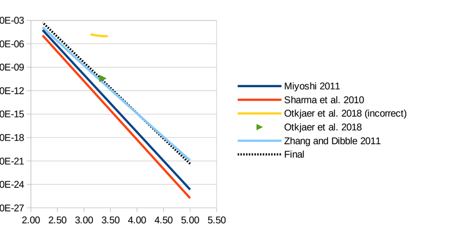
Aliphatic RO2

1,4 Hshift

P1 1.26E+12 5.6E+11 5.67E+13 1.00E-02
P2 16930 0.2 1.88E+04 4.007
P3 34.2 5.26E+08 12964
Ea shift -1.12E+03

-CH2OO. | -CH3

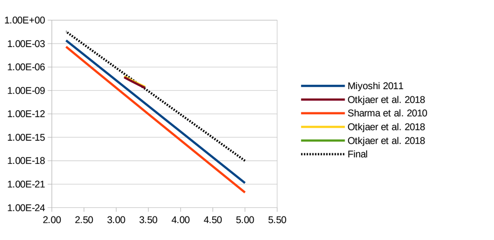
T	Miyoshi 2011	Sharma et al.	Otkjaer et al.	Otkjaer et al.	Zhang and Dibble 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200	2.17E-25	1.71E-26			1.17E-21	1.63E-24		4.34E-22	5.00	5.00E-03	-2.30E+00	-2.14E+01	A		3.97E-22
225	2.64E-21	2.49E-22			2.53E-18	1.18E-20		1.69E-18	4.44	4.44E-03	-2.35E+00	-1.78E+01		1.48E+11	0.92
250	4.90E-18	5.34E-19			1.23E-15	1.47E-17		1.28E-15	4.00	4.00E-03	-2.40E+00	-1.49E+01	Ea		
260	6.62E-17	7.60E-18			1.05E-14	1.74E-16		1.28E-14	3.85	3.85E-03	-2.41E+00	-1.39E+01		1.50E+04	
270	7.39E-16	8.90E-17			7.77E-14	1.72E-15		1.08E-13	3.70	3.70E-03	-2.43E+00	-1.30E+01			1.03
280	6.94E-15	8.73E-16			4.99E-13	1.45E-14		7.79E-13	3.57	3.57E-03	-2.45E+00	-1.21E+01			8.03E-13
290	5.58E-14	7.32E-15	9.24E-06		2.84E-12	1.05E-13		4.93E-12	3.45	3.45E-03	-2.46E+00	-1.13E+01		-1.40E+00	
298	2.67E-13	3.62E-14	9.71E-06	3.72E-11	1.05E-11	4.67E-13	1.98E-11	1.98E-11	3.36	3.36E-03	-2.47E+00	-1.07E+01		-6.33E+03	
310	2.41E-12	3.42E-13	1.21E-05		6.63E-11	3.79E-12		1.39E-10	3.23	3.23E-03	-2.49E+00	-9.86E+00		7.08E+00	
320	1.33E-11	1.95E-12	1.62E-05		2.78E-10	1.93E-11		6.32E-10	3.13	3.13E-03	-2.51E+00	-9.20E+00		#N/A	
330	6.60E-11	1.00E-11			1.07E-09	8.92E-11		2.63E-09	3.03	3.03E-03	-2.52E+00	-8.58E+00		#N/A	
340	2.99E-10	4.67E-11			3.84E-09	3.77E-10		1.00E-08	2.94	2.94E-03	-2.53E+00	-8.00E+00	A		1.00E-08
350	1.24E-09	1.99E-10			1.28E-08	1.47E-09		3.56E-08	2.86	2.86E-03	-2.54E+00	-7.45E+00		1.21E+07	1.00
375	3.11E-08	5.37E-09			2.00E-07	3.22E-08		6.32E-07	2.67	2.67E-03	-2.57E+00	-6.20E+00	n		
400	5.23E-07	9.57E-08			2.25E-06	4.83E-07		7.86E-06	2.50	2.50E-03	-2.60E+00	-5.10E+00		1.40	
425	6.31E-06	1.22E-06			1.93E-05	5.29E-06		7.31E-05	2.35	2.35E-03	-2.63E+00	-4.14E+00	Ea		1.00
450	5.77E-05	1.17E-05			1.32E-04	4.46E-05		5.33E-04	2.22	2.22E-03	-2.65E+00	-3.27E+00		14586	5.33E-04



P1 1.02E+12 4E+11 4.77E+12 6.53E+12 4.67E+12
P2 15130 1.1 1.68E+04 1.70E+04 1.69E+04
P3 30.1 2.21E+08 2.28E+08 2.23E+08
Ea shift -1.59E+03

-CH2OO. | -CH2-

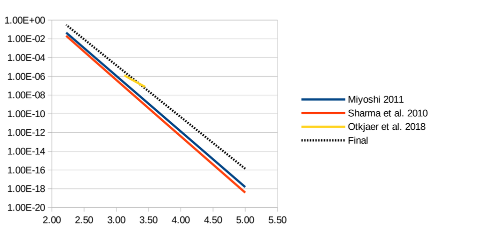
T	Miyoshi 2011	Sharma et al.	Otkjaer et al.	Otkjaer et al.	Otkjaer et al. 2018	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200	1.43E-21	8.68E-23				3.52E-22		9.90E-19	5.00	5.00E-03	-2.30E+00	-1.80E+01	A		9.56E-19
225	6.38E-18	4.47E-19				1.69E-18		1.96E-15	4.44	4.44E-03	-2.35E+00	-1.47E+01		5.73E+11	0.97
250	5.31E-15	4.21E-16				1.50E-15		8.59E-13	4.00	4.00E-03	-2.40E+00	-1.21E+01	Ea		
260	5.45E-14	4.52E-15				1.57E-14		7.06E-12	3.85	3.85E-03	-2.41E+00	-1.12E+01		1.37E+04	
270	4.70E-13	4.08E-14				1.38E-13		4.97E-11	3.70	3.70E-03	-2.43E+00	-1.03E+01			1.01
280	3.48E-12	3.15E-13				1.05E-12		3.04E-10	3.57	3.57E-03	-2.45E+00	-9.52E+00			3.08E-10
290	2.24E-11	2.11E-12	2.85E-09	2.61E-09	2.14E-09	6.88E-12		1.65E-09	3.45	3.45E-03	-2.46E+00	-8.78E+00		-5.50E-01	
298	9.09E-11	8.85E-12	6.63E-09	6.05E-09	5.01E-09	2.84E-11	5.86E-09	5.86E-09	3.36	3.36E-03	-2.47E+00	-8.23E+00		-5.89E+03	
310	6.49E-10	6.61E-11	2.31E-08	2.10E-08	1.75E-08	2.07E-10		3.48E-08	3.23	3.23E-03	-2.49E+00	-7.46E+00		1.02E+01	
320	2.98E-09	3.15E-10	6.41E-08	5.82E-08	4.88E-08	9.70E-10		1.39E-07	3.13	3.13E-03	-2.51E+00	-6.86E+00		#N/A	
330	1.25E-08	1.37E-09				4.14E-09		5.09E-07	3.03	3.03E-03	-2.52E+00	-6.29E+00		#N/A	
340	4.81E-08	5.46E-09				1.62E-08		1.73E-06	2.94	2.94E-03	-2.53E+00	-5.76E+00	A		1.73E-06
350	1.72E-07	2.01E-08				5.88E-08		5.50E-06	2.86	2.86E-03	-2.54E+00	-5.26E+00		1.43E+10	1.00
375	3.06E-06	3.89E-07				1.09E-06		7.54E-05	2.67	2.67E-03	-2.57E+00	-4.12E+00	n		
400	3.81E-05	5.21E-06				1.41E-05		7.48E-04	2.50	2.50E-03	-2.60E+00	-3.13E+00		0.55	
425	3.53E-04	5.17E-05				1.35E-04		5.67E-03	2.35	2.35E-03	-2.63E+00	-2.25E+00	Ea		1.00
450	2.55E-03	3.99E-04				1.01E-03		3.44E-02	2.22	2.22E-03	-2.65E+00	-1.46E+00		13551	3.44E-02



P1 6.95E+11 5.8E+11 1.94E+12
P2 13660 0.8 1.54E+04
P3 27.1 2.05E+08
Ea shift -1.03E+03

-CH2OO. | >CH-

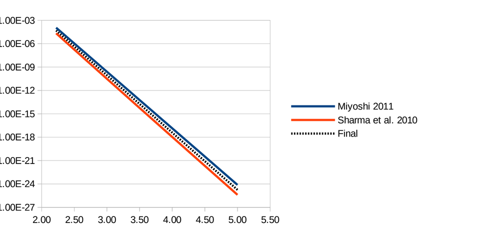
T	Miyoshi 2011	Sharma et al.	Otkjaer et al. 2018	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200	1.51E-18	3.88E-19		7.66E-19		1.35E-16	5.00	5.00E-03	-2.30E+00	-1.59E+01	A		1.32E-16
225	2.99E-15	8.32E-16		1.58E-15		1.57E-13	4.44	4.44E-03	-2.35E+00	-1.28E+01		5.86E+11	0.98
250	1.29E-12	3.88E-13		7.09E-13		4.45E-11	4.00	4.00E-03	-2.40E+00	-1.04E+01	Ea		
260	1.06E-11	3.27E-12		5.88E-12		3.15E-10	3.85	3.85E-03	-2.41E+00	-9.50E+00		1.27E+04	
270	7.41E-11	2.35E-11		4.17E-11		1.93E-09	3.70	3.70E-03	-2.43E+00	-8.71E+00			1.01
280	4.51E-10	1.47E-10		2.57E-10		1.04E-08	3.57	3.57E-03	-2.45E+00	-7.98E+00			1.05E-08
290	2.43E-09	8.10E-10	7.51E-08	1.40E-09		4.97E-08	3.45	3.45E-03	-2.46E+00	-7.30E+00		-4.00E-01	
298	8.60E-09	2.93E-09	1.62E-07	5.02E-09	1.62E-07	1.62E-07	3.36	3.36E-03	-2.47E+00	-6.79E+00		-5.48E+03	
310	5.07E-08	1.78E-08	5.03E-07	3.00E-08		8.46E-07	3.23	3.23E-03	-2.49E+00	-6.07E+00		1.06E+01	
320	2.01E-07	7.20E-08	1.27E-06	1.20E-07		3.05E-06	3.13	3.13E-03	-2.51E+00	-5.52E+00		#N/A	
330	7.33E-07	2.69E-07		4.44E-07		1.02E-05	3.03	3.03E-03	-2.52E+00	-4.99E+00		#N/A	
340	2.47E-06	9.28E-07		1.52E-06		3.18E-05	2.94	2.94E-03	-2.53E+00	-4.50E+00	A		3.18E-05
350	7.80E-06	2.99E-06		4.83E-06		9.29E-05	2.86	2.86E-03	-2.54E+00	-4.03E+00		4.01E+10	1.00
375	1.05E-04	4.24E-05		6.68E-05		1.06E-03	2.67	2.67E-03	-2.57E+00	-2.98E+00	n		
400	1.03E-03	4.34E-04		6.67E-04		8.86E-03	2.50	2.50E-03	-2.60E+00	-2.05E+00		0.40	
425	7.64E-03	3.38E-03		5.08E-03		5.81E-02	2.35	2.35E-03	-2.63E+00	-1.24E+00	Ea		1.00
450	4.56E-02	2.11E-02		3.10E-02		3.09E-01	2.22	2.22E-03	-2.65E+00	-5.10E-01		12614	3.09E-01



P1 1.54E+12 9.70E+11
P2 16720.0 1.1
P3 33.5
Ea shift 0.00E+00

>CHOO. | -CH3

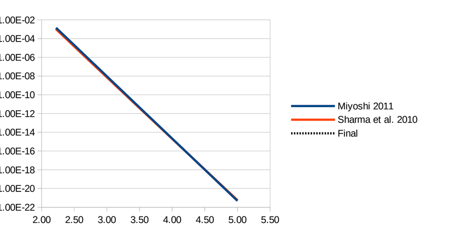
T	Miyoshi 2011	Sharma et al. 2010	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200	7.59E-25	4.05E-26	1.75E-25		1.75E-25	5.00	5.00E-03	-2.30E+00	-2.48E+01	A		1.70E-25
225	8.22E-21	5.39E-22	2.10E-21		2.10E-21	4.44	4.44E-03	-2.35E+00	-2.07E+01		1.10E+12	0.97
250	1.39E-17	1.09E-18	3.88E-18		3.88E-18	4.00	4.00E-03	-2.40E+00	-1.74E+01	Ea		
260	1.82E-16	1.52E-17	5.25E-17		5.25E-17	3.85	3.85E-03	-2.41E+00	-1.63E+01		1.70E+04	
270	1.97E-15	1.75E-16	5.86E-16		5.86E-16	3.70	3.70E-03	-2.43E+00	-1.52E+01			1.01
280	1.79E-14	1.69E-15	5.51E-15		5.51E-15	3.57	3.57E-03	-2.45E+00	-1.43E+01			5.58E-15
290	1.41E-13	1.40E-14	4.44E-14		4.44E-14	3.45	3.45E-03	-2.46E+00	-1.34E+01		-5.50E-01	
298	6.61E-13	6.88E-14	2.13E-13	2.13E-13	2.13E-13	3.36	3.36E-03	-2.47E+00	-1.27E+01		-7.29E+03	
310	5.80E-12	6.42E-13	1.93E-12		1.93E-12	3.23	3.23E-03	-2.49E+00	-1.17E+01		1.04E+01	
320	3.13E-11	3.64E-12	1.07E-11		1.07E-11	3.13	3.13E-03	-2.51E+00	-1.10E+01		#N/A	
330	1.52E-10	1.86E-11	5.32E-11		5.32E-11	3.03	3.03E-03	-2.52E+00	-1.03E+01		#N/A	
340	6.77E-10	8.63E-11	2.42E-10		2.42E-10	2.94	2.94E-03	-2.53E+00	-9.62E+00	A		2.42E-10
350	2.76E-09	3.67E-10	1.01E-09		1.01E-09	2.86	2.86E-03	-2.54E+00	-9.00E+00		2.74E+10	1.00
375	6.66E-08	9.84E-09	2.56E-08		2.56E-08	2.67	2.67E-03	-2.57E+00	-7.59E+00	n		
400	1.08E-06	1.75E-07	4.36E-07		4.36E-07	2.50	2.50E-03	-2.60E+00	-6.36E+00		0.55	
425	1.26E-05	2.24E-06	5.32E-06		5.32E-06	2.35	2.35E-03	-2.63E+00	-5.27E+00	Ea		1.00
450	1.12E-04	2.16E-05	4.93E-05		4.93E-05	2.22	2.22E-03	-2.65E+00	-4.31E+00		16790	4.93E-05



P1 8.50E+11 4.3E+11
P2 15310 0.9
P3 29.5
Ea shift 0.00E+00

>CHOO. | -CH2-

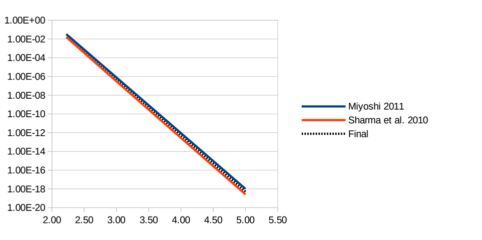
T	Miyoshi 2011	Sharma et al. 2010	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200	4.83E-22	5.83E-22	5.31E-22		5.31E-22	5.00	5.00E-03	-2.30E+00	-2.13E+01	A		5.16E-22
225	2.39E-18	2.48E-18	2.43E-18		2.43E-18	4.44	4.44E-03	-2.35E+00	-1.76E+01		5.53E+11	0.97
250	2.15E-15	2.00E-15	2.07E-15		2.07E-15	4.00	4.00E-03	-2.40E+00	-1.47E+01	Ea		
260	2.27E-14	2.03E-14	2.15E-14		2.15E-14	3.85	3.85E-03	-2.41E+00	-1.37E+01		1.52E+04	
270	2.01E-13	1.74E-13	1.87E-13		1.87E-13	3.70	3.70E-03	-2.43E+00	-1.27E+01			1.01
280	1.52E-12	1.28E-12	1.40E-12		1.40E-12	3.57	3.57E-03	-2.45E+00	-1.19E+01			1.41E-12
290	1.00E-11	8.24E-12	9.10E-12		9.10E-12	3.45	3.45E-03	-2.46E+00	-1.10E+01		-4.50E-01	
298	4.14E-11	3.34E-11	3.72E-11	3.72E-11	3.72E-11	3.36	3.36E-03	-2.47E+00	-1.04E+01		-6.55E+03	
310	3.03E-10	2.38E-10	2.68E-10		2.68E-10	3.23	3.23E-03	-2.49E+00	-9.57E+00		1.04E+01	
320	1.42E-09	1.09E-09	1.24E-09		1.24E-09	3.13	3.13E-03	-2.51E+00	-8.90E+00		#N/A	
330	6.04E-09	4.59E-09	5.26E-09		5.26E-09	3.03	3.03E-03	-2.52E+00	-8.28E+00		#N/A	
340	2.36E-08	1.77E-08	2.04E-08		2.04E-08	2.94	2.94E-03	-2.53E+00	-7.69E+00	A		2.04E-08
350	8.55E-08	6.32E-08	7.35E-08		7.35E-08	2.86	2.86E-03	-2.54E+00	-7.13E+00		2.70E+10	1.00
375	1.58E-06	1.14E-06	1.34E-06		1.34E-06	2.67	2.67E-03	-2.57E+00	-5.87E+00	n		
400	2.03E-05	1.43E-05	1.70E-05		1.70E-05	2.50	2.50E-03	-2.60E+00	-4.77E+00		0.45	
425	1.93E-04	1.34E-04	1.61E-04		1.61E-04	2.35	2.35E-03	-2.63E+00	-3.79E+00	Ea		1.00
450	1.42E-03	9.84E-04	1.18E-03		1.18E-03	2.22	2.22E-03	-2.65E+00	-2.93E+00		15078	1.18E-03



P1 5.41E+11 4.7E+11
P2 13690 0.6
P3 27.3
Ea shift 0.00E+00

>CHOO. | >CH-

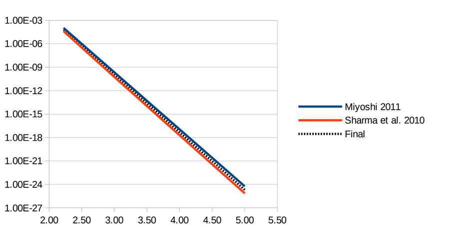
T	Miyoshi 2011	Sharma et al. 2010	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200	1.01E-18	2.62E-19	5.15E-19		5.15E-19	5.00	5.00E-03	-2.30E+00	-1.83E+01	A		5.06E-19
225	2.04E-15	5.81E-16	1.09E-15		1.09E-15	4.44	4.44E-03	-2.35E+00	-1.50E+01		4.75E+11	0.98
250	8.94E-13	2.77E-13	4.98E-13		4.98E-13	4.00	4.00E-03	-2.40E+00	-1.23E+01	Ea		
260	7.34E-12	2.35E-12	4.16E-12		4.16E-12	3.85	3.85E-03	-2.41E+00	-1.14E+01		1.38E+04	
270	5.16E-11	1.70E-11	2.97E-11		2.97E-11	3.70	3.70E-03	-2.43E+00	-1.05E+01			1.01
280	3.16E-10	1.07E-10	1.84E-10		1.84E-10	3.57	3.57E-03	-2.45E+00	-9.74E+00			1.85E-10
290	1.70E-09	5.94E-10	1.01E-09		1.01E-09	3.45	3.45E-03	-2.46E+00	-9.00E+00		-3.00E-01	
298	6.05E-09	2.16E-09	3.61E-09	3.61E-09	3.61E-09	3.36	3.36E-03	-2.47E+00	-8.44E+00		-5.96E+03	
310	3.58E-08	1.31E-08	2.17E-08		2.17E-08	3.23	3.23E-03	-2.49E+00	-7.66E+00		1.08E+01	
320	1.42E-07	5.35E-08	8.73E-08		8.73E-08	3.13	3.13E-03	-2.51E+00	-7.06E+00		#N/A	
330	5.21E-07	2.00E-07	3.23E-07		3.23E-07	3.03	3.03E-03	-2.52E+00	-6.49E+00		#N/A	
340	1.76E-06	6.94E-07	1.11E-06		1.11E-06	2.94	2.94E-03	-2.53E+00	-5.96E+00	A		1.11E-06
350	5.57E-06	2.24E-06	3.53E-06		3.53E-06	2.86	2.86E-03	-2.54E+00	-5.45E+00		6.35E+10	1.00
375	7.56E-05	3.20E-05	4.92E-05		4.92E-05	2.67	2.67E-03	-2.57E+00	-4.31E+00	n		
400	7.40E-04	3.28E-04	4.93E-04		4.93E-04	2.50	2.50E-03	-2.60E+00	-3.31E+00		0.30	
425	5.54E-03	2.57E-03	3.77E-03		3.77E-03	2.35	2.35E-03	-2.63E+00	-2.42E+00	Ea		1.00
450	3.32E-02	1.60E-02	2.30E-02		2.30E-02	2.22	2.22E-03	-2.65E+00	-1.64E+00		13715	2.30E-02



P1 1.80E+12 2E+12
P2 16810 1.2
P3 33.5
Ea shift 0.00E+00

>C(OO.)- | -CH3

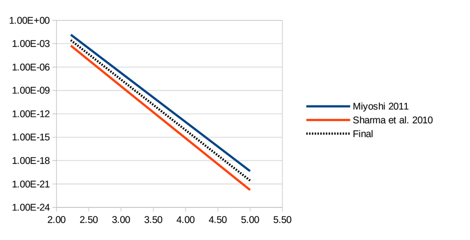
T	Miyoshi 2011	Sharma et al. 2010	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	5.66E-25	7.11E-26	2.01E-25		2.01E-25	5.00	5.00E-03	-2.30E+00	-2.47E+01	A		1.93E-25
225	6.44E-21	9.58E-22	2.48E-21		2.48E-21	4.44	4.44E-03	-2.35E+00	-2.06E+01		1.68E+12	0.96
250	1.13E-17	1.95E-18	4.70E-18		4.70E-18	4.00	4.00E-03	-2.40E+00	-1.73E+01	Ea		
260	1.50E-16	2.74E-17	6.41E-17		6.41E-17	3.85	3.85E-03	-2.41E+00	-1.62E+01		1.70E+04	
270	1.65E-15	3.16E-16	7.21E-16		7.21E-16	3.70	3.70E-03	-2.43E+00	-1.51E+01			1.01
280	1.52E-14	3.07E-15	6.84E-15		6.84E-15	3.57	3.57E-03	-2.45E+00	-1.42E+01			6.93E-15
290	1.21E-13	2.56E-14	5.55E-14		5.55E-14	3.45	3.45E-03	-2.46E+00	-1.33E+01		-6.00E-01	
298	5.71E-13	1.26E-13	2.68E-13	2.68E-13	2.68E-13	3.36	3.36E-03	-2.47E+00	-1.26E+01		-7.31E+03	
310	5.07E-12	1.18E-12	2.44E-12		2.44E-12	3.23	3.23E-03	-2.49E+00	-1.16E+01		1.05E+01	
320	2.76E-11	6.70E-12	1.36E-11		1.36E-11	3.13	3.13E-03	-2.51E+00	-1.09E+01		#N/A	
330	1.36E-10	3.43E-11	6.82E-11		6.82E-11	3.03	3.03E-03	-2.52E+00	-1.02E+01		#N/A	
340	6.07E-10	1.60E-10	3.11E-10		3.11E-10	2.94	2.94E-03	-2.53E+00	-9.51E+00	A		3.11E-10
350	2.49E-09	6.82E-10	1.30E-09		1.30E-09	2.86	2.86E-03	-2.54E+00	-8.88E+00		3.01E+10	1.00
375	6.13E-08	1.84E-08	3.36E-08		3.36E-08	2.67	2.67E-03	-2.57E+00	-7.47E+00	n		
400	1.01E-06	3.30E-07	5.77E-07		5.77E-07	2.50	2.50E-03	-2.60E+00	-6.24E+00		0.60	
425	1.20E-05	4.23E-06	7.12E-06		7.12E-06	2.35	2.35E-03	-2.63E+00	-5.15E+00	Ea		1.00
450	1.08E-04	4.11E-05	6.65E-05		6.65E-05	2.22	2.22E-03	-2.65E+00	-4.18E+00		16835	6.65E-05



P1 1.44E+12 4.1E+11
P2 14510 0.7
P3 30.1
Ea shift 0.00E+00

>C(OO.)- | -CH2-

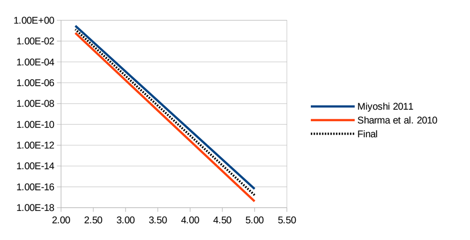
T	Miyoshi 2011	Sharma et al. 2010	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	4.47E-20	1.69E-22	2.75E-21		2.75E-21	5.00	5.00E-03	-2.30E+00	-2.06E+01	A		2.69E-21
225	1.42E-16	8.31E-19	1.09E-17		1.09E-17	4.44	4.44E-03	-2.35E+00	-1.70E+01		7.17E+11	0.98
250	8.95E-14	7.51E-16	8.20E-15		8.20E-15	4.00	4.00E-03	-2.40E+00	-1.41E+01	Ea		
260	8.34E-13	7.94E-15	8.14E-14		8.14E-14	3.85	3.85E-03	-2.41E+00	-1.31E+01		1.49E+04	
270	6.59E-12	7.05E-14	6.82E-13		6.82E-13	3.70	3.70E-03	-2.43E+00	-1.22E+01			1.01
280	4.49E-11	5.37E-13	4.91E-12		4.91E-12	3.57	3.57E-03	-2.45E+00	-1.13E+01			4.95E-12
290	2.68E-10	3.55E-12	3.09E-11		3.09E-11	3.45	3.45E-03	-2.46E+00	-1.05E+01		-3.50E-01	
298	1.03E-09	1.47E-11	1.23E-10	1.23E-10	1.23E-10	3.36	3.36E-03	-2.47E+00	-9.91E+00		-6.44E+03	
310	6.77E-09	1.08E-10	8.56E-10		8.56E-10	3.23	3.23E-03	-2.49E+00	-9.07E+00		1.08E+01	
320	2.92E-08	5.10E-10	3.86E-09		3.86E-09	3.13	3.13E-03	-2.51E+00	-8.41E+00		#N/A	
330	1.15E-07	2.19E-09	1.59E-08		1.59E-08	3.03	3.03E-03	-2.52E+00	-7.80E+00		#N/A	
340	4.21E-07	8.61E-09	6.02E-08		6.02E-08	2.94	2.94E-03	-2.53E+00	-7.22E+00	A		6.02E-08
350	1.42E-06	3.14E-08	2.11E-07		2.11E-07	2.86	2.86E-03	-2.54E+00	-6.67E+00		6.85E+10	1.00
375	2.26E-05	5.90E-07	3.65E-06		3.65E-06	2.67	2.67E-03	-2.57E+00	-5.44E+00	n		
400	2.54E-04	7.71E-06	4.42E-05		4.42E-05	2.50	2.50E-03	-2.60E+00	-4.35E+00		0.35	
425	2.14E-03	7.46E-05	4.00E-04		4.00E-04	2.35	2.35E-03	-2.63E+00	-3.40E+00	Ea		1.00
450	1.43E-02	5.63E-04	2.83E-03		2.83E-03	2.22	2.22E-03	-2.65E+00	-2.55E+00		14829	2.83E-03



P1 9.76E+11 5.5E+11
P2 12980 0.4
P3 26.4
Ea shift 0.00E+00

>C(OO.)- | >CH-

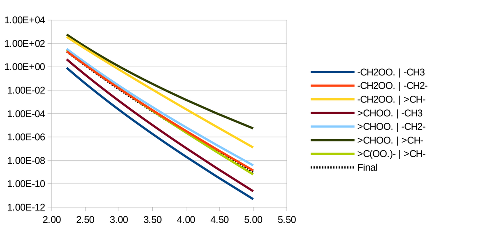
T	Miyoshi 2011	Sharma et al. 2010	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	6.36E-17	4.07E-18	1.61E-17		1.61E-17	5.00	5.00E-03	-2.30E+00	-1.68E+01	A		1.59E-17
225	8.62E-14	6.85E-15	2.43E-14		2.43E-14	4.44	4.44E-03	-2.35E+00	-1.36E+01		7.04E+11	0.99
250	2.76E-11	2.62E-12	8.51E-12		8.51E-12	4.00	4.00E-03	-2.40E+00	-1.11E+01	Ea		
260	2.03E-10	2.06E-11	6.47E-11		6.47E-11	3.85	3.85E-03	-2.41E+00	-1.02E+01		1.32E+04	
270	1.29E-09	1.39E-10	4.23E-10		4.23E-10	3.70	3.70E-03	-2.43E+00	-9.37E+00			1.00
280	7.19E-09	8.15E-10	2.42E-09		2.42E-09	3.57	3.57E-03	-2.45E+00	-8.62E+00			2.43E-09
290	3.56E-08	4.25E-09	1.23E-08		1.23E-08	3.45	3.45E-03	-2.46E+00	-7.91E+00		-2.00E-01	
298	1.18E-07	1.47E-08	4.17E-08	4.17E-08	4.17E-08	3.36	3.36E-03	-2.47E+00	-7.38E+00		-5.70E+03	
310	6.38E-07	8.38E-08	2.31E-07		2.31E-07	3.23	3.23E-03	-2.49E+00	-6.64E+00		1.13E+01	
320	2.36E-06	3.24E-07	8.75E-07		8.75E-07	3.13	3.13E-03	-2.51E+00	-6.06E+00		#N/A	
330	8.08E-06	1.15E-06	3.05E-06		3.05E-06	3.03	3.03E-03	-2.52E+00	-5.52E+00		#N/A	
340	2.57E-05	3.82E-06	9.90E-06		9.90E-06	2.94	2.94E-03	-2.53E+00	-5.00E+00	A		9.90E-06
350	7.64E-05	1.18E-05	3.00E-05		3.00E-05	2.86	2.86E-03	-2.54E+00	-4.52E+00		1.84E+11	1.00
375	9.06E-04	1.52E-04	3.71E-04		3.71E-04	2.67	2.67E-03	-2.57E+00	-3.43E+00	n		
400	7.88E-03	1.43E-03	3.36E-03		3.36E-03	2.50	2.50E-03	-2.60E+00	-2.47E+00		0.20	
425	5.32E-02	1.03E-02	2.35E-02		2.35E-02	2.35	2.35E-03	-2.63E+00	-1.63E+00	Ea		1.00
450	2.90E-01	6.01E-02	1.32E-01		1.32E-01	2.22	2.22E-03	-2.65E+00	-8.79E-01		13133	1.32E-01



1,5 Hshift

Average Temperature dependence
1.45E+02

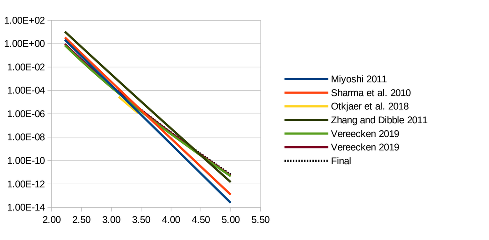
T	-CH2OO. | -C	-CH2OO. | -CI	-CH2OO. | >C	>CHOO. | -CH	>CHOO. | -CH	>CHOO. | >CI	>C(OO.)- | >CH-	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log()		log(T)	Replicate
200	4.82E-12	1.36E-09	1.26E-07	2.29E-11	3.73E-09	5.39E-06	6.25E-10	2.18E-09		1.06E-09	5.00	5.00E-03	-2.30E+00	-8.97E+00	A		5.39E-10
225	4.59E-10	9.63E-08	8.09E-06	2.38E-09	2.23E-07	1.12E-04	5.72E-08	1.43E-07		7.51E-08	4.44	4.44E-03	-2.35E+00	-7.12E+00		2.11E+09	0.51
250	2.05E-08	3.25E-06	2.37E-04	1.12E-07	6.66E-06	1.50E-03	2.34E-06	4.57E-06		2.56E-06	4.00	4.00E-03	-2.40E+00	-5.59E+00	Ea		
260	7.93E-08	1.13E-05	7.74E-04	4.41E-07	2.23E-05	3.84E-03	8.66E-06	1.56E-05		8.95E-06	3.85	3.85E-03	-2.41E+00	-5.05E+00		8.56E+03	
270	2.83E-07	3.62E-05	2.33E-03	1.59E-06	6.92E-05	9.37E-03	2.95E-05	4.95E-05		2.90E-05	3.70	3.70E-03	-2.43E+00	-4.54E+00			1.27
280	9.41E-07	1.08E-04	6.50E-03	5.34E-06	2.01E-04	2.19E-02	9.28E-05	1.47E-04		8.74E-05	3.57	3.57E-03	-2.45E+00	-4.06E+00			1.11E-04
290	2.93E-06	3.05E-04	1.70E-02	1.67E-05	5.51E-04	4.90E-02	2.73E-04	4.08E-04		2.48E-04	3.45	3.45E-03	-2.46E+00	-3.61E+00		-1.08E+01	
298	6.95E-06	6.68E-04	3.52E-02	3.99E-05	1.19E-03	9.11E-02	6.20E-04	8.88E-04	5.47E-04	5.47E-04	3.36	3.36E-03	-2.47E+00	-3.26E+00		-2.34E+03	
310	2.38E-05	2.03E-03	9.81E-02	1.37E-04	3.54E-03	2.21E-01	1.98E-03	2.69E-03		1.68E-03	3.23	3.23E-03	-2.49E+00	-2.77E+00		-2.21E+01	
320	6.29E-05	4.88E-03	2.19E-01	3.62E-04	8.35E-03	4.49E-01	4.92E-03	6.42E-03		4.08E-03	3.13	3.13E-03	-2.51E+00	-2.39E+00		#N/A	
330	1.59E-04	1.12E-02	4.66E-01	9.13E-04	1.89E-02	8.84E-01	1.17E-02	1.47E-02		9.47E-03	3.03	3.03E-03	-2.52E+00	-2.02E+00		#N/A	
340	3.84E-04	2.47E-02	9.53E-01	2.21E-03	4.12E-02	1.69E+00	2.65E-02	3.23E-02		2.11E-02	2.94	2.94E-03	-2.53E+00	-1.68E+00	A		2.11E-02
350	8.94E-04	5.25E-02	1.88E+00	5.12E-03	8.68E-02	3.17E+00	5.78E-02	6.86E-02		4.54E-02	2.86	2.86E-03	-2.54E+00	-1.34E+00		7.45E-23	1.00
375	6.35E-03	3.00E-01	8.87E+00	3.59E-02	4.87E-01	1.38E+01	3.49E-01	3.92E-01		2.66E-01	2.67	2.67E-03	-2.57E+00	-5.74E-01	n		
400	3.74E-02	1.43E+00	3.52E+01	2.08E-01	2.31E+00	5.30E+01	1.75E+00	1.88E+00		1.31E+00	2.50	2.50E-03	-2.60E+00	1.18E-01		10.79	
425	1.88E-01	5.91E+00	1.20E+02	1.03E+00	9.50E+00	1.84E+02	7.47E+00	7.83E+00		5.57E+00	2.35	2.35E-03	-2.63E+00	7.46E-01	Ea		1.00
450	8.29E-01	2.15E+01	3.65E+02	4.42E+00	3.46E+01	5.85E+02	2.79E+01	2.88E+01		2.09E+01	2.22	2.22E-03	-2.65E+00	1.32E+00		5382	2.09E+01



P1 3.07E+11 2.45E+11 3.87E+11 6.20E-34 1.63825E-31 1.80E+06
P2 11560 1.366666667 1.27E+04 1.43E+01 13.55030662 1.729
P3 21.36666667 8.36E+07 5108.248122 5380.744254 10167
Ea shift -5.00E+01

-CH2OO. | -CH3

T	Miyoshi 2011	Sharma et al.	Otkjaer et al.	Vereecken 20	Vereecken 20	Zhang and Dibble 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200	2.43E-14	1.21E-13		4.54E-12	5.13E-12	1.43E-12	4.82E-12		6.19E-12	5.00	5.00E-03	-2.30E+00	-1.12E+01	A		2.59E-12
225	1.49E-11	5.60E-11		4.19E-10	5.03E-10	4.98E-10	4.59E-10		5.73E-10	4.44	4.44E-03	-2.35E+00	-9.24E+00		4.08E+08	0.42
250	2.54E-09	7.69E-09		1.83E-08	2.29E-08	5.48E-08	2.05E-08		2.50E-08	4.00	4.00E-03	-2.40E+00	-7.60E+00	Ea		
260	1.51E-08	4.24E-08		7.06E-08	8.92E-08	2.80E-07	7.93E-08		9.62E-08	3.85	3.85E-03	-2.41E+00	-7.02E+00		9.30E+03	
270	7.81E-08	2.07E-07		2.51E-07	3.20E-07	1.27E-06	2.83E-07		3.41E-07	3.70	3.70E-03	-2.43E+00	-6.47E+00			1.36
280	3.61E-07	9.01E-07		8.30E-07	1.07E-06	5.20E-06	9.41E-07		1.13E-06	3.57	3.57E-03	-2.45E+00	-5.95E+00			1.53E-06
290	1.50E-06	3.55E-06	1.14E-06	2.57E-06	3.33E-06	1.93E-05	2.93E-06		3.48E-06	3.45	3.45E-03	-2.46E+00	-5.46E+00		-1.39E+01	
298	4.37E-06	9.98E-06	2.83E-06	6.10E-06	7.93E-06	5.19E-05	6.95E-06	8.22E-06	8.22E-06	3.36	3.36E-03	-2.47E+00	-5.08E+00		-2.26E+03	
310	1.96E-05	4.26E-05	1.03E-05	2.08E-05	2.72E-05	2.08E-04	2.38E-05		2.80E-05	3.23	3.23E-03	-2.49E+00	-4.55E+00		-3.20E+01	
320	6.28E-05	1.31E-04	2.88E-05	5.50E-05	7.20E-05	6.13E-04	6.29E-05		7.36E-05	3.13	3.13E-03	-2.51E+00	-4.13E+00		#N/A	
330	1.88E-04	3.80E-04		1.39E-04	1.82E-04	1.69E-03	1.59E-04		1.85E-04	3.03	3.03E-03	-2.52E+00	-3.73E+00		#N/A	
340	5.26E-04	1.03E-03		3.35E-04	4.40E-04	4.41E-03	3.84E-04		4.45E-04	2.94	2.94E-03	-2.53E+00	-3.35E+00	A		4.45E-04
350	1.39E-03	2.65E-03		7.80E-04	1.02E-03	1.09E-02	8.94E-04		1.03E-03	2.86	2.86E-03	-2.54E+00	-2.99E+00		1.01E-32	1.00
375	1.26E-02	2.26E-02		5.54E-03	7.27E-03	8.52E-02	6.35E-03		7.25E-03	2.67	2.67E-03	-2.57E+00	-2.14E+00	n		
400	8.63E-02	1.48E-01		3.27E-02	4.28E-02	5.19E-01	3.74E-02		4.24E-02	2.50	2.50E-03	-2.60E+00	-1.37E+00		13.94	
425	4.72E-01	7.81E-01		1.65E-01	2.15E-01	2.57E+00	1.88E-01		2.12E-01	2.35	2.35E-03	-2.63E+00	-6.74E-01	Ea		1.00
450	2.14E+00	3.45E+00		7.31E-01	9.40E-01	1.07E+01	8.29E-01		9.26E-01	2.22	2.22E-03	-2.65E+00	-3.33E-02		5195	9.26E-01

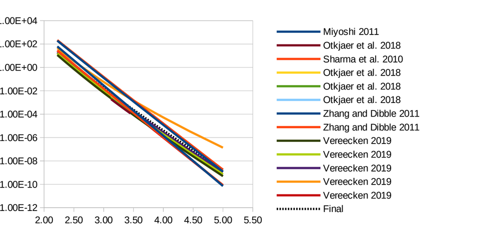


P1 2.24E+11 54000000000 5.34E+11 7.56E+11 4.14E+11 6.64E-22 1.69474E-20 1.97E-19 6.89E-40 205.3062848 4.62E+06 7.60E+06
P2 9900 1.3 1.12E+04 1.14E+04 1.14E+04 1.04E+01 9.960499537 9.61E+00 1.62E+01 2.848689071 1.558 1.472
P3 18.2 8.01E+07 8.15E+07 8.56E+07 5556.292019 5659.922503 5689.57293 2325.84103 8723.405749 8821 8756
Ea shift -5.75E+01

-CH2OO. | -CH2-

T	Miyoshi 2011	Sharma et al.	Otkjaer et al.	Otkjaer et al.	Otkjaer et al.	Vereecken 20	Vereecken 20	Vereecken 20	Vereecken 20	Vereecken 20	Zhang and Dit	Zhang and Dit	T-dependence	Target	Final
200	7.12E-11	8.59E-11				4.99E-10	7.21E-10	1.12E-09	1.37E-07	8.41E-11	1.24E-09	1.80E-09	1.36E-09		1.81E-09
225	1.74E-08	1.62E-08				3.72E-08	5.41E-08	8.17E-08	3.37E-06	1.50E-08	2.01E-07	2.77E-07	9.63E-08		1.24E-07
250	1.42E-06	1.09E-06				1.32E-06	1.91E-06	2.82E-06	5.23E-05	9.76E-07	1.19E-05	1.58E-05	3.25E-06		4.09E-06
260	6.51E-06	4.70E-06				4.65E-06	6.75E-06	9.86E-06	1.42E-04	4.17E-06	4.93E-05	6.45E-05	1.13E-05		1.41E-05
270	2.67E-05	1.82E-05				1.52E-05	2.20E-05	3.19E-05	3.64E-04	1.61E-05	1.84E-04	2.38E-04	3.62E-05		4.48E-05
280	9.88E-05	6.41E-05				4.63E-05	6.69E-05	9.60E-05	8.93E-04	5.66E-05	6.24E-04	7.98E-04	1.08E-04		1.33E-04
290	3.34E-04	2.07E-04	2.41E-04	1.81E-04	1.17E-04	1.32E-04	1.90E-04	2.71E-04	2.10E-03	1.83E-04	1.95E-03	2.47E-03	3.05E-04		3.74E-04
298	8.36E-04	5.01E-04	5.24E-04	4.00E-04	2.56E-04	2.93E-04	4.22E-04	5.96E-04	4.05E-03	4.44E-04	4.61E-03	5.78E-03	6.68E-04	8.10E-04	8.10E-04
310	3.03E-03	1.73E-03	1.60E-03	1.25E-03	7.84E-04	9.11E-04	1.30E-03	1.82E-03	1.04E-02	1.54E-03	1.54E-02	1.91E-02	2.03E-03		2.45E-03
320	8.21E-03	4.55E-03	3.88E-03	3.07E-03	1.90E-03	2.22E-03	3.16E-03	4.39E-03	2.20E-02	4.07E-03	3.94E-02	4.84E-02	4.88E-03		5.84E-03
330	2.10E-02	1.13E-02				5.17E-03	7.35E-03	1.01E-02	4.52E-02	1.02E-02	9.53E-02	1.16E-01	1.12E-02		1.33E-02
340	5.07E-02	2.65E-02				1.16E-02	1.64E-02	2.24E-02	9.03E-02	2.40E-02	2.19E-01	2.65E-01	2.47E-02		2.93E-02
350	1.16E-01	5.94E-02				2.50E-02	3.52E-02	4.77E-02	1.76E-01	5.44E-02	4.81E-01	5.77E-01	5.25E-02		6.19E-02
375	7.67E-01	3.72E-01				1.47E-01	2.06E-01	2.73E-01	8.39E-01	3.49E-01	2.88E+00	3.38E+00	3.00E-01		3.50E-01
400	3.99E+00	1.86E+00				7.29E-01	1.00E+00	1.31E+00	3.52E+00	1.79E+00	1.38E+01	1.60E+01	1.43E+00		1.66E+00
425	1.71E+01	7.75E+00				3.10E+00	4.22E+00	5.42E+00	1.33E+01	7.69E+00	5.56E+01	6.34E+01	5.91E+00		6.77E+00
450	6.25E+01	2.77E+01				1.16E+01	1.56E+01	1.98E+01	4.55E+01	2.83E+01	1.93E+02	2.17E+02	2.15E+01		2.45E+01

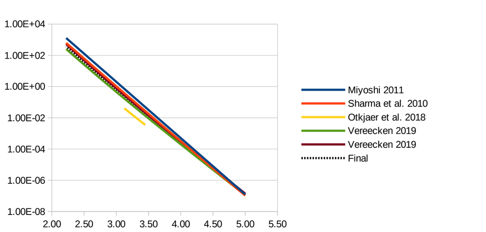
T	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200	5.00	5.00E-03	-2.30E+00	-8.74E+00	A		9.80E-10
225	4.44	4.44E-03	-2.35E+00	-6.91E+00		1.93E+09	0.54
250	4.00	4.00E-03	-2.40E+00	-5.39E+00	Ea		
260	3.85	3.85E-03	-2.41E+00	-4.85E+00		8.42E+03	
270	3.70	3.70E-03	-2.43E+00	-4.35E+00			1.24
280	3.57	3.57E-03	-2.45E+00	-3.88E+00			1.65E-04
290	3.45	3.45E-03	-2.46E+00	-3.43E+00		-9.81E+00	
298	3.36	3.36E-03	-2.47E+00	-3.09E+00		-2.40E+03	
310	3.23	3.23E-03	-2.49E+00	-2.61E+00		-1.93E+01	
320	3.13	3.13E-03	-2.51E+00	-2.23E+00		#N/A	
330	3.03	3.03E-03	-2.52E+00	-1.88E+00		#N/A	
340	2.94	2.94E-03	-2.53E+00	-1.53E+00	A		2.93E-02
350	2.86	2.86E-03	-2.54E+00	-1.21E+00		5.00E-20	1.00
375	2.67	2.67E-03	-2.57E+00	-4.57E-01	n		
400	2.50	2.50E-03	-2.60E+00	2.19E-01		9.81	
425	2.35	2.35E-03	-2.63E+00	8.31E-01	Ea		1.00
450	2.22	2.22E-03	-2.65E+00	1.39E+00		5534	2.45E+01



P1 1.31E+11 49000000000 2.34E+11 1.25E-02 0.000252313
P2 8300 1.2 1.02E+04 4.02E+00 4.763106869
P3 15.4 8.16E+07 6576.708248 6546.824892
Ea shift 1.40E+00

-CH2OO. | >CH-

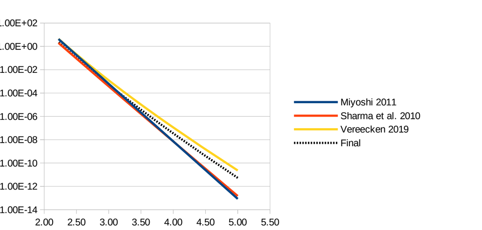
T	Miyoshi 2011	Sharma et al.	Otkjaer et al.	Vereecken 20	Vereecken 2019	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200	1.24E-07	1.05E-07		1.13E-07	1.40E-07	1.26E-07		1.25E-07	5.00	5.00E-03	-2.30E+00	-6.90E+00	A		9.50E-08
225	1.25E-05	8.98E-06		7.03E-06	9.31E-06	8.09E-06		8.04E-06	4.44	4.44E-03	-2.35E+00	-5.09E+00		1.09E+10	0.76
250	5.00E-04	3.19E-04		2.00E-04	2.82E-04	2.37E-04		2.36E-04	4.00	4.00E-03	-2.40E+00	-3.63E+00	Ea		
260	1.79E-03	1.10E-03		6.43E-04	9.31E-04	7.74E-04		7.70E-04	3.85	3.85E-03	-2.41E+00	-3.11E+00		7.86E+03	
270	5.84E-03	3.48E-03		1.91E-03	2.83E-03	2.33E-03		2.32E-03	3.70	3.70E-03	-2.43E+00	-2.64E+00			1.10
280	1.75E-02	1.01E-02		5.27E-03	8.01E-03	6.50E-03		6.46E-03	3.57	3.57E-03	-2.45E+00	-2.19E+00			7.12E-03
290	4.87E-02	2.74E-02	3.52E-03	1.36E-02	2.12E-02	1.70E-02		1.69E-02	3.45	3.45E-03	-2.46E+00	-1.77E+00		-4.39E+00	
298	1.05E-01	5.81E-02	6.97E-03	2.80E-02	4.42E-02	3.52E-02	3.50E-02	3.50E-02	3.36	3.36E-03	-2.47E+00	-1.46E+00		-2.85E+03	
310	3.09E-01	1.67E-01	1.86E-02	7.70E-02	1.25E-01	9.81E-02		9.77E-02	3.23	3.23E-03	-2.49E+00	-1.01E+00		-2.75E+00	
320	7.12E-01	3.78E-01	4.05E-02	1.70E-01	2.81E-01	2.19E-01		2.18E-01	3.13	3.13E-03	-2.51E+00	-6.62E-01		#N/A	
330	1.56E+00	8.18E-01		3.58E-01	6.05E-01	4.66E-01		4.64E-01	3.03	3.03E-03	-2.52E+00	-3.34E-01		#N/A	
340	3.28E+00	1.69E+00		7.26E-01	1.25E+00	9.53E-01		9.49E-01	2.94	2.94E-03	-2.53E+00	-2.29E-02	A		9.49E-01
350	6.58E+00	3.36E+00		1.42E+00	2.49E+00	1.88E+00		1.87E+00	2.86	2.86E-03	-2.54E+00	2.72E-01		1.77E-03	1.00
375	3.20E+01	1.60E+01		6.54E+00	1.20E+01	8.87E+00		8.84E+00	2.67	2.67E-03	-2.57E+00	9.46E-01	n		
400	1.28E+02	6.28E+01		2.54E+01	4.87E+01	3.52E+01		3.50E+01	2.50	2.50E-03	-2.60E+00	1.54E+00		4.39	
425	4.32E+02	2.11E+02		8.51E+01	1.70E+02	1.20E+02		1.20E+02	2.35	2.35E-03	-2.63E+00	2.08E+00	Ea		1.00
450	1.28E+03	6.23E+02		2.53E+02	5.26E+02	3.65E+02		3.64E+02	2.22	2.22E-03	-2.65E+00	2.56E+00		6563	3.64E+02



P1 3.92E+11 76000000000 1.31E-27
P2 11360 1.4 1.25E+01
P3 20.8 5.72E+03
Ea shift 2.92E+02

>CHOO. | -CH3

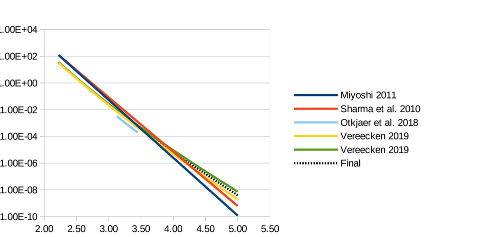
T	Miyoshi 2011	Sharma et al.	Vereecken 2019	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200	8.42E-14	1.48E-13	2.29E-11	2.29E-11		5.33E-12	5.00	5.00E-03	-2.30E+00	-1.13E+01	A		2.44E-12
225	4.64E-11	5.87E-11	2.38E-09	2.38E-09		6.51E-10	4.44	4.44E-03	-2.35E+00	-9.19E+00		2.57E+09	0.46
250	7.23E-09	7.13E-09	1.12E-07	1.12E-07		3.50E-08	4.00	4.00E-03	-2.40E+00	-7.46E+00	Ea		
260	4.15E-08	3.77E-08	4.41E-07	4.41E-07		1.44E-07	3.85	3.85E-03	-2.41E+00	-6.84E+00		9.68E+03	
270	2.09E-07	1.77E-07	1.59E-06	1.59E-06		5.42E-07	3.70	3.70E-03	-2.43E+00	-6.27E+00			1.31
280	9.40E-07	7.42E-07	5.34E-06	5.34E-06		1.89E-06	3.57	3.57E-03	-2.45E+00	-5.72E+00			2.48E-06
290	3.81E-06	2.83E-06	1.67E-05	1.67E-05		6.12E-06	3.45	3.45E-03	-2.46E+00	-5.21E+00		-1.25E+01	
298	1.09E-05	7.74E-06	3.99E-05	3.99E-05	1.50E-05	1.50E-05	3.36	3.36E-03	-2.47E+00	-4.82E+00		-2.61E+03	
310	4.77E-05	3.19E-05	1.37E-04	1.37E-04		5.35E-05	3.23	3.23E-03	-2.49E+00	-4.27E+00		-2.69E+01	
320	1.50E-04	9.57E-05	3.62E-04	3.62E-04		1.46E-04	3.13	3.13E-03	-2.51E+00	-3.84E+00		#N/A	
330	4.40E-04	2.69E-04	9.13E-04	9.13E-04		3.77E-04	3.03	3.03E-03	-2.52E+00	-3.42E+00		#N/A	
340	1.21E-03	7.14E-04	2.21E-03	2.21E-03		9.35E-04	2.94	2.94E-03	-2.53E+00	-3.03E+00	A		9.35E-04
350	3.14E-03	1.79E-03	5.12E-03	5.12E-03		2.22E-03	2.86	2.86E-03	-2.54E+00	-2.65E+00		1.31E-27	1.00
375	2.74E-02	1.45E-02	3.59E-02	3.59E-02		1.65E-02	2.67	2.67E-03	-2.57E+00	-1.78E+00	n		
400	1.82E-01	9.08E-02	2.08E-01	2.08E-01		1.00E-01	2.50	2.50E-03	-2.60E+00	-9.98E-01		12.46	
425	9.66E-01	4.61E-01	1.03E+00	1.03E+00		5.17E-01	2.35	2.35E-03	-2.63E+00	-2.86E-01	Ea		1.00
450	4.26E+00	1.96E+00	4.42E+00	4.42E+00		2.31E+00	2.22	2.22E-03	-2.65E+00	3.64E-01		6010	2.31E+00



P1 5.26E+11 1.4E+11 6.18E+11 8.68E-19 1.00E-29
P2 9970 0.2 1.13E+04 9.46E+00 1.31E+01
P3 18.5 8.00E+07 5.72E+03 4.23E+03
Ea shift -1.03E+01

>CHOO. | -CH2-

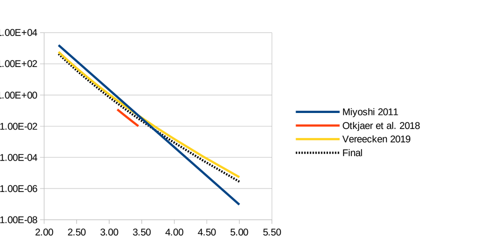
T	Miyoshi 2011	Sharma et al.	Otkjaer et al.	Vereecken 20	Vereecken 2019	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200	1.18E-10	6.15E-10		1.92E-09	7.21E-09	3.73E-09		3.92E-09	5.00	5.00E-03	-2.30E+00	-8.41E+00	A		1.94E-09
225	3.00E-08	1.11E-07		1.40E-07	3.53E-07	2.23E-07		2.33E-07	4.44	4.44E-03	-2.35E+00	-6.63E+00		1.89E+09	0.49
250	2.52E-06	7.11E-06		4.83E-06	9.19E-06	6.66E-06		6.94E-06	4.00	4.00E-03	-2.40E+00	-5.16E+00	Ea		
260	1.17E-05	3.00E-05		1.69E-05	2.94E-05	2.23E-05		2.32E-05	3.85	3.85E-03	-2.41E+00	-4.64E+00		8.28E+03	
270	4.83E-05	1.14E-04		5.44E-05	8.80E-05	6.92E-05		7.19E-05	3.70	3.70E-03	-2.43E+00	-4.14E+00			1.28
280	1.81E-04	3.93E-04		1.63E-04	2.48E-04	2.01E-04		2.09E-04	3.57	3.57E-03	-2.45E+00	-3.68E+00			2.67E-04
290	6.17E-04	1.25E-03	1.96E-04	4.61E-04	6.60E-04	5.51E-04		5.71E-04	3.45	3.45E-03	-2.46E+00	-3.24E+00		-1.13E+01	
298	1.55E-03	2.97E-03	4.32E-04	1.01E-03	1.39E-03	1.19E-03	1.23E-03	1.23E-03	3.36	3.36E-03	-2.47E+00	-2.91E+00		-2.16E+03	
310	5.67E-03	1.00E-02	1.34E-03	3.09E-03	4.05E-03	3.54E-03		3.65E-03	3.23	3.23E-03	-2.49E+00	-2.44E+00		-2.35E+01	
320	1.55E-02	2.58E-02	3.28E-03	7.42E-03	9.39E-03	8.35E-03		8.62E-03	3.13	3.13E-03	-2.51E+00	-2.06E+00		#N/A	
330	3.98E-02	6.26E-02		1.71E-02	2.10E-02	1.89E-02		1.95E-02	3.03	3.03E-03	-2.52E+00	-1.71E+00		#N/A	
340	9.68E-02	1.44E-01		3.76E-02	4.52E-02	4.12E-02		4.25E-02	2.94	2.94E-03	-2.53E+00	-1.37E+00	A		4.25E-02
350	2.24E-01	3.18E-01		8.01E-02	9.41E-02	8.68E-02		8.94E-02	2.86	2.86E-03	-2.54E+00	-1.05E+00		2.95E-24	1.00
375	1.49E+00	1.90E+00		4.57E-01	5.19E-01	4.87E-01		5.01E-01	2.67	2.67E-03	-2.57E+00	-3.01E-01	n		
400	7.87E+00	9.07E+00		2.18E+00	2.44E+00	2.31E+00		2.37E+00	2.50	2.50E-03	-2.60E+00	3.75E-01		11.26	
425	3.41E+01	3.61E+01		8.97E+00	1.01E+01	9.50E+00		9.73E+00	2.35	2.35E-03	-2.63E+00	9.88E-01	Ea		1.00
450	1.26E+02	1.23E+02		3.25E+01	3.69E+01	3.46E+01		3.54E+01	2.22	2.22E-03	-2.65E+00	1.55E+00		4966	3.54E+01



P1 2.42E+11 5.79E+11 1.64E-35
P2 8480 1.01E+04 1.50E+01
P3 7.69E+07 2285.956585
Ea shift 1.35E+02

>CHOO. | >CH-

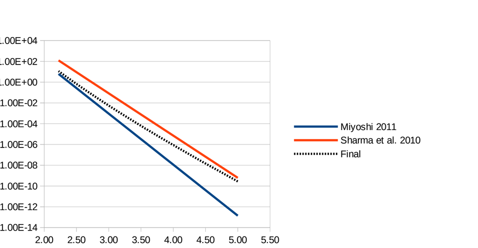
T	Miyoshi 2011	Otkjaer et al.	Vereecken 2019	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200	9.33E-08		5.39E-06	5.39E-06		2.75E-06	5.00	5.00E-03	-2.30E+00	-5.56E+00	A		1.08E-06
225	1.04E-05		1.12E-04	1.12E-04		6.17E-05	4.44	4.44E-03	-2.35E+00	-4.21E+00		7.54E+08	0.39
250	4.49E-04		1.50E-03	1.50E-03		8.77E-04	4.00	4.00E-03	-2.40E+00	-3.06E+00	Ea		
260	1.66E-03		3.84E-03	3.84E-03		2.29E-03	3.85	3.85E-03	-2.41E+00	-2.64E+00		6.84E+03	
270	5.54E-03		9.37E-03	9.37E-03		5.69E-03	3.70	3.70E-03	-2.43E+00	-2.24E+00			1.39
280	1.70E-02		2.19E-02	2.19E-02		1.35E-02	3.57	3.57E-03	-2.45E+00	-1.87E+00			1.88E-02
290	4.84E-02	1.02E-02	4.90E-02	4.90E-02		3.08E-02	3.45	3.45E-03	-2.46E+00	-1.51E+00		-1.50E+01	
298	1.06E-01	2.02E-02	9.11E-02	9.11E-02	5.80E-02	5.80E-02	3.36	3.36E-03	-2.47E+00	-1.24E+00		-1.05E+03	
310	3.19E-01	5.42E-02	2.21E-01	2.21E-01		1.43E-01	3.23	3.23E-03	-2.49E+00	-8.43E-01		-3.48E+01	
320	7.50E-01	1.19E-01	4.49E-01	4.49E-01		2.95E-01	3.13	3.13E-03	-2.51E+00	-5.31E-01		#N/A	
330	1.67E+00		8.84E-01	8.84E-01		5.88E-01	3.03	3.03E-03	-2.52E+00	-2.31E-01		#N/A	
340	3.56E+00		1.69E+00	1.69E+00		1.14E+00	2.94	2.94E-03	-2.53E+00	5.72E-02	A		1.14E+00
350	7.27E+00		3.17E+00	3.17E+00		2.16E+00	2.86	2.86E-03	-2.54E+00	3.34E-01		1.64E-35	1.00
375	3.66E+01		1.38E+01	1.38E+01		9.63E+00	2.67	2.67E-03	-2.57E+00	9.83E-01	n		
400	1.50E+02		5.30E+01	5.30E+01		3.79E+01	2.50	2.50E-03	-2.60E+00	1.58E+00		14.99	
425	5.23E+02		1.84E+02	1.84E+02		1.34E+02	2.35	2.35E-03	-2.63E+00	2.13E+00	Ea		1.00
450	1.58E+03		5.85E+02	5.85E+02		4.34E+02	2.22	2.22E-03	-2.65E+00	2.64E+00		2420	4.34E+02



P1 5.05E+11 1.4E+11
P2 11310 0.2
P3 18.5
Ea shift 4.13E+02

>C(OO.)- | -CH3

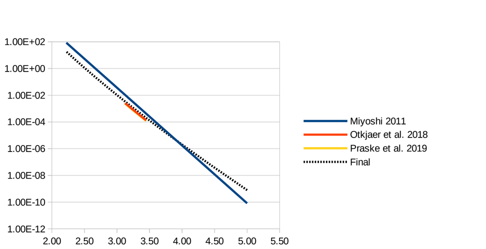
T	Miyoshi 2011	Sharma et al. 2010	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	1.39E-13	6.15E-10	2.18E-09		2.77E-10	5.00	5.00E-03	-2.30E+00	-9.56E+00	A		1.41E-10
225	7.46E-11	1.11E-07	1.43E-07		2.29E-08	4.44	4.44E-03	-2.35E+00	-7.64E+00		2.11E+09	0.51
250	1.14E-08	7.11E-06	4.57E-06		8.75E-07	4.00	4.00E-03	-2.40E+00	-6.06E+00	Ea		
260	6.48E-08	3.00E-05	1.56E-05		3.19E-06	3.85	3.85E-03	-2.41E+00	-5.50E+00		8.83E+03	
270	3.24E-07	1.14E-04	4.95E-05		1.07E-05	3.70	3.70E-03	-2.43E+00	-4.97E+00			1.27
280	1.45E-06	3.93E-04	1.47E-04		3.35E-05	3.57	3.57E-03	-2.45E+00	-4.48E+00			4.24E-05
290	5.83E-06	1.25E-03	4.08E-04		9.81E-05	3.45	3.45E-03	-2.46E+00	-4.01E+00		-1.08E+01	
298	1.66E-05	2.97E-03	8.88E-04	2.22E-04	2.22E-04	3.36	3.36E-03	-2.47E+00	-3.65E+00		-2.45E+03	
310	7.22E-05	1.00E-02	2.69E-03		7.08E-04	3.23	3.23E-03	-2.49E+00	-3.15E+00		-2.21E+01	
320	2.26E-04	2.58E-02	6.42E-03		1.76E-03	3.13	3.13E-03	-2.51E+00	-2.75E+00		#N/A	
330	6.59E-04	6.26E-02	1.47E-02		4.20E-03	3.03	3.03E-03	-2.52E+00	-2.38E+00		#N/A	
340	1.81E-03	1.44E-01	3.23E-02		9.59E-03	2.94	2.94E-03	-2.53E+00	-2.02E+00	A		9.59E-03
350	4.67E-03	3.18E-01	6.86E-02		2.11E-02	2.86	2.86E-03	-2.54E+00	-1.68E+00		7.45E-23	1.00
375	4.03E-02	1.90E+00	3.92E-01		1.30E-01	2.67	2.67E-03	-2.57E+00	-8.85E-01	n		
400	2.65E-01	9.07E+00	1.88E+00		6.70E-01	2.50	2.50E-03	-2.60E+00	-1.74E-01		10.79	
425	1.40E+00	3.61E+01	7.83E+00		2.96E+00	2.35	2.35E-03	-2.63E+00	4.71E-01	Ea		1.00
450	6.14E+00	1.23E+02	2.88E+01		1.15E+01	2.22	2.22E-03	-2.65E+00	1.06E+00		5650	1.15E+01



P1 3.48E+11 1.43E+12 1.43E+12
P2 9960 1.16E+04 1.16E+04
P3 7.53E+07 7.53E+07
Ea shift 2.04E+02

>C(OO.)- | -CH2-

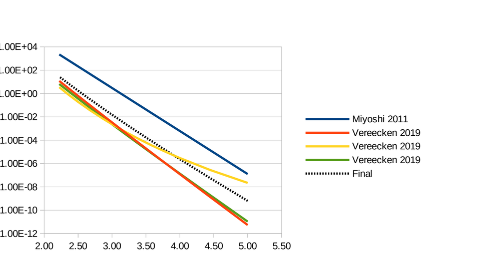
T	Miyoshi 2011	Otkjaer et al.	Praske et al. 2019	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	8.20E-11			2.18E-09		7.89E-10	5.00	5.00E-03	-2.30E+00	-9.10E+00	A		4.02E-10
225	2.07E-08			1.43E-07		5.78E-08	4.44	4.44E-03	-2.35E+00	-7.24E+00		2.11E+09	0.51
250	1.73E-06			4.57E-06		2.02E-06	4.00	4.00E-03	-2.40E+00	-5.69E+00	Ea		
260	8.03E-06			1.56E-05		7.14E-06	3.85	3.85E-03	-2.41E+00	-5.15E+00		8.62E+03	
270	3.32E-05			4.95E-05		2.33E-05	3.70	3.70E-03	-2.43E+00	-4.63E+00			1.27
280	1.24E-04			1.47E-04		7.08E-05	3.57	3.57E-03	-2.45E+00	-4.15E+00			8.97E-05
290	4.22E-04	1.33E-04	1.21E-04	4.08E-04		2.02E-04	3.45	3.45E-03	-2.46E+00	-3.69E+00		-1.08E+01	
298	1.06E-03	3.06E-04	2.78E-04	8.88E-04	4.49E-04	4.49E-04	3.36	3.36E-03	-2.47E+00	-3.35E+00		-2.36E+03	
310	3.87E-03	1.00E-03	9.16E-04	2.69E-03		1.39E-03	3.23	3.23E-03	-2.49E+00	-2.86E+00		-2.21E+01	
320	1.06E-02	2.57E-03	2.35E-03	6.42E-03		3.40E-03	3.13	3.13E-03	-2.51E+00	-2.47E+00		#N/A	
330	2.72E-02			1.47E-02		7.93E-03	3.03	3.03E-03	-2.52E+00	-2.10E+00		#N/A	
340	6.60E-02			3.23E-02		1.78E-02	2.94	2.94E-03	-2.53E+00	-1.75E+00	A		1.78E-02
350	1.52E-01			6.86E-02		3.84E-02	2.86	2.86E-03	-2.54E+00	-1.42E+00		7.45E-23	1.00
375	1.02E+00			3.92E-01		2.28E-01	2.67	2.67E-03	-2.57E+00	-6.42E-01	n		
400	5.34E+00			1.88E+00		1.13E+00	2.50	2.50E-03	-2.60E+00	5.39E-02		10.79	
425	2.31E+01			7.83E+00		4.85E+00	2.35	2.35E-03	-2.63E+00	6.86E-01	Ea		1.00
450	8.50E+01			2.88E+01		1.83E+01	2.22	2.22E-03	-2.65E+00	1.26E+00		5440	1.83E+01



P1 3.57E+11 245.1515933 2.33385E-74 0.001225092
P2 8500 2.92027375 27.50948792 4.483441502
P3 9386.415698 -1229.47022 8464.981889
Ea shift 0.00E+00

>C(OO.)- | >CH-

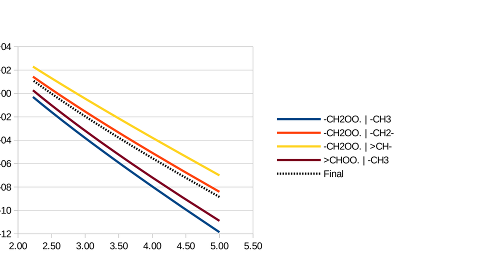
T	Miyoshi 2011	Vereecken 20	Vereecken 20	Vereecken 2019	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	1.24E-07	5.33E-12	2.18E-08	1.05E-11	6.25E-10		6.25E-10	5.00	5.00E-03	-2.30E+00	-9.20E+00	A		3.62E-10
225	1.40E-05	1.38E-09	2.81E-07	1.97E-09	5.72E-08		5.72E-08	4.44	4.44E-03	-2.35E+00	-7.24E+00		6.05E+09	0.58
250	6.12E-04	1.22E-07	2.95E-06	1.36E-07	2.34E-06		2.34E-06	4.00	4.00E-03	-2.40E+00	-5.63E+00	Ea		
260	2.26E-03	5.80E-07	7.18E-06	5.97E-07	8.66E-06		8.66E-06	3.85	3.85E-03	-2.41E+00	-5.06E+00		8.85E+03	
270	7.59E-03	2.46E-06	1.70E-05	2.36E-06	2.95E-05		2.95E-05	3.70	3.70E-03	-2.43E+00	-4.53E+00			1.21
280	2.34E-02	9.48E-06	3.94E-05	8.52E-06	9.28E-05		9.28E-05	3.57	3.57E-03	-2.45E+00	-4.03E+00			1.12E-04
290	6.66E-02	3.34E-05	8.88E-05	2.83E-05	2.73E-04		2.73E-04	3.45	3.45E-03	-2.46E+00	-3.56E+00		-8.73E+00	
298	1.46E-01	8.62E-05	1.68E-04	6.99E-05	6.20E-04	6.20E-04	6.20E-04	3.36	3.36E-03	-2.47E+00	-3.21E+00		-2.73E+03	
310	4.41E-01	3.27E-04	4.23E-04	2.51E-04	1.98E-03		1.98E-03	3.23	3.23E-03	-2.49E+00	-2.70E+00		-1.57E+01	
320	1.04E+00	9.25E-04	8.96E-04	6.78E-04	4.92E-03		4.92E-03	3.13	3.13E-03	-2.51E+00	-2.31E+00		#N/A	
330	2.32E+00	2.46E-03	1.86E-03	1.74E-03	1.17E-02		1.17E-02	3.03	3.03E-03	-2.52E+00	-1.93E+00		#N/A	
340	4.96E+00	6.20E-03	3.79E-03	4.22E-03	2.65E-02		2.65E-02	2.94	2.94E-03	-2.53E+00	-1.58E+00	A		2.65E-02
350	1.01E+01	1.49E-02	7.58E-03	9.79E-03	5.78E-02		5.78E-02	2.86	2.86E-03	-2.54E+00	-1.24E+00		2.24E-16	1.00
375	5.11E+01	1.09E-01	4.00E-02	6.69E-02	3.49E-01		3.49E-01	2.67	2.67E-03	-2.57E+00	-4.57E-01	n		
400	2.11E+02	6.27E-01	1.92E-01	3.66E-01	1.75E+00		1.75E+00	2.50	2.50E-03	-2.60E+00	2.42E-01		8.73	
425	7.36E+02	2.97E+00	8.51E-01	1.67E+00	7.47E+00		7.47E+00	2.35	2.35E-03	-2.63E+00	8.73E-01	Ea		1.00
450	2.24E+03	1.20E+01	3.49E+00	6.52E+00	2.79E+01		2.79E+01	2.22	2.22E-03	-2.65E+00	1.45E+00		6280	2.79E+01



1,6 Hshift

Average Temperature dependence
1.14E+02

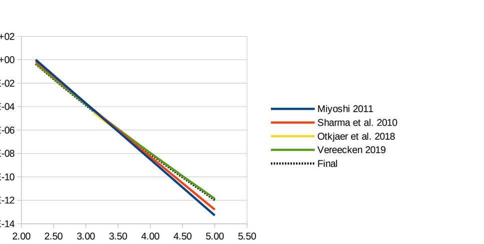
T	-CH2OO. | -C	-CH2OO. | -CI	-CH2OO. | >C	>CHOO. | -CH	>CHOO. | >CH-	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log()		log(T)	Replicate
200	1.36E-12	3.88E-09	9.86E-08	1.28E-11	1.45E-05	2.49E-09		1.41E-09	5.00	5.00E-03	-2.30E+00	-8.85E+00	A		7.99E-10
225	1.92E-10	2.64E-07	5.94E-06	1.37E-09	2.16E-04	1.55E-07		9.32E-08	4.44	4.44E-03	-2.35E+00	-7.03E+00		8.23E+08	0.57
250	1.11E-08	8.36E-06	1.65E-04	6.50E-08	2.21E-03	4.66E-06		2.95E-06	4.00	4.00E-03	-2.40E+00	-5.53E+00	Ea		
260	4.61E-08	2.82E-05	5.29E-04	2.54E-07	5.16E-03	1.55E-05		1.00E-05	3.85	3.85E-03	-2.41E+00	-5.00E+00		8.30E+03	
270	1.75E-07	8.78E-05	1.56E-03	9.14E-07	1.15E-02	4.79E-05		3.14E-05	3.70	3.70E-03	-2.43E+00	-4.50E+00			1.22
280	6.10E-07	2.55E-04	4.30E-03	3.04E-06	2.48E-02	1.38E-04		9.18E-05	3.57	3.57E-03	-2.45E+00	-4.04E+00			1.12E-04
290	1.97E-06	6.92E-04	1.11E-02	9.42E-06	5.15E-02	3.74E-04		2.52E-04	3.45	3.45E-03	-2.46E+00	-3.60E+00		-9.05E+00	
298	4.80E-06	1.48E-03	2.26E-02	2.22E-05	9.03E-02	7.97E-04	5.43E-04	5.43E-04	3.36	3.36E-03	-2.47E+00	-3.26E+00		-2.44E+03	
310	1.69E-05	4.31E-03	6.21E-02	7.53E-05	2.03E-01	2.33E-03		1.61E-03	3.23	3.23E-03	-2.49E+00	-2.79E+00		-1.75E+01	
320	4.54E-05	9.99E-03	1.37E-01	1.96E-04	3.85E-01	5.42E-03		3.79E-03	3.13	3.13E-03	-2.51E+00	-2.42E+00		#N/A	
330	1.16E-04	2.22E-02	2.87E-01	4.87E-04	7.15E-01	1.21E-02		8.54E-03	3.03	3.03E-03	-2.52E+00	-2.07E+00		#N/A	
340	2.81E-04	4.72E-02	5.81E-01	1.16E-03	1.30E+00	2.59E-02		1.85E-02	2.94	2.94E-03	-2.53E+00	-1.73E+00	A		1.85E-02
350	6.55E-04	9.68E-02	1.13E+00	2.64E-03	2.30E+00	5.34E-02		3.85E-02	2.86	2.86E-03	-2.54E+00	-1.41E+00		3.47E-18	1.00
375	4.57E-03	5.05E-01	5.21E+00	1.77E-02	8.85E+00	2.85E-01		2.10E-01	2.67	2.67E-03	-2.57E+00	-6.77E-01	n		
400	2.59E-02	2.21E+00	2.02E+01	9.81E-02	3.06E+01	1.28E+00		9.64E-01	2.50	2.50E-03	-2.60E+00	-1.61E-02		9.05	
425	1.24E-01	8.34E+00	6.77E+01	4.61E-01	9.65E+01	4.99E+00		3.82E+00	2.35	2.35E-03	-2.63E+00	5.82E-01	Ea		1.00
450	5.10E-01	2.78E+01	2.01E+02	1.89E+00	2.81E+02	1.72E+01		1.34E+01	2.22	2.22E-03	-2.65E+00	1.13E+00		5628	1.34E+01



P1 43600000000 13000000000 1.30E+11 5.66E-17
P2 11020 1.5 1.23E+04 8.59E+00
P3 20 8.04E+07 7085.723305
Ea shift 5.17E+01

-CH2OO. | -CH3

T	Miyoshi 2011	Sharma et al.	Otkjaer et al.	Vereecken 2019	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200	5.13E-14	1.62E-13		1.36E-12	1.36E-12		1.05E-12	5.00	5.00E-03	-2.30E+00	-1.20E+01	A		6.14E-13
225	2.34E-11	5.18E-11		1.92E-10	1.92E-10		1.52E-10	4.44	4.44E-03	-2.35E+00	-9.82E+00		6.08E+08	0.58
250	3.13E-09	5.31E-09		1.11E-08	1.11E-08		8.99E-09	4.00	4.00E-03	-2.40E+00	-8.05E+00	Ea		
260	1.71E-08	2.65E-08		4.61E-08	4.61E-08		3.78E-08	3.85	3.85E-03	-2.41E+00	-7.42E+00		9.67E+03	
270	8.20E-08	1.18E-07		1.75E-07	1.75E-07		1.44E-07	3.70	3.70E-03	-2.43E+00	-6.84E+00			1.21
280	3.52E-07	4.71E-07		6.10E-07	6.10E-07		5.07E-07	3.57	3.57E-03	-2.45E+00	-6.29E+00			6.12E-07
290	1.37E-06	1.71E-06	1.34E-06	1.97E-06	1.97E-06		1.65E-06	3.45	3.45E-03	-2.46E+00	-5.78E+00		-8.59E+00	
298	3.80E-06	4.53E-06	3.22E-06	4.80E-06	4.80E-06	4.04E-06	4.04E-06	3.36	3.36E-03	-2.47E+00	-5.39E+00		-3.10E+03	
310	1.59E-05	1.78E-05	1.13E-05	1.69E-05	1.69E-05		1.43E-05	3.23	3.23E-03	-2.49E+00	-4.84E+00		-1.62E+01	
320	4.82E-05	5.14E-05	3.06E-05	4.54E-05	4.54E-05		3.86E-05	3.13	3.13E-03	-2.51E+00	-4.41E+00		#N/A	
330	1.37E-04	1.40E-04		1.16E-04	1.16E-04		9.90E-05	3.03	3.03E-03	-2.52E+00	-4.00E+00		#N/A	
340	3.66E-04	3.58E-04		2.81E-04	2.81E-04		2.42E-04	2.94	2.94E-03	-2.53E+00	-3.62E+00	A		2.42E-04
350	9.23E-04	8.72E-04		6.55E-04	6.55E-04		5.65E-04	2.86	2.86E-03	-2.54E+00	-3.25E+00		5.66E-17	1.00
375	7.53E-03	6.58E-03		4.57E-03	4.57E-03		3.98E-03	2.67	2.67E-03	-2.57E+00	-2.40E+00	n		
400	4.73E-02	3.88E-02		2.59E-02	2.59E-02		2.28E-02	2.50	2.50E-03	-2.60E+00	-1.64E+00		8.59	
425	2.39E-01	1.87E-01		1.24E-01	1.24E-01		1.09E-01	2.35	2.35E-03	-2.63E+00	-9.61E-01	Ea		1.00
450	1.01E+00	7.58E-01		5.10E-01	5.10E-01		4.54E-01	2.22	2.22E-03	-2.65E+00	-3.43E-01		7137	4.54E-01

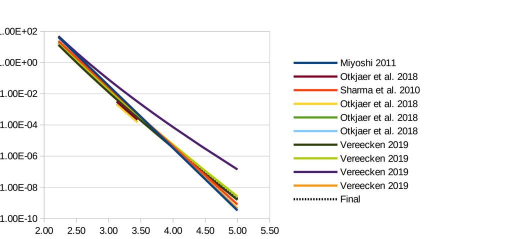


P1 33900000000 7400000000 1.17E+11 1.17E+11 1.39E+11 8.32E-15 1.37863E-13 1.59E-27 4.33E+06
P2 9220 1.2 1.09E+04 1.09E+04 1.08E+04 7.90E+00 7.505214771 1.20E+01 1.32E+00
P3 16.6 8.07E+07 8.07E+07 7.69E+07 5.94E+03 5990.300956 3576.375604 8771.966922
Ea shift 1.53E+02

-CH2OO. | -CH2-

T	Miyoshi 2011	Sharma et al.	Otkjaer et al.	Otkjaer et al.	Otkjaer et al.	Vereecken 20	Vereecken 20	Vereecken 20	Vereecken 2019	T-dependence	Target	Final
200	3.23E-10	7.75E-10				1.55E-09	2.52E-09	1.39E-07	4.20E-10	3.88E-09		1.81E-09
225	5.42E-08	9.26E-08				1.07E-07	1.70E-07	4.17E-06	6.42E-08	2.64E-07		1.34E-07
250	3.26E-06	4.30E-06				3.44E-06	5.37E-06	7.27E-05	3.64E-06	8.36E-06		4.53E-06
260	1.35E-05	1.63E-05				1.17E-05	1.81E-05	2.02E-04	1.48E-05	2.82E-05		1.56E-05
270	5.01E-05	5.61E-05				3.67E-05	5.65E-05	5.30E-04	5.41E-05	8.78E-05		4.98E-05
280	1.70E-04	1.77E-04				1.07E-04	1.64E-04	1.32E-03	1.81E-04	2.55E-04		1.47E-04
290	5.28E-04	5.16E-04	1.52E-04	1.52E-04	2.18E-04	2.94E-04	4.46E-04	3.12E-03	5.59E-04	6.92E-04		4.08E-04
298	1.24E-03	1.16E-03	3.22E-04	3.22E-04	4.63E-04	6.32E-04	9.53E-04	6.04E-03	1.31E-03	1.48E-03	8.83E-04	8.83E-04
310	4.11E-03	3.59E-03	9.42E-04	9.42E-04	1.36E-03	1.87E-03	2.79E-03	1.55E-02	4.30E-03	4.31E-03		2.63E-03
320	1.04E-02	8.65E-03	2.21E-03	2.21E-03	3.20E-03	4.37E-03	6.48E-03	3.25E-02	1.09E-02	9.99E-03		6.19E-03
330	2.49E-02	1.98E-02				9.78E-03	1.44E-02	6.60E-02	2.59E-02	2.22E-02		1.39E-02
340	5.66E-02	4.32E-02				2.10E-02	3.07E-02	1.30E-01	5.90E-02	4.72E-02		3.01E-02
350	1.23E-01	9.03E-02				4.35E-02	6.31E-02	2.49E-01	1.28E-01	9.68E-02		6.25E-02
375	7.12E-01	4.82E-01				2.33E-01	3.32E-01	1.13E+00	7.45E-01	5.05E-01		3.36E-01
400	3.31E+00	2.09E+00				1.04E+00	1.46E+00	4.46E+00	3.50E+00	2.21E+00		1.51E+00
425	1.28E+01	7.70E+00				4.04E+00	5.56E+00	1.57E+01	1.38E+01	8.34E+00		5.82E+00
450	4.29E+01	2.46E+01				1.38E+01	1.87E+01	4.97E+01	4.68E+01	2.78E+01		1.98E+01

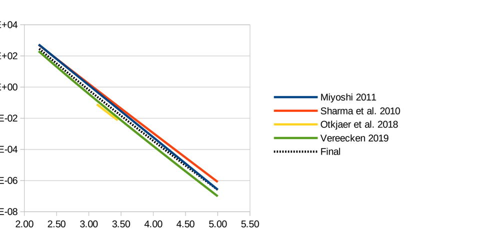
T	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200	5.00	5.00E-03	-2.30E+00	-8.74E+00	A		1.15E-09
225	4.44	4.44E-03	-2.35E+00	-6.87E+00		1.50E+09	0.64
250	4.00	4.00E-03	-2.40E+00	-5.34E+00	Ea		
260	3.85	3.85E-03	-2.41E+00	-4.81E+00		8.34E+03	
270	3.70	3.70E-03	-2.43E+00	-4.30E+00			1.17
280	3.57	3.57E-03	-2.45E+00	-3.83E+00			1.72E-04
290	3.45	3.45E-03	-2.46E+00	-3.39E+00		-7.19E+00	
298	3.36	3.36E-03	-2.47E+00	-3.05E+00		-2.70E+03	
310	3.23	3.23E-03	-2.49E+00	-2.58E+00		-1.18E+01	
320	3.13	3.13E-03	-2.51E+00	-2.21E+00		#N/A	
330	3.03	3.03E-03	-2.52E+00	-1.86E+00		#N/A	
340	2.94	2.94E-03	-2.53E+00	-1.52E+00	A		3.01E-02
350	2.86	2.86E-03	-2.54E+00	-1.20E+00		1.68E-12	1.00
375	2.67	2.67E-03	-2.57E+00	-4.74E-01	n		
400	2.50	2.50E-03	-2.60E+00	1.78E-01		7.19	
425	2.35	2.35E-03	-2.63E+00	7.65E-01	Ea		1.00
450	2.22	2.22E-03	-2.65E+00	1.30E+00		6223	1.98E+01



P1 15300000000 6800000000 9.59E+10 1.88E-03
P2 7720 1.2 9.62E+03 4.25E+00
P3 13.8 7.32E+07 6476.062651
Ea shift -1.91E+02

-CH2OO. | >CH-

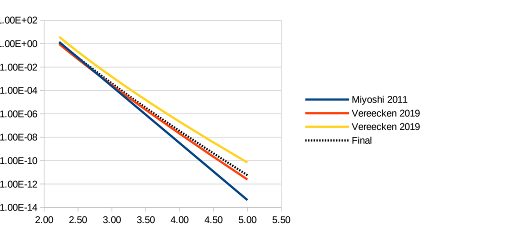
T	Miyoshi 2011	Sharma et al.	Otkjaer et al.	Vereecken 2019	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200	2.64E-07	8.18E-07		9.86E-08	9.86E-08		2.56E-07	5.00	5.00E-03	-2.30E+00	-6.59E+00	A		1.96E-07
225	1.92E-05	4.46E-05		5.94E-06	5.94E-06		1.39E-05	4.44	4.44E-03	-2.35E+00	-4.86E+00		4.59E+09	0.77
250	5.94E-04	1.11E-03		1.65E-04	1.65E-04		3.55E-04	4.00	4.00E-03	-2.40E+00	-3.45E+00	Ea		
260	1.95E-03	3.39E-03		5.29E-04	5.29E-04		1.10E-03	3.85	3.85E-03	-2.41E+00	-2.96E+00		7.54E+03	
270	5.85E-03	9.53E-03		1.56E-03	1.56E-03		3.17E-03	3.70	3.70E-03	-2.43E+00	-2.50E+00			1.10
280	1.62E-02	2.49E-02		4.30E-03	4.30E-03		8.49E-03	3.57	3.57E-03	-2.45E+00	-2.07E+00			9.32E-03
290	4.20E-02	6.12E-02	7.56E-03	1.11E-02	1.11E-02		2.14E-02	3.45	3.45E-03	-2.46E+00	-1.67E+00		-4.25E+00	
298	8.59E-02	1.20E-01	1.46E-02	2.26E-02	2.26E-02	4.30E-02	4.30E-02	3.36	3.36E-03	-2.47E+00	-1.37E+00		-2.73E+03	
310	2.34E-01	3.11E-01	3.73E-02	6.21E-02	6.21E-02		1.15E-01	3.23	3.23E-03	-2.49E+00	-9.40E-01		-2.73E+00	
320	5.10E-01	6.50E-01	7.87E-02	1.37E-01	1.37E-01		2.48E-01	3.13	3.13E-03	-2.51E+00	-6.06E-01		#N/A	
330	1.06E+00	1.30E+00		2.87E-01	2.87E-01		5.12E-01	3.03	3.03E-03	-2.52E+00	-2.90E-01		#N/A	
340	2.11E+00	2.51E+00		5.81E-01	5.81E-01		1.02E+00	2.94	2.94E-03	-2.53E+00	7.92E-03	A		1.02E+00
350	4.03E+00	4.65E+00		1.13E+00	1.13E+00		1.95E+00	2.86	2.86E-03	-2.54E+00	2.91E-01		1.88E-03	1.00
375	1.75E+01	1.90E+01		5.21E+00	5.21E+00		8.67E+00	2.67	2.67E-03	-2.57E+00	9.38E-01	n		
400	6.35E+01	6.52E+01		2.02E+01	2.02E+01		3.25E+01	2.50	2.50E-03	-2.60E+00	1.51E+00		4.25	
425	1.98E+02	1.95E+02		6.77E+01	6.77E+01		1.06E+02	2.35	2.35E-03	-2.63E+00	2.03E+00	Ea		1.00
450	5.42E+02	5.17E+02		2.01E+02	2.01E+02		3.08E+02	2.22	2.22E-03	-2.65E+00	2.49E+00		6285	3.08E+02



P1 92700000000 7.28043E-16 6.75E-29
P2 11210 8.306557086 1.27E+01
P3 7182.783983 5.20E+03
Ea shift 1.64E+02

>CHOO. | -CH3

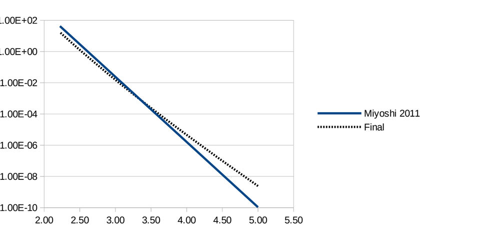
T	Miyoshi 2011	Vereecken 20	Vereecken 2019	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200	4.22E-14	2.39E-12	6.81E-11	1.28E-11		5.62E-12	5.00	5.00E-03	-2.30E+00	-1.13E+01	A		2.91E-12
225	2.14E-11	3.44E-10	5.47E-09	1.37E-09		6.61E-10	4.44	4.44E-03	-2.35E+00	-9.18E+00		9.77E+08	0.52
250	3.11E-09	2.01E-08	2.10E-07	6.50E-08		3.37E-08	4.00	4.00E-03	-2.40E+00	-7.47E+00	Ea		
260	1.75E-08	8.40E-08	7.71E-07	2.54E-07		1.35E-07	3.85	3.85E-03	-2.41E+00	-6.87E+00		9.45E+03	
270	8.63E-08	3.20E-07	2.61E-06	9.14E-07		4.98E-07	3.70	3.70E-03	-2.43E+00	-6.30E+00			1.26
280	3.80E-07	1.12E-06	8.25E-06	3.04E-06		1.69E-06	3.57	3.57E-03	-2.45E+00	-5.77E+00			2.13E-06
290	1.51E-06	3.63E-06	2.45E-05	9.42E-06		5.35E-06	3.45	3.45E-03	-2.46E+00	-5.27E+00		-1.05E+01	
298	4.27E-06	8.84E-06	5.59E-05	2.22E-05	1.28E-05	1.28E-05	3.36	3.36E-03	-2.47E+00	-4.89E+00		-2.76E+03	
310	1.83E-05	3.12E-05	1.82E-04	7.53E-05		4.43E-05	3.23	3.23E-03	-2.49E+00	-4.35E+00		-2.17E+01	
320	5.67E-05	8.38E-05	4.59E-04	1.96E-04		1.17E-04	3.13	3.13E-03	-2.51E+00	-3.93E+00		#N/A	
330	1.64E-04	2.14E-04	1.11E-03	4.87E-04		2.96E-04	3.03	3.03E-03	-2.52E+00	-3.53E+00		#N/A	
340	4.45E-04	5.19E-04	2.58E-03	1.16E-03		7.15E-04	2.94	2.94E-03	-2.53E+00	-3.15E+00	A		7.15E-04
350	1.14E-03	1.21E-03	5.78E-03	2.64E-03		1.65E-03	2.86	2.86E-03	-2.54E+00	-2.78E+00		2.22E-22	1.00
375	9.65E-03	8.41E-03	3.74E-02	1.77E-02		1.15E-02	2.67	2.67E-03	-2.57E+00	-1.94E+00	n		
400	6.25E-02	4.76E-02	2.02E-01	9.81E-02		6.51E-02	2.50	2.50E-03	-2.60E+00	-1.19E+00		10.52	
425	3.25E-01	2.27E-01	9.39E-01	4.61E-01		3.14E-01	2.35	2.35E-03	-2.63E+00	-5.04E-01	Ea		1.00
450	1.41E+00	9.31E-01	3.83E+00	1.89E+00		1.31E+00	2.22	2.22E-03	-2.65E+00	1.18E-01		6353	1.31E+00



P1 79300000000
P2 9610
P3
Ea shift 5.28E+00

>CHOO. | -CH2-

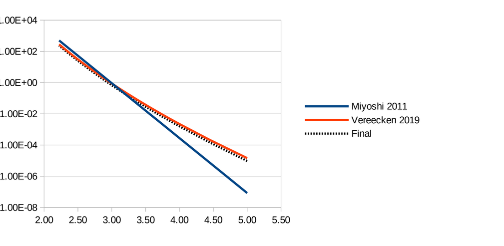
T	Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200	1.08E-10	2.49E-09		2.43E-09	5.00	5.00E-03	-2.30E+00	-8.61E+00	A		1.38E-09
225	2.24E-08	1.55E-07		1.51E-07	4.44	4.44E-03	-2.35E+00	-6.82E+00		8.23E+08	0.57
250	1.60E-06	4.66E-06		4.56E-06	4.00	4.00E-03	-2.40E+00	-5.34E+00	Ea		
260	7.03E-06	1.55E-05		1.52E-05	3.85	3.85E-03	-2.41E+00	-4.82E+00		8.19E+03	
270	2.76E-05	4.79E-05		4.70E-05	3.70	3.70E-03	-2.43E+00	-4.33E+00			1.22
280	9.86E-05	1.38E-04		1.36E-04	3.57	3.57E-03	-2.45E+00	-3.87E+00			1.65E-04
290	3.22E-04	3.74E-04		3.67E-04	3.45	3.45E-03	-2.46E+00	-3.43E+00		-9.05E+00	
298	7.83E-04	7.97E-04	7.83E-04	7.83E-04	3.36	3.36E-03	-2.47E+00	-3.11E+00		-2.40E+03	
310	2.73E-03	2.33E-03		2.29E-03	3.23	3.23E-03	-2.49E+00	-2.64E+00		-1.75E+01	
320	7.19E-03	5.42E-03		5.33E-03	3.13	3.13E-03	-2.51E+00	-2.27E+00		#N/A	
330	1.79E-02	1.21E-02		1.19E-02	3.03	3.03E-03	-2.52E+00	-1.93E+00		#N/A	
340	4.21E-02	2.59E-02		2.55E-02	2.94	2.94E-03	-2.53E+00	-1.59E+00	A		2.55E-02
350	9.44E-02	5.34E-02		5.26E-02	2.86	2.86E-03	-2.54E+00	-1.28E+00		3.47E-18	1.00
375	5.89E-01	2.85E-01		2.81E-01	2.67	2.67E-03	-2.57E+00	-5.51E-01	n		
400	2.92E+00	1.28E+00		1.27E+00	2.50	2.50E-03	-2.60E+00	1.02E-01		9.05	
425	1.20E+01	4.99E+00		4.93E+00	2.35	2.35E-03	-2.63E+00	6.93E-01	Ea		1.00
450	4.21E+01	1.72E+01		1.70E+01	2.22	2.22E-03	-2.65E+00	1.23E+00		5519	1.70E+01



P1 32800000000 1.28E-35
P2 8100 1.47E+01
P3 1746.57242
Ea shift 8.39E+01

>CHOO. | >CH-

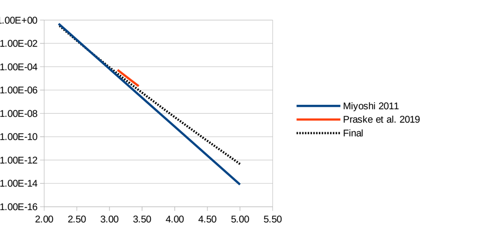
T	Miyoshi 2011	Vereecken 2019	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200	8.45E-08	1.45E-05	1.45E-05		9.53E-06	5.00	5.00E-03	-2.30E+00	-5.02E+00	A		3.79E-06
225	7.61E-06	2.16E-04	2.16E-04		1.49E-04	4.44	4.44E-03	-2.35E+00	-3.83E+00		9.25E+07	0.40
250	2.78E-04	2.21E-03	2.21E-03		1.58E-03	4.00	4.00E-03	-2.40E+00	-2.80E+00	Ea		
260	9.68E-04	5.16E-03	5.16E-03		3.73E-03	3.85	3.85E-03	-2.41E+00	-2.43E+00		6.17E+03	
270	3.07E-03	1.15E-02	1.15E-02		8.44E-03	3.70	3.70E-03	-2.43E+00	-2.07E+00			1.38
280	8.96E-03	2.48E-02	2.48E-02		1.84E-02	3.57	3.57E-03	-2.45E+00	-1.74E+00			2.54E-02
290	2.43E-02	5.15E-02	5.15E-02		3.86E-02	3.45	3.45E-03	-2.46E+00	-1.41E+00		-1.47E+01	
298	5.14E-02	9.03E-02	9.03E-02	6.82E-02	6.82E-02	3.36	3.36E-03	-2.47E+00	-1.17E+00		-7.95E+02	
310	1.47E-01	2.03E-01	2.03E-01		1.55E-01	3.23	3.23E-03	-2.49E+00	-8.11E-01		-3.49E+01	
320	3.33E-01	3.85E-01	3.85E-01		2.96E-01	3.13	3.13E-03	-2.51E+00	-5.28E-01		#N/A	
330	7.18E-01	7.15E-01	7.15E-01		5.54E-01	3.03	3.03E-03	-2.52E+00	-2.56E-01		#N/A	
340	1.48E+00	1.30E+00	1.30E+00		1.01E+00	2.94	2.94E-03	-2.53E+00	5.40E-03	A		1.01E+00
350	2.92E+00	2.30E+00	2.30E+00		1.81E+00	2.86	2.86E-03	-2.54E+00	2.57E-01		1.28E-35	1.00
375	1.36E+01	8.85E+00	8.85E+00		7.07E+00	2.67	2.67E-03	-2.57E+00	8.50E-01	n		
400	5.27E+01	3.06E+01	3.06E+01		2.48E+01	2.50	2.50E-03	-2.60E+00	1.39E+00		14.71	
425	1.73E+02	9.65E+01	9.65E+01		7.92E+01	2.35	2.35E-03	-2.63E+00	1.90E+00	Ea		1.00
450	5.00E+02	2.81E+02	2.81E+02		2.33E+02	2.22	2.22E-03	-2.65E+00	2.37E+00		1831	2.33E+02



P1 50400000000 4.50E+11
P2 11420 12528
P3 8.12E+07
Ea shift 1.72E+03

>C(OO.)- | -CH3

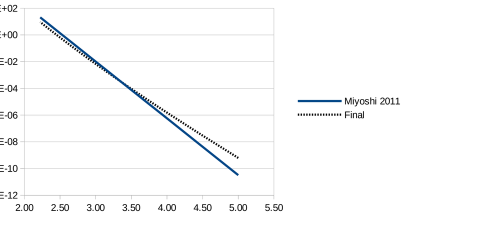
T	Miyoshi 2011	Praske et al. 2019	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	8.02E-15		2.49E-09		4.57E-13	5.00	5.00E-03	-2.30E+00	-1.23E+01	A		2.59E-13
225	4.57E-12		1.55E-07		7.38E-11	4.44	4.44E-03	-2.35E+00	-1.01E+01		8.23E+08	0.57
250	7.31E-10		4.66E-06		4.77E-09	4.00	4.00E-03	-2.40E+00	-8.32E+00	Ea		
260	4.24E-09		1.55E-05		2.07E-08	3.85	3.85E-03	-2.41E+00	-7.68E+00		9.90E+03	
270	2.15E-08		4.79E-05		8.17E-08	3.70	3.70E-03	-2.43E+00	-7.09E+00			1.22
280	9.76E-08		1.38E-04		2.96E-07	3.57	3.57E-03	-2.45E+00	-6.53E+00			3.61E-07
290	3.98E-07	2.18E-06	3.74E-04		9.90E-07	3.45	3.45E-03	-2.46E+00	-6.00E+00		-9.05E+00	
298	1.15E-06	5.34E-06	7.97E-04	2.48E-06	2.48E-06	3.36	3.36E-03	-2.47E+00	-5.61E+00		-3.14E+03	
310	5.05E-06	1.93E-05	2.33E-03		9.06E-06	3.23	3.23E-03	-2.49E+00	-5.04E+00		-1.75E+01	
320	1.60E-05	5.33E-05	5.42E-03		2.50E-05	3.13	3.13E-03	-2.51E+00	-4.60E+00		#N/A	
330	4.71E-05		1.21E-02		6.56E-05	3.03	3.03E-03	-2.52E+00	-4.18E+00		#N/A	
340	1.30E-04		2.59E-02		1.64E-04	2.94	2.94E-03	-2.53E+00	-3.79E+00	A		1.64E-04
350	3.40E-04		5.34E-02		3.91E-04	2.86	2.86E-03	-2.54E+00	-3.41E+00		3.47E-18	1.00
375	3.00E-03		2.85E-01		2.90E-03	2.67	2.67E-03	-2.57E+00	-2.54E+00	n		
400	2.01E-02		1.28E+00		1.74E-02	2.50	2.50E-03	-2.60E+00	-1.76E+00		9.05	
425	1.08E-01		4.99E+00		8.70E-02	2.35	2.35E-03	-2.63E+00	-1.06E+00	Ea		1.00
450	4.80E-01		1.72E+01		3.76E-01	2.22	2.22E-03	-2.65E+00	-4.25E-01		7235	3.76E-01



P1 57800000000
P2 9790
P3
Ea shift 2.80E+02

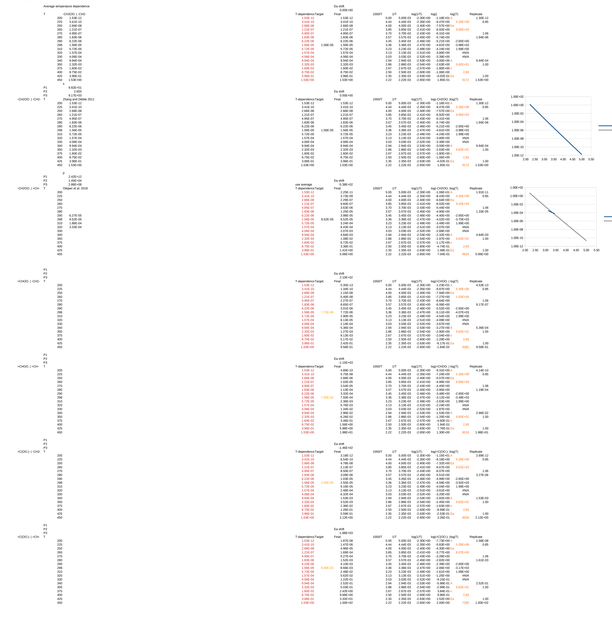
>C(OO.)- | -CH2-

T	Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	3.19E-11	2.49E-09		6.16E-10	5.00	5.00E-03	-2.30E+00	-9.21E+00	A		3.50E-10
225	7.33E-09	1.55E-07		4.47E-08	4.44	4.44E-03	-2.35E+00	-7.35E+00		8.23E+08	0.57
250	5.69E-07	4.66E-06		1.52E-06	4.00	4.00E-03	-2.40E+00	-5.82E+00	Ea		
260	2.56E-06	1.55E-05		5.30E-06	3.85	3.85E-03	-2.41E+00	-5.28E+00		8.46E+03	
270	1.03E-05	4.79E-05		1.70E-05	3.70	3.70E-03	-2.43E+00	-4.77E+00			1.22
280	3.78E-05	1.38E-04		5.09E-05	3.57	3.57E-03	-2.45E+00	-4.29E+00			6.21E-05
290	1.26E-04	3.74E-04		1.43E-04	3.45	3.45E-03	-2.46E+00	-3.85E+00		-9.05E+00	
298	3.12E-04	7.97E-04	3.12E-04	3.12E-04	3.36	3.36E-03	-2.47E+00	-3.51E+00		-2.52E+03	
310	1.11E-03	2.33E-03		9.47E-04	3.23	3.23E-03	-2.49E+00	-3.02E+00		-1.75E+01	
320	2.99E-03	5.42E-03		2.26E-03	3.13	3.13E-03	-2.51E+00	-2.65E+00		#N/A	
330	7.55E-03	1.21E-02		5.18E-03	3.03	3.03E-03	-2.52E+00	-2.29E+00		#N/A	

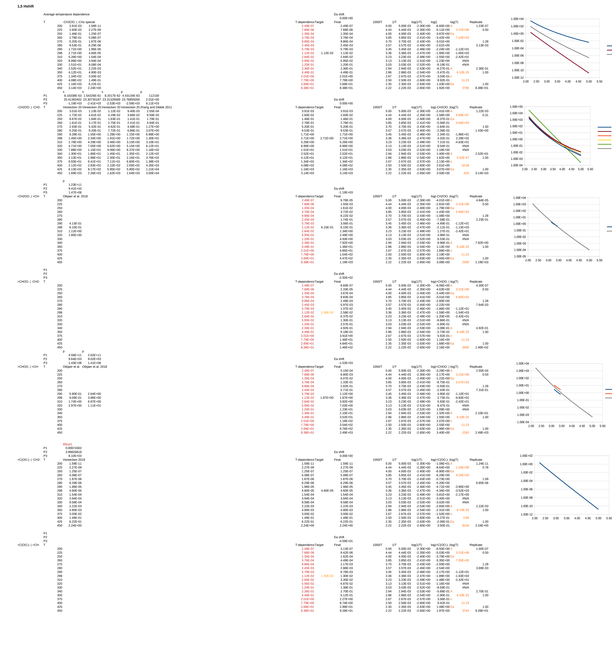


Unsaturated RO2 with exo-cyclic double bond

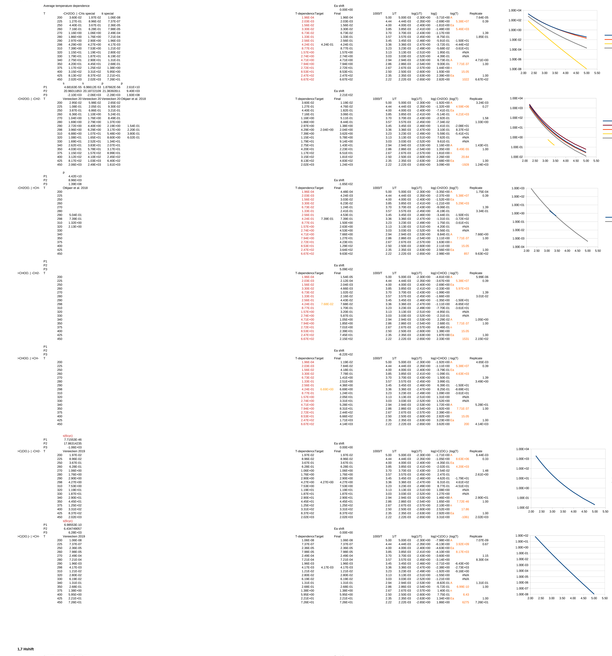
L1-Hulsh



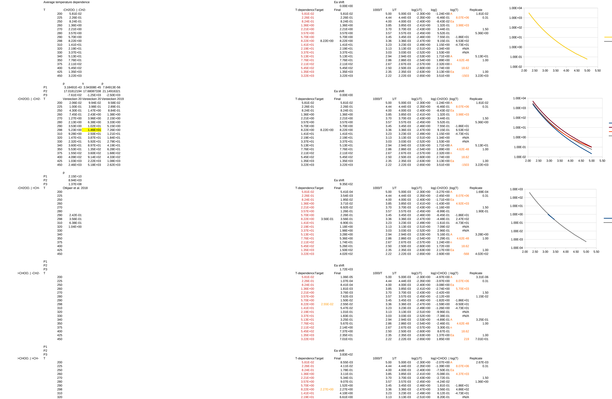
L2-Hulsh



L3-Hulsh



L4-Hulsh



L5-Hulsh

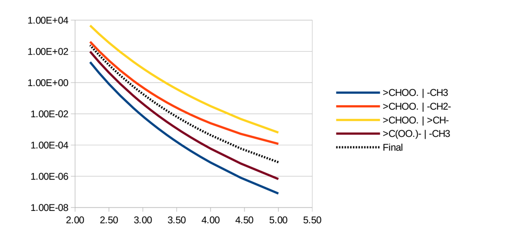
282			1.54E-01		3.67	3.57E-03	2.45E+00	8.12E-01	2.22E-01
290			2.75E-01		5.45	5.46E-03	2.46E+00	5.61E-01	1.95E+01
298			4.90E-01		8.10	8.34E-03	2.47E+00	3.88E-01	1.73E+01
306			8.27E-01		12.03	1.27E-02	2.48E+00	2.68E-01	1.54E+01
314			1.39E+00		17.87	1.94E-02	2.49E+00	1.85E-01	1.37E+01
322			2.34E+00		26.54	2.96E-02	2.50E+00	1.28E-01	1.22E+01
330			3.94E+00		39.42	4.51E-02	2.51E+00	8.85E-02	1.08E+01
338			6.64E+00		58.55	6.88E-02	2.52E+00	6.12E-02	9.57E+00
346			1.12E+01		86.97	1.05E-01	2.53E+00	4.23E-02	8.47E+00
354			1.89E+01		129.20	1.60E-01	2.54E+00	2.92E-02	7.49E+00
362			3.18E+01		191.93	2.44E-01	2.55E+00	2.02E-02	6.63E+00
370			5.36E+01		285.13	3.72E-01	2.56E+00	1.39E-02	5.86E+00
378			9.03E+01		423.67	5.67E-01	2.57E+00	9.62E-03	5.19E+00
386			1.52E+02		629.44	8.64E-01	2.58E+00	6.65E-03	4.59E+00
394			2.56E+02		935.31	1.32E+00	2.59E+00	4.59E-03	4.06E+00
402			4.32E+02		1389.68	2.01E+00	2.60E+00	3.17E-03	3.59E+00
410			7.27E+02		2064.50	3.07E+00	2.61E+00	2.19E-03	3.18E+00
418			1.22E+03		3067.61	4.68E+00	2.62E+00	1.51E-03	2.81E+00
426			2.06E+03		4557.58	7.14E+00	2.63E+00	1.04E-03	2.49E+00
434			3.47E+03		6770.49	1.09E+01	2.64E+00	7.19E-04	2.20E+00
442			5.85E+03		10061.00	1.66E+01	2.65E+00	4.96E-04	1.95E+00
450			9.87E+03		14948.00	2.53E+01	2.66E+00	3.42E-04	1.72E+00
458			1.66E+04		22210.00	3.86E+01	2.67E+00	2.36E-04	1.52E+00
466			2.80E+04		33000.00	5.89E+01	2.68E+00	1.63E-04	1.35E+00
474			4.72E+04		49040.00	8.98E+01	2.69E+00	1.12E-04	1.19E+00
482			7.96E+04		72870.00	1.37E+02	2.70E+00	7.75E-05	1.06E+00
490			1.34E+05		108300.00	2.09E+02	2.71E+00	5.34E-05	9.39E-01
498			2.26E+05		160900.00	3.18E+02	2.72E+00	3.68E-05	8.32E-01
506			3.81E+05		239100.00	4.85E+02	2.73E+00	2.53E-05	7.37E-01
514			6.43E+05		355300.00	7.40E+02	2.74E+00	1.74E-05	6.53E-01
522			1.08E+06		527900.00	1.13E+03	2.75E+00	1.20E-05	5.78E-01
530			1.82E+06		784400.00	1.72E+03	2.76E+00	8.24E-06	5.12E-01
538			3.07E+06		1165000.00	2.63E+03	2.77E+00	5.67E-06	4.53E-01
546			5.18E+06		1731000.00	4.01E+03	2.78E+00	3.90E-06	4.02E-01
554			8.74E+06		2572000.00	6.13E+03	2.79E+00	2.68E-06	3.56E-01
562			1.47E+07		3822000.00	9.36E+03	2.80E+00	1.85E-06	3.16E-01
570			2.49E+07		5680000.00	1.43E+04	2.81E+00	1.27E-06	2.80E-01
578			4.20E+07		8439000.00	2.18E+04	2.82E+00	8.76E-07	2.49E-01
586			7.09E+07		12540000.00	3.33E+04	2.83E+00	6.03E-07	2.21E-01
594			1.20E+08		18630000.00	5.08E+04	2.84E+00	4.15E-07	1.96E-01
602			2.02E+08		27680000.00	7.76E+04	2.85E+00	2.86E-07	1.74E-01
610			3.42E+08		41130000.00	1.18E+05	2.86E+00	1.97E-07	1.54E-01
618			5.77E+08		61130000.00	1.81E+05	2.87E+00	1.36E-07	1.37E-01
626			9.74E+08		90850000.00	2.76E+05	2.88E+00	9.36E-08	1.21E-01
634			1.64E+09		135000000.00	4.22E+05	2.89E+00	6.45E-08	1.08E-01
642			2.77E+09		200600000.00	6.44E+05	2.90E+00	4.44E-08	9.56E-02
650			4.67E+09		298100000.00	9.84E+05	2.91E+00	3.06E-08	8.46E-02
658			7.89E+09		443000000.00	1.50E+06	2.92E+00	2.11E-08	7.49E-02
666			1.33E+10		658400000.00	2.29E+06	2.93E+00	1.45E-08	6.63E-02
674			2.25E+10		978600000.00	3.50E+06	2.94E+00	1.00E-08	5.87E-02
682			3.80E+10		1454000000.00	5.34E+06	2.95E+00	6.89E-09	5.19E-02
690			6.41E+10		2161000000.00	8.16E+06	2.96E+00	4.75E-09	4.60E-02
698			1.08E+11		3212000000.00	1.25E+07	2.97E+00	3.27E-09	4.07E-02
706			1.82E+11		4774000000.00	1.91E+07	2.98E+00	2.25E-09	3.60E-02
714			3.07E+11		7096000000.00	2.92E+07	2.99E+00	1.55E-09	3.19E-02
722			5.18E+11		10550000000.00	4.46E+07	3.00E+00	1.07E-09	2.82E-02
730			8.74E+11		15680000000.00	6.82E+07	3.01E+00	7.36E-10	2.50E-02
738			1.47E+12		23310000000.00	1.04E+08	3.02E+00	5.07E-10	2.21E-02
746			2.49E+12		34660000000.00	1.59E+08	3.03E+00	3.49E-10	1.96E-02
754			4.20E+12		51530000000.00	2.43E+08	3.04E+00	2.41E-10	1.73E-02
762			7.09E+12		76610000000.00	3.71E+08	3.05E+00	1.66E-10	1.53E-02
770			1.20E+13		113900000000.00	5.66E+08	3.06E+00	1.14E-10	1.35E-02
778			2.02E+13		169400000000.00	8.64E+08	3.07E+00	7.85E-11	1.19E-02
786			3.42E+13		251900000000.00	1.32E+09	3.08E+00	5.41E-11	1.05E-02
794			5.77E+13		374600000000.00	2.01E+09	3.09E+00	3.73E-11	9.27E-03
802			9.74E+13		557000000000.00	3.07E+09	3.10E+00	2.57E-11	8.18E-03
810			1.64E+14		828400000000.00	4.69E+09	3.11E+00	1.77E-11	7.22E-03
818			2.77E+14		1232000000000.00	7.16E+09	3.12E+00	1.22E-11	6.37E-03
826			4.67E+14		1832000000000.00	1.09E+10	3.13E+00	8.40E-12	5.62E-03
834			7.89E+14		2724000000000.00	1.67E+10	3.14E+00	5.79E-12	4.96E-03
842			1.33E+15		4051000000000.00	2.54E+10	3.15E+00	3.99E-12	4.38E-03
850			2.25E+15		6024000000000.00	3.88E+10	3.16E+00	2.75E-12	3.86E-03
858			3.80E+15		8957000000000.00	5.92E+10	3.17E+00	1.89E-12	3.41E-03
866			6.41E+15		1.33E+13	9.04E+10	3.18E+00	1.30E-12	3.00E-03
874			1.08E+16		1.98E+13	1.38E+11	3.19E+00	8.97E-13	2.65E-03
882			1.82E+16		2.94E+13	2.10E+11	3.20E+00	6.18E-13	2.33E-03
890			3.07E+16		4.37E+13	3.21E+11	3.21E+00	4.26E-13	2.06E-03
898			5.18E+16		6.49E+13	4.89E+11	3.22E+00	2.93E-13	1.81E-03
906			8.74E+16		9.64E+13	7.46E+11	3.23E+00	2.02E-13	1.60E-03
914			1.47E+17		1.43E+14	1.14E+12	3.24E+00	1.39E-13	1.41E-03
922			2.49E+17		2.13E+14	1.73E+12	3.25E+00	9.59E-14	1.24E-03
930			4.20E+17		3.16E+14	2.64E+12	3.26E+00	6.61E-14	1.10E-03
938			7.09E+17		4.70E+14	4.02E+12	3.27E+00	4.56E-14	9.67E-04
946			1.20E+18		6.98E+14	6.12E+12	3.28E+00	3.14E-14	8.52E-04
954			2.02E+18		1.04E+15	9.32E+12	3.29E+00	2.17E-14	7.51E-04
962			3.42E+18		1.54E+15	1.42E+13	3.30E+00	1.49E-14	6.61E-04
970			5.77E+18		2.29E+15	2.16E+13	3.31E+00	1.03E-14	5.82E-04
978			9.74E+18		3.40E+15	3.29E+13	3.32E+00	7.08E-15	5.13E-04
986			1.64E+19		5.05E+15	5.00E+13	3.33E+00	4.88E-15	4.51E-04
994			2.77E+19		7.50E+15	7.61E+13	3.34E+00	3.36E-15	3.97E-04
1002			4.67E+19		1.11E+16	1.16E+14	3.35E+00	2.31E-15	3.50E-04
1010			7.89E+19		1.66E+16	1.76E+14	3.36E+00	1.59E-15	3.08E-04
1018			1.33E+20		2.46E+16	2.68E+14	3.37E+00	1.09E-15	2.71E-04
1026			2.25E+20		3.65E+16	4.07E+14	3.38E+00	7.52E-16	2.39E-04
1034			3.80E+20		5.41E+16	6.18E+14	3.39E+00	5.18E-16	2.10E-04
1042			6.41E+20		8.02E+16	9.38E+14	3.40E+00	3.57E-16	1.85E-04
1050			1.08E+21		1.19E+17	1.42E+15	3.41E+00	2.46E-16	1.63E-04
1058			1.82E+21		1.76E+17	2.16E+15	3.42E+00	1.69E-16	1.43E-04
1066			3.07E+21		2.61E+17	3.27E+15	3.43E+00	1.17E-16	1.26E-04
1074			5.18E+21		3.87E+17	4.96E+15	3.44E+00	8.05E-17	1.11E-04
1082			8.74E+21		5.73E+17	7.52E+15	3.45E+00	5.54E-17	9.76E-05
1090			1.47E+22		8.49E+17	1.14E+16	3.46E+00	3.82E-17	8.59E-05
1098			2.49E+22		1.26E+18	1.73E+16	3.47E+00	2.63E-17	7.56E-05
1106			4.20E+22		1.86E+18	2.62E+16	3.48E+00	1.81E-17	6.65E-05
1114			7.09E+22		2.76E+18	3.97E+16	3.49E+00	1.25E-17	5.85E-05
1122			1.20E+23		4.09E+18	6.02E+16	3.50E+00	8.59E-18	5.15E-05
1130			2.02E+23		6.06E+18	9.12E+16	3.51E+00	5.91E-18	4.53E-05
1138			3.42E+23		8.98E+18	1.38E+17	3.52E+00	4.07E-18	3.98E-05
1146			5.77E+23		1.33E+19	2.09E+17	3.53E+00	2.80E-18	3.50E-05
1154			9.74E+23		1.97E+19	3.16E+17	3.54E+00	1.93E-18	3.08E-05
1162			1.64E+24		2.92E+19	4.78E+17	3.55E+00	1.33E-18	2.71E-05
1170			2.77E+24		4.32E+19	7.23E+17	3.56E+00	9.14E-19	2.38E-05
1178			4.67E+24		6.40E+19	1.09E+18	3.57E+00	6.29E-19	2.09E-05
1186			7.89E+24		9.48E+19	1.65E+18	3.58E+00	4.33E-19	1.84E-05
1194			1.33E+25		1.40E+20	2.49E+18	3.59E+00	2.98E-19	1.62E-05
1202			2.25E+25		2.08E+20	3.77E+18	3.60E+00	2.05E-19	1.42E-05
1210			3.80E+25		3.08E+20	5.70E+18	3.61E+00	1.41E-19	1.25E-05
1218			6.41E+25		4.56E+20	8.62E+18	3.62E+00	9.71E-20	1.10E-05
1226			1.08E+26		6.75E+20	1.30E+19	3.63E+00	6.69E-20	9.66E-06
1234			1.82E+26		1.00E+21	1.97E+19	3.64E+00	4.61E-20	8.50E-06
1242			3.07E+26		1.48E+21	2.97E+19	3.65E+00	3.17E-20	7.48E-06
1250			5.18E+26		2.19E+21	4.49E+19	3.66E+00	2.18E-20	6.58E-06
1258			8.74E+26		3.24E+21	6.78E+19	3.67E+00	1.50E-20	5.79E-06
1266			1.47E+27		4.79E+21	1.02E+20	3.68E+00	1.03E-20	5.09E-06
1274			2.49E+27		7.09E+21	1.54E+20	3.69E+00	7.09E-21	4.48E-06
1282			4.20E+27		1.05E+22	2.32E+20	3.70E+00	4.88E-21	3.94E-06
1290			7.09E+27		1.55E+22	3.50E+20	3.71E+00	3.36E-21	3.47E-06
1298			1.20E+28		2.30E+22	5.28E+20	3.72E+00	2.31E-21	3.05E-06
1306			2.02E+28		3.40E+22	7.96E+20	3.73E+00	1.59E-21	2.68E-06
1314			3.42E+28		5.03E+22	1.20E+21	3.74E+00	1.09E-21	2.36E-06
1322			5.77E+28		7.44E+22	1.81E+21	3.75E+00	7.51E-22	2.07E-06
1330			9.74E+28		1.10E+23	2.72E+21	3.76E+00	5.16E-22	1.82E-06
1338			1.64E+29		1.63E+23	4.10E+21	3.77E+00	3.54E-22	1.60E-06
1346			2.77E+29		2.41E+23	6.17E+21	3.78E+00	2.43E-22	1.41E-06
1354			4.67E+29		3.56E+23	9.29E+21	3.79E+00	1.67E-22	1.24E-06
1362			7.89E+29		5.26E+23	1.40E+22	3.80E+00	1.15E-22	1.09E-06
1370			1.33E+30		7.78E+23	2.10E+22	3.81E+00	7.90E-23	9.59E-07
1378			2.25E+30		1.15E+24	3.16E+22	3.82E+00	5.43E-23	8.43E-07
1386			3.80E+30		1.70E+24	4.76E+22	3.83E+00	3.73E-23	7.41E-07
1394			6.41E+30		2.51E+24	7.16E+22	3.84E+00	2.56E-23	6.52E-07
1402			1.08E+31		3.71E+24	1.08E+23	3.85E+00	1.76E-23	5.73E-07
1410			1.82E+31		5.48E+24	1.62E+23	3.86E+00	1.21E-23	5.04E-07
1418			3.07E+31		8.10E+24	2.44E+23	3.87E+00	8.31E-24	4.43E-07
1426			5.18E+31		1.20E+25	3.67E+23	3.88E+00	5.71E-24	3.89E-07
1434			8.74E+31		1.77E+25	5.52E+23	3.89E+00	3.92E-24	3.42E-07
1442			1.47E+32		2.62E+25	8.30E+23	3.90E+00	2.69E-24	3.01E-07
1450			2.49E+32		3.87E+25	1.25E+24	3.91E+00	1.85E-24	2.64E-07
1458			4.20E+32		5.72E+25	1.87E+24	3.92E+00	1.27E-24	2.32E-07
1466			7.09E+32		8.45E+25	2.82E+24	3.93E+00	8.73E-25	2.04E-07
1474			1.20E+33		1.25E+26	4.24E+24	3.94E+00	6.00E-25	1.79E-07
1482			2.02E+33		1.85E+26	6.38E+24	3.95E+00	4.12E-25	1.57E-07
1490			3.42E+33		2.73E+26	9.60E+24	3.96E+00	2.83E-25	1.38E-07
1498			5.77E+33		4.03E+26	1.44E+25	3.97E+00	1.94E-25	1.21E-07
1506			9.74E+33		5.96E+26	2.17E+25	3.98E+00	1.33E-25	1.06E-07
1514			1.64E+34		8.80E+26	3.26E+25	3.99E+00	9.14E-26	9.31E-08
1522			2.77E+34		1.30E+27	4.91E+25	4.00E+00	6.28E-26	8.17E-08
1530			4.67E+34		1.92E+27	7.39E+25	4.01E+00	4.31E-26	7.17E-08
1538			7.89E+34		2.84E+27	1.11E+26	4.02E+00	2.96E-26	6.29E-08
1546			1.33E+35		4.19E+27	1.67E+26	4.03E+00	2.03E-26	5.52E-08
1554			2.25E+35		6.19E+27	2.51E+26	4.04E+00	1.39E-26	4.84E-08
1562			3.80E+35		9.14E+27	3.78E+26	4.05E+00	9.55E-27	4.25E-08
1570			6.41E+35		1.35E+28	5.68E+26	4.06E+00	6.55E-27	3.73E-08
1578			1.08E+36		1.99E+28	8.54E+26	4.07E+00	4.49E-27	3.27E-08
1586			1.82E+36		2.94E+28	1.28E+27	4.08E+00	3.08E-27	2.87E-08
1594			3.07E+36		4.34E+28	1.92E+27	4.09E+00	2.11E-27	2.52E-08
1602			5.18E+36		6.41E+28	2.89E+27	4.10E+00	1.45E-27	2.21E-08
1610			8.74E+36		9.46E+28	4.34E+27	4.11E+00	9.93E-28	1.94E-08
1618			1.47E+37		1.40E+29	6.53E+27	4.12E+00	6.81E-28	1.70E-08
1626			2.49E+37		2.06E+29	9.82E+27	4.13E+00	4.67E-28	1.49E-08
1634			4.20E+37		3.04E+29	1.48E+28	4.14E+00	3.20E-28	1.31E-08
1642			7.09E+37		4.49E+29	2.22E+28	4.15E+00	2.20E-28	1.15E-08
1650			1.20E+38		6.63E+29	3.34E+28	4.16E+00	1.51E-28	1.01E-08
1658			2.02E+38		9.79E+29	5.02E+28	4.17E+00	1.03E-28	8.85E-09
1666			3.42E+38		1.45E+30	7.55E+28	4.18E+00	7.09E-29	7.76E-09
1674			5.77E+38		2.14E+30	1.13E+29	4.19E+00	4.86E-29	6.80E-09
1682			9.74E+38		3.16E+30	1.70E+29	4.20E+00	3.34E-29	5.96E-09
1690			1.64E+39		4.66E+30	2.55E+29	4.21E+00	2.29E-29	5.22E-09
1698			2.77E+39		6.88E+30	3.84E+29	4.22E+00	1.57E-29	4.57E-09
1706			4.67E+39		1.02E+31	5.77E+29	4.23E+00	1.08E-29	4.00E-09
1714			7.89E+39		1.50E+31	8.67E+29	4.24E+00	7.40E-30	3.50E-09
1722			1.33E+40		2.22E+31	1.30E+30	4.25E+00	5.08E-30	3.07E-09
1730			2.25E+40		3.27E+31	1.96E+30	4.26E+00	3.48E-30	2.68E-09
1738			3.80E+40		4.83E+31	2.94E+30	4.27E+00	2.39E-30	2.35E-09
1746			6.41E+40		7.13E+31	4.42E+30	4.28E+00	1.64E-30	2.05E-09
1754			1.08E+41		1.05E+32	6.64E+30	4.29E+00	1.12E-30	1.80E-09
1762			1.82E+41		1.55E+32	9.98E+30	4.30E+00	7.71E-31	1.57E-09
1770			3.07E+41		2.28E+32	1.50E+31	4.31E+00	5.29E-31	1.38E-09
1778			5.18E+41		3.36E+32	2.25E+31	4.32E+00	3.63E-31	1.21E-09
1786			8.74E+41		4.96E+32	3.38E+31	4.33E+00	2.49E-31	1.06E-09
1794			1.47E+42		7.32E+32	5.08E+31	4.34E+00	1.71E-31	9.29E-10
1802			2.49E+42		1.08E+33	7.63E+31	4.35E+00	1.17E-31	8.14E-10
1810			4.20E+42		1.59E+33	1.15E+32	4.36E+00	8.05E-32	7.13E-10
1818			7.09E+42		2.35E+33	1.72E+32	4.37E+00	5.52E-32	6.24E-10
1826			1.20E+43		3.46E+33	2.59E+32	4.38E+00	3.79E-32	5.47E-10
1834			2.02E+43		5.11E+33	3.89E+32	4.39E+00	2.60E-32	4.79E-10
1842			3.42E+43		7.54E+33	5.84E+32	4.40E+00	1.78E-32	4.19E-10
1850			5.77E+43		1.11E+34	8.77E+32	4.41E+00	1.22E-32	3.67E-10
1858			9.74E+43		1.64E+34	1.32E+33	4.42E+00	8.38E-33	3.21E-10
1866			1.64E+44		2.42E+34	1.97E+33	4.43E+00	5.75E-33	2.81E-10
1874			2.77E+44		3.57E+34	2.96E+33	4.44E+00	3.94E-33	2.46E-10
1882			4.67E+44		5.26E+34	4.44E+33	4.45E+00	2.70E-33	2.15E-10
1890			7.89E+44		7.76E+34	6.66E+33	4.46E+00	1.85E-33	1.88E-10
1898			1.33E+45		1.14E+35	9.99E+33	4.47E+00	1.27E-33	1.65E-10
1906			2.25E+45		1.68E+35	1.50E+34	4.48E+00	8.70E-34	1.44E-10
1914			3.80E+45		2.47E+35	2.24E+34	4.49E+00	5.96E-34	1.26E-10
1922			6.41E+45		3.64E+35	3.37E+34	4.50E+00	4.09E-34	1.10E-10
1930			1.08E+46		5.36E+35	5.05E+34	4.51E+00	2.80E-34	9.64E-11
1938			1.82E+46		7.89E+35	7.58E+34	4.52E+00	1.92E-34	8.43E-11
1946			3.07E+46		1.16E+36	1.14E+35	4.53E+00	1.32E-34	7.37E-11
1954			5.18E+46		1.71E+36	1.70E+35	4.54E+00	9.04E-35	6.44E-11
1962			8.74E+46		2.51E+36	2.55E+35	4.55E+00	6.20E-35	5.63E-11
1970			1.47E+47		3.70E+36	3.82E+35	4.56E+00	4.25E-35	4.92E-11
1978			2.49E+47		5.44E+36	5.73E+35	4.57E+00	2.91E-35	4.30E-11
1986			4.20E+47		8.00E+36	8.59E+35	4.58E+00	2.00E-35	3.76E-11
1994			7.09E+47		1.18E+37	1.29E+36	4.59E+00	1.37E-35	3.28E-11
2002			1.20E+48		1.73E+37	1.93E+36	4.60E+00	9.41E-36	2.87E-11
2010			2.02E+48		2.55E+37	2.90E+36	4.61E+00	6.46E-36	2.50E-11
2018			3.42E+48		3.75E+37	4.34E+36	4.62E+00	4.43E-36	2.19E-11
2026			5.77E+48		5.52E+37	6.51E+36	4.63E+00	3.04E-36	1.91E-11
2034			9.74E+48		8.12E+37	9.76E+36	4.64E+00	2.08E-36	1.67E-11
2042			1.64E+49		1.19E+38	1.46E+37	4.65E+00	1.43E-36	1.46E-11
2050			2.77E+49		1.76E+38	2.19E+37	4.66E+00	9.80E-37	1.27E-11
2058			4.67E+49		2.58E+38	3.28E+37	4.67E+00	6.72E-37	1.11E-11
2066			7.89E+49		3.80E+38	4.92E+37	4.68E+00	4.61E-37	9.68E-12
2074			1.33E+50		5.58E+38	7.38E+37	4.69E+00	3.16E-37	8.44E-12
2082			2.25E+50		8.21E+38	1.11E+38	4.70E+00	2.17E-37	7.36E-12
2090			3.80E+50		1.21E+39	1.66E+38	4.71E+00	1.49E-37	6.41E-12
2098			6.41E+50		1.77E+39	2.49E+38	4.72E+00	1.02E-37	5.59E-12
2106			1.08E+51		2.61E+39	3.73E+38	4.73E+00	7.01E-38	4.87E-12
2114			1.82E+51		3.84E+39	5.59E+38	4.74E+00	4.81E-38	4.25E-12
2122			3.07E+51		5.65E+39	8.38E+38	4.75E+00	3.30E-38	3.70E-12
2130			5.18E+51		8.31E+39	1.26E+39	4.76E+00	2.26E-38	3.23E-12
2138			8.74E+51		1.22E+40	1.88E+39	4.77E+00	1.55E-38	2.81E-12
2146			1.47E+52		1.80E+40	2.82E+39	4.78E+00	1.06E-38	2.45E-12
2154			2.49E+52		2.64E+40	4.22E+39	4.79E+00	7.28E-39	2.13E-12
2162			4.20E+52		3.88E+40	6.32E+39	4.80E+00	4.99E-39	1.86E-12
2170			7.09E+52		5.70E+40	9.46E+39	4.81E+00	3.42E-39	1.62E-12
2178			1.20E+53		8.38E+40	1.42E+40	4.82E+00	2.34E-39	1.41E-12
2186			2.02E+53		1.23E+41	2.12E+40	4.83E+00	1.61E-39	1.23E-12
2194			3.42E+53		1.81E+41	3.17E+40	4.84E+00	1.10E-39	1.07E-12
2202			5.77E+53		2.66E+41	4.75E+40	4.85E+00	7.56E-40	9.31E-13
2210			9.74E+53		3.91E+41	7.11E+40	4.86E+00	5.19E-40	8.10E-13
2218			1.64E+54		5.75E+41	1.06E+41	4.87E+00	3.56E-40	7.04E-13
2226			2.77E+54		8.45E+41	1.59E+41	4.88E+00	2.44E-40	6.12E-13
2234			4.67E+54		1.24E+42	2.38E+41	4.89E+00	1.68E-40	5.32E-13
2242			7.89E+54		1.82E+42	3.56E+41	4.90E+00	1.15E-40	4.62E-13
2250			1.33E+55		2.68E+42	5.33E+41	4.91E+00	7.92E-41	4.02E-13
2258			2.25E+55		3.94E+42	7.98E+41	4.92E+00	5.44E-41	3.49E-13
2266			3.80E+55		5.79E+42	1.19E+42	4.93E+00	3.73E-41	3.04E-13
2274			6.41E+55		8.51E+42	1.79E+42	4.94E+00	2.57E-41	2.64E-13
2282			1.08E+56		1.25E+43	2.67E+42	4.95E+00	1.76E-41	2.30E-13
2290			1.82E+56		1.84E+43	4.00E+42	4

Unsaturated RO2 with endo-cyclic double bond

1,5 Hshift

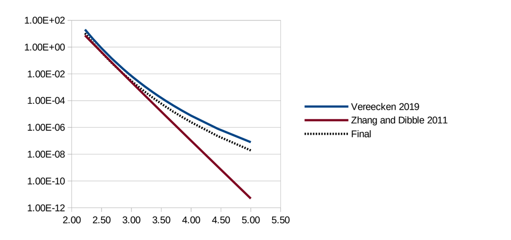
Average temperature dependence

T	>CHOO. | -CH3	>CHOO. | -CH2-	>CHOO. | >CH-	>C(OO.)- | -CH3	T-dependence	Target	Ea shift 0.00E+00 Final	1000/T	1/T	log(1/T)	log()		log(T)	Replicate
200	7.88E-08	1.19E-04	6.33E-04	6.69E-07	7.94E-06		7.94E-06	5.00	5.00E-03	-2.30E+00	-5.10E+00	A		1.06E-06
225	8.03E-07	5.21E-04	4.69E-03	6.56E-06	5.99E-05		5.99E-05	4.44	4.44E-03	-2.35E+00	-4.22E+00		5.02E+07	0.13
250	7.59E-06	2.49E-03	3.11E-02	5.89E-05	4.31E-04		4.31E-04	4.00	4.00E-03	-2.40E+00	-3.37E+00	Ea		
260	1.82E-05	4.72E-03	6.42E-02	1.38E-04	9.34E-04		9.34E-04	3.85	3.85E-03	-2.41E+00	-3.03E+00		6.30E+03	
270	4.29E-05	8.93E-03	1.31E-01	3.19E-04	2.00E-03		2.00E-03	3.70	3.70E-03	-2.43E+00	-2.70E+00			2.02
280	9.98E-05	1.69E-02	2.61E-01	7.23E-04	4.23E-03		4.23E-03	3.57	3.57E-03	-2.45E+00	-2.37E+00			8.56E-03
290	2.29E-04	3.20E-02	5.14E-01	1.62E-03	8.83E-03		8.83E-03	3.45	3.45E-03	-2.46E+00	-2.05E+00		-3.22E+01	
298	4.39E-04	5.32E-02	8.73E-01	3.04E-03	1.58E-02	1.58E-02	1.58E-02	3.36	3.36E-03	-2.47E+00	-1.80E+00		1.39E+03	
310	1.15E-03	1.14E-01	1.90E+00	7.71E-03	3.72E-02		3.72E-02	3.23	3.23E-03	-2.49E+00	-1.43E+00		-8.61E+01	
320	2.51E-03	2.12E-01	3.58E+00	1.65E-02	7.49E-02		7.49E-02	3.13	3.13E-03	-2.51E+00	-1.13E+00		#N/A	
330	5.43E-03	3.96E-01	6.65E+00	3.47E-02	1.49E-01		1.49E-01	3.03	3.03E-03	-2.52E+00	-8.26E-01		#N/A	
340	1.16E-02	7.32E-01	1.22E+01	7.20E-02	2.94E-01		2.94E-01	2.94	2.94E-03	-2.53E+00	-5.32E-01	A		2.94E-01
350	2.43E-02	1.35E+00	2.21E+01	1.47E-01	5.71E-01		5.71E-01	2.86	2.86E-03	-2.54E+00	-2.43E-01		7.61E-87	1.00
375	1.46E-01	6.00E+00	9.22E+01	8.34E-01	2.87E+00		2.87E+00	2.67	2.67E-03	-2.57E+00	4.57E-01	n		
400	8.17E-01	2.57E+01	3.59E+02	4.36E+00	1.35E+01		1.35E+01	2.50	2.50E-03	-2.60E+00	1.13E+00		32.20	
425	4.23E+00	1.05E+02	1.31E+03	2.12E+01	5.93E+01		5.93E+01	2.35	2.35E-03	-2.63E+00	1.77E+00	Ea		1.00
450	2.05E+01	4.11E+02	4.51E+03	9.66E+01	2.46E+02		2.46E+02	2.22	2.22E-03	-2.65E+00	2.39E+00		-3190	2.46E+02



		CHOOH	CHOOH
	P1	1.91458E-95	3966
	P2	35.01289326	2.392
	P3	-3.25E+03	9.40E+03

>CHOO. | -CH3 T	Vereecken 2019	Zhang and Dibble 2011	T-dependence	Target	Ea shift 2.83E+02 Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200	7.88E-08	4.90E-12	7.88E-08		1.92E-08	5.00	5.00E-03	-2.30E+00	-7.72E+00	A		2.14E-09
225	8.03E-07	1.20E-09	8.03E-07		2.28E-07	4.44	4.44E-03	-2.35E+00	-6.64E+00		2.00E+07	0.11
250	7.59E-06	1.01E-07	7.59E-06		2.45E-06	4.00	4.00E-03	-2.40E+00	-5.61E+00	Ea		
260	1.82E-05	4.72E-07	1.82E-05		6.12E-06	3.85	3.85E-03	-2.41E+00	-5.21E+00		7.35E+03	
270	4.29E-05	1.97E-06	4.29E-05		1.50E-05	3.70	3.70E-03	-2.43E+00	-4.82E+00			2.15
280	9.98E-05	7.45E-06	9.98E-05		3.63E-05	3.57	3.57E-03	-2.45E+00	-4.44E+00			7.82E-05
290	2.29E-04	2.58E-05	2.29E-04		8.62E-05	3.45	3.45E-03	-2.46E+00	-4.06E+00		-3.50E+01	
298	4.39E-04	6.57E-05	4.39E-04	1.70E-04	1.70E-04	3.36	3.36E-03	-2.47E+00	-3.77E+00		1.29E+03	
310	1.15E-03	2.45E-04	1.15E-03		4.60E-04	3.23	3.23E-03	-2.49E+00	-3.34E+00		-9.47E+01	
320	2.51E-03	6.81E-04	2.51E-03		1.04E-03	3.13	3.13E-03	-2.51E+00	-2.98E+00		#N/A	
330	5.43E-03	1.79E-03	5.43E-03		2.30E-03	3.03	3.03E-03	-2.52E+00	-2.64E+00		#N/A	
340	1.16E-02	4.43E-03	1.16E-02		5.03E-03	2.94	2.94E-03	-2.53E+00	-2.30E+00	A		5.03E-03
350	2.43E-02	1.05E-02	2.43E-02		1.08E-02	2.86	2.86E-03	-2.54E+00	-1.97E+00		1.91E-95	1.00
375	1.46E-01	7.40E-02	1.46E-01		6.89E-02	2.67	2.67E-03	-2.57E+00	-1.16E+00	n		
400	8.17E-01	4.14E-01	8.17E-01		4.03E-01	2.50	2.50E-03	-2.60E+00	-3.95E-01		35.01	
425	4.23E+00	1.90E+00	4.23E+00		2.18E+00	2.35	2.35E-03	-2.63E+00	3.38E-01	Ea		1.00
450	2.05E+01	7.46E+00	2.05E+01		1.09E+01	2.22	2.22E-03	-2.65E+00	1.04E+00		-2963	1.09E+01



		CHOOH	CHOOH
	P1	2.30646E-94	67920
	P2	34.57662412	2.058
	P3	-4.67E+03	8.31E+03

>CHOO. | -CH2- T Vereecken 2019 Zhang and Dibble 2011 — Ea shift 3.14E+02

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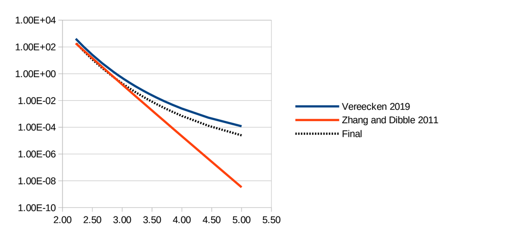

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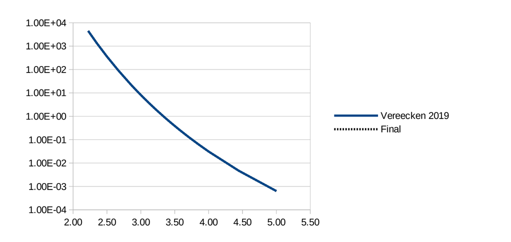

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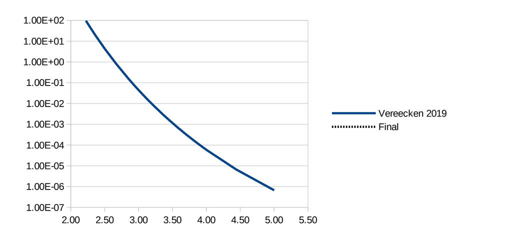
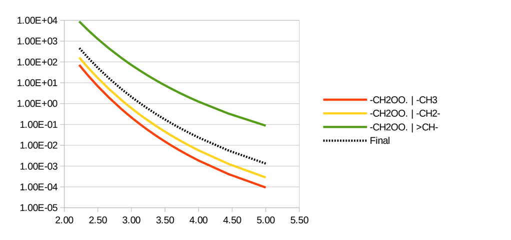


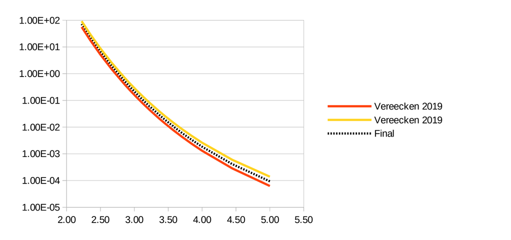
[illegible]

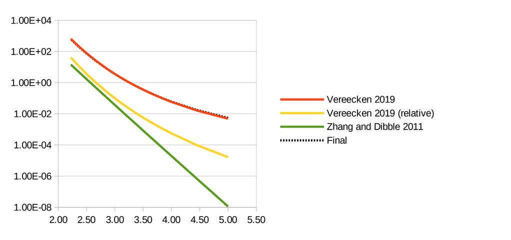
1,6 Hshift

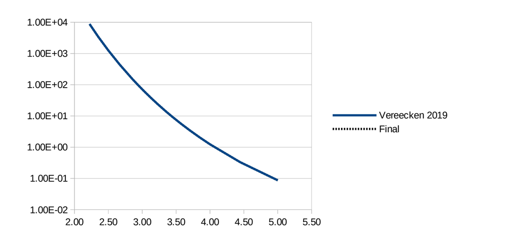
Average temperature dependence

[illegible]







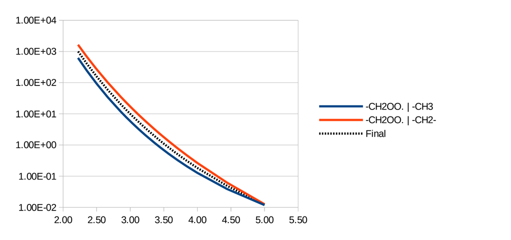


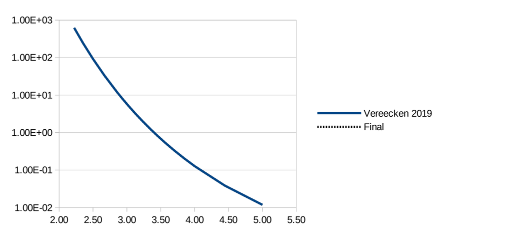
[illegible]

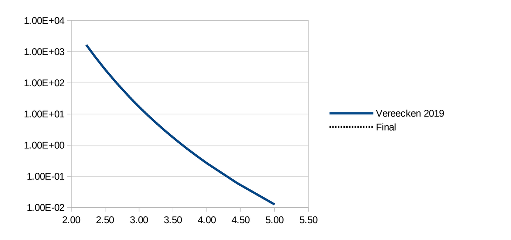
1,7 Hshift

Average temperature dependence

[illegible]





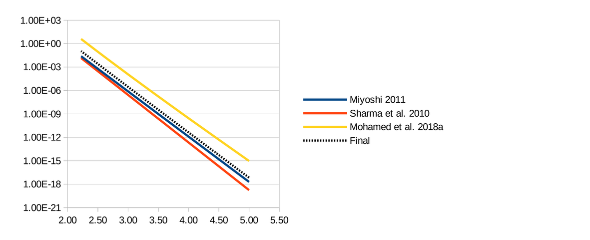


[illegible]

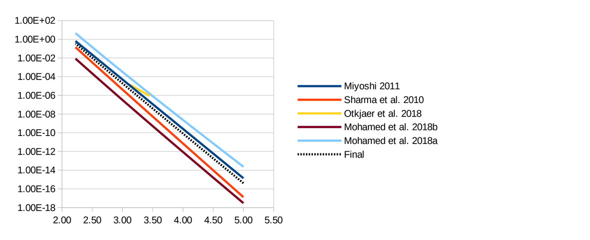
RO2 migration of α-OOH hydrogen atoms

1,4 Hshift

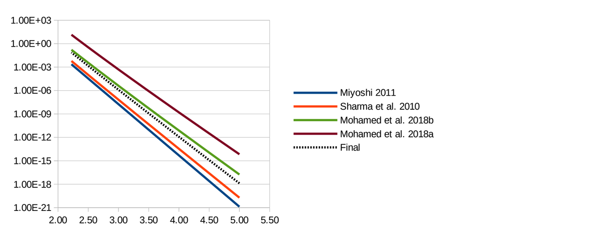
	P0			2		T-dependence	Target	Final	1000/T
	P1	1.83E+11	4.70E+11	-4.79E+00					
	P2	1.33E+04	-2.40E-01	5.07				Ea shift	
	P3		28	2.28E+01				0.00E+00	
-CH2OO. | -CH2-	T	Miyoshi 2011	Sharma et al.	Mohamed et al. 2018a		T-dependence	Target	Final	1000/T
	200	1.97E-18	1.74E-19	9.34E-16		6.84E-18		6.84E-18	5.00
	225	3.26E-15	4.25E-16	9.96E-13		1.11E-14		1.11E-14	4.44
	250	1.23E-12	2.17E-13	2.79E-10		4.20E-12		4.20E-12	4.00
	260	9.55E-12	1.88E-12	1.99E-09		3.29E-11		3.29E-11	3.85
	270	6.38E-11	1.39E-11	1.23E-08		2.22E-10		2.22E-10	3.70
	280	3.73E-10	8.87E-11	6.76E-08		1.31E-09		1.31E-09	3.57
	290	1.93E-09	4.99E-10	3.32E-07		6.83E-09		6.83E-09	3.45
	298	6.63E-09	1.83E-09	1.10E-06		2.37E-08	2.37E-08	2.37E-08	3.36
	310	3.75E-08	1.13E-08	5.98E-06		1.36E-07		1.36E-07	3.23
	320	1.44E-07	4.64E-08	2.23E-05		5.30E-07		5.30E-07	3.13
	330	5.09E-07	1.75E-07	7.74E-05		1.90E-06		1.90E-06	3.03
	340	1.67E-06	6.09E-07	2.50E-04		6.34E-06		6.34E-06	2.94
	350	5.12E-06	1.98E-06	7.60E-04		1.98E-05		1.98E-05	2.86
	375	6.50E-05	2.85E-05	9.60E-03		2.61E-04		2.61E-04	2.67
	400	6.01E-04	2.94E-04	9.01E-02		2.51E-03		2.51E-03	2.50
	425	4.27E-03	2.30E-03	6.62E-01		1.87E-02		1.87E-02	2.35
	450	2.44E-02	1.43E-02	3.97E+00		1.12E-01		1.12E-01	2.22

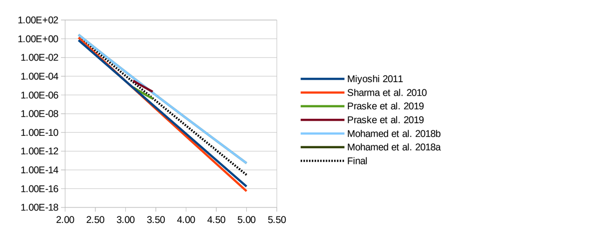


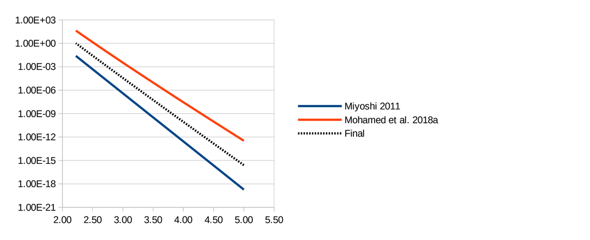
	P0				1	1			
	P1	3.49E+11	1.1E+12	4.10E+12	2.03E+00	-2.97E+00			
	P2	1.22E+04	1.2	1.48E+04	3.21	4.56		Ea shift	
	P3		25.7	1.97E+08	2.36E+01	2.09E+01		-1.56E+02	
-CH2OO. | >CH-	T	Miyoshi 2011	Sharma et al.	Otkjaer et al.	Mohamed et a	Mohamed et al. 2018a	T-dependence / Target	Final	1000/T
	200	1.37E-15	1.31E-17		3.00E-18	2.30E-14	1.88E-16	4.09E-16	5.00
	225	1.18E-12	1.99E-14		3.21E-15	1.36E-11	1.79E-13	3.58E-13	4.44
	250	2.62E-10	7.08E-12		8.83E-13	2.36E-09	4.43E-11	8.28E-11	4.00
	260	1.70E-09	5.43E-11		6.23E-12	1.42E-08	3.01E-10	5.48E-10	3.85
	270	9.63E-09	3.59E-10		3.82E-11	7.56E-08	1.78E-09	3.17E-09	3.70
	280	4.81E-08	2.07E-09		2.06E-10	3.59E-07	9.27E-09	1.62E-08	3.57
	290	2.15E-07	1.06E-08	9.05E-07	9.98E-10	1.54E-06	4.33E-08	7.41E-08	3.45
	298	6.63E-07	3.64E-08	1.89E-06	3.27E-09	4.61E-06	1.38E-07 / 2.33E-07	2.33E-07	3.36
	310	3.22E-06	2.05E-07	5.63E-06	1.74E-08	2.16E-05	7.05E-07	1.17E-06	3.23
	320	1.10E-05	7.83E-07	1.37E-05	6.36E-08	7.22E-05	2.51E-06	4.08E-06	3.13
	330	3.47E-05	2.77E-06		2.16E-07	2.25E-04	8.26E-06	1.33E-05	3.03
	340	1.02E-04	9.08E-06		6.86E-07	6.58E-04	2.55E-05	4.03E-05	2.94
	350	2.85E-04	2.79E-05		2.04E-06	1.82E-03	7.37E-05	1.15E-04	2.86
	375	2.88E-03	3.56E-04		2.45E-05	1.85E-02	8.25E-04	1.25E-03	2.67
	400	2.19E-02	3.32E-03		2.18E-04	1.43E-01	6.90E-03	1.02E-02	2.50
	425	1.31E-01	2.39E-02		1.52E-03	8.86E-01	4.53E-02	6.54E-02	2.35
	450	6.42E-01	1.39E-01		8.62E-03	4.54E+00	2.43E-01	3.44E-01	2.22

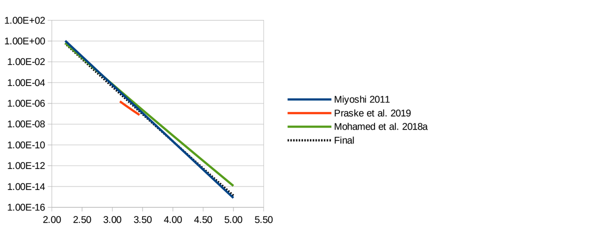


	P0			2	2				
	P1	8.96E+11	7.7E+11	-1.12E+00	-3.79E+00				
	P2	1.51E+04	1.6	4.15	5.02			Ea shift	
	P3		27.9	2.39E+01	2.23E+01			0.00E+00	
>CHOO. | -CH2-	T	Miyoshi 2011	Sharma et al.	Mohamed et a	Mohamed et al. 2018a	T-dependence	Target	Final	1000/T
	200	1.32E-21	1.90E-20	1.76E-17	6.85E-15	1.32E-18		1.32E-18	5.00
	225	5.86E-18	5.59E-17	2.29E-14	6.32E-12	2.62E-15		2.62E-15	4.44
	250	4.85E-15	3.40E-14	7.43E-12	1.57E-09	1.18E-12		1.18E-12	4.00
	260	4.97E-14	3.14E-13	5.56E-11	1.08E-08	9.83E-12		9.83E-12	3.85
	270	4.28E-13	2.46E-12	3.61E-10	6.43E-08	7.03E-11		7.03E-11	3.70

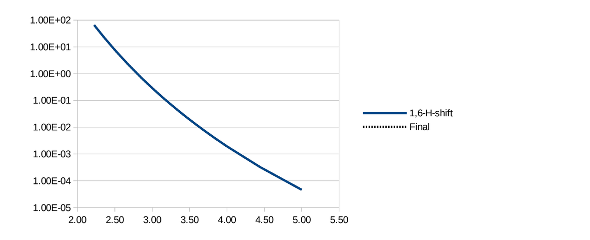


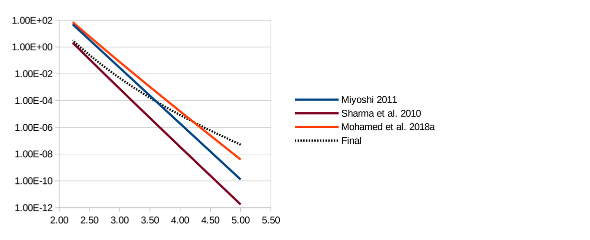


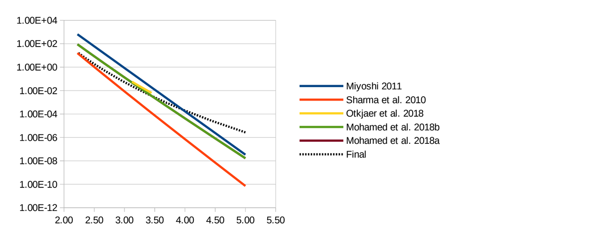


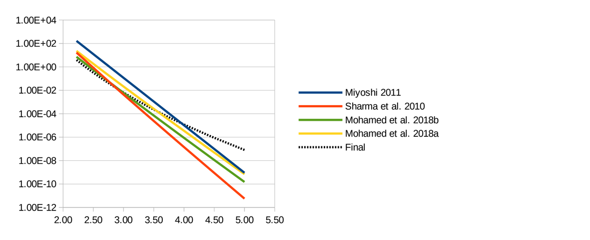


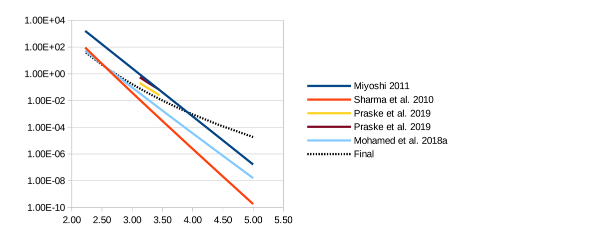
1,5 Hshift

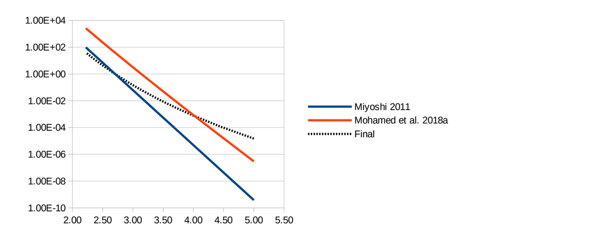


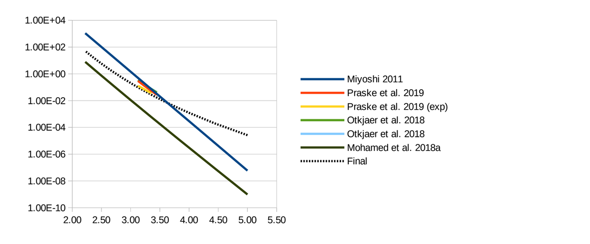




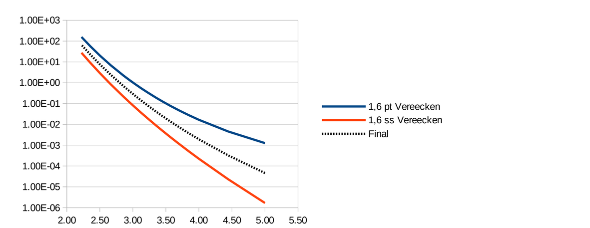


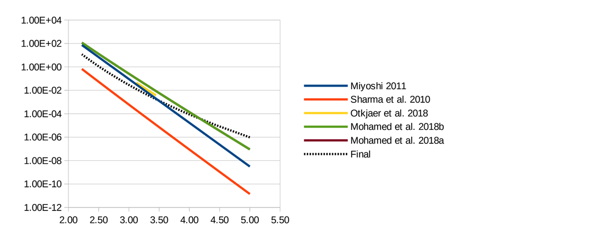


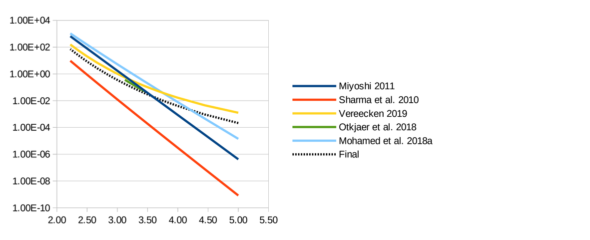


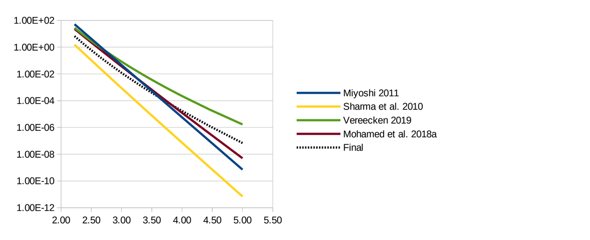


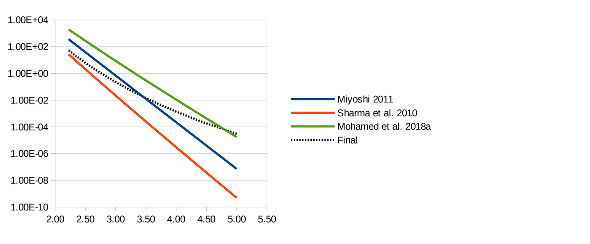
1,6 Hshift

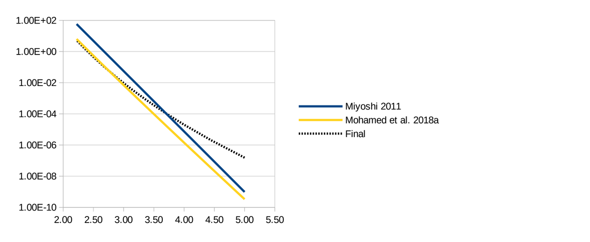


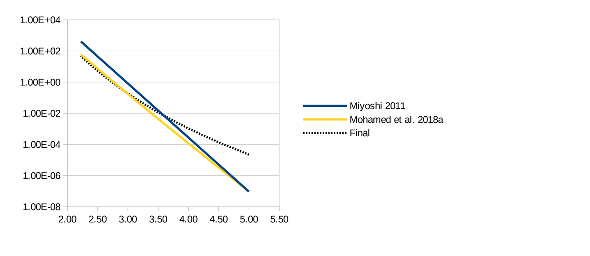




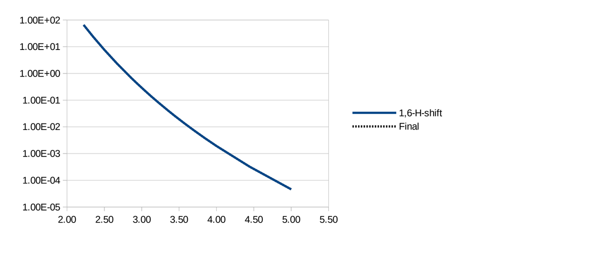


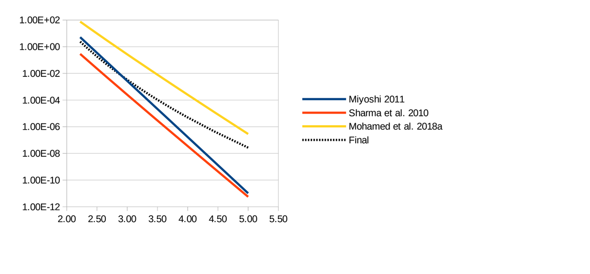


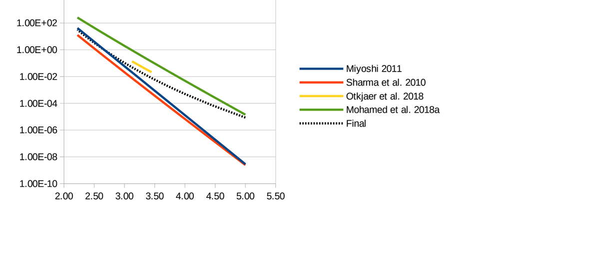


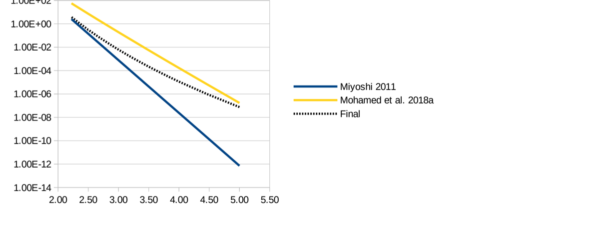


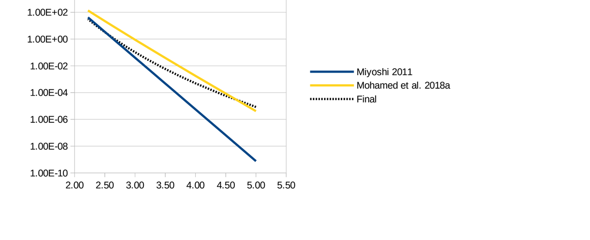
1,7 Hshift

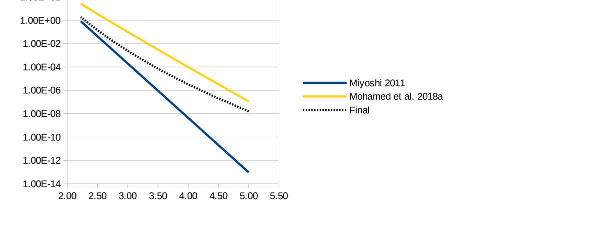


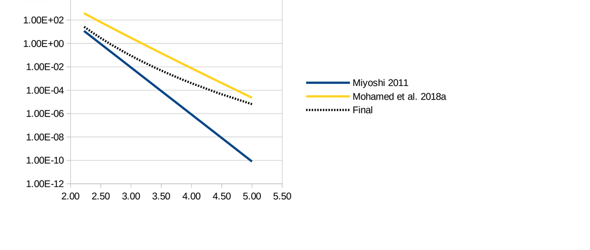










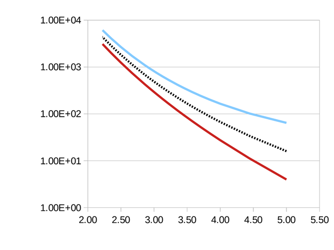


Scrambling -OOH hydrogen atoms

Average temperature dependence

Ea shift 0.00E+00

T	Vereecken 1,8	Vereecken 1,8 sp	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log()		log(T)	Replicate
200	6.43E+01	3.97E+00	1.60E+01		1.60E+01	5.00	5.00E-03	-2.30E+00	1.20E+00	A		9.41E+00
225	1.02E+02	1.11E+01	3.37E+01		3.37E+01	4.44	4.44E-03	-2.35E+00	1.53E+00		2.55E+05	0.59
250	1.65E+02	2.74E+01	6.72E+01		6.72E+01	4.00	4.00E-03	-2.40E+00	1.83E+00	Ea		
260	2.00E+02	3.82E+01	8.74E+01		8.74E+01	3.85	3.85E-03	-2.41E+00	1.94E+00		2.04E+03	
270	2.43E+02	5.23E+01	1.13E+02		1.13E+02	3.70	3.70E-03	-2.43E+00	2.05E+00			1.20
280	2.95E+02	7.07E+01	1.44E+02		1.44E+02	3.57	3.57E-03	-2.45E+00	2.16E+00			1.74E+02
290	3.58E+02	9.45E+01	1.84E+02		1.84E+02	3.45	3.45E-03	-2.46E+00	2.26E+00		-8.46E+00	
298	4.17E+02	1.18E+02	2.22E+02	2.22E+02	2.22E+02	3.36	3.36E-03	-2.47E+00	2.35E+00		1.96E+02	
310	5.25E+02	1.63E+02	2.92E+02		2.92E+02	3.23	3.23E-03	-2.49E+00	2.47E+00		-1.92E+01	
320	6.34E+02	2.11E+02	3.66E+02		3.66E+02	3.13	3.13E-03	-2.51E+00	2.56E+00		#N/A	
330	7.64E+02	2.70E+02	4.54E+02		4.54E+02	3.03	3.03E-03	-2.52E+00	2.66E+00		#N/A	
340	9.20E+02	3.43E+02	5.62E+02		5.62E+02	2.94	2.94E-03	-2.53E+00	2.75E+00	A		5.62E+02
350	1.10E+03	4.33E+02	6.91E+02		6.91E+02	2.86	2.86E-03	-2.54E+00	2.84E+00		5.64E-20	1.00
375	1.73E+03	7.48E+02	1.14E+03		1.14E+03	2.67	2.67E-03	-2.57E+00	3.06E+00	n		
400	2.67E+03	1.24E+03	1.82E+03		1.82E+03	2.50	2.50E-03	-2.60E+00	3.26E+00		8.46	
425	4.07E+03	1.99E+03	2.85E+03		2.85E+03	2.35	2.35E-03	-2.63E+00	3.45E+00	Ea		1.00
450	6.12E+03	3.10E+03	4.35E+03		4.35E+03	2.22	2.22E-03	-2.65E+00	3.64E+00		-452	4.35E+03



1,6 Hshift

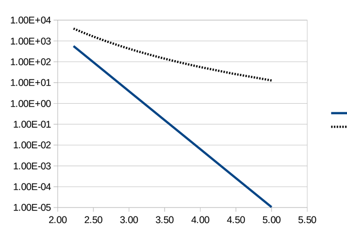
Scaling: 4.80E+02

P1 8.69E+08
P2 6.41E+03
P3

-CH2OO. | -CH3

Ea shift 4.66E+01

T	Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200	1.05E-05	1.60E+01		1.27E+01	5.00	5.00E-03	-2.30E+00	1.10E+00	A		7.45E+00
225	3.69E-04	3.37E+01		2.74E+01	4.44	4.44E-03	-2.35E+00	1.44E+00		2.55E+05	0.59
250	6.36E-03	6.72E+01		5.58E+01	4.00	4.00E-03	-2.40E+00	1.75E+00	Ea		
260	1.71E-02	8.74E+01		7.30E+01	3.85	3.85E-03	-2.41E+00	1.86E+00		2.09E+03	
270	4.25E-02	1.13E+02		9.49E+01	3.70	3.70E-03	-2.43E+00	1.98E+00			1.20
280	9.93E-02	1.44E+02		1.22E+02	3.57	3.57E-03	-2.45E+00	2.09E+00			1.47E+02
290	2.19E-01	1.84E+02		1.57E+02	3.45	3.45E-03	-2.46E+00	2.19E+00		-8.46E+00	
298	3.96E-01	2.22E+02	1.90E+02	1.90E+02	3.36	3.36E-03	-2.47E+00	2.28E+00		1.76E+02	
310	9.10E-01	2.92E+02		2.52E+02	3.23	3.23E-03	-2.49E+00	2.40E+00		-1.92E+01	
320	1.74E+00	3.66E+02		3.16E+02	3.13	3.13E-03	-2.51E+00	2.50E+00		#N/A	
330	3.19E+00	4.54E+02		3.95E+02	3.03	3.03E-03	-2.52E+00	2.60E+00		#N/A	
340	5.64E+00	5.62E+02		4.90E+02	2.94	2.94E-03	-2.53E+00	2.69E+00	A		4.90E+02
350	9.67E+00	6.91E+02		6.05E+02	2.86	2.86E-03	-2.54E+00	2.78E+00		5.64E-20	1.00
375	3.28E+01	1.14E+03		1.00E+03	2.67	2.67E-03	-2.57E+00	3.00E+00	n		
400	9.54E+01	1.82E+03		1.62E+03	2.50	2.50E-03	-2.60E+00	3.21E+00		8.46	
425	2.45E+02	2.85E+03		2.55E+03	2.35	2.35E-03	-2.63E+00	3.41E+00	Ea		1.00
450	5.66E+02	4.35E+03		3.92E+03	2.22	2.22E-03	-2.65E+00	3.59E+00		-405	3.92E+03

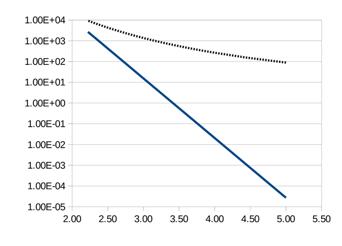


P0
P1 6.75E+09
P2 6.63E+03
P3

-CH2OO. | -CH2-

Ea shift -3.44E+02

T	Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200	2.71E-05	1.60E+01		8.94E+01	5.00	5.00E-03	-2.30E+00	1.95E+00	A		5.26E+01
225	1.08E-03	3.37E+01		1.56E+02	4.44	4.44E-03	-2.35E+00	2.19E+00		2.55E+05	0.59
250	2.05E-02	6.72E+01		2.66E+02	4.00	4.00E-03	-2.40E+00	2.43E+00	Ea		
260	5.69E-02	8.74E+01		3.28E+02	3.85	3.85E-03	-2.41E+00	2.52E+00		1.70E+03	
270	1.46E-01	1.13E+02		4.04E+02	3.70	3.70E-03	-2.43E+00	2.61E+00			1.20
280	3.51E-01	1.44E+02		4.94E+02	3.57	3.57E-03	-2.45E+00	2.69E+00			5.95E+02
290	7.95E-01	1.84E+02		6.03E+02	3.45	3.45E-03	-2.46E+00	2.78E+00		-8.46E+00	
298	1.47E+00	2.22E+02	7.05E+02	7.05E+02	3.36	3.36E-03	-2.47E+00	2.85E+00		3.46E+02	
310	3.48E+00	2.92E+02		8.88E+02	3.23	3.23E-03	-2.49E+00	2.95E+00		-1.92E+01	
320	6.78E+00	3.66E+02		1.07E+03	3.13	3.13E-03	-2.51E+00	3.03E+00		#N/A	
330	1.27E+01	4.54E+02		1.29E+03	3.03	3.03E-03	-2.52E+00	3.11E+00		#N/A	
340	2.29E+01	5.62E+02		1.55E+03	2.94	2.94E-03	-2.53E+00	3.19E+00	A		1.55E+03
350	4.00E+01	6.91E+02		1.85E+03	2.86	2.86E-03	-2.54E+00	3.27E+00		5.64E-20	1.00
375	1.42E+02	1.14E+03		2.85E+03	2.67	2.67E-03	-2.57E+00	3.45E+00	n		
400	4.27E+02	1.82E+03		4.31E+03	2.50	2.50E-03	-2.60E+00	3.63E+00		8.46	
425	1.13E+03	2.85E+03		6.40E+03	2.35	2.35E-03	-2.63E+00	3.81E+00	Ea		1.00
450	2.70E+03	4.35E+03		9.35E+03	2.22	2.22E-03	-2.65E+00	3.97E+00		-796	9.35E+03

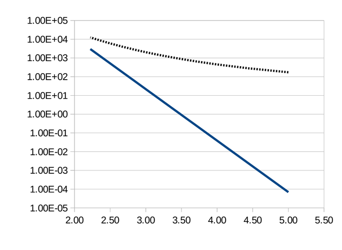


P1 3840000000
P2 6330
P3

-CH2OO. | >CH-

Ea shift -4.76E+02

T	Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200	6.90E-05	1.60E+01		1.73E+02	5.00	5.00E-03	-2.30E+00	2.24E+00	A		1.02E+02
225	2.32E-03	3.37E+01		2.80E+02	4.44	4.44E-03	-2.35E+00	2.45E+00		2.55E+05	0.59
250	3.87E-02	6.72E+01		4.51E+02	4.00	4.00E-03	-2.40E+00	2.65E+00	Ea		
260	1.03E-01	8.74E+01		5.45E+02	3.85	3.85E-03	-2.41E+00	2.74E+00		1.57E+03	
270	2.53E-01	1.13E+02		6.58E+02	3.70	3.70E-03	-2.43E+00	2.82E+00			1.20
280	5.84E-01	1.44E+02		7.91E+02	3.57	3.57E-03	-2.45E+00	2.90E+00			9.53E+02
290	1.27E+00	1.84E+02		9.50E+02	3.45	3.45E-03	-2.46E+00	2.98E+00		-8.46E+00	
298	2.29E+00	2.22E+02	1.10E+03	1.10E+03	3.36	3.36E-03	-2.47E+00	3.04E+00		4.03E+02	
310	5.20E+00	2.92E+02		1.36E+03	3.23	3.23E-03	-2.49E+00	3.13E+00		-1.92E+01	
320	9.85E+00	3.66E+02		1.62E+03	3.13	3.13E-03	-2.51E+00	3.21E+00		#N/A	
330	1.79E+01	4.54E+02		1.92E+03	3.03	3.03E-03	-2.52E+00	3.28E+00		#N/A	
340	3.15E+01	5.62E+02		2.28E+03	2.94	2.94E-03	-2.53E+00	3.36E+00	A		2.28E+03
350	5.37E+01	6.91E+02		2.70E+03	2.86	2.86E-03	-2.54E+00	3.43E+00		5.64E-20	1.00
375	1.79E+02	1.14E+03		4.05E+03	2.67	2.67E-03	-2.57E+00	3.61E+00	n		
400	5.15E+02	1.82E+03		5.99E+03	2.50	2.50E-03	-2.60E+00	3.78E+00		8.46	
425	1.31E+03	2.85E+03		8.73E+03	2.35	2.35E-03	-2.63E+00	3.94E+00	Ea		1.00
450	2.99E+03	4.35E+03		1.25E+04	2.22	2.22E-03	-2.65E+00	4.10E+00		-928	1.25E+04

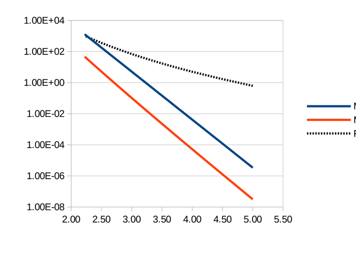


P0 1
P1 9340000000 2.02E+00
P2 7110 2.77
P3 1.35E+01

>CHOO. | -CH3

Ea shift 6.49E+02

T	Miyoshi 2011	Mohamed et al. 2018b	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200	3.40E-06	3.15E-08	1.60E+01		6.22E-01	5.00	5.00E-03	-2.30E+00	-2.07E-01	A		3.66E-01
225	1.76E-04	1.90E-06	3.37E+01		1.88E+00	4.44	4.44E-03	-2.35E+00	2.74E-01		2.55E+05	0.59
250	4.16E-03	5.21E-05	6.72E+01		5.00E+00	4.00	4.00E-03	-2.40E+00	6.99E-01	Ea		
260	1.24E-02	1.65E-04	8.74E+01		7.19E+00	3.85	3.85E-03	-2.41E+00	8.57E-01		2.69E+03	
270	3.42E-02	4.83E-04	1.13E+02		1.02E+01	3.70	3.70E-03	-2.43E+00	1.01E+00			1.20
280	8.76E-02	1.31E-03	1.44E+02		1.42E+01	3.57	3.57E-03	-2.45E+00	1.15E+00			1.71E+01
290	2.10E-01	3.34E-03	1.84E+02		1.96E+01	3.45	3.45E-03	-2.46E+00	1.29E+00		-8.46E+00	
298	4.06E-01	6.75E-03	2.22E+02	2.51E+01	2.51E+01	3.36	3.36E-03	-2.47E+00	1.40E+00		-8.58E+01	
310	1.02E+00	1.82E-02	2.92E+02		3.60E+01	3.23	3.23E-03	-2.49E+00	1.56E+00		-1.92E+01	
320	2.09E+00	3.94E-02	3.66E+02		4.80E+01	3.13	3.13E-03	-2.51E+00	1.68E+00		#N/A	
330	4.10E+00	8.17E-02	4.54E+02		6.35E+01	3.03	3.03E-03	-2.52E+00	1.80E+00		#N/A	
340	7.74E+00	1.63E-01	5.62E+02		8.32E+01	2.94	2.94E-03	-2.53E+00	1.92E+00	A		8.32E+01
350	1.41E+01	3.12E-01	6.91E+02		1.08E+02	2.86	2.86E-03	-2.54E+00	2.03E+00		5.64E-20	1.00
375	5.45E+01	1.38E+00	1.14E+03		2.01E+02	2.67	2.67E-03	-2.57E+00	2.30E+00	n		
400	1.78E+02	5.11E+00	1.82E+03		3.59E+02	2.50	2.50E-03	-2.60E+00	2.56E+00		8.46	
425	5.07E+02	1.64E+01	2.85E+03		6.18E+02	2.35	2.35E-03	-2.63E+00	2.79E+00	Ea		1.00
450	1.28E+03	4.67E+01	4.35E+03		1.03E+03	2.22	2.22E-03	-2.65E+00	3.01E+00		198	1.03E+03

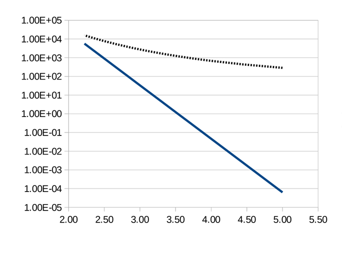


P1 12900000000
P2 6590
P3

>CHOO. | -CH2-

Ea shift -5.77E+02

T	Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200	6.32E-05	1.60E+01		2.86E+02	5.00	5.00E-03	-2.30E+00	2.46E+00	A		1.67E+02
225	2.46E-03	3.37E+01		4.38E+02	4.44	4.44E-03	-2.35E+00	2.64E+00		2.55E+05	0.59
250	4.60E-02	6.72E+01		6.77E+02	4.00	4.00E-03	-2.40E+00	2.83E+00	Ea		
260	1.27E-01	8.74E+01		8.05E+02	3.85	3.85E-03	-2.41E+00	2.91E+00		1.46E+03	
270	3.24E-01	1.13E+02		9.57E+02	3.70	3.70E-03	-2.43E+00	2.98E+00			1.20
280	7.75E-01	1.44E+02		1.14E+03	3.57	3.57E-03	-2.45E+00	3.06E+00			1.37E+03
290	1.74E+00	1.84E+02		1.35E+03	3.45	3.45E-03	-2.46E+00	3.13E+00		-8.46E+00	
298	3.21E+00	2.22E+02	1.54E+03	1.54E+03	3.36	3.36E-03	-2.47E+00	3.19E+00		4.47E+02	
310	7.56E+00	2.92E+02		1.88E+03	3.23	3.23E-03	-2.49E+00	3.27E+00		-1.92E+01	
320	1.47E+01	3.66E+02		2.22E+03	3.13	3.13E-03	-2.51E+00	3.35E+00		#N/A	
330	2.74E+01	4.54E+02		2.61E+03	3.03	3.03E-03	-2.52E+00	3.42E+00		#N/A	
340	4.93E+01	5.62E+02		3.07E+03	2.94	2.94E-03	-2.53E+00	3.49E+00	A		3.07E+03
350	8.58E+01	6.91E+02		3.60E+03	2.86	2.86E-03	-2.54E+00	3.56E+00		5.64E-20	1.00
375	3.01E+02	1.14E+03		5.30E+03	2.67	2.67E-03	-2.57E+00	3.72E+00	n		
400	9.03E+02	1.82E+03		7.71E+03	2.50	2.50E-03	-2.60E+00	3.89E+00		8.46	
425	2.38E+03	2.85E+03		1.11E+04	2.35	2.35E-03	-2.63E+00	4.04E+00	Ea		1.00
450	5.63E+03	4.35E+03		1.57E+04	2.22	2.22E-03	-2.65E+00	4.20E+00		-1029	1.57E+04

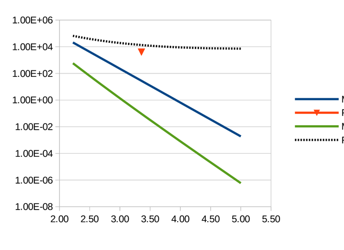


P0 1
P1 9060000000 -5.20E-01
P2 5840 3.47
P3 1.28E+01

>CHOO. | >CH-

Ea shift -1.22E+03

T	Miyoshi 2011	Praske et al.	Mohamed et al. 2018b	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200	1.89E-03		5.89E-07	1.60E+01		7.20E+03	5.00	5.00E-03	-2.30E+00	3.86E+00	A		4.24E+03
225	4.84E-02		3.18E-05	3.37E+01		7.69E+03	4.44	4.44E-03	-2.35E+00	3.89E+00		2.55E+05	0.59
250	6.49E-01		8.02E-04	6.72E+01		8.92E+03	4.00	4.00E-03	-2.40E+00	3.95E+00	Ea		
260	1.59E+00		2.48E-03	8.74E+01		9.61E+03	3.85	3.85E-03	-2.41E+00	3.98E+00		8.20E+02	
270	3.66E+00		7.07E-03	1.13E+02		1.04E+04	3.70	3.70E-03	-2.43E+00	4.02E+00			1.20
280	7.92E+00		1.88E-02	1.44E+02		1.14E+04	3.57	3.57E-03	-2.45E+00	4.06E+00			1.37E+04
290	1.63E+01		4.69E-02	1.84E+02		1.24E+04	3.45	3.45E-03	-2.46E+00	4.09E+00		-8.46E+00	
298	2.79E+01	4.00E+03	9.37E-02	2.22E+02	1.34E+04	1.34E+04	3.36	3.36E-03	-2.47E+00	4.13E+00		7.27E+02	
310	5.96E+01		2.48E-01	2.92E+02		1.51E+04	3.23	3.23E-03	-2.49E+00	4.18E+00		-1.92E+01	
320	1.07E+02		5.30E-01	3.66E+02		1.67E+04	3.13	3.13E-03	-2.51E+00	4.22E+00		#N/A	
330	1.87E+02		1.09E+00	4.54E+02		1.84E+04	3.03	3.03E-03	-2.52E+00	4.27E+00		#N/A	
340	3.14E+02		2.14E+00	5.62E+02		2.04E+04	2.94	2.94E-03	-2.53E+00	4.31E+00	A		2.04E+04
350	5.14E+02		4.06E+00	6.91E+02		2.27E+04	2.86	2.86E-03	-2.54E+00	4.36E+00		5.64E-20	1.00
375	1.56E+03		1.76E+01	1.14E+03		2.96E+04	2.67	2.67E-03	-2.57E+00	4.47E+00	n		
400	4.13E+03		6.44E+01	1.82E+03		3.87E+04	2.50	2.50E-03	-2.60E+00	4.59E+00		8.46	
425	9.76E+03		2.05E+02	2.85E+03		5.05E+04	2.35	2.35E-03	-2.63E+00	4.70E+00	Ea		1.00
450	2.09E+04		5.80E+02	4.35E+03		6.58E+04	2.22	2.22E-03	-2.65E+00	4.82E+00		-1674	6.58E+04

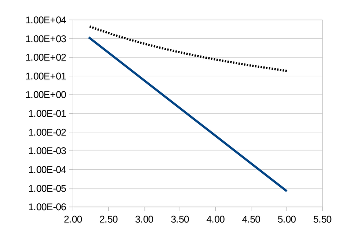


P1 4480000000
P2 6820
P3

>C(OO.)- | -CH3

Ea shift -3.22E+01

T	Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	6.95E-06	1.60E+01		1.88E+01	5.00	5.00E-03	-2.30E+00	1.27E+00	A		1.10E+01
225	3.07E-04	3.37E+01		3.89E+01	4.44	4.44E-03	-2.35E+00	1.59E+00		2.55E+05	0.59
250	6.36E-03	6.72E+01		7.64E+01	4.00	4.00E-03	-2.40E+00	1.88E+00	Ea		
260	1.82E-02	8.74E+01		9.89E+01	3.85	3.85E-03	-2.41E+00	2.00E+00		2.01E+03	
270	4.80E-02	1.13E+02		1.27E+02	3.70	3.70E-03	-2.43E+00	2.10E+00			1.20
280	1.18E-01	1.44E+02		1.62E+02	3.57	3.57E-03	-2.45E+00	2.21E+00			1.95E+02
290	2.74E-01	1.84E+02		2.05E+02	3.45	3.45E-03	-2.46E+00	2.31E+00		-8.46E+00	
298	5.15E-01	2.22E+02	2.47E+02	2.47E+02	3.36	3.36E-03	-2.47E+00	2.39E+00		2.10E+02	
310	1.25E+00	2.92E+02		3.24E+02	3.23	3.23E-03	-2.49E+00	2.51E+00		-1.92E+01	
320	2.49E+00	3.66E+02		4.04E+02	3.13	3.13E-03	-2.51E+00	2.61E+00		#N/A	
330	4.74E+00	4.54E+02		5.01E+02	3.03	3.03E-03	-2.52E+00	2.70E+00		#N/A	
340	8.71E+00	5.62E+02		6.18E+02	2.94	2.94E-03	-2.53E+00	2.79E+00	A		6.18E+02
350	1.54E+01	6.91E+02		7.58E+02	2.86	2.86E-03	-2.54E+00	2.88E+00		5.64E-20	1.00
375	5.66E+01	1.14E+03		1.24E+03	2.67	2.67E-03	-2.57E+00	3.09E+00	n		
400	1.76E+02	1.82E+03		1.97E+03	2.50	2.50E-03	-2.60E+00	3.30E+00		8.46	
425	4.81E+02	2.85E+03		3.07E+03	2.35	2.35E-03	-2.63E+00	3.49E+00	Ea		1.00
450	1.17E+03	4.35E+03		4.67E+03	2.22	2.22E-03	-2.65E+00	3.67E+00		-484	4.67E+03

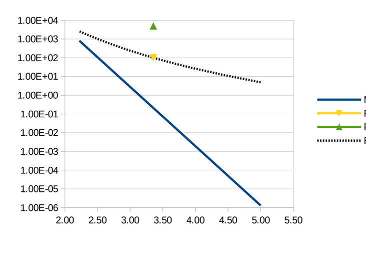


P1 8780000000
P2 7290
P3

>C(OO.)- | -CH2-

Ea shift 2.37E+02

T	Miyoshi 2011	Praske 2019 (	Praske 2019	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	1.30E-06			1.60E+01		4.88E+00	5.00	5.00E-03	-2.30E+00	6.88E-01	A		2.87E+00
225	7.45E-05			3.37E+01		1.17E+01	4.44	4.44E-03	-2.35E+00	1.07E+00		2.55E+05	0.59
250	1.90E-03			6.72E+01		2.60E+01	4.00	4.00E-03	-2.40E+00	1.42E+00	Ea		
260	5.84E-03			8.74E+01		3.51E+01	3.85	3.85E-03	-2.41E+00	1.54E+00		2.28E+03	
270	1.65E-02			1.13E+02		4.68E+01	3.70	3.70E-03	-2.43E+00	1.67E+00			1.20
280	4.33E-02			1.44E+02		6.19E+01	3.57	3.57E-03	-2.45E+00	1.79E+00			7.45E+01
290	1.06E-01			1.84E+02		8.11E+01	3.45	3.45E-03	-2.46E+00	1.91E+00		-8.46E+00	
298	2.09E-01	1.00E+02	4.90E+03	2.22E+02	1.00E+02	1.00E+02	3.36	3.36E-03	-2.47E+00	2.00E+00		9.31E+01	
310	5.38E-01			2.92E+02		1.36E+02	3.23	3.23E-03	-2.49E+00	2.13E+00		-1.92E+01	
320	1.12E+00			3.66E+02		1.74E+02	3.13	3.13E-03	-2.51E+00	2.24E+00		#N/A	
330	2.24E+00			4.54E+02		2.21E+02	3.03	3.03E-03	-2.52E+00	2.35E+00		#N/A	
340	4.28E+00			5.62E+02		2.80E+02	2.94	2.94E-03	-2.53E+00	2.45E+00	A		2.80E+02
350	7.90E+00			6.91E+02		3.51E+02	2.86	2.86E-03	-2.54E+00	2.55E+00		5.64E-20	1.00
375	3.17E+01			1.14E+03		6.04E+02	2.67	2.67E-03	-2.57E+00	2.78E+00	n		
400	1.07E+02			1.82E+03		1.01E+03	2.50	2.50E-03	-2.60E+00	3.00E+00		8.46	
425	3.12E+02			2.85E+03		1.63E+03	2.35	2.35E-03	-2.63E+00	3.21E+00	Ea		1.00
450	8.09E+02			4.35E+03		2.57E+03	2.22	2.22E-03	-2.65E+00	3.41E+00		-214	2.57E+03

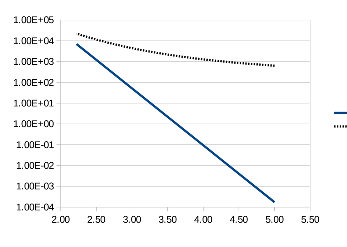


P1 8570000000
P2 6310
P3

>C(OO.)- | >CH-

Ea shift -7.35E+02

T	Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	1.70E-04	1.60E+01		6.32E+02	5.00	5.00E-03	-2.30E+00	2.80E+00	A		3.72E+02
225	5.67E-03	3.37E+01		8.85E+02	4.44	4.44E-03	-2.35E+00	2.95E+00		2.55E+05	0.59
250	9.36E-02	6.72E+01		1.27E+03	4.00	4.00E-03	-2.40E+00	3.10E+00	Ea		
260	2.47E-01	8.74E+01		1.48E+03	3.85	3.85E-03	-2.41E+00	3.17E+00		1.31E+03	
270	6.07E-01	1.13E+02		1.72E+03	3.70	3.70E-03	-2.43E+00	3.24E+00			1.20
280	1.40E+00	1.44E+02		2.00E+03	3.57	3.57E-03	-2.45E+00	3.30E+00			2.40E+03
290	3.04E+00	1.84E+02		2.32E+03	3.45	3.45E-03	-2.46E+00	3.37E+00		-8.46E+00	
298	5.46E+00	2.22E+02	2.62E+03	2.62E+03	3.36	3.36E-03	-2.47E+00	3.42E+00		5.16E+02	
310	1.24E+01	2.92E+02		3.14E+03	3.23	3.23E-03	-2.49E+00	3.50E+00		-1.92E+01	
320	2.34E+01	3.66E+02		3.64E+03	3.13	3.13E-03	-2.51E+00	3.56E+00		#N/A	
330	4.25E+01	4.54E+02		4.22E+03	3.03	3.03E-03	-2.52E+00	3.63E+00		#N/A	
340	7.46E+01	5.62E+02		4.89E+03	2.94	2.94E-03	-2.53E+00	3.69E+00	A		4.89E+03
350	1.27E+02	6.91E+02		5.65E+03	2.86	2.86E-03	-2.54E+00	3.75E+00		5.64E-20	1.00
375	4.22E+02	1.14E+03		8.08E+03	2.67	2.67E-03	-2.57E+00	3.91E+00	n		
400	1.21E+03	1.82E+03		1.15E+04	2.50	2.50E-03	-2.60E+00	4.06E+00		8.46	
425	3.05E+03	2.85E+03		1.61E+04	2.35	2.35E-03	-2.63E+00	4.21E+00	Ea		1.00
450	6.97E+03	4.35E+03		2.23E+04	2.22	2.22E-03	-2.65E+00	4.35E+00		-1187	2.23E+04



1,7 Hshift

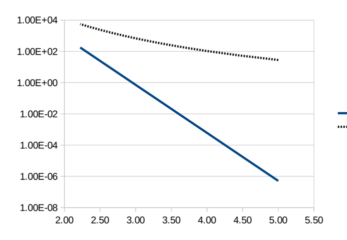
Scaling: 5.60E+03

P1 1.21E+09
P2 7080
P3

-CH2OO. | -CH3

Ea shift -1.14E+02

T	Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200	5.11E-07	1.60E+01		2.83E+01	5.00	5.00E-03	-2.30E+00	1.45E+00	A		1.67E+01
225	2.61E-05	3.37E+01		5.59E+01	4.44	4.44E-03	-2.35E+00	1.75E+00		2.55E+05	0.59
250	6.08E-04	6.72E+01		1.06E+02	4.00	4.00E-03	-2.40E+00	2.03E+00	Ea		
260	1.81E-03	8.74E+01		1.36E+02	3.85	3.85E-03	-2.41E+00	2.13E+00		1.93E+03	
270	4.95E-03	1.13E+02		1.72E+02	3.70	3.70E-03	-2.43E+00	2.24E+00			1.20
280	1.26E-02	1.44E+02		2.17E+02	3.57	3.57E-03	-2.45E+00	2.34E+00			2.61E+02
290	3.02E-02	1.84E+02		2.73E+02	3.45	3.45E-03	-2.46E+00	2.44E+00		-8.46E+00	
298	5.82E-02	2.22E+02	3.26E+02	3.26E+02	3.36	3.36E-03	-2.47E+00	2.51E+00		2.46E+02	
310	1.46E-01	2.92E+02		4.23E+02	3.23	3.23E-03	-2.49E+00	2.63E+00		-1.92E+01	
320	2.98E-01	3.66E+02		5.22E+02	3.13	3.13E-03	-2.51E+00	2.72E+00		#N/A	
330	5.82E-01	4.54E+02		6.42E+02	3.03	3.03E-03	-2.52E+00	2.81E+00		#N/A	
340	1.09E+00	5.62E+02		7.86E+02	2.94	2.94E-03	-2.53E+00	2.90E+00	A		7.86E+02
350	1.98E+00	6.91E+02		9.58E+02	2.86	2.86E-03	-2.54E+00	2.98E+00		5.64E-20	1.00
375	7.64E+00	1.14E+03		1.54E+03	2.67	2.67E-03	-2.57E+00	3.19E+00	n		
400	2.49E+01	1.82E+03		2.42E+03	2.50	2.50E-03	-2.60E+00	3.38E+00		8.46	
425	7.05E+01	2.85E+03		3.72E+03	2.35	2.35E-03	-2.63E+00	3.57E+00	Ea		1.00
450	1.78E+02	4.35E+03		5.61E+03	2.22	2.22E-03	-2.65E+00	3.75E+00		-566	5.61E+03

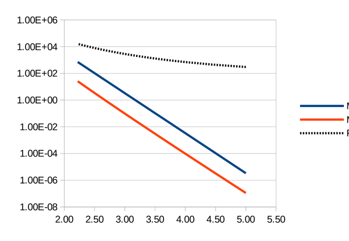


P0 1
P1 3.22E+09 2.63E+00
P2 6900 2.37
P3 1.24E+01

-CH2OO. | -CH2-

Ea shift -5.86E+02

T	Miyoshi 2011	Mohamed et al. 2018b	average T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200	3.35E-06	1.11E-07	1.60E+01		2.99E+02	5.00	5.00E-03	-2.30E+00	2.48E+00	A		1.76E+02
225	1.55E-04	4.69E-06	3.37E+01		4.55E+02	4.44	4.44E-03	-2.35E+00	2.66E+00		2.55E+05	0.59
250	3.32E-03	9.65E-05	6.72E+01		7.00E+02	4.00	4.00E-03	-2.40E+00	2.85E+00	Ea		
260	9.60E-03	2.76E-04	8.74E+01		8.32E+02	3.85	3.85E-03	-2.41E+00	2.92E+00		1.46E+03	
270	2.57E-02	7.36E-04	1.13E+02		9.87E+02	3.70	3.70E-03	-2.43E+00	2.99E+00			1.20
280	6.39E-02	1.83E-03	1.44E+02		1.17E+03	3.57	3.57E-03	-2.45E+00	3.07E+00			1.41E+03
290	1.50E-01	4.29E-03	1.84E+02		1.39E+03	3.45	3.45E-03	-2.46E+00	3.14E+00		-8.46E+00	
298	2.83E-01	8.15E-03	2.22E+02	1.59E+03	1.59E+03	3.36	3.36E-03	-2.47E+00	3.20E+00		4.51E+02	
310	6.94E-01	2.01E-02	2.92E+02		1.94E+03	3.23	3.23E-03	-2.49E+00	3.29E+00		-1.92E+01	
320	1.39E+00	4.07E-02	3.66E+02		2.28E+03	3.13	3.13E-03	-2.51E+00	3.36E+00		#N/A	
330	2.67E+00	7.91E-02	4.54E+02		2.68E+03	3.03	3.03E-03	-2.52E+00	3.43E+00		#N/A	
340	4.95E+00	1.48E-01	5.62E+02		3.15E+03	2.94	2.94E-03	-2.53E+00	3.50E+00	A		3.15E+03
350	8.83E+00	2.68E-01	6.91E+02		3.69E+03	2.86	2.86E-03	-2.54E+00	3.57E+00		5.64E-20	1.00
375	3.29E+01	1.04E+00	1.14E+03		5.42E+03	2.67	2.67E-03	-2.57E+00	3.73E+00	n		
400	1.04E+02	3.42E+00	1.82E+03		7.88E+03	2.50	2.50E-03	-2.60E+00	3.90E+00		8.46	
425	2.86E+02	9.87E+00	2.85E+03		1.13E+04	2.35	2.35E-03	-2.63E+00	4.05E+00	Ea		1.00
450	7.06E+02	2.56E+01	4.35E+03		1.60E+04	2.22	2.22E-03	-2.65E+00	4.20E+00		-1038	1.60E+04

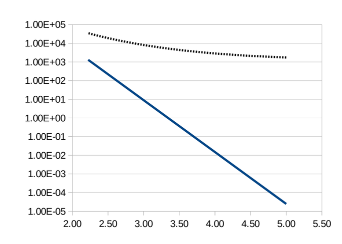


P1 1.95E+09
P2 6400
P3

-CH2OO. | >CH-

Ea shift -9.36E+02

T	Miyoshi 2011	average T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200	2.47E-05	1.60E+01		1.73E+03	5.00	5.00E-03	-2.30E+00	3.24E+00	A		1.02E+03
225	8.65E-04	3.37E+01		2.16E+03	4.44	4.44E-03	-2.35E+00	3.33E+00		2.55E+05	0.59
250	1.49E-02	6.72E+01		2.84E+03	4.00	4.00E-03	-2.40E+00	3.45E+00	Ea		
260	3.98E-02	8.74E+01		3.20E+03	3.85	3.85E-03	-2.41E+00	3.51E+00		1.11E+03	
270	9.90E-02	1.13E+02		3.62E+03	3.70	3.70E-03	-2.43E+00	3.56E+00			1.20
280	2.31E-01	1.44E+02		4.09E+03	3.57	3.57E-03	-2.45E+00	3.61E+00			4.93E+03
290	5.08E-01	1.84E+02		4.64E+03	3.45	3.45E-03	-2.46E+00	3.67E+00		-8.46E+00	
298	9.18E-01	2.22E+02	5.14E+03	5.14E+03	3.36	3.36E-03	-2.47E+00	3.71E+00		6.03E+02	
310	2.11E+00	2.92E+02		6.00E+03	3.23	3.23E-03	-2.49E+00	3.78E+00		-1.92E+01	
320	4.02E+00	3.66E+02		6.82E+03	3.13	3.13E-03	-2.51E+00	3.83E+00		#N/A	
330	7.37E+00	4.54E+02		7.76E+03	3.03	3.03E-03	-2.52E+00	3.89E+00		#N/A	
340	1.30E+01	5.62E+02		8.83E+03	2.94	2.94E-03	-2.53E+00	3.95E+00	A		8.83E+03
350	2.23E+01	6.91E+02		1.00E+04	2.86	2.86E-03	-2.54E+00	4.00E+00		5.64E-20	1.00
375	7.55E+01	1.14E+03		1.38E+04	2.67	2.67E-03	-2.57E+00	4.14E+00	n		
400	2.19E+02	1.82E+03		1.89E+04	2.50	2.50E-03	-2.60E+00	4.28E+00		8.46	
425	5.62E+02	2.85E+03		2.58E+04	2.35	2.35E-03	-2.63E+00	4.41E+00	Ea		1.00
450	1.30E+03	4.35E+03		3.49E+04	2.22	2.22E-03	-2.65E+00	4.54E+00		-1388	3.49E+04

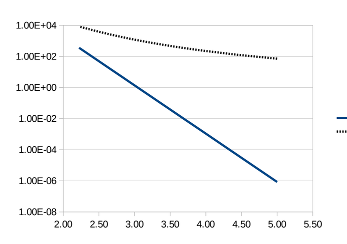


P1 2.85E+09
P2 7150
P3

>CHOO. | -CH3

Ea shift -2.99E+02

T	Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200	8.49E-07	1.60E+01		7.14E+01	5.00	5.00E-03	-2.30E+00	1.85E+00	A		4.21E+01
225	4.51E-05	3.37E+01		1.27E+02	4.44	4.44E-03	-2.35E+00	2.11E+00		2.55E+05	0.59
250	1.08E-03	6.72E+01		2.23E+02	4.00	4.00E-03	-2.40E+00	2.35E+00	Ea		
260	3.25E-03	8.74E+01		2.76E+02	3.85	3.85E-03	-2.41E+00	2.44E+00		1.74E+03	
270	9.00E-03	1.13E+02		3.42E+02	3.70	3.70E-03	-2.43E+00	2.53E+00			1.20
280	2.32E-02	1.44E+02		4.21E+02	3.57	3.57E-03	-2.45E+00	2.62E+00			5.07E+02
290	5.59E-02	1.84E+02		5.17E+02	3.45	3.45E-03	-2.46E+00	2.71E+00		-8.46E+00	
298	1.08E-01	2.22E+02	6.07E+02	6.07E+02	3.36	3.36E-03	-2.47E+00	2.78E+00		3.26E+02	
310	2.74E-01	2.92E+02		7.68E+02	3.23	3.23E-03	-2.49E+00	2.89E+00		-1.92E+01	
320	5.64E-01	3.66E+02		9.32E+02	3.13	3.13E-03	-2.51E+00	2.97E+00		#N/A	
330	1.11E+00	4.54E+02		1.13E+03	3.03	3.03E-03	-2.52E+00	3.05E+00		#N/A	
340	2.10E+00	5.62E+02		1.36E+03	2.94	2.94E-03	-2.53E+00	3.13E+00	A		1.36E+03
350	3.83E+00	6.91E+02		1.63E+03	2.86	2.86E-03	-2.54E+00	3.21E+00		5.64E-20	1.00
375	1.49E+01	1.14E+03		2.53E+03	2.67	2.67E-03	-2.57E+00	3.40E+00	n		
400	4.92E+01	1.82E+03		3.85E+03	2.50	2.50E-03	-2.60E+00	3.59E+00		8.46	
425	1.41E+02	2.85E+03		5.76E+03	2.35	2.35E-03	-2.63E+00	3.76E+00	Ea		1.00
450	3.58E+02	4.35E+03		8.47E+03	2.22	2.22E-03	-2.65E+00	3.93E+00		-751	8.47E+03

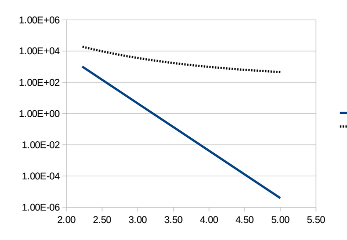


P1 5540000000
P2 6980
P3

>CHOO. | -CH2-

Ea shift -6.68E+02

T	Miyoshi 2011	average T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200	3.86E-06	1.60E+01		4.50E+02	5.00	5.00E-03	-2.30E+00	2.65E+00	A		2.65E+02
225	1.87E-04	3.37E+01		6.54E+02	4.44	4.44E-03	-2.35E+00	2.82E+00		2.55E+05	0.59
250	4.15E-03	6.72E+01		9.71E+02	4.00	4.00E-03	-2.40E+00	2.99E+00	Ea		
260	1.21E-02	8.74E+01		1.14E+03	3.85	3.85E-03	-2.41E+00	3.06E+00		1.37E+03	
270	3.28E-02	1.13E+02		1.34E+03	3.70	3.70E-03	-2.43E+00	3.13E+00			1.20
280	8.26E-02	1.44E+02		1.57E+03	3.57	3.57E-03	-2.45E+00	3.20E+00			1.89E+03
290	1.95E-01	1.84E+02		1.84E+03	3.45	3.45E-03	-2.46E+00	3.26E+00		-8.46E+00	
298	3.72E-01	2.22E+02	2.09E+03	2.09E+03	3.36	3.36E-03	-2.47E+00	3.32E+00		4.86E+02	
310	9.22E-01	2.92E+02		2.52E+03	3.23	3.23E-03	-2.49E+00	3.40E+00		-1.92E+01	
320	1.86E+00	3.66E+02		2.94E+03	3.13	3.13E-03	-2.51E+00	3.47E+00		#N/A	
330	3.61E+00	4.54E+02		3.44E+03	3.03	3.03E-03	-2.52E+00	3.54E+00		#N/A	
340	6.73E+00	5.62E+02		4.00E+03	2.94	2.94E-03	-2.53E+00	3.60E+00	A		4.00E+03
350	1.21E+01	6.91E+02		4.66E+03	2.86	2.86E-03	-2.54E+00	3.67E+00		5.64E-20	1.00
375	4.57E+01	1.14E+03		6.75E+03	2.67	2.67E-03	-2.57E+00	3.83E+00	n		
400	1.46E+02	1.82E+03		9.66E+03	2.50	2.50E-03	-2.60E+00	3.99E+00		8.46	
425	4.08E+02	2.85E+03		1.37E+04	2.35	2.35E-03	-2.63E+00	4.14E+00	Ea		1.00
450	1.02E+03	4.35E+03		1.92E+04	2.22	2.22E-03	-2.65E+00	4.28E+00		-1119	1.92E+04

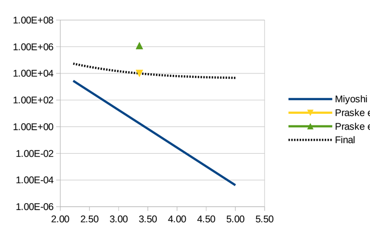


P1 5090000000
P2 6490
P3

>CHOO. | >CH-

Ea shift -1.13E+03

T	Miyoshi 2011	Praske et al.	Praske et al. 2019	average T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200	4.11E-05			1.60E+01		4.59E+03	5.00	5.00E-03	-2.30E+00	3.66E+00	A		2.71E+03
225	1.51E-03			3.37E+01		5.16E+03	4.44	4.44E-03	-2.35E+00	3.71E+00		2.55E+05	0.59
250	2.71E-02			6.72E+01		6.23E+03	4.00	4.00E-03	-2.40E+00	3.79E+00	Ea		
260	7.35E-02			8.74E+01		6.80E+03	3.85	3.85E-03	-2.41E+00	3.83E+00		9.10E+02	
270	1.85E-01			1.13E+02		7.47E+03	3.70	3.70E-03	-2.43E+00	3.87E+00			1.20
280	4.37E-01			1.44E+02		8.24E+03	3.57	3.57E-03	-2.45E+00	3.92E+00			9.92E+03
290	9.72E-01			1.84E+02		9.13E+03	3.45	3.45E-03	-2.46E+00	3.96E+00		-8.46E+00	
298	1.77E+00	1.00E+04	1.20E+06	2.22E+02	9.92E+03	9.92E+03	3.36	3.36E-03	-2.47E+00	4.00E+00		6.88E+02	
310	4.12E+00			2.92E+02		1.13E+04	3.23	3.23E-03	-2.49E+00	4.05E+00		-1.92E+01	
320	7.92E+00			3.66E+02		1.26E+04	3.13	3.13E-03	-2.51E+00	4.10E+00		#N/A	
330	1.46E+01			4.54E+02		1.40E+04	3.03	3.03E-03	-2.52E+00	4.15E+00		#N/A	
340	2.61E+01			5.62E+02		1.57E+04	2.94	2.94E-03	-2.53E+00	4.20E+00	A		1.57E+04
350	4.50E+01			6.91E+02		1.76E+04	2.86	2.86E-03	-2.54E+00	4.24E+00		5.64E-20	1.00
375	1.55E+02			1.14E+03		2.33E+04	2.67	2.67E-03	-2.57E+00	4.37E+00	n		
400	4.57E+02			1.82E+03		3.09E+04	2.50	2.50E-03	-2.60E+00	4.49E+00		8.46	
425	1.19E+03			2.85E+03		4.09E+04	2.35	2.35E-03	-2.63E+00	4.61E+00	Ea		1.00
450	2.77E+03			4.35E+03		5.39E+04	2.22	2.22E-03	-2.65E+00	4.73E+00		-1584	5.39E+04

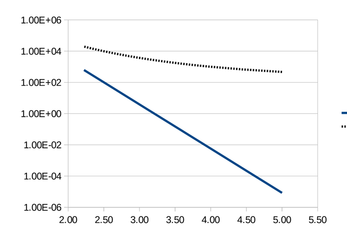


P1 1210000000
P2 6520
P3

>C(OO.)- | -CH3

Ea shift -6.74E+02

T	Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	8.41E-06	1.60E+01		4.65E+02	5.00	5.00E-03	-2.30E+00	2.67E+00	A		2.74E+02
225	3.15E-04	3.37E+01		6.74E+02	4.44	4.44E-03	-2.35E+00	2.83E+00		2.55E+05	0.59
250	5.71E-03	6.72E+01		9.97E+02	4.00	4.00E-03	-2.40E+00	3.00E+00	Ea		
260	1.56E-02	8.74E+01		1.17E+03	3.85	3.85E-03	-2.41E+00	3.07E+00		1.37E+03	
270	3.94E-02	1.13E+02		1.37E+03	3.70	3.70E-03	-2.43E+00	3.14E+00			1.20
280	9.33E-02	1.44E+02		1.60E+03	3.57	3.57E-03	-2.45E+00	3.21E+00			1.93E+03
290	2.08E-01	1.84E+02		1.88E+03	3.45	3.45E-03	-2.46E+00	3.27E+00		-8.46E+00	
298	3.81E-01	2.22E+02	2.13E+03	2.13E+03	3.36	3.36E-03	-2.47E+00	3.33E+00		4.89E+02	
310	8.88E-01	2.92E+02		2.57E+03	3.23	3.23E-03	-2.49E+00	3.41E+00		-1.92E+01	
320	1.71E+00	3.66E+02		3.01E+03	3.13	3.13E-03	-2.51E+00	3.48E+00		#N/A	
330	3.18E+00	4.54E+02		3.51E+03	3.03	3.03E-03	-2.52E+00	3.54E+00		#N/A	
340	5.68E+00	5.62E+02		4.08E+03	2.94	2.94E-03	-2.53E+00	3.61E+00	A		4.08E+03
350	9.83E+00	6.91E+02		4.75E+03	2.86	2.86E-03	-2.54E+00	3.68E+00		5.64E-20	1.00
375	3.40E+01	1.14E+03		6.87E+03	2.67	2.67E-03	-2.57E+00	3.84E+00	n		
400	1.01E+02	1.82E+03		9.83E+03	2.50	2.50E-03	-2.60E+00	3.99E+00		8.46	
425	2.63E+02	2.85E+03		1.39E+04	2.35	2.35E-03	-2.63E+00	4.14E+00	Ea		1.00
450	6.17E+02	4.35E+03		1.95E+04	2.22	2.22E-03	-2.65E+00	4.29E+00		-1126	1.95E+04

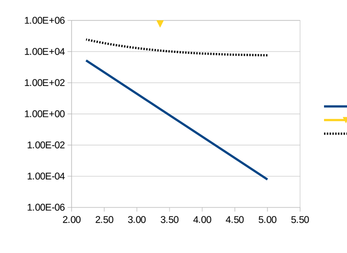


P1 3470000000
P2 6330
P3

>C(OO.)- | -CH2-

Ea shift -1.18E+03

T	Miyoshi 2011	Praske et al. 2019	average T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	6.24E-05		1.60E+01		5.78E+03	5.00	5.00E-03	-2.30E+00	3.76E+00	A		3.40E+03
225	2.10E-03		3.37E+01		6.33E+03	4.44	4.44E-03	-2.35E+00	3.80E+00		2.55E+05	0.59
250	3.50E-02		6.72E+01		7.48E+03	4.00	4.00E-03	-2.40E+00	3.87E+00	Ea		
260	9.27E-02		8.74E+01		8.11E+03	3.85	3.85E-03	-2.41E+00	3.91E+00		8.64E+02	
270	2.28E-01		1.13E+02		8.85E+03	3.70	3.70E-03	-2.43E+00	3.95E+00			1.20
280	5.27E-01		1.44E+02		9.71E+03	3.57	3.57E-03	-2.45E+00	3.99E+00			1.17E+04
290	1.15E+00		1.84E+02		1.07E+04	3.45	3.45E-03	-2.46E+00	4.03E+00		-8.46E+00	
298	2.07E+00	6.00E+05	2.22E+02	1.16E+04	1.16E+04	3.36	3.36E-03	-2.47E+00	4.06E+00		7.08E+02	
310	4.70E+00		2.92E+02		1.31E+04	3.23	3.23E-03	-2.49E+00	4.12E+00		-1.92E+01	
320	8.90E+00		3.66E+02		1.45E+04	3.13	3.13E-03	-2.51E+00	4.16E+00		#N/A	
330	1.62E+01		4.54E+02		1.61E+04	3.03	3.03E-03	-2.52E+00	4.21E+00		#N/A	
340	2.85E+01		5.62E+02		1.80E+04	2.94	2.94E-03	-2.53E+00	4.25E+00	A		1.80E+04
350	4.85E+01		6.91E+02		2.00E+04	2.86	2.86E-03	-2.54E+00	4.30E+00		5.64E-20	1.00
375	1.62E+02		1.14E+03		2.63E+04	2.67	2.67E-03	-2.57E+00	4.42E+00	n		
400	4.65E+02		1.82E+03		3.46E+04	2.50	2.50E-03	-2.60E+00	4.54E+00		8.46	
425	1.18E+03		2.85E+03		4.55E+04	2.35	2.35E-03	-2.63E+00	4.66E+00	Ea		1.00
450	2.70E+03		4.35E+03		5.97E+04	2.22	2.22E-03	-2.65E+00	4.78E+00		-1630	5.97E+04

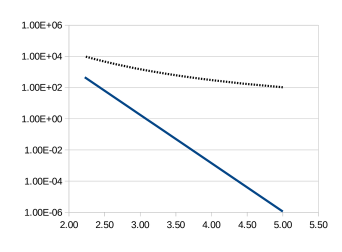


P1 3560000000
P2 7140
P3

>C(OO.)- | >CH-

Ea shift -3.76E+02

T	Miyoshi 2011	average T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	1.11E-06	1.60E+01		1.05E+02	5.00	5.00E-03	-2.30E+00	2.02E+00	A		6.16E+01
225	5.89E-05	3.37E+01		1.79E+02	4.44	4.44E-03	-2.35E+00	2.25E+00		2.55E+05	0.59
250	1.41E-03	6.72E+01		3.02E+02	4.00	4.00E-03	-2.40E+00	2.48E+00	Ea		
260	4.22E-03	8.74E+01		3.71E+02	3.85	3.85E-03	-2.41E+00	2.57E+00		1.67E+03	
270	1.17E-02	1.13E+02		4.53E+02	3.70	3.70E-03	-2.43E+00	2.66E+00			1.20
280	3.00E-02	1.44E+02		5.53E+02	3.57	3.57E-03	-2.45E+00	2.74E+00			6.65E+02
290	7.22E-02	1.84E+02		6.72E+02	3.45	3.45E-03	-2.46E+00	2.83E+00		-8.46E+00	
298	1.40E-01	2.22E+02	7.84E+02	7.84E+02	3.36	3.36E-03	-2.47E+00	2.89E+00		3.59E+02	
310	3.54E-01	2.92E+02		9.83E+02	3.23	3.23E-03	-2.49E+00	2.99E+00		-1.92E+01	
320	7.27E-01	3.66E+02		1.18E+03	3.13	3.13E-03	-2.51E+00	3.07E+00		#N/A	
330	1.43E+00	4.54E+02		1.42E+03	3.03	3.03E-03	-2.52E+00	3.15E+00		#N/A	
340	2.70E+00	5.62E+02		1.70E+03	2.94	2.94E-03	-2.53E+00	3.23E+00	A		1.70E+03
350	4.92E+00	6.91E+02		2.02E+03	2.86	2.86E-03	-2.54E+00	3.31E+00		5.64E-20	1.00
375	1.92E+01	1.14E+03		3.10E+03	2.67	2.67E-03	-2.57E+00	3.49E+00	n		
400	6.30E+01	1.82E+03		4.66E+03	2.50	2.50E-03	-2.60E+00	3.67E+00		8.46	
425	1.80E+02	2.85E+03		6.89E+03	2.35	2.35E-03	-2.63E+00	3.84E+00	Ea		1.00
450	4.58E+02	4.35E+03		1.00E+04	2.22	2.22E-03	-2.65E+00	4.00E+00		-827	1.00E+04



1,8 Hshift

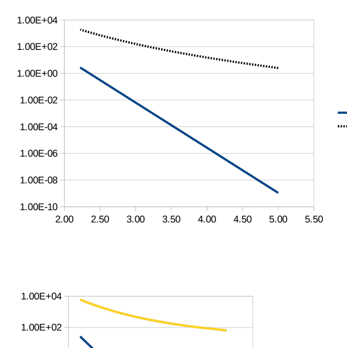
Scaling: 1.60E+05

P1 9.04E+07
P2 7.79E+03
P3

-CH2OO. | -CH3

Ea shift 3.70E+02

T	Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200	1.10E-09	1.60E+01		2.51E+00	5.00	5.00E-03	-2.30E+00	4.00E-01	A		1.48E+00
225	8.32E-08	3.37E+01		6.51E+00	4.44	4.44E-03	-2.35E+00	8.13E-01		2.55E+05	0.59
250	2.65E-06	6.72E+01		1.53E+01	4.00	4.00E-03	-2.40E+00	1.18E+00	Ea		
260	8.79E-06	8.74E+01		2.11E+01	3.85	3.85E-03	-2.41E+00	1.32E+00		2.41E+03	
270	2.67E-05	1.13E+02		2.87E+01	3.70	3.70E-03	-2.43E+00	1.46E+00			1.20
280	7.47E-05	1.44E+02		3.86E+01	3.57	3.57E-03	-2.45E+00	1.59E+00			4.64E+01
290	1.95E-04	1.84E+02		5.14E+01	3.45	3.45E-03	-2.46E+00	1.71E+00		-8.46E+00	
298	4.01E-04	2.22E+02	6.42E+01	6.42E+01	3.36	3.36E-03	-2.47E+00	1.81E+00		3.55E+01	
310	1.10E-03	2.92E+02		8.87E+01	3.23	3.23E-03	-2.49E+00	1.95E+00		-1.92E+01	
320	2.42E-03	3.66E+02		1.15E+02	3.13	3.13E-03	-2.51E+00	2.06E+00		#N/A	
330	5.06E-03	4.54E+02		1.48E+02	3.03	3.03E-03	-2.52E+00	2.17E+00		#N/A	
340	1.01E-02	5.62E+02		1.89E+02	2.94	2.94E-03	-2.53E+00	2.28E+00	A		1.89E+02
350	1.95E-02	6.91E+02		2.40E+02	2.86	2.86E-03	-2.54E+00	2.38E+00		5.64E-20	1.00
375	8.60E-02	1.14E+03		4.24E+02	2.67	2.67E-03	-2.57E+00	2.63E+00	n		
400	3.15E-01	1.82E+03		7.22E+02	2.50	2.50E-03	-2.60E+00	2.86E+00		8.46	
425	9.90E-01	2.85E+03		1.19E+03	2.35	2.35E-03	-2.63E+00	3.08E+00	Ea		1.00
450	2.74E+00	4.35E+03		1.91E+03	2.22	2.22E-03	-2.65E+00	3.28E+00		-82	1.91E+03

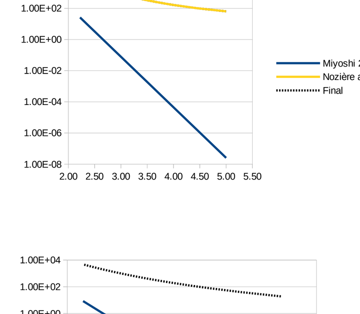


P1 4.22E+08 3.48E-25
P2 7.47E+03 1.02E+01
P3 -1326.6652

-CH2OO. | -CH2-

Ea shift 0.00E+00

T	Miyoshi 2011	Nozière and Vereecken 2019	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200	2.54E-08	6.43E+01	6.43E+01		6.43E+01	5.00	5.00E-03	-2.30E+00	1.81E+00	A		3.40E+01
225	1.61E-06	1.02E+02	1.02E+02		1.02E+02	4.44	4.44E-03	-2.35E+00	2.01E+00		1.43E+05	0.53
250	4.45E-05	1.65E+02	1.65E+02		1.65E+02	4.00	4.00E-03	-2.40E+00	2.22E+00	Ea		
260	1.41E-04	2.00E+02	2.00E+02		2.00E+02	3.85	3.85E-03	-2.41E+00	2.30E+00		1.67E+03	
270	4.07E-04	2.43E+02	2.43E+02		2.43E+02	3.70	3.70E-03	-2.43E+00	2.39E+00			1.25
280	1.09E-03	2.95E+02	2.95E+02		2.95E+02	3.57	3.57E-03	-2.45E+00	2.47E+00			3.69E+02
290	2.74E-03	3.58E+02	3.58E+02		3.58E+02	3.45	3.45E-03	-2.46E+00	2.55E+00		-1.02E+01	
298	5.48E-03	4.17E+02	4.17E+02	4.17E+02	4.17E+02	3.36	3.36E-03	-2.47E+00	2.62E+00		5.76E+02	
310	1.45E-02	5.25E+02	5.25E+02		5.25E+02	3.23	3.23E-03	-2.49E+00	2.72E+00		-2.45E+01	
320	3.07E-02	6.34E+02	6.34E+02		6.34E+02	3.13	3.13E-03	-2.51E+00	2.80E+00		#N/A	
330	6.23E-02	7.64E+02	7.64E+02		7.64E+02	3.03	3.03E-03	-2.52E+00	2.88E+00		#N/A	
340	1.21E-01	9.20E+02	9.20E+02		9.20E+02	2.94	2.94E-03	-2.53E+00	2.96E+00	A		9.20E+02
350	2.27E-01	1.10E+03	1.10E+03		1.10E+03	2.86	2.86E-03	-2.54E+00	3.04E+00		3.48E-25	1.00
375	9.42E-01	1.73E+03	1.73E+03		1.73E+03	2.67	2.67E-03	-2.57E+00	3.24E+00	n		
400	3.27E+00	2.67E+03	2.67E+03		2.67E+03	2.50	2.50E-03	-2.60E+00	3.43E+00		10.16	
425	9.82E+00	4.07E+03	4.07E+03		4.07E+03	2.35	2.35E-03	-2.63E+00	3.61E+00	Ea		1.00
450	2.61E+01	6.12E+03	6.12E+03		6.12E+03	2.22	2.22E-03	-2.65E+00	3.79E+00		-1327	6.12E+03

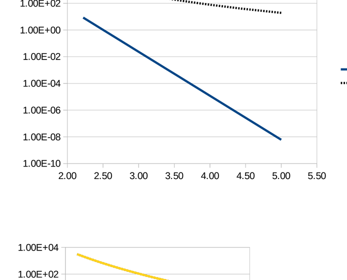


P1 1.75E+08
P2 7.58E+03
P3

-CH2OO. | >CH-

Ea shift -3.70E+01

T	Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200	6.07E-09	1.60E+01		1.92E+01	5.00	5.00E-03	-2.30E+00	1.28E+00	A		1.13E+01
225	4.09E-07	3.37E+01		3.97E+01	4.44	4.44E-03	-2.35E+00	1.60E+00		2.55E+05	0.59
250	1.19E-05	6.72E+01		7.79E+01	4.00	4.00E-03	-2.40E+00	1.89E+00	Ea		
260	3.82E-05	8.74E+01		1.01E+02	3.85	3.85E-03	-2.41E+00	2.00E+00		2.00E+03	
270	1.12E-04	1.13E+02		1.29E+02	3.70	3.70E-03	-2.43E+00	2.11E+00			1.20
280	3.06E-04	1.44E+02		1.65E+02	3.57	3.57E-03	-2.45E+00	2.22E+00			1.98E+02
290	7.79E-04	1.84E+02		2.09E+02	3.45	3.45E-03	-2.46E+00	2.32E+00		-8.46E+00	
298	1.57E-03	2.22E+02	2.51E+02	2.51E+02	3.36	3.36E-03	-2.47E+00	2.40E+00		2.12E+02	
310	4.21E-03	2.92E+02		3.29E+02	3.23	3.23E-03	-2.49E+00	2.52E+00		-1.92E+01	
320	9.03E-03	3.66E+02		4.10E+02	3.13	3.13E-03	-2.51E+00	2.61E+00		#N/A	
330	1.85E-02	4.54E+02		5.08E+02	3.03	3.03E-03	-2.52E+00	2.71E+00		#N/A	
340	3.64E-02	5.62E+02		6.26E+02	2.94	2.94E-03	-2.53E+00	2.80E+00	A		6.26E+02
350	6.88E-02	6.91E+02		7.68E+02	2.86	2.86E-03	-2.54E+00	2.89E+00		5.64E-20	1.00
375	2.91E-01	1.14E+03		1.26E+03	2.67	2.67E-03	-2.57E+00	3.10E+00	n		
400	1.03E+00	1.82E+03		2.00E+03	2.50	2.50E-03	-2.60E+00	3.30E+00		8.46	
425	3.14E+00	2.85E+03		3.11E+03	2.35	2.35E-03	-2.63E+00	3.49E+00	Ea		1.00
450	8.46E+00	4.35E+03		4.73E+03	2.22	2.22E-03	-2.65E+00	3.67E+00		-489	4.73E+03

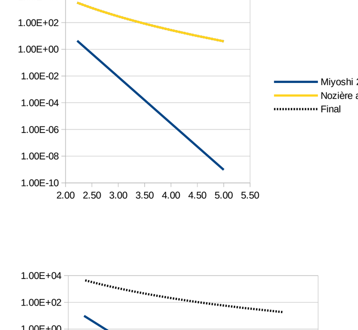


P1 234000000 9.14E-15
P2 8010 6.76E+00
P3 423.3439512

>CHOO. | -CH3

Ea shift 0.00E+00

T	Miyoshi 2011	Nozière and Vereecken 2019	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200	9.46E-10	3.97E+00	3.97E+00		3.97E+00	5.00	5.00E-03	-2.30E+00	5.99E-01	A		2.60E+00
225	8.10E-08	1.11E+01	1.11E+01		1.11E+01	4.44	4.44E-03	-2.35E+00	1.05E+00		4.58E+05	0.65
250	2.85E-06	2.74E+01	2.74E+01		2.74E+01	4.00	4.00E-03	-2.40E+00	1.44E+00	Ea		
260	9.76E-06	3.82E+01	3.82E+01		3.82E+01	3.85	3.85E-03	-2.41E+00	1.58E+00		2.42E+03	
270	3.06E-05	5.23E+01	5.23E+01		5.23E+01	3.70	3.70E-03	-2.43E+00	1.72E+00			1.16
280	8.82E-05	7.07E+01	7.07E+01		7.07E+01	3.57	3.57E-03	-2.45E+00	1.85E+00			8.20E+01
290	2.36E-04	9.45E+01	9.45E+01		9.45E+01	3.45	3.45E-03	-2.46E+00	1.98E+00		-6.76E+00	
298	4.96E-04	1.18E+02	1.18E+02	1.18E+02	1.18E+02	3.36	3.36E-03	-2.47E+00	2.07E+00		-1.84E+02	
310	1.40E-03	1.63E+02	1.63E+02		1.63E+02	3.23	3.23E-03	-2.49E+00	2.21E+00		-1.40E+01	
320	3.15E-03	2.11E+02	2.11E+02		2.11E+02	3.13	3.13E-03	-2.51E+00	2.32E+00		#N/A	
330	6.73E-03	2.70E+02	2.70E+02		2.70E+02	3.03	3.03E-03	-2.52E+00	2.43E+00		#N/A	
340	1.37E-02	3.43E+02	3.43E+02		3.43E+02	2.94	2.94E-03	-2.53E+00	2.54E+00	A		3.43E+02
350	2.69E-02	4.33E+02	4.33E+02		4.33E+02	2.86	2.86E-03	-2.54E+00	2.64E+00		9.14E-15	1.00
375	1.24E-01	7.48E+02	7.48E+02		7.48E+02	2.67	2.67E-03	-2.57E+00	2.87E+00	n		
400	4.70E-01	1.24E+03	1.24E+03		1.24E+03	2.50	2.50E-03	-2.60E+00	3.09E+00		6.76	
425	1.53E+00	1.99E+03	1.99E+03		1.99E+03	2.35	2.35E-03	-2.63E+00	3.30E+00	Ea		1.00
450	4.35E+00	3.10E+03	3.10E+03		3.10E+03	2.22	2.22E-03	-2.65E+00	3.49E+00		423	3.10E+03

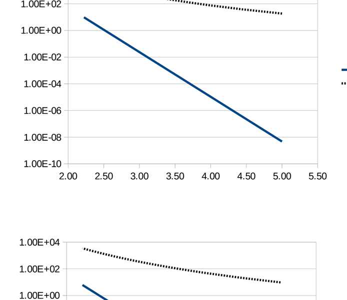


P1 274000000
P2 7720
P3

>CHOO. | -CH2-

Ea shift -3.06E+01

T	Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200	4.72E-09	1.60E+01		1.86E+01	5.00	5.00E-03	-2.30E+00	1.27E+00	A		1.10E+01
225	3.44E-07	3.37E+01		3.86E+01	4.44	4.44E-03	-2.35E+00	1.59E+00		2.55E+05	0.59
250	1.06E-05	6.72E+01		7.59E+01	4.00	4.00E-03	-2.40E+00	1.88E+00	Ea		
260	3.49E-05	8.74E+01		9.83E+01	3.85	3.85E-03	-2.41E+00	1.99E+00		2.01E+03	
270	1.05E-04	1.13E+02		1.26E+02	3.70	3.70E-03	-2.43E+00	2.10E+00			1.20
280	2.91E-04	1.44E+02		1.61E+02	3.57	3.57E-03	-2.45E+00	2.21E+00			1.94E+02
290	7.53E-04	1.84E+02		2.04E+02	3.45	3.45E-03	-2.46E+00	2.31E+00		-8.46E+00	
298	1.54E-03	2.22E+02	2.46E+02	2.46E+02	3.36	3.36E-03	-2.47E+00	2.39E+00		2.09E+02	
310	4.19E-03	2.92E+02		3.23E+02	3.23	3.23E-03	-2.49E+00	2.51E+00		-1.92E+01	
320	9.13E-03	3.66E+02		4.02E+02	3.13	3.13E-03	-2.51E+00	2.60E+00		#N/A	
330	1.90E-02	4.54E+02		4.99E+02	3.03	3.03E-03	-2.52E+00	2.70E+00		#N/A	
340	3.77E-02	5.62E+02		6.15E+02	2.94	2.94E-03	-2.53E+00	2.79E+00	A		6.15E+02
350	7.22E-02	6.91E+02		7.55E+02	2.86	2.86E-03	-2.54E+00	2.88E+00		5.64E-20	1.00
375	3.14E-01	1.14E+03		1.23E+03	2.67	2.67E-03	-2.57E+00	3.09E+00	n		
400	1.14E+00	1.82E+03		1.97E+03	2.50	2.50E-03	-2.60E+00	3.29E+00		8.46	
425	3.54E+00	2.85E+03		3.06E+03	2.35	2.35E-03	-2.63E+00	3.49E+00	Ea		1.00
450	9.71E+00	4.35E+03		4.66E+03	2.22	2.22E-03	-2.65E+00	3.67E+00		-482	4.66E+03

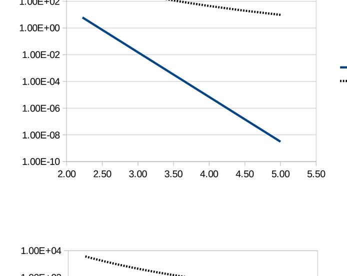


P1 170000000
P2 7710
P3

>CHOO. | >CH-

Ea shift 1.02E+02

T	Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200	3.08E-09	1.60E+01		9.61E+00	5.00	5.00E-03	-2.30E+00	9.83E-01	A		5.66E+00
225	2.23E-07	3.37E+01		2.14E+01	4.44	4.44E-03	-2.35E+00	1.33E+00		2.55E+05	0.59
250	6.87E-06	6.72E+01		4.47E+01	4.00	4.00E-03	-2.40E+00	1.65E+00	Ea		
260	2.25E-05	8.74E+01		5.91E+01	3.85	3.85E-03	-2.41E+00	1.77E+00		2.14E+03	
270	6.74E-05	1.13E+02		7.74E+01	3.70	3.70E-03	-2.43E+00	1.89E+00			1.20
280	1.87E-04	1.44E+02		1.00E+02	3.57	3.57E-03	-2.45E+00	2.00E+00			1.21E+02
290	4.83E-04	1.84E+02		1.30E+02	3.45	3.45E-03	-2.46E+00	2.11E+00		-8.46E+00	
298	9.87E-04	2.22E+02	1.58E+02	1.58E+02	3.36	3.36E-03	-2.47E+00	2.20E+00		1.52E+02	
310	2.69E-03	2.92E+02		2.11E+02	3.23	3.23E-03	-2.49E+00	2.32E+00		-1.92E+01	
320	5.84E-03	3.66E+02		2.66E+02	3.13	3.13E-03	-2.51E+00	2.42E+00		#N/A	
330	1.21E-02	4.54E+02		3.34E+02	3.03	3.03E-03	-2.52E+00	2.52E+00		#N/A	
340	2.41E-02	5.62E+02		4.17E+02	2.94	2.94E-03	-2.53E+00	2.62E+00	A		4.17E+02
350	4.61E-02	6.91E+02		5.17E+02	2.86	2.86E-03	-2.54E+00	2.71E+00		5.64E-20	1.00
375	2.00E-01	1.14E+03		8.67E+02	2.67	2.67E-03	-2.57E+00	2.94E+00	n		
400	7.23E-01	1.82E+03		1.41E+03	2.50	2.50E-03	-2.60E+00	3.15E+00		8.46	
425	2.25E+00	2.85E+03		2.24E+03	2.35	2.35E-03	-2.63E+00	3.35E+00	Ea		1.00
450	6.16E+00	4.35E+03		3.47E+03	2.22	2.22E-03	-2.65E+00	3.54E+00		-350	3.47E+03

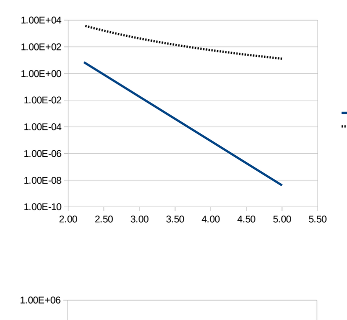


P1 169000000
P2 7650
P3

>C(OO.)- | -CH3

Ea shift 4.34E+01

T	Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	4.13E-09	1.60E+01		1.29E+01	5.00	5.00E-03	-2.30E+00	1.11E+00	A		7.57E+00
225	2.90E-07	3.37E+01		2.78E+01	4.44	4.44E-03	-2.35E+00	1.44E+00		2.55E+05	0.59
250	8.68E-06	6.72E+01		5.65E+01	4.00	4.00E-03	-2.40E+00	1.75E+00	Ea		
260	2.82E-05	8.74E+01		7.39E+01	3.85	3.85E-03	-2.41E+00	1.87E+00		2.09E+03	
270	8.37E-05	1.13E+02		9.60E+01	3.70	3.70E-03	-2.43E+00	1.98E+00			1.20
280	2.30E-04	1.44E+02		1.24E+02	3.57	3.57E-03	-2.45E+00	2.09E+00			1.49E+02
290	5.91E-04	1.84E+02		1.58E+02	3.45	3.45E-03	-2.46E+00	2.20E+00		-8.46E+00	
298	1.20E-03	2.22E+02	1.92E+02	1.92E+02	3.36	3.36E-03	-2.47E+00	2.28E+00		1.77E+02	
310	3.24E-03	2.92E+02		2.54E+02	3.23	3.23E-03	-2.49E+00	2.41E+00		-1.92E+01	
320	7.01E-03	3.66E+02		3.19E+02	3.13	3.13E-03	-2.51E+00	2.50E+00		#N/A	
330	1.45E-02	4.54E+02		3.98E+02	3.03	3.03E-03	-2.52E+00	2.60E+00		#N/A	
340	2.86E-02	5.62E+02		4.95E+02	2.94	2.94E-03	-2.53E+00	2.69E+00	A		4.95E+02
350	5.44E-02	6.91E+02		6.11E+02	2.86	2.86E-03	-2.54E+00	2.79E+00		5.64E-20	1.00
375	2.33E-01	1.14E+03		1.01E+03	2.67	2.67E-03	-2.57E+00	3.01E+00	n		
400	8.36E-01	1.82E+03		1.63E+03	2.50	2.50E-03	-2.60E+00	3.21E+00		8.46	
425	2.57E+00	2.85E+03		2.57E+03	2.35	2.35E-03	-2.63E+00	3.41E+00	Ea		1.00
450	7.00E+00	4.35E+03		3.95E+03	2.22	2.22E-03	-2.65E+00	3.60E+00		-408	3.95E+03

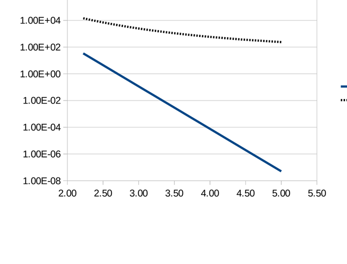


P1 395000000
P2 7320
P3

>C(OO.)- | -CH2-

Ea shift -5.40E+02

T	Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	5.03E-08	1.60E+01		2.37E+02	5.00	5.00E-03	-2.30E+00	2.38E+00	A		1.40E+02
225	2.93E-06	3.37E+01		3.71E+02	4.44	4.44E-03	-2.35E+00	2.57E+00		2.55E+05	0.59
250	7.59E-05	6.72E+01		5.82E+02	4.00	4.00E-03	-2.40E+00	2.76E+00	Ea		
260	2.34E-04	8.74E+01		6.96E+02	3.85	3.85E-03	-2.41E+00	2.84E+00		1.50E+03	
270	6.64E-04	1.13E+02		8.32E+02	3.70	3.70E-03	-2.43E+00	2.92E+00			1.20
280	1.75E-03	1.44E+02		9.92E+02	3.57	3.57E-03	-2.45E+00	3.00E+00			1.19E+03
290	4.31E-03	1.84E+02		1.18E+03	3.45	3.45E-03	-2.46E+00	3.07E+00		-8.46E+00	
298	8.49E-03	2.22E+02	1.36E+03	1.36E+03	3.36	3.36E-03	-2.47E+00	3.13E+00		4.30E+02	
310	2.20E-02	2.92E+02		1.67E+03	3.23	3.23E-03	-2.49E+00	3.22E+00		-1.92E+01	
320	4.59E-02	3.66E+02		1.97E+03	3.13	3.13E-03	-2.51E+00	3.30E+00		#N/A	
330	9.19E-02	4.54E+02		2.33E+03	3.03	3.03E-03	-2.52E+00	3.37E+00		#N/A	
340	1.76E-01	5.62E+02		2.75E+03	2.94	2.94E-03	-2.53E+00	3.44E+00	A		2.75E+03
350	3.26E-01	6.91E+02		3.23E+03	2.86	2.86E-03	-2.54E+00	3.51E+00		5.64E-20	1.00
375	1.32E+00	1.14E+03		4.80E+03	2.67	2.67E-03	-2.57E+00	3.68E+00	n		
400	4.46E+00	1.82E+03		7.02E+03	2.50	2.50E-03	-2.60E+00	3.85E+00		8.46	
425	1.31E+01	2.85E+03		1.01E+04	2.35	2.35E-03	-2.63E+00	4.01E+00	Ea		1.00
450	3.40E+01	4.35E+03		1.44E+04	2.22	2.22E-03	-2.65E+00	4.16E+00		-991	1.44E+04

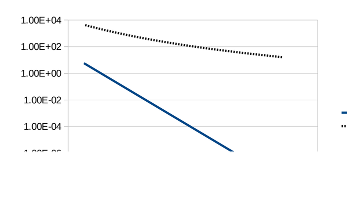


P1 70000000
P2 7340
P3

>C(OO.)- | >CH-

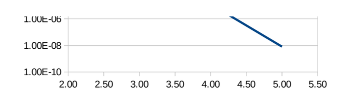
Ea shift -3.94E+00

T	Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	8.06E-09	1.60E+01		1.63E+01	5.00	5.00E-03	-2.30E+00	1.21E+00	A		9.59E+00
225	4.76E-07	3.37E+01		3.43E+01	4.44	4.44E-03	-2.35E+00	1.53E+00		2.55E+05	0.59
250	1.24E-05	6.72E+01		6.83E+01	4.00	4.00E-03	-2.40E+00	1.83E+00	Ea		
260	3.84E-05	8.74E+01		8.87E+01	3.85	3.85E-03	-2.41E+00	1.95E+00		2.04E+03	
270	1.09E-04	1.13E+02		1.14E+02	3.70	3.70E-03	-2.43E+00	2.06E+00			1.20
280	2.89E-04	1.44E+02		1.47E+02	3.57	3.57E-03	-2.45E+00	2.17E+00			1.76E+02
290	7.13E-04	1.84E+02		1.86E+02	3.45	3.45E-03	-2.46E+00	2.27E+00		-8.46E+00	
298	1.41E-03	2.22E+02	2.25E+02	2.25E+02	3.36	3.36E-03	-2.47E+00	2.35E+00		1.98E+02	
310	3.65E-03	2.92E+02		2.96E+02	3.23	3.23E-03	-2.49E+00	2.47E+00		-1.92E+01	
320	7.65E-03	3.66E+02		3.70E+02	3.13	3.13E-03	-2.51E+00	2.57E+00		#N/A	
330	1.53E-02	4.54E+02		4.60E+02	3.03	3.03E-03	-2.52E+00	2.66E+00		#N/A	



Plot OOHscrambling

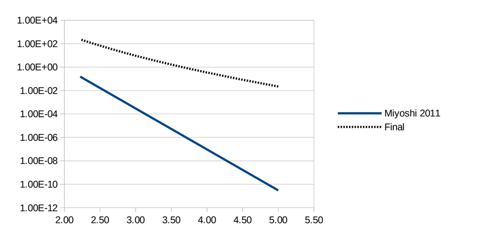
		340	2.95E-02	5.62E+02		5.68E+02	2.94	2.94E-03	-2.53E+00	2.75E+00	A		5.68E+02
		350	5.46E-02	6.91E+02		6.99E+02	2.86	2.86E-03	-2.54E+00	2.84E+00		5.64E-20	1.00
		375	2.21E-01	1.14E+03		1.15E+03	2.67	2.67E-03	-2.57E+00	3.06E+00	n		
		400	7.51E-01	1.82E+03		1.84E+03	2.50	2.50E-03	-2.60E+00	3.26E+00		8.46	
		425	2.21E+00	2.85E+03		2.87E+03	2.35	2.35E-03	-2.63E+00	3.46E+00	Ea		1.00
		450	5.77E+00	4.35E+03		4.39E+03	2.22	2.22E-03	-2.65E+00	3.64E+00		-456	4.39E+03



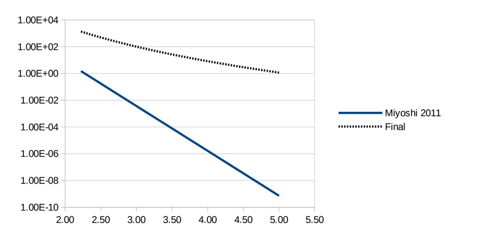
Scaling: 1.60E+05

1,9 Hshift

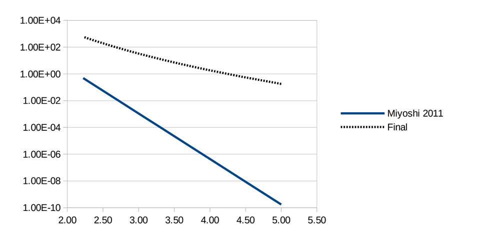
	P1		9.04E+06										
	P2		8.05E+03			Ea shift							
	P3					1.32E+03							
-CH2OO. | -CH3	T		Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
		200	2.99E-11	1.60E+01		2.22E-02	5.00	5.00E-03	-2.30E+00	-1.65E+00	A		1.31E-02
		225	2.62E-09	3.37E+01		9.71E-02	4.44	4.44E-03	-2.35E+00	-1.01E+00		2.55E+05	0.59
		250	9.37E-08	6.72E+01		3.48E-01	4.00	4.00E-03	-2.40E+00	-4.59E-01	Ea		
		260	3.23E-07	8.74E+01		5.53E-01	3.85	3.85E-03	-2.41E+00	-2.57E-01		3.36E+03	
		270	1.02E-06	1.13E+02		8.62E-01	3.70	3.70E-03	-2.43E+00	-6.47E-02			1.20
		280	2.95E-06	1.44E+02		1.31E+00	3.57	3.57E-03	-2.45E+00	1.19E-01			1.58E+00
		290	7.96E-06	1.84E+02		1.97E+00	3.45	3.45E-03	-2.46E+00	2.94E-01		-8.46E+00	
		298	1.68E-05	2.22E+02	2.68E+00	2.68E+00	3.36	3.36E-03	-2.47E+00	4.29E-01		-3.75E+02	
		310	4.77E-05	2.92E+02		4.19E+00	3.23	3.23E-03	-2.49E+00	6.22E-01		-1.92E+01	
		320	1.07E-04	3.66E+02		5.98E+00	3.13	3.13E-03	-2.51E+00	7.77E-01		#N/A	
		330	2.30E-04	4.54E+02		8.42E+00	3.03	3.03E-03	-2.52E+00	9.26E-01		#N/A	
		340	4.72E-04	5.62E+02		1.17E+01	2.94	2.94E-03	-2.53E+00	1.07E+00	A		1.17E+01
		350	9.28E-04	6.91E+02		1.61E+01	2.86	2.86E-03	-2.54E+00	1.21E+00		5.64E-20	1.00
		375	4.30E-03	1.14E+03		3.40E+01	2.67	2.67E-03	-2.57E+00	1.53E+00	n		
		400	1.64E-02	1.82E+03		6.78E+01	2.50	2.50E-03	-2.60E+00	1.83E+00		8.46	
		425	5.37E-02	2.85E+03		1.29E+02	2.35	2.35E-03	-2.63E+00	2.11E+00	Ea		1.00
		450	1.54E-01	4.35E+03		2.34E+02	2.22	2.22E-03	-2.65E+00	2.37E+00		864	2.34E+02



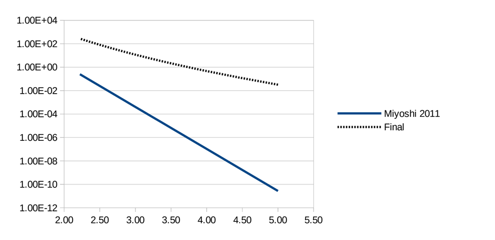
	P1		4.22E+07										
	P2		7.72E+03			Ea shift							
	P3					5.27E+02							
-CH2OO. | -CH2-	T		Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
		200	7.27E-10	1.60E+01		1.15E+00	5.00	5.00E-03	-2.30E+00	5.94E-02	A		6.75E-01
		225	5.30E-08	3.37E+01		3.24E+00	4.44	4.44E-03	-2.35E+00	5.10E-01		2.55E+05	0.59
		250	1.64E-06	6.72E+01		8.17E+00	4.00	4.00E-03	-2.40E+00	9.12E-01	Ea		
		260	5.37E-06	8.74E+01		1.15E+01	3.85	3.85E-03	-2.41E+00	1.06E+00		2.57E+03	
		270	1.61E-05	1.13E+02		1.60E+01	3.70	3.70E-03	-2.43E+00	1.20E+00			1.20
		280	4.48E-05	1.44E+02		2.20E+01	3.57	3.57E-03	-2.45E+00	1.34E+00			2.65E+01
		290	1.16E-04	1.84E+02		2.99E+01	3.45	3.45E-03	-2.46E+00	1.48E+00		-8.46E+00	
		298	2.37E-04	2.22E+02	3.79E+01	3.79E+01	3.36	3.36E-03	-2.47E+00	1.58E+00		-3.27E+01	
		310	6.46E-04	2.92E+02		5.34E+01	3.23	3.23E-03	-2.49E+00	1.73E+00		-1.92E+01	
		320	1.41E-03	3.66E+02		7.04E+01	3.13	3.13E-03	-2.51E+00	1.85E+00		#N/A	
		330	2.92E-03	4.54E+02		9.21E+01	3.03	3.03E-03	-2.52E+00	1.96E+00		#N/A	
		340	5.81E-03	5.62E+02		1.19E+02	2.94	2.94E-03	-2.53E+00	2.08E+00	A		1.19E+02
		350	1.11E-02	6.91E+02		1.53E+02	2.86	2.86E-03	-2.54E+00	2.19E+00		5.64E-20	1.00
		375	4.84E-02	1.14E+03		2.79E+02	2.67	2.67E-03	-2.57E+00	2.45E+00	n		
		400	1.75E-01	1.82E+03		4.88E+02	2.50	2.50E-03	-2.60E+00	2.69E+00		8.46	
		425	5.45E-01	2.85E+03		8.24E+02	2.35	2.35E-03	-2.63E+00	2.92E+00	Ea		1.00
		450	1.50E+00	4.35E+03		1.35E+03	2.22	2.22E-03	-2.65E+00	3.13E+00		75	1.35E+03



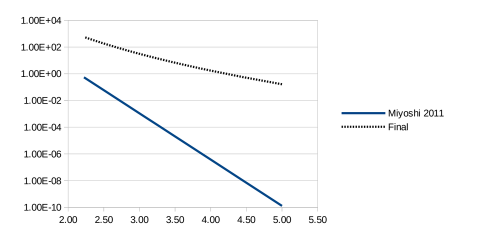
	P1		1.75E+07										
	P2		7.83E+03			Ea shift							
	P3					8.99E+02							
-CH2OO. | >CH-	T		Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
		200	1.74E-10	1.60E+01		1.78E-01	5.00	5.00E-03	-2.30E+00	-7.49E-01	A		1.05E-01
		225	1.35E-08	3.37E+01		6.19E-01	4.44	4.44E-03	-2.35E+00	-2.08E-01		2.55E+05	0.59
		250	4.37E-07	6.72E+01		1.84E+00	4.00	4.00E-03	-2.40E+00	2.65E-01	Ea		
		260	1.46E-06	8.74E+01		2.75E+00	3.85	3.85E-03	-2.41E+00	4.39E-01		2.94E+03	
		270	4.45E-06	1.13E+02		4.03E+00	3.70	3.70E-03	-2.43E+00	6.06E-01			1.20
		280	1.25E-05	1.44E+02		5.82E+00	3.57	3.57E-03	-2.45E+00	7.65E-01			7.01E+00
		290	3.29E-05	1.84E+02		8.28E+00	3.45	3.45E-03	-2.46E+00	9.18E-01		-8.46E+00	
		298	6.79E-05	2.22E+02	1.09E+01	1.09E+01	3.36	3.36E-03	-2.47E+00	1.04E+00		-1.94E+02	
		310	1.88E-04	2.92E+02		1.61E+01	3.23	3.23E-03	-2.49E+00	1.21E+00		-1.92E+01	
		320	4.13E-04	3.66E+02		2.20E+01	3.13	3.13E-03	-2.51E+00	1.34E+00		#N/A	
		330	8.68E-04	4.54E+02		2.98E+01	3.03	3.03E-03	-2.52E+00	1.47E+00		#N/A	
		340	1.74E-03	5.62E+02		3.99E+01	2.94	2.94E-03	-2.53E+00	1.60E+00	A		3.99E+01
		350	3.37E-03	6.91E+02		5.30E+01	2.86	2.86E-03	-2.54E+00	1.72E+00		5.64E-20	1.00
		375	1.50E-02	1.14E+03		1.03E+02	2.67	2.67E-03	-2.57E+00	2.01E+00	n		
		400	5.52E-02	1.82E+03		1.92E+02	2.50	2.50E-03	-2.60E+00	2.28E+00		8.46	
		425	1.75E-01	2.85E+03		3.43E+02	2.35	2.35E-03	-2.63E+00	2.54E+00	Ea		1.00
		450	4.86E-01	4.35E+03		5.90E+02	2.22	2.22E-03	-2.65E+00	2.77E+00		448	5.90E+02



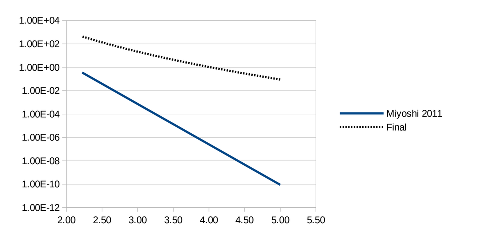
	P1		23400000										
	P2		8260			Ea shift							
	P3					1.24E+03							
>CHOO. | -CH3	T		Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
		200	2.71E-11	1.60E+01		3.20E-02	5.00	5.00E-03	-2.30E+00	-1.49E+00	A		1.88E-02
		225	2.67E-09	3.37E+01		1.35E-01	4.44	4.44E-03	-2.35E+00	-8.71E-01		2.55E+05	0.59
		250	1.05E-07	6.72E+01		4.66E-01	4.00	4.00E-03	-2.40E+00	-3.31E-01	Ea		
		260	3.73E-07	8.74E+01		7.34E-01	3.85	3.85E-03	-2.41E+00	-1.34E-01		3.28E+03	
		270	1.21E-06	1.13E+02		1.13E+00	3.70	3.70E-03	-2.43E+00	5.34E-02			1.20
		280	3.61E-06	1.44E+02		1.71E+00	3.57	3.57E-03	-2.45E+00	2.32E-01			2.06E+00
		290	9.98E-06	1.84E+02		2.53E+00	3.45	3.45E-03	-2.46E+00	4.04E-01		-8.46E+00	
		298	2.14E-05	2.22E+02	3.43E+00	3.43E+00	3.36	3.36E-03	-2.47E+00	5.36E-01		-3.43E+02	
		310	6.27E-05	2.92E+02		5.31E+00	3.23	3.23E-03	-2.49E+00	7.25E-01		-1.92E+01	
		320	1.44E-04	3.66E+02		7.53E+00	3.13	3.13E-03	-2.51E+00	8.77E-01		#N/A	
		330	3.15E-04	4.54E+02		1.05E+01	3.03	3.03E-03	-2.52E+00	1.02E+00		#N/A	
		340	6.58E-04	5.62E+02		1.45E+01	2.94	2.94E-03	-2.53E+00	1.16E+00	A		1.45E+01
		350	1.32E-03	6.91E+02		1.99E+01	2.86	2.86E-03	-2.54E+00	1.30E+00		5.64E-20	1.00
		375	6.36E-03	1.14E+03		4.14E+01	2.67	2.67E-03	-2.57E+00	1.62E+00	n		
		400	2.52E-02	1.82E+03		8.15E+01	2.50	2.50E-03	-2.60E+00	1.91E+00		8.46	
		425	8.48E-02	2.85E+03		1.53E+02	2.35	2.35E-03	-2.63E+00	2.18E+00	Ea		1.00
		450	2.50E-01	4.35E+03		2.75E+02	2.22	2.22E-03	-2.65E+00	2.44E+00		791	2.75E+02



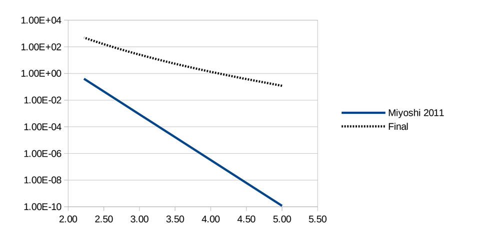
	P1		27400000										
	P2		7980			Ea shift							
	P3					9.16E+02							
>CHOO. | -CH2-	T		Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
		200	1.29E-10	1.60E+01		1.64E-01	5.00	5.00E-03	-2.30E+00	-7.85E-01	A		9.67E-02
		225	1.08E-08	3.37E+01		5.76E-01	4.44	4.44E-03	-2.35E+00	-2.40E-01		2.55E+05	0.59
		250	3.76E-07	6.72E+01		1.73E+00	4.00	4.00E-03	-2.40E+00	2.37E-01	Ea		
		260	1.28E-06	8.74E+01		2.58E+00	3.85	3.85E-03	-2.41E+00	4.12E-01		2.96E+03	
		270	4.00E-06	1.13E+02		3.80E+00	3.70	3.70E-03	-2.43E+00	5.79E-01			1.20
		280	1.15E-05	1.44E+02		5.49E+00	3.57	3.57E-03	-2.45E+00	7.40E-01			6.61E+00
		290	3.07E-05	1.84E+02		7.82E+00	3.45	3.45E-03	-2.46E+00	8.93E-01		-8.46E+00	
		298	6.43E-05	2.22E+02	1.03E+01	1.03E+01	3.36	3.36E-03	-2.47E+00	1.01E+00		-2.01E+02	
		310	1.81E-04	2.92E+02		1.53E+01	3.23	3.23E-03	-2.49E+00	1.18E+00		-1.92E+01	
		320	4.05E-04	3.66E+02		2.09E+01	3.13	3.13E-03	-2.51E+00	1.32E+00		#N/A	
		330	8.62E-04	4.54E+02		2.83E+01	3.03	3.03E-03	-2.52E+00	1.45E+00		#N/A	
		340	1.76E-03	5.62E+02		3.80E+01	2.94	2.94E-03	-2.53E+00	1.58E+00	A		3.80E+01
		350	3.43E-03	6.91E+02		5.05E+01	2.86	2.86E-03	-2.54E+00	1.70E+00		5.64E-20	1.00
		375	1.57E-02	1.14E+03		9.90E+01	2.67	2.67E-03	-2.57E+00	2.00E+00	n		
		400	5.94E-02	1.82E+03		1.85E+02	2.50	2.50E-03	-2.60E+00	2.27E+00		8.46	
		425	1.92E-01	2.85E+03		3.30E+02	2.35	2.35E-03	-2.63E+00	2.52E+00	Ea		1.00
		450	5.45E-01	4.35E+03		5.69E+02	2.22	2.22E-03	-2.65E+00	2.76E+00		464	5.69E+02



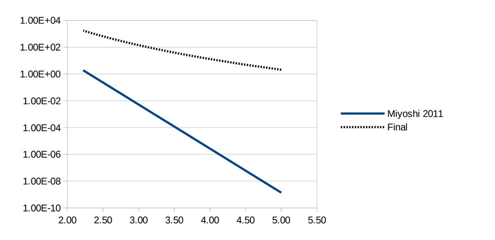
	P1		17000000										
	P2		7960			Ea shift							
	P3					1.04E+03							
>CHOO. | >CH-	T		Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
		200	8.82E-11	1.60E+01		8.91E-02	5.00	5.00E-03	-2.30E+00	-1.05E+00	A		5.25E-02
		225	7.35E-09	3.37E+01		3.34E-01	4.44	4.44E-03	-2.35E+00	-4.76E-01		2.55E+05	0.59
		250	2.53E-07	6.72E+01		1.06E+00	4.00	4.00E-03	-2.40E+00	2.45E-02	Ea		
		260	8.60E-07	8.74E+01		1.61E+00	3.85	3.85E-03	-2.41E+00	2.08E-01		3.08E+03	
		270	2.67E-06	1.13E+02		2.41E+00	3.70	3.70E-03	-2.43E+00	3.83E-01			1.20
		280	7.66E-06	1.44E+02		3.55E+00	3.57	3.57E-03	-2.45E+00	5.50E-01			4.27E+00
		290	2.04E-05	1.84E+02		5.13E+00	3.45	3.45E-03	-2.46E+00	7.10E-01		-8.46E+00	
		298	4.26E-05	2.22E+02	6.82E+00	6.82E+00	3.36	3.36E-03	-2.47E+00	8.34E-01		-2.55E+02	
		310	1.20E-04	2.92E+02		1.03E+01	3.23	3.23E-03	-2.49E+00	1.01E+00		-1.92E+01	
		320	2.68E-04	3.66E+02		1.43E+01	3.13	3.13E-03	-2.51E+00	1.15E+00		#N/A	
		330	5.69E-04	4.54E+02		1.96E+01	3.03	3.03E-03	-2.52E+00	1.29E+00		#N/A	
		340	1.16E-03	5.62E+02		2.65E+01	2.94	2.94E-03	-2.53E+00	1.42E+00	A		2.65E+01
		350	2.26E-03	6.91E+02		3.56E+01	2.86	2.86E-03	-2.54E+00	1.55E+00		5.64E-20	1.00
		375	1.03E-02	1.14E+03		7.14E+01	2.67	2.67E-03	-2.57E+00	1.85E+00	n		
		400	3.87E-02	1.82E+03		1.36E+02	2.50	2.50E-03	-2.60E+00	2.13E+00		8.46	
		425	1.25E-01	2.85E+03		2.48E+02	2.35	2.35E-03	-2.63E+00	2.39E+00	Ea		1.00
		450	3.53E-01	4.35E+03		4.34E+02	2.22	2.22E-03	-2.65E+00	2.64E+00		586	4.34E+02



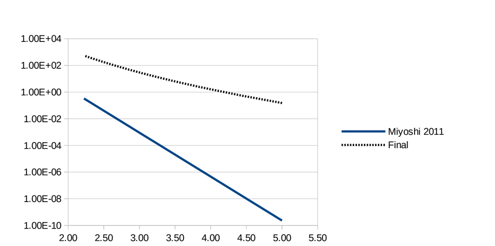
	P1		16900000										
	P2		7900			Ea shift							
	P3					9.80E+02							
>C(OO.)- | -CH3	T		Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
		200	1.18E-10	1.60E+01		1.19E-01	5.00	5.00E-03	-2.30E+00	-9.24E-01	A		7.02E-02
		225	9.54E-09	3.37E+01		4.33E-01	4.44	4.44E-03	-2.35E+00	-3.63E-01		2.55E+05	0.59
		250	3.19E-07	6.72E+01		1.34E+00	4.00	4.00E-03	-2.40E+00	1.26E-01	Ea		
		260	1.08E-06	8.74E+01		2.02E+00	3.85	3.85E-03	-2.41E+00	3.05E-01		3.02E+03	
		270	3.32E-06	1.13E+02		3.00E+00	3.70	3.70E-03	-2.43E+00	4.76E-01			1.20
		280	9.43E-06	1.44E+02		4.37E+00	3.57	3.57E-03	-2.45E+00	6.40E-01			5.26E+00
		290	2.50E-05	1.84E+02		6.27E+00	3.45	3.45E-03	-2.46E+00	7.98E-01		-8.46E+00	
		298	5.18E-05	2.22E+02	8.30E+00	8.30E+00	3.36	3.36E-03	-2.47E+00	9.19E-01		-2.29E+02	
		310	1.45E-04	2.92E+02		1.24E+01	3.23	3.23E-03	-2.49E+00	1.09E+00		-1.92E+01	
		320	3.21E-04	3.66E+02		1.71E+01	3.13	3.13E-03	-2.51E+00	1.23E+00		#N/A	
		330	6.78E-04	4.54E+02		2.33E+01	3.03	3.03E-03	-2.52E+00	1.37E+00		#N/A	
		340	1.37E-03	5.62E+02		3.15E+01	2.94	2.94E-03	-2.53E+00	1.50E+00	A		3.15E+01
		350	2.66E-03	6.91E+02		4.21E+01	2.86	2.86E-03	-2.54E+00	1.62E+00		5.64E-20	1.00
		375	1.20E-02	1.14E+03		8.35E+01	2.67	2.67E-03	-2.57E+00	1.92E+00	n		
		400	4.47E-02	1.82E+03		1.57E+02	2.50	2.50E-03	-2.60E+00	2.20E+00		8.46	
		425	1.43E-01	2.85E+03		2.84E+02	2.35	2.35E-03	-2.63E+00	2.45E+00	Ea		1.00
		450	4.01E-01	4.35E+03		4.94E+02	2.22	2.22E-03	-2.65E+00	2.69E+00		528	4.94E+02



	P1		39500000										
	P2		7580			Ea shift							
	P3					4.07E+02							
>C(OO.)- | -CH2-	T		Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
		200	1.37E-09	1.60E+01		2.09E+00	5.00	5.00E-03	-2.30E+00	3.21E-01	A		1.23E+00
		225	9.24E-08	3.37E+01		5.53E+00	4.44	4.44E-03	-2.35E+00	7.43E-01		2.55E+05	0.59
		250	2.68E-06	6.72E+01		1.32E+01	4.00	4.00E-03	-2.40E+00	1.12E+00	Ea		
		260	8.61E-06	8.74E+01		1.83E+01	3.85	3.85E-03	-2.41E+00	1.26E+00		2.45E+03	
		270	2.54E-05	1.13E+02		2.50E+01	3.70	3.70E-03	-2.43E+00	1.40E+00			1.20
		280	6.91E-05	1.44E+02		3.38E+01	3.57	3.57E-03	-2.45E+00	1.53E+00			4.07E+01
		290	1.76E-04	1.84E+02		4.53E+01	3.45	3.45E-03	-2.46E+00	1.66E+00		-8.46E+00	
		298	3.55E-04	2.22E+02	5.67E+01	5.67E+01	3.36	3.36E-03	-2.47E+00	1.75E+00		1.96E+01	
		310	9.49E-04	2.92E+02		7.88E+01	3.23	3.23E-03	-2.49E+00	1.90E+00		-1.92E+01	
		320	2.04E-03	3.66E+02		1.03E+02	3.13	3.13E-03	-2.51E+00	2.01E+00		#N/A	
		330	4.18E-03	4.54E+02		1.33E+02	3.03	3.03E-03	-2.52E+00	2.12E+00		#N/A	
		340	8.21E-03	5.62E+02		1.70E+02	2.94	2.94E-03	-2.53E+00	2.23E+00	A		1.70E+02
		350	1.55E-02	6.91E+02		2.16E+02	2.86	2.86E-03	-2.54E+00	2.34E+00		5.64E-20	1.00
		375	6.58E-02	1.14E+03		3.85E+02	2.67	2.67E-03	-2.57E+00	2.59E+00	n		
		400	2.33E-01	1.82E+03		6.59E+02	2.50	2.50E-03	-2.60E+00	2.82E+00		8.46	
		425	7.09E-01	2.85E+03		1.09E+03	2.35	2.35E-03	-2.63E+00	3.04E+00	Ea		1.00
		450	1.91E+00	4.35E+03		1.76E+03	2.22	2.22E-03	-2.65E+00	3.25E+00		-45	1.76E+03



	P1		7000000										
	P2		7590			Ea shift							
	P3					9.32E+02							
>C(OO.)- | >CH-	T		Miyoshi 2011	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
		200	2.31E-10	1.60E+01		1.51E-01	5.00	5.00E-03	-2.30E+00	-8.21E-01	A		8.90E-02
		225	1.57E-08	3.37E+01		5.35E-01	4.44	4.44E-03	-2.35E+00	-2.72E-01		2.55E+05	0.59
		250	4.57E-07	6.72E+01		1.61E+00	4.00	4.00E-03	-2.40E+00	2.08E-01	Ea		
		260	1.47E-06	8.74E+01		2.42E+00	3.85	3.85E-03	-2.41E+00	3.84E-01		2.97E+03	
		270	4.33E-06	1.13E+02		3.57E+00	3.70	3.70E-03	-2.43E+00	5.53E-01			1.20
		280	1.18E-05	1.44E+02		5.17E+00	3.57	3.57E-03	-2.45E+00	7.14E-01			6.23E+00
		290	3.01E-05	1.84E+02		7.39E+00	3.45	3.45E-03	-2.46E+00	8.68E-01		-8.46E+00	
		298	6.08E-05	2.22E+02	9.72E+00	9.72E+00	3.36	3.36E-03	-2.47E+00	9.88E-01		-2.09E+02	
		310	1.63E-04	2.92E+02		1.45E+01	3.23	3.23E-03	-2.49E+00	1.16E+00		-1.92E+01	
		320	3.50E-04	3.66E+02		1.98E+01	3.13	3.13E-03	-2.51E+00	1.30E+00		#N/A	
		330	7.18E-04	4.54E+02		2.70E+01	3.03	3.03E-03	-2.52E+00	1.43E+00		#N/A	
		340	1.41E-03	5.62E+02		3.62E+01	2.94	2.94E-03	-2.53E+00	1.56E+00	A		3.62E+01
		350	2.67E-03	6.91E+02		4.82E+01	2.86	2.86E-03	-2.54E+00	1.68E+00		5.64E-20	1.00
		375	1.13E-02	1.14E+03		9.47E+01	2.67	2.67E-03	-2.57E+00	1.98E+00	n		
		400	4.02E-02	1.82E+03		1.77E+02	2.50	2.50E-03	-2.60E+00	2.25E+00		8.46	
		425	1.23E-01	2.85E+03		3.17E+02	2.35	2.35E-03	-2.63E+00	2.50E+00	Ea		1.00
		450	3.31E-01	4.35E+03		5.48E+02	2.22	2.22E-03	-2.65E+00	2.74E+00		481	5.48E+02

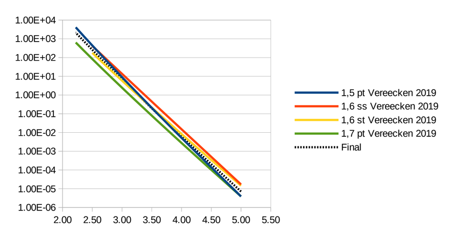


Plot O2QOH

RO2 migration of α-OH hydrogen atoms

1,4 Hshift

Average temperature dependence



Ea shift -1.21E+02

T	1,5 pt Vereec	1,6 ss Vereec (Different T)	1,6 st Vereec (Different T)	1,7 pt Vereecken 2019	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log()		log(T)	Replicate
200	3.89E-06	1.70E-05	1.46E-05	3.89E-06	3.89E-06		7.12E-06	5.00	5.00E-03	-2.30E+00	-5.15E+00	A		5.61E-06
225	2.06E-04	7.32E-04	4.85E-04	1.46E-04	1.74E-04		2.97E-04	4.44	4.44E-03	-2.35E+00	-3.53E+00		1.05E+10	0.79
250	5.18E-03	1.49E-02	8.30E-03	2.77E-03	3.79E-03		6.14E-03	4.00	4.00E-03	-2.40E+00	-2.21E+00	Ea		
260	1.60E-02	4.24E-02	2.24E-02	7.73E-03	1.11E-02		1.77E-02	3.85	3.85E-03	-2.41E+00	-1.75E+00		7.03E+03	
270	4.57E-02	1.12E-01	5.64E-02	2.01E-02	3.03E-02		4.75E-02	3.70	3.70E-03	-2.43E+00	-1.32E+00			1.09
280	1.22E-01	2.75E-01	1.34E-01	4.91E-02	7.73E-02		1.19E-01	3.57	3.57E-03	-2.45E+00	-9.24E-01			1.30E-01
290	3.05E-01	6.36E-01	2.99E-01	1.13E-01	1.86E-01		2.82E-01	3.45	3.45E-03	-2.46E+00	-5.50E-01		-3.81E+00	
298	6.10E-01	1.19E+00	5.51E-01	2.13E-01	3.60E-01	5.40E-01	5.40E-01	3.36	3.36E-03	-2.47E+00	-2.67E-01		-2.57E+03	
310	1.62E+00	2.90E+00	1.30E+00	5.18E-01	9.16E-01		1.35E+00	3.23	3.23E-03	-2.49E+00	1.32E-01		-1.09E+00	
320	3.48E+00	5.76E+00	2.54E+00	1.04E+00	1.90E+00		2.77E+00	3.13	3.13E-03	-2.51E+00	4.43E-01		#N/A	
330	7.16E+00	1.10E+01	4.79E+00	2.00E+00	3.78E+00		5.45E+00	3.03	3.03E-03	-2.52E+00	7.37E-01		#N/A	
340	1.42E+01	2.02E+01	8.73E+00	3.71E+00	7.25E+00		1.04E+01	2.94	2.94E-03	-2.53E+00	1.01E+00	A		1.04E+01
350	2.70E+01	3.59E+01	1.54E+01	6.68E+00	1.34E+01		1.90E+01	2.86	2.86E-03	-2.54E+00	1.28E+00		8.05E-02	1.00
375	1.19E+02	1.32E+02	5.64E+01	2.56E+01	5.52E+01		7.62E+01	2.67	2.67E-03	-2.57E+00	1.88E+00	n		
400	4.41E+02	4.15E+02	1.78E+02	8.43E+01	1.93E+02		2.61E+02	2.50	2.50E-03	-2.60E+00	2.42E+00		3.81	
425	1.42E+03			2.44E+02	5.90E+02		7.84E+02	2.35	2.35E-03	-2.63E+00	2.89E+00	Ea		1.00
450	4.09E+03			6.35E+02	1.61E+03		2.11E+03	2.22	2.22E-03	-2.65E+00	3.32E+00		5909	2.11E+03

P1
P2
P3

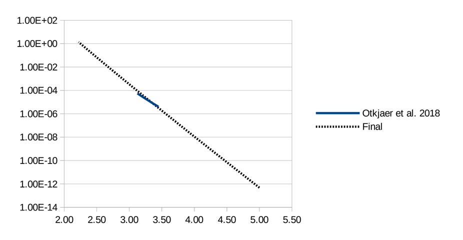
-CH2OO. | -CH2-

Ea shift 1.76E+03

T	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200	3.89E-06		5.85E-10	5.00	5.00E-03	-2.30E+00	-9.23E+00	A		4.61E-10
225	1.74E-04		6.94E-08	4.44	4.44E-03	-2.35E+00	-7.16E+00		1.05E+10	0.79
250	3.79E-03		3.31E-06	4.00	4.00E-03	-2.40E+00	-5.48E+00	Ea		
260	1.11E-02		1.27E-05	3.85	3.85E-03	-2.41E+00	-4.89E+00		8.91E+03	
270	3.03E-02		4.47E-05	3.70	3.70E-03	-2.43E+00	-4.35E+00			1.09
280	7.73E-02		1.44E-04	3.57	3.57E-03	-2.45E+00	-3.84E+00			1.56E-04
290	1.86E-01		4.29E-04	3.45	3.45E-03	-2.46E+00	-3.37E+00		-3.81E+00	
298	3.60E-01	9.79E-04	9.79E-04	3.36	3.36E-03	-2.47E+00	-3.01E+00		-3.38E+03	
310	9.16E-01		3.13E-03	3.23	3.23E-03	-2.49E+00	-2.50E+00		-1.09E+00	
320	1.90E+00		7.75E-03	3.13	3.13E-03	-2.51E+00	-2.11E+00		#N/A	
330	3.78E+00		1.82E-02	3.03	3.03E-03	-2.52E+00	-1.74E+00		#N/A	
340	7.25E+00		4.09E-02	2.94	2.94E-03	-2.53E+00	-1.39E+00	A		4.09E-02
350	1.34E+01		8.79E-02	2.86	2.86E-03	-2.54E+00	-1.06E+00		8.05E-02	1.00
375	5.52E+01		5.04E-01	2.67	2.67E-03	-2.57E+00	-2.97E-01	n		
400	1.93E+02		2.36E+00	2.50	2.50E-03	-2.60E+00	3.73E-01		3.81	
425	5.90E+02		9.36E+00	2.35	2.35E-03	-2.63E+00	9.71E-01	Ea		1.00
450	1.61E+03		3.22E+01	2.22	2.22E-03	-2.65E+00	1.51E+00		7790	3.22E+01

P0
P1 1.38E+12
P2 1.38E+04
P3 1.76E+08

-CH2OO. | >CH-

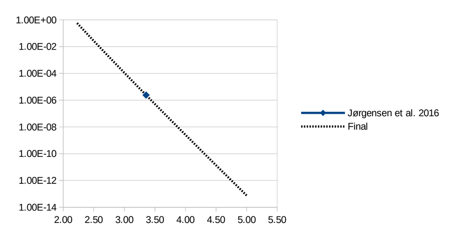


Ea shift 3.18E+03

T	Otkjaer et al. 2018	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200		3.89E-06		4.75E-13	5.00	5.00E-03	-2.30E+00	-1.23E+01	A		3.74E-13
225		1.74E-04		1.24E-10	4.44	4.44E-03	-2.35E+00	-9.91E+00		1.05E+10	0.79
250		3.79E-03		1.12E-08	4.00	4.00E-03	-2.40E+00	-7.95E+00	Ea		
260		1.11E-02		5.35E-08	3.85	3.85E-03	-2.41E+00	-7.27E+00		1.03E+04	
270		3.03E-02		2.29E-07	3.70	3.70E-03	-2.43E+00	-6.64E+00			1.09
280		7.73E-02		8.92E-07	3.57	3.57E-03	-2.45E+00	-6.05E+00			9.69E-07
290	4.05E-06	1.86E-01		3.17E-06	3.45	3.45E-03	-2.46E+00	-5.50E+00		-3.81E+00	
298	8.25E-06	3.60E-01	8.25E-06	8.25E-06	3.36	3.36E-03	-2.47E+00	-5.08E+00		-4.00E+03	
310	2.36E-05	9.16E-01		3.18E-05	3.23	3.23E-03	-2.49E+00	-4.50E+00		-1.09E+00	
320	5.54E-05	1.90E+00		9.07E-05	3.13	3.13E-03	-2.51E+00	-4.04E+00		#N/A	
330		3.78E+00		2.44E-04	3.03	3.03E-03	-2.52E+00	-3.61E+00		#N/A	
340		7.25E+00		6.22E-04	2.94	2.94E-03	-2.53E+00	-3.21E+00	A		6.22E-04
350		1.34E+01		1.51E-03	2.86	2.86E-03	-2.54E+00	-2.82E+00		8.05E-02	1.00
375		5.52E+01		1.13E-02	2.67	2.67E-03	-2.57E+00	-1.95E+00	n		
400		1.93E+02		6.73E-02	2.50	2.50E-03	-2.60E+00	-1.17E+00		3.81	
425		5.90E+02		3.29E-01	2.35	2.35E-03	-2.63E+00	-4.83E-01	Ea		1.00
450		1.61E+03		1.36E+00	2.22	2.22E-03	-2.65E+00	1.35E-01		9213	1.36E+00

P0
P1
P2
P3

>CHOO. | -CH2-

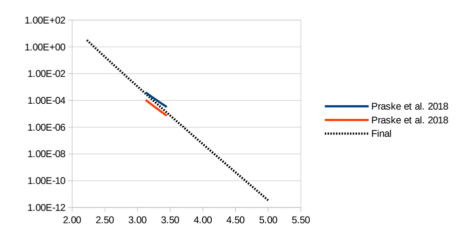


Ea shift 3.55E+03

T	Jørgensen et al. 2016	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200		3.89E-06		7.54E-14	5.00	5.00E-03	-2.30E+00	-1.31E+01	A		5.94E-14
225		1.74E-04		2.42E-11	4.44	4.44E-03	-2.35E+00	-1.06E+01		1.05E+10	0.79
250		3.79E-03		2.56E-09	4.00	4.00E-03	-2.40E+00	-8.59E+00	Ea		
260		1.11E-02		1.30E-08	3.85	3.85E-03	-2.41E+00	-7.89E+00		1.07E+04	
270		3.03E-02		5.87E-08	3.70	3.70E-03	-2.43E+00	-7.23E+00			1.09
280		7.73E-02		2.40E-07	3.57	3.57E-03	-2.45E+00	-6.62E+00			2.60E-07
290		1.86E-01		8.91E-07	3.45	3.45E-03	-2.46E+00	-6.05E+00		-3.81E+00	
298	2.40E-06	3.60E-01	2.40E-06	2.40E-06	3.36	3.36E-03	-2.47E+00	-5.62E+00		-4.16E+03	
310		9.16E-01		9.69E-06	3.23	3.23E-03	-2.49E+00	-5.01E+00		-1.09E+00	
320		1.90E+00		2.87E-05	3.13	3.13E-03	-2.51E+00	-4.54E+00		#N/A	
330		3.78E+00		8.00E-05	3.03	3.03E-03	-2.52E+00	-4.10E+00		#N/A	
340		7.25E+00		2.11E-04	2.94	2.94E-03	-2.53E+00	-3.68E+00	A		2.11E-04
350		1.34E+01		5.26E-04	2.86	2.86E-03	-2.54E+00	-3.28E+00		8.05E-02	1.00
375		5.52E+01		4.25E-03	2.67	2.67E-03	-2.57E+00	-2.37E+00	n		
400		1.93E+02		2.68E-02	2.50	2.50E-03	-2.60E+00	-1.57E+00		3.81	
425		5.90E+02		1.38E-01	2.35	2.35E-03	-2.63E+00	-8.59E-01	Ea		1.00
450		1.61E+03		6.02E-01	2.22	2.22E-03	-2.65E+00	-2.20E-01		9581	6.02E-01

P0		
P1	1.50E+12	1.75E+12
P2	13091	13488
P3	1.65E+08	1.58E+08

>CHOO. | >CH-



Ea shift 2.79E+03

T	Praske et al.	Praske et al. 2018	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200			3.89E-06		3.46E-12	5.00	5.00E-03	-2.30E+00	-1.15E+01	A		2.73E-12
225			1.74E-04		7.27E-10	4.44	4.44E-03	-2.35E+00	-9.14E+00		1.05E+10	0.79
250			3.79E-03		5.47E-08	4.00	4.00E-03	-2.40E+00	-7.26E+00	Ea		
260			1.11E-02		2.46E-07	3.85	3.85E-03	-2.41E+00	-6.61E+00		9.94E+03	
270			3.03E-02		9.99E-07	3.70	3.70E-03	-2.43E+00	-6.00E+00			1.09
280			7.73E-02		3.68E-06	3.57	3.57E-03	-2.45E+00	-5.43E+00			4.01E-06
290	3.24E-05	7.30E-06	1.86E-01		1.25E-05	3.45	3.45E-03	-2.46E+00	-4.90E+00		-3.81E+00	
298	6.41E-05	1.53E-05	3.60E-01	3.13E-05	3.13E-05	3.36	3.36E-03	-2.47E+00	-4.50E+00		-3.83E+03	
310	1.75E-04	4.52E-05	9.16E-01		1.14E-04	3.23	3.23E-03	-2.49E+00	-3.94E+00		-1.09E+00	
320	3.96E-04	1.09E-04	1.90E+00		3.14E-04	3.13	3.13E-03	-2.51E+00	-3.50E+00		#N/A	
330			3.78E+00		8.14E-04	3.03	3.03E-03	-2.52E+00	-3.09E+00		#N/A	
340			7.25E+00		2.00E-03	2.94	2.94E-03	-2.53E+00	-2.70E+00	A		2.00E-03
350			1.34E+01		4.69E-03	2.86	2.86E-03	-2.54E+00	-2.33E+00		8.05E-02	1.00
375			5.52E+01		3.27E-02	2.67	2.67E-03	-2.57E+00	-1.49E+00	n		
400			1.93E+02		1.82E-01	2.50	2.50E-03	-2.60E+00	-7.40E-01		3.81	
425			5.90E+02		8.38E-01	2.35	2.35E-03	-2.63E+00	-7.69E-02	Ea		1.00
450			1.61E+03		3.30E+00	2.22	2.22E-03	-2.65E+00	5.18E-01		8816	3.30E+00

P0
P1
P2
P3

>C(OO.)- | -CH2-

Ea shift 2.91E+03

T	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	3.89E-06		1.85E-12	5.00	5.00E-03	-2.30E+00	-1.17E+01	A		1.46E-12
225	1.74E-04		4.17E-10	4.44	4.44E-03	-2.35E+00	-9.38E+00		1.05E+10	0.79
250	3.79E-03		3.31E-08	4.00	4.00E-03	-2.40E+00	-7.48E+00	Ea		
260	1.11E-02		1.52E-07	3.85	3.85E-03	-2.41E+00	-6.82E+00		1.01E+04	
270	3.03E-02		6.28E-07	3.70	3.70E-03	-2.43E+00	-6.20E+00			1.09
280	7.73E-02		2.36E-06	3.57	3.57E-03	-2.45E+00	-5.63E+00			2.56E-06
290	1.86E-01		8.10E-06	3.45	3.45E-03	-2.46E+00	-5.09E+00		-3.81E+00	
298	3.60E-01	2.06E-05	2.06E-05	3.36	3.36E-03	-2.47E+00	-4.69E+00		-3.88E+03	
310	9.16E-01		7.64E-05	3.23	3.23E-03	-2.49E+00	-4.12E+00		-1.09E+00	
320	1.90E+00		2.12E-04	3.13	3.13E-03	-2.51E+00	-3.67E+00		#N/A	
330	3.78E+00		5.57E-04	3.03	3.03E-03	-2.52E+00	-3.25E+00		#N/A	
340	7.25E+00		1.38E-03	2.94	2.94E-03	-2.53E+00	-2.86E+00	A		1.38E-03
350	1.34E+01		3.28E-03	2.86	2.86E-03	-2.54E+00	-2.48E+00		8.05E-02	1.00
375	5.52E+01		2.34E-02	2.67	2.67E-03	-2.57E+00	-1.63E+00	n		
400	1.93E+02		1.33E-01	2.50	2.50E-03	-2.60E+00	-8.76E-01		3.81	
425	5.90E+02		6.24E-01	2.35	2.35E-03	-2.63E+00	-2.05E-01	Ea		1.00
450	1.61E+03		2.50E+00	2.22	2.22E-03	-2.65E+00	3.97E-01		8941	2.50E+00

P1
P2
P3

>C(OO.)- | >CH-

Ea shift 1.18E+03

T	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	3.89E-06		1.09E-08	5.00	5.00E-03	-2.30E+00	-7.96E+00	A		8.58E-09
225	1.74E-04		9.35E-07	4.44	4.44E-03	-2.35E+00	-6.03E+00		1.05E+10	0.79
250	3.79E-03		3.44E-05	4.00	4.00E-03	-2.40E+00	-4.46E+00	Ea		
260	1.11E-02		1.21E-04	3.85	3.85E-03	-2.41E+00	-3.92E+00		8.33E+03	
270	3.03E-02		3.90E-04	3.70	3.70E-03	-2.43E+00	-3.41E+00			1.09
280	7.73E-02		1.16E-03	3.57	3.57E-03	-2.45E+00	-2.94E+00			1.26E-03
290	1.86E-01		3.22E-03	3.45	3.45E-03	-2.46E+00	-2.49E+00		-3.81E+00	
298	3.60E-01	6.97E-03	6.97E-03	3.36	3.36E-03	-2.47E+00	-2.16E+00		-3.13E+03	
310	9.16E-01		2.07E-02	3.23	3.23E-03	-2.49E+00	-1.69E+00		-1.09E+00	
320	1.90E+00		4.82E-02	3.13	3.13E-03	-2.51E+00	-1.32E+00		#N/A	
330	3.78E+00		1.07E-01	3.03	3.03E-03	-2.52E+00	-9.70E-01		#N/A	
340	7.25E+00		2.28E-01	2.94	2.94E-03	-2.53E+00	-6.41E-01	A		2.28E-01
350	1.34E+01		4.67E-01	2.86	2.86E-03	-2.54E+00	-3.30E-01		8.05E-02	1.00
375	5.52E+01		2.40E+00	2.67	2.67E-03	-2.57E+00	3.80E-01	n		
400	1.93E+02		1.02E+01	2.50	2.50E-03	-2.60E+00	1.01E+00		3.81	
425	5.90E+02		3.71E+01	2.35	2.35E-03	-2.63E+00	1.57E+00	Ea		1.00
450	1.61E+03		1.18E+02	2.22	2.22E-03	-2.65E+00	2.07E+00		7205	1.18E+02

1,5 Hshift

P1
P2
P3

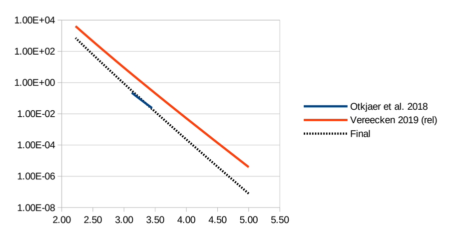
-CH2OO. | -CH2-

Ea shift 1.12E+03

T	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200	3.89E-06		1.44E-08	5.00	5.00E-03	-2.30E+00	-7.84E+00	A		1.13E-08
225	1.74E-04		1.20E-06	4.44	4.44E-03	-2.35E+00	-5.92E+00		1.05E+10	0.79
250	3.79E-03		4.29E-05	4.00	4.00E-03	-2.40E+00	-4.37E+00	Ea		
260	1.11E-02		1.50E-04	3.85	3.85E-03	-2.41E+00	-3.83E+00		8.27E+03	
270	3.03E-02		4.78E-04	3.70	3.70E-03	-2.43E+00	-3.32E+00			1.09
280	7.73E-02		1.41E-03	3.57	3.57E-03	-2.45E+00	-2.85E+00			1.54E-03
290	1.86E-01		3.90E-03	3.45	3.45E-03	-2.46E+00	-2.41E+00		-3.81E+00	
298	3.60E-01	8.39E-03	8.39E-03	3.36	3.36E-03	-2.47E+00	-2.08E+00		-3.11E+03	
310	9.16E-01		2.47E-02	3.23	3.23E-03	-2.49E+00	-1.61E+00		-1.09E+00	
320	1.90E+00		5.73E-02	3.13	3.13E-03	-2.51E+00	-1.24E+00		#N/A	
330	3.78E+00		1.27E-01	3.03	3.03E-03	-2.52E+00	-8.97E-01		#N/A	
340	7.25E+00		2.69E-01	2.94	2.94E-03	-2.53E+00	-5.71E-01	A		2.69E-01
350	1.34E+01		5.47E-01	2.86	2.86E-03	-2.54E+00	-2.62E-01		8.05E-02	1.00
375	5.52E+01		2.78E+00	2.67	2.67E-03	-2.57E+00	4.44E-01	n		
400	1.93E+02		1.17E+01	2.50	2.50E-03	-2.60E+00	1.07E+00		3.81	
425	5.90E+02		4.22E+01	2.35	2.35E-03	-2.63E+00	1.63E+00	Ea		1.00
450	1.61E+03		1.34E+02	2.22	2.22E-03	-2.65E+00	2.13E+00		7150	1.34E+02

P0		
P1	5.78E+11	5.54E-02
P2	1.01E+04	4.12E+00
P3	9.77E+07	6276.862412

-CH2OO. | >CH-



Ea shift 7.82E+02

T	Otkjaer et al.	Vereecken 2019 (rel)	average T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200		3.89E-06	3.89E-06		7.80E-08	5.00	5.00E-03	-2.30E+00	-7.11E+00	A		6.03E-08
225		2.06E-04	2.06E-04		6.39E-06	4.44	4.44E-03	-2.35E+00	-5.19E+00		5.53E+10	0.77
250		5.18E-03	5.18E-03		2.27E-04	4.00	4.00E-03	-2.40E+00	-3.64E+00	Ea		
260		1.60E-02	1.60E-02		7.92E-04	3.85	3.85E-03	-2.41E+00	-3.10E+00		8.27E+03	
270		4.57E-02	4.57E-02		2.53E-03	3.70	3.70E-03	-2.43E+00	-2.60E+00			1.09
280		1.22E-01	1.22E-01		7.47E-03	3.57	3.57E-03	-2.45E+00	-2.13E+00			8.17E-03
290	2.38E-02	3.05E-01	3.05E-01		2.06E-02	3.45	3.45E-03	-2.46E+00	-1.69E+00		-4.12E+00	
298	4.42E-02	6.10E-01	6.10E-01	4.42E-02	4.42E-02	3.36	3.36E-03	-2.47E+00	-1.35E+00		-3.07E+03	
310	1.09E-01	1.62E+00	1.62E+00		1.30E-01	3.23	3.23E-03	-2.49E+00	-8.85E-01		-1.26E+00	
320	2.24E-01	3.48E+00	3.48E+00		3.02E-01	3.13	3.13E-03	-2.51E+00	-5.19E-01		#N/A	
330		7.16E+00	7.16E+00		6.70E-01	3.03	3.03E-03	-2.52E+00	-1.74E-01		#N/A	
340		1.42E+01	1.42E+01		1.42E+00	2.94	2.94E-03	-2.53E+00	1.52E-01	A		1.42E+00
350		2.70E+01	2.70E+01		2.90E+00	2.86	2.86E-03	-2.54E+00	4.62E-01		5.54E-02	1.00
375		1.19E+02	1.19E+02		1.48E+01	2.67	2.67E-03	-2.57E+00	1.17E+00	n		
400		4.41E+02	4.41E+02		6.25E+01	2.50	2.50E-03	-2.60E+00	1.80E+00		4.12	
425		1.42E+03	1.42E+03		2.26E+02	2.35	2.35E-03	-2.63E+00	2.35E+00	Ea		1.00
450		4.09E+03	4.09E+03		7.21E+02	2.22	2.22E-03	-2.65E+00	2.86E+00		7059	7.21E+02

P0
P1
P2
P3

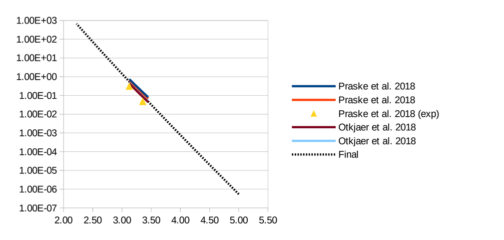
>CHOO. | -CH2-

Ea shift 9.96E+02

T	average T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200	3.89E-06		2.68E-08	5.00	5.00E-03	-2.30E+00	-7.57E+00	A		2.11E-08
225	1.74E-04		2.08E-06	4.44	4.44E-03	-2.35E+00	-5.68E+00		1.05E+10	0.79
250	3.79E-03		7.05E-05	4.00	4.00E-03	-2.40E+00	-4.15E+00	Ea		
260	1.11E-02		2.41E-04	3.85	3.85E-03	-2.41E+00	-3.62E+00		8.15E+03	
270	3.03E-02		7.58E-04	3.70	3.70E-03	-2.43E+00	-3.12E+00			1.09
280	7.73E-02		2.21E-03	3.57	3.57E-03	-2.45E+00	-2.66E+00			2.40E-03
290	1.86E-01		5.99E-03	3.45	3.45E-03	-2.46E+00	-2.22E+00		-3.81E+00	
298	3.60E-01	1.27E-02	1.27E-02	3.36	3.36E-03	-2.47E+00	-1.89E+00		-3.05E+03	
310	9.16E-01		3.69E-02	3.23	3.23E-03	-2.49E+00	-1.43E+00		-1.09E+00	
320	1.90E+00		8.45E-02	3.13	3.13E-03	-2.51E+00	-1.07E+00		#N/A	
330	3.78E+00		1.85E-01	3.03	3.03E-03	-2.52E+00	-7.33E-01		#N/A	
340	7.25E+00		3.88E-01	2.94	2.94E-03	-2.53E+00	-4.12E-01	A		3.88E-01
350	1.34E+01		7.81E-01	2.86	2.86E-03	-2.54E+00	-1.07E-01		8.05E-02	1.00
375	5.52E+01		3.87E+00	2.67	2.67E-03	-2.57E+00	5.88E-01	n		
400	1.93E+02		1.60E+01	2.50	2.50E-03	-2.60E+00	1.20E+00		3.81	
425	5.90E+02		5.66E+01	2.35	2.35E-03	-2.63E+00	1.75E+00	Ea		1.00
450	1.61E+03		1.76E+02	2.22	2.22E-03	-2.65E+00	2.25E+00		7026	1.76E+02

P1	5.02E+11	1.94E+12		1.02E+12	3.10E+11
P2	9517.1	10084		9.99E+03	9.49E+03
P3	8.19E+07	9.27E+07		8.99E+07	8.20E+07

>CHOO. | >CH-



Ea shift 3.96E+02

T	Praske et al.	Praske et al.	Praske et al.	Otkjaer et al.	Otkjaer et al. 2018	average T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200						3.89E-06		5.38E-07	5.00	5.00E-03	-2.30E+00	-6.27E+00	A		4.24E-07
225						1.74E-04		3.00E-05	4.44	4.44E-03	-2.35E+00	-4.52E+00		1.05E+10	0.79
250						3.79E-03		7.79E-04	4.00	4.00E-03	-2.40E+00	-3.11E+00	Ea		
260						1.11E-02		2.43E-03	3.85	3.85E-03	-2.41E+00	-2.61E+00		7.55E+03	
270						3.03E-02		7.01E-03	3.70	3.70E-03	-2.43E+00	-2.15E+00			1.09
280						7.73E-02		1.88E-02	3.57	3.57E-03	-2.45E+00	-1.73E+00			2.05E-02
290	8.08E-02	6.86E-02		4.45E-02	5.49E-02	1.86E-01		4.75E-02	3.45	3.45E-03	-2.46E+00	-1.32E+00		-3.81E+00	
298	1.50E-01	1.29E-01	4.80E-02	8.41E-02	1.02E-01	3.60E-01	9.55E-02	9.55E-02	3.36	3.36E-03	-2.47E+00	-1.02E+00		-2.79E+03	
310	3.65E-01	3.24E-01		2.11E-01	2.46E-01	9.16E-01		2.56E-01	3.23	3.23E-03	-2.49E+00	-5.92E-01		-1.09E+00	
320	7.42E-01	6.76E-01	3.10E-01	4.38E-01	5.00E-01	1.90E+00		5.52E-01	3.13	3.13E-03	-2.51E+00	-2.58E-01		#N/A	
330						3.78E+00		1.14E+00	3.03	3.03E-03	-2.52E+00	5.71E-02		#N/A	
340						7.25E+00		2.27E+00	2.94	2.94E-03	-2.53E+00	3.55E-01	A		2.27E+00
350						1.34E+01		4.34E+00	2.86	2.86E-03	-2.54E+00	6.38E-01		8.05E-02	1.00
375						5.52E+01		1.92E+01	2.67	2.67E-03	-2.57E+00	1.28E+00	n		
400						1.93E+02		7.17E+01	2.50	2.50E-03	-2.60E+00	1.86E+00		3.81	
425						5.90E+02		2.32E+02	2.35	2.35E-03	-2.63E+00	2.37E+00	Ea		1.00
450						1.61E+03		6.70E+02	2.22	2.22E-03	-2.65E+00	2.83E+00		6425	6.70E+02

P1
P2
P3

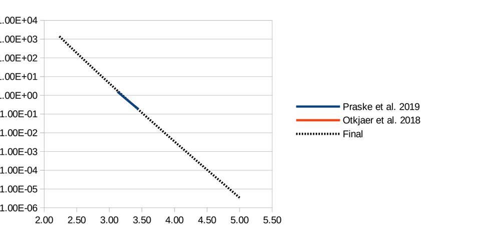
>C(OO.)- | -CH2-

Ea shift 1.30E+03

T	average T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	3.89E-06		5.96E-09	5.00	5.00E-03	-2.30E+00	-8.22E+00	A		4.69E-09
225	1.74E-04		5.47E-07	4.44	4.44E-03	-2.35E+00	-6.26E+00		1.05E+10	0.79
250	3.79E-03		2.12E-05	4.00	4.00E-03	-2.40E+00	-4.67E+00	Ea		
260	1.11E-02		7.60E-05	3.85	3.85E-03	-2.41E+00	-4.12E+00		8.45E+03	
270	3.03E-02		2.49E-04	3.70	3.70E-03	-2.43E+00	-3.60E+00			1.09
280	7.73E-02		7.55E-04	3.57	3.57E-03	-2.45E+00	-3.12E+00			8.21E-04
290	1.86E-01		2.13E-03	3.45	3.45E-03	-2.46E+00	-2.67E+00		-3.81E+00	
298	3.60E-01	4.65E-03	4.65E-03	3.36	3.36E-03	-2.47E+00	-2.33E+00		-3.18E+03	
310	9.16E-01		1.40E-02	3.23	3.23E-03	-2.49E+00	-1.85E+00		-1.09E+00	
320	1.90E+00		3.31E-02	3.13	3.13E-03	-2.51E+00	-1.48E+00		#N/A	
330	3.78E+00		7.44E-02	3.03	3.03E-03	-2.52E+00	-1.13E+00		#N/A	
340	7.25E+00		1.60E-01	2.94	2.94E-03	-2.53E+00	-7.95E-01	A		1.60E-01
350	1.34E+01		3.31E-01	2.86	2.86E-03	-2.54E+00	-4.80E-01		8.05E-02	1.00
375	5.52E+01		1.74E+00	2.67	2.67E-03	-2.57E+00	2.40E-01	n		
400	1.93E+02		7.54E+00	2.50	2.50E-03	-2.60E+00	8.78E-01		3.81	
425	5.90E+02		2.79E+01	2.35	2.35E-03	-2.63E+00	1.45E+00	Ea		1.00
450	1.61E+03		9.05E+01	2.22	2.22E-03	-2.65E+00	1.96E+00		7326	9.05E+01

P1	9.52E+11	9.52E+11
P2	9543.6	9.54E+03
P3	8.82E+07	8.82E+07

>C(OO.)- | >CH-



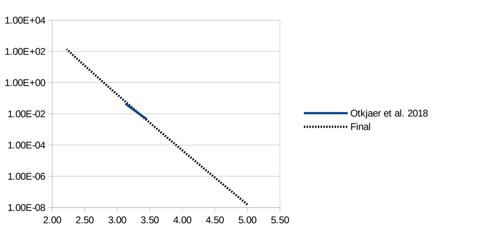
Ea shift 2.49E+01

T	Praske et al.	Otkjaer et al. 2018	average T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200			3.89E-06		3.44E-06	5.00	5.00E-03	-2.30E+00	-5.46E+00	A		2.71E-06
225			1.74E-04		1.56E-04	4.44	4.44E-03	-2.35E+00	-3.81E+00		1.05E+10	0.79
250			3.79E-03		3.43E-03	4.00	4.00E-03	-2.40E+00	-2.46E+00	Ea		
260			1.11E-02		1.01E-02	3.85	3.85E-03	-2.41E+00	-2.00E+00		7.18E+03	
270			3.03E-02		2.77E-02	3.70	3.70E-03	-2.43E+00	-1.56E+00			1.09
280			7.73E-02		7.08E-02	3.57	3.57E-03	-2.45E+00	-1.15E+00			7.69E-02
290	1.81E-01	1.83E-01	1.86E-01		1.70E-01	3.45	3.45E-03	-2.46E+00	-7.68E-01		-3.81E+00	
298	3.29E-01	3.33E-01	3.60E-01	3.31E-01	3.31E-01	3.36	3.36E-03	-2.47E+00	-4.80E-01		-2.63E+03	
310	7.84E-01	7.93E-01	9.16E-01		8.46E-01	3.23	3.23E-03	-2.49E+00	-7.28E-02		-1.09E+00	
320	1.57E+00	1.59E+00	1.90E+00		1.76E+00	3.13	3.13E-03	-2.51E+00	2.45E-01		#N/A	
330			3.78E+00		3.51E+00	3.03	3.03E-03	-2.52E+00	5.45E-01		#N/A	
340			7.25E+00		6.74E+00	2.94	2.94E-03	-2.53E+00	8.29E-01	A		6.74E+00
350			1.34E+01		1.25E+01	2.86	2.86E-03	-2.54E+00	1.10E+00		8.05E-02	1.00
375			5.52E+01		5.16E+01	2.67	2.67E-03	-2.57E+00	1.71E+00	n		
400			1.93E+02		1.81E+02	2.50	2.50E-03	-2.60E+00	2.26E+00		3.81	
425			5.90E+02		5.56E+02	2.35	2.35E-03	-2.63E+00	2.75E+00	Ea		1.00
450			1.61E+03		1.53E+03	2.22	2.22E-03	-2.65E+00	3.18E+00		6055	1.53E+03

1,6 Hshift

P1 4.80E+10
P2 9.71E+03
P3 8.63E+07

-CH2OO. | -CH2-

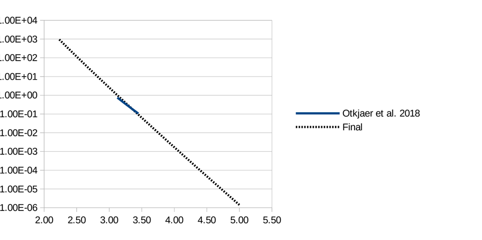


Ea shift 1.10E+03

T	Otkjaer et al. 2018	average T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200		3.89E-06		1.55E-08	5.00	5.00E-03	-2.30E+00	-7.81E+00	A		1.22E-08
225		1.74E-04		1.28E-06	4.44	4.44E-03	-2.35E+00	-5.89E+00		1.05E+10	0.79
250		3.79E-03		4.56E-05	4.00	4.00E-03	-2.40E+00	-4.34E+00	Ea		
260		1.11E-02		1.59E-04	3.85	3.85E-03	-2.41E+00	-3.80E+00		8.26E+03	
270		3.03E-02		5.07E-04	3.70	3.70E-03	-2.43E+00	-3.30E+00			1.09
280		7.73E-02		1.50E-03	3.57	3.57E-03	-2.45E+00	-2.83E+00			1.63E-03
290	4.75E-03	1.86E-01		4.12E-03	3.45	3.45E-03	-2.46E+00	-2.39E+00		-3.81E+00	
298	8.84E-03	3.60E-01	8.84E-03	8.84E-03	3.36	3.36E-03	-2.47E+00	-2.05E+00		-3.10E+03	
310	2.17E-02	9.16E-01		2.60E-02	3.23	3.23E-03	-2.49E+00	-1.59E+00		-1.09E+00	
320	4.44E-02	1.90E+00		6.02E-02	3.13	3.13E-03	-2.51E+00	-1.22E+00		#N/A	
330		3.78E+00		1.33E-01	3.03	3.03E-03	-2.52E+00	-8.76E-01		#N/A	
340		7.25E+00		2.81E-01	2.94	2.94E-03	-2.53E+00	-5.51E-01	A		2.81E-01
350		1.34E+01		5.72E-01	2.86	2.86E-03	-2.54E+00	-2.42E-01		8.05E-02	1.00
375		5.52E+01		2.90E+00	2.67	2.67E-03	-2.57E+00	4.62E-01	n		
400		1.93E+02		1.22E+01	2.50	2.50E-03	-2.60E+00	1.09E+00		3.81	
425		5.90E+02		4.38E+01	2.35	2.35E-03	-2.63E+00	1.64E+00	Ea		1.00
450		1.61E+03		1.38E+02	2.22	2.22E-03	-2.65E+00	2.14E+00		7134	1.38E+02

P1 3.23E+10
P2 8.60E+03
P3 7.83E+07

-CH2OO. | >CH-

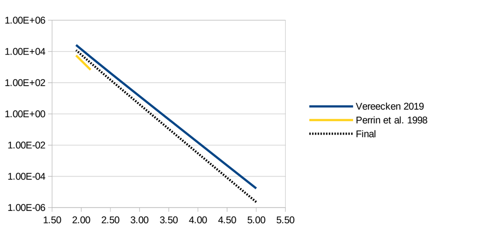


Ea shift 2.03E+02

T	Otkjaer et al. 2018	average T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200		3.89E-06		1.41E-06	5.00	5.00E-03	-2.30E+00	-5.85E+00	A		1.11E-06
225		1.74E-04		7.05E-05	4.44	4.44E-03	-2.35E+00	-4.15E+00		1.05E+10	0.79
250		3.79E-03		1.68E-03	4.00	4.00E-03	-2.40E+00	-2.77E+00	Ea		
260		1.11E-02		5.10E-03	3.85	3.85E-03	-2.41E+00	-2.29E+00		7.36E+03	
270		3.03E-02		1.43E-02	3.70	3.70E-03	-2.43E+00	-1.84E+00			1.09
280		7.73E-02		3.75E-02	3.57	3.57E-03	-2.45E+00	-1.43E+00			4.07E-02
290	1.06E-01	1.86E-01		9.23E-02	3.45	3.45E-03	-2.46E+00	-1.03E+00		-3.81E+00	
298	1.82E-01	3.60E-01	1.82E-01	1.82E-01	3.36	3.36E-03	-2.47E+00	-7.39E-01		-2.71E+03	
310	4.00E-01	9.16E-01		4.76E-01	3.23	3.23E-03	-2.49E+00	-3.22E-01		-1.09E+00	
320	7.50E-01	1.90E+00		1.01E+00	3.13	3.13E-03	-2.51E+00	3.31E-03		#N/A	
330		3.78E+00		2.04E+00	3.03	3.03E-03	-2.52E+00	3.11E-01		#N/A	
340		7.25E+00		3.99E+00	2.94	2.94E-03	-2.53E+00	6.01E-01	A		3.99E+00
350		1.34E+01		7.53E+00	2.86	2.86E-03	-2.54E+00	8.77E-01		8.05E-02	1.00
375		5.52E+01		3.21E+01	2.67	2.67E-03	-2.57E+00	1.51E+00	n		
400		1.93E+02		1.16E+02	2.50	2.50E-03	-2.60E+00	2.06E+00		3.81	
425		5.90E+02		3.66E+02	2.35	2.35E-03	-2.63E+00	2.56E+00	Ea		1.00
450		1.61E+03		1.03E+03	2.22	2.22E-03	-2.65E+00	3.01E+00		6233	1.03E+03

P1	3.54E+08	6.40E+10
P2	5.02E-01	1.69E+01
P3	6665.244042	

>CHOO. | -CH2-

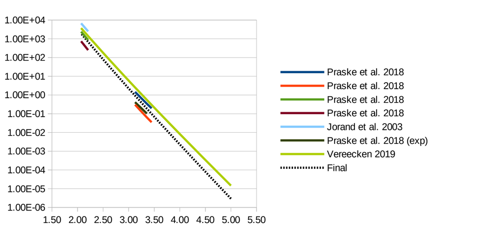


Ea shift 4.02E+02

T	Vereecken 20	Perrin et al. 1998	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200	1.70E-05		1.70E-05		2.27E-06	5.00	5.00E-03	-2.30E+00	-5.64E+00	A		2.15E-06
225	7.32E-04		7.32E-04		1.22E-04	4.44	4.44E-03	-2.35E+00	-3.91E+00		1.11E+10	0.94
250	1.49E-02		1.49E-02		2.99E-03	4.00	4.00E-03	-2.40E+00	-2.53E+00	Ea		
260	4.24E-02		4.24E-02		9.03E-03	3.85	3.85E-03	-2.41E+00	-2.04E+00		7.24E+03	
270	1.12E-01		1.12E-01		2.52E-02	3.70	3.70E-03	-2.43E+00	-1.60E+00			1.01
280	2.75E-01		2.75E-01		6.53E-02	3.57	3.57E-03	-2.45E+00	-1.18E+00			6.62E-02
290	6.36E-01		6.36E-01		1.59E-01	3.45	3.45E-03	-2.46E+00	-7.99E-01		-8.56E-01	
298	1.19E+00		1.19E+00		**3.10E-01**	3.36	3.36E-03	-2.47E+00	-5.09E-01		-3.03E+03	
310	2.90E+00		2.90E+00		7.91E-01	3.23	3.23E-03	-2.49E+00	-1.02E-01		7.53E+00	
320	5.76E+00		5.76E+00		1.64E+00	3.13	3.13E-03	-2.51E+00	2.15E-01		#N/A	
330	1.10E+01		1.10E+01		3.25E+00	3.03	3.03E-03	-2.52E+00	5.12E-01		#N/A	
340	2.02E+01		2.02E+01		6.19E+00	2.94	2.94E-03	-2.53E+00	7.92E-01	A		6.21E+00
350	3.59E+01		3.59E+01		1.14E+01	2.86	2.86E-03	-2.54E+00	1.06E+00		3.41E+07	1.00
375	1.32E+02		1.32E+02		4.53E+01	2.67	2.67E-03	-2.57E+00	1.66E+00	n		
400	4.15E+02		4.15E+02		1.52E+02	2.50	2.50E-03	-2.60E+00	2.18E+00		0.86	
463	4.45E+03	6.73E+02	4.45E+03		1.87E+03	2.16	2.16E-03	-2.67E+00	3.27E+00	Ea		0.98
523	2.58E+04	5.54E+03	2.58E+04	1.20E+04	1.20E+04	1.91	1.91E-03	-2.72E+00	4.08E+00		6972	1.17E+04

P1	9.10E+10	7.73E+10					2.51E-01
P2	8688	9144.2					3.42E+00
P3	7.55E+07	7.59E+07					5577.021247

>CHOO. | >CH-



Ea shift 3.20E+02

T	Praske et al.	Praske et al.	Praske et al.	Praske et al.	Jorand et al.	Praske et al.	Vereecken 2019	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200							1.46E-05	1.46E-05		2.95E-06	5.00	5.00E-03	-2.30E+00	-5.53E+00	A		2.31E-06
225							4.85E-04	4.85E-04		1.17E-04	4.44	4.44E-03	-2.35E+00	-3.93E+00		2.58E+09	0.78
250							8.30E-03	8.30E-03		2.31E-03	4.00	4.00E-03	-2.40E+00	-2.64E+00	Ea		
260							2.24E-02	2.24E-02		6.53E-03	3.85	3.85E-03	-2.41E+00	-2.18E+00		6.93E+03	
270							5.64E-02	5.64E-02		1.72E-02	3.70	3.70E-03	-2.43E+00	-1.76E+00			1.08
280							1.34E-01	1.34E-01		4.25E-02	3.57	3.57E-03	-2.45E+00	-1.37E+00			4.60E-02
290	1.96E-01	3.51E-02					2.99E-01	2.99E-01		9.92E-02	3.45	3.45E-03	-2.46E+00	-1.00E+00		-3.39E+00	
298	3.44E-01	6.42E-02				0.102761861	5.51E-01	5.51E-01	1.88E-01	1.88E-01	3.36	3.36E-03	-2.47E+00	-7.26E-01		-2.56E+03	
310	7.73E-01	1.53E-01					1.30E+00	1.30E+00		4.63E-01	3.23	3.23E-03	-2.49E+00	-3.35E-01		-5.19E-01	
320	1.47E+00	3.05E-01				0.414716771	2.54E+00	2.54E+00		9.35E-01	3.13	3.13E-03	-2.51E+00	-2.92E-02		#N/A	
330							4.79E+00	4.79E+00		1.82E+00	3.03	3.03E-03	-2.52E+00	2.59E-01		#N/A	
340							8.73E+00	8.73E+00		3.40E+00	2.94	2.94E-03	-2.53E+00	5.32E-01	A		3.40E+00
350							1.54E+01	1.54E+01		6.17E+00	2.86	2.86E-03	-2.54E+00	7.90E-01		3.03E-01	1.00
375							5.64E+01	5.64E+01		2.40E+01	2.67	2.67E-03	-2.57E+00	1.38E+00	n		
400							1.78E+02	1.78E+02		8.00E+01	2.50	2.50E-03	-2.60E+00	1.90E+00		3.39	
453			8.60E+02	2.50E+02	2.50E+03		1.39E+03	1.39E+03		6.87E+02	2.21	2.21E-03	-2.66E+00	2.84E+00	Ea		1.00
483			2.40E+03	7.40E+02	6.70E+03		3.71E+03	3.71E+03		1.91E+03	2.07	2.07E-03	-2.68E+00	3.28E+00		5905	1.92E+03

P1
P2
P3

>C(OO.)- | -CH2-

Ea shift 1.30E+03

T	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	3.89E-06		5.83E-09	5.00	5.00E-03	-2.30E+00	-8.23E+00	A		4.59E-09
225	1.74E-04		5.36E-07	4.44	4.44E-03	-2.35E+00	-6.27E+00		1.05E+10	0.79
250	3.79E-03		2.08E-05	4.00	4.00E-03	-2.40E+00	-4.68E+00	Ea		
260	1.11E-02		7.47E-05	3.85	3.85E-03	-2.41E+00	-4.13E+00		8.45E+03	
270	3.03E-02		2.45E-04	3.70	3.70E-03	-2.43E+00	-3.61E+00			1.09
280	7.73E-02		7.43E-04	3.57	3.57E-03	-2.45E+00	-3.13E+00			8.07E-04
290	1.86E-01		2.09E-03	3.45	3.45E-03	-2.46E+00	-2.68E+00		-3.81E+00	
298	3.60E-01	4.58E-03	4.58E-03	3.36	3.36E-03	-2.47E+00	-2.34E+00		-3.18E+03	
310	9.16E-01		1.38E-02	3.23	3.23E-03	-2.49E+00	-1.86E+00		-1.09E+00	
320	1.90E+00		3.26E-02	3.13	3.13E-03	-2.51E+00	-1.49E+00		#N/A	
330	3.78E+00		7.34E-02	3.03	3.03E-03	-2.52E+00	-1.13E+00		#N/A	
340	7.25E+00		1.58E-01	2.94	2.94E-03	-2.53E+00	-8.01E-01	A		1.58E-01
350	1.34E+01		3.27E-01	2.86	2.86E-03	-2.54E+00	-4.86E-01		8.05E-02	1.00
375	5.52E+01		1.72E+00	2.67	2.67E-03	-2.57E+00	2.35E-01	n		
400	1.93E+02		7.46E+00	2.50	2.50E-03	-2.60E+00	8.73E-01		3.81	
425	5.90E+02		2.76E+01	2.35	2.35E-03	-2.63E+00	1.44E+00	Ea		1.00
450	1.61E+03		8.96E+01	2.22	2.22E-03	-2.65E+00	1.95E+00		7330	8.96E+01

P1
P2
P3

>C(OO.)- | >CH-

Ea shift 5.13E-01

T	average T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	3.89E-06		3.88E-06	5.00	5.00E-03	-2.30E+00	-5.41E+00	A		3.06E-06
225	1.74E-04		1.73E-04	4.44	4.44E-03	-2.35E+00	-3.76E+00		1.05E+10	0.79
250	3.79E-03		3.78E-03	4.00	4.00E-03	-2.40E+00	-2.42E+00	Ea		
260	1.11E-02		1.11E-02	3.85	3.85E-03	-2.41E+00	-1.95E+00		7.15E+03	
270	3.03E-02		3.03E-02	3.70	3.70E-03	-2.43E+00	-1.52E+00			1.09
280	7.73E-02		7.72E-02	3.57	3.57E-03	-2.45E+00	-1.11E+00			8.39E-02
290	1.86E-01		1.85E-01	3.45	3.45E-03	-2.46E+00	-7.32E-01		-3.81E+00	
298	3.60E-01	3.60E-01	3.60E-01	3.36	3.36E-03	-2.47E+00	-4.44E-01		-2.62E+03	
310	9.16E-01		9.15E-01	3.23	3.23E-03	-2.49E+00	-3.87E-02		-1.09E+00	
320	1.90E+00		1.90E+00	3.13	3.13E-03	-2.51E+00	2.78E-01		#N/A	
330	3.78E+00		3.77E+00	3.03	3.03E-03	-2.52E+00	5.77E-01		#N/A	
340	7.25E+00		7.24E+00	2.94	2.94E-03	-2.53E+00	8.60E-01	A		7.24E+00
350	1.34E+01		1.34E+01	2.86	2.86E-03	-2.54E+00	1.13E+00		8.05E-02	1.00
375	5.52E+01		5.51E+01	2.67	2.67E-03	-2.57E+00	1.74E+00	n		
400	1.93E+02		1.92E+02	2.50	2.50E-03	-2.60E+00	2.28E+00		3.81	
425	5.90E+02		5.89E+02	2.35	2.35E-03	-2.63E+00	2.77E+00	Ea		1.00
450	1.61E+03		1.61E+03	2.22	2.22E-03	-2.65E+00	3.21E+00		6030	1.61E+03

1,7 Hshift

P1
P2
P3

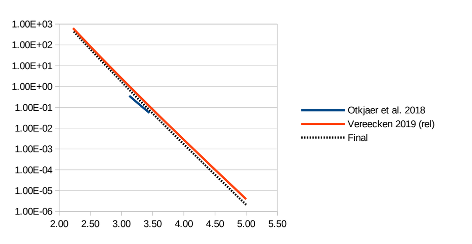
-CH2OO. | -CH2-

Ea shift 1.87E+03

T	average T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200	3.89E-06		3.44E-10	5.00	5.00E-03	-2.30E+00	-9.46E+00	A		2.71E-10
225	1.74E-04		4.33E-08	4.44	4.44E-03	-2.35E+00	-7.36E+00		1.05E+10	0.79
250	3.79E-03		2.17E-06	4.00	4.00E-03	-2.40E+00	-5.66E+00	Ea		
260	1.11E-02		8.48E-06	3.85	3.85E-03	-2.41E+00	-5.07E+00		9.02E+03	
270	3.03E-02		3.01E-05	3.70	3.70E-03	-2.43E+00	-4.52E+00			1.09
280	7.73E-02		9.84E-05	3.57	3.57E-03	-2.45E+00	-4.01E+00			1.07E-04
290	1.86E-01		2.98E-04	3.45	3.45E-03	-2.46E+00	-3.53E+00		-3.81E+00	
298	3.60E-01	6.86E-04	6.86E-04	3.36	3.36E-03	-2.47E+00	-3.16E+00		-3.43E+03	
310	9.16E-01		2.22E-03	3.23	3.23E-03	-2.49E+00	-2.65E+00		-1.09E+00	
320	1.90E+00		5.56E-03	3.13	3.13E-03	-2.51E+00	-2.25E+00		#N/A	
330	3.78E+00		1.32E-02	3.03	3.03E-03	-2.52E+00	-1.88E+00		#N/A	
340	7.25E+00		2.99E-02	2.94	2.94E-03	-2.53E+00	-1.52E+00	A		2.99E-02
350	1.34E+01		6.49E-02	2.86	2.86E-03	-2.54E+00	-1.19E+00		8.05E-02	1.00
375	5.52E+01		3.80E-01	2.67	2.67E-03	-2.57E+00	-4.20E-01	n		
400	1.93E+02		1.81E+00	2.50	2.50E-03	-2.60E+00	2.58E-01		3.81	
425	5.90E+02		7.29E+00	2.35	2.35E-03	-2.63E+00	8.63E-01	Ea		1.00
450	1.61E+03		2.55E+01	2.22	2.22E-03	-2.65E+00	1.41E+00		7896	2.55E+01

P1	5.09E+09	1.17E-01
P2	8.19E+03	3.51E+00
P3	7.28E+07	5782.474959

-CH2OO. | >CH-



Ea shift 1.24E+02

T	Otkjaer et al.	Vereecken 2019 (rel)	average T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |		log(T)	Replicate
200		3.89E-06	3.89E-06		2.09E-06	5.00	5.00E-03	-2.30E+00	-5.68E+00	A		1.68E-06
225		1.46E-04	1.46E-04		8.42E-05	4.44	4.44E-03	-2.35E+00	-4.07E+00		1.99E+09	0.80
250		2.77E-03	2.77E-03		1.68E-03	4.00	4.00E-03	-2.40E+00	-2.77E+00	Ea		
260		7.73E-03	7.73E-03		4.79E-03	3.85	3.85E-03	-2.41E+00	-2.32E+00		6.94E+03	
270		2.01E-02	2.01E-02		1.27E-02	3.70	3.70E-03	-2.43E+00	-1.90E+00			1.08
280		4.91E-02	4.91E-02		3.15E-02	3.57	3.57E-03	-2.45E+00	-1.50E+00			3.40E-02
290	5.47E-02	1.13E-01	1.13E-01		7.37E-02	3.45	3.45E-03	-2.46E+00	-1.13E+00		-3.51E+00	
298	9.24E-02	2.13E-01	2.13E-01	1.40E-01	1.40E-01	3.36	3.36E-03	-2.47E+00	-8.53E-01		-2.57E+03	
310	1.97E-01	5.18E-01	5.18E-01		3.47E-01	3.23	3.23E-03	-2.49E+00	-4.60E-01		-9.32E-01	
320	3.60E-01	1.04E+00	1.04E+00		7.03E-01	3.13	3.13E-03	-2.51E+00	-1.53E-01		#N/A	
330		2.00E+00	2.00E+00		1.37E+00	3.03	3.03E-03	-2.52E+00	1.37E-01		#N/A	
340		3.71E+00	3.71E+00		2.58E+00	2.94	2.94E-03	-2.53E+00	4.11E-01	A		2.58E+00
350		6.68E+00	6.68E+00		4.69E+00	2.86	2.86E-03	-2.54E+00	6.71E-01		1.17E-01	1.00
375		2.56E+01	2.56E+01		1.84E+01	2.67	2.67E-03	-2.57E+00	1.26E+00	n		
400		8.43E+01	8.43E+01		6.18E+01	2.50	2.50E-03	-2.60E+00	1.79E+00		3.51	
425		2.44E+02	2.44E+02		1.82E+02	2.35	2.35E-03	-2.63E+00	2.26E+00	Ea		1.00
450		6.35E+02	6.35E+02		4.82E+02	2.22	2.22E-03	-2.65E+00	2.68E+00		5907	4.82E+02

P1
P2
P3

>CHOO. | -CH2-

Ea shift 2.33E+03

T	average T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200	3.89E-06		3.43E-11	5.00	5.00E-03	-2.30E+00	-1.05E+01	A		2.70E-11
225	1.74E-04		5.58E-09	4.44	4.44E-03	-2.35E+00	-8.25E+00		1.05E+10	0.79
250	3.79E-03		3.42E-07	4.00	4.00E-03	-2.40E+00	-6.47E+00	Ea		
260	1.11E-02		1.44E-06	3.85	3.85E-03	-2.41E+00	-5.84E+00		9.48E+03	
270	3.03E-02		5.46E-06	3.70	3.70E-03	-2.43E+00	-5.26E+00			1.09
280	7.73E-02		1.90E-05	3.57	3.57E-03	-2.45E+00	-4.72E+00			2.06E-05
290	1.86E-01		6.07E-05	3.45	3.45E-03	-2.46E+00	-4.22E+00		-3.81E+00	
298	3.60E-01	1.46E-04	1.46E-04	3.36	3.36E-03	-2.47E+00	-3.84E+00		-3.63E+03	
310	9.16E-01		5.02E-04	3.23	3.23E-03	-2.49E+00	-3.30E+00		-1.09E+00	
320	1.90E+00		1.32E-03	3.13	3.13E-03	-2.51E+00	-2.88E+00		#N/A	
330	3.78E+00		3.27E-03	3.03	3.03E-03	-2.52E+00	-2.49E+00		#N/A	
340	7.25E+00		7.71E-03	2.94	2.94E-03	-2.53E+00	-2.11E+00	A		7.71E-03
350	1.34E+01		1.74E-02	2.86	2.86E-03	-2.54E+00	-1.76E+00		8.05E-02	1.00
375	5.52E+01		1.11E-01	2.67	2.67E-03	-2.57E+00	-9.54E-01	n		
400	1.93E+02		5.72E-01	2.50	2.50E-03	-2.60E+00	-2.42E-01		3.81	
425	5.90E+02		2.46E+00	2.35	2.35E-03	-2.63E+00	3.92E-01	Ea		1.00
450	1.61E+03		9.14E+00	2.22	2.22E-03	-2.65E+00	9.61E-01		8358	9.14E+00

P1
P2
P3

>CHOO. | >CH-

Ea shift 9.90E+02

T	average T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |		log(T)	Replicate
200	3.89E-06		2.76E-08	5.00	5.00E-03	-2.30E+00	-7.56E+00	A		2.18E-08
225	1.74E-04		2.14E-06	4.44	4.44E-03	-2.35E+00	-5.67E+00		1.05E+10	0.79
250	3.79E-03		7.23E-05	4.00	4.00E-03	-2.40E+00	-4.14E+00	Ea		
260	1.11E-02		2.47E-04	3.85	3.85E-03	-2.41E+00	-3.61E+00		8.14E+03	
270	3.03E-02		7.76E-04	3.70	3.70E-03	-2.43E+00	-3.11E+00			1.09
280	7.73E-02		2.26E-03	3.57	3.57E-03	-2.45E+00	-2.65E+00			2.45E-03
290	1.86E-01		6.12E-03	3.45	3.45E-03	-2.46E+00	-2.21E+00		-3.81E+00	
298	3.60E-01	1.30E-02	1.30E-02	3.36	3.36E-03	-2.47E+00	-1.89E+00		-3.05E+03	
310	9.16E-01		3.76E-02	3.23	3.23E-03	-2.49E+00	-1.42E+00		-1.09E+00	
320	1.90E+00		8.62E-02	3.13	3.13E-03	-2.51E+00	-1.06E+00		#N/A	
330	3.78E+00		1.88E-01	3.03	3.03E-03	-2.52E+00	-7.25E-01		#N/A	
340	7.25E+00		3.95E-01	2.94	2.94E-03	-2.53E+00	-4.04E-01	A		3.95E-01
350	1.34E+01		7.95E-01	2.86	2.86E-03	-2.54E+00	-9.94E-02		8.05E-02	1.00
375	5.52E+01		3.94E+00	2.67	2.67E-03	-2.57E+00	5.96E-01	n		
400	1.93E+02		1.62E+01	2.50	2.50E-03	-2.60E+00	1.21E+00		3.81	
425	5.90E+02		5.75E+01	2.35	2.35E-03	-2.63E+00	1.76E+00	Ea		1.00
450	1.61E+03		1.79E+02	2.22	2.22E-03	-2.65E+00	2.25E+00		7019	1.79E+02

P1
P2
P3

>C(OO.)- | -CH2-

Ea shift 2.77E+03

T	average T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	3.89E-06		3.68E-12	5.00	5.00E-03	-2.30E+00	-1.14E+01	A		2.90E-12
225	1.74E-04		7.68E-10	4.44	4.44E-03	-2.35E+00	-9.11E+00		1.05E+10	0.79
250	3.79E-03		5.75E-08	4.00	4.00E-03	-2.40E+00	-7.24E+00	Ea		
260	1.11E-02		2.59E-07	3.85	3.85E-03	-2.41E+00	-6.59E+00		9.93E+03	
270	3.03E-02		1.05E-06	3.70	3.70E-03	-2.43E+00	-5.98E+00			1.09
280	7.73E-02		3.85E-06	3.57	3.57E-03	-2.45E+00	-5.41E+00			4.19E-06
290	1.86E-01		1.30E-05	3.45	3.45E-03	-2.46E+00	-4.89E+00		-3.81E+00	
298	3.60E-01	3.26E-05	3.26E-05	3.36	3.36E-03	-2.47E+00	-4.49E+00		-3.82E+03	
310	9.16E-01		1.19E-04	3.23	3.23E-03	-2.49E+00	-3.92E+00		-1.09E+00	
320	1.90E+00		3.26E-04	3.13	3.13E-03	-2.51E+00	-3.49E+00		#N/A	
330	3.78E+00		8.45E-04	3.03	3.03E-03	-2.52E+00	-3.07E+00		#N/A	
340	7.25E+00		2.08E-03	2.94	2.94E-03	-2.53E+00	-2.68E+00	A		2.08E-03
350	1.34E+01		4.86E-03	2.86	2.86E-03	-2.54E+00	-2.31E+00		8.05E-02	1.00
375	5.52E+01		3.38E-02	2.67	2.67E-03	-2.57E+00	-1.47E+00	n		
400	1.93E+02		1.88E-01	2.50	2.50E-03	-2.60E+00	-7.27E-01		3.81	
425	5.90E+02		8.63E-01	2.35	2.35E-03	-2.63E+00	-6.42E-02	Ea		1.00
450	1.61E+03		3.39E+00	2.22	2.22E-03	-2.65E+00	5.30E-01		8804	3.39E+00

P1
P2
P3

>C(OO.)- | >CH-

Ea shift 1.49E+03

T	average T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |		log(T)	Replicate
200	3.89E-06		2.31E-09	5.00	5.00E-03	-2.30E+00	-8.64E+00	A		1.82E-09
225	1.74E-04		2.36E-07	4.44	4.44E-03	-2.35E+00	-6.63E+00		1.05E+10	0.79
250	3.79E-03		9.95E-06	4.00	4.00E-03	-2.40E+00	-5.00E+00	Ea		
260	1.11E-02		3.67E-05	3.85	3.85E-03	-2.41E+00	-4.44E+00		8.64E+03	
270	3.03E-02		1.24E-04	3.70	3.70E-03	-2.43E+00	-3.91E+00			1.09
280	7.73E-02		3.84E-04	3.57	3.57E-03	-2.45E+00	-3.42E+00			4.17E-04
290	1.86E-01		1.11E-03	3.45	3.45E-03	-2.46E+00	-2.96E+00		-3.81E+00	
298	3.60E-01	2.46E-03	2.46E-03	3.36	3.36E-03	-2.47E+00	-2.61E+00		-3.26E+03	
310	9.16E-01		7.60E-03	3.23	3.23E-03	-2.49E+00	-2.12E+00		-1.09E+00	
320	1.90E+00		1.83E-02	3.13	3.13E-03	-2.51E+00	-1.74E+00		#N/A	
330	3.78E+00		4.19E-02	3.03	3.03E-03	-2.52E+00	-1.38E+00		#N/A	
340	7.25E+00		9.18E-02	2.94	2.94E-03	-2.53E+00	-1.04E+00	A		9.18E-02
350	1.34E+01		1.93E-01	2.86	2.86E-03	-2.54E+00	-7.15E-01		8.05E-02	1.00
375	5.52E+01		1.05E+00	2.67	2.67E-03	-2.57E+00	2.11E-02	n		
400	1.93E+02		4.70E+00	2.50	2.50E-03	-2.60E+00	6.72E-01		3.81	
425	5.90E+02		1.79E+01	2.35	2.35E-03	-2.63E+00	1.25E+00	Ea		1.00
450	1.61E+03		5.94E+01	2.22	2.22E-03	-2.65E+00	1.77E+00		7515	5.94E+01

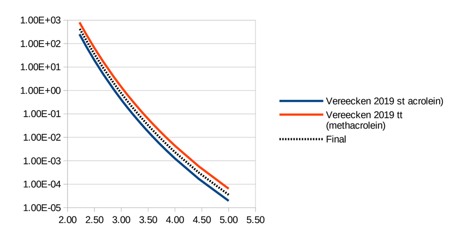
RO2 migration of aldehydic hydrogen atoms

1,4 Hshift

Average temperature dependence

Ea shift 0.00E+00

T	Vereecken 20	Vereecken 2019 tt (methacrolein)	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log()	log(T)	Replicate
200	1.94E-05	6.39E-05	3.52E-05		3.52E-05	5.00	5.00E-03	-2.30E+00	-4.45E+00	A	7.49E-06
225	1.68E-04	5.74E-04	3.10E-04		3.10E-04	4.44	4.44E-03	-2.35E+00	-3.51E+00	6.57E+07	0.21
250	1.25E-03	4.35E-03	2.33E-03		2.33E-03	4.00	4.00E-03	-2.40E+00	-2.63E+00	Ea	
260	2.67E-03	9.37E-03	5.00E-03		5.00E-03	3.85	3.85E-03	-2.41E+00	-2.30E+00	5.96E+03	
270	5.62E-03	1.98E-02	1.05E-02		1.05E-02	3.70	3.70E-03	-2.43E+00	-1.98E+00		1.72
280	1.16E-02	4.08E-02	2.17E-02		2.17E-02	3.57	3.57E-03	-2.45E+00	-1.66E+00		3.74E-02
290	2.34E-02	8.24E-02	4.39E-02		4.39E-02	3.45	3.45E-03	-2.46E+00	-1.36E+00	-2.47E+01	
298	4.06E-02	1.43E-01	7.62E-02	7.62E-02	7.62E-02	3.36	3.36E-03	-2.47E+00	-1.12E+00	5.78E+02	
310	9.09E-02	3.19E-01	1.70E-01		1.70E-01	3.23	3.23E-03	-2.49E+00	-7.69E-01	-6.43E+01	
320	1.75E-01	6.10E-01	3.26E-01		3.26E-01	3.13	3.13E-03	-2.51E+00	-4.86E-01	#N/A	
330	3.30E-01	1.15E+00	6.16E-01		6.16E-01	3.03	3.03E-03	-2.52E+00	-2.10E-01	#N/A	
340	6.15E-01	2.13E+00	1.15E+00		1.15E+00	2.94	2.94E-03	-2.53E+00	5.90E-02	A	1.15E+00
350	1.13E+00	3.90E+00	2.10E+00		2.10E+00	2.86	2.86E-03	-2.54E+00	3.22E-01	5.24E-65	1.00
375	4.87E+00	1.66E+01	8.98E+00		8.98E+00	2.67	2.67E-03	-2.57E+00	9.53E-01	n	
400	1.94E+01	6.49E+01	3.55E+01		3.55E+01	2.50	2.50E-03	-2.60E+00	1.55E+00	24.74	
425	7.23E+01	2.37E+02	1.31E+02		1.31E+02	2.35	2.35E-03	-2.63E+00	2.12E+00	Ea	1.00
450	2.52E+02	8.11E+02	4.52E+02		4.52E+02	2.22	2.22E-03	-2.65E+00	2.66E+00	-1331	4.52E+02



P1
P2
P3

Ea shift -1.05E+03

-CH2OO. | >CH-

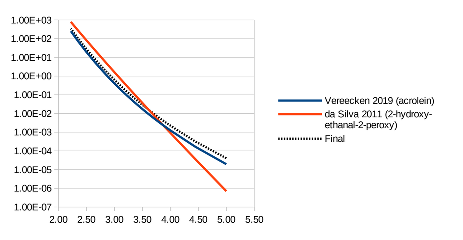
T	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |	log(T)	Replicate
200	3.52E-05		6.64E-03	5.00	5.00E-03	-2.30E+00	-2.18E+00	A	1.41E-03
225	3.10E-04		3.27E-02	4.44	4.44E-03	-2.35E+00	-1.49E+00	6.57E+07	0.21
250	2.33E-03		1.54E-01	4.00	4.00E-03	-2.40E+00	-8.13E-01	Ea	
260	5.00E-03		2.82E-01	3.85	3.85E-03	-2.41E+00	-5.50E-01	4.91E+03	
270	1.05E-02		5.11E-01	3.70	3.70E-03	-2.43E+00	-2.92E-01		1.72
280	2.17E-02		9.17E-01	3.57	3.57E-03	-2.45E+00	-3.78E-02		1.58E+00
290	4.39E-02		1.63E+00	3.45	3.45E-03	-2.46E+00	2.12E-01	-2.47E+01	
298	7.62E-02	2.56E+00	2.56E+00	3.36	3.36E-03	-2.47E+00	4.09E-01	1.03E+03	
310	1.70E-01		5.00E+00	3.23	3.23E-03	-2.49E+00	6.99E-01	-6.43E+01	
320	3.26E-01		8.63E+00	3.13	3.13E-03	-2.51E+00	9.36E-01	#N/A	
330	6.16E-01		1.47E+01	3.03	3.03E-03	-2.52E+00	1.17E+00	#N/A	
340	1.15E+00		2.50E+01	2.94	2.94E-03	-2.53E+00	1.40E+00	A	2.50E+01
350	2.10E+00		4.19E+01	2.86	2.86E-03	-2.54E+00	1.62E+00	5.24E-65	1.00
375	8.98E+00		1.47E+02	2.67	2.67E-03	-2.57E+00	2.17E+00	n	
400	3.55E+01		4.88E+02	2.50	2.50E-03	-2.60E+00	2.69E+00	24.74	
425	1.31E+02		1.54E+03	2.35	2.35E-03	-2.63E+00	3.19E+00	Ea	1.00
450	4.52E+02		4.64E+03	2.22	2.22E-03	-2.65E+00	3.67E+00	-2379	4.64E+03

P1 1.08E-66 1.26E-04
P2 2.52E+01 4.782
P3 -1469.76604 6104.680423

Ea shift -1.46E+02

>CHOO. | >CH-

T	Vereecken 20	da Silva 2011 (2-hydroxy-ethanal-2-peroxy)	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |	log(T)	Replicate
200	1.94E-05	7.04E-07	1.94E-05		4.04E-05	5.00	5.00E-03	-2.30E+00	-4.39E+00	A	8.32E-06
225	1.68E-04	3.68E-05	1.68E-04		3.21E-04	4.44	4.44E-03	-2.35E+00	-3.49E+00	3.61E+07	0.21
250	1.25E-03	9.17E-04	1.25E-03		2.24E-03	4.00	4.00E-03	-2.40E+00	-2.65E+00	Ea	
260	2.67E-03	2.83E-03	2.67E-03		4.69E-03	3.85	3.85E-03	-2.41E+00	-2.33E+00	5.82E+03	
270	5.62E-03	8.09E-03	5.62E-03		9.66E-03	3.70	3.70E-03	-2.43E+00	-2.02E+00		1.74
280	1.16E-02	2.16E-02	1.16E-02		1.95E-02	3.57	3.57E-03	-2.45E+00	-1.71E+00		3.39E-02
290	2.34E-02	5.41E-02	2.34E-02		3.88E-02	3.45	3.45E-03	-2.46E+00	-1.41E+00	-2.52E+01	
298	4.06E-02	1.08E-01	4.06E-02	6.64E-02	6.64E-02	3.36	3.36E-03	-2.47E+00	-1.18E+00	7.02E+02	
310	9.09E-02	2.90E-01	9.09E-02		1.46E-01	3.23	3.23E-03	-2.49E+00	-8.36E-01	-6.60E+01	
320	1.75E-01	6.24E-01	1.75E-01		2.76E-01	3.13	3.13E-03	-2.51E+00	-5.59E-01	#N/A	
330	3.30E-01	1.29E+00	3.30E-01		5.15E-01	3.03	3.03E-03	-2.52E+00	-2.89E-01	#N/A	
340	6.15E-01	2.56E+00	6.15E-01		9.46E-01	2.94	2.94E-03	-2.53E+00	-2.40E-02	A	9.46E-01
350	1.13E+00	4.91E+00	1.13E+00		1.72E+00	2.86	2.86E-03	-2.54E+00	2.35E-01	1.08E-66	1.00
375	4.87E+00	2.18E+01	4.87E+00		7.20E+00	2.67	2.67E-03	-2.57E+00	8.57E-01	n	
400	1.94E+01	8.23E+01	1.94E+01		2.80E+01	2.50	2.50E-03	-2.60E+00	1.45E+00	25.23	
425	7.23E+01	2.70E+02	7.23E+01		1.02E+02	2.35	2.35E-03	-2.63E+00	2.01E+00	Ea	1.00
450	2.52E+02	7.88E+02	2.52E+02		3.49E+02	2.22	2.22E-03	-2.65E+00	2.54E+00	-1616	3.49E+02

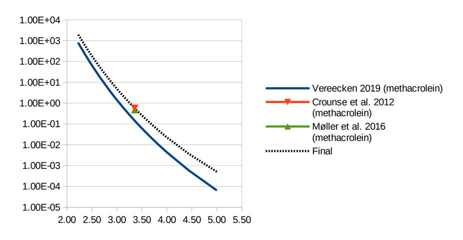


P1 2.54E-63
P2 2.43E+01
P3 -1192.62405

Ea shift -4.12E+02

>C(OO.)- | >CH-

T	Vereecken 20	Crounse et al.	Møller et al. 2016 (methacrolein)	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |	log(T)	Replicate
200	6.39E-05			6.39E-05		5.03E-04	5.00	5.00E-03	-2.30E+00	-3.30E+00	A	1.10E-04
225	5.74E-04			5.74E-04		3.59E-03	4.44	4.44E-03	-2.35E+00	-2.45E+00	1.19E+08	0.22
250	4.35E-03			4.35E-03		2.26E-02	4.00	4.00E-03	-2.40E+00	-1.65E+00	Ea	
260	9.37E-03			9.37E-03		4.58E-02	3.85	3.85E-03	-2.41E+00	-1.34E+00	5.54E+03	
270	1.98E-02			1.98E-02		9.10E-02	3.70	3.70E-03	-2.43E+00	-1.04E+00		1.70
280	4.08E-02			4.08E-02		1.78E-01	3.57	3.57E-03	-2.45E+00	-7.50E-01		3.03E-01
290	8.24E-02			8.24E-02		3.42E-01	3.45	3.45E-03	-2.46E+00	-4.66E-01	-2.43E+01	
298	1.43E-01	5.70E-01	4.80E-01	1.43E-01	5.70E-01	5.70E-01	3.36	3.36E-03	-2.47E+00	-2.44E-01	6.97E+02	
310	3.19E-01			3.19E-01		1.21E+00	3.23	3.23E-03	-2.49E+00	8.12E-02	-6.26E+01	
320	6.10E-01			6.10E-01		2.21E+00	3.13	3.13E-03	-2.51E+00	3.45E-01	#N/A	
330	1.15E+00			1.15E+00		4.01E+00	3.03	3.03E-03	-2.52E+00	6.03E-01	#N/A	
340	2.13E+00			2.13E+00		7.17E+00	2.94	2.94E-03	-2.53E+00	8.56E-01	A	7.17E+00
350	3.90E+00			3.90E+00		1.27E+01	2.86	2.86E-03	-2.54E+00	1.10E+00	2.54E-63	1.00
375	1.66E+01			1.66E+01		4.97E+01	2.67	2.67E-03	-2.57E+00	1.70E+00	n	
400	6.49E+01			6.49E+01		1.82E+02	2.50	2.50E-03	-2.60E+00	2.26E+00	24.25	
425	2.37E+02			2.37E+02		6.26E+02	2.35	2.35E-03	-2.63E+00	2.80E+00	Ea	1.00
450	8.11E+02			8.11E+02		2.03E+03	2.22	2.22E-03	-2.65E+00	3.31E+00	-1605	2.03E+03

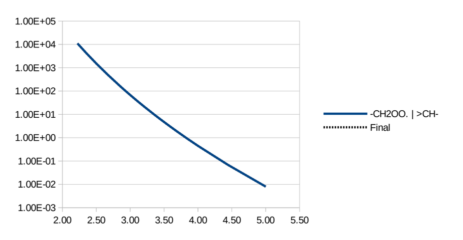


1,5 Hshift

Average temperature dependence

Ea shift 0.00E+00

T	-CH2OO. | >CH-	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log()	log(T)	Replicate
200	8.02E-03	8.02E-03		8.02E-03	5.00	5.00E-03	-2.30E+00	-2.10E+00	A	3.05E-03
225	6.81E-02	6.81E-02		6.81E-02	4.44	4.44E-03	-2.35E+00	-1.17E+00	4.21E+08	0.38
250	4.48E-01	4.48E-01		4.48E-01	4.00	4.00E-03	-2.40E+00	-3.48E-01	Ea	
260	8.98E-01	8.98E-01		8.98E-01	3.85	3.85E-03	-2.41E+00	-4.66E-02	5.13E+03	
270	1.75E+00	1.75E+00		1.75E+00	3.70	3.70E-03	-2.43E+00	2.42E-01		1.40
280	3.31E+00	3.31E+00		3.31E+00	3.57	3.57E-03	-2.45E+00	5.20E-01		4.64E+00
290	6.11E+00	6.11E+00		6.11E+00	3.45	3.45E-03	-2.46E+00	7.86E-01	-1.55E+01	
298	9.81E+00	9.81E+00	9.81E+00	9.81E+00	3.36	3.36E-03	-2.47E+00	9.92E-01	-2.49E+02	
310	1.95E+01	1.95E+01		1.95E+01	3.23	3.23E-03	-2.49E+00	1.29E+00	-3.64E+01	
320	3.37E+01	3.37E+01		3.37E+01	3.13	3.13E-03	-2.51E+00	1.53E+00	#N/A	
330	5.72E+01	5.72E+01		5.72E+01	3.03	3.03E-03	-2.52E+00	1.76E+00	#N/A	
340	9.56E+01	9.56E+01		9.56E+01	2.94	2.94E-03	-2.53E+00	1.98E+00	A	9.56E+01
350	1.57E+02	1.57E+02		1.57E+02	2.86	2.86E-03	-2.54E+00	2.20E+00	3.66E-37	1.00
375	5.09E+02	5.09E+02		5.09E+02	2.67	2.67E-03	-2.57E+00	2.71E+00	n	
400	1.52E+03	1.52E+03		1.52E+03	2.50	2.50E-03	-2.60E+00	3.18E+00	15.46	
425	4.22E+03	4.22E+03		4.22E+03	2.35	2.35E-03	-2.63E+00	3.63E+00	Ea	1.00
450	1.10E+04	1.10E+04		1.10E+04	2.22	2.22E-03	-2.65E+00	4.04E+00	573	1.10E+04

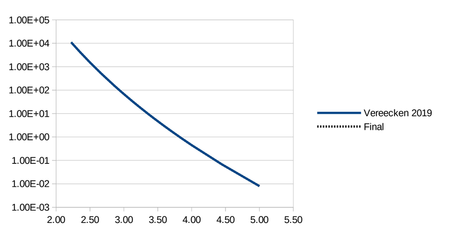


P1 3.66E-37
P2 1.55E+01
P3 5.73E+02

Ea shift 0.00E+00

-CH2OO. | >CH-

T	Vereecken 2019	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |	log(T)	Replicate
200	8.02E-03	8.02E-03		8.02E-03	5.00	5.00E-03	-2.30E+00	-2.10E+00	A	3.05E-03
225	6.81E-02	6.81E-02		6.81E-02	4.44	4.44E-03	-2.35E+00	-1.17E+00	4.21E+08	0.38
250	4.48E-01	4.48E-01		4.48E-01	4.00	4.00E-03	-2.40E+00	-3.48E-01	Ea	
260	8.98E-01	8.98E-01		8.98E-01	3.85	3.85E-03	-2.41E+00	-4.66E-02	5.13E+03	
270	1.75E+00	1.75E+00		1.75E+00	3.70	3.70E-03	-2.43E+00	2.42E-01		1.40
280	3.31E+00	3.31E+00		3.31E+00	3.57	3.57E-03	-2.45E+00	5.20E-01		4.64E+00
290	6.11E+00	6.11E+00		6.11E+00	3.45	3.45E-03	-2.46E+00	7.86E-01	-1.55E+01	
298	9.81E+00	9.81E+00	9.81E+00	9.81E+00	3.36	3.36E-03	-2.47E+00	9.92E-01	-2.49E+02	
310	1.95E+01	1.95E+01		1.95E+01	3.23	3.23E-03	-2.49E+00	1.29E+00	-3.64E+01	
320	3.37E+01	3.37E+01		3.37E+01	3.13	3.13E-03	-2.51E+00	1.53E+00	#N/A	
330	5.72E+01	5.72E+01		5.72E+01	3.03	3.03E-03	-2.52E+00	1.76E+00	#N/A	
340	9.56E+01	9.56E+01		9.56E+01	2.94	2.94E-03	-2.53E+00	1.98E+00	A	9.56E+01
350	1.57E+02	1.57E+02		1.57E+02	2.86	2.86E-03	-2.54E+00	2.20E+00	3.66E-37	1.00
375	5.09E+02	5.09E+02		5.09E+02	2.67	2.67E-03	-2.57E+00	2.71E+00	n	
400	1.52E+03	1.52E+03		1.52E+03	2.50	2.50E-03	-2.60E+00	3.18E+00	15.46	
425	4.22E+03	4.22E+03		4.22E+03	2.35	2.35E-03	-2.63E+00	3.63E+00	Ea	1.00
450	1.10E+04	1.10E+04		1.10E+04	2.22	2.22E-03	-2.65E+00	4.04E+00	573	1.10E+04



P1
P2
P3

Ea shift -1.50E+02

>CHOO. | >CH-

T	Møller et al. 2016 (3-OH-propanal-3-peroxy)	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |	log(T)	Replicate
200		8.02E-03		1.70E-02	5.00	5.00E-03	-2.30E+00	-1.77E+00	A	6.46E-03
225		6.81E-02		1.33E-01	4.44	4.44E-03	-2.35E+00	-8.76E-01	4.21E+08	0.38
250		4.48E-01		8.18E-01	4.00	4.00E-03	-2.40E+00	-8.71E-02	Ea	
260		8.98E-01		1.60E+00	3.85	3.85E-03	-2.41E+00	2.05E-01	4.98E+03	
270		1.75E+00		3.05E+00	3.70	3.70E-03	-2.43E+00	4.84E-01		1.40
280		3.31E+00		5.66E+00	3.57	3.57E-03	-2.45E+00	7.53E-01		7.94E+00
290		6.11E+00		1.03E+01	3.45	3.45E-03	-2.46E+00	1.01E+00	-1.55E+01	
298	1.92E-03	9.81E+00	1.62E+01	1.62E+01	3.36	3.36E-03	-2.47E+00	1.21E+00	-1.84E+02	
310		1.95E+01		3.16E+01	3.23	3.23E-03	-2.49E+00	1.50E+00	-3.64E+01	
320		3.37E+01		5.39E+01	3.13	3.13E-03	-2.51E+00	1.73E+00	#N/A	
330		5.72E+01		9.03E+01	3.03	3.03E-03	-2.52E+00	1.96E+00	#N/A	
340		9.56E+01		1.49E+02	2.94	2.94E-03	-2.53E+00	2.17E+00	A	1.49E+02
350		1.57E+02		2.41E+02	2.86	2.86E-03	-2.54E+00	2.38E+00	3.66E-37	1.00
375		5.09E+02		7.60E+02	2.67	2.67E-03	-2.57E+00	2.88E+00	n	
400		1.52E+03		2.21E+03	2.50	2.50E-03	-2.60E+00	3.34E+00	15.46	
425		4.22E+03		6.01E+03	2.35	2.35E-03	-2.63E+00	3.78E+00	Ea	1.00
450		1.10E+04		1.54E+04	2.22	2.22E-03	-2.65E+00	4.19E+00	423	1.54E+04

P1
P2
P3

Ea shift 1.20E+03

>C(OO.)- | >CH-

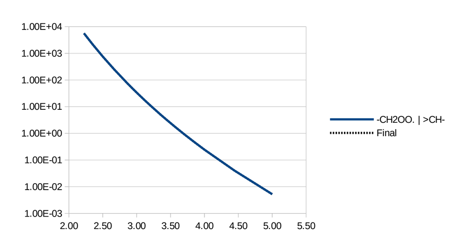
T	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |	log(T)	Replicate
200	8.02E-03		1.97E-05	5.00	5.00E-03	-2.30E+00	-4.71E+00	A	7.47E-06
225	6.81E-02		3.26E-04	4.44	4.44E-03	-2.35E+00	-3.49E+00	4.21E+08	0.38
250	4.48E-01		3.66E-03	4.00	4.00E-03	-2.40E+00	-2.44E+00	Ea	
260	8.98E-01		8.82E-03	3.85	3.85E-03	-2.41E+00	-2.05E+00	6.33E+03	
270	1.75E+00		2.04E-02	3.70	3.70E-03	-2.43E+00	-1.69E+00		1.40
280	3.31E+00		4.52E-02	3.57	3.57E-03	-2.45E+00	-1.34E+00		6.34E-02
290	6.11E+00		9.68E-02	3.45	3.45E-03	-2.46E+00	-1.01E+00	-1.55E+01	
298	9.81E+00	1.74E-01	1.74E-01	3.36	3.36E-03	-2.47E+00	-7.60E-01	-7.71E+02	
310	1.95E+01		4.03E-01	3.23	3.23E-03	-2.49E+00	-3.95E-01	-3.64E+01	
320	3.37E+01		7.87E-01	3.13	3.13E-03	-2.51E+00	-1.04E-01	#N/A	
330	5.72E+01		1.50E+00	3.03	3.03E-03	-2.52E+00	1.76E-01	#N/A	
340	9.56E+01		2.79E+00	2.94	2.94E-03	-2.53E+00	4.45E-01	A	2.79E+00
350	1.57E+02		5.06E+00	2.86	2.86E-03	-2.54E+00	7.04E-01	3.66E-37	1.00
375	5.09E+02		2.06E+01	2.67	2.67E-03	-2.57E+00	1.31E+00	n	
400	1.52E+03		7.53E+01	2.50	2.50E-03	-2.60E+00	1.88E+00	15.46	
425	4.22E+03		2.50E+02	2.35	2.35E-03	-2.63E+00	2.40E+00	Ea	1.00
450	1.10E+04		7.62E+02	2.22	2.22E-03	-2.65E+00	2.88E+00	1775	7.62E+02

1,6 Hshift

Average temperature dependence

Ea shift 0.00E+00

T	-CH2OO. | >CH-	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log()	log(T)	Replicate
200	5.22E-03	5.22E-03		5.22E-03	5.00	5.00E-03	-2.30E+00	-2.28E+00	A	1.83E-03
225	3.99E-02	3.99E-02		3.99E-02	4.44	4.44E-03	-2.35E+00	-1.40E+00	1.67E+08	0.35
250	2.45E-01	2.45E-01		2.45E-01	4.00	4.00E-03	-2.40E+00	-6.12E-01	Ea	
260	4.80E-01	4.80E-01		4.80E-01	3.85	3.85E-03	-2.41E+00	-3.19E-01	5.05E+03	
270	9.17E-01	9.17E-01		9.17E-01	3.70	3.70E-03	-2.43E+00	-3.76E-02		1.44
280	1.71E+00	1.71E+00		1.71E+00	3.57	3.57E-03	-2.45E+00	2.33E-01		2.47E+00
290	3.12E+00	3.12E+00		3.12E+00	3.45	3.45E-03	-2.46E+00	4.95E-01	-1.68E+01	
298	4.98E+00	4.98E+00	4.98E+00	4.98E+00	3.36	3.36E-03	-2.47E+00	6.97E-01	-4.38E+01	
310	9.79E+00	9.79E+00		9.79E+00	3.23	3.23E-03	-2.49E+00	9.91E-01	-4.07E+01	
320	1.68E+01	1.68E+01		1.68E+01	3.13	3.13E-03	-2.51E+00	1.23E+00	#N/A	
330	2.85E+01	2.85E+01		2.85E+01	3.03	3.03E-03	-2.52E+00	1.45E+00	#N/A	
340	4.75E+01	4.75E+01		4.75E+01	2.94	2.94E-03	-2.53E+00	1.68E+00	A	4.75E+01
350	7.79E+01	7.79E+01		7.79E+01	2.86	2.86E-03	-2.54E+00	1.89E+00	2.03E-41	1.00
375	2.53E+02	2.53E+02		2.53E+02	2.67	2.67E-03	-2.57E+00	2.40E+00	n	
400	7.60E+02	7.60E+02		7.60E+02	2.50	2.50E-03	-2.60E+00	2.88E+00	16.79	
425	2.13E+03	2.13E+03		2.13E+03	2.35	2.35E-03	-2.63E+00	3.33E+00	Ea	1.00
450	5.65E+03	5.65E+03		5.65E+03	2.22	2.22E-03	-2.65E+00	3.75E+00	101	5.65E+03

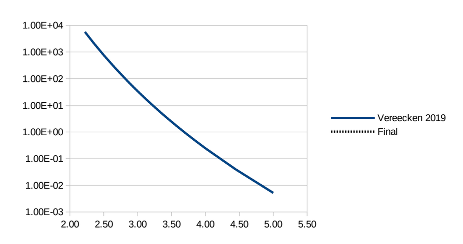


P1 2.03E-41
P2 1.68E+01
P3 1.01E+02

Ea shift 0.00E+00

-CH2OO. | >CH-

T	Vereecken 2019	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |	log(T)	Replicate
200	5.22E-03	5.22E-03		5.22E-03	5.00	5.00E-03	-2.30E+00	-2.28E+00	A	1.83E-03
225	3.99E-02	3.99E-02		3.99E-02	4.44	4.44E-03	-2.35E+00	-1.40E+00	1.67E+08	0.35
250	2.45E-01	2.45E-01		2.45E-01	4.00	4.00E-03	-2.40E+00	-6.12E-01	Ea	
260	4.80E-01	4.80E-01		4.80E-01	3.85	3.85E-03	-2.41E+00	-3.19E-01	5.05E+03	
270	9.17E-01	9.17E-01		9.17E-01	3.70	3.70E-03	-2.43E+00	-3.76E-02		1.44
280	1.71E+00	1.71E+00		1.71E+00	3.57	3.57E-03	-2.45E+00	2.33E-01		2.47E+00
290	3.12E+00	3.12E+00		3.12E+00	3.45	3.45E-03	-2.46E+00	4.95E-01	-1.68E+01	
298	4.98E+00	4.98E+00	4.98E+00	4.98E+00	3.36	3.36E-03	-2.47E+00	6.97E-01	-4.38E+01	
310	9.79E+00	9.79E+00		9.79E+00	3.23	3.23E-03	-2.49E+00	9.91E-01	-4.07E+01	
320	1.68E+01	1.68E+01		1.68E+01	3.13	3.13E-03	-2.51E+00	1.23E+00	#N/A	
330	2.85E+01	2.85E+01		2.85E+01	3.03	3.03E-03	-2.52E+00	1.45E+00	#N/A	
340	4.75E+01	4.75E+01		4.75E+01	2.94	2.94E-03	-2.53E+00	1.68E+00	A	4.75E+01
350	7.79E+01	7.79E+01		7.79E+01	2.86	2.86E-03	-2.54E+00	1.89E+00	2.03E-41	1.00
375	2.53E+02	2.53E+02		2.53E+02	2.67	2.67E-03	-2.57E+00	2.40E+00	n	
400	7.60E+02	7.60E+02		7.60E+02	2.50	2.50E-03	-2.60E+00	2.88E+00	16.79	
425	2.13E+03	2.13E+03		2.13E+03	2.35	2.35E-03	-2.63E+00	3.33E+00	Ea	1.00
450	5.65E+03	5.65E+03		5.65E+03	2.22	2.22E-03	-2.65E+00	3.75E+00	101	5.65E+03



P1
P2
P3

Ea shift -1.38E+02

>CHOO. | >CH-

T	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |	log(T)	Replicate
200	5.22E-03		1.04E-02	5.00	5.00E-03	-2.30E+00	-1.98E+00	A	3.63E-03
225	3.99E-02		7.35E-02	4.44	4.44E-03	-2.35E+00	-1.13E+00	1.67E+08	0.35
250	2.45E-01		4.24E-01	4.00	4.00E-03	-2.40E+00	-3.73E-01	Ea	
260	4.80E-01		8.15E-01	3.85	3.85E-03	-2.41E+00	-8.91E-02	4.91E+03	
270	9.17E-01		1.53E+00	3.70	3.70E-03	-2.43E+00	1.84E-01		1.44
280	1.71E+00		2.80E+00	3.57	3.57E-03	-2.45E+00	4.47E-01		4.04E+00
290	3.12E+00		5.02E+00	3.45	3.45E-03	-2.46E+00	7.01E-01	-1.68E+01	
298	4.98E+00	7.90E+00	7.90E+00	3.36	3.36E-03	-2.47E+00	8.98E-01	1.60E+01	
310	9.79E+00		1.53E+01	3.23	3.23E-03	-2.49E+00	1.18E+00	-4.07E+01	
320	1.68E+01		2.59E+01	3.13	3.13E-03	-2.51E+00	1.41E+00	#N/A	
330	2.85E+01		4.33E+01	3.03	3.03E-03	-2.52E+00	1.64E+00	#N/A	
340	4.75E+01		7.12E+01	2.94	2.94E-03	-2.53E+00	1.85E+00	A	7.12E+01
350	7.79E+01		1.15E+02	2.86	2.86E-03	-2.54E+00	2.06E+00	2.03E-41	1.00
375	2.53E+02		3.65E+02	2.67	2.67E-03	-2.57E+00	2.56E+00	n	
400	7.60E+02		1.07E+03	2.50	2.50E-03	-2.60E+00	3.03E+00	16.79	
425	2.13E+03		2.95E+03	2.35	2.35E-03	-2.63E+00	3.47E+00	Ea	1.00
450	5.65E+03		7.67E+03	2.22	2.22E-03	-2.65E+00	3.88E+00	-37	7.67E+03

P1
P2
P3

Ea shift 1.67E+02

>C(OO.)- | >CH-

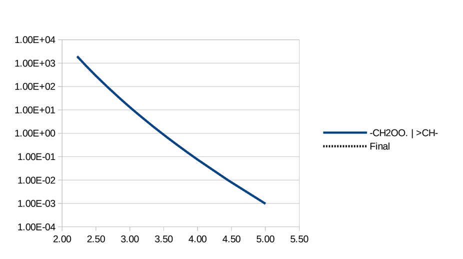
T	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |	log(T)	Replicate
200	5.22E-03		2.26E-03	5.00	5.00E-03	-2.30E+00	-2.65E+00	A	7.91E-04
225	3.99E-02		1.90E-02	4.44	4.44E-03	-2.35E+00	-1.72E+00	1.67E+08	0.35
250	2.45E-01		1.25E-01	4.00	4.00E-03	-2.40E+00	-9.02E-01	Ea	
260	4.80E-01		2.52E-01	3.85	3.85E-03	-2.41E+00	-5.98E-01	5.22E+03	
270	9.17E-01		4.94E-01	3.70	3.70E-03	-2.43E+00	-3.07E-01		1.44
280	1.71E+00		9.42E-01	3.57	3.57E-03	-2.45E+00	-2.60E-02		1.36E+00
290	3.12E+00		1.75E+00	3.45	3.45E-03	-2.46E+00	2.44E-01	-1.68E+01	
298	4.98E+00	2.84E+00	2.84E+00	3.36	3.36E-03	-2.47E+00	4.53E-01	-1.16E+02	
310	9.79E+00		5.71E+00	3.23	3.23E-03	-2.49E+00	7.56E-01	-4.07E+01	
320	1.68E+01		9.99E+00	3.13	3.13E-03	-2.51E+00	1.00E+00	#N/A	
330	2.85E+01		1.72E+01	3.03	3.03E-03	-2.52E+00	1.23E+00	#N/A	
340	4.75E+01		2.90E+01	2.94	2.94E-03	-2.53E+00	1.46E+00	A	2.90E+01
350	7.79E+01		4.83E+01	2.86	2.86E-03	-2.54E+00	1.68E+00	2.03E-41	1.00
375	2.53E+02		1.62E+02	2.67	2.67E-03	-2.57E+00	2.21E+00	n	
400	7.60E+02		5.00E+02	2.50	2.50E-03	-2.60E+00	2.70E+00	16.79	
425	2.13E+03		1.44E+03	2.35	2.35E-03	-2.63E+00	3.16E+00	Ea	1.00
450	5.65E+03		3.89E+03	2.22	2.22E-03	-2.65E+00	3.59E+00	268	3.89E+03

1,7 Hshift

Average temperature dependence

Ea shift 0.00E+00

T	-CH2OO. | >CH-	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log()	log(T)	Replicate
200	9.75E-04	9.75E-04		9.75E-04	5.00	5.00E-03	-2.30E+00	-3.01E+00	A	4.35E-04
225	1.00E-02	1.00E-02		1.00E-02	4.44	4.44E-03	-2.35E+00	-2.00E+00	1.15E+08	0.45
250	7.46E-02	7.46E-02		7.46E-02	4.00	4.00E-03	-2.40E+00	-1.13E+00	Ea	
260	1.55E-01	1.55E-01		1.55E-01	3.85	3.85E-03	-2.41E+00	-8.10E-01	5.26E+03	
270	3.10E-01	3.10E-01		3.10E-01	3.70	3.70E-03	-2.43E+00	-5.08E-01		1.33
280	6.02E-01	6.02E-01		6.02E-01	3.57	3.57E-03	-2.45E+00	-2.21E-01		7.98E-01
290	1.13E+00	1.13E+00		1.13E+00	3.45	3.45E-03	-2.46E+00	5.40E-02	-1.29E+01	
298	1.84E+00	1.84E+00	1.84E+00	1.84E+00	3.36	3.36E-03	-2.47E+00	2.65E-01	-6.33E+02	
310	3.70E+00	3.70E+00		3.70E+00	3.23	3.23E-03	-2.49E+00	5.69E-01	-2.95E+01	
320	6.46E+00	6.46E+00		6.46E+00	3.13	3.13E-03	-2.51E+00	8.10E-01	#N/A	
330	1.10E+01	1.10E+01		1.10E+01	3.03	3.03E-03	-2.52E+00	1.04E+00	#N/A	
340	1.85E+01	1.85E+01		1.85E+01	2.94	2.94E-03	-2.53E+00	1.27E+00	A	1.85E+01
350	3.04E+01	3.04E+01		3.04E+01	2.86	2.86E-03	-2.54E+00	1.48E+00	2.91E-30	1.00
375	9.76E+01	9.76E+01		9.76E+01	2.67	2.67E-03	-2.57E+00	1.99E+00	n	
400	2.86E+02	2.86E+02		2.86E+02	2.50	2.50E-03	-2.60E+00	2.46E+00	12.90	
425	7.76E+02	7.76E+02		7.76E+02	2.35	2.35E-03	-2.63E+00	2.89E+00	Ea	1.00
450	1.96E+03	1.96E+03		1.96E+03	2.22	2.22E-03	-2.65E+00	3.29E+00	1458	1.96E+03

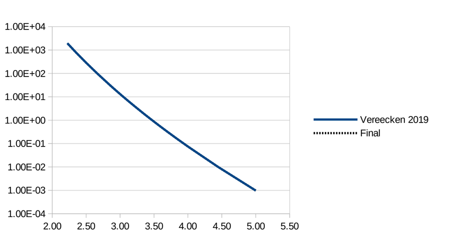


P1 2.91E-30
P2 1.29E+01
P3 1.46E+03

Ea shift 0.00E+00

-CH2OO. | >CH-

T	Vereecken 2019	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(-CH2OO. |	log(T)	Replicate
200	9.75E-04	9.75E-04		9.75E-04	5.00	5.00E-03	-2.30E+00	-3.01E+00	A	4.35E-04
225	1.00E-02	1.00E-02		1.00E-02	4.44	4.44E-03	-2.35E+00	-2.00E+00	1.15E+08	0.45
250	7.46E-02	7.46E-02		7.46E-02	4.00	4.00E-03	-2.40E+00	-1.13E+00	Ea	
260	1.55E-01	1.55E-01		1.55E-01	3.85	3.85E-03	-2.41E+00	-8.10E-01	5.26E+03	
270	3.10E-01	3.10E-01		3.10E-01	3.70	3.70E-03	-2.43E+00	-5.08E-01		1.33
280	6.02E-01	6.02E-01		6.02E-01	3.57	3.57E-03	-2.45E+00	-2.21E-01		7.98E-01
290	1.13E+00	1.13E+00		1.13E+00	3.45	3.45E-03	-2.46E+00	5.40E-02	-1.29E+01	
298	1.84E+00	1.84E+00	1.84E+00	1.84E+00	3.36	3.36E-03	-2.47E+00	2.65E-01	-6.33E+02	
310	3.70E+00	3.70E+00		3.70E+00	3.23	3.23E-03	-2.49E+00	5.69E-01	-2.95E+01	
320	6.46E+00	6.46E+00		6.46E+00	3.13	3.13E-03	-2.51E+00	8.10E-01	#N/A	
330	1.10E+01	1.10E+01		1.10E+01	3.03	3.03E-03	-2.52E+00	1.04E+00	#N/A	
340	1.85E+01	1.85E+01		1.85E+01	2.94	2.94E-03	-2.53E+00	1.27E+00	A	1.85E+01
350	3.04E+01	3.04E+01		3.04E+01	2.86	2.86E-03	-2.54E+00	1.48E+00	2.91E-30	1.00
375	9.76E+01	9.76E+01		9.76E+01	2.67	2.67E-03	-2.57E+00	1.99E+00	n	
400	2.86E+02	2.86E+02		2.86E+02	2.50	2.50E-03	-2.60E+00	2.46E+00	12.90	
425	7.76E+02	7.76E+02		7.76E+02	2.35	2.35E-03	-2.63E+00	2.89E+00	Ea	1.00
450	1.96E+03	1.96E+03		1.96E+03	2.22	2.22E-03	-2.65E+00	3.29E+00	1458	1.96E+03



P1
P2
P3

Ea shift 7.08E+02

>CHOO. | >CH-

T	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>CHOO. |	log(T)	Replicate
200	9.75E-04		2.82E-05	5.00	5.00E-03	-2.30E+00	-4.55E+00	A	1.26E-05
225	1.00E-02		4.30E-04	4.44	4.44E-03	-2.35E+00	-3.37E+00	1.15E+08	0.45
250	7.46E-02		4.39E-03	4.00	4.00E-03	-2.40E+00	-2.36E+00	Ea	
260	1.55E-01		1.02E-02	3.85	3.85E-03	-2.41E+00	-1.99E+00	5.97E+03	
270	3.10E-01		2.25E-02	3.70	3.70E-03	-2.43E+00	-1.65E+00		1.33
280	6.02E-01		4.79E-02	3.57	3.57E-03	-2.45E+00	-1.32E+00		6.36E-02
290	1.13E+00		9.84E-02	3.45	3.45E-03	-2.46E+00	-1.01E+00	-1.29E+01	
298	1.84E+00	1.71E-01	1.71E-01	3.36	3.36E-03	-2.47E+00	-7.67E-01	-9.41E+02	
310	3.70E+00		3.77E-01	3.23	3.23E-03	-2.49E+00	-4.24E-01	-2.95E+01	
320	6.46E+00		7.06E-01	3.13	3.13E-03	-2.51E+00	-1.51E-01	#N/A	
330	1.10E+01		1.29E+00	3.03	3.03E-03	-2.52E+00	1.11E-01	#N/A	
340	1.85E+01		2.30E+00	2.94	2.94E-03	-2.53E+00	3.62E-01	A	2.30E+00
350	3.04E+01		4.01E+00	2.86	2.86E-03	-2.54E+00	6.03E-01	2.91E-30	1.00
375	9.76E+01		1.48E+01	2.67	2.67E-03	-2.57E+00	1.17E+00	n	
400	2.86E+02		4.87E+01	2.50	2.50E-03	-2.60E+00	1.69E+00	12.90	
425	7.76E+02		1.46E+02	2.35	2.35E-03	-2.63E+00	2.17E+00	Ea	1.00
450	1.96E+03		4.07E+02	2.22	2.22E-03	-2.65E+00	2.61E+00	2167	4.07E+02

P1
P2
P3

Ea shift 1.20E+03

>C(OO.)- | >CH-

T	T-dependence	Target	Final	1000/T	1/T	log(1/T)	log(>C(OO.)- |	log(T)	Replicate
200	9.75E-04		2.36E-06	5.00	5.00E-03	-2.30E+00	-5.63E+00	A	1.05E-06
225	1.00E-02		4.74E-05	4.44	4.44E-03	-2.35E+00	-4.32E+00	1.15E+08	0.45
250	7.46E-02		6.03E-04	4.00	4.00E-03	-2.40E+00	-3.22E+00	Ea	
260	1.55E-01		1.51E-03	3.85	3.85E-03	-2.41E+00	-2.82E+00	6.47E+03	
270	3.10E-01		3.59E-03	3.70	3.70E-03	-2.43E+00	-2.45E+00		1.33
280	6.02E-01		8.15E-03	3.57	3.57E-03	-2.45E+00	-2.09E+00		1.08E-02
290	1.13E+00		1.78E-02	3.45	3.45E-03	-2.46E+00	-1.75E+00	-1.29E+01	
298	1.84E+00	3.24E-02	3.24E-02	3.36	3.36E-03	-2.47E+00	-1.49E+00	-1.16E+03	
310	3.70E+00		7.61E-02	3.23	3.23E-03	-2.49E+00	-1.12E+00	-2.95E+01	
320	6.46E+00		1.50E-01	3.13	3.13E-03	-2.51E+00	-8.24E-01	#N/A	
330	1.10E+01		2.87E-01	3.03	3.03E-03	-2.52E+00	-5.42E-01	#N/A	
340	1.85E+01		5.35E-01	2.94	2.94E-03	-2.53E+00	-2.72E-01	A	5.35E-01
350	3.04E+01		9.72E-01	2.86	2.86E-03	-2.54E+00	-1.22E-02	2.91E-30	1.00
375	9.76E+01		3.93E+00	2.67	2.67E-03	-2.57E+00	5.95E-01	n	
400	2.86E+02		1.41E+01	2.50	2.50E-03	-2.60E+00	1.15E+00	12.90	
425	7.76E+02		4.56E+01	2.35	2.35E-03	-2.63E+00	1.66E+00	Ea	1.00
450	1.96E+03		1.35E+02	2.22	2.22E-03	-2.65E+00	2.13E+00	2663	1.35E+02