+04	8.70e-14
270.00	4.77e-19	1.63	1.05e+05	8.16e-14
275.00	3.67e-19	1.59	1.35e+05	7.89e-14
280.00	2.86e-19	1.56	1.72e+05	7.69e-14
290.00	1.78e-19	1.51	2.71e+05	7.30e-14
298.00	1.25e-19	1.48	3.81e+05	7.05e-14
300.00	1.14e-19	1.47	4.14e+05	6.94e-14
310.00	7.59e-20	1.43	6.14e+05	6.67e-14
325.00	4.31e-20	1.38	1.06e+06	6.29e-14
3 + H₂O TS1a vtst				
225.00	8.67e-18	2.23	9.11e+03	1.76e-13
230.00	5.92e-18	2.15	1.30e+04	1.65e-13
240.00	2.91e-18	2.00	2.53e+04	1.48e-13
250.00	1.51e-18	1.89	4.65e+04	1.33e-13
260.00	8.29e-19	1.80	8.15e+04	1.22e-13
270.00	4.77e-19	1.72	1.37e+05	1.12e-13
275.00	3.67e-19	1.69	1.74e+05	1.08e-13
280.00	2.86e-19	1.65	2.20e+05	1.04e-13
290.00	1.78e-19	1.60	3.43e+05	9.75e-14
298.00	1.25e-19	1.55	4.79e+05	9.30e-14
300.00	1.14e-19	1.54	5.19e+05	9.13e-14
310.00	7.59e-20	1.50	7.62e+05	8.65e-14
325.00	4.31e-20	1.45	1.29e+06	8.06e-14
3 + H₂O TS1b vtst				
225.00	8.67e-18	2.41	2.79e+03	5.83e-14
230.00	5.92e-18	2.32	4.10e+03	5.63e-14
240.00	2.91e-18	2.16	8.44e+03	5.30e-14
250.00	1.51e-18	2.01	1.64e+04	4.98e-14
260.00	8.29e-19	1.91	3.01e+04	4.76e-14

270.00	4.77e-19	1.82	5.28e+04	4.57e-14
275.00	3.67e-19	1.77	6.88e+04	4.48e-14
280.00	2.86e-19	1.73	8.88e+04	4.40e-14
290.00	1.78e-19	1.67	1.44e+05	4.27e-14
298.00	1.25e-19	1.62	2.07e+05	4.19e-14
300.00	1.14e-19	1.61	2.26e+05	4.15e-14
310.00	7.59e-20	1.56	3.43e+05	4.06e-14
325.00	4.31e-20	1.50	6.11e+05	3.94e-14
4 + H₂O TS1a ctst				
225.00	4.66e-18	3.23	4.33e-01	6.52e-18
230.00	3.20e-18	2.97	7.67e-01	7.30e-18
240.00	1.58e-18	2.61	2.24e+00	9.24e-18
250.00	8.29e-19	2.37	5.99e+00	1.18e-17
260.00	4.58e-19	2.20	1.48e+01	1.49e-17
270.00	2.65e-19	2.04	3.43e+01	1.86e-17
275.00	2.05e-19	1.98	5.09e+01	2.07e-17
280.00	1.60e-19	1.93	7.45e+01	2.30e-17
290.00	1.00e-19	1.84	1.53e+02	2.81e-17
298.00	7.04e-20	1.77	2.63e+02	3.28e-17
300.00	6.47e-20	1.76	3.00e+02	3.41e-17
310.00	4.31e-20	1.69	5.62e+02	4.09e-17
325.00	2.47e-20	1.60	1.34e+03	5.31e-17
4 + H₂O TS1b ctst				
225.00	4.66e-18	3.39	4.40e-02	6.94e-19
230.00	3.20e-18	3.05	8.23e-02	8.03e-19
240.00	1.58e-18	2.62	2.66e-01	1.10e-18
250.00	8.29e-19	2.36	7.79e-01	1.53e-18
260.00	4.58e-19	2.18	2.10e+00	2.10e-18
270.00	2.65e-19	2.04	5.25e+00	2.84e-18
275.00	2.05e-19	1.98	8.09e+00	3.28e-18
280.00	1.60e-19	1.92	1.23e+01	3.78e-18
290.00	1.00e-19	1.83	2.70e+01	4.94e-18
298.00	7.04e-20	1.76	4.89e+01	6.06e-18
300.00	6.47e-20	1.75	5.64e+01	6.38e-18
310.00	4.31e-20	1.68	1.12e+02	8.10e-18
325.00	2.47e-20	1.59	2.90e+02	1.14e-17
4 + H₂O TS2a ctst				
225.00	4.66e-18	6512.61	1.19e-04	3.61e-18
230.00	3.20e-18	3364.71	2.55e-04	2.75e-18
240.00	1.58e-18	1037.74	1.06e-03	1.74e-18
250.00	8.29e-19	385.79	3.94e-03	1.26e-18
260.00	4.58e-19	170.45	1.32e-02	1.03e-18
270.00	2.65e-19	87.84	4.03e-02	9.38e-19
275.00	2.05e-19	66.03	6.83e-02	9.25e-19
280.00	1.60e-19	50.88	1.14e-01	9.28e-19
290.00	1.00e-19	32.79	2.97e-01	9.74e-19
298.00	7.04e-20	24.35	6.12e-01	1.05e-18
300.00	6.47e-20	22.63	7.29e-01	1.07e-18
310.00	4.31e-20	16.69	1.69e+00	1.22e-18
325.00	2.47e-20	11.49	5.37e+00	1.52e-18

4 + H₂O TS2b ctst				
225.00	4.66e-18	7268.45	6.37e-05	2.16e-18
230.00	3.20e-18	3722.63	1.37e-04	1.63e-18
240.00	1.58e-18	1132.87	5.72e-04	1.02e-18
250.00	8.29e-19	415.02	2.13e-03	7.33e-19
260.00	4.58e-19	181.82	7.15e-03	5.95e-19
270.00	2.65e-19	92.24	2.19e-02	5.35e-19
275.00	2.05e-19	69.00	3.71e-02	5.25e-19
280.00	1.60e-19	53.07	6.18e-02	5.25e-19
290.00	1.00e-19	33.83	1.62e-01	5.48e-19
298.00	7.04e-20	25.00	3.34e-01	5.88e-19
300.00	6.47e-20	23.32	3.98e-01	6.00e-19
310.00	4.31e-20	17.14	9.22e-01	6.81e-19
325.00	2.47e-20	11.66	2.95e+00	8.50e-19
4 + H₂O TS1a vtst				
225.00	4.66e-18	2.74	1.61e-01	2.06e-18
230.00	3.20e-18	2.61	2.92e-01	2.44e-18
240.00	1.58e-18	2.39	8.90e-01	3.37e-18
250.00	8.29e-19	2.22	2.48e+00	4.57e-18
260.00	4.58e-19	2.09	6.36e+00	6.09e-18
270.00	2.65e-19	1.97	1.52e+01	7.92e-18
275.00	2.05e-19	1.92	2.29e+01	9.02e-18
280.00	1.60e-19	1.87	3.41e+01	1.02e-17
290.00	1.00e-19	1.78	7.23e+01	1.29e-17
298.00	7.04e-20	1.73	1.27e+02	1.55e-17
300.00	6.47e-20	1.72	1.45e+02	1.62e-17
310.00	4.31e-20	1.65	2.80e+02	2.00e-17
325.00	2.47e-20	1.58	6.89e+02	2.69e-17
4 + H₂O TS1b vtst				
225.00	4.66e-18	3.96	1.67e-02	3.08e-19
230.00	3.20e-18	3.69	3.20e-02	3.78e-19
240.00	1.58e-18	3.29	1.08e-01	5.61e-19
250.00	8.29e-19	2.97	3.30e-01	8.12e-19
260.00	4.58e-19	2.72	9.23e-01	1.15e-18
270.00	2.65e-19	2.51	2.39e+00	1.59e-18
275.00	2.05e-19	2.43	3.74e+00	1.86e-18
280.00	1.60e-19	2.34	5.77e+00	2.16e-18
290.00	1.00e-19	2.21	1.31e+01	2.89e-18
298.00	7.04e-20	2.11	2.42e+01	3.60e-18
300.00	6.47e-20	2.09	2.81e+01	3.79e-18
310.00	4.31e-20	1.99	5.73e+01	4.91e-18
325.00	2.47e-20	1.86	1.54e+02	7.06e-18
4 + H₂O TS2a vtst				
225.00	4.66e-18	8343.69	9.66e-05	3.76e-18
230.00	3.20e-18	5288.46	2.08e-04	3.52e-18
240.00	1.58e-18	2342.14	8.71e-04	3.22e-18
250.00	8.29e-19	1147.69	3.25e-03	3.09e-18
260.00	4.58e-19	612.84	1.09e-02	3.06e-18
270.00	2.65e-19	348.21	3.36e-02	3.10e-18
275.00	2.05e-19	270.18	5.70e-02	3.16e-18

280.00	1.60e-19	212.63	9.50e-02	3.23e-18
290.00	1.00e-19	136.40	2.50e-01	3.41e-18
298.00	7.04e-20	99.22	5.16e-01	3.60e-18
300.00	6.47e-20	92.03	6.15e-01	3.66e-18
310.00	4.31e-20	64.41	1.43e+00	3.97e-18
325.00	2.47e-20	40.48	4.57e+00	4.57e-18
4 + H₂O TS2b vtst				
225.00	4.66e-18	4692.83	5.86e-05	1.28e-18
230.00	3.20e-18	2992.06	1.26e-04	1.21e-18
240.00	1.58e-18	1332.70	5.29e-04	1.11e-18
250.00	8.29e-19	656.57	1.98e-03	1.08e-18
260.00	4.58e-19	357.89	6.65e-03	1.09e-18
270.00	2.65e-19	208.82	2.04e-02	1.13e-18
275.00	2.05e-19	163.11	3.47e-02	1.16e-18
280.00	1.60e-19	129.76	5.78e-02	1.20e-18
290.00	1.00e-19	85.53	1.52e-01	1.30e-18
298.00	7.04e-20	63.06	3.14e-01	1.39e-18
300.00	6.47e-20	58.82	3.74e-01	1.42e-18
310.00	4.31e-20	42.17	8.68e-01	1.58e-18
325.00	2.47e-20	27.45	2.78e+00	1.88e-18
5 + H₂O TS1a ctst				
225.00	4.81e-19	16.27	3.81e-03	2.98e-20
230.00	3.51e-19	11.95	7.43e-03	3.12e-20
240.00	1.95e-19	7.72	2.59e-02	3.90e-20
250.00	1.13e-19	5.77	8.18e-02	5.33e-20
260.00	6.91e-20	4.70	2.36e-01	7.67e-20
270.00	4.38e-20	3.99	6.27e-01	1.09e-19
275.00	3.53e-20	3.72	9.96e-01	1.31e-19
280.00	2.87e-20	3.52	1.55e+00	1.56e-19
290.00	1.94e-20	3.16	3.61e+00	2.21e-19
298.00	1.45e-20	2.91	6.81e+00	2.87e-19
300.00	1.35e-20	2.86	7.94e+00	3.06e-19
310.00	9.66e-21	2.64	1.65e+01	4.21e-19
325.00	6.08e-21	2.39	4.57e+01	6.63e-19
5 + H₂O TS1b ctst				
225.00	4.81e-19	27.20	1.18e-04	1.54e-21
230.00	3.51e-19	17.02	2.48e-04	1.48e-21
240.00	1.95e-19	8.87	9.97e-04	1.72e-21
250.00	1.13e-19	6.05	3.57e-03	2.44e-21
260.00	6.91e-20	4.74	1.16e-02	3.80e-21
270.00	4.38e-20	3.98	3.44e-02	6.00e-21
275.00	3.53e-20	3.72	5.76e-02	7.55e-21
280.00	2.87e-20	3.48	9.45e-02	9.44e-21
290.00	1.94e-20	3.12	2.41e-01	1.46e-20
298.00	1.45e-20	2.89	4.88e-01	2.04e-20
300.00	1.35e-20	2.83	5.79e-01	2.21e-20
310.00	9.66e-21	2.62	1.31e+00	3.31e-20
325.00	6.08e-21	2.36	4.06e+00	5.82e-20
5 + H₂O TS2a ctst				
225.00	4.81e-19	18863.64	2.20e-06	2.00e-20

230.00	3.51e-19	9009.90	5.05e-06	1.60e-20
240.00	1.95e-19	2387.50	2.40e-05	1.12e-20
250.00	1.13e-19	778.00	1.00e-04	8.79e-21
260.00	6.91e-20	304.00	3.75e-04	7.88e-21
270.00	4.38e-20	141.73	1.27e-03	7.88e-21
275.00	3.53e-20	102.21	2.26e-03	8.15e-21
280.00	2.87e-20	76.34	3.93e-03	8.61e-21
290.00	1.94e-20	45.75	1.13e-02	1.00e-20
298.00	1.45e-20	32.66	2.48e-02	1.17e-20
300.00	1.35e-20	30.27	3.00e-02	1.23e-20
310.00	9.66e-21	21.36	7.49e-02	1.55e-20
325.00	6.08e-21	14.06	2.66e-01	2.27e-20

5 + H₂O TS2b ctst

225.00	4.81e-19	17798.74	3.18e-06	2.72e-20
230.00	3.51e-19	8577.35	7.24e-06	2.18e-20
240.00	1.95e-19	2312.68	3.39e-05	1.53e-20
250.00	1.13e-19	769.78	1.39e-04	1.21e-20
260.00	6.91e-20	303.50	5.14e-04	1.08e-20
270.00	4.38e-20	142.44	1.72e-03	1.07e-20
275.00	3.53e-20	103.29	3.04e-03	1.11e-20
280.00	2.87e-20	77.00	5.26e-03	1.16e-20
290.00	1.94e-20	46.51	1.49e-02	1.34e-20
298.00	1.45e-20	33.23	3.25e-02	1.57e-20
300.00	1.35e-20	30.61	3.92e-02	1.62e-20
310.00	9.66e-21	21.75	9.70e-02	2.04e-20
325.00	6.08e-21	14.28	3.39e-01	2.94e-20

6 + H₂O TS1a ctst

225.00	9.30e-19	5.70	5.63e-02	2.99e-19
230.00	6.74e-19	4.93	1.02e-01	3.39e-19
240.00	3.70e-19	3.97	3.10e-01	4.55e-19
250.00	2.14e-19	3.40	8.58e-01	6.25e-19
260.00	1.29e-19	3.00	2.20e+00	8.53e-19
270.00	8.11e-20	2.71	5.24e+00	1.15e-18
275.00	6.52e-20	2.60	7.89e+00	1.34e-18
280.00	5.28e-20	2.50	1.17e+01	1.54e-18
290.00	3.55e-20	2.31	2.48e+01	2.04e-18
298.00	2.64e-20	2.20	4.34e+01	2.52e-18
300.00	2.46e-20	2.17	4.97e+01	2.66e-18
310.00	1.74e-20	2.05	9.54e+01	3.41e-18
325.00	1.09e-20	1.90	2.35e+02	4.87e-18

6 + H₂O TS1b ctst

225.00	9.30e-19	13.53	1.70e-03	2.14e-20
230.00	6.74e-19	10.09	3.31e-03	2.25e-20
240.00	3.70e-19	6.69	1.15e-02	2.85e-20
250.00	2.14e-19	5.14	3.60e-02	3.96e-20
260.00	1.29e-19	4.25	1.03e-01	5.65e-20
270.00	8.11e-20	3.66	2.73e-01	8.10e-20
275.00	6.52e-20	3.44	4.33e-01	9.71e-20
280.00	5.28e-20	3.23	6.74e-01	1.15e-19
290.00	3.55e-20	2.93	1.56e+00	1.62e-19

298.00	2.64e-20	2.73	2.93e+00	2.11e-19
300.00	2.46e-20	2.69	3.41e+00	2.25e-19
310.00	1.74e-20	2.49	7.08e+00	3.06e-19
325.00	1.09e-20	2.26	1.94e+01	4.79e-19
6 + H₂O TS2a ctst				
225.00	9.30e-19	11010.64	1.88e-05	1.93e-19
230.00	6.74e-19	5555.56	4.05e-05	1.52e-19
240.00	3.70e-19	1623.53	1.70e-04	1.02e-19
250.00	2.14e-19	570.08	6.35e-04	7.75e-20
260.00	1.29e-19	238.32	2.14e-03	6.58e-20
270.00	8.11e-20	116.44	6.57e-03	6.20e-20
275.00	6.52e-20	85.27	1.12e-02	6.23e-20
280.00	5.28e-20	65.05	1.86e-02	6.39e-20
290.00	3.55e-20	40.08	4.89e-02	6.96e-20
298.00	2.64e-20	29.11	1.01e-01	7.76e-20
300.00	2.46e-20	27.08	1.20e-01	8.00e-20
310.00	1.74e-20	19.39	2.80e-01	9.45e-20
325.00	1.09e-20	12.96	8.95e-01	1.26e-19
6 + H₂O TS2b ctst				
225.00	9.30e-19	9776.95	2.69e-05	2.45e-19
230.00	6.74e-19	4965.16	5.74e-05	1.92e-19
240.00	3.70e-19	1485.23	2.37e-04	1.30e-19
250.00	2.14e-19	533.33	8.70e-04	9.93e-20
260.00	1.29e-19	226.64	2.89e-03	8.45e-20
270.00	8.11e-20	112.36	8.74e-03	7.96e-20
275.00	6.52e-20	82.99	1.47e-02	7.95e-20
280.00	5.28e-20	63.11	2.44e-02	8.13e-20
290.00	3.55e-20	39.43	6.34e-02	8.87e-20
298.00	2.64e-20	28.62	1.30e-01	9.82e-20
300.00	2.46e-20	26.69	1.54e-01	1.01e-19
310.00	1.74e-20	19.27	3.54e-01	1.19e-19
325.00	1.09e-20	12.86	1.12e+00	1.57e-19
7 + H₂O TS1a ctst				
225.00	1.91e-19	4.15	1.82e-01	1.44e-19
230.00	1.49e-19	3.77	3.13e-01	1.76e-19
240.00	9.47e-20	3.21	8.65e-01	2.63e-19
250.00	6.25e-20	2.84	2.20e+00	3.91e-19
260.00	4.27e-20	2.58	5.20e+00	5.72e-19
270.00	3.01e-20	2.37	1.15e+01	8.19e-19
275.00	2.55e-20	2.27	1.68e+01	9.74e-19
280.00	2.18e-20	2.21	2.40e+01	1.16e-18
290.00	1.62e-20	2.07	4.77e+01	1.60e-18
298.00	1.29e-20	1.98	7.97e+01	2.04e-18
300.00	1.23e-20	1.96	9.02e+01	2.18e-18
310.00	9.49e-21	1.87	1.64e+02	2.90e-18
325.00	6.69e-21	1.75	3.73e+02	4.38e-18
7 + H₂O TS1b ctst				
225.00	1.91e-19	4.57	1.25e-01	1.09e-19
230.00	1.49e-19	4.09	2.17e-01	1.32e-19
240.00	9.47e-20	3.44	6.10e-01	1.99e-19

250.00	6.25e-20	3.01	1.58e+00	2.98e-19
260.00	4.27e-20	2.72	3.78e+00	4.40e-19
270.00	3.01e-20	2.48	8.50e+00	6.35e-19
275.00	2.55e-20	2.40	1.24e+01	7.57e-19
280.00	2.18e-20	2.29	1.80e+01	9.00e-19
290.00	1.62e-20	2.15	3.61e+01	1.26e-18
298.00	1.29e-20	2.05	6.09e+01	1.61e-18
300.00	1.23e-20	2.03	6.91e+01	1.72e-18
310.00	9.49e-21	1.92	1.27e+02	2.32e-18
325.00	6.69e-21	1.80	2.93e+02	3.53e-18

8 + H₂O TS1a ctst

225.00	8.07e-19	8.05	2.36e-01	1.53e-18
230.00	5.89e-19	6.78	4.16e-01	1.66e-18
240.00	3.28e-19	5.25	1.19e+00	2.05e-18
250.00	1.91e-19	4.32	3.15e+00	2.60e-18
260.00	1.17e-19	3.70	7.70e+00	3.33e-18
270.00	7.42e-20	3.26	1.76e+01	4.26e-18
275.00	5.99e-20	3.10	2.59e+01	4.81e-18
280.00	4.88e-20	2.94	3.78e+01	5.42e-18
290.00	3.31e-20	2.69	7.69e+01	6.85e-18
298.00	2.48e-20	2.53	1.31e+02	8.21e-18
300.00	2.31e-20	2.49	1.49e+02	8.57e-18
310.00	1.65e-20	2.32	2.77e+02	1.06e-17
325.00	1.04e-20	2.14	6.51e+02	1.45e-17

8 + H₂O TS1b ctst

225.00	8.07e-19	6.31	4.15e-01	2.11e-18
230.00	5.89e-19	5.50	7.15e-01	2.31e-18
240.00	3.28e-19	4.41	1.98e+00	2.86e-18
250.00	1.91e-19	3.75	5.02e+00	3.59e-18
260.00	1.17e-19	3.27	1.19e+01	4.55e-18
270.00	7.42e-20	2.94	2.62e+01	5.72e-18
275.00	5.99e-20	2.81	3.81e+01	6.41e-18
280.00	4.88e-20	2.67	5.47e+01	7.12e-18
290.00	3.31e-20	2.48	1.08e+02	8.87e-18
298.00	2.48e-20	2.33	1.81e+02	1.05e-17
300.00	2.31e-20	2.30	2.05e+02	1.09e-17
310.00	1.65e-20	2.17	3.71e+02	1.33e-17
325.00	1.04e-20	2.00	8.43e+02	1.76e-17

9 + H₂O TS1a ctst

225.00	8.07e-19	8.05	2.36e-01	1.53e-18
230.00	5.89e-19	6.78	4.16e-01	1.66e-18
240.00	3.28e-19	5.25	1.19e+00	2.05e-18
250.00	1.91e-19	4.32	3.15e+00	2.60e-18
260.00	1.17e-19	3.70	7.70e+00	3.33e-18
270.00	7.42e-20	3.26	1.76e+01	4.26e-18
275.00	5.99e-20	3.10	2.59e+01	4.81e-18
280.00	4.88e-20	2.94	3.78e+01	5.42e-18
290.00	3.31e-20	2.69	7.69e+01	6.85e-18
298.00	2.48e-20	2.53	1.31e+02	8.21e-18
300.00	2.31e-20	2.49	1.49e+02	8.57e-18

310.00	1.65e-20	2.32	2.77e+02	1.06e-17
325.00	1.04e-20	2.14	6.51e+02	1.45e-17
9 + H₂O TS1b ctst				
225.00	8.07e-19	6.31	4.15e-01	2.11e-18
230.00	5.89e-19	5.50	7.15e-01	2.31e-18
240.00	3.28e-19	4.41	1.98e+00	2.86e-18
250.00	1.91e-19	3.75	5.02e+00	3.59e-18
260.00	1.17e-19	3.27	1.19e+01	4.55e-18
270.00	7.42e-20	2.94	2.62e+01	5.72e-18
275.00	5.99e-20	2.81	3.81e+01	6.41e-18
280.00	4.88e-20	2.67	5.47e+01	7.12e-18
290.00	3.31e-20	2.48	1.08e+02	8.87e-18
298.00	2.48e-20	2.33	1.81e+02	1.05e-17
300.00	2.31e-20	2.30	2.05e+02	1.09e-17
310.00	1.65e-20	2.17	3.71e+02	1.33e-17
325.00	1.04e-20	2.00	8.43e+02	1.76e-17
10 + H₂O TS1a ctst				
225.00	2.14e-19	3.07	7.48e-01	4.92e-19
230.00	1.58e-19	2.85	1.30e+00	5.85e-19
240.00	9.01e-20	2.53	3.64e+00	8.30e-19
250.00	5.37e-20	2.30	9.38e+00	1.16e-18
260.00	3.34e-20	2.14	2.24e+01	1.60e-18
270.00	2.16e-20	2.01	5.02e+01	2.18e-18
275.00	1.76e-20	1.95	7.34e+01	2.52e-18
280.00	1.44e-20	1.90	1.06e+02	2.89e-18
290.00	9.93e-21	1.80	2.12e+02	3.79e-18
298.00	7.51e-21	1.74	3.56e+02	4.66e-18
300.00	7.02e-21	1.73	4.04e+02	4.90e-18
310.00	5.09e-21	1.67	7.38e+02	6.26e-18
325.00	3.27e-21	1.58	1.70e+03	8.80e-18
10 + H₂O TS1b ctst				
225.00	2.14e-19	2.55	3.43e-01	1.87e-19
230.00	1.58e-19	2.40	6.01e-01	2.28e-19
240.00	9.01e-20	2.17	1.72e+00	3.37e-19
250.00	5.37e-20	2.02	4.51e+00	4.89e-19
260.00	3.34e-20	1.89	1.10e+01	6.95e-19
270.00	2.16e-20	1.80	2.49e+01	9.68e-19
275.00	1.76e-20	1.75	3.67e+01	1.13e-18
280.00	1.44e-20	1.72	5.33e+01	1.32e-18
290.00	9.93e-21	1.65	1.08e+02	1.77e-18
298.00	7.51e-21	1.60	1.84e+02	2.21e-18
300.00	7.02e-21	1.59	2.09e+02	2.33e-18
310.00	5.09e-21	1.54	3.86e+02	3.02e-18
325.00	3.27e-21	1.48	9.01e+02	4.35e-18
11 + H₂O TS1a ctst				
225.00	3.97e-20	2.68	5.79e-02	6.15e-21
230.00	3.22e-20	2.50	1.01e-01	8.15e-21
240.00	2.17e-20	2.27	2.85e-01	1.40e-20
250.00	1.52e-20	2.10	7.39e-01	2.36e-20
260.00	1.09e-20	1.96	1.78e+00	3.79e-20

270.00	8.08e-21	1.85	4.00e+00	5.98e-20
275.00	7.01e-21	1.81	5.87e+00	7.43e-20
280.00	6.12e-21	1.76	8.48e+00	9.12e-20
290.00	4.74e-21	1.69	1.70e+01	1.37e-19
298.00	3.92e-21	1.64	2.88e+01	1.85e-19
300.00	3.74e-21	1.63	3.26e+01	1.99e-19
310.00	3.01e-21	1.57	5.99e+01	2.83e-19
325.00	2.23e-21	1.51	1.38e+02	4.64e-19

11 + H₂O TS1b ctst

225.00	3.97e-20	3.08	6.94e-03	8.50e-22
230.00	3.22e-20	2.81	1.27e-02	1.15e-21
240.00	2.17e-20	2.45	3.96e-02	2.11e-21
250.00	1.52e-20	2.23	1.12e-01	3.80e-21
260.00	1.09e-20	2.08	2.92e-01	6.61e-21
270.00	8.08e-21	1.95	7.08e-01	1.12e-20
275.00	7.01e-21	1.91	1.07e+00	1.43e-20
280.00	6.12e-21	1.84	1.61e+00	1.82e-20
290.00	4.74e-21	1.76	3.44e+00	2.88e-20
298.00	3.92e-21	1.70	6.10e+00	4.08e-20
300.00	3.74e-21	1.68	7.01e+00	4.41e-20
310.00	3.01e-21	1.63	1.36e+01	6.65e-20
325.00	2.23e-21	1.55	3.40e+01	1.18e-19

12 + H₂O TS1a ctst

225.00	2.10e-18	3.04	3.03e+03	1.94e-14
230.00	1.53e-18	2.87	4.25e+03	1.87e-14
240.00	8.42e-19	2.58	8.00e+03	1.73e-14
250.00	4.89e-19	2.36	1.43e+04	1.65e-14
260.00	2.97e-19	2.19	2.43e+04	1.58e-14
270.00	1.88e-19	2.05	3.97e+04	1.53e-14
275.00	1.51e-19	1.99	5.01e+04	1.50e-14
280.00	1.23e-19	1.93	6.26e+04	1.49e-14
290.00	8.28e-20	1.84	9.53e+04	1.45e-14
298.00	6.17e-20	1.77	1.31e+05	1.43e-14
300.00	5.75e-20	1.76	1.41e+05	1.43e-14
310.00	4.10e-20	1.69	2.03e+05	1.41e-14
325.00	2.57e-20	1.60	3.36e+05	1.39e-14

12 + H₂O TS1b ctst

225.00	2.10e-18	4.73	2.02e+02	2.01e-15
230.00	1.53e-18	4.30	3.02e+02	1.99e-15
240.00	8.42e-19	3.65	6.41e+02	1.97e-15
250.00	4.89e-19	3.20	1.28e+03	2.00e-15
260.00	2.97e-19	2.88	2.41e+03	2.06e-15
270.00	1.88e-19	2.60	4.34e+03	2.12e-15
275.00	1.51e-19	2.52	5.72e+03	2.17e-15
280.00	1.23e-19	2.41	7.46e+03	2.21e-15
290.00	8.28e-20	2.26	1.23e+04	2.30e-15
298.00	6.17e-20	2.14	1.80e+04	2.38e-15
300.00	5.75e-20	2.12	1.97e+04	2.40e-15
310.00	4.10e-20	2.01	3.05e+04	2.51e-15
325.00	2.57e-20	1.86	5.58e+04	2.67e-15

Table S4: Calculated values at different temperatures (T in K) of equilibrium constants (K_{eq} in $\text{cm}^3 \text{ molecule}^{-1}$), tunneling parameters, κ , unimolecular rate constants (k_2 in s^{-1}), rate constants (k_T in $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) for all elementary reactions between the different carbonyl oxides investigated and water dimer.

T	K_{eq}	κ	k_2	k_T
1 + (H₂O)₂ TS1a ctst				
225.00	4.18e-17	1.24	1.19e+08	6.14e-09
230.00	2.45e-17	1.23	1.36e+08	4.09e-09
240.00	9.05e-18	1.20	1.76e+08	1.92e-09
250.00	3.62e-18	1.18	2.22e+08	9.52e-10
260.00	1.56e-18	1.17	2.73e+08	4.99e-10
270.00	7.13e-19	1.15	3.31e+08	2.72e-10
275.00	4.93e-19	1.15	3.61e+08	2.05e-10
280.00	3.46e-19	1.15	3.93e+08	1.56e-10
290.00	1.77e-19	1.13	4.61e+08	9.26e-11
298.00	1.07e-19	1.13	5.19e+08	6.25e-11
300.00	9.45e-20	1.12	5.34e+08	5.67e-11
310.00	5.27e-20	1.11	6.11e+08	3.59e-11
325.00	2.35e-20	1.10	7.33e+08	1.90e-11
1 + (H₂O)₂ TS1b ctst				
225.00	4.27e-17	1.23	1.95e+08	1.02e-08
230.00	2.48e-17	1.22	2.23e+08	6.72e-09
240.00	8.97e-18	1.19	2.87e+08	3.07e-09
250.00	3.52e-18	1.18	3.59e+08	1.49e-09
260.00	1.49e-18	1.16	4.41e+08	7.63e-10
270.00	6.72e-19	1.15	5.32e+08	4.10e-10
275.00	4.61e-19	1.14	5.80e+08	3.06e-10
280.00	3.21e-19	1.14	6.31e+08	2.30e-10
290.00	1.62e-19	1.13	7.37e+08	1.34e-10
298.00	9.67e-20	1.12	8.27e+08	8.95e-11
300.00	8.54e-20	1.12	8.50e+08	8.11e-11
310.00	4.70e-20	1.11	9.70e+08	5.08e-11
325.00	2.07e-20	1.09	1.16e+09	2.63e-11
1 + (H₂O)₂ TS1c ctst				
225.00	2.62e-17	1.32	2.16e+07	7.49e-10
230.00	1.56e-17	1.31	2.55e+07	5.23e-10
240.00	5.90e-18	1.28	3.49e+07	2.64e-10
250.00	2.42e-18	1.25	4.64e+07	1.41e-10
260.00	1.06e-18	1.23	6.01e+07	7.84e-11
270.00	4.96e-19	1.21	7.60e+07	4.57e-11
275.00	3.47e-19	1.20	8.49e+07	3.54e-11
280.00	2.45e-19	1.20	9.43e+07	2.77e-11
290.00	1.28e-19	1.18	1.15e+08	1.74e-11
298.00	7.81e-20	1.17	1.33e+08	1.22e-11
300.00	6.94e-20	1.17	1.38e+08	1.12e-11
310.00	3.93e-20	1.15	1.63e+08	7.39e-12
325.00	1.79e-20	1.14	2.05e+08	4.17e-12

$1 + (\text{H}_2\text{O})_2$ TS1d ctst				
225.00	4.45e-17	1.27	1.33e+08	7.52e-09
230.00	2.58e-17	1.25	1.54e+08	4.95e-09
240.00	9.23e-18	1.22	2.01e+08	2.27e-09
250.00	3.60e-18	1.21	2.55e+08	1.11e-09
260.00	1.51e-18	1.19	3.17e+08	5.69e-10
270.00	6.76e-19	1.17	3.87e+08	3.07e-10
275.00	4.63e-19	1.16	4.25e+08	2.29e-10
280.00	3.21e-19	1.16	4.64e+08	1.73e-10
290.00	1.61e-19	1.15	5.48e+08	1.01e-10
298.00	9.58e-20	1.14	6.20e+08	6.77e-11
300.00	8.45e-20	1.14	6.39e+08	6.14e-11
310.00	4.63e-20	1.13	7.35e+08	3.84e-11
325.00	2.02e-20	1.12	8.90e+08	2.01e-11
$1 + (\text{H}_2\text{O})_2$ TS1a ctst CBS				
225.00	2.00e-16	1.24	4.35e+07	1.08e-08
230.00	1.14e-16	1.23	5.10e+07	7.13e-09
240.00	3.93e-17	1.21	6.85e+07	3.25e-09
250.00	1.48e-17	1.18	8.96e+07	1.57e-09
260.00	6.04e-18	1.18	1.14e+08	8.09e-10
270.00	2.63e-18	1.15	1.43e+08	4.34e-10
275.00	1.78e-18	1.15	1.59e+08	3.26e-10
280.00	1.22e-18	1.15	1.75e+08	2.45e-10
290.00	5.96e-19	1.14	2.11e+08	1.43e-10
298.00	3.48e-19	1.13	2.43e+08	9.54e-11
300.00	3.06e-19	1.12	2.51e+08	8.63e-11
310.00	1.64e-19	1.12	2.94e+08	5.38e-11
325.00	6.96e-20	1.10	3.65e+08	2.80e-11
$1 + (\text{H}_2\text{O})_2$ TS1b ctst CBS				
225.00	1.96e-16	1.23	7.46e+07	1.79e-08
230.00	1.10e-16	1.22	8.72e+07	1.17e-08
240.00	3.74e-17	1.20	1.16e+08	5.20e-09
250.00	1.39e-17	1.18	1.51e+08	2.47e-09
260.00	5.56e-18	1.16	1.92e+08	1.24e-09
270.00	2.39e-18	1.15	2.39e+08	6.55e-10
275.00	1.60e-18	1.14	2.64e+08	4.83e-10
280.00	1.09e-18	1.14	2.91e+08	3.61e-10
290.00	5.27e-19	1.13	3.50e+08	2.08e-10
298.00	3.05e-19	1.12	4.00e+08	1.37e-10
300.00	2.67e-19	1.12	4.13e+08	1.23e-10
310.00	1.42e-19	1.11	4.83e+08	7.61e-11
325.00	5.92e-20	1.10	5.96e+08	3.88e-11
$1 + (\text{H}_2\text{O})_2$ TS1c ctst CBS				
225.00	1.18e-16	1.33	6.45e+06	1.01e-09
230.00	6.77e-17	1.31	7.84e+06	6.97e-10
240.00	2.41e-17	1.28	1.13e+07	3.49e-10
250.00	9.32e-18	1.26	1.56e+07	1.84e-10
260.00	3.89e-18	1.24	2.11e+07	1.02e-10
270.00	1.73e-18	1.22	2.78e+07	5.85e-11
275.00	1.18e-18	1.21	3.16e+07	4.50e-11

280.00	8.19e-19	1.20	3.57e+07	3.51e-11
290.00	4.08e-19	1.18	4.50e+07	2.17e-11
298.00	2.42e-19	1.17	5.35e+07	1.52e-11
300.00	2.14e-19	1.17	5.57e+07	1.40e-11
310.00	1.17e-19	1.16	6.78e+07	9.18e-12
325.00	5.07e-20	1.14	8.87e+07	5.12e-12

1 + (H₂O)₂ TS1d ctst CBS

225.00	2.04e-16	1.27	4.36e+07	1.13e-08
230.00	1.14e-16	1.26	5.15e+07	7.38e-09
240.00	3.85e-17	1.23	7.03e+07	3.33e-09
250.00	1.42e-17	1.21	9.33e+07	1.60e-09
260.00	5.63e-18	1.19	1.21e+08	8.11e-10
270.00	2.40e-18	1.18	1.52e+08	4.30e-10
275.00	1.61e-18	1.17	1.70e+08	3.20e-10
280.00	1.09e-18	1.16	1.89e+08	2.40e-10
290.00	5.24e-19	1.15	2.30e+08	1.39e-10
298.00	3.02e-19	1.14	2.67e+08	9.18e-11
300.00	2.65e-19	1.14	2.76e+08	8.35e-11
310.00	1.40e-19	1.13	3.27e+08	5.17e-11
325.00	5.79e-20	1.12	4.10e+08	2.65e-11

1 + (H₂O)₂ TS1a vtst

225.00	4.18e-17	1.26	7.00e+07	3.69e-09
230.00	2.45e-17	1.25	8.19e+07	2.50e-09
240.00	9.05e-18	1.22	1.10e+08	1.21e-09
250.00	3.62e-18	1.20	1.43e+08	6.19e-10
260.00	1.56e-18	1.18	1.82e+08	3.34e-10
270.00	7.13e-19	1.16	2.26e+08	1.87e-10
275.00	4.93e-19	1.15	2.51e+08	1.42e-10
280.00	3.46e-19	1.14	2.77e+08	1.09e-10
290.00	1.77e-19	1.13	3.33e+08	6.66e-11
298.00	1.07e-19	1.12	3.82e+08	4.58e-11
300.00	9.45e-20	1.12	3.95e+08	4.17e-11
310.00	5.27e-20	1.11	4.62e+08	2.70e-11
325.00	2.35e-20	1.09	5.72e+08	1.47e-11

1 + (H₂O)₂ TS1b vtst

225.00	4.27e-17	1.25	1.14e+08	6.11e-09
230.00	2.48e-17	1.24	1.33e+08	4.09e-09
240.00	8.97e-18	1.21	1.77e+08	1.93e-09
250.00	3.52e-18	1.20	2.29e+08	9.64e-10
260.00	1.49e-18	1.18	2.91e+08	5.10e-10
270.00	6.72e-19	1.16	3.61e+08	2.81e-10
275.00	4.61e-19	1.15	3.99e+08	2.12e-10
280.00	3.21e-19	1.14	4.40e+08	1.61e-10
290.00	1.62e-19	1.13	5.28e+08	9.67e-11
298.00	9.67e-20	1.12	6.04e+08	6.56e-11
300.00	8.54e-20	1.12	6.24e+08	5.97e-11
310.00	4.70e-20	1.11	7.29e+08	3.80e-11
325.00	2.07e-20	1.10	9.00e+08	2.04e-11

1 + (H₂O)₂ TS1c vtst

225.00	2.62e-17	1.43	1.01e+07	3.77e-10
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230.00	1.56e-17	1.40	1.23e+07	2.68e-10
240.00	5.90e-18	1.36	1.77e+07	1.42e-10
250.00	2.42e-18	1.32	2.45e+07	7.84e-11
260.00	1.06e-18	1.29	3.31e+07	4.54e-11
270.00	4.96e-19	1.27	4.35e+07	2.74e-11
275.00	3.47e-19	1.26	4.95e+07	2.16e-11
280.00	2.45e-19	1.24	5.60e+07	1.71e-11
290.00	1.28e-19	1.23	7.06e+07	1.11e-11
298.00	7.81e-20	1.22	8.38e+07	7.97e-12
300.00	6.94e-20	1.21	8.74e+07	7.36e-12
310.00	3.93e-20	1.20	1.06e+08	4.99e-12
325.00	1.79e-20	1.17	1.39e+08	2.92e-12

1 + (H₂O)₂ TS1d vtst

225.00	4.45e-17	1.33	7.24e+07	4.27e-09
230.00	2.58e-17	1.31	8.53e+07	2.89e-09
240.00	9.23e-18	1.28	1.16e+08	1.37e-09
250.00	3.60e-18	1.25	1.53e+08	6.88e-10
260.00	1.51e-18	1.23	1.96e+08	3.64e-10
270.00	6.76e-19	1.21	2.47e+08	2.01e-10
275.00	4.63e-19	1.20	2.75e+08	1.53e-10
280.00	3.21e-19	1.19	3.05e+08	1.17e-10
290.00	1.61e-19	1.18	3.70e+08	7.00e-11
298.00	9.58e-20	1.16	4.28e+08	4.76e-11
300.00	8.45e-20	1.16	4.43e+08	4.34e-11
310.00	4.63e-20	1.15	5.22e+08	2.78e-11
325.00	2.02e-20	1.13	6.54e+08	1.49e-11

2 + (H₂O)₂ TS1a ctst

225.00	9.99e-16	2.21	9.45e+03	2.09e-11
230.00	5.59e-16	2.12	1.28e+04	1.52e-11
240.00	1.88e-16	1.98	2.25e+04	8.37e-12
250.00	6.94e-17	1.86	3.77e+04	4.86e-12
260.00	2.77e-17	1.77	6.04e+04	2.96e-12
270.00	1.18e-17	1.69	9.31e+04	1.85e-12
275.00	7.93e-18	1.65	1.14e+05	1.49e-12
280.00	5.39e-18	1.62	1.39e+05	1.21e-12
290.00	2.59e-18	1.56	2.01e+05	8.11e-13
298.00	1.50e-18	1.52	2.64e+05	6.03e-13
300.00	1.31e-18	1.51	2.82e+05	5.59e-13
310.00	6.96e-19	1.47	3.87e+05	3.97e-13
325.00	2.90e-19	1.42	5.98e+05	2.46e-13

2 + (H₂O)₂ TS1b ctst

225.00	6.98e-16	2.10	7.82e+03	1.14e-11
230.00	3.97e-16	2.02	1.06e+04	8.50e-12
240.00	1.38e-16	1.89	1.86e+04	4.86e-12
250.00	5.23e-17	1.79	3.12e+04	2.91e-12
260.00	2.14e-17	1.70	5.00e+04	1.82e-12
270.00	9.37e-18	1.63	7.72e+04	1.18e-12
275.00	6.35e-18	1.60	9.46e+04	9.59e-13
280.00	4.36e-18	1.57	1.15e+05	7.89e-13
290.00	2.15e-18	1.52	1.66e+05	5.44e-13

298.00	1.26e-18	1.48	2.19e+05	4.10e-13
300.00	1.11e-18	1.47	2.34e+05	3.83e-13
310.00	5.99e-19	1.44	3.21e+05	2.76e-13
325.00	2.56e-19	1.39	4.96e+05	1.76e-13
2 + (H₂O)₂ TS1c ctst				
225.00	6.98e-16	2.39	1.68e+02	2.80e-13
230.00	3.97e-16	2.28	2.46e+02	2.23e-13
240.00	1.38e-16	2.10	5.00e+02	1.45e-13
250.00	5.23e-17	1.97	9.59e+02	9.88e-14
260.00	2.14e-17	1.86	1.74e+03	6.91e-14
270.00	9.37e-18	1.77	3.01e+03	4.98e-14
275.00	6.35e-18	1.73	3.90e+03	4.27e-14
280.00	4.36e-18	1.69	4.99e+03	3.68e-14
290.00	2.15e-18	1.63	7.98e+03	2.80e-14
298.00	1.26e-18	1.58	1.13e+04	2.26e-14
300.00	1.11e-18	1.57	1.23e+04	2.14e-14
310.00	5.99e-19	1.52	1.84e+04	1.68e-14
325.00	2.56e-19	1.46	3.21e+04	1.20e-14
2 + (H₂O)₂ TS1d ctst				
225.00	9.99e-16	2.33	3.28e+03	7.63e-12
230.00	5.59e-16	2.22	4.51e+03	5.59e-12
240.00	1.88e-16	2.06	8.14e+03	3.16e-12
250.00	6.94e-17	1.94	1.39e+04	1.87e-12
260.00	2.77e-17	1.83	2.28e+04	1.16e-12
270.00	1.18e-17	1.74	3.59e+04	7.38e-13
275.00	7.93e-18	1.70	4.44e+04	6.00e-13
280.00	5.39e-18	1.67	5.45e+04	4.90e-13
290.00	2.59e-18	1.61	8.02e+04	3.34e-13
298.00	1.50e-18	1.56	1.07e+05	2.50e-13
300.00	1.31e-18	1.55	1.15e+05	2.33e-13
310.00	6.96e-19	1.50	1.60e+05	1.67e-13
325.00	2.90e-19	1.44	2.52e+05	1.06e-13
2 + (H₂O)₂ TS2a ctst				
225.00	9.99e-16	571.43	2.10e-04	1.20e-16
230.00	5.59e-16	324.58	4.19e-04	7.60e-17
240.00	1.88e-16	124.34	1.52e-03	3.55e-17
250.00	6.94e-17	58.23	4.98e-03	2.01e-17
260.00	2.77e-17	32.50	1.48e-02	1.33e-17
270.00	1.18e-17	20.72	4.04e-02	9.88e-18
275.00	7.93e-18	17.10	6.49e-02	8.80e-18
280.00	5.39e-18	14.61	1.02e-01	8.03e-18
290.00	2.59e-18	10.91	2.43e-01	6.86e-18
298.00	1.50e-18	9.03	4.64e-01	6.29e-18
300.00	1.31e-18	8.65	5.42e-01	6.14e-18
310.00	6.96e-19	7.09	1.15e+00	5.67e-18
325.00	2.90e-19	5.59	3.22e+00	5.22e-18
2 + (H₂O)₂ TS2b ctst				
225.00	9.99e-16	191.71	9.65e-06	1.85e-18
230.00	5.59e-16	114.49	2.07e-05	1.32e-18
240.00	1.88e-16	51.16	8.60e-05	8.27e-19

250.00	6.94e-17	28.55	3.18e-04	6.30e-19
260.00	2.77e-17	18.49	1.06e-03	5.43e-19
270.00	1.18e-17	13.27	3.21e-03	5.03e-19
275.00	7.93e-18	11.51	5.42e-03	4.95e-19
280.00	5.39e-18	10.13	8.98e-03	4.90e-19
290.00	2.59e-18	8.11	2.33e-02	4.90e-19
298.00	1.50e-18	6.95	4.78e-02	4.98e-19
300.00	1.31e-18	6.71	5.68e-02	4.99e-19
310.00	6.96e-19	5.71	1.30e-01	5.16e-19
325.00	2.90e-19	4.65	4.09e-01	5.51e-19

2 + (H₂O)₂ TS2c ctst

225.00	6.98e-16	809.03	4.87e-05	2.75e-17
230.00	3.97e-16	441.44	9.99e-05	1.75e-17
240.00	1.38e-16	156.40	3.83e-04	8.27e-18
250.00	5.23e-17	69.24	1.31e-03	4.74e-18
260.00	2.14e-17	36.67	4.09e-03	3.21e-18
270.00	9.37e-18	22.84	1.16e-02	2.48e-18
275.00	6.35e-18	18.64	1.91e-02	2.26e-18
280.00	4.36e-18	15.64	3.07e-02	2.09e-18
290.00	2.15e-18	11.60	7.54e-02	1.88e-18
298.00	1.26e-18	9.53	1.48e-01	1.78e-18
300.00	1.11e-18	9.08	1.74e-01	1.75e-18
310.00	5.99e-19	7.40	3.81e-01	1.69e-18
325.00	2.56e-19	5.76	1.12e+00	1.65e-18

2 + (H₂O)₂ TS2d ctst

225.00	6.98e-16	920.70	4.54e-05	2.92e-17
230.00	3.97e-16	496.28	9.41e-05	1.85e-17
240.00	1.38e-16	172.48	3.67e-04	8.74e-18
250.00	5.23e-17	74.77	1.28e-03	5.01e-18
260.00	2.14e-17	39.36	4.04e-03	3.40e-18
270.00	9.37e-18	23.93	1.17e-02	2.62e-18
275.00	6.35e-18	19.64	1.92e-02	2.39e-18
280.00	4.36e-18	16.37	3.11e-02	2.22e-18
290.00	2.15e-18	12.05	7.75e-02	2.01e-18
298.00	1.26e-18	9.87	1.53e-01	1.90e-18
300.00	1.11e-18	9.39	1.81e-01	1.89e-18
310.00	5.99e-19	7.64	3.99e-01	1.83e-18
325.00	2.56e-19	5.92	1.19e+00	1.80e-18

2 + (H₂O)₂ TS1a vtst

225.00	9.99e-16	2.54	2.35e+03	5.96e-12
230.00	5.59e-16	2.44	3.31e+03	4.51e-12
240.00	1.88e-16	2.25	6.30e+03	2.67e-12
250.00	6.94e-17	2.12	1.13e+04	1.66e-12
260.00	2.77e-17	1.99	1.94e+04	1.07e-12
270.00	1.18e-17	1.88	3.19e+04	7.09e-13
275.00	7.93e-18	1.84	4.02e+04	5.87e-13
280.00	5.39e-18	1.80	5.03e+04	4.88e-13
290.00	2.59e-18	1.72	7.67e+04	3.42e-13
298.00	1.50e-18	1.68	1.05e+05	2.64e-13
300.00	1.31e-18	1.67	1.13e+05	2.48e-13

310.00	6.96e-19	1.61	1.63e+05	1.82e-13
325.00	2.90e-19	1.54	2.69e+05	1.20e-13
2 + (H₂O)₂ TS1b vtst				
225.00	6.98e-16	2.62	2.09e+03	3.82e-12
230.00	3.97e-16	2.51	2.94e+03	2.93e-12
240.00	1.38e-16	2.31	5.58e+03	1.78e-12
250.00	5.23e-17	2.17	1.00e+04	1.13e-12
260.00	2.14e-17	2.04	1.71e+04	7.47e-13
270.00	9.37e-18	1.94	2.80e+04	5.08e-13
275.00	6.35e-18	1.89	3.53e+04	4.24e-13
280.00	4.36e-18	1.84	4.42e+04	3.55e-13
290.00	2.15e-18	1.77	6.72e+04	2.56e-13
298.00	1.26e-18	1.72	9.20e+04	1.99e-13
300.00	1.11e-18	1.70	9.93e+04	1.88e-13
310.00	5.99e-19	1.64	1.43e+05	1.40e-13
325.00	2.56e-19	1.57	2.35e+05	9.42e-14
2 + (H₂O)₂ TS1c vtst				
225.00	6.98e-16	2.97	4.78e+01	9.91e-14
230.00	3.97e-16	2.82	7.31e+01	8.18e-14
240.00	1.38e-16	2.58	1.61e+02	5.74e-14
250.00	5.23e-17	2.39	3.32e+02	4.14e-14
260.00	2.14e-17	2.22	6.44e+02	3.06e-14
270.00	9.37e-18	2.09	1.19e+03	2.33e-14
275.00	6.35e-18	2.04	1.58e+03	2.04e-14
280.00	4.36e-18	1.99	2.08e+03	1.81e-14
290.00	2.15e-18	1.89	3.51e+03	1.43e-14
298.00	1.26e-18	1.82	5.19e+03	1.19e-14
300.00	1.11e-18	1.81	5.70e+03	1.14e-14
310.00	5.99e-19	1.74	8.94e+03	9.34e-15
325.00	2.56e-19	1.66	1.66e+04	7.04e-15
2 + (H₂O)₂ TS1d vtst				
225.00	9.99e-16	3.32	1.86e+01	6.16e-14
230.00	5.59e-16	3.13	2.90e+01	5.08e-14
240.00	1.88e-16	2.83	6.65e+01	3.53e-14
250.00	6.94e-17	2.59	1.42e+02	2.55e-14
260.00	2.77e-17	2.41	2.84e+02	1.89e-14
270.00	1.18e-17	2.24	5.39e+02	1.43e-14
275.00	7.93e-18	2.18	7.28e+02	1.26e-14
280.00	5.39e-18	2.13	9.73e+02	1.12e-14
290.00	2.59e-18	2.02	1.68e+03	8.78e-15
298.00	1.50e-18	1.94	2.53e+03	7.37e-15
300.00	1.31e-18	1.92	2.80e+03	7.03e-15
310.00	6.96e-19	1.84	4.49e+03	5.74e-15
325.00	2.90e-19	1.73	8.61e+03	4.32e-15
2 + (H₂O)₂ TS2a vtst				
225.00	9.99e-16	4285.71	5.25e-05	2.25e-16
230.00	5.59e-16	3287.04	1.08e-04	1.98e-16
240.00	1.88e-16	2021.69	4.15e-04	1.58e-16
250.00	6.94e-17	1300.70	1.43e-03	1.29e-16
260.00	2.77e-17	871.91	4.45e-03	1.07e-16

270.00	1.18e-17	607.09	1.27e-02	9.10e-17
275.00	7.93e-18	514.42	2.08e-02	8.49e-17
280.00	5.39e-18	435.82	3.35e-02	7.87e-17
290.00	2.59e-18	321.21	8.25e-02	6.86e-17
298.00	1.50e-18	256.79	1.62e-01	6.24e-17
300.00	1.31e-18	242.41	1.91e-01	6.07e-17
310.00	6.96e-19	187.53	4.17e-01	5.44e-17
325.00	2.90e-19	131.71	1.23e+00	4.70e-17

2 + (H₂O)₂ TS2b vtst

225.00	9.99e-16	18097.75	7.57e-06	7.56e-21
230.00	5.59e-16	11533.74	1.63e-05	9.11e-21
240.00	1.88e-16	5391.30	6.90e-05	1.30e-20
250.00	6.94e-17	2903.47	2.59e-04	1.80e-20
260.00	2.77e-17	1727.69	8.74e-04	2.42e-20
270.00	1.18e-17	1096.65	2.69e-03	3.17e-20
275.00	7.93e-18	892.54	4.56e-03	3.62e-20
280.00	5.39e-18	734.21	7.60e-03	4.10e-20
290.00	2.59e-18	512.56	1.99e-02	5.15e-20
298.00	1.50e-18	396.59	4.11e-02	6.16e-20
300.00	1.31e-18	371.43	4.90e-02	6.42e-20
310.00	6.96e-19	276.99	1.13e-01	7.86e-20
325.00	2.90e-19	185.87	3.61e-01	1.05e-19

2 + (H₂O)₂ TS2c vtst

225.00	6.98e-16	23956.04	2.73e-05	4.56e-16
230.00	3.97e-16	15334.51	5.68e-05	3.46e-16
240.00	1.38e-16	7187.50	2.24e-04	2.22e-16
250.00	5.23e-17	3865.65	7.89e-04	1.60e-16
260.00	2.14e-17	2270.92	2.51e-03	1.22e-16
270.00	9.37e-18	1422.71	7.31e-03	9.74e-17
275.00	6.35e-18	1157.02	1.21e-02	8.89e-17
280.00	4.36e-18	944.16	1.97e-02	8.11e-17
290.00	2.15e-18	653.14	4.93e-02	6.92e-17
298.00	1.26e-18	498.47	9.81e-02	6.16e-17
300.00	1.11e-18	466.38	1.16e-01	6.01e-17
310.00	5.99e-19	344.36	2.57e-01	5.30e-17
325.00	2.56e-19	227.68	7.73e-01	4.51e-17

2 + (H₂O)₂ TS2d vtst

225.00	6.98e-16	7666.67	2.70e-05	1.88e-20
230.00	3.97e-16	5167.55	5.67e-05	2.25e-20
240.00	1.38e-16	2625.55	2.27e-04	3.13e-20
250.00	5.23e-17	1490.15	8.12e-04	4.25e-20
260.00	2.14e-17	908.40	2.62e-03	5.61e-20
270.00	9.37e-18	589.91	7.73e-03	7.24e-20
275.00	6.35e-18	482.95	1.29e-02	8.19e-20
280.00	4.36e-18	402.38	2.10e-02	9.16e-20
290.00	2.15e-18	283.30	5.33e-02	1.15e-19
298.00	1.26e-18	220.56	1.07e-01	1.35e-19
300.00	1.11e-18	207.09	1.27e-01	1.41e-19
310.00	5.99e-19	155.99	2.84e-01	1.70e-19
325.00	2.56e-19	106.47	8.66e-01	2.22e-19

3 + (H₂O)₂ TS1a ctst				
225.00	6.43e-14	1.59	4.78e+05	4.89e-08
230.00	3.24e-14	1.56	6.04e+05	3.05e-08
240.00	8.95e-15	1.50	9.36e+05	1.25e-08
250.00	2.75e-15	1.45	1.39e+06	5.55e-09
260.00	9.24e-16	1.41	2.00e+06	2.60e-09
270.00	3.38e-16	1.37	2.80e+06	1.29e-09
275.00	2.10e-16	1.35	3.27e+06	9.28e-10
280.00	1.33e-16	1.34	3.80e+06	6.76e-10
290.00	5.58e-17	1.31	5.04e+06	3.68e-10
298.00	2.91e-17	1.29	6.22e+06	2.33e-10
300.00	2.49e-17	1.28	6.55e+06	2.09e-10
310.00	1.17e-17	1.26	8.34e+06	1.23e-10
325.00	4.12e-18	1.24	1.16e+07	5.93e-11
3 + (H₂O)₂ TS1b ctst				
225.00	4.47e-14	1.58	1.10e+06	7.78e-08
230.00	2.30e-14	1.55	1.34e+06	4.78e-08
240.00	6.63e-15	1.49	1.95e+06	1.92e-08
250.00	2.11e-15	1.44	2.73e+06	8.29e-09
260.00	7.36e-16	1.40	3.72e+06	3.83e-09
270.00	2.78e-16	1.36	4.92e+06	1.87e-09
275.00	1.76e-16	1.35	5.62e+06	1.33e-09
280.00	1.13e-16	1.33	6.38e+06	9.59e-10
290.00	4.87e-17	1.31	8.09e+06	5.16e-10
298.00	2.60e-17	1.28	9.65e+06	3.22e-10
300.00	2.23e-17	1.28	1.01e+07	2.88e-10
310.00	1.08e-17	1.26	1.23e+07	1.67e-10
325.00	3.93e-18	1.23	1.63e+07	7.90e-11
3 + (H₂O)₂ TS1c ctst				
225.00	4.47e-14	1.93	1.37e+05	1.18e-08
230.00	2.30e-14	1.86	1.75e+05	7.50e-09
240.00	6.63e-15	1.76	2.75e+05	3.21e-09
250.00	2.11e-15	1.67	4.16e+05	1.47e-09
260.00	7.36e-16	1.60	6.06e+05	7.15e-10
270.00	2.78e-16	1.54	8.56e+05	3.67e-10
275.00	1.76e-16	1.51	1.01e+06	2.69e-10
280.00	1.13e-16	1.49	1.18e+06	1.99e-10
290.00	4.87e-17	1.45	1.58e+06	1.12e-10
298.00	2.60e-17	1.42	1.96e+06	7.25e-11
300.00	2.23e-17	1.41	2.07e+06	6.51e-11
310.00	1.08e-17	1.38	2.66e+06	3.96e-11
325.00	3.93e-18	1.34	3.75e+06	1.97e-11
3 + (H₂O)₂ TS1d ctst				
225.00	6.43e-14	1.69	1.16e+06	1.26e-07
230.00	3.24e-14	1.64	1.43e+06	7.61e-08
240.00	8.95e-15	1.58	2.10e+06	2.96e-08
250.00	2.75e-15	1.52	2.99e+06	1.25e-08
260.00	9.24e-16	1.47	4.13e+06	5.60e-09
270.00	3.38e-16	1.42	5.55e+06	2.67e-09
275.00	2.10e-16	1.41	6.37e+06	1.88e-09

280.00	1.33e-16	1.39	7.28e+06	1.34e-09
290.00	5.58e-17	1.35	9.34e+06	7.03e-10
298.00	2.91e-17	1.34	1.12e+07	4.36e-10
300.00	2.49e-17	1.32	1.18e+07	3.88e-10
310.00	1.17e-17	1.30	1.45e+07	2.21e-10
325.00	4.12e-18	1.27	1.95e+07	1.02e-10

3 + (H₂O)₂ TS1a vtst

225.00	6.43e-14	1.69	2.24e+05	2.43e-08
230.00	3.24e-14	1.64	2.94e+05	1.56e-08
240.00	8.95e-15	1.55	4.88e+05	6.78e-09
250.00	2.75e-15	1.47	7.73e+05	3.14e-09
260.00	9.24e-16	1.42	1.18e+06	1.54e-09
270.00	3.38e-16	1.36	1.74e+06	8.01e-10
275.00	2.10e-16	1.34	2.08e+06	5.86e-10
280.00	1.33e-16	1.31	2.48e+06	4.34e-10
290.00	5.58e-17	1.27	3.45e+06	2.44e-10
298.00	2.91e-17	1.24	4.41e+06	1.59e-10
300.00	2.49e-17	1.23	4.67e+06	1.43e-10
310.00	1.17e-17	1.20	6.20e+06	8.67e-11
325.00	4.12e-18	1.14	9.12e+06	4.28e-11

3 + (H₂O)₂ TS1b vtst

225.00	4.47e-14	1.69	3.47e+05	2.62e-08
230.00	2.30e-14	1.64	4.41e+05	1.67e-08
240.00	6.63e-15	1.57	6.86e+05	7.16e-09
250.00	2.11e-15	1.50	1.03e+06	3.27e-09
260.00	7.36e-16	1.45	1.49e+06	1.59e-09
270.00	2.78e-16	1.41	2.08e+06	8.15e-10
275.00	1.76e-16	1.39	2.44e+06	5.95e-10
280.00	1.13e-16	1.36	2.85e+06	4.38e-10
290.00	4.87e-17	1.33	3.79e+06	2.45e-10
298.00	2.60e-17	1.30	4.70e+06	1.59e-10
300.00	2.23e-17	1.30	4.94e+06	1.43e-10
310.00	1.08e-17	1.27	6.32e+06	8.67e-11
325.00	3.93e-18	1.23	8.85e+06	4.28e-11

3 + (H₂O)₂ TS1c vtst

225.00	4.47e-14	2.16	5.24e+04	5.05e-09
230.00	2.30e-14	2.07	6.95e+04	3.31e-09
240.00	6.63e-15	1.92	1.18e+05	1.51e-09
250.00	2.11e-15	1.81	1.90e+05	7.26e-10
260.00	7.36e-16	1.72	2.95e+05	3.72e-10
270.00	2.78e-16	1.63	4.41e+05	2.00e-10
275.00	1.76e-16	1.60	5.33e+05	1.50e-10
280.00	1.13e-16	1.56	6.39e+05	1.13e-10
290.00	4.87e-17	1.50	9.00e+05	6.57e-11
298.00	2.60e-17	1.46	1.16e+06	4.39e-11
300.00	2.23e-17	1.44	1.24e+06	3.99e-11
310.00	1.08e-17	1.39	1.66e+06	2.49e-11
325.00	3.93e-18	0.84	2.43e+06	7.98e-12

3 + (H₂O)₂ TS1d vtst

225.00	6.43e-14	1.86	3.81e+05	4.55e-08
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230.00	3.24e-14	1.81	4.87e+05	2.85e-08
240.00	8.95e-15	1.71	7.70e+05	1.18e-08
250.00	2.75e-15	1.64	1.17e+06	5.28e-09
260.00	9.24e-16	1.58	1.71e+06	2.50e-09
270.00	3.38e-16	1.53	2.43e+06	1.25e-09
275.00	2.10e-16	1.50	2.86e+06	9.03e-10
280.00	1.33e-16	1.48	3.35e+06	6.60e-10
290.00	5.58e-17	1.44	4.50e+06	3.62e-10
298.00	2.91e-17	1.41	5.62e+06	2.31e-10
300.00	2.49e-17	1.40	5.93e+06	2.07e-10
310.00	1.17e-17	1.37	7.64e+06	1.23e-10
325.00	4.12e-18	1.33	1.08e+07	5.93e-11

4 + (H₂O)₂ TS1a ctst

225.00	3.44e-14	4.93	9.75e+01	1.65e-11
230.00	1.74e-14	4.46	1.46e+02	1.13e-11
240.00	4.83e-15	3.79	3.09e+02	5.65e-12
250.00	1.49e-15	3.31	6.14e+02	3.02e-12
260.00	5.03e-16	2.96	1.15e+03	1.71e-12
270.00	1.85e-16	2.68	2.06e+03	1.02e-12
275.00	1.15e-16	2.57	2.71e+03	8.00e-13
280.00	7.30e-17	2.47	3.52e+03	6.36e-13
290.00	3.08e-17	2.30	5.79e+03	4.10e-13
298.00	1.61e-17	2.19	8.41e+03	2.96e-13
300.00	1.38e-17	2.16	9.20e+03	2.75e-13
310.00	6.51e-18	2.05	1.41e+04	1.88e-13
325.00	2.31e-18	1.90	2.56e+04	1.12e-13

4 + (H₂O)₂ TS1b ctst

225.00	2.65e-14	4.79	7.48e+01	9.49e-12
230.00	1.37e-14	4.33	1.11e+02	6.59e-12
240.00	3.97e-15	3.70	2.30e+02	3.38e-12
250.00	1.28e-15	3.24	4.50e+02	1.87e-12
260.00	4.48e-16	2.89	8.33e+02	1.08e-12
270.00	1.70e-16	2.63	1.47e+03	6.58e-13
275.00	1.08e-16	2.53	1.92e+03	5.24e-13
280.00	6.95e-17	2.43	2.48e+03	4.19e-13
290.00	3.02e-17	2.27	4.02e+03	2.76e-13
298.00	1.62e-17	2.16	5.78e+03	2.02e-13
300.00	1.39e-17	2.14	6.31e+03	1.88e-13
310.00	6.76e-18	2.02	9.59e+03	1.31e-13
325.00	2.49e-18	1.88	1.71e+04	7.99e-14

4 + (H₂O)₂ TS1c ctst

225.00	2.65e-14	7.02	2.45e+00	4.56e-13
230.00	1.37e-14	6.09	3.89e+00	3.25e-13
240.00	3.97e-15	4.89	9.20e+00	1.79e-13
250.00	1.28e-15	4.10	2.03e+01	1.06e-13
260.00	4.48e-16	3.56	4.18e+01	6.68e-14
270.00	1.70e-16	3.17	8.16e+01	4.40e-14
275.00	1.08e-16	3.00	1.12e+02	3.63e-14
280.00	6.95e-17	2.87	1.51e+02	3.02e-14
290.00	3.02e-17	2.63	2.68e+02	2.13e-14

298.00	1.62e-17	2.48	4.12e+02	1.65e-14
300.00	1.39e-17	2.43	4.57e+02	1.54e-14
310.00	6.76e-18	2.28	7.50e+02	1.16e-14
325.00	2.49e-18	2.10	1.48e+03	7.74e-15
4 + (H₂O)₂ TS1d ctst				
225.00	3.44e-14	5.30	5.32e+01	9.70e-12
230.00	1.74e-14	4.78	8.00e+01	6.65e-12
240.00	4.83e-15	3.99	1.72e+02	3.31e-12
250.00	1.49e-15	3.47	3.46e+02	1.79e-12
260.00	5.03e-16	3.07	6.57e+02	1.02e-12
270.00	1.85e-16	2.77	1.19e+03	6.10e-13
275.00	1.15e-16	2.66	1.57e+03	4.80e-13
280.00	7.30e-17	2.55	2.05e+03	3.82e-13
290.00	3.08e-17	2.37	3.40e+03	2.48e-13
298.00	1.61e-17	2.25	4.97e+03	1.80e-13
300.00	1.38e-17	2.22	5.44e+03	1.67e-13
310.00	6.51e-18	2.09	8.43e+03	1.15e-13
325.00	2.31e-18	1.94	1.54e+04	6.91e-14
4 + (H₂O)₂ TS2a ctst				
225.00	3.44e-14	2040.82	1.47e-05	1.03e-15
230.00	1.74e-14	1059.94	3.17e-05	5.85e-16
240.00	4.83e-15	337.31	1.34e-04	2.18e-16
250.00	1.49e-15	134.73	5.01e-04	1.01e-16
260.00	5.03e-16	65.68	1.69e-03	5.58e-17
270.00	1.85e-16	37.26	5.18e-03	3.57e-17
275.00	1.15e-16	29.55	8.80e-03	2.99e-17
280.00	7.30e-17	24.04	1.46e-02	2.56e-17
290.00	3.08e-17	16.85	3.84e-02	1.99e-17
298.00	1.61e-17	13.24	7.93e-02	1.69e-17
300.00	1.38e-17	12.61	9.44e-02	1.64e-17
310.00	6.51e-18	9.91	2.18e-01	1.41e-17
325.00	2.31e-18	7.37	6.95e-01	1.18e-17
4 + (H₂O)₂ TS2b ctst				
225.00	3.44e-14	7155.43	3.41e-07	8.39e-17
230.00	1.74e-14	3275.00	8.00e-07	4.56e-17
240.00	4.83e-15	822.34	3.94e-06	1.56e-17
250.00	1.49e-15	263.53	1.70e-05	6.68e-18
260.00	5.03e-16	107.18	6.55e-05	3.53e-18
270.00	1.85e-16	53.74	2.27e-04	2.26e-18
275.00	1.15e-16	40.59	4.09e-04	1.91e-18
280.00	7.30e-17	31.67	7.20e-04	1.66e-18
290.00	3.08e-17	20.95	2.10e-03	1.36e-18
298.00	1.61e-17	15.98	4.70e-03	1.21e-18
300.00	1.38e-17	15.05	5.70e-03	1.18e-18
310.00	6.51e-18	11.45	1.45e-02	1.08e-18
325.00	2.31e-18	8.30	5.24e-02	1.00e-18
4 + (H₂O)₂ TS2c ctst				
225.00	2.65e-14	3798.28	2.33e-06	2.35e-16
230.00	1.37e-14	1874.52	5.18e-06	1.33e-16
240.00	3.97e-15	543.48	2.30e-05	4.96e-17

250.00	1.28e-15	197.57	9.06e-05	2.29e-17
260.00	4.48e-16	89.34	3.19e-04	1.28e-17
270.00	1.70e-16	47.94	1.02e-03	8.31e-18
275.00	1.08e-16	36.89	1.77e-03	7.05e-18
280.00	6.95e-17	29.37	3.00e-03	6.12e-18
290.00	3.02e-17	19.98	8.16e-03	4.92e-18
298.00	1.62e-17	15.38	1.73e-02	4.31e-18
300.00	1.39e-17	14.54	2.07e-02	4.18e-18
310.00	6.76e-18	11.21	4.94e-02	3.75e-18
325.00	2.49e-18	8.17	1.64e-01	3.34e-18

4 + (H₂O)₂ TS2d ctst

225.00	2.65e-14	3036.92	3.25e-06	2.62e-16
230.00	1.37e-14	1511.79	7.21e-06	1.49e-16
240.00	3.97e-15	446.88	3.20e-05	5.68e-17
250.00	1.28e-15	165.87	1.26e-04	2.68e-17
260.00	4.48e-16	76.52	4.43e-04	1.52e-17
270.00	1.70e-16	41.83	1.42e-03	1.01e-17
275.00	1.08e-16	32.78	2.45e-03	8.67e-18
280.00	6.95e-17	26.20	4.16e-03	7.58e-18
290.00	3.02e-17	18.14	1.13e-02	6.19e-18
298.00	1.62e-17	14.18	2.39e-02	5.49e-18
300.00	1.39e-17	13.38	2.87e-02	5.34e-18
310.00	6.76e-18	10.41	6.84e-02	4.81e-18
325.00	2.49e-18	7.67	2.27e-01	4.33e-18

4 + (H₂O)₂ TS1a vtst

225.00	3.44e-14	3.90	3.44e+01	4.61e-12
230.00	1.74e-14	3.67	5.32e+01	3.39e-12
240.00	4.83e-15	3.28	1.20e+02	1.90e-12
250.00	1.49e-15	2.97	2.54e+02	1.12e-12
260.00	5.03e-16	2.74	5.03e+02	6.94e-13
270.00	1.85e-16	2.54	9.46e+02	4.44e-13
275.00	1.15e-16	2.46	1.27e+03	3.59e-13
280.00	7.30e-17	2.37	1.69e+03	2.93e-13
290.00	3.08e-17	2.23	2.91e+03	2.00e-13
298.00	1.61e-17	2.13	4.36e+03	1.50e-13
300.00	1.38e-17	2.10	4.80e+03	1.39e-13
310.00	6.51e-18	2.01	7.66e+03	1.00e-13
325.00	2.31e-18	1.88	1.46e+04	6.33e-14

4 + (H₂O)₂ TS1b vtst

225.00	2.65e-14	4.67	2.25e+01	2.78e-12
230.00	1.37e-14	4.38	3.45e+01	2.07e-12
240.00	3.97e-15	3.88	7.68e+01	1.18e-12
250.00	1.28e-15	3.48	1.60e+02	7.13e-13
260.00	4.48e-16	3.18	3.13e+02	4.46e-13
270.00	1.70e-16	2.93	5.81e+02	2.89e-13
275.00	1.08e-16	2.81	7.78e+02	2.37e-13
280.00	6.95e-17	2.72	1.03e+03	1.95e-13
290.00	3.02e-17	2.54	1.75e+03	1.34e-13
298.00	1.62e-17	2.42	2.60e+03	1.02e-13
300.00	1.39e-17	2.40	2.86e+03	9.54e-14

310.00	6.76e-18	2.27	4.53e+03	6.96e-14
325.00	2.49e-18	2.11	8.50e+03	4.46e-14
4 + (H₂O)₂ TS1c vtst				
225.00	2.65e-14	5.28	8.87e-01	1.24e-13
230.00	1.37e-14	4.91	1.44e+00	9.69e-14
240.00	3.97e-15	4.29	3.57e+00	6.07e-14
250.00	1.28e-15	3.83	8.19e+00	4.02e-14
260.00	4.48e-16	3.45	1.76e+01	2.72e-14
270.00	1.70e-16	3.15	3.55e+01	1.90e-14
275.00	1.08e-16	3.01	4.95e+01	1.61e-14
280.00	6.95e-17	2.91	6.80e+01	1.38e-14
290.00	3.02e-17	2.70	1.24e+02	1.01e-14
298.00	1.62e-17	2.56	1.95e+02	8.08e-15
300.00	1.39e-17	2.52	2.18e+02	7.63e-15
310.00	6.76e-18	2.38	3.66e+02	5.88e-15
325.00	2.49e-18	2.19	7.52e+02	4.11e-15
4 + (H₂O)₂ TS1d vtst				
225.00	3.44e-14	5.41	1.85e+01	3.44e-12
230.00	1.74e-14	5.05	2.89e+01	2.54e-12
240.00	4.83e-15	4.44	6.65e+01	1.42e-12
250.00	1.49e-15	3.95	1.43e+02	8.42e-13
260.00	5.03e-16	3.59	2.87e+02	5.18e-13
270.00	1.85e-16	3.27	5.48e+02	3.31e-13
275.00	1.15e-16	3.14	7.43e+02	2.68e-13
280.00	7.30e-17	3.02	9.95e+02	2.19e-13
290.00	3.08e-17	2.80	1.73e+03	1.49e-13
298.00	1.61e-17	2.65	2.62e+03	1.12e-13
300.00	1.38e-17	2.62	2.89e+03	1.05e-13
310.00	6.51e-18	2.47	4.66e+03	7.49e-14
325.00	2.31e-18	2.28	9.00e+03	4.74e-14
4 + (H₂O)₂ TS2a vtst				
225.00	3.44e-14	340.81	4.46e-06	5.23e-17
230.00	1.74e-14	256.36	9.83e-06	4.38e-17
240.00	4.83e-15	153.83	4.31e-05	3.20e-17
250.00	1.49e-15	99.40	1.67e-04	2.47e-17
260.00	5.03e-16	68.04	5.82e-04	1.99e-17
270.00	1.85e-16	48.75	1.84e-03	1.66e-17
275.00	1.15e-16	41.96	3.17e-03	1.53e-17
280.00	7.30e-17	36.26	5.35e-03	1.42e-17
290.00	3.08e-17	27.99	1.44e-02	1.24e-17
298.00	1.61e-17	23.20	3.03e-02	1.13e-17
300.00	1.38e-17	22.21	3.62e-02	1.11e-17
310.00	6.51e-18	18.01	8.55e-02	1.00e-17
325.00	2.31e-18	13.70	2.81e-01	8.89e-18
4 + (H₂O)₂ TS2b vtst				
225.00	3.44e-14	362.50	1.36e-07	1.70e-18
230.00	1.74e-14	264.51	3.24e-07	1.49e-18
240.00	4.83e-15	152.12	1.65e-06	1.21e-18
250.00	1.49e-15	95.12	7.37e-06	1.04e-18
260.00	5.03e-16	63.36	2.92e-05	9.31e-19

270.00	1.85e-16	44.62	1.04e-04	8.58e-19
275.00	1.15e-16	38.00	1.90e-04	8.30e-19
280.00	7.30e-17	32.84	3.38e-04	8.10e-19
290.00	3.08e-17	24.95	1.01e-03	7.76e-19
298.00	1.61e-17	20.48	2.30e-03	7.58e-19
300.00	1.38e-17	19.61	2.80e-03	7.58e-19
310.00	6.51e-18	15.86	7.25e-03	7.49e-19
325.00	2.31e-18	11.93	2.70e-02	7.44e-19

4 + (H₂O)₂ TS2c vtst

225.00	2.65e-14	423.98	8.09e-07	9.09e-18
230.00	1.37e-14	311.48	1.83e-06	7.81e-18
240.00	3.97e-15	181.07	8.45e-06	6.07e-18
250.00	1.28e-15	113.66	3.44e-05	5.00e-18
260.00	4.48e-16	76.24	1.25e-04	4.27e-18
270.00	1.70e-16	53.77	4.11e-04	3.76e-18
275.00	1.08e-16	45.84	7.22e-04	3.57e-18
280.00	6.95e-17	39.52	1.24e-03	3.41e-18
290.00	3.02e-17	30.14	3.45e-03	3.14e-18
298.00	1.62e-17	24.70	7.45e-03	2.98e-18
300.00	1.39e-17	23.63	8.97e-03	2.95e-18
310.00	6.76e-18	19.04	2.18e-02	2.81e-18
325.00	2.49e-18	14.32	7.47e-02	2.66e-18

4 + (H₂O)₂ TS2d vtst

225.00	2.65e-14	659.46	1.11e-06	1.94e-17
230.00	1.37e-14	474.10	2.51e-06	1.63e-17
240.00	3.97e-15	265.22	1.15e-05	1.21e-17
250.00	1.28e-15	160.26	4.68e-05	9.60e-18
260.00	4.48e-16	103.53	1.70e-04	7.88e-18
270.00	1.70e-16	70.79	5.58e-04	6.72e-18
275.00	1.08e-16	59.57	9.77e-04	6.29e-18
280.00	6.95e-17	50.54	1.68e-03	5.90e-18
290.00	3.02e-17	37.47	4.67e-03	5.28e-18
298.00	1.62e-17	30.20	1.01e-02	4.94e-18
300.00	1.39e-17	28.84	1.21e-02	4.85e-18
310.00	6.76e-18	22.79	2.94e-02	4.53e-18
325.00	2.49e-18	16.80	1.00e-01	4.18e-18

5 + (H₂O)₂ TS1a ctst

225.00	2.15e-17	12.70	8.27e+00	2.26e-15
230.00	1.29e-17	10.62	1.30e+01	1.78e-15
240.00	4.99e-18	7.82	3.03e+01	1.18e-15
250.00	2.08e-18	6.19	6.58e+01	8.47e-16
260.00	9.32e-19	5.11	1.34e+02	6.38e-16
270.00	4.43e-19	4.36	2.59e+02	5.01e-16
275.00	3.12e-19	4.06	3.52e+02	4.46e-16
280.00	2.23e-19	3.82	4.74e+02	4.04e-16
290.00	1.18e-19	3.41	8.33e+02	3.35e-16
298.00	7.29e-20	3.15	1.27e+03	2.92e-16
300.00	6.49e-20	3.08	1.41e+03	2.82e-16
310.00	3.73e-20	2.83	2.29e+03	2.42e-16
325.00	1.74e-20	2.54	4.49e+03	1.98e-16

5 + (H₂O)₂ TS1b ctst				
225.00	7.35e-17	15.12	2.52e+00	2.80e-15
230.00	4.39e-17	12.40	4.00e+00	2.18e-15
240.00	1.67e-17	8.92	9.54e+00	1.42e-15
250.00	6.89e-18	6.92	2.11e+01	1.01e-15
260.00	3.05e-18	5.62	4.38e+01	7.50e-16
270.00	1.43e-18	4.73	8.60e+01	5.82e-16
275.00	1.01e-18	4.41	1.18e+02	5.25e-16
280.00	7.14e-19	4.12	1.60e+02	4.71e-16
290.00	3.74e-19	3.65	2.85e+02	3.89e-16
298.00	2.30e-19	3.34	4.40e+02	3.38e-16
300.00	2.05e-19	3.28	4.88e+02	3.28e-16
310.00	1.17e-19	2.99	8.05e+02	2.82e-16
325.00	5.37e-20	2.67	1.60e+03	2.29e-16
5 + (H₂O)₂ TS1c ctst				
225.00	7.35e-17	22.71	6.21e-02	1.04e-16
230.00	4.39e-17	17.48	1.07e-01	8.21e-17
240.00	1.67e-17	11.48	2.97e-01	5.69e-17
250.00	6.89e-18	8.38	7.55e-01	4.36e-17
260.00	3.05e-18	6.57	1.78e+00	3.57e-17
270.00	1.43e-18	5.41	3.94e+00	3.05e-17
275.00	1.01e-18	4.96	5.73e+00	2.87e-17
280.00	7.14e-19	4.59	8.21e+00	2.69e-17
290.00	3.74e-19	4.02	1.62e+01	2.43e-17
298.00	2.30e-19	3.66	2.70e+01	2.27e-17
300.00	2.05e-19	3.57	3.05e+01	2.23e-17
310.00	1.17e-19	3.22	5.52e+01	2.08e-17
325.00	5.37e-20	2.83	1.25e+02	1.90e-17
5 + (H₂O)₂ TS1d ctst				
225.00	2.15e-17	15.34	6.91e+00	2.28e-15
230.00	1.29e-17	12.57	1.09e+01	1.77e-15
240.00	4.99e-18	9.02	2.56e+01	1.15e-15
250.00	2.08e-18	6.97	5.58e+01	8.09e-16
260.00	9.32e-19	5.68	1.14e+02	6.04e-16
270.00	4.43e-19	4.77	2.22e+02	4.70e-16
275.00	3.12e-19	4.42	3.03e+02	4.18e-16
280.00	2.23e-19	4.13	4.09e+02	3.77e-16
290.00	1.18e-19	3.66	7.21e+02	3.12e-16
298.00	7.29e-20	3.37	1.10e+03	2.70e-16
300.00	6.49e-20	3.30	1.22e+03	2.61e-16
310.00	3.73e-20	3.00	2.00e+03	2.24e-16
325.00	1.74e-20	2.66	3.94e+03	1.83e-16
5 + (H₂O)₂ TS2a ctst				
225.00	2.15e-17	2330.28	2.18e-05	1.09e-18
230.00	1.29e-17	1241.23	4.56e-05	7.30e-19
240.00	4.99e-18	412.64	1.82e-04	3.75e-19
250.00	2.08e-18	168.73	6.46e-04	2.27e-19
260.00	9.32e-19	82.13	2.07e-03	1.58e-19
270.00	4.43e-19	46.14	6.09e-03	1.24e-19
275.00	3.12e-19	36.34	1.01e-02	1.15e-19

280.00	2.23e-19	29.21	1.65e-02	1.07e-19
290.00	1.18e-19	20.10	4.17e-02	9.89e-20
298.00	7.29e-20	15.69	8.35e-02	9.55e-20
300.00	6.49e-20	14.78	9.88e-02	9.48e-20
310.00	3.73e-20	11.45	2.21e-01	9.44e-20
325.00	1.74e-20	8.35	6.71e-01	9.74e-20

5 + (H₂O)₂ TS2b ctst

225.00	7.35e-17	4753.02	9.11e-07	3.18e-19
230.00	4.39e-17	2334.98	2.03e-06	2.08e-19
240.00	1.67e-17	671.46	9.04e-06	1.01e-19
250.00	6.89e-18	241.85	3.56e-05	5.93e-20
260.00	3.05e-18	107.14	1.26e-04	4.12e-20
270.00	1.43e-18	56.19	4.04e-04	3.25e-20
275.00	1.01e-18	43.00	7.00e-04	3.04e-20
280.00	7.14e-19	33.87	1.19e-03	2.88e-20
290.00	3.74e-19	22.62	3.24e-03	2.74e-20
298.00	2.30e-19	17.32	6.87e-03	2.74e-20
300.00	2.05e-19	16.26	8.24e-03	2.75e-20
310.00	1.17e-19	12.39	1.97e-02	2.85e-20
325.00	5.37e-20	8.87	6.57e-02	3.13e-20

5 + (H₂O)₂ TS2c ctst

225.00	7.35e-17	4597.70	3.48e-06	1.18e-18
230.00	4.39e-17	2324.97	7.57e-06	7.73e-19
240.00	1.67e-17	700.62	3.24e-05	3.79e-19
250.00	6.89e-18	259.35	1.23e-04	2.20e-19
260.00	3.05e-18	116.39	4.21e-04	1.49e-19
270.00	1.43e-18	61.45	1.31e-03	1.15e-19
275.00	1.01e-18	47.09	2.23e-03	1.06e-19
280.00	7.14e-19	36.90	3.74e-03	9.85e-20
290.00	3.74e-19	24.47	9.93e-03	9.09e-20
298.00	2.30e-19	18.69	2.06e-02	8.85e-20
300.00	2.05e-19	17.52	2.46e-02	8.84e-20
310.00	1.17e-19	13.23	5.75e-02	8.90e-20
325.00	5.37e-20	9.46	1.85e-01	9.40e-20

5 + (H₂O)₂ TS2d ctst

225.00	2.15e-17	5711.76	1.70e-06	2.09e-19
230.00	1.29e-17	2804.23	3.78e-06	1.37e-19
240.00	4.99e-18	798.82	1.69e-05	6.74e-20
250.00	2.08e-18	284.86	6.67e-05	3.95e-20
260.00	9.32e-19	123.31	2.36e-04	2.71e-20
270.00	4.43e-19	63.77	7.59e-04	2.14e-20
275.00	3.12e-19	48.18	1.32e-03	1.98e-20
280.00	2.23e-19	37.72	2.24e-03	1.88e-20
290.00	1.18e-19	24.88	6.11e-03	1.79e-20
298.00	7.29e-20	18.77	1.30e-02	1.78e-20
300.00	6.49e-20	17.63	1.56e-02	1.78e-20
310.00	3.73e-20	13.27	3.73e-02	1.85e-20
325.00	1.74e-20	9.36	1.25e-01	2.04e-20

6 + (H₂O)₂ TS1a ctst

225.00	3.23e-17	6.79	7.54e+02	1.65e-13
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230.00	1.94e-17	6.04	1.05e+03	1.23e-13
240.00	7.44e-18	4.95	1.94e+03	7.15e-14
250.00	3.09e-18	4.22	3.39e+03	4.42e-14
260.00	1.38e-18	3.69	5.67e+03	2.88e-14
270.00	6.51e-19	3.28	9.11e+03	1.95e-14
275.00	4.58e-19	3.11	1.14e+04	1.62e-14
280.00	3.26e-19	2.96	1.41e+04	1.36e-14
290.00	1.71e-19	2.72	2.11e+04	9.82e-15
298.00	1.06e-19	2.55	2.86e+04	7.74e-15
300.00	9.42e-20	2.52	3.07e+04	7.29e-15
310.00	5.39e-20	2.37	4.35e+04	5.55e-15
325.00	2.50e-20	2.16	7.03e+04	3.80e-15

6 + (H₂O)₂ TS1b ctst

225.00	1.29e-16	8.21	6.52e+01	6.90e-14
230.00	7.53e-17	7.17	9.41e+01	5.08e-14
240.00	2.73e-17	5.72	1.87e+02	2.92e-14
250.00	1.08e-17	4.76	3.49e+02	1.79e-14
260.00	4.57e-18	4.08	6.20e+02	1.16e-14
270.00	2.07e-18	3.59	1.05e+03	7.80e-15
275.00	1.42e-18	3.39	1.35e+03	6.49e-15
280.00	9.94e-19	3.22	1.71e+03	5.48e-15
290.00	5.03e-19	2.93	2.69e+03	3.96e-15
298.00	3.02e-19	2.72	3.78e+03	3.11e-15
300.00	2.67e-19	2.68	4.10e+03	2.94e-15
310.00	1.48e-19	2.50	6.05e+03	2.23e-15
325.00	6.53e-20	2.26	1.04e+04	1.53e-15

6 + (H₂O)₂ TS1c ctst

225.00	1.29e-16	18.25	2.69e-01	6.33e-16
230.00	7.53e-17	14.50	4.40e-01	4.80e-16
240.00	2.73e-17	10.00	1.11e+00	3.03e-16
250.00	1.08e-17	7.52	2.58e+00	2.10e-16
260.00	4.57e-18	6.00	5.63e+00	1.54e-16
270.00	2.07e-18	5.02	1.15e+01	1.19e-16
275.00	1.42e-18	4.62	1.62e+01	1.06e-16
280.00	9.94e-19	4.30	2.24e+01	9.57e-17
290.00	5.03e-19	3.79	4.14e+01	7.90e-17
298.00	3.02e-19	3.46	6.56e+01	6.86e-17
300.00	2.67e-19	3.40	7.33e+01	6.65e-17
310.00	1.48e-19	3.08	1.25e+02	5.70e-17
325.00	6.53e-20	2.73	2.60e+02	4.64e-17

6 + (H₂O)₂ TS1d ctst

225.00	3.23e-17	10.46	7.36e+01	2.49e-14
230.00	1.94e-17	8.93	1.09e+02	1.89e-14
240.00	7.44e-18	6.92	2.24e+02	1.15e-14
250.00	3.09e-18	5.60	4.36e+02	7.54e-15
260.00	1.38e-18	4.69	8.03e+02	5.20e-15
270.00	6.51e-19	4.06	1.41e+03	3.72e-15
275.00	4.58e-19	3.82	1.83e+03	3.20e-15
280.00	3.26e-19	3.60	2.36e+03	2.77e-15
290.00	1.71e-19	3.25	3.82e+03	2.12e-15

298.00	1.06e-19	2.99	5.48e+03	1.74e-15
300.00	9.42e-20	2.94	5.98e+03	1.66e-15
310.00	5.39e-20	2.72	9.06e+03	1.33e-15
325.00	2.50e-20	2.44	1.61e+04	9.82e-16
6 + (H₂O)₂ TS2a ctst				
225.00	3.23e-17	872.79	6.21e-04	1.75e-17
230.00	1.94e-17	512.61	1.19e-03	1.18e-17
240.00	7.44e-18	202.72	4.04e-03	6.09e-18
250.00	3.09e-18	95.16	1.24e-02	3.65e-18
260.00	1.38e-18	52.16	3.47e-02	2.50e-18
270.00	6.51e-19	32.03	8.96e-02	1.87e-18
275.00	4.58e-19	26.14	1.40e-01	1.68e-18
280.00	3.26e-19	21.62	2.16e-01	1.52e-18
290.00	1.71e-19	15.64	4.88e-01	1.30e-18
298.00	1.06e-19	12.57	8.99e-01	1.20e-18
300.00	9.42e-20	12.02	1.04e+00	1.18e-18
310.00	5.39e-20	9.48	2.12e+00	1.08e-18
325.00	2.50e-20	7.19	5.62e+00	1.01e-18
6 + (H₂O)₂ TS2b ctst				
225.00	1.29e-16	2568.53	9.85e-06	3.26e-18
230.00	7.53e-17	1346.34	2.05e-05	2.08e-18
240.00	2.73e-17	436.57	8.04e-05	9.58e-19
250.00	1.08e-17	173.05	2.82e-04	5.27e-19
260.00	4.57e-18	82.44	8.94e-04	3.37e-19
270.00	2.07e-18	45.77	2.60e-03	2.46e-19
275.00	1.42e-18	35.90	4.29e-03	2.19e-19
280.00	9.94e-19	28.74	6.96e-03	1.99e-19
290.00	5.03e-19	19.71	1.74e-02	1.73e-19
298.00	3.02e-19	15.32	3.46e-02	1.60e-19
300.00	2.67e-19	14.46	4.08e-02	1.58e-19
310.00	1.48e-19	11.17	9.04e-02	1.49e-19
325.00	6.53e-20	8.19	2.71e-01	1.45e-19
6 + (H₂O)₂ TS2c ctst				
225.00	1.29e-16	2353.54	1.98e-05	6.01e-18
230.00	7.53e-17	1250.61	4.07e-05	3.83e-18
240.00	2.73e-17	415.48	1.55e-04	1.76e-18
250.00	1.08e-17	167.23	5.31e-04	9.59e-19
260.00	4.57e-18	80.61	1.65e-03	6.08e-19
270.00	2.07e-18	45.09	4.68e-03	4.37e-19
275.00	1.42e-18	35.42	7.65e-03	3.85e-19
280.00	9.94e-19	28.46	1.23e-02	3.48e-19
290.00	5.03e-19	19.60	3.01e-02	2.97e-19
298.00	3.02e-19	15.25	5.91e-02	2.72e-19
300.00	2.67e-19	14.39	6.95e-02	2.67e-19
310.00	1.48e-19	11.19	1.51e-01	2.50e-19
325.00	6.53e-20	8.15	4.44e-01	2.36e-19
6 + (H₂O)₂ TS2d ctst				
225.00	3.23e-17	2025.32	2.37e-05	1.55e-18
230.00	1.94e-17	1080.08	4.87e-05	1.02e-18
240.00	7.44e-18	359.57	1.88e-04	5.03e-19

250.00	3.09e-18	146.52	6.47e-04	2.93e-19
260.00	1.38e-18	71.29	2.02e-03	1.99e-19
270.00	6.51e-19	40.55	5.77e-03	1.52e-19
275.00	4.58e-19	32.00	9.47e-03	1.39e-19
280.00	3.26e-19	25.82	1.53e-02	1.29e-19
290.00	1.71e-19	17.96	3.77e-02	1.16e-19
298.00	1.06e-19	14.17	7.41e-02	1.11e-19
300.00	9.42e-20	13.40	8.73e-02	1.10e-19
310.00	5.39e-20	10.47	1.91e-01	1.08e-19
325.00	2.50e-20	7.72	5.65e-01	1.09e-19

7 + (H₂O)₂ TS1a ctst

225.00	6.38e-16	12.72	4.00e+00	3.25e-14
230.00	3.62e-16	10.52	6.39e+00	2.43e-14
240.00	1.25e-16	7.66	1.54e+01	1.48e-14
250.00	4.72e-17	6.06	3.43e+01	9.82e-15
260.00	1.92e-17	4.99	7.17e+01	6.87e-15
270.00	8.39e-18	4.25	1.42e+02	5.07e-15
275.00	5.68e-18	3.98	1.95e+02	4.41e-15
280.00	3.89e-18	3.74	2.66e+02	3.87e-15
290.00	1.91e-18	3.34	4.76e+02	3.04e-15
298.00	1.12e-18	3.09	7.37e+02	2.55e-15
300.00	9.83e-19	3.03	8.19e+02	2.44e-15
310.00	5.29e-19	2.78	1.36e+03	2.00e-15
325.00	2.25e-19	2.50	2.72e+03	1.53e-15

7 + (H₂O)₂ TS1b ctst

225.00	4.58e-16	16.78	2.67e-01	2.05e-15
230.00	2.68e-16	13.33	4.41e-01	1.58e-15
240.00	9.79e-17	9.29	1.12e+00	1.02e-15
250.00	3.89e-17	7.02	2.65e+00	7.24e-16
260.00	1.66e-17	5.65	5.84e+00	5.48e-16
270.00	7.59e-18	4.73	1.21e+01	4.34e-16
275.00	5.24e-18	4.39	1.70e+01	3.91e-16
280.00	3.67e-18	4.09	2.37e+01	3.56e-16
290.00	1.87e-18	3.63	4.41e+01	2.99e-16
298.00	1.13e-18	3.32	7.04e+01	2.64e-16
300.00	9.99e-19	3.26	7.88e+01	2.57e-16
310.00	5.56e-19	2.98	1.35e+02	2.24e-16
325.00	2.48e-19	2.64	2.85e+02	1.87e-16

7 + (H₂O)₂ TS1c ctst

225.00	4.58e-16	8.97	4.16e+00	1.71e-14
230.00	2.68e-16	7.66	6.54e+00	1.34e-14
240.00	9.79e-17	5.94	1.52e+01	8.84e-15
250.00	3.89e-17	4.86	3.29e+01	6.22e-15
260.00	1.66e-17	4.14	6.69e+01	4.60e-15
270.00	7.59e-18	3.61	1.29e+02	3.54e-15
275.00	5.24e-18	3.41	1.75e+02	3.13e-15
280.00	3.67e-18	3.22	2.36e+02	2.79e-15
290.00	1.87e-18	2.94	4.12e+02	2.26e-15
298.00	1.13e-18	2.74	6.27e+02	1.94e-15
300.00	9.99e-19	2.69	6.94e+02	1.87e-15

310.00	5.56e-19	2.50	1.13e+03	1.57e-15
325.00	2.48e-19	2.27	2.20e+03	1.24e-15
7 + (H₂O)₂ TS1d ctst				
225.00	6.38e-16	11.82	7.73e-01	5.83e-15
230.00	3.62e-16	9.76	1.27e+00	4.49e-15
240.00	1.25e-16	7.21	3.23e+00	2.91e-15
250.00	4.72e-17	5.70	7.59e+00	2.04e-15
260.00	1.92e-17	4.75	1.66e+01	1.51e-15
270.00	8.39e-18	4.08	3.43e+01	1.17e-15
275.00	5.68e-18	3.82	4.82e+01	1.05e-15
280.00	3.89e-18	3.59	6.69e+01	9.34e-16
290.00	1.91e-18	3.23	1.24e+02	7.64e-16
298.00	1.12e-18	2.98	1.98e+02	6.61e-16
300.00	9.83e-19	2.92	2.22e+02	6.38e-16
310.00	5.29e-19	2.69	3.79e+02	5.40e-16
325.00	2.25e-19	2.42	7.96e+02	4.34e-16
8 + (H₂O)₂ TS1a ctst				
225.00	3.34e-15	9.40	3.34e+01	1.05e-12
230.00	1.82e-15	8.07	5.03e+01	7.39e-13
240.00	5.85e-16	6.27	1.08e+02	3.96e-13
250.00	2.06e-16	5.12	2.17e+02	2.29e-13
260.00	7.90e-17	4.36	4.13e+02	1.42e-13
270.00	3.26e-17	3.79	7.46e+02	9.23e-14
275.00	2.14e-17	3.57	9.86e+02	7.53e-14
280.00	1.43e-17	3.37	1.29e+03	6.22e-14
290.00	6.67e-18	3.05	2.14e+03	4.36e-14
298.00	3.76e-18	2.84	3.13e+03	3.34e-14
300.00	3.28e-18	2.79	3.43e+03	3.14e-14
310.00	1.69e-18	2.58	5.31e+03	2.32e-14
325.00	6.76e-19	2.35	9.71e+03	1.54e-14
8 + (H₂O)₂ TS1b ctst				
225.00	3.19e-15	13.13	1.66e+00	6.95e-14
230.00	1.76e-15	10.79	2.66e+00	5.05e-14
240.00	5.76e-16	7.87	6.44e+00	2.92e-14
250.00	2.07e-16	6.20	1.44e+01	1.85e-14
260.00	8.05e-17	5.08	3.03e+01	1.24e-14
270.00	3.37e-17	4.34	6.01e+01	8.80e-15
275.00	2.23e-17	4.05	8.30e+01	7.49e-15
280.00	1.50e-17	3.81	1.13e+02	6.45e-15
290.00	7.09e-18	3.38	2.04e+02	4.89e-15
298.00	4.04e-18	3.13	3.16e+02	4.00e-15
300.00	3.53e-18	3.08	3.51e+02	3.81e-15
310.00	1.84e-18	2.83	5.84e+02	3.04e-15
325.00	7.49e-19	2.52	1.18e+03	2.22e-15
8 + (H₂O)₂ TS1c ctst				
225.00	3.19e-15	7.83	3.22e+00	8.04e-14
230.00	1.76e-15	6.77	5.07e+00	6.04e-14
240.00	5.76e-16	5.34	1.19e+01	3.66e-14
250.00	2.07e-16	4.42	2.60e+01	2.38e-14
260.00	8.05e-17	3.82	5.31e+01	1.63e-14

270.00	3.37e-17	3.37	1.03e+02	1.17e-14
275.00	2.23e-17	3.20	1.40e+02	9.99e-15
280.00	1.50e-17	3.04	1.89e+02	8.61e-15
290.00	7.09e-18	2.77	3.33e+02	6.54e-15
298.00	4.04e-18	2.59	5.09e+02	5.33e-15
300.00	3.53e-18	2.55	5.64e+02	5.08e-15
310.00	1.84e-18	2.38	9.21e+02	4.03e-15
325.00	7.49e-19	2.18	1.81e+03	2.95e-15

8 + (H₂O)₂ TS1d ctst

225.00	3.34e-15	11.01	1.89e+00	6.95e-14
230.00	1.82e-15	9.22	3.06e+00	5.13e-14
240.00	5.85e-16	6.89	7.53e+00	3.04e-14
250.00	2.06e-16	5.49	1.72e+01	1.95e-14
260.00	7.90e-17	4.62	3.66e+01	1.34e-14
270.00	3.26e-17	3.98	7.37e+01	9.55e-15
275.00	2.14e-17	3.74	1.02e+02	8.15e-15
280.00	1.43e-17	3.50	1.41e+02	7.05e-15
290.00	6.67e-18	3.16	2.56e+02	5.39e-15
298.00	3.76e-18	2.92	4.01e+02	4.40e-15
300.00	3.28e-18	2.89	4.47e+02	4.23e-15
310.00	1.69e-18	2.65	7.51e+02	3.36e-15
325.00	6.76e-19	2.39	1.54e+03	2.49e-15

9 + (H₂O)₂ TS1a ctst

225.00	1.12e-15	5.20	2.75e+02	1.60e-12
230.00	6.35e-16	4.70	4.06e+02	1.21e-12
240.00	2.18e-16	3.95	8.42e+02	7.26e-13
250.00	8.18e-17	3.45	1.64e+03	4.62e-13
260.00	3.31e-17	3.06	3.03e+03	3.07e-13
270.00	1.44e-17	2.78	5.32e+03	2.13e-13
275.00	9.69e-18	2.65	6.94e+03	1.78e-13
280.00	6.63e-18	2.54	8.96e+03	1.51e-13
290.00	3.23e-18	2.37	1.45e+04	1.11e-13
298.00	1.89e-18	2.25	2.08e+04	8.83e-14
300.00	1.66e-18	2.22	2.27e+04	8.37e-14
310.00	8.87e-19	2.09	3.45e+04	6.40e-14
325.00	3.75e-19	1.94	6.13e+04	4.46e-14

9 + (H₂O)₂ TS1b ctst

225.00	3.70e-15	4.95	9.36e+02	1.71e-11
230.00	2.00e-15	4.50	1.35e+03	1.21e-11
240.00	6.34e-16	3.81	2.68e+03	6.47e-12
250.00	2.20e-16	3.34	5.00e+03	3.67e-12
260.00	8.32e-17	2.98	8.88e+03	2.20e-12
270.00	3.38e-17	2.70	1.51e+04	1.38e-12
275.00	2.21e-17	2.60	1.93e+04	1.11e-12
280.00	1.47e-17	2.49	2.45e+04	8.98e-13
290.00	6.77e-18	2.32	3.86e+04	6.05e-13
298.00	3.79e-18	2.20	5.41e+04	4.51e-13
300.00	3.29e-18	2.18	5.86e+04	4.21e-13
310.00	1.68e-18	2.06	8.66e+04	2.99e-13
325.00	6.62e-19	1.92	1.48e+05	1.88e-13

9 + (H₂O)₂ TS1c ctst				
225.00	3.70e-15	4.62	4.46e+02	7.62e-12
230.00	2.00e-15	4.19	6.56e+02	5.50e-12
240.00	6.34e-16	3.60	1.34e+03	3.06e-12
250.00	2.20e-16	3.16	2.59e+03	1.80e-12
260.00	8.32e-17	2.83	4.73e+03	1.11e-12
270.00	3.38e-17	2.59	8.23e+03	7.20e-13
275.00	2.21e-17	2.49	1.07e+04	5.88e-13
280.00	1.47e-17	2.40	1.37e+04	4.84e-13
290.00	6.77e-18	2.23	2.21e+04	3.34e-13
298.00	3.79e-18	2.13	3.14e+04	2.54e-13
300.00	3.29e-18	2.10	3.43e+04	2.37e-13
310.00	1.68e-18	2.00	5.16e+04	1.73e-13
325.00	6.62e-19	1.86	9.07e+04	1.12e-13
9 + (H₂O)₂ TS1d ctst				
225.00	3.70e-15	3.76	1.43e+04	1.99e-10
230.00	2.00e-15	3.51	1.90e+04	1.33e-10
240.00	6.34e-16	3.08	3.25e+04	6.34e-11
250.00	2.20e-16	2.77	5.30e+04	3.23e-11
260.00	8.32e-17	2.53	8.30e+04	1.75e-11
270.00	3.38e-17	2.34	1.25e+05	9.90e-12
275.00	2.21e-17	2.26	1.52e+05	7.58e-12
280.00	1.47e-17	2.19	1.83e+05	5.88e-12
290.00	6.77e-18	2.05	2.60e+05	3.62e-12
298.00	3.79e-18	1.97	3.37e+05	2.52e-12
300.00	3.29e-18	1.95	3.59e+05	2.31e-12
310.00	1.68e-18	1.86	4.86e+05	1.52e-12
325.00	6.62e-19	1.76	7.35e+05	8.54e-13
10 + (H₂O)₂ TS1a ctst				
225.00	2.11e-16	4.02	2.04e+02	1.73e-13
230.00	1.22e-16	3.70	2.97e+02	1.34e-13
240.00	4.42e-17	3.22	6.00e+02	8.53e-14
250.00	1.73e-17	2.87	1.14e+03	5.66e-14
260.00	7.32e-18	2.61	2.05e+03	3.92e-14
270.00	3.30e-18	2.40	3.53e+03	2.79e-14
275.00	2.27e-18	2.31	4.55e+03	2.38e-14
280.00	1.58e-18	2.23	5.82e+03	2.05e-14
290.00	7.96e-19	2.10	9.24e+03	1.54e-14
298.00	4.77e-19	2.00	1.31e+04	1.25e-14
300.00	4.21e-19	1.99	1.42e+04	1.19e-14
310.00	2.32e-19	1.89	2.12e+04	9.30e-15
325.00	1.02e-19	1.78	3.67e+04	6.65e-15
10 + (H₂O)₂ TS1b ctst				
225.00	6.94e-17	3.90	1.78e+02	4.82e-14
230.00	4.13e-17	3.62	2.60e+02	3.88e-14
240.00	1.56e-17	3.15	5.31e+02	2.61e-14
250.00	6.38e-18	2.81	1.02e+03	1.83e-14
260.00	2.80e-18	2.55	1.86e+03	1.33e-14
270.00	1.31e-18	2.36	3.22e+03	9.94e-15
275.00	9.16e-19	2.28	4.17e+03	8.69e-15

280.00	6.48e-19	2.21	5.35e+03	7.65e-15
290.00	3.37e-19	2.07	8.57e+03	5.96e-15
298.00	2.07e-19	1.98	1.22e+04	4.99e-15
300.00	1.84e-19	1.95	1.33e+04	4.78e-15
310.00	1.04e-19	1.87	1.99e+04	3.87e-15
325.00	4.77e-20	1.76	3.48e+04	2.91e-15

10 + (H₂O)₂ TS1c ctst

225.00	6.94e-17	3.65	4.16e+02	1.05e-13
230.00	4.13e-17	3.39	6.01e+02	8.43e-14
240.00	1.56e-17	2.99	1.19e+03	5.55e-14
250.00	6.38e-18	2.69	2.23e+03	3.83e-14
260.00	2.80e-18	2.46	3.97e+03	2.73e-14
270.00	1.31e-18	2.27	6.74e+03	2.00e-14
275.00	9.16e-19	2.20	8.65e+03	1.74e-14
280.00	6.48e-19	2.13	1.10e+04	1.52e-14
290.00	3.37e-19	2.00	1.73e+04	1.17e-14
298.00	2.07e-19	1.93	2.42e+04	9.65e-15
300.00	1.84e-19	1.90	2.63e+04	9.20e-15
310.00	1.04e-19	1.82	3.88e+04	7.34e-15
325.00	4.77e-20	1.72	6.63e+04	5.44e-15

10 + (H₂O)₂ TS1d ctst

225.00	2.11e-16	3.55	2.60e+03	1.95e-12
230.00	1.22e-16	3.31	3.59e+03	1.45e-12
240.00	4.42e-17	2.93	6.52e+03	8.44e-13
250.00	1.73e-17	2.63	1.13e+04	5.14e-13
260.00	7.32e-18	2.41	1.86e+04	3.29e-13
270.00	3.30e-18	2.25	2.94e+04	2.18e-13
275.00	2.27e-18	2.17	3.66e+04	1.80e-13
280.00	1.58e-18	2.10	4.50e+04	1.50e-13
290.00	7.96e-19	1.98	6.66e+04	1.05e-13
298.00	4.77e-19	1.90	8.93e+04	8.11e-14
300.00	4.21e-19	1.89	9.59e+04	7.62e-14
310.00	2.32e-19	1.81	1.34e+05	5.64e-14
325.00	1.02e-19	1.70	2.14e+05	3.71e-14

11+ (H₂O)₂ TS1a ctst

225.00	1.72e-17	5.62	6.07e+01	5.87e-15
230.00	1.04e-17	5.03	9.31e+01	4.87e-15
240.00	4.04e-18	4.17	2.07e+02	3.49e-15
250.00	1.70e-18	3.58	4.30e+02	2.62e-15
260.00	7.63e-19	3.17	8.41e+02	2.04e-15
270.00	3.65e-19	2.86	1.56e+03	1.63e-15
275.00	2.58e-19	2.73	2.09e+03	1.47e-15
280.00	1.85e-19	2.62	2.76e+03	1.34e-15
290.00	9.79e-20	2.41	4.68e+03	1.11e-15
298.00	6.09e-20	2.28	6.96e+03	9.68e-16
300.00	5.43e-20	2.26	7.65e+03	9.39e-16
310.00	3.14e-20	2.13	1.21e+04	8.10e-16
325.00	1.47e-20	1.98	2.26e+04	6.57e-16

11+ (H₂O)₂ TS1b ctst

225.00	1.72e-17	6.17	3.58e+00	3.80e-16
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230.00	1.04e-17	5.41	5.88e+00	3.31e-16
240.00	4.04e-18	4.40	1.48e+01	2.63e-16
250.00	1.70e-18	3.73	3.46e+01	2.19e-16
260.00	7.63e-19	3.28	7.53e+01	1.88e-16
270.00	3.65e-19	2.94	1.54e+02	1.65e-16
275.00	2.58e-19	2.81	2.16e+02	1.56e-16
280.00	1.85e-19	2.68	2.99e+02	1.48e-16
290.00	9.79e-20	2.47	5.54e+02	1.34e-16
298.00	6.09e-20	2.34	8.77e+02	1.25e-16
300.00	5.43e-20	2.31	9.80e+02	1.23e-16
310.00	3.14e-20	2.16	1.67e+03	1.13e-16
325.00	1.47e-20	2.00	3.47e+03	1.02e-16

11+ (H₂O)₂ TS1c ctst

225.00	3.92e-17	5.19	2.06e+01	4.19e-15
230.00	2.37e-17	4.65	3.18e+01	3.51e-15
240.00	9.21e-18	3.88	7.13e+01	2.55e-15
250.00	3.87e-18	3.38	1.49e+02	1.95e-15
260.00	1.74e-18	3.00	2.94e+02	1.53e-15
270.00	8.34e-19	2.72	5.48e+02	1.24e-15
275.00	5.89e-19	2.60	7.35e+02	1.12e-15
280.00	4.21e-19	2.50	9.75e+02	1.03e-15
290.00	2.24e-19	2.33	1.66e+03	8.65e-16
298.00	1.39e-19	2.21	2.48e+03	7.60e-16
300.00	1.24e-19	2.18	2.73e+03	7.38e-16
310.00	7.17e-20	2.06	4.32e+03	6.39e-16
325.00	3.36e-20	1.91	8.16e+03	5.24e-16

11+ (H₂O)₂ TS1d ctst

225.00	9.33e-17	6.75	5.11e+00	3.22e-15
230.00	5.60e-17	5.93	7.97e+00	2.65e-15
240.00	2.15e-17	4.78	1.83e+01	1.88e-15
250.00	8.93e-18	4.04	3.91e+01	1.41e-15
260.00	3.98e-18	3.52	7.84e+01	1.10e-15
270.00	1.89e-18	3.13	1.49e+02	8.83e-16
275.00	1.33e-18	2.97	2.02e+02	7.98e-16
280.00	9.45e-19	2.83	2.70e+02	7.23e-16
290.00	4.97e-19	2.61	4.67e+02	6.06e-16
298.00	3.08e-19	2.46	7.04e+02	5.33e-16
300.00	2.74e-19	2.42	7.77e+02	5.15e-16
310.00	1.57e-19	2.26	1.25e+03	4.44e-16
325.00	7.29e-20	2.09	2.40e+03	3.65e-16

12+ (H₂O)₂ TS1a ctst

225.00	2.24e-15	3.44	5.23e+04	4.03e-10
230.00	1.23e-15	3.20	6.74e+04	2.66e-10
240.00	4.04e-16	2.85	1.08e+05	1.24e-10
250.00	1.45e-16	2.59	1.65e+05	6.21e-11
260.00	5.62e-17	2.39	2.44e+05	3.27e-11
270.00	2.35e-17	2.22	3.49e+05	1.82e-11
275.00	1.56e-17	2.15	4.13e+05	1.39e-11
280.00	1.05e-17	2.08	4.86e+05	1.06e-11
290.00	4.93e-18	1.98	6.58e+05	6.41e-12

298.00	2.80e-18	1.89	8.26e+05	4.37e-12
300.00	2.45e-18	1.88	8.72e+05	4.02e-12
310.00	1.27e-18	1.80	1.13e+06	2.58e-12
325.00	5.17e-19	1.69	1.62e+06	1.42e-12
12+ (H₂O)₂ TS1b ctst				
225.00	9.93e-16	4.69	5.57e+03	2.59e-11
230.00	5.48e-16	4.27	7.65e+03	1.79e-11
240.00	1.80e-16	3.67	1.38e+04	9.13e-12
250.00	6.50e-17	3.22	2.38e+04	4.99e-12
260.00	2.54e-17	2.90	3.90e+04	2.87e-12
270.00	1.06e-17	2.65	6.15e+04	1.73e-12
275.00	7.06e-18	2.53	7.62e+04	1.36e-12
280.00	4.76e-18	2.45	9.36e+04	1.09e-12
290.00	2.25e-18	2.28	1.38e+05	7.06e-13
298.00	1.28e-18	2.16	1.85e+05	5.12e-13
300.00	1.12e-18	2.14	1.98e+05	4.75e-13
310.00	5.85e-19	2.03	2.77e+05	3.28e-13
325.00	2.38e-19	1.89	4.39e+05	1.97e-13
12+ (H₂O)₂ TS1c ctst				
225.00	9.93e-16	2.56	3.81e+05	9.68e-10
230.00	5.48e-16	2.44	4.76e+05	6.36e-10
240.00	1.80e-16	2.25	7.20e+05	2.92e-10
250.00	6.50e-17	2.09	1.05e+06	1.42e-10
260.00	2.54e-17	1.97	1.48e+06	7.39e-11
270.00	1.06e-17	1.86	2.03e+06	4.00e-11
275.00	7.06e-18	1.81	2.36e+06	3.01e-11
280.00	4.76e-18	1.77	2.72e+06	2.29e-11
290.00	2.25e-18	1.70	3.55e+06	1.35e-11
298.00	1.28e-18	1.64	4.33e+06	9.11e-12
300.00	1.12e-18	1.63	4.54e+06	8.31e-12
310.00	5.85e-19	1.58	5.71e+06	5.28e-12
325.00	2.38e-19	1.51	7.80e+06	2.81e-12
12+ (H₂O)₂ TS1d ctst				
225.00	1.15e-15	2.56	2.62e+05	7.72e-10
230.00	6.41e-16	2.44	3.28e+05	5.13e-10
240.00	2.14e-16	2.24	4.99e+05	2.40e-10
250.00	7.80e-17	2.08	7.30e+05	1.19e-10
260.00	3.08e-17	1.96	1.03e+06	6.22e-11
270.00	1.31e-17	1.86	1.42e+06	3.46e-11
275.00	8.71e-18	1.81	1.65e+06	2.60e-11
280.00	5.89e-18	1.77	1.90e+06	1.98e-11
290.00	2.82e-18	1.69	2.49e+06	1.19e-11
298.00	1.62e-18	1.64	3.05e+06	8.12e-12
300.00	1.42e-18	1.63	3.20e+06	7.41e-12
310.00	7.45e-19	1.58	4.03e+06	4.74e-12
325.00	3.07e-19	1.51	5.52e+06	2.56e-12

Table S5: Calculated values, at different temperatures (T in Kelvin), of rate constants (k_M , and k_D (both in $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$), and the fitted rate constants (k_{fit} in cm^3

molecule⁻¹ s⁻¹) for the reaction of carbonyl oxides with water and with water dimer for the reactions of carbonyl oxides **1**, **3**, **7**, **8**, **9**, **10**, **11**, and **12** with H₂O and with (H₂O)₂. The Arrhenius parameters are also given.

T	K _M /k _D	k _{fit}
1 + H₂O ctst		
Arrhenius equation A 3.53e-14 Ea -1.37 r**2 -0.99979		
225.00	1.69e-15	1.67e-15
230.00	1.79e-15	1.78e-15
240.00	2.02e-15	2.02e-15
250.00	2.26e-15	2.26e-15
260.00	2.50e-15	2.52e-15
270.00	2.76e-15	2.77e-15
275.00	2.89e-15	2.91e-15
280.00	3.02e-15	3.04e-15
290.00	3.31e-15	3.31e-15
298.00	3.52e-15	3.52e-15
300.00	3.58e-15	3.58e-15
310.00	3.86e-15	3.85e-15
325.00	4.32e-15	4.27e-15
1 + H₂O vtst		
# Arrhenius equation A 3.33e-14 Ea -1.42 r**2 -0.99951		
225.00	1.43e-15	1.40e-15
230.00	1.51e-15	1.50e-15
240.00	1.70e-15	1.71e-15
250.00	1.91e-15	1.92e-15
260.00	2.13e-15	2.15e-15
270.00	2.35e-15	2.38e-15
275.00	2.47e-15	2.49e-15
280.00	2.59e-15	2.61e-15
290.00	2.84e-15	2.85e-15
298.00	3.05e-15	3.05e-15
300.00	3.09e-15	3.10e-15
310.00	3.36e-15	3.34e-15
325.00	3.79e-15	3.72e-15
1 + (H₂O)₂ ctst		
# Arrhenius equation A 1.30e-16 Ea 8.53 r**2 1.00000		
225.00	2.46e-08	2.48e-08
230.00	1.63e-08	1.64e-08
240.00	7.52e-09	7.52e-09
250.00	3.69e-09	3.68e-09
260.00	1.91e-09	1.90e-09
270.00	1.03e-09	1.03e-09
275.00	7.75e-10	7.73e-10
280.00	5.86e-10	5.85e-10
290.00	3.46e-10	3.45e-10
298.00	2.32e-10	2.32e-10
300.00	2.10e-10	2.11e-10
310.00	1.32e-10	1.33e-10
325.00	6.95e-11	7.01e-11

1 + (H₂O)₂ vtst

Arrhenius equation A 1.76e-16 Ea 8.15 r**2 1.00000

225.00	1.44e-08	1.45e-08
230.00	9.75e-09	9.76e-09
240.00	4.65e-09	4.64e-09
250.00	2.35e-09	2.34e-09
260.00	1.25e-09	1.25e-09
270.00	6.96e-10	6.95e-10
275.00	5.28e-10	5.27e-10
280.00	4.04e-10	4.04e-10
290.00	2.44e-10	2.44e-10
298.00	1.67e-10	1.67e-10
300.00	1.52e-10	1.52e-10
310.00	9.77e-11	9.79e-11
325.00	5.30e-11	5.32e-11

3 + H₂O ctst

Arrhenius equation A 2.43e-14 Ea 1.34 r**2 0.99918

225.00	5.00e-13	4.90e-13
230.00	4.64e-13	4.59e-13
240.00	4.05e-13	4.06e-13
250.00	3.59e-13	3.63e-13
260.00	3.23e-13	3.27e-13
270.00	2.94e-13	2.97e-13
275.00	2.80e-13	2.84e-13
280.00	2.69e-13	2.72e-13
290.00	2.49e-13	2.50e-13
298.00	2.36e-13	2.35e-13
300.00	2.31e-13	2.31e-13
310.00	2.17e-13	2.15e-13
325.00	1.99e-13	1.95e-13

3+ H₂O vtst

Arrhenius equation A 2.58e-14 Ea 0.98 r**2 0.99846

225.00	2.34e-13	2.30e-13
230.00	2.21e-13	2.19e-13
240.00	2.00e-13	2.01e-13
250.00	1.83e-13	1.85e-13
260.00	1.69e-13	1.71e-13
270.00	1.58e-13	1.60e-13
275.00	1.53e-13	1.54e-13
280.00	1.48e-13	1.50e-13
290.00	1.40e-13	1.41e-13
298.00	1.35e-13	1.35e-13
300.00	1.33e-13	1.33e-13
310.00	1.27e-13	1.26e-13
325.00	1.20e-13	1.17e-13

3 + (H₂O)₂ ctst

Arrhenius equation A 4.43e-17 Ea 10.07 r**2 1.00000

225.00	2.64e-07	2.64e-07
230.00	1.62e-07	1.62e-07
240.00	6.46e-08	6.47e-08

250.00	2.78e-08	2.78e-08
260.00	1.27e-08	1.28e-08
270.00	6.20e-09	6.20e-09
275.00	4.41e-09	4.41e-09
280.00	3.18e-09	3.17e-09
290.00	1.70e-09	1.70e-09
298.00	1.06e-09	1.06e-09
300.00	9.51e-10	9.50e-10
310.00	5.51e-10	5.51e-10
325.00	2.60e-10	2.59e-10

3 + (H₂O)₂ vtst

Arrhenius equation A 7.51e-17 Ea 9.40 r**2 0.99999

225.00	1.01e-07	1.02e-07
230.00	6.41e-08	6.44e-08
240.00	2.73e-08	2.73e-08
250.00	1.24e-08	1.24e-08
260.00	6.01e-09	6.00e-09
270.00	3.07e-09	3.06e-09
275.00	2.23e-09	2.22e-09
280.00	1.64e-09	1.64e-09
290.00	9.18e-10	9.13e-10
298.00	5.93e-10	5.89e-10
300.00	5.34e-10	5.30e-10
310.00	3.21e-10	3.19e-10
325.00	1.53e-10	1.58e-10

7 + H₂O ctst

Arrhenius equation A 1.74e-14 Ea -5.02 r**2 -0.99925

225.00	2.53e-19	2.34e-19
230.00	3.08e-19	2.98e-19
240.00	4.62e-19	4.71e-19
250.00	6.88e-19	7.18e-19
260.00	1.01e-18	1.06e-18
270.00	1.45e-18	1.52e-18
275.00	1.73e-18	1.80e-18
280.00	2.06e-18	2.12e-18
290.00	2.86e-18	2.89e-18
298.00	3.65e-18	3.65e-18
300.00	3.90e-18	3.86e-18
310.00	5.22e-18	5.06e-18
325.00	7.91e-18	7.37e-18

7 + (H₂O)₂ ctst

Arrhenius equation A 5.42e-18 Ea 4.09 r**2 0.99675

225.00	5.74e-14	5.03e-14
230.00	4.38e-14	4.12e-14
240.00	2.75e-14	2.84e-14
250.00	1.88e-14	2.02e-14
260.00	1.35e-14	1.47e-14
270.00	1.02e-14	1.10e-14
275.00	8.98e-15	9.55e-15
280.00	7.95e-15	8.36e-15

290.00	6.36e-15	6.49e-15
298.00	5.42e-15	5.36e-15
300.00	5.20e-15	5.12e-15
310.00	4.33e-15	4.11e-15
325.00	3.39e-15	3.02e-15

8 + H₂O ctst

Arrhenius equation A 4.01e-15 Ea -3.19 r**2 -0.99591

225.00	3.65e-18	3.24e-18
230.00	3.98e-18	3.78e-18
240.00	4.91e-18	5.05e-18
250.00	6.19e-18	6.60e-18
260.00	7.89e-18	8.45e-18
270.00	9.98e-18	1.06e-17
275.00	1.12e-17	1.18e-17
280.00	1.25e-17	1.31e-17
290.00	1.57e-17	1.60e-17
298.00	1.87e-17	1.85e-17
300.00	1.95e-17	1.92e-17
310.00	2.39e-17	2.28e-17
325.00	3.20e-17	2.90e-17

8 + (H₂O)₂ ctst

Arrhenius equation A 2.56e-18 Ea 5.81 r**2 0.99880

225.00	1.27e-12	1.13e-12
230.00	9.01e-13	8.55e-13
240.00	4.92e-13	5.03e-13
250.00	2.90e-13	3.09e-13
260.00	1.84e-13	1.97e-13
270.00	1.22e-13	1.30e-13
275.00	1.01e-13	1.07e-13
280.00	8.43e-14	8.82e-14
290.00	6.04e-14	6.15e-14
298.00	4.71e-14	4.69e-14
300.00	4.45e-14	4.40e-14
310.00	3.36e-14	3.21e-14
325.00	2.31e-14	2.08e-14

9 + H₂O ctst

Arrhenius equation A 9.05e-15 Ea -0.68 r**2 -0.94056

225.00	2.19e-15	2.00e-15
230.00	2.16e-15	2.06e-15
240.00	2.15e-15	2.20e-15
250.00	2.21e-15	2.32e-15
260.00	2.31e-15	2.45e-15
270.00	2.44e-15	2.57e-15
275.00	2.50e-15	2.63e-15
280.00	2.58e-15	2.69e-15
290.00	2.76e-15	2.80e-15
298.00	2.91e-15	2.89e-15
300.00	2.94e-15	2.91e-15
310.00	3.14e-15	3.02e-15
325.00	3.48e-15	3.18e-15

9 + (H₂O)₂ ctst

Arrhenius equation A 8.58e-18 Ea 7.62 r**2 0.99986

225.00	2.25e-10	2.15e-10
230.00	1.52e-10	1.49e-10
240.00	7.37e-11	7.42e-11
250.00	3.83e-11	3.91e-11
260.00	2.11e-11	2.17e-11
270.00	1.22e-11	1.26e-11
275.00	9.45e-12	9.71e-12
280.00	7.41e-12	7.57e-12
290.00	4.66e-12	4.72e-12
298.00	3.31e-12	3.31e-12
300.00	3.05e-12	3.04e-12
310.00	2.05e-12	2.01e-12
325.00	1.20e-12	1.14e-12

10 + H₂O ctst

Arrhenius equation A 1.00e-14 Ea -4.32 r**2 -0.99960

225.00	6.79e-19	6.45e-19
230.00	8.12e-19	7.96e-19
240.00	1.17e-18	1.18e-18
250.00	1.65e-18	1.69e-18
260.00	2.30e-18	2.37e-18
270.00	3.15e-18	3.22e-18
275.00	3.65e-18	3.73e-18
280.00	4.21e-18	4.30e-18
290.00	5.56e-18	5.61e-18
298.00	6.87e-18	6.86e-18
300.00	7.23e-18	7.20e-18
310.00	9.28e-18	9.10e-18
325.00	1.31e-17	1.26e-17

10 + (H₂O)₂ ctst

Arrhenius equation A 1.02e-17 Ea 5.49 r**2 0.99981

225.00	2.27e-12	2.19e-12
230.00	1.71e-12	1.67e-12
240.00	1.01e-12	1.02e-12
250.00	6.27e-13	6.41e-13
260.00	4.08e-13	4.19e-13
270.00	2.76e-13	2.83e-13
275.00	2.30e-13	2.35e-13
280.00	1.93e-13	1.96e-13
290.00	1.38e-13	1.40e-13
298.00	1.08e-13	1.08e-13
300.00	1.02e-13	1.02e-13
310.00	7.69e-14	7.55e-14
325.00	5.21e-14	5.01e-14

11 + H₂O ctst

Arrhenius equation A 1.16e-14 Ea -6.43 r**2 -0.99979

225.00	7.00e-21	6.65e-21
230.00	9.30e-21	9.09e-21
240.00	1.61e-20	1.63e-20

250.00	2.74e-20	2.80e-20
260.00	4.45e-20	4.60e-20
270.00	7.09e-20	7.30e-20
275.00	8.86e-20	9.07e-20
280.00	1.09e-19	1.12e-19
290.00	1.65e-19	1.67e-19
298.00	2.25e-19	2.25e-19
300.00	2.43e-19	2.42e-19
310.00	3.50e-19	3.42e-19
325.00	5.81e-19	5.54e-19

11 + (H₂O)₂ ctst

Arrhenius equation A 1.35e-17 Ea 3.06 r**2 0.99838

225.00	1.37e-14	1.28e-14
230.00	1.14e-14	1.10e-14
240.00	8.18e-15	8.31e-15
250.00	6.19e-15	6.43e-15
260.00	4.86e-15	5.07e-15
270.00	3.92e-15	4.07e-15
275.00	3.55e-15	3.67e-15
280.00	3.23e-15	3.32e-15
290.00	2.71e-15	2.75e-15
298.00	2.39e-15	2.38e-15
300.00	2.32e-15	2.30e-15
310.00	2.01e-15	1.95e-15
325.00	1.65e-15	1.55e-15

12 + H₂O ctst

Arrhenius equation A 8.81e-15 Ea 0.38 r**2 0.95939

225.00	2.14e-14	2.05e-14
230.00	2.07e-14	2.02e-14
240.00	1.93e-14	1.95e-14
250.00	1.85e-14	1.89e-14
260.00	1.79e-14	1.83e-14
270.00	1.74e-14	1.78e-14
275.00	1.72e-14	1.76e-14
280.00	1.71e-14	1.74e-14
290.00	1.68e-14	1.70e-14
298.00	1.67e-14	1.67e-14
300.00	1.67e-14	1.66e-14
310.00	1.66e-14	1.63e-14
325.00	1.65e-14	1.58e-14

12 + (H₂O)₂ ctst

Arrhenius equation A 1.70e-17 Ea 8.34 r**2 0.99999

225.00	2.17e-09	2.14e-09
230.00	1.43e-09	1.42e-09
240.00	6.65e-10	6.66e-10
250.00	3.28e-10	3.31e-10
260.00	1.72e-10	1.73e-10
270.00	9.45e-11	9.54e-11
275.00	7.14e-11	7.19e-11
280.00	5.44e-11	5.48e-11

290.00	3.26e-11	3.27e-11
298.00	2.21e-11	2.21e-11
300.00	2.02e-11	2.02e-11
310.00	1.29e-11	1.28e-11
325.00	6.98e-12	6.87e-12

Table S6: Calculated values, at different temperatures (T in K), of rate constants (k_{TS1M} , k_{TS2M} , k_{TS1D} and k_{TS2D} in $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$), the overall rate constant k_{M} , and k_{D} ($k_{\text{M}} = k_{\text{TS1M}} + k_{\text{TS2M}}$, $k_{\text{D}} = k_{\text{TS1D}} + k_{\text{TS2D}}$, both in $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$), the fitted rate constants (k_{fit} in $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) for the reaction of carbonyl oxides with water and with water dimer for the reactions of carbonyl oxides **2**, **4**, **5**, and **6** with H_2O and with $(\text{H}_2\text{O})_2$. The branching ration for reaction 2 (Γ in %) and the Arrhenius parameters are also given.

T	$k_{\text{TS1M}}/k_{\text{TS1D}}$	$k_{\text{TS2M}}/k_{\text{TS2D}}$	$k_{\text{M}}/k_{\text{D}}$	k_{fit}	Γ
2 + H₂O ctst					
# Arrhenius equation A 5.85e-17 Ea -1.88 r**2 -0.77766					
225.00	1.19e-19	1.46e-18	1.58e-18	8.72e-19	7.55
230.00	1.50e-19	1.14e-18	1.29e-18	9.55e-19	11.62
240.00	2.37e-19	7.66e-19	1.00e-18	1.13e-18	23.64
250.00	3.64e-19	5.75e-19	9.39e-19	1.33e-18	38.74
260.00	5.47e-19	4.84e-19	1.03e-18	1.54e-18	53.05
270.00	8.00e-19	4.49e-19	1.25e-18	1.76e-18	64.02
275.00	9.58e-19	4.46e-19	1.40e-18	1.87e-18	68.24
280.00	1.14e-18	4.52e-19	1.59e-18	1.99e-18	71.65
290.00	1.59e-18	4.83e-19	2.08e-18	2.24e-18	76.76
298.00	2.06e-18	5.25e-19	2.58e-18	2.44e-18	79.68
300.00	2.18e-18	5.41e-19	2.72e-18	2.50e-18	80.15
310.00	2.94e-18	6.22e-19	3.56e-18	2.76e-18	82.53
325.00	4.45e-18	8.01e-19	5.25e-18	3.18e-18	84.73
2 + H₂O vtst					
# Arrhenius equation A 1.78e-16 Ea -2.44 r**2 -0.96014					
225.00	7.34e-20	8.99e-19	9.72e-19	7.53e-19	7.55
230.00	9.47e-20	8.78e-19	9.72e-19	8.48e-19	9.73
240.00	1.53e-19	8.77e-19	1.03e-18	1.06e-18	14.85
250.00	2.39e-19	9.04e-19	1.14e-18	1.30e-18	20.88
260.00	3.63e-19	9.66e-19	1.33e-18	1.57e-18	27.33
270.00	5.37e-19	1.06e-18	1.59e-18	1.87e-18	33.71
275.00	6.45e-19	1.11e-18	1.75e-18	2.03e-18	36.75
280.00	7.74e-19	1.17e-18	1.95e-18	2.20e-18	39.76
290.00	1.09e-18	1.33e-18	2.42e-18	2.56e-18	45.18
298.00	1.42e-18	1.47e-18	2.89e-18	2.87e-18	49.09
300.00	1.52e-18	1.51e-18	3.03e-18	2.95e-18	50.03
310.00	2.06e-18	1.74e-18	3.80e-18	3.37e-18	54.21
325.00	3.17e-18	2.18e-18	5.34e-18	4.05e-18	59.26
2 + (H₂O)₂ ctst					
# Arrhenius equation A 3.26e-17 Ea 6.27 r**2 0.99999					
225.00	4.02e-11	1.78e-16	4.02e-11	3.98e-11	100.00
230.00	2.95e-11	1.13e-16	2.95e-11	2.93e-11	100.00
240.00	1.65e-11	5.34e-17	1.65e-11	1.66e-11	100.00

250.00	9.74e-12	3.05e-17	9.74e-12	9.80e-12	100.00
260.00	6.01e-12	2.05e-17	6.01e-12	6.03e-12	100.00
270.00	3.82e-12	1.55e-17	3.82e-12	3.85e-12	100.00
275.00	3.09e-12	1.40e-17	3.09e-12	3.11e-12	100.00
280.00	2.53e-12	1.28e-17	2.53e-12	2.54e-12	100.00
290.00	1.72e-12	1.12e-17	1.72e-12	1.72e-12	100.00
298.00	1.29e-12	1.05e-17	1.29e-12	1.28e-12	100.00
300.00	1.20e-12	1.03e-17	1.20e-12	1.20e-12	100.00
310.00	8.57e-13	9.70e-18	8.57e-13	8.53e-13	100.00
325.00	5.40e-13	9.22e-18	5.40e-13	5.33e-13	100.00

2 + (H₂O)₂ vtst

Arrhenius equation A 4.44e-17 Ea 5.50 r**2 0.99999

225.00	9.94e-12	9.63e-16	9.94e-12	9.84e-12	99.99
230.00	7.57e-12	7.66e-16	7.57e-12	7.53e-12	99.99
240.00	4.54e-12	5.32e-16	4.54e-12	4.56e-12	99.99
250.00	2.86e-12	4.04e-16	2.86e-12	2.87e-12	99.99
260.00	1.87e-12	3.22e-16	1.87e-12	1.88e-12	99.98
270.00	1.25e-12	2.66e-16	1.25e-12	1.26e-12	99.98
275.00	1.04e-12	2.46e-16	1.04e-12	1.05e-12	99.98
280.00	8.72e-13	2.27e-16	8.73e-13	8.77e-13	99.97
290.00	6.21e-13	1.97e-16	6.21e-13	6.23e-13	99.97
298.00	4.82e-13	1.78e-16	4.83e-13	4.82e-13	99.96
300.00	4.54e-13	1.74e-16	4.54e-13	4.53e-13	99.96
310.00	3.38e-13	1.56e-16	3.38e-13	3.37e-13	99.95
325.00	2.26e-13	1.35e-16	2.26e-13	2.23e-13	99.94

4 + H₂O ctst

Arrhenius equation A 2.72e-15 Ea -2.50 r**2 -0.97517

225.00	7.22e-18	5.77e-18	1.30e-17	1.01e-17	55.58
230.00	8.10e-18	4.38e-18	1.25e-17	1.14e-17	64.91
240.00	1.03e-17	2.76e-18	1.31e-17	1.43e-17	78.93
250.00	1.33e-17	1.99e-18	1.53e-17	1.76e-17	86.97
260.00	1.70e-17	1.63e-18	1.86e-17	2.14e-17	91.26
270.00	2.14e-17	1.47e-18	2.29e-17	2.56e-17	93.56
275.00	2.40e-17	1.45e-18	2.54e-17	2.79e-17	94.30
280.00	2.68e-17	1.45e-18	2.83e-17	3.02e-17	94.86
290.00	3.30e-17	1.52e-18	3.46e-17	3.53e-17	95.60
298.00	3.89e-17	1.64e-18	4.05e-17	3.97e-17	95.96
300.00	4.05e-17	1.67e-18	4.21e-17	4.08e-17	96.04
310.00	4.90e-17	1.90e-18	5.09e-17	4.67e-17	96.27
325.00	6.45e-17	2.37e-18	6.69e-17	5.64e-17	96.45

4 + H₂O vtst

Arrhenius equation A 1.60e-15 Ea -2.49 r**2 -0.98016

225.00	2.36e-18	5.04e-18	7.40e-18	6.08e-18	31.93
230.00	2.82e-18	4.73e-18	7.55e-18	6.86e-18	37.36
240.00	3.93e-18	4.34e-18	8.26e-18	8.61e-18	47.51
250.00	5.38e-18	4.17e-18	9.55e-18	1.06e-17	56.33
260.00	7.24e-18	4.15e-18	1.14e-17	1.29e-17	63.57
270.00	9.51e-18	4.23e-18	1.37e-17	1.54e-17	69.22
275.00	1.09e-17	4.32e-18	1.52e-17	1.67e-17	71.59
280.00	1.24e-17	4.43e-18	1.68e-17	1.82e-17	73.62

290.00	1.58e-17	4.71e-18	2.05e-17	2.12e-17	77.02
298.00	1.91e-17	5.00e-18	2.41e-17	2.38e-17	79.25
300.00	2.00e-17	5.09e-18	2.51e-17	2.45e-17	79.70
310.00	2.49e-17	5.55e-18	3.04e-17	2.80e-17	81.76
325.00	3.40e-17	6.45e-18	4.04e-17	3.38e-17	84.04

4 + (H₂O)₂ ctst

Arrhenius equation A 4.17e-18 Ea 7.12 r**2 0.99980

225.00	3.62e-11	1.61e-15	3.62e-11	3.42e-11	100.00
230.00	2.49e-11	9.13e-16	2.49e-11	2.42e-11	100.00
240.00	1.25e-11	3.40e-16	1.25e-11	1.27e-11	100.00
250.00	6.79e-12	1.57e-16	6.79e-12	6.97e-12	100.00
260.00	3.87e-12	8.73e-17	3.87e-12	4.02e-12	100.00
270.00	2.34e-12	5.64e-17	2.34e-12	2.41e-12	100.00
275.00	1.84e-12	4.75e-17	1.84e-12	1.89e-12	100.00
280.00	1.47e-12	4.10e-17	1.47e-12	1.50e-12	100.00
290.00	9.55e-13	3.24e-17	9.55e-13	9.66e-13	100.00
298.00	6.96e-13	2.79e-17	6.96e-13	6.93e-13	100.00
300.00	6.45e-13	2.71e-17	6.45e-13	6.40e-13	100.00
310.00	4.45e-13	2.37e-17	4.45e-13	4.35e-13	99.99
325.00	2.69e-13	2.05e-17	2.69e-13	2.55e-13	99.99

4 + (H₂O)₂ vtst

Arrhenius equation A 1.14e-17 Ea 6.15 r**2 0.99998

225.00	1.10e-11	8.25e-17	1.10e-11	1.08e-11	100.00
230.00	8.10e-12	6.95e-17	8.10e-12	8.03e-12	100.00
240.00	4.57e-12	5.14e-17	4.57e-12	4.58e-12	100.00
250.00	2.72e-12	4.04e-17	2.72e-12	2.73e-12	100.00
260.00	1.69e-12	3.30e-17	1.69e-12	1.70e-12	100.00
270.00	1.08e-12	2.79e-17	1.08e-12	1.09e-12	100.00
275.00	8.79e-13	2.60e-17	8.79e-13	8.87e-13	100.00
280.00	7.20e-13	2.43e-17	7.20e-13	7.25e-13	100.00
290.00	4.93e-13	2.16e-17	4.93e-13	4.95e-13	100.00
298.00	3.72e-13	2.00e-17	3.72e-13	3.72e-13	99.99
300.00	3.47e-13	1.97e-17	3.47e-13	3.47e-13	99.99
310.00	2.51e-13	1.81e-17	2.51e-13	2.49e-13	99.99
325.00	1.59e-13	1.65e-17	1.59e-13	1.57e-13	99.99

5 + H₂O ctst

Arrhenius equation A 1.17e-16 Ea -3.50 r**2 -0.94379

225.00	3.14e-20	4.72e-20	7.86e-20	1.00e+00	39.93
230.00	3.27e-20	3.78e-20	7.04e-20	1.00e+00	46.37
240.00	4.07e-20	2.65e-20	6.72e-20	1.00e+00	60.61
250.00	5.58e-20	2.09e-20	7.67e-20	1.00e+00	72.76
260.00	8.05e-20	1.87e-20	9.92e-20	1.00e+00	81.18
270.00	1.16e-19	1.86e-20	1.34e-19	1.00e+00	86.12
275.00	1.39e-19	1.92e-20	1.58e-19	1.00e+00	87.80
280.00	1.66e-19	2.02e-20	1.86e-19	1.00e+00	89.13
290.00	2.36e-19	2.35e-20	2.59e-19	1.00e+00	90.95
298.00	3.08e-19	2.74e-20	3.35e-19	1.00e+00	91.82
300.00	3.29e-19	2.85e-20	3.57e-19	1.00e+00	92.03
310.00	4.54e-19	3.58e-20	4.90e-19	1.00e+00	92.69
325.00	7.21e-19	5.22e-20	7.73e-19	1.00e+00	93.25

5 + (H₂O)₂ ctst					
# Arrhenius equation A 2.21e-18 Ea 3.57 r**2 0.99516					
225.00	7.44e-15	2.80e-18	7.44e-15	6.47e-15	99.96
230.00	5.81e-15	1.85e-18	5.81e-15	5.44e-15	99.97
240.00	3.81e-15	9.23e-19	3.81e-15	3.93e-15	99.98
250.00	2.71e-15	5.45e-19	2.71e-15	2.91e-15	99.98
260.00	2.03e-15	3.76e-19	2.03e-15	2.21e-15	99.98
270.00	1.58e-15	2.94e-19	1.58e-15	1.71e-15	99.98
275.00	1.42e-15	2.71e-19	1.42e-15	1.52e-15	99.98
280.00	1.28e-15	2.54e-19	1.28e-15	1.35e-15	99.98
290.00	1.06e-15	2.35e-19	1.06e-15	1.08e-15	99.98
298.00	9.23e-16	2.29e-19	9.23e-16	9.16e-16	99.98
300.00	8.93e-16	2.28e-19	8.93e-16	8.80e-16	99.97
310.00	7.69e-16	2.30e-19	7.69e-16	7.26e-16	99.97
325.00	6.29e-16	2.43e-19	6.30e-16	5.55e-16	99.96
6 + H₂O ctst					
# Arrhenius equation A 5.05e-16 Ea -3.07 r**2 -0.96294					
225.00	3.20e-19	4.37e-19	7.57e-19	1.00e+00	42.26
230.00	3.62e-19	3.44e-19	7.05e-19	1.00e+00	51.26
240.00	4.84e-19	2.32e-19	7.16e-19	1.00e+00	67.54
250.00	6.64e-19	1.77e-19	8.41e-19	1.00e+00	78.99
260.00	9.09e-19	1.50e-19	1.06e-18	1.00e+00	85.82
270.00	1.23e-18	1.42e-19	1.37e-18	1.00e+00	89.69
275.00	1.43e-18	1.42e-19	1.58e-18	1.00e+00	91.00
280.00	1.66e-18	1.45e-19	1.80e-18	1.00e+00	91.94
290.00	2.20e-18	1.58e-19	2.36e-18	1.00e+00	93.29
298.00	2.73e-18	1.76e-19	2.91e-18	1.00e+00	93.95
300.00	2.88e-18	1.81e-19	3.06e-18	1.00e+00	94.09
310.00	3.72e-18	2.13e-19	3.93e-18	1.00e+00	94.58
325.00	5.35e-18	2.83e-19	5.63e-18	1.00e+00	94.97
6 + (H₂O)₂ ctst					
# Arrhenius equation A 1.40e-18 Ea 5.39 r**2 0.99939					
225.00	2.60e-13	2.83e-17	2.60e-13	2.42e-13	99.99
230.00	1.93e-13	1.88e-17	1.93e-13	1.86e-13	99.99
240.00	1.13e-13	9.31e-18	1.13e-13	1.14e-13	99.99
250.00	6.99e-14	5.43e-18	6.99e-14	7.25e-14	99.99
260.00	4.58e-14	3.64e-18	4.58e-14	4.78e-14	99.99
270.00	3.11e-14	2.70e-18	3.11e-14	3.25e-14	99.99
275.00	2.60e-14	2.42e-18	2.60e-14	2.70e-14	99.99
280.00	2.20e-14	2.20e-18	2.20e-14	2.27e-14	99.99
290.00	1.60e-14	1.89e-18	1.60e-14	1.62e-14	99.99
298.00	1.27e-14	1.74e-18	1.27e-14	1.26e-14	99.99
300.00	1.20e-14	1.71e-18	1.20e-14	1.19e-14	99.99
310.00	9.17e-15	1.59e-18	9.17e-15	8.87e-15	99.98
325.00	6.36e-15	1.50e-18	6.36e-15	5.93e-15	99.98

Table S7: Relative reaction rates (v₂/v₁) according equation 11 of the main text) computed at different temperatures (T in Kelvin) and at different relative humidities (RH). ^a

T (K)	20% RH	40% RH	60% RH	80% RH	100% RH
Entry 1					
275.00	2.71e+01	5.43e+01	8.13e+01	1.09e+02	1.36e+02
280.00	2.47e+01	4.94e+01	7.42e+01	9.90e+01	1.23e+02
290.00	2.12e+01	4.25e+01	6.38e+01	8.50e+01	1.06e+02
298.00	1.92e+01	3.85e+01	5.78e+01	7.69e+01	9.61e+01
300.00	1.86e+01	3.72e+01	5.58e+01	7.45e+01	9.28e+01
310.00	1.62e+01	3.25e+01	4.88e+01	6.47e+01	8.10e+01
Entry 2					
275.00	7.54e+01	1.51e+02	2.26e+02	3.02e+02	3.78e+02
280.00	7.10e+01	1.42e+02	2.13e+02	2.84e+02	3.55e+02
290.00	6.34e+01	1.27e+02	1.91e+02	2.54e+02	3.17e+02
298.00	5.88e+01	1.18e+02	1.77e+02	2.35e+02	2.94e+02
300.00	5.68e+01	1.14e+02	1.70e+02	2.27e+02	2.83e+02
310.00	4.95e+01	9.90e+01	1.49e+02	1.97e+02	2.47e+02
Entry 3					
275.00	1.85e+00	3.72e+00	5.56e+00	7.43e+00	9.29e+00
280.00	1.76e+00	3.51e+00	5.27e+00	7.04e+00	8.78e+00
290.00	1.62e+00	3.24e+00	4.86e+00	6.47e+00	8.09e+00
298.00	1.55e+00	3.10e+00	4.65e+00	6.19e+00	7.74e+00
300.00	1.52e+00	3.05e+00	4.57e+00	6.09e+00	7.59e+00
310.00	1.41e+00	2.82e+00	4.24e+00	5.62e+00	7.03e+00
Entry 4					
275.00	7.34e+00	1.47e+01	2.20e+01	2.94e+01	3.67e+01
280.00	6.79e+00	1.36e+01	2.04e+01	2.72e+01	3.39e+01
290.00	5.94e+00	1.19e+01	1.79e+01	2.38e+01	2.98e+01
298.00	5.43e+00	1.09e+01	1.63e+01	2.17e+01	2.71e+01
300.00	5.25e+00	1.05e+01	1.57e+01	2.10e+01	2.62e+01
310.00	4.60e+00	9.19e+00	1.38e+01	1.83e+01	2.29e+01
Entry 5					
275.00	1.14e+00	2.28e+00	3.42e+00	4.56e+00	5.71e+00
280.00	1.09e+00	2.18e+00	3.26e+00	4.36e+00	5.43e+00
290.00	1.01e+00	2.02e+00	3.04e+00	4.04e+00	5.06e+00
298.00	9.70e-01	1.94e+00	2.91e+00	3.88e+00	4.85e+00
300.00	9.48e-01	1.90e+00	2.84e+00	3.79e+00	4.72e+00
310.00	8.75e-01	1.75e+00	2.63e+00	3.49e+00	4.36e+00
Entry 6					
275.00	2.09e+00	4.20e+00	6.28e+00	8.38e+00	1.05e+01
280.00	1.93e+00	3.86e+00	5.79e+00	7.73e+00	9.64e+00
290.00	1.67e+00	3.35e+00	5.03e+00	6.70e+00	8.38e+00
298.00	1.53e+00	3.07e+00	4.60e+00	6.13e+00	7.66e+00
300.00	1.48e+00	2.96e+00	4.43e+00	5.91e+00	7.37e+00
310.00	1.30e+00	2.60e+00	3.91e+00	5.19e+00	6.49e+00
Entry 7					
275.00	6.57e-01	1.32e+00	1.97e+00	2.63e+00	3.29e+00
280.00	6.13e-01	1.22e+00	1.84e+00	2.45e+00	3.06e+00
290.00	5.50e-01	1.10e+00	1.65e+00	2.20e+00	2.75e+00
298.00	5.23e-01	1.05e+00	1.57e+00	2.09e+00	2.61e+00
300.00	5.05e-01	1.01e+00	1.52e+00	2.02e+00	2.52e+00
310.00	4.63e-01	9.26e-01	1.39e+00	1.85e+00	2.31e+00

Entry 8					
275.00	1.14e+00	2.29e+00	3.42e+00	4.57e+00	5.71e+00
280.00	1.07e+00	2.13e+00	3.19e+00	4.26e+00	5.32e+00
290.00	9.48e-01	1.90e+00	2.85e+00	3.80e+00	4.75e+00
298.00	8.88e-01	1.78e+00	2.67e+00	3.55e+00	4.44e+00
300.00	8.66e-01	1.73e+00	2.60e+00	3.46e+00	4.32e+00
310.00	7.84e-01	1.57e+00	2.36e+00	3.13e+00	3.91e+00
Entry 9					
275.00	4.79e-01	9.61e-01	1.44e+00	1.92e+00	2.40e+00
280.00	4.55e-01	9.08e-01	1.36e+00	1.82e+00	2.27e+00
290.00	4.17e-01	8.36e-01	1.26e+00	1.67e+00	2.09e+00
298.00	4.01e-01	8.03e-01	1.20e+00	1.60e+00	2.00e+00
300.00	3.93e-01	7.85e-01	1.18e+00	1.57e+00	1.96e+00
310.00	3.65e-01	7.29e-01	1.10e+00	1.45e+00	1.82e+00
Entry 10					
275.00	7.99e+00	1.60e+01	2.40e+01	3.20e+01	4.00e+01
280.00	7.26e+00	1.45e+01	2.18e+01	2.91e+01	3.62e+01
290.00	6.13e+00	1.23e+01	1.85e+01	2.46e+01	3.07e+01
298.00	5.54e+00	1.11e+01	1.66e+01	2.22e+01	2.77e+01
300.00	5.35e+00	1.07e+01	1.60e+01	2.14e+01	2.66e+01
310.00	4.62e+00	9.24e+00	1.39e+01	1.84e+01	2.30e+01
Entry 11					
275.00	5.08e+00	1.02e+01	1.52e+01	2.03e+01	2.54e+01
280.00	4.69e+00	9.36e+00	1.41e+01	1.88e+01	2.34e+01
290.00	4.05e+00	8.12e+00	1.22e+01	1.62e+01	2.03e+01
298.00	3.73e+00	7.47e+00	1.12e+01	1.49e+01	1.86e+01
300.00	3.61e+00	7.23e+00	1.08e+01	1.45e+01	1.80e+01
310.00	3.20e+00	6.40e+00	9.62e+00	1.28e+01	1.60e+01
Entry 12					
275.00	5.26e-01	1.05e+00	1.58e+00	2.11e+00	2.63e+00
280.00	5.04e-01	1.01e+00	1.51e+00	2.02e+00	2.52e+00
290.00	4.79e-01	9.60e-01	1.44e+00	1.92e+00	2.40e+00
298.00	4.66e-01	9.34e-01	1.40e+00	1.86e+00	2.33e+00
300.00	4.60e-01	9.19e-01	1.38e+00	1.84e+00	2.29e+00
310.00	4.34e-01	8.67e-01	1.30e+00	1.73e+00	2.16e+00

a) For entries **1, 2, 3,** and **4** these values are computed using VTST rate constants;
For entries **5, 6, 7, 8,** and **9** these values are computed using CTST rate constants

Table S8: Effective rate constants (k_{eff} in $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$), computed at different temperatures (T in Kelvin), and at different relative humidities (RH), for the reaction of carbonyl oxides with water. ^a These values have been computed according equation 13 of the main text.

T (K)	20% RH	40% RH	60% RH	80% RH	100% RH
Entry 1					
275.00	6.94e-14	1.37e-13	2.03e-13	2.70e-13	3.38e-13

280.00	6.67e-14	1.31e-13	1.95e-13	2.59e-13	3.22e-13
290.00	6.32e-14	1.24e-13	1.84e-13	2.44e-13	3.05e-13
298.00	6.18e-14	1.21e-13	1.79e-13	2.38e-13	2.97e-13
300.00	6.07e-14	1.18e-13	1.76e-13	2.34e-13	2.90e-13
310.00	5.78e-14	1.12e-13	1.67e-13	2.21e-13	2.75e-13

Entry 2

275.00	1.34e-16	2.67e-16	3.99e-16	5.31e-16	6.64e-16
280.00	1.40e-16	2.78e-16	4.17e-16	5.55e-16	6.92e-16
290.00	1.56e-16	3.10e-16	4.64e-16	6.16e-16	7.70e-16
298.00	1.73e-16	3.43e-16	5.13e-16	6.82e-16	8.52e-16
300.00	1.75e-16	3.47e-16	5.19e-16	6.91e-16	8.60e-16
310.00	1.92e-16	3.81e-16	5.70e-16	7.55e-16	9.43e-16

Entry 3

275.00	4.36e-13	7.20e-13	1.00e-12	1.29e-12	1.57e-12
280.00	4.09e-13	6.69e-13	9.30e-13	1.19e-12	1.45e-12
290.00	3.67e-13	5.94e-13	8.22e-13	1.05e-12	1.27e-12
298.00	3.44e-13	5.53e-13	7.62e-13	9.69e-13	1.18e-12
300.00	3.35e-13	5.37e-13	7.40e-13	9.42e-13	1.14e-12
310.00	3.06e-13	4.85e-13	6.66e-13	8.42e-13	1.02e-12

Entry 4

275.00	1.27e-16	2.39e-16	3.50e-16	4.62e-16	5.74e-16
280.00	1.31e-16	2.45e-16	3.59e-16	4.74e-16	5.86e-16
290.00	1.42e-16	2.65e-16	3.87e-16	5.08e-16	6.31e-16
298.00	1.55e-16	2.86e-16	4.17e-16	5.47e-16	6.78e-16
300.00	1.56e-16	2.88e-16	4.19e-16	5.51e-16	6.80e-16
310.00	1.70e-16	3.10e-16	4.51e-16	5.88e-16	7.27e-16

Entry 5

275.00	3.38e-19	5.18e-19	6.97e-19	8.78e-19	1.06e-18
280.00	3.89e-19	5.91e-19	7.93e-19	9.97e-19	1.20e-18
290.00	5.21e-19	7.84e-19	1.05e-18	1.31e-18	1.57e-18
298.00	6.60e-19	9.86e-19	1.31e-18	1.63e-18	1.96e-18
300.00	6.95e-19	1.03e-18	1.37e-18	1.71e-18	2.04e-18
310.00	9.19e-19	1.35e-18	1.78e-18	2.20e-18	2.63e-18

Entry 6

275.00	4.87e-18	8.19e-18	1.15e-17	1.48e-17	1.81e-17
280.00	5.28e-18	8.76e-18	1.22e-17	1.57e-17	1.92e-17
290.00	6.30e-18	1.03e-17	1.42e-17	1.82e-17	2.21e-17
298.00	7.36e-18	1.18e-17	1.63e-17	2.07e-17	2.52e-17
300.00	7.59e-18	1.21e-17	1.66e-17	2.12e-17	2.56e-17
310.00	9.04e-18	1.42e-17	1.93e-17	2.43e-17	2.94e-17

Entry 7

275.00	2.87e-18	4.01e-18	5.15e-18	6.29e-18	7.43e-18
280.00	3.32e-18	4.57e-18	5.83e-18	7.10e-18	8.34e-18
290.00	4.43e-18	6.01e-18	7.58e-18	9.15e-18	1.07e-17
298.00	5.56e-18	7.48e-18	9.38e-18	1.13e-17	1.32e-17
300.00	5.87e-18	7.84e-18	9.81e-18	1.18e-17	1.37e-17
310.00	7.63e-18	1.01e-17	1.25e-17	1.49e-17	1.73e-17

Entry 8

275.00	2.40e-17	3.69e-17	4.96e-17	6.25e-17	7.53e-17
280.00	2.59e-17	3.92e-17	5.26e-17	6.60e-17	7.92e-17

290.00	3.06e-17	4.56e-17	6.06e-17	7.54e-17	9.04e-17
298.00	3.53e-17	5.19e-17	6.85e-17	8.50e-17	1.02e-16
300.00	3.63e-17	5.32e-17	7.01e-17	8.69e-17	1.04e-16
310.00	4.26e-17	6.14e-17	8.02e-17	9.86e-17	1.17e-16
Entry 9					
275.00	3.70e-15	4.90e-15	6.09e-15	7.30e-15	8.50e-15
280.00	3.76e-15	4.93e-15	6.11e-15	7.29e-15	8.45e-15
290.00	3.91e-15	5.07e-15	6.23e-15	7.37e-15	8.53e-15
298.00	4.08e-15	5.25e-15	6.41e-15	7.57e-15	8.74e-15
300.00	4.09e-15	5.25e-15	6.40e-15	7.56e-15	8.70e-15
310.00	4.29e-15	5.43e-15	6.59e-15	7.71e-15	8.86e-15
Entry 10					
275.00	3.28e-17	6.21e-17	9.11e-17	1.20e-16	1.50e-16
280.00	3.48e-17	6.53e-17	9.59e-17	1.27e-16	1.57e-16
290.00	3.97e-17	7.39e-17	1.08e-16	1.42e-16	1.76e-16
298.00	4.50e-17	8.32e-17	1.21e-16	1.59e-16	1.97e-16
300.00	4.59e-17	8.45e-17	1.23e-16	1.62e-16	2.00e-16
310.00	5.22e-17	9.50e-17	1.38e-16	1.80e-16	2.23e-16
Entry 11					
275.00	5.39e-19	9.91e-19	1.44e-18	1.89e-18	2.34e-18
280.00	6.22e-19	1.13e-18	1.65e-18	2.16e-18	2.67e-18
290.00	8.35e-19	1.51e-18	2.18e-18	2.85e-18	3.52e-18
298.00	1.07e-18	1.91e-18	2.75e-18	3.58e-18	4.42e-18
300.00	1.12e-18	2.00e-18	2.87e-18	3.75e-18	4.61e-18
310.00	1.47e-18	2.59e-18	3.71e-18	4.81e-18	5.93e-18
Entry 12					
275.00	2.63e-14	3.54e-14	4.44e-14	5.35e-14	6.26e-14
280.00	2.57e-14	3.43e-14	4.30e-14	5.16e-14	6.01e-14
290.00	2.48e-14	3.29e-14	4.10e-14	4.90e-14	5.71e-14
298.00	2.45e-14	3.23e-14	4.01e-14	4.78e-14	5.56e-14
300.00	2.43e-14	3.20e-14	3.96e-14	4.73e-14	5.48e-14
310.00	2.38e-14	3.10e-14	3.83e-14	4.54e-14	5.25e-14

- a) For entries **1**, **2**, **3**, and **4** these values are computed using VTST rate constants;
for entries **5**, **6**, **7**, **8**, and **9** these values are computed using CTST rate constants.