Understanding the kinetics of thermal decomposition of 2,3-epoxy-2,3-dimethylbutane using RRKM theory

Abolfazl Shiroudi[a,b,*], Ehsan Zahedi[c]

[a] Center of Molecular and Materials Modelling, Hasselt University, Agoralaan, Gebouw D, B-3590 Diepenbeek, Belgium

[b] Young Researchers and Elite Club, East Tehran Branch, Islamic Azad University, Tehran, Iran

[c] Chemistry Department, Shahrood Branch, Islamic Azad University, Shahrood, Iran

Electronic Supplementary Information

Table S1: Unimolecular rate constants for all reaction steps involved in the reported chemical pathways (results obtained by means of RRKM theory at different pressures and temperatures, according to the computed UM06-2*x*/aug-cc-pVTZ energy profiles).

Table S1*a*: [T = 661.5 K]

P (bar)	k_{uni} (R→P1)	k_{uni} (R→P3)	k_{uni} (R→P2)	log P	log k_{uni} (R→P1)	log k_{uni} (R→P3)	log k_{uni} (R→P2)
1.00E+02	1.83E-07	7.82E-07	6.60E-10	2	-6.74	-6.11	-9.18
1.00E+00	1.83E-07	7.82E-07	6.60E-10	0	-6.74	-6.11	-9.18
1.00E-02	1.83E-07	7.82E-07	6.60E-10	-2	-6.74	-6.11	-9.18
1.00E-04	1.83E-07	7.82E-07	6.60E-10	-4	-6.74	-6.11	-9.18
1.00E-06	1.77E-07	7.42E-07	6.58E-10	-6	-6.75	-6.13	-9.18
1.00E-08	1.16E-07	4.42E-07	5.95E-10	-8	-6.94	-6.35	-9.23
1.00E-10	2.87E-08	9.41E-08	2.99E-10	-10	-7.54	-7.03	-9.52
1.00E-12	2.55E-09	7.33E-09	5.52E-11	-12	-8.59	-8.13	-10.26

Table S1*b*: [T = 672.2 K]

P (bar)	k_{uni} (R→P1)	k_{uni} (R→P3)	k_{uni} (R→P2)	log P	log k_{uni} (R→P1)	log k_{uni} (R→P3)	log k_{uni} (R→P2)
1.00E+02	3.73E-07	1.55E-06	1.44E-09	2	-6.43	-5.81	-8.84
1.00E+00	3.73E-07	1.55E-06	1.44E-09	0	-6.43	-5.81	-8.84
1.00E-02	3.73E-07	1.55E-06	1.44E-09	-2	-6.43	-5.81	-8.84
1.00E-04	3.73E-07	1.55E-06	1.44E-09	-4	-6.43	-5.81	-8.84
1.00E-06	3.57E-07	1.46E-06	1.44E-09	-6	-6.45	-5.84	-8.84
1.00E-08	2.24E-07	8.30E-07	1.28E-09	-8	-6.65	-6.08	-8.89
1.00E-10	5.21E-08	1.65E-07	6.10E-10	-10	-7.28	-6.78	-9.21
1.00E-12	4.39E-09	1.22E-08	1.06E-10	-12	-8.36	-7.91	-9.97

* Corresponding author: E-mails: abolfazl.shiroudi@uhasselt.be (A. Shiroudi)

Table S1*c*: [T = 681.1 K]

P (bar)	k_{uni} (R→P1)	k_{uni} (R→P3)	k_{uni} (R→P2)	log P	log k_{uni} (R→P1)	log k_{uni} (R→P3)	log k_{uni} (R→P2)
1.00E+02	6.62E-07	2.70E-06	2.72E-09	2	-6.18	-5.57	-8.57
1.00E+00	6.62E-07	2.70E-06	2.72E-09	0	-6.18	-5.57	-8.57
1.00E-02	6.62E-07	2.70E-06	2.72E-09	-2	-6.18	-5.57	-8.57
1.00E-04	6.61E-07	2.70E-06	2.72E-09	-4	-6.18	-5.57	-8.57
1.00E-06	6.30E-07	2.52E-06	2.71E-09	-6	-6.20	-5.60	-8.57
1.00E-08	3.81E-07	1.37E-06	2.38E-09	-8	-6.42	-5.86	-8.62
1.00E-10	8.40E-08	2.59E-07	1.08E-09	-10	-7.08	-6.59	-8.97
1.00E-12	6.76E-09	1.83E-08	1.78E-10	-12	-8.17	-7.74	-9.75

Table S1*d*: [T = 689.1 K]

P (bar)	k_{uni} (R→P1)	k_{uni} (R→P3)	k_{uni} (R→P2)	log P	log k_{uni} (R→P1)	log k_{uni} (R→P3)	log k_{uni} (R→P2)
1.00E+02	1.09E-06	4.39E-06	4.73E-09	2	-5.96	-5.36	-8.33
1.00E+00	1.09E-06	4.39E-06	4.73E-09	0	-5.96	-5.36	-8.33
1.00E-02	1.09E-06	4.39E-06	4.73E-09	-2	-5.96	-5.36	-8.33
1.00E-04	1.09E-06	4.38E-06	4.73E-09	-4	-5.96	-5.36	-8.33
1.00E-06	1.04E-06	4.05E-06	4.71E-09	-6	-5.98	-5.39	-8.33
1.00E-08	6.07E-07	2.14E-06	4.08E-09	-8	-6.22	-5.67	-8.39
1.00E-10	1.27E-07	3.84E-07	1.78E-09	-10	-6.90	-6.42	-8.75
1.00E-12	9.85E-09	2.61E-08	2.81E-10	-12	-8.01	-7.58	-9.55

Table S1*e*: [T = 696.3 K]

P (bar)	k_{uni} (R→P1)	k_{uni} (R→P3)	k_{uni} (R→P2)	log P	log k_{uni} (R→P1)	log k_{uni} (R→P3)	log k_{uni} (R→P2)
1.00E+02	1.71E-06	6.73E-06	7.72E-09	2	-5.77	-5.17	-8.11
1.00E+00	1.71E-06	6.73E-06	7.72E-09	0	-5.77	-5.17	-8.11
1.00E-02	1.71E-06	6.73E-06	7.72E-09	-2	-5.77	-5.17	-8.11
1.00E-04	1.70E-06	6.71E-06	7.71E-09	-4	-5.77	-5.17	-8.11
1.00E-06	1.60E-06	6.16E-06	7.67E-09	-6	-5.80	-5.21	-8.12
1.00E-08	9.11E-07	3.14E-06	6.56E-09	-8	-6.04	-5.50	-8.18
1.00E-10	1.83E-07	5.41E-07	2.76E-09	-10	-6.74	-6.27	-8.56
1.00E-12	1.37E-08	3.55E-08	4.17E-10	-12	-7.86	-7.45	-9.38

Table S1*f*: [T = 704.2 K]

P (bar)	k_{uni} (R→P1)	k_{uni} (R→P3)	k_{uni} (R→P2)	log P	log k_{uni} (R→P1)	log k_{uni} (R→P3)	log k_{uni} (R→P2)
1.00E+02	2.75E-06	1.07E-05	1.30E-08	2	-5.56	-4.97	-7.89
1.00E+00	2.75E-06	1.07E-05	1.30E-08	0	-5.56	-4.97	-7.89
1.00E-02	2.75E-06	1.07E-05	1.30E-08	-2	-5.56	-4.97	-7.89
1.00E-04	2.74E-06	1.06E-05	1.30E-08	-4	-5.56	-4.97	-7.89
1.00E-06	2.56E-06	9.66E-06	1.29E-08	-6	-5.59	-5.02	-7.89
1.00E-08	1.41E-06	4.74E-06	1.09E-08	-8	-5.85	-5.32	-7.96
1.00E-10	2.70E-07	7.79E-07	4.41E-09	-10	-6.57	-6.11	-8.36
1.00E-12	1.94E-08	4.93E-08	6.37E-10	-12	-7.71	-7.31	-9.20

Table S1*g*: [T =713.2 K]

P (bar)	k_{uni} (R→P1)	k_{uni} (R→P3)	k_{uni} (R→P2)	log P	log k_{uni} (R→P1)	log k_{uni} (R→P3)	log k_{uni} (R→P2)
1.00E+02	4.66E-06	1.77E-05	2.34E-08	2	-5.33	-4.75	-7.63
1.00E+00	4.66E-06	1.77E-05	2.34E-08	0	-5.33	-4.75	-7.63
1.00E-02	4.66E-06	1.77E-05	2.34E-08	-2	-5.33	-4.75	-7.63
1.00E-04	4.66E-06	1.77E-05	2.34E-08	-4	-5.33	-4.75	-7.63
1.00E-06	4.31E-06	1.59E-05	2.32E-08	-6	-5.37	-4.80	-7.64
1.00E-08	2.27E-06	7.46E-06	1.91E-08	-8	-5.64	-5.13	-7.72
1.00E-10	4.13E-07	1.16E-06	7.39E-09	-10	-6.38	-5.93	-8.13
1.00E-12	2.85E-08	7.07E-08	1.01E-09	-12	-7.55	-7.15	-8.99

Table S1*h*: [T =721.2 K]

P (bar)	k_{uni} (R→P1)	k_{uni} (R→P3)	k_{uni} (R→P2)	log P	log k_{uni} (R→P1)	log k_{uni} (R→P3)	log k_{uni} (R→P2)
1.00E+02	7.39E-06	2.77E-05	3.88E-08	2.00	-5.13	-4.56	-7.41
1.00E+00	7.39E-06	2.77E-05	3.88E-08	0.00	-5.13	-4.56	-7.41
1.00E-02	7.39E-06	2.77E-05	3.88E-08	-2.00	-5.13	-4.56	-7.41
1.00E-04	7.37E-06	2.76E-05	3.88E-08	-4.00	-5.13	-4.56	-7.41
1.00E-06	6.76E-06	2.45E-05	3.84E-08	-6.00	-5.17	-4.61	-7.42
1.00E-08	3.44E-06	1.11E-05	3.12E-08	-8.00	-5.46	-4.95	-7.51
1.00E-10	5.96E-07	1.65E-06	1.15E-08	-10.00	-6.22	-5.78	-7.94
1.00E-12	3.97E-08	9.63E-08	1.52E-09	-12.00	-7.40	-7.02	-8.82

Table S1*i*: [T = 729.1 K]

P (bar)	k_{uni} (R→P1)	k_{uni} (R→P3)	k_{uni} (R→P2)	log P	log k_{uni} (R→P1)	log k_{uni} (R→P3)	log k_{uni} (R→P2)
1.00E+02	1.15E-05	4.24E-05	6.32E-08	2.00	-4.94	-4.37	-7.20
1.00E+00	1.15E-05	4.24E-05	6.32E-08	0.00	-4.94	-4.37	-7.20
1.00E-02	1.15E-05	4.24E-05	6.32E-08	-2.00	-4.94	-4.37	-7.20
1.00E-04	1.15E-05	4.23E-05	6.32E-08	-4.00	-4.94	-4.37	-7.20
1.00E-06	1.04E-05	3.71E-05	6.25E-08	-6.00	-4.98	-4.43	-7.20
1.00E-08	5.12E-06	1.61E-05	4.98E-08	-8.00	-5.29	-4.79	-7.30
1.00E-10	8.48E-07	2.29E-06	1.77E-08	-10.00	-6.07	-5.64	-7.75
1.00E-12	5.44E-08	1.29E-07	2.23E-09	-12.00	-7.26	-6.89	-8.65

Table S2: Kinetic rate constants (in s^{-1}), and branching ratios in the reported chemical pathways at different pressures and temperatures using the RRKM theory, according to the computed UM06-2*x*/aug-cc-pVTZ energy profiles.

Table S2*a*:

Parameter / Temperature (K)	***P* = 10² bar**					
	Unimolecular rate constant, k_{uni} (s^{-1})			Branching ratio (R)		
	R →P1	R →P3	R →P2	R(1)	R(3)	R(2)
661.5	1.83E-07	7.82E-07	6.60E-10	18.95	80.98	0.07
672.2	3.73E-07	1.55E-06	1.44E-09	19.38	80.54	0.07
681.1	6.62E-07	2.70E-06	2.72E-09	19.67	80.24	0.08
689.1	1.09E-06	4.39E-06	4.73E-09	19.87	80.04	0.09
696.3	1.71E-06	6.73E-06	7.72E-09	20.24	79.67	0.09
704.2	2.75E-06	1.07E-05	1.30E-08	20.43	79.48	0.10
713.2	4.66E-06	1.77E-05	2.34E-08	20.82	79.08	0.10
721.2	7.39E-06	2.77E-05	3.88E-08	21.04	78.85	0.11
729.1	1.15E-05	4.24E-05	6.32E-08	21.31	78.57	0.12

Table S2*b*:

Parameter / Temperature (K)	***P* = 10⁰ bar**					
	Unimolecular rate constant, k_{uni} (s^{-1})			Branching ratio (R)		
	R →P1	R →P3	R →P2	R(1)	R(3)	R(2)
661.5	1.83E-07	7.82E-07	6.60E-10	18.95	80.98	0.07
672.2	3.73E-07	1.55E-06	1.44E-09	19.38	80.54	0.07
681.1	6.62E-07	2.70E-06	2.72E-09	19.67	80.24	0.08
689.1	1.09E-06	4.39E-06	4.73E-09	19.87	80.04	0.09
696.3	1.71E-06	6.73E-06	7.72E-09	20.24	79.67	0.09
704.2	2.75E-06	1.07E-05	1.30E-08	20.43	79.48	0.10
713.2	4.66E-06	1.77E-05	2.34E-08	20.82	79.08	0.10
721.2	7.39E-06	2.77E-05	3.88E-08	21.04	78.85	0.11
729.1	1.15E-05	4.24E-05	6.32E-08	21.31	78.57	0.12

Table S2*c*:

Parameter / Temperature (K)	$P = 10^{-2}$ bar					
	Unimolecular rate constant, k_{uni} (s^{-1})			Branching ratio (R)		
	R →P1	R →P3	R →P2	R(1)	R(3)	R(2)
661.5	1.83E-07	7.82E-07	6.60E-10	18.95	80.98	0.07
672.2	3.73E-07	1.55E-06	1.44E-09	19.38	80.54	0.07
681.1	6.62E-07	2.70E-06	2.72E-09	19.67	80.24	0.08
689.1	1.09E-06	4.39E-06	4.73E-09	19.87	80.04	0.09
696.3	1.71E-06	6.73E-06	7.72E-09	20.24	79.67	0.09
704.2	2.75E-06	1.07E-05	1.30E-08	20.43	79.48	0.10
713.2	4.66E-06	1.77E-05	2.34E-08	20.82	79.08	0.10
721.2	7.39E-06	2.77E-05	3.88E-08	21.04	78.85	0.11
729.1	1.15E-05	4.24E-05	6.32E-08	21.31	78.57	0.12

Table S2*d*:

Parameter / Temperature (K)	$P = 10^{-4}$ bar					
	Unimolecular rate constant, k_{uni} (s^{-1})			Branching ratio (R)		
	R →P1	R →P3	R →P2	R(1)	R(3)	R(2)
661.5	1.83E-07	7.82E-07	6.60E-10	18.95	80.98	0.07
672.2	3.73E-07	1.55E-06	1.44E-09	19.38	80.54	0.07
681.1	6.61E-07	2.70E-06	2.72E-09	19.65	80.27	0.08
689.1	1.09E-06	4.38E-06	4.73E-09	19.91	80.00	0.09
696.3	1.70E-06	6.71E-06	7.71E-09	20.20	79.71	0.09
704.2	2.74E-06	1.06E-05	1.30E-08	20.52	79.38	0.10
713.2	4.66E-06	1.77E-05	2.34E-08	20.82	79.08	0.10
721.2	7.37E-06	2.76E-05	3.88E-08	21.05	78.84	0.11
729.1	1.15E-05	4.23E-05	6.32E-08	21.35	78.53	0.12

Table S2*e*:

Parameter / Temperature (K)	$P = 10^{-6}$ bar					
	Unimolecular rate constant, k_{uni} (s^{-1})			Branching ratio (R)		
	R →P1	R →P3	R →P2	R(1)	R(3)	R(2)
661.5	1.77E-07	7.42E-07	6.58E-10	19.25	80.68	0.07
672.2	3.57E-07	1.46E-06	1.44E-09	19.63	80.29	0.08
681.1	6.30E-07	2.52E-06	2.71E-09	19.98	79.93	0.09
689.1	1.04E-06	4.05E-06	4.71E-09	20.41	79.49	0.09
696.3	1.60E-06	6.16E-06	7.67E-09	20.60	79.30	0.10
704.2	2.56E-06	9.66E-06	1.29E-08	20.93	78.97	0.11
713.2	4.31E-06	1.59E-05	2.32E-08	21.30	78.58	0.11
721.2	6.76E-06	2.45E-05	3.84E-08	21.60	78.28	0.12
729.1	1.04E-05	3.71E-05	6.25E-08	21.87	78.00	0.13

Table S2*f*:

Parameter / Temperature (K)	$P = 10^{-8}$ bar					
	Unimolecular rate constant, k_{uni} (s^{-1})			Branching ratio (R)		
	R →P1	R →P3	R →P2	R(1)	R(3)	R(2)
661.5	1.16E-07	4.42E-07	5.95E-10	20.77	79.13	0.11
672.2	2.24E-07	8.30E-07	1.28E-09	21.23	78.65	0.12
681.1	3.81E-07	1.37E-06	2.38E-09	21.73	78.13	0.14
689.1	6.07E-07	2.14E-06	4.08E-09	22.06	77.79	0.15
696.3	9.11E-07	3.14E-06	6.56E-09	22.45	77.39	0.16
704.2	1.41E-06	4.74E-06	1.09E-08	22.89	76.94	0.18
713.2	2.27E-06	7.46E-06	1.91E-08	23.28	76.52	0.20
721.2	3.44E-06	1.11E-05	3.12E-08	23.61	76.18	0.21
729.1	5.12E-06	1.61E-05	4.98E-08	24.07	75.69	0.23

Table S2*g*:

Parameter / Temperature (K)	$P = 10^{-10}$ bar					
	Unimolecular rate constant, k_{uni} (s^{-1})			Branching ratio (R)		
	R →P1	R →P3	R →P2	R(1)	R(3)	R(2)
661.5	2.87E-08	9.41E-08	2.99E-10	23.31	76.44	0.24
672.2	5.21E-08	1.65E-07	6.10E-10	23.93	75.79	0.28
681.1	8.40E-08	2.59E-07	1.08E-09	24.41	75.27	0.31
689.1	1.27E-07	3.84E-07	1.78E-09	24.77	74.89	0.35
696.3	1.83E-07	5.41E-07	2.76E-09	25.18	74.44	0.38
704.2	2.70E-07	7.79E-07	4.41E-09	25.63	73.95	0.42
713.2	4.13E-07	1.16E-06	7.39E-09	26.13	73.40	0.47
721.2	5.96E-07	1.65E-06	1.15E-08	26.40	73.09	0.51
729.1	8.48E-07	2.29E-06	1.77E-08	26.87	72.57	0.56

Table S2*h*:

Parameter / Temperature (K)	$P = 10^{-12}$ bar					
	Unimolecular rate constant, k_{uni} (s^{-1})			Branching ratio (R)		
	R →P1	R →P3	R →P2	R(1)	R(3)	R(2)
661.5	2.55E-09	7.33E-09	5.52E-11	25.67	73.78	0.56
672.2	4.39E-09	1.22E-08	1.06E-10	26.29	73.07	0.63
681.1	6.76E-09	1.83E-08	1.78E-10	26.79	72.51	0.71
689.1	1.04E-05	3.71E-05	6.25E-08	21.87	78.00	0.13
696.3	1.37E-08	3.55E-08	4.17E-10	27.61	71.55	0.84
704.2	1.94E-08	4.93E-08	6.37E-10	27.98	71.10	0.92
713.2	2.85E-08	7.07E-08	1.01E-09	28.44	70.55	1.01
721.2	3.97E-08	9.63E-08	1.52E-09	28.87	70.03	1.11
729.1	5.44E-08	1.29E-07	2.23E-09	29.31	69.49	1.20

Table S3: Dependence upon the pressure and temperature of the regioselectivities [RSI= $R(\mathbf{3})$–$[R(\mathbf{1})+R(\mathbf{2})]/R(\mathbf{1})+R(\mathbf{2})+R(\mathbf{3})]$ of thermal decomposition of 2,3-epoxy-2,3-dimethylbutane, according to the RRKM estimates of unimolecular rate constants [$k_{uni}(\mathbf{1})$, $k_{uni}(\mathbf{2})$, $k_{uni}(\mathbf{3})$] based on UM06-2*x*/aug-cc-pVTZ energy profiles.

Table S3*a*: [T = 661.5 K]

P (bar)	k_{uni} (**1**)	k_{uni} (**2**)	k_{uni} (**3**)	k_{uni} [(**1**)+(**3**)+(**2**)]	R(**1**)	R(**2**)	R(**3**)	log P	{R(**3**)–[R(**1**)+R(**2**)]} / [R(**1**)+R(**1**)+R(**3**)]
1.00E+02	1.83E-07	6.60E-10	7.82E-07	9.66E-07	18.96	0.07	80.97	2	0.6195
1.00E+00	1.83E-07	6.60E-10	7.82E-07	9.66E-07	18.96	0.07	80.97	0	0.6195
1.00E-02	1.83E-07	6.60E-10	7.82E-07	9.66E-07	18.96	0.07	80.97	-2	0.6195
1.00E-04	1.83E-07	6.60E-10	7.82E-07	9.65E-07	18.96	0.07	80.97	-4	0.6194
1.00E-06	1.77E-07	6.58E-10	7.42E-07	9.19E-07	19.21	0.07	80.72	-6	0.6144
1.00E-08	1.16E-07	5.95E-10	4.42E-07	5.58E-07	20.70	0.11	79.20	-8	0.5839
1.00E-10	2.87E-08	2.99E-10	9.41E-08	1.23E-07	23.32	0.24	76.44	-10	0.5287
1.00E-12	2.55E-09	5.52E-11	7.33E-09	9.94E-09	25.67	0.55	73.78	-12	0.4755

Table S3*b*: [T = 681.1 K]

P (bar)	k_{uni} (**1**)	k_{uni} (**2**)	k_{uni} (**3**)	k_{uni} [(**1**)+(**3**)+(**2**)]	R(**1**)	R(**2**)	R(**3**)	log P	{R(**3**)–[R(**1**)+R(**2**)]} / [R(**1**)+R(**1**)+R(**3**)]
1.00E+02	6.62E-07	2.72E-09	2.70E-06	3.36E-06	19.67	0.08	80.25	2	0.6050
1.00E+00	6.62E-07	2.72E-09	2.70E-06	3.36E-06	19.67	0.08	80.25	0	0.6050
1.00E-02	6.62E-07	2.72E-09	2.70E-06	3.36E-06	19.67	0.08	80.25	-2	0.6050
1.00E-04	6.61E-07	2.72E-09	2.70E-06	3.36E-06	19.68	0.08	80.24	-4	0.6048
1.00E-06	6.30E-07	2.71E-09	2.52E-06	3.15E-06	20.01	0.09	79.91	-6	0.5982
1.00E-08	3.81E-07	2.38E-09	1.37E-06	1.76E-06	21.69	0.14	78.18	-8	0.5635
1.00E-10	8.40E-08	1.08E-09	2.59E-07	3.45E-07	24.39	0.31	75.30	-10	0.5060
1.00E-12	6.76E-09	1.78E-10	1.83E-08	2.53E-08	26.76	0.71	72.54	-12	0.4508

Table S3*c*: [T = 696.3 K]

P (bar)	k_{uni} (**1**)	k_{uni} (**2**)	k_{uni} (**3**)	k_{uni} [(**1**)+(**3**)+(**2**)]	R(**1**)	R(**2**)	R(**3**)	log P	{R(**3**)–[R(**1**)+R(**2**)]} / [R(**1**)+R(**1**)+R(**3**)]
1.00E+02	1.71E-06	7.72E-09	6.73E-06	8.44E-06	20.21	0.09	79.70	2	0.5940
1.00E+00	1.71E-06	7.72E-09	6.73E-06	8.44E-06	20.21	0.09	79.70	0	0.5940
1.00E-02	1.71E-06	7.72E-09	6.73E-06	8.44E-06	20.21	0.09	79.70	-2	0.5940
1.00E-04	1.70E-06	7.71E-09	6.71E-06	8.43E-06	20.22	0.09	79.69	-4	0.5937
1.00E-06	1.60E-06	7.67E-09	6.16E-06	7.77E-06	20.62	0.10	79.28	-6	0.5857
1.00E-08	9.11E-07	6.56E-09	3.14E-06	4.06E-06	22.45	0.16	77.39	-8	0.5477
1.00E-10	1.83E-07	2.76E-09	5.41E-07	7.27E-07	25.19	0.38	74.43	-10	0.4885
1.00E-12	1.37E-08	4.17E-10	3.55E-08	4.96E-08	27.57	0.84	71.59	-12	0.4318

Table S3*d*: [T = 713.2 K]

P (bar)	k_{uni} (**1**)	k_{uni} (**2**)	k_{uni} (**3**)	k_{uni} [(**1**)+(**3**)+(**2**)]	R(**1**)	R(**2**)	R(**3**)	log P	{R(**3**)–[R(**1**)+R(**2**)]} / [R(**1**)+R(**1**)+R(**3**)]
1.00E+02	4.66E-06	2.34E-08	1.77E-05	2.24E-05	20.79	0.10	79.11	2	0.5821
1.00E+00	4.66E-06	2.34E-08	1.77E-05	2.24E-05	20.79	0.10	79.11	0	0.5821
1.00E-02	4.66E-06	2.34E-08	1.77E-05	2.24E-05	20.79	0.10	79.11	-2	0.5821
1.00E-04	4.66E-06	2.34E-08	1.77E-05	2.24E-05	20.81	0.10	79.09	-4	0.5818
1.00E-06	4.31E-06	2.32E-08	1.59E-05	2.02E-05	21.30	0.11	78.59	-6	0.5718
1.00E-08	2.27E-06	1.91E-08	7.46E-06	9.76E-06	23.29	0.20	76.51	-8	0.5302
1.00E-10	4.13E-07	7.39E-09	1.16E-06	1.58E-06	26.06	0.47	73.47	-10	0.4695
1.00E-12	2.85E-08	1.01E-09	7.07E-08	1.00E-07	28.45	1.01	70.54	-12	0.4108

Table S3*e*: [T = 729.1 K]

P (bar)	k_{uni} (**1**)	k_{uni} (**2**)	k_{uni} (**3**)	k_{uni} [(**1**)+(**3**)+(**2**)]	R(**1**)	R(**2**)	R(**3**)	log P	{R(**3**)–[R(**1**)+R(**2**)]} / [R(**1**)+R(**1**)+R(**3**)]
1.00E+02	1.15E-05	6.32E-08	4.24E-05	5.40E-05	21.32	0.12	78.56	2	0.5712
1.00E+00	1.15E-05	6.32E-08	4.24E-05	5.40E-05	21.32	0.12	78.56	0	0.5712
1.00E-02	1.15E-05	6.32E-08	4.24E-05	5.40E-05	21.32	0.12	78.56	-2	0.5712
1.00E-04	1.15E-05	6.32E-08	4.23E-05	5.38E-05	21.35	0.12	78.54	-4	0.5707
1.00E-06	1.04E-05	6.25E-08	3.71E-05	4.76E-05	21.93	0.13	77.94	-6	0.5588
1.00E-08	5.12E-06	4.98E-08	1.61E-05	2.13E-05	24.08	0.23	75.69	-8	0.5138
1.00E-10	8.48E-07	1.77E-08	2.29E-06	3.16E-06	26.85	0.56	72.59	-10	0.4518
1.00E-12	5.44E-08	2.23E-09	1.29E-07	1.86E-07	29.24	1.20	69.56	-12	0.3912