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Atmospheric oxidation reactions of imidazole initiated by hydroxyl radicals: Kinetics and mechanism reactions and atmospheric implications

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Electronic Supplementary Information (ESI)

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Table S1: Kinetic rate constants for the reactions involved in the reaction pathways **1**–**3** by means of RRKM theory at different pressure and temperatures, according to the computed M06-2*x* energy profiles. (*x*=2,3)

Table S1a: *T*= 297 K.

P	Equilibrium constants (bar^{-1})		Unimolecular rate constants (s^{-1})			Effective rate constants ($cm^3\ molecule^{-1}\ s^{-1}$)			
	$K_{P(1)}$	$K_{P(X),x=2,3}$	k_2 (**1**)	k_2 (**2**)	k_2 (**3**)	k_{eff}(**1**)	k_{eff}(**2**)	k_{eff}(**3**)	k_{eff} [(**1**)+(**3**)+(**2**)]
1.00E+08	9.22E-04	7.39E-04	3.13E+09	6.90E+07	7.89E+10	1.19E-13	2.09E-15	2.39E-12	2.51E-12
1.00E+06	9.22E-04	7.39E-04	3.13E+09	6.90E+07	7.89E+10	1.19E-13	2.09E-15	2.39E-12	2.51E-12
1.00E+04	9.22E-04	7.39E-04	3.13E+09	6.90E+07	7.84E+10	1.18E-13	2.09E-15	2.38E-12	2.50E-12
1.00E+02	9.22E-04	7.39E-04	2.88E+09	6.85E+07	5.08E+10	1.09E-13	2.08E-15	1.54E-12	1.65E-12
1.00E+00	9.22E-04	7.39E-04	4.49E+08	4.33E+07	1.57E+09	1.70E-14	1.31E-15	4.77E-14	6.60E-14
1.00E-02	9.22E-04	7.39E-04	5.94E+06	1.89E+06	1.62E+07	2.24E-16	5.74E-17	4.90E-16	7.72E-16
1.00E-04	9.22E-04	7.39E-04	5.96E+04	2.03E+04	1.62E+05	2.25E-18	6.15E-19	4.90E-18	7.77E-18
1.00E-06	9.22E-04	7.39E-04	5.96E+02	2.03E+02	1.62E+03	2.25E-20	6.15E-21	4.90E-20	7.77E-20
1.00E-08	9.22E-04	7.39E-04	5.96E+00	2.03E+00	1.62E+01	2.25E-22	6.15E-23	4.90E-22	7.77E-22
1.00E-10	9.22E-04	7.39E-04	5.96E-02	2.03E-02	1.62E-01	2.25E-24	6.15E-25	4.90E-24	7.77E-24

Table S1b: T= 316 K.

P	Equilibrium constants (bar^{-1})		Unimolecular rate constants (s^{-1})			Effective rate constants ($cm^3\ molecule^{-1}\ s^{-1}$)			
	$K_{P(1)}$	$K_{P(X),x=2,3}$	k_2 (**1**)	k_2 (**2**)	k_2 (**3**)	k_{eff} (**1**)	k_{eff} (**2**)	k_{eff} (**3**)	k_{eff} [(**1**)+(**3**)+(**2**)]
1.00E+08	6.66E-04	5.70E-04	4.31E+09	1.13E+08	8.72E+10	1.25E-13	2.80E-15	2.17E-12	2.30E-12
1.00E+06	6.66E-04	5.70E-04	4.31E+09	1.13E+08	8.72E+10	1.25E-13	2.80E-15	2.17E-12	2.30E-12
1.00E+04	6.66E-04	5.70E-04	4.31E+09	1.13E+08	8.66E+10	1.25E-13	2.80E-15	2.15E-12	2.28E-12
1.00E+02	6.66E-04	5.70E-04	3.91E+09	1.11E+08	5.40E+10	1.14E-13	2.77E-15	1.34E-12	1.46E-12
1.00E+00	6.66E-04	5.70E-04	5.38E+08	6.57E+07	1.55E+09	1.56E-14	1.64E-15	3.86E-14	5.58E-14
1.00E-02	6.66E-04	5.70E-04	6.89E+06	2.57E+06	1.59E+07	2.00E-16	6.39E-17	3.95E-16	6.59E-16
1.00E-04	6.66E-04	5.70E-04	6.91E+04	2.73E+04	1.59E+05	2.01E-18	6.78E-19	3.95E-18	6.64E-18
1.00E-06	6.66E-04	5.70E-04	6.91E+02	2.73E+02	1.59E+03	2.01E-20	6.79E-21	3.95E-20	6.64E-20
1.00E-08	6.66E-04	5.70E-04	6.91E+00	2.73E+00	1.59E+01	2.01E-22	6.79E-23	3.95E-22	6.64E-22
1.00E-10	6.66E-04	5.70E-04	6.91E-02	2.73E-02	1.59E-01	2.01E-24	6.79E-25	3.95E-24	6.64E-24

Table S1c: T= 331 K.

P	Equilibrium constants (bar^{-1})		Unimolecular rate constants (s^{-1})			Effective rate constants ($cm^3\ molecule^{-1}\ s^{-1}$)			
	$K_{P(1)}$	$K_{P(X),x=2,3}$	k_2 (**1**)	k_2 (**2**)	k_2 (**3**)	k_{eff} (**1**)	k_{eff} (**2**)	k_{eff} (**3**)	k_{eff} [(**1**)+(**3**)+(**2**)]
1.00E+08	5.30E-04	4.75E-04	5.40E+09	1.59E+08	9.35E+10	1.31E-13	3.45E-15	2.03E-12	2.17E-12
1.00E+06	5.30E-04	4.75E-04	5.40E+09	1.59E+08	9.35E+10	1.31E-13	3.45E-15	2.03E-12	2.16E-12
1.00E+04	5.30E-04	4.75E-04	5.40E+09	1.59E+08	9.29E+10	1.31E-13	3.45E-15	2.02E-12	2.15E-12
1.00E+02	5.30E-04	4.75E-04	4.84E+09	1.57E+08	5.62E+10	1.17E-13	3.41E-15	1.22E-12	1.34E-12
1.00E+00	5.30E-04	4.75E-04	6.05E+08	8.76E+07	1.53E+09	1.47E-14	1.90E-15	3.32E-14	4.97E-14
1.00E-02	5.30E-04	4.75E-04	7.57E+06	3.15E+06	1.56E+07	1.83E-16	6.83E-17	3.39E-16	5.91E-16
1.00E-04	5.30E-04	4.75E-04	7.60E+04	3.32E+04	1.56E+05	1.84E-18	7.21E-19	3.39E-18	5.95E-18
1.00E-06	5.30E-04	4.75E-04	7.60E+02	3.32E+02	1.56E+03	1.84E-20	7.22E-21	3.39E-20	5.95E-20
1.00E-08	5.30E-04	4.75E-04	7.60E+00	3.32E+00	1.56E+01	1.84E-22	7.22E-23	3.39E-22	5.95E-22
1.00E-10	5.30E-04	4.75E-04	7.60E-02	3.32E-02	1.56E-01	1.84E-24	7.22E-25	3.39E-24	5.95E-24

Table S1d: T= 344 K.

P	Equilibrium constants (bar^{-1})		Unimolecular rate constants (s^{-1})			Effective rate constants ($cm^3\ molecule^{-1}\ s^{-1}$)			
	$K_{P(1)}$	$K_{P(X),x=2,3}$	k_2 (**1**)	k_2 (**2**)	k_2 (**3**)	k_{eff} (**1**)	k_{eff} (**2**)	k_{eff} (**3**)	k_{eff} [(**1**)+(**3**)+(**2**)]
1.00E+08	4.43E-04	4.12E-04	6.47E+09	2.09E+08	9.89E+10	1.36E-13	4.09E-15	1.94E-12	2.08E-12
1.00E+06	4.43E-04	4.12E-04	6.47E+09	2.09E+08	9.89E+10	1.36E-13	4.09E-15	1.94E-12	2.08E-12
1.00E+04	4.43E-04	4.12E-04	6.46E+09	2.09E+08	9.82E+10	1.36E-13	4.09E-15	1.92E-12	2.06E-12
1.00E+02	4.43E-04	4.12E-04	5.72E+09	2.07E+08	5.79E+10	1.20E-13	4.04E-15	1.13E-12	1.26E-12
1.00E+00	4.43E-04	4.12E-04	6.59E+08	1.09E+08	1.50E+09	1.39E-14	2.14E-15	2.95E-14	4.55E-14
1.00E-02	4.43E-04	4.12E-04	8.11E+06	3.67E+06	1.53E+07	1.71E-16	7.17E-17	3.00E-16	5.43E-16
1.00E-04	4.43E-04	4.12E-04	8.13E+04	3.85E+04	1.53E+05	1.71E-18	7.54E-19	3.00E-18	5.47E-18
1.00E-06	4.43E-04	4.12E-04	8.13E+02	3.85E+02	1.53E+03	1.71E-20	7.54E-21	3.00E-20	5.47E-20
1.00E-08	4.43E-04	4.12E-04	8.13E+00	3.85E+00	1.53E+01	1.71E-22	7.54E-23	3.00E-22	5.47E-22
1.00E-10	4.43E-04	4.12E-04	8.13E-02	3.85E-02	1.53E-01	1.71E-24	7.54E-25	3.00E-24	5.47E-24

Table S1e: T= 353 K.

P	Equilibrium constants (bar^{-1})		Unimolecular rate constants (s^{-1})			Effective rate constants (cm^3 $molecule^{-1}$ s^{-1})			
	$K_{P(1)}$	$K_{P(X),x=2,3}$	k_2 (**1**)	k_2 (**2**)	k_2 (**3**)	k_{eff} (**1**)	k_{eff} (**2**)	k_{eff} (**3**)	k_{eff} [(**1**)+(**3**)+(**2**)]
1.00E+08	3.95E-04	3.75E-04	7.26E+09	2.50E+08	1.03E+11	1.40E-13	4.57E-15	1.87E-12	2.02E-12
1.00E+06	3.95E-04	3.75E-04	7.26E+09	2.50E+08	1.03E+11	1.40E-13	4.57E-15	1.87E-12	2.02E-12
1.00E+04	3.95E-04	3.75E-04	7.25E+09	2.50E+08	1.02E+11	1.40E-13	4.57E-15	1.86E-12	2.00E-12
1.00E+02	3.95E-04	3.75E-04	6.37E+09	2.47E+08	5.89E+10	1.23E-13	4.51E-15	1.08E-12	1.20E-12
1.00E+00	3.95E-04	3.75E-04	6.95E+08	1.26E+08	1.49E+09	1.34E-14	2.30E-15	2.72E-14	4.29E-14
1.00E-02	3.95E-04	3.75E-04	8.45E+06	4.03E+06	1.52E+07	1.63E-16	7.37E-17	2.77E-16	5.13E-16
1.00E-04	3.95E-04	3.75E-04	8.47E+04	4.22E+04	1.52E+05	1.63E-18	7.72E-19	2.77E-18	5.17E-18
1.00E-06	3.95E-04	3.75E-04	8.47E+02	4.22E+02	1.52E+03	1.63E-20	7.72E-21	2.77E-20	5.18E-20
1.00E-08	3.95E-04	3.75E-04	8.47E+00	4.22E+00	1.52E+01	1.63E-22	7.72E-23	2.77E-22	5.18E-22
1.00E-10	3.95E-04	3.75E-04	8.47E-02	4.22E-02	1.52E-01	1.63E-24	7.72E-25	2.77E-24	5.18E-24

Table S1f: T= 362 K.

P	Equilibrium constants (bar^{-1})		Unimolecular rate constants (s^{-1})			Effective rate constants ($cm^3\ molecule^{-1}\ s^{-1}$)			
	$K_{P(1)}$	$K_{P(X),x=2,3}$	k_2 (**1**)	k_2 (**2**)	k_2 (**3**)	k_{eff} (**1**)	k_{eff} (**2**)	k_{eff} (**3**)	k_{eff} [(**1**)+(**3**)+(**2**)]
1.00E+08	3.54E-04	3.44E-04	8.11E+09	2.96E+08	1.06E+11	1.43E-13	5.09E-15	1.82E-12	1.97E-12
1.00E+06	3.54E-04	3.44E-04	8.11E+09	2.96E+08	1.06E+11	1.43E-13	5.09E-15	1.82E-12	1.97E-12
1.00E+04	3.54E-04	3.44E-04	8.09E+09	2.96E+08	1.05E+11	1.43E-13	5.09E-15	1.81E-12	1.96E-12
1.00E+02	3.54E-04	3.44E-04	7.06E+09	2.92E+08	5.98E+10	1.25E-13	5.02E-15	1.03E-12	1.16E-12
1.00E+00	3.54E-04	3.44E-04	7.28E+08	1.44E+08	1.47E+09	1.29E-14	2.47E-15	2.53E-14	4.06E-14
1.00E-02	3.54E-04	3.44E-04	8.76E+06	4.39E+06	1.50E+07	1.55E-16	7.55E-17	2.57E-16	4.88E-16
1.00E-04	3.54E-04	3.44E-04	8.78E+04	4.59E+04	1.50E+05	1.55E-18	7.89E-19	2.57E-18	4.92E-18
1.00E-06	3.54E-04	3.44E-04	8.78E+02	4.59E+02	1.50E+03	1.55E-20	7.90E-21	2.57E-20	4.92E-20
1.00E-08	3.54E-04	3.44E-04	8.78E+00	4.59E+00	1.50E+01	1.55E-22	7.90E-23	2.57E-22	4.92E-22
1.00E-10	3.54E-04	3.44E-04	8.78E-02	4.59E-02	1.50E-01	1.55E-24	7.90E-25	2.57E-24	4.92E-24

Table S1g: T= 386 K.

P	Equilibrium constants (bar^{-1})		Unimolecular rate constants (s^{-1})			Effective rate constants ($cm^3\ molecule^{-1}\ s^{-1}$)			
	$K_{P(1)}$	$K_{P(X),x=2,3}$	k_2 (**1**)	k_2 (**2**)	k_2 (**3**)	k_{eff} (**1**)	k_{eff} (**2**)	k_{eff} (**3**)	k_{eff} [(**1**)+(**3**)+(**2**)]
1.00E+08	2.72E-04	2.79E-04	1.06E+10	4.47E+08	1.15E+11	1.54E-13	6.64E-15	1.71E-12	1.87E-12
1.00E+06	2.72E-04	2.79E-04	1.06E+10	4.47E+08	1.15E+11	1.54E-13	6.64E-15	1.71E-12	1.87E-12
1.00E+04	2.72E-04	2.79E-04	1.06E+10	4.47E+08	1.14E+11	1.53E-13	6.64E-15	1.70E-12	1.86E-12
1.00E+02	2.72E-04	2.79E-04	9.00E+09	4.39E+08	6.19E+10	1.31E-13	6.53E-15	9.21E-13	1.06E-12
1.00E+00	2.72E-04	2.79E-04	8.07E+08	1.95E+08	1.42E+09	1.17E-14	2.90E-15	2.11E-14	3.57E-14
1.00E-02	2.72E-04	2.79E-04	9.46E+06	5.34E+06	1.44E+07	1.37E-16	7.94E-17	2.15E-16	4.31E-16
1.00E-04	2.72E-04	2.79E-04	9.48E+04	5.54E+04	1.44E+05	1.37E-18	8.24E-19	2.15E-18	4.35E-18
1.00E-06	2.72E-04	2.79E-04	9.48E+02	5.54E+02	1.44E+03	1.37E-20	8.24E-21	2.15E-20	4.35E-20
1.00E-08	2.72E-04	2.79E-04	9.48E+00	5.54E+00	1.44E+01	1.37E-22	8.24E-23	2.15E-22	4.35E-22
1.00E-10	2.72E-04	2.79E-04	9.48E-02	5.54E-02	1.44E-01	1.37E-24	8.24E-25	2.15E-24	4.35E-24

Table S1h: T= 402 K.

P	Equilibrium constants (bar^{-1})		Unimolecular rate constants (s^{-1})			Effective rate constants ($cm^3\ molecule^{-1}\ s^{-1}$)			
	$K_{P(1)}$	$K_{P(X),x=2,3}$	k_2 (**1**)	k_2 (**2**)	k_2 (**3**)	k_{eff} (**1**)	k_{eff} (**2**)	k_{eff} (**3**)	k_{eff} [(**1**)+(**3**)+(**2**)]
1.00E+08	2.32E-04	2.47E-04	1.24E+10	5.72E+08	1.21E+11	1.60E-13	7.84E-15	1.66E-12	1.83E-12
1.00E+06	2.32E-04	2.47E-04	1.24E+10	5.72E+08	1.21E+11	1.60E-13	7.84E-15	1.66E-12	1.83E-12
1.00E+04	2.32E-04	2.47E-04	1.24E+10	5.72E+08	1.20E+11	1.60E-13	7.84E-15	1.64E-12	1.81E-12
1.00E+02	2.32E-04	2.47E-04	1.04E+10	5.60E+08	6.30E+10	1.34E-13	7.68E-15	8.64E-13	1.01E-12
1.00E+00	2.32E-04	2.47E-04	8.50E+08	2.32E+08	1.39E+09	1.09E-14	3.19E-15	1.90E-14	3.32E-14
1.00E-02	2.32E-04	2.47E-04	9.81E+06	5.93E+06	1.41E+07	1.26E-16	8.13E-17	1.93E-16	4.01E-16
1.00E-04	2.32E-04	2.47E-04	9.83E+04	6.13E+04	1.41E+05	1.27E-18	8.41E-19	1.93E-18	4.04E-18
1.00E-06	2.32E-04	2.47E-04	9.83E+02	6.13E+02	1.41E+03	1.27E-20	8.41E-21	1.93E-20	4.04E-20
1.00E-08	2.32E-04	2.47E-04	9.83E+00	6.13E+00	1.41E+01	1.27E-22	8.41E-23	1.93E-22	4.04E-22
1.00E-10	2.32E-04	2.47E-04	9.83E-02	6.13E-02	1.41E-01	1.27E-24	8.41E-25	1.93E-24	4.04E-24

Table S1i: T= 425 K.

P	Equilibrium constants (bar^{-1})		Unimolecular rate constants (s^{-1})			Effective rate constants ($cm^3\ molecule^{-1}\ s^{-1}$)			
	$K_{P(1)}$	$K_{P(X),x=2,3}$	k_2 (**1**)	k_2 (**2**)	k_2 (**3**)	k_{eff} (**1**)	k_{eff} (**2**)	k_{eff} (**3**)	k_{eff} [(**1**)+(**3**)+(**2**)]
1.00E+08	1.90E-04	2.11E-04	1.53E+10	7.89E+08	1.29E+11	1.71E-13	9.77E-15	1.60E-12	1.78E-12
1.00E+06	1.90E-04	2.11E-04	1.53E+10	7.89E+08	1.29E+11	1.71E-13	9.77E-15	1.60E-12	1.78E-12
1.00E+04	1.90E-04	2.11E-04	1.53E+10	7.88E+08	1.28E+11	1.70E-13	9.76E-15	1.58E-12	1.76E-12
1.00E+02	1.90E-04	2.11E-04	1.25E+10	7.69E+08	6.42E+10	1.39E-13	9.52E-15	7.95E-13	9.44E-13
1.00E+00	1.90E-04	2.11E-04	9.00E+08	2.88E+08	1.34E+09	1.00E-14	3.57E-15	1.66E-14	3.02E-14
1.00E-02	1.90E-04	2.11E-04	1.02E+07	6.70E+06	1.36E+07	1.14E-16	8.30E-17	1.68E-16	3.65E-16
1.00E-04	1.90E-04	2.11E-04	1.02E+05	6.90E+04	1.36E+05	1.14E-18	8.54E-19	1.68E-18	3.67E-18
1.00E-06	1.90E-04	2.11E-04	1.02E+03	6.90E+02	1.36E+03	1.14E-20	8.54E-21	1.68E-20	3.67E-20
1.00E-08	1.90E-04	2.11E-04	1.02E+01	6.90E+00	1.36E+01	1.14E-22	8.54E-23	1.68E-22	3.67E-22
1.00E-10	1.90E-04	2.11E-04	1.02E-01	6.90E-02	1.36E-01	1.14E-24	8.54E-25	1.68E-24	3.67E-24

Table S1j: T= 440 K.

P	Equilibrium constants (bar^{-1})		Unimolecular rate constants (s^{-1})			Effective rate constants ($cm^3\ molecule^{-1}\ s^{-1}$)			
	$K_{P(1)}$	$K_{P(X),x=2,3}$	k_2 (**1**)	k_2 (**2**)	k_2 (**3**)	k_{eff} (**1**)	k_{eff} (**2**)	k_{eff} (**3**)	k_{eff} [(**1**)+(**3**)+(**2**)]
1.00E+08	1.69E-04	1.92E-04	1.74E+10	9.55E+08	1.34E+11	1.78E-13	1.11E-14	1.56E-12	1.75E-12
1.00E+06	1.69E-04	1.92E-04	1.73E+10	9.55E+08	1.34E+11	1.78E-13	1.11E-14	1.56E-12	1.75E-12
1.00E+04	1.69E-04	1.92E-04	1.73E+10	9.54E+08	1.33E+11	1.78E-13	1.11E-14	1.55E-12	1.74E-12
1.00E+02	1.69E-04	1.92E-04	1.39E+10	9.28E+08	6.48E+10	1.42E-13	1.08E-14	7.56E-13	9.09E-13
1.00E+00	1.69E-04	1.92E-04	9.25E+08	3.25E+08	1.31E+09	9.50E-15	3.79E-15	1.53E-14	2.86E-14
1.00E-02	1.69E-04	1.92E-04	1.04E+07	7.15E+06	1.33E+07	1.06E-16	8.34E-17	1.55E-16	3.44E-16
1.00E-04	1.69E-04	1.92E-04	1.04E+05	7.33E+04	1.33E+05	1.06E-18	8.56E-19	1.55E-18	3.47E-18
1.00E-06	1.69E-04	1.92E-04	1.04E+03	7.34E+02	1.33E+03	1.06E-20	8.56E-21	1.55E-20	3.47E-20
1.00E-08	1.69E-04	1.92E-04	1.04E+01	7.34E+00	1.33E+01	1.06E-22	8.56E-23	1.55E-22	3.47E-22
1.00E-10	1.69E-04	1.92E-04	1.04E-01	7.34E-02	1.33E-01	1.06E-24	8.56E-25	1.55E-24	3.47E-24

Table S2: Kinetic rate constants (k) for OH attack onto C_2, C_4, and C_5 positions of imidazole for different addition products by means of TST (P =1 bar). (x=2,3)

T (K)	k_f (cm^3 $molecule^{-1}$ s^{-1})			k_f[OH] (s^{-1})			k_r (s^{-1})		
	R→P1 k_{1f}(**1**)	R→P2 k_{2f}(**2**)	R→P3 k_{3f}(**3**)	R→P1 k_{1f}(**1**)	R→P2 k_{2f}(**2**)	R→P3 k_{3f}(**3**)	P1→R k_{1r}(**1**)	P2→R k_{1r}(**2**)	P3→R k_{1r}(**3**)
297	6.61E-14	1.15E-15	1.22E-12	1.32E-07	2.30E-09	2.44E-06	7.63E-06	1.90E+00	1.09E-02
316	6.88E-14	1.52E-15	1.10E-12	1.38E-07	3.04E-09	2.20E-06	9.72E-05	1.13E+01	9.35E-02
331	7.11E-14	1.85E-15	1.03E-12	1.42E-07	3.70E-09	2.06E-06	5.90E-04	4.02E+01	4.30E-01
344	7.32E-14	2.18E-15	9.75E-13	1.46E-07	4.36E-09	1.95E-06	2.49E-03	1.10E+02	1.45E+00
353	7.49E-14	2.42E-15	9.42E-13	1.50E-07	4.84E-09	1.88E-06	6.33E-03	2.13E+02	3.20E+00
362	7.64E-14	2.69E-15	9.15E-13	1.53E-07	5.38E-09	1.83E-06	1.54E-02	3.97E+02	6.79E+00
386	8.40E-14	4.08E-15	8.28E-13	1.68E-07	8.16E-09	1.66E-06	1.35E-01	1.82E+03	4.25E+01
402	8.40E-14	4.08E-15	8.28E-13	1.68E-07	8.16E-09	1.66E-06	4.97E-01	4.54E+03	1.28E+02
425	8.89E-14	5.05E-15	7.96E-13	1.78E-07	1.01E-08	1.59E-06	2.73E+00	1.50E+04	5.43E+02
440	9.24E-14	5.74E-15	7.78E-13	1.85E-07	1.15E-08	1.56E-06	7.56E+00	3.07E+04	1.28E+03

Table S3: Effective bimolecular rate constants (cm^3 $molecule^{-1}$ s^{-1}), branching ratios (%) and regioselectivity for the pathways **1**–**3** (***x***=**1**,**2**) at different pressures and temperatures, using RRKM theory, and according to the computed M06-2*x* energy profiles.

Table S3a: *T*= 297 K.

P	Effective rate constants			Branching ratios			Regioselectivity				
	k_{eff}(**1**)	k_{eff}(**2**)	k_{eff}(**3**)	*R*(**1**)	*R*(**2**)	*R*(**3**)	LogP	{R(**3**)–[R(**1**)+R(**2**)]/ [R(**1**)+R(**1**)+R(**3**)]}	logk_{eff}(**1**)	logk_{eff}(**2**)	logk_{eff}(**3**)
1.00E+08	1.19E-13	2.09E-15	2.39E-12	4.72	0.08	95.20	8	0.9039	-12.926	-14.679	-11.621
1.00E+06	1.19E-13	2.09E-15	2.39E-12	4.72	0.08	95.20	6	0.9039	-12.926	-14.679	-11.621
1.00E+04	1.18E-13	2.09E-15	2.38E-12	4.74	0.08	95.18	4	0.9035	-12.927	-14.679	-11.624
1.00E+02	1.09E-13	2.08E-15	1.54E-12	6.60	0.13	93.28	2	0.8656	-12.963	-14.683	-11.812
1.00E+00	1.70E-14	1.31E-15	4.77E-14	25.72	1.99	72.29	0	0.4458	-13.770	-14.882	-13.321
1.00E-02	2.24E-16	5.74E-17	4.90E-16	29.08	7.43	63.49	-2	0.2697	-15.649	-16.241	-15.310
1.00E-04	2.25E-18	6.15E-19	4.90E-18	29.01	7.91	63.08	-4	0.2617	-17.647	-18.211	-17.310
1.00E-06	2.25E-20	6.15E-21	4.90E-20	29.01	7.92	63.08	-6	0.2616	-19.647	-20.211	-19.310
1.00E-08	2.25E-22	6.15E-23	4.90E-22	29.01	7.92	63.08	-8	0.2616	-21.647	-22.211	-21.310
1.00E-10	2.25E-24	6.15E-25	4.90E-24	29.01	7.92	63.08	-10	0.2616	-23.647	-24.211	-23.310

Table S3b: T= 316 K.

P	Effective rate constants			Branching ratios			Regioselectivity				
	k_{eff}(**1**)	k_{eff}(**2**)	k_{eff}(**3**)	R(**1**)	R(**2**)	R(**3**)	LogP	{R(**3**)−[R(**1**)+R(**2**)]/ [R(**1**)+R(**1**)+R(**3**)]}	logk_{eff}(**1**)	logk_{eff}(**2**)	logk_{eff}(**3**)
1.00E+08	1.25E-13	2.80E-15	2.17E-12	5.46	0.12	94.42	8	0.8884	-12.902	-14.553	-11.664
1.00E+06	1.25E-13	2.80E-15	2.17E-12	5.46	0.12	94.42	6	0.8884	-12.902	-14.553	-11.664
1.00E+04	1.25E-13	2.80E-15	2.15E-12	5.49	0.12	94.39	4	0.8878	-12.902	-14.553	-11.667
1.00E+02	1.14E-13	2.77E-15	1.34E-12	7.78	0.19	92.03	2	0.8406	-12.945	-14.557	-11.872
1.00E+00	1.56E-14	1.64E-15	3.86E-14	27.99	2.93	69.08	0	0.3817	-13.806	-14.786	-13.414
1.00E-02	2.00E-16	6.39E-17	3.95E-16	30.37	9.69	59.93	-2	0.1986	-15.699	-16.195	-15.403
1.00E-04	2.01E-18	6.78E-19	3.95E-18	30.26	10.22	59.52	-4	0.1903	-17.697	-18.168	-17.403
1.00E-06	2.01E-20	6.79E-21	3.95E-20	30.26	10.23	59.51	-6	0.1902	-19.697	-20.168	-19.403
1.00E-08	2.01E-22	6.79E-23	3.95E-22	30.26	10.23	59.51	-8	0.1902	-21.697	-22.168	-21.403
1.00E-10	2.01E-24	6.79E-25	3.95E-24	30.26	10.23	59.51	-10	0.1902	-23.697	-24.168	-23.403

Table S3c: T= 331 K.

P	Effective rate constants			Branching ratios			Regioselectivity				
	k_{eff}(**1**)	k_{eff}(**2**)	k_{eff}(**3**)	R(**1**)	R(**2**)	R(**3**)	LogP	{R(**3**)−[R(**1**)+R(**2**)]/ [R(**1**)+R(**1**)+R(**3**)]}	logk_{eff}(**1**)	logk_{eff}(**2**)	logk_{eff}(**3**)
1.00E+08	1.31E-13	3.45E-15	2.03E-12	6.05	0.16	93.79	8	0.8758	-12.883	-14.462	-11.692
1.00E+06	1.31E-13	3.45E-15	2.03E-12	6.05	0.16	93.79	6	0.8758	-12.883	-14.462	-11.692
1.00E+04	1.31E-13	3.45E-15	2.02E-12	6.08	0.16	93.76	4	0.8752	-12.883	-14.462	-11.695
1.00E+02	1.17E-13	3.41E-15	1.22E-12	8.74	0.25	91.00	2	0.8201	-12.931	-14.467	-11.914
1.00E+00	1.47E-14	1.90E-15	3.32E-14	29.47	3.83	66.71	0	0.3342	-13.834	-14.721	-13.479
1.00E-02	1.83E-16	6.83E-17	3.39E-16	31.06	11.57	57.37	-2	0.1474	-15.736	-16.165	-15.470
1.00E-04	1.84E-18	7.21E-19	3.39E-18	30.93	12.12	56.95	-4	0.1390	-17.735	-18.142	-17.470
1.00E-06	1.84E-20	7.22E-21	3.39E-20	30.93	12.13	56.95	-6	0.1390	-19.735	-20.142	-19.470
1.00E-08	1.84E-22	7.22E-23	3.39E-22	30.93	12.13	56.95	-8	0.1390	-21.735	-22.142	-21.470
1.00E-10	1.84E-24	7.22E-25	3.39E-24	30.93	12.13	56.95	-10	0.1390	-23.735	-24.142	-23.470

Table S3d: T= 344 K.

P	Effective rate constants			Branching ratios			Regioselectivity				
	k_{eff}(**1**)	k_{eff}(**2**)	k_{eff}(**3**)	R(**1**)	R(**2**)	R(**3**)	LogP	{R(**3**)−[R(**1**)+R(**2**)]/ [R(**1**)+R(**1**)+R(**3**)]}	logk_{eff}(**1**)	logk_{eff}(**2**)	logk_{eff}(**3**)
1.00E+08	1.36E-13	4.09E-15	1.94E-12	6.56	0.20	93.25	8	0.8649	-12.866	-14.388	-11.713
1.00E+06	1.36E-13	4.09E-15	1.94E-12	6.56	0.20	93.25	6	0.8649	-12.866	-14.388	-11.713
1.00E+04	1.36E-13	4.09E-15	1.92E-12	6.59	0.20	93.21	4	0.8642	-12.867	-14.388	-11.716
1.00E+02	1.20E-13	4.04E-15	1.13E-12	9.58	0.32	90.10	2	0.8019	-12.919	-14.393	-11.946
1.00E+00	1.39E-14	2.14E-15	2.95E-14	30.52	4.71	64.77	0	0.2955	-13.858	-14.669	-13.531
1.00E-02	1.71E-16	7.17E-17	3.00E-16	31.45	13.22	55.34	-2	0.1067	-15.768	-16.144	-15.522
1.00E-04	1.71E-18	7.54E-19	3.00E-18	31.29	13.78	54.92	-4	0.0985	-17.767	-18.123	-17.522
1.00E-06	1.71E-20	7.54E-21	3.00E-20	31.29	13.79	54.92	-6	0.0984	-19.767	-20.122	-19.522
1.00E-08	1.71E-22	7.54E-23	3.00E-22	31.29	13.79	54.92	-8	0.0984	-21.767	-22.122	-21.522
1.00E-10	1.71E-24	7.54E-25	3.00E-24	31.29	13.79	54.92	-10	0.0984	-23.767	-24.122	-23.522

Table S3e: T= 353 K.

P	Effective rate constants			Branching ratios			Regioselectivity				
	k_{eff}(**1**)	k_{eff}(**2**)	k_{eff}(**3**)	R(**1**)	R(**2**)	R(**3**)	LogP	{R(**3**)−[R(**1**)+R(**2**)]/ [R(**1**)+R(**1**)+R(**3**)]}	logk_{eff}(**1**)	logk_{eff}(**2**)	logk_{eff}(**3**)
1.00E+08	1.40E-13	4.57E-15	1.87E-12	6.93	0.23	92.85	8	0.8569	-12.854	-14.340	-11.727
1.00E+06	1.40E-13	4.57E-15	1.87E-12	6.93	0.23	92.85	6	0.8569	-12.854	-14.340	-11.727
1.00E+04	1.40E-13	4.57E-15	1.86E-12	6.97	0.23	92.81	4	0.8561	-12.855	-14.340	-11.731
1.00E+02	1.23E-13	4.51E-15	1.08E-12	10.20	0.37	89.43	2	0.7886	-12.911	-14.346	-11.968
1.00E+00	1.34E-14	2.30E-15	2.72E-14	31.20	5.37	63.43	0	0.2686	-13.874	-14.638	-13.565
1.00E-02	1.63E-16	7.37E-17	2.77E-16	31.69	14.35	53.97	-2	0.0793	-15.789	-16.133	-15.557
1.00E-04	1.63E-18	7.72E-19	2.77E-18	31.53	14.92	53.56	-4	0.0711	-17.787	-18.112	-17.557
1.00E-06	1.63E-20	7.72E-21	2.77E-20	31.52	14.92	53.55	-6	0.0711	-19.787	-20.112	-19.557
1.00E-08	1.63E-22	7.72E-23	2.77E-22	31.52	14.92	53.55	-8	0.0711	-21.787	-22.112	-21.557
1.00E-10	1.63E-24	7.72E-25	2.77E-24	31.52	14.92	53.55	-10	0.0711	-23.787	-24.112	-23.557

Table S3f: T= 362 K.

P	Effective rate constants			Branching ratios			Regioselectivity				
	k_{eff}(**1**)	k_{eff}(**2**)	k_{eff}(**3**)	R(**1**)	R(**2**)	R(**3**)	LogP	{R(**3**)−[R(**1**)+R(**2**)]/ [R(**1**)+R(**1**)+R(**3**)]}	logk_{eff}(**1**)	logk_{eff}(**2**)	logk_{eff}(**3**)
1.00E+08	1.43E-13	5.09E-15	1.82E-12	7.27	0.26	92.47	8	0.8494	-12.843	-14.293	-11.739
1.00E+06	1.43E-13	5.09E-15	1.82E-12	7.27	0.26	92.47	6	0.8494	-12.843	-14.293	-11.739
1.00E+04	1.43E-13	5.09E-15	1.81E-12	7.31	0.26	92.43	4	0.8485	-12.844	-14.293	-11.742
1.00E+02	1.25E-13	5.02E-15	1.03E-12	10.78	0.43	88.79	2	0.7758	-12.904	-14.300	-11.988
1.00E+00	1.29E-14	2.47E-15	2.53E-14	31.71	6.08	62.21	0	0.2442	-13.890	-14.607	-13.597
1.00E-02	1.55E-16	7.55E-17	2.57E-16	31.78	15.48	52.74	-2	0.0548	-15.810	-16.122	-15.589
1.00E-04	1.55E-18	7.89E-19	2.57E-18	31.61	16.05	52.34	-4	0.0468	-17.808	-18.103	-17.589
1.00E-06	1.55E-20	7.90E-21	2.57E-20	31.61	16.06	52.34	-6	0.0467	-19.808	-20.102	-19.589
1.00E-08	1.55E-22	7.90E-23	2.57E-22	31.61	16.06	52.34	-8	0.0467	-21.808	-22.102	-21.589
1.00E-10	1.55E-24	7.90E-25	2.57E-24	31.61	16.06	52.34	-10	0.0467	-23.808	-24.102	-23.589

Table S3g: T= 386 K.

P	Effective rate constants			Branching ratios			Regioselectivity				
	k_{eff}(**1**)	k_{eff}(**2**)	k_{eff}(**3**)	R(**1**)	R(**2**)	R(**3**)	LogP	{R(**3**)−[R(**1**)+R(**2**)]/ [R(**1**)+R(**1**)+R(**3**)]}	logk_{eff}(**1**)	logk_{eff}(**2**)	logk_{eff}(**3**)
1.00E+08	1.54E-13	6.64E-15	1.71E-12	8.20	0.35	91.45	8	0.8290	-12.814	-14.178	-11.766
1.00E+06	1.54E-13	6.64E-15	1.71E-12	8.20	0.35	91.45	6	0.8290	-12.814	-14.178	-11.766
1.00E+04	1.53E-13	6.64E-15	1.70E-12	8.25	0.36	91.39	4	0.8278	-12.814	-14.178	-11.770
1.00E+02	1.31E-13	6.53E-15	9.21E-13	12.34	0.62	87.04	2	0.7409	-12.884	-14.185	-12.036
1.00E+00	1.17E-14	2.90E-15	2.11E-14	32.73	8.12	59.15	0	0.1830	-13.932	-14.537	-13.675
1.00E-02	1.37E-16	7.94E-17	2.15E-16	31.80	18.41	49.79	-2	-0.0042	-15.863	-16.100	-15.668
1.00E-04	1.37E-18	8.24E-19	2.15E-18	31.62	18.97	49.42	-4	-0.0117	-17.862	-18.084	-17.668
1.00E-06	1.37E-20	8.24E-21	2.15E-20	31.62	18.97	49.41	-6	-0.0118	-19.862	-20.084	-19.668
1.00E-08	1.37E-22	8.24E-23	2.15E-22	31.62	18.97	49.41	-8	-0.0118	-21.862	-22.084	-21.668
1.00E-10	1.37E-24	8.24E-25	2.15E-24	31.62	18.97	49.41	-10	-0.0118	-23.862	-24.084	-23.668

Table S3h: T= 402 K.

P	Effective rate constants			Branching ratios			Regioselectivity				
	k_{eff}(**1**)	k_{eff}(**2**)	k_{eff}(**3**)	R(**1**)	R(**2**)	R(**3**)	LogP	{R(**3**)–[R(**1**)+R(**2**)]/ [R(**1**)+R(**1**)+R(**3**)]}	logk_{eff}(**1**)	logk_{eff}(**2**)	logk_{eff}(**3**)
1.00E+08	1.60E-13	7.84E-15	1.66E-12	8.76	0.43	90.81	8	0.8162	-12.795	-14.106	-11.780
1.00E+06	1.60E-13	7.84E-15	1.66E-12	8.76	0.43	90.81	6	0.8162	-12.795	-14.106	-11.780
1.00E+04	1.60E-13	7.84E-15	1.64E-12	8.82	0.43	90.75	4	0.8149	-12.796	-14.106	-11.784
1.00E+02	1.34E-13	7.68E-15	8.64E-13	13.31	0.76	85.93	2	0.7186	-12.873	-14.115	-12.063
1.00E+00	1.09E-14	3.19E-15	1.90E-14	33.01	9.61	57.38	0	0.1477	-13.961	-14.496	-13.720
1.00E-02	1.26E-16	8.13E-17	1.93E-16	31.54	20.29	48.17	-2	-0.0365	-15.898	-16.090	-15.714
1.00E-04	1.27E-18	8.41E-19	1.93E-18	31.36	20.82	47.82	-4	-0.0436	-17.898	-18.075	-17.714
1.00E-06	1.27E-20	8.41E-21	1.93E-20	31.36	20.83	47.81	-6	-0.0437	-19.898	-20.075	-19.714
1.00E-08	1.27E-22	8.41E-23	1.93E-22	31.36	20.83	47.81	-8	-0.0437	-21.898	-22.075	-21.714
1.00E-10	1.27E-24	8.41E-25	1.93E-24	31.36	20.83	47.81	-10	-0.0437	-23.898	-24.075	-23.714

Table S3i: T= 425 K.

P	Effective rate constants			Branching ratios			Regioselectivity				
	k_{eff}(**1**)	k_{eff}(**2**)	k_{eff}(**3**)	R(**1**)	R(**2**)	R(**3**)	LogP	{R(**3**)−[R(**1**)+R(**2**)]/ [R(**1**)+R(**1**)+R(**3**)]}	logk_{eff}(**1**)	logk_{eff}(**2**)	logk_{eff}(**3**)
1.00E+08	1.71E-13	9.77E-15	1.60E-12	9.60	0.55	89.85	8	0.7969	-12.767	-14.010	-11.796
1.00E+06	1.71E-13	9.77E-15	1.60E-12	9.60	0.55	89.85	6	0.7970	-12.767	-14.010	-11.796
1.00E+04	1.70E-13	9.76E-15	1.58E-12	9.67	0.55	89.77	4	0.7955	-12.768	-14.010	-11.801
1.00E+02	1.39E-13	9.52E-15	7.95E-13	14.73	1.01	84.26	2	0.6852	-12.857	-14.021	-12.099
1.00E+00	1.00E-14	3.57E-15	1.66E-14	33.23	11.82	54.96	0	0.0991	-13.998	-14.447	-13.780
1.00E-02	1.14E-16	8.30E-17	1.68E-16	31.15	22.75	46.09	-2	-0.0782	-15.945	-16.081	-15.774
1.00E-04	1.14E-18	8.54E-19	1.68E-18	30.98	23.25	45.77	-4	-0.0846	-17.944	-18.069	-17.774
1.00E-06	1.14E-20	8.54E-21	1.68E-20	30.98	23.26	45.77	-6	-0.0847	-19.944	-20.068	-19.774
1.00E-08	1.14E-22	8.54E-23	1.68E-22	30.98	23.26	45.77	-8	-0.0847	-21.944	-22.068	-21.774
1.00E-10	1.14E-24	8.54E-25	1.68E-24	30.98	23.26	45.77	-10	-0.0847	-23.944	-24.068	-23.774

Table S3j: T= 440 K.

P	Effective rate constants			Branching ratios			Regioselectivity				
	k_{eff}(**1**)	k_{eff}(**2**)	k_{eff}(**3**)	R(**1**)	R(**2**)	R(**3**)	LogP	{R(**3**)−[R(**1**)+R(**2**)]/ [R(**1**)+R(**1**)+R(**3**)]}	logk_{eff}(**1**)	logk_{eff}(**2**)	logk_{eff}(**3**)
1.00E+08	1.78E-13	1.11E-14	1.56E-12	10.16	0.64	89.21	8	0.7841	-12.749	-13.953	-11.806
1.00E+06	1.78E-13	1.11E-14	1.56E-12	10.16	0.64	89.21	6	0.7841	-12.749	-13.953	-11.806
1.00E+04	1.78E-13	1.11E-14	1.55E-12	10.23	0.64	89.12	4	0.7825	-12.750	-13.953	-11.810
1.00E+02	1.42E-13	1.08E-14	7.56E-13	15.66	1.19	83.15	2	0.6630	-12.846	-13.965	-12.121
1.00E+00	9.50E-15	3.79E-15	1.53E-14	33.24	13.28	53.48	0	0.0696	-14.022	-14.421	-13.816
1.00E-02	1.06E-16	8.34E-17	1.55E-16	30.89	24.21	44.90	-2	-0.1020	-15.973	-16.079	-15.811
1.00E-04	1.06E-18	8.56E-19	1.55E-18	30.72	24.68	44.60	-4	-0.1080	-17.973	-18.068	-17.811
1.00E-06	1.06E-20	8.56E-21	1.55E-20	30.72	24.69	44.60	-6	-0.1080	-19.973	-20.068	-19.811
1.00E-08	1.06E-22	8.56E-23	1.55E-22	30.72	24.69	44.60	-8	-0.1080	-21.973	-22.068	-21.811
1.00E-10	1.06E-24	8.56E-25	1.55E-24	30.72	24.69	44.60	-10	-0.1080	-23.973	-24.068	-23.811