Supporting Information

Modeling the kinetics of hydrogen abstraction reactions in nitrogen-containing compounds via group additivity

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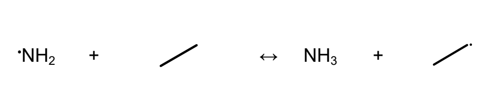
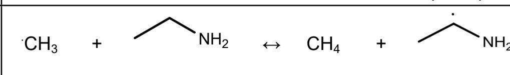
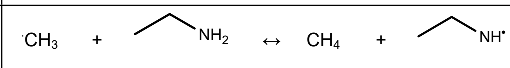
1. CBS-QB3 methodology: Experimental validation

Table S1: Experimental validation of the CBS-QB3 methodology: Source and kinetic parameters for the modified Arrhenius expression, i.e. k=A·T^n·exp(-E_a/RT). The pre-exponential factor is expressed in m^3 mol^{-1} s^{-1} and E_a is expressed in kJ mol^{-1}.

No.	Reaction	Ref	Temperature [K]	*A*	*n*	E_a
1	H + NH_3 ↔ H_2 + $^{\bullet}NH_2$	[1]	490 – 960	7.29E+07	0.0	57.5
		[2]	524 - 714	4.00E+06	0.0	41.8
		[3]	863 - 963	4.09E+07	0.0	57.3
		[4]	673 – 1000	8.07E+07	0.0	60.9
		[5]	500 - 1800	6.36E-01	2.39	42.6
		[6]	908 - 1780	3.44E+08	0.0	67.1
2	$^{\bullet}NH_2$ + CH_4 ↔ NH_3 + $^{\bullet}CH_3$	[7]	300 - 520	4.94E+05	0.0	43.9
		[8]	743 - 1020	4.70E+06	0.0	38.9
		[9]	1500 – 2100	1.20E+07	0.0	63.4
		[10]	1591 – 2084	7.05E+07	0.0	71.3
3		[7]	300 - 520	3.70E+05	0.0	29.9
		[11]	600 – 970	9.70E+06	0.0	44.4
		[9]	1500 – 2100	9.70E+06	0.0	48.0
4	$^{\bullet}CH_3$ + —NH_2 ↔ CH_4 + $^{\bullet}$—NH_2	[12]	380 - 450	9.76E+04	0.0	36.4
5	$^{\bullet}CH_3$ + —NH_2 ↔ CH_4 + —$NH^{\bullet}$	[12]	380 - 450	3.55E+03	0.0	23.9
6		[13]	400 - 450	6.31E+10	0.0	26.8
7		[14]	380 – 450	1.50E+05	0.0	33.9
8		[14]	380 - 450	7.59E+03	0.0	27.1

2. H-H-N hydrogen abstractions

2.1. Single-event Arrhenius parameters for reference reaction

Table S2: Intrinsic Arrhenius parameters over the temperature range 300-1800 K for the reference reaction of H-H-N hydrogen abstraction reactions, i.e. H· + NH_3 → H_2 + ·NH_2. The single-event pre-exponential factor is expressed in m^3 mol^{-1} s^{-1} and E_a is expressed in kJ mol^{-1}.

Temperature [K]	Forward		Reverse	
	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a
300	7.124	57.7	6.048	48.2
400	7.203	58.2	6.040	48.1
500	7.249	58.5	6.069	48.3
600	7.355	59.6	6.140	49.0
700	7.462	60.9	6.235	50.1
800	7.563	62.3	6.339	51.6
900	7.658	63.8	6.444	53.2
1000	7.746	65.4	6.545	55.1
1100	7.826	67.0	6.642	57.0
1200	7.900	68.6	6.733	59.0
1300	7.967	70.2	6.818	61.0
1400	8.030	71.8	6.896	63.0
1500	8.087	73.4	6.969	65.0
1600	8.140	75.0	7.037	67.0
1700	8.190	76.5	7.100	69.0
1800	8.236	78.1	7.158	71.0

2.2. Rate coefficients between 300 and 1800 K

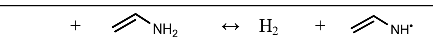
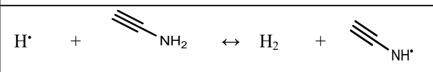
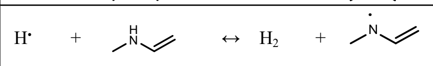
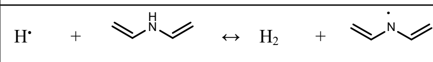
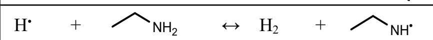
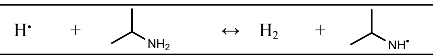
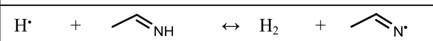
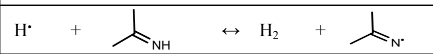
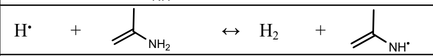
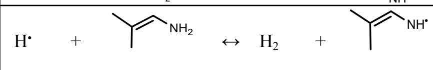
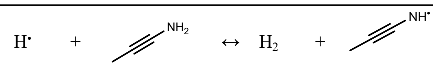
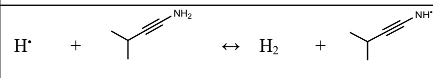
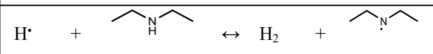
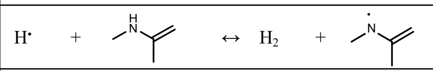
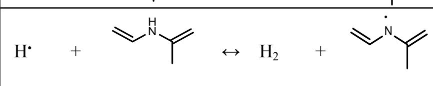
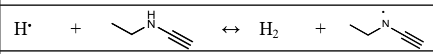
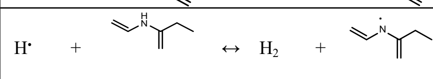
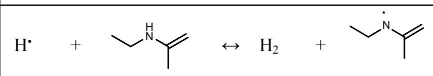
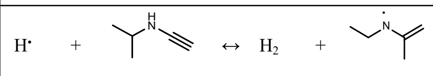
Table S3: Rate coefficients [m^3 mol^{-1} s^{-1}] in the temperature range 300-1800 K for the reactions presented in Table S4. The rate coefficients do not include tunneling contributions.

No.		300 K	400 K	500 K	600 K	700 K	800 K	900 K	1000 K	1100 K	1200 K	1300 K	1400 K	1500 K	1600 K	1700 K	1800 K
1	→	3.6E-03	1.2E+00	3.9E+01	4.2E+02	2.4E+03	9.1E+03	2.6E+04	6.3E+04	1.3E+05	2.4E+05	4.2E+05	6.7E+05	1.0E+06	1.5E+06	2.1E+06	2.8E+06
1	←	1.9E-02	2.3E+00	4.1E+01	2.9E+02	1.2E+03	3.6E+03	8.8E+03	1.8E+04	3.4E+04	5.8E+04	9.2E+04	1.4E+05	2.0E+05	2.8E+05	3.8E+05	5.0E+05
2	→	2.1E+00	1.2E+02	1.5E+03	7.9E+03	2.8E+04	7.3E+04	1.6E+05	3.0E+05	5.2E+05	8.2E+05	1.2E+06	1.8E+06	2.4E+06	3.2E+06	4.2E+06	5.3E+06
2	←	2.5E-05	1.3E-02	5.9E-01	7.8E+00	5.1E+01	2.1E+02	6.8E+02	1.7E+03	3.9E+03	7.6E+03	1.4E+04	2.3E+04	3.7E+04	5.6E+04	8.2E+04	1.2E+05
3	→	1.8E+04	9.2E+04	2.7E+05	5.7E+05	1.0E+06	1.6E+06	2.4E+06	3.3E+06	4.4E+06	5.7E+06	7.1E+06	8.7E+06	1.0E+07	1.2E+07	1.5E+07	1.7E+07
3	←	6.1E-10	4.9E-06	1.1E-03	4.2E-02	5.9E-01	4.4E+00	2.2E+01	7.9E+01	2.3E+02	5.8E+02	1.3E+03	2.6E+03	4.8E+03	8.2E+03	1.3E+04	2.1E+04
4	→	3.3E+00	1.3E+02	1.2E+03	6.0E+03	2.0E+04	4.9E+04	1.0E+05	1.9E+05	3.3E+05	5.1E+05	7.7E+05	1.1E+06	1.5E+06	2.0E+06	2.6E+06	3.3E+06
4	←	1.1E-13	5.4E-09	3.8E-06	3.2E-04	8.0E-03	9.4E-02	6.6E-01	3.2E+00	1.2E+01	3.7E+01	9.8E+01	2.3E+02	4.8E+02	9.2E+02	1.7E+03	2.8E+03
5	→	1.5E+01	5.1E+02	4.4E+03	1.9E+04	5.8E+04	1.4E+05	2.7E+05	4.8E+05	7.7E+05	1.2E+06	1.7E+06	2.3E+06	3.1E+06	4.1E+06	5.2E+06	6.4E+06
5	←	4.6E-14	3.9E-09	3.6E-06	3.5E-04	9.6E-03	1.2E-01	8.7E-01	4.4E+00	1.7E+01	5.2E+01	1.4E+02	3.2E+02	6.9E+02	1.3E+03	2.4E+03	4.2E+03
6	→	2.4E+02	4.0E+03	2.2E+04	7.4E+04	1.8E+05	3.6E+05	6.4E+05	1.0E+06	1.5E+06	2.2E+06	2.9E+06	3.8E+06	4.9E+06	6.1E+06	7.5E+06	9.0E+06
6	←	8.7E-08	1.6E-04	1.6E-02	3.6E-01	3.5E+00	2.0E+01	8.2E+01	2.6E+02	6.8E+02	1.5E+03	3.1E+03	5.9E+03	1.0E+04	1.7E+04	2.6E+04	4.0E+04
7	→	3.4E+01	6.6E+02	4.2E+03	1.5E+04	4.1E+04	8.8E+04	1.7E+05	2.8E+05	4.4E+05	6.5E+05	9.2E+05	1.3E+06	1.6E+06	2.1E+06	2.6E+06	3.3E+06
7	←	2.2E-14	2.2E-09	2.4E-06	2.7E-04	8.6E-03	1.2E-01	9.7E-01	5.3E+00	2.2E+01	7.4E+01	2.1E+02	5.2E+02	1.1E+03	2.3E+03	4.4E+03	7.8E+03
8	→	9.4E-01	4.8E+01	5.2E+02	2.6E+03	8.4E+03	2.1E+04	4.3E+04	7.8E+04	1.3E+05	2.0E+05	2.9E+05	4.0E+05	5.3E+05	6.9E+05	8.7E+05	1.1E+06
8	←	7.9E-19	1.9E-12	1.3E-08	4.9E-06	3.4E-04	8.4E-03	1.0E-01	7.5E-01	3.9E+00	1.6E+01	5.0E+01	1.4E+02	3.3E+02	7.3E+02	1.5E+03	2.7E+03
9	→	2.6E+02	3.5E+03	1.8E+04	5.4E+04	1.3E+05	2.4E+05	4.2E+05	6.7E+05	9.8E+05	1.4E+06	1.9E+06	2.5E+06	3.1E+06	3.9E+06	4.8E+06	5.7E+06
9	←	3.9E-15	5.2E-10	6.6E-07	8.1E-05	2.6E-03	3.8E-02	3.0E-01	1.7E+00	6.9E+00	2.3E+01	6.4E+01	1.6E+02	3.5E+02	7.0E+02	1.3E+03	2.3E+03
10	→	3.9E+00	1.9E+02	2.1E+03	1.1E+04	3.7E+04	9.4E+04	2.0E+05	3.7E+05	6.3E+05	9.9E+05	1.5E+06	2.1E+06	2.9E+06	3.8E+06	4.9E+06	6.2E+06
10	←	4.5E-05	2.0E-02	8.4E-01	1.0E+01	6.5E+01	2.7E+02	8.2E+02	2.1E+03	4.6E+03	9.0E+03	1.6E+04	2.7E+04	4.3E+04	6.4E+04	9.4E+04	1.3E+05
11	→	1.2E+00	7.9E+01	1.0E+03	5.8E+03	2.1E+04	5.7E+04	1.3E+05	2.5E+05	4.3E+05	6.9E+05	1.0E+06	1.5E+06	2.1E+06	2.8E+06	3.7E+06	4.7E+06
11	←	9.6E-05	3.3E-02	1.2E+00	1.3E+01	7.6E+01	3.0E+02	8.9E+02	2.2E+03	4.7E+03	9.0E+03	1.6E+04	2.6E+04	4.1E+04	6.2E+04	8.9E+04	1.2E+05
12	→	3.5E+00	1.8E+02	2.0E+03	1.0E+04	3.5E+04	9.1E+04	1.9E+05	3.7E+05	6.2E+05	9.9E+05	1.5E+06	2.1E+06	2.9E+06	3.8E+06	5.0E+06	6.3E+06
12	←	2.6E-05	1.4E-02	6.4E-01	8.5E+00	5.6E+01	2.4E+02	7.6E+02	2.0E+03	4.4E+03	8.7E+03	1.6E+04	2.7E+04	4.3E+04	6.5E+04	9.5E+04	1.3E+05
13	→	9.4E+03	5.7E+04	1.8E+05	4.0E+05	7.5E+05	1.2E+06	1.9E+06	2.6E+06	3.6E+06	4.7E+06	5.9E+06	7.4E+06	9.0E+06	1.1E+07	1.3E+07	1.5E+07
13	←	2.8E-09	1.2E-05	1.8E-03	5.5E-02	6.5E-01	4.3E+00	1.9E+01	6.6E+01	1.8E+02	4.4E+02	9.5E+02	1.8E+03	3.3E+03	5.6E+03	8.9E+03	1.4E+04
14	→	3.5E+03	2.7E+04	9.6E+04	2.4E+05	4.7E+05	8.1E+05	1.3E+06	1.9E+06	2.6E+06	3.4E+06	4.5E+06	5.6E+06	6.9E+06	8.4E+06	1.0E+07	1.2E+07

14	←	3.7E-09	1.7E-05	2.8E-03	8.6E-02	1.0E+00	7.0E+00	3.2E+01	1.1E+02	3.1E+02	7.4E+02	1.6E+03	3.1E+03	5.6E+03	9.5E+03	1.5E+04	2.4E+04
15	→	3.2E+01	7.5E+02	5.3E+03	2.1E+04	5.7E+04	1.3E+05	2.5E+05	4.2E+05	6.8E+05	1.0E+06	1.5E+06	2.0E+06	2.7E+06	3.5E+06	4.5E+06	5.5E+06
15	←	2.4E-12	6.7E-08	3.3E-05	2.2E-03	4.7E-02	4.9E-01	3.2E+00	1.5E+01	5.2E+01	1.5E+02	3.9E+02	8.9E+02	1.8E+03	3.5E+03	6.2E+03	1.0E+04
16	→	5.5E+02	6.9E+03	3.3E+04	9.8E+04	2.2E+05	4.2E+05	7.0E+05	1.1E+06	1.6E+06	2.2E+06	3.0E+06	3.9E+06	4.9E+06	6.1E+06	7.4E+06	8.9E+06
16	←	1.5E-14	2.3E-09	3.2E-06	4.1E-04	1.4E-02	2.1E-01	1.7E+00	9.8E+00	4.1E+01	1.4E+02	4.0E+02	9.9E+02	2.2E+03	4.5E+03	8.5E+03	1.5E+04
17	→	4.3E+01	8.9E+02	5.7E+03	2.1E+04	5.4E+04	1.1E+05	2.1E+05	3.5E+05	5.3E+05	7.7E+05	1.1E+06	1.4E+06	1.9E+06	2.4E+06	2.9E+06	3.6E+06
17	←	2.0E-14	1.9E-09	1.9E-06	2.0E-04	5.7E-03	7.4E-02	5.5E-01	2.8E+00	1.1E+01	3.5E+01	9.4E+01	2.2E+02	4.8E+02	9.4E+02	1.7E+03	3.0E+03
18	→	1.4E+02	2.8E+03	1.8E+04	6.4E+04	1.7E+05	3.5E+05	6.4E+05	1.1E+06	1.6E+06	2.3E+06	3.2E+06	4.3E+06	5.6E+06	7.1E+06	8.8E+06	1.1E+07
18	←	1.1E-13	1.0E-08	1.1E-05	1.1E-03	3.2E-02	4.2E-01	3.1E+00	1.6E+01	6.3E+01	2.0E+02	5.4E+02	1.3E+03	2.7E+03	5.4E+03	9.9E+03	1.7E+04
19	→	5.9E+01	1.3E+03	9.0E+03	3.4E+04	9.1E+04	2.0E+05	3.6E+05	6.1E+05	9.4E+05	1.4E+06	1.9E+06	2.6E+06	3.4E+06	4.3E+06	5.3E+06	6.5E+06
19	←	2.0E-08	5.1E-05	6.1E-03	1.6E-01	1.7E+00	1.0E+01	4.4E+01	1.5E+02	3.9E+02	9.2E+02	1.9E+03	3.7E+03	6.5E+03	1.1E+04	1.7E+04	2.6E+04
20	→	2.9E+02	4.2E+03	2.1E+04	6.6E+04	1.5E+05	2.9E+05	5.0E+05	7.8E+05	1.1E+06	1.6E+06	2.1E+06	2.7E+06	3.4E+06	4.2E+06	5.1E+06	6.1E+06
20	←	9.9E-08	1.6E-04	1.5E-02	3.1E-01	2.8E+00	1.5E+01	5.9E+01	1.8E+02	4.6E+02	1.0E+03	2.0E+03	3.7E+03	6.3E+03	1.0E+04	1.6E+04	2.3E+04
21	→	1.9E+02	2.6E+03	1.3E+04	4.0E+04	9.3E+04	1.8E+05	3.1E+05	5.0E+05	7.4E+05	1.1E+06	1.4E+06	1.9E+06	2.5E+06	3.1E+06	3.8E+06	4.6E+06
21	←	3.6E-12	6.7E-08	2.6E-05	1.5E-03	2.8E-02	2.7E-01	1.7E+00	7.3E+00	2.5E+01	7.3E+01	1.8E+02	4.0E+02	8.2E+02	1.5E+03	2.7E+03	4.5E+03
22	→	2.6E-02	3.9E+00	8.3E+01	6.7E+02	3.1E+03	1.0E+04	2.7E+04	5.8E+04	1.1E+05	1.9E+05	3.1E+05	4.8E+05	6.9E+05	9.6E+05	1.3E+06	1.7E+06
22	←	1.3E-18	2.3E-12	1.3E-08	4.0E-06	2.5E-04	5.8E-03	6.7E-02	4.8E-01	2.4E+00	9.6E+00	3.1E+01	8.4E+01	2.0E+02	4.4E+02	8.8E+02	1.6E+03
23	→	1.6E+02	2.2E+03	1.1E+04	3.4E+04	8.0E+04	1.6E+05	2.7E+05	4.2E+05	6.2E+05	8.8E+05	1.2E+06	1.5E+06	2.0E+06	2.5E+06	3.0E+06	3.6E+06
23	←	3.8E-15	5.0E-10	6.2E-07	7.6E-05	2.5E-03	3.5E-02	2.9E-01	1.6E+00	6.5E+00	2.2E+01	6.1E+01	1.5E+02	3.3E+02	6.7E+02	1.3E+03	2.2E+03
24	→	1.3E+01	3.9E+02	3.2E+03	1.4E+04	4.1E+04	9.6E+04	1.9E+05	3.4E+05	5.5E+05	8.4E+05	1.2E+06	1.7E+06	2.2E+06	2.9E+06	3.6E+06	4.4E+06
24	←	3.0E-16	9.3E-11	1.9E-07	3.3E-05	1.3E-03	2.2E-02	2.1E-01	1.2E+00	5.5E+00	1.9E+01	5.7E+01	1.4E+02	3.3E+02	6.8E+02	1.3E+03	2.3E+03
25	→	1.7E+02	2.3E+03	1.2E+04	3.5E+04	8.2E+04	1.6E+05	2.8E+05	4.4E+05	6.5E+05	9.3E+05	1.3E+06	1.7E+06	2.1E+06	2.7E+06	3.3E+06	4.0E+06
25	←	1.1E-12	3.6E-08	2.0E-05	1.4E-03	3.1E-02	3.4E-01	2.3E+00	1.1E+01	3.9E+01	1.2E+02	3.1E+02	7.1E+02	1.5E+03	2.9E+03	5.2E+03	8.8E+03
26	→	1.7E+02	2.5E+03	1.3E+04	4.1E+04	9.7E+04	1.9E+05	3.3E+05	5.3E+05	7.8E+05	1.1E+06	1.5E+06	2.0E+06	2.5E+06	3.2E+06	3.9E+06	4.7E+06
26	←	8.5E-15	9.0E-10	9.8E-07	1.1E-04	3.3E-03	4.5E-02	3.5E-01	1.9E+00	7.6E+00	2.5E+01	6.9E+01	1.7E+02	3.6E+02	7.3E+02	1.4E+03	2.4E+03

2.3. Arrhenius parameters regressed at 1000 K

Table S4: Standard reaction enthalpy [kJ mol^{-1}], pre-exponential factor [m^3 mol^{-1} s^{-1}], activation energy [kJ mol^{-1}], rate coefficient [m^3 mol^{-1} s^{-1}] and deviation factor at 1000 K for 25 H-H-N hydrogen abstraction reactions in the training (T) and validation dataset (V). The Arrhenius parameters exclude tunneling.

No.		Reaction	ΔH_r°	Forward			Reverse			ρ (1000 K)	
				$logA$	E_a	k_{for}	$logA$	E_a	k_{rev}	*for*	*rev*
1	T	H· + NH_3 ↔ H_2 + NH_2·	12.4	8.223	65.4	6.3E+04	7.147	55.1	1.8E+04	-	-
2	T	H· + —NH_2 ↔ H_2 + —NH·	-21.3	8.010	48.3	3.0E+05	6.972	71.2	1.7E+03	1.1	1.1
3	T	H· + =NH ↔ H_2 + =N·	-72.5	7.835	25.0	3.3E+06	6.998	97.5	7.9E+01	1.3	1.7
4	T		-69.8	7.742	46.9	1.9E+05	6.749	119.3	3.2E+00	2.3	1.9
5	T		-77.2	7.933	43.0	4.8E+05	6.982	121.2	4.4E+00	1.4	1.2
6	T		-46.1	7.872	35.5	1.0E+06	6.937	86.4	2.6E+02	1.3	1.4
7	T		-81.2	7.540	39.9	2.8E+05	7.429	128.1	5.3E+00	1.4	1.4
8	T		-105.9	7.241	44.9	7.8E+04	7.720	150.1	7.5E-01	1.5	1.0
9	T		-91.1	7.636	34.5	6.7E+05	6.915	127.9	1.7E+00	1.3	1.0
10	V		-21.1	8.032	46.9	3.7E+05	6.992	70.1	2.1E+03	1.2	1.0
11	V		-15.9	7.992	49.7	2.5E+05	6.899	67.9	2.2E+03	1.3	1.1
12	V		-23.1	8.060	47.6	3.7E+05	7.049	71.7	2.0E+03	1.2	1.0
13	V		-64.7	7.820	26.6	2.6E+06	6.656	92.4	6.6E+01	1.0	1.0
14	V		-63.3	7.786	28.9	1.9E+06	6.908	93.1	1.1E+02	1.4	1.7
15	V		-69.6	7.810	41.6	4.2E+05	7.157	114.5	1.5E+01	1.1	1.2
16	V		-90.1	7.786	33.3	1.1E+06	7.782	129.8	9.8E+00	2.4	1.3
17	V		-83.4	7.539	38.1	3.5E+05	6.885	122.9	2.8E+00	2.0	2.6
18	V		-82.8	8.007	37.9	1.1E+06	7.650	123.1	1.6E+01	1.5	2.2
19	V		-46.3	7.826	38.9	6.1E+05	6.845	89.4	1.5E+02	1.3	1.3
20	V		-49.9	7.651	33.5	7.8E+05	6.630	83.6	1.8E+02	1.0	1.0
21	V		-76.1	7.545	35.2	5.0E+05	6.689	111.3	7.3E+00	1.3	1.0
22	V		-99.1	7.824	58.5	5.8E+04	7.412	147.9	4.8E-01	2.0	1.6
23	V		-90.7	7.434	34.5	4.2E+05	6.897	128.1	1.6E+00	1.3	1.1
24	V		-86.0	7.786	43.0	3.4E+05	7.143	134.8	1.2E+00	2.9	1.6
25	V		-76.1	7.485	35.1	4.4E+05	7.144	116.8	1.1E+01	1.1	1.4
26	V		-88.0	7.564	35.1	5.3E+05	6.861	125.9	1.9E+00	1.0	1.1

2.4. Reaction path degeneracy

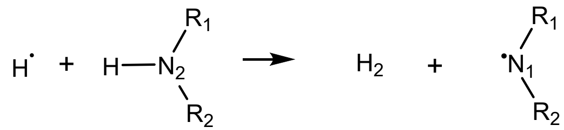
Table S5: External and internal symmetry numbers, number of optical isomers and number of single events n_e for all H-H-N hydrogen abstractions of Table S4.

No.		Reactant 1 R˙			Reactant 2 RH			Transition state			Reaction path degeneracy
		σ_{ext}	σ_{int}	n_{op}	σ_{ext}	σ_{int}	n_{op}	σ_{ext}	σ_{int}	n_{opt}	n_e
1	→	1	1	1	3	1	1	1	1	1	3
1	←	2	1	1	1	1	3	1	1	1	4
2	←	1	1	1	1	3	1	1	3	2	2
2	→	2	1	1	1	1	2	1	3	2	4
3	←	1	1	1	1	1	1	1	1	1	1
3	→	2	1	1	2	1	1	1	1	1	4
4	←	1	1	1	1	1	1	1	1	2	2
4	→	2	1	1	1	1	2	1	1	2	4
5	←	1	1	1	1	1	1	1	1	1	1
5	→	2	1	1	1	1	1	1	1	1	2
6	←	1	1	1	1	9	1	1	9	1	1
6	→	2	1	1	9	1	1	1	9	1	4
7	←	1	1	1	1	3	2	1	3	2	1
7	→	2	1	1	3	1	1	1	3	2	4
8	←	1	1	1	1	1	1	1	1	1	1
8	→	2	1	1	2	1	1	1	1	1	4
9	←	1	1	1	1	3	2	1	3	2	1
9	→	2	1	1	3	1	1	1	3	2	4
10	←	1	1	1	1	3	1	1	3	2	2
10	→	2	1	1	3	1	2	1	3	2	4
11	←	1	1	1	1	9	1	1	9	2	2
11	→	2	1	1	9	1	2	1	9	2	4
12	←	1	1	1	1	9	1	1	9	2	2
12	→	2	1	1	9	1	2	1	9	2	4
13	←	1	1	1	1	3	1	1	3	1	1
13	→	2	1	1	3	1	1	1	3	1	2
14	←	1	1	1	1	9	1	1	9	1	1
14	→	2	1	1	9	1	1	1	9	1	2
15	←	1	1	1	1	3	1	1	3	2	2
15	→	2	1	1	6	1	2	1	3	2	8
16	←	1	1	1	1	9	1	1	9	2	2
16	→	2	1	1	9	1	2	1	9	2	8
17	←	1	1	1	1	3	1	1	3	2	2
17	→	2	1	1	3	1	2	1	3	2	4
18	←	1	1	1	1	9	1	1	9	2	2
18	→	2	1	1	9	1	2	1	9	2	4
19	←	1	1	1	1	9	2	1	9	2	1
19	→	2	1	1	9	1	1	1	9	2	4
20	←	1	1	1	1	9	1	1	9	1	1
20	→	2	1	1	9	1	1	1	9	1	4
21	←	1	1	1	1	9	2	1	9	2	1
21	→	2	1	1	9	1	1	1	9	2	4
22	←	1	1	1	1	3	2	1	3	2	1
22	→	2	1	1	3	1	1	1	3	2	4
23	←	1	1	1	1	3	2	1	3	2	1
23	→	2	1	1	3	1	1	1	3	2	4
24	→	1	1	1	1	3	2	1	3	2	1
24	←	2	1	1	3	1	1	1	3	2	4
25	→	1	1	1	1	9	2	1	9	2	1
25	←	2	1	1	9	1	1	1	9	2	4
26	→	1	1	1	1	9	2	1	9	2	1

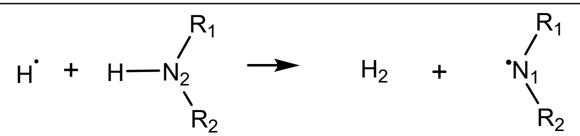
26	←	2	1	1	9	1	1	1	9	2	4

2.5. Group additivity values between 300 and 1800 K

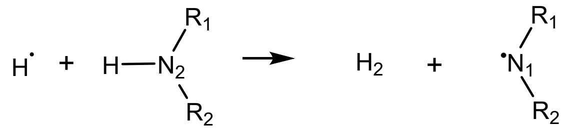
Table S6: Primary standard group additivity values ΔGAV°s between 300 and 1800 K for abstraction of a hydrogen atom from N-H by a hydrogen atom, deduced from the combined training and test set. For the reference reaction, the single-event pre-exponential factor is expressed in m^3 mol^{-1} s^{-1} and E_a is expressed in kJ mol^{-1}.



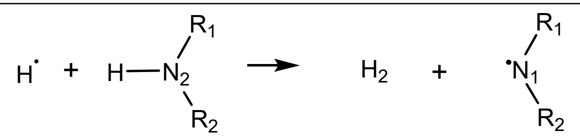
		300 K				**400 K**				**500 K**				**600 K**			
		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)	
No.	**Group**	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a
	Reference:	7.124	57.7	6.048	48.2	7.203	58.2	6.040	48.1	7.249	58.5	6.069	48.3	7.355	59.6	6.140	49.0
1	**N_i-(C)(H)**	-0.374	13.1	-0.094	-17.9	-0.302	13.6	-0.055	-17.6	-0.283	13.7	-0.048	-17.5	-0.242	14.1	-0.035	-17.4
2	**$N_{i,I}$**	-0.250	37.6	-0.062	-39.7	-0.195	38.0	-0.002	-39.3	-0.181	38.1	0.011	-39.2	-0.150	38.4	0.038	-38.9
3	**N_i-(C_d)(H)**	-0.476	61.3	-0.444	-26.8	-0.335	62.2	-0.400	-26.5	-0.293	62.6	-0.385	-26.4	-0.199	63.5	-0.353	-26.1
4	**N_i-(C_t)(H)**	-0.011	66.0	-0.150	-26.0	0.038	66.3	-0.134	-25.9	0.051	66.4	-0.132	-25.8	0.079	66.7	-0.127	-25.8
5	**N_i-$(C)_2$**	-0.745	27.3	0.007	-29.5	-0.599	28.3	0.046	-29.2	-0.562	28.6	0.049	-29.2	-0.481	29.4	0.055	-29.1
6	**N_i-(C_d)(C)**	-0.632	57.3	-0.361	-30.4	-0.489	58.3	-0.349	-30.4	-0.440	58.6	-0.341	-30.3	-0.330	59.7	-0.319	-30.1
7	**N_i-$(C_d)_2$**	0.303	90.3	-0.159	-16.8	0.378	90.9	-0.140	-16.6	0.386	90.9	-0.134	-16.6	0.398	91.0	-0.122	-16.5
8	**N_i-(C_t)(C)**	-0.597	68.7	-0.308	-31.8	-0.485	69.4	-0.268	-31.5	-0.453	69.7	-0.258	-31.4	-0.382	70.4	-0.237	-31.2



		700 K				800 K				900 K				1000 K			
		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)	
No.	**Group**	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a
	Reference:	7.462	60.9	6.235	50.1	7.563	62.3	6.339	51.6	7.658	63.8	6.444	53.2	7.746	65.4	6.545	55.1
1	**N_i-(C)(H)**	-0.214	14.5	-0.030	-17.4	-0.195	14.8	-0.025	-17.3	-0.181	15.0	-0.024	-17.2	-0.169	15.2	-0.024	-17.2
2	**$N_{i,I}$**	-0.129	38.6	0.052	-38.8	-0.114	38.9	0.061	-38.6	-0.102	39.1	0.065	-38.6	-0.092	39.2	0.068	-38.5
3	**N_i-(C_d)(H)**	-0.132	64.3	-0.326	-25.7	-0.083	65.1	-0.302	-25.4	-0.047	65.6	-0.283	-25.1	-0.018	66.1	-0.268	-24.8
4	**N_i-(C_t)(H)**	0.097	66.9	-0.125	-25.8	0.109	67.1	-0.122	-25.7	0.118	67.2	-0.121	-25.7	0.126	67.4	-0.120	-25.7
5	**N_i-$(C)_2$**	-0.428	30.1	0.052	-29.1	-0.391	30.6	0.049	-29.2	-0.364	31.0	0.043	-29.3	-0.343	31.4	0.037	-29.4
6	**N_i-(C_d)(C)**	-0.241	60.8	-0.293	-29.8	-0.167	61.8	-0.266	-29.4	-0.108	62.8	-0.242	-29.0	-0.060	63.6	-0.223	-28.7
7	**N_i-$(C_d)_2$**	0.383	90.9	-0.117	-16.4	0.352	90.4	-0.115	-16.4	0.315	89.9	-0.120	-16.5	0.278	89.2	-0.129	-16.6
8	**N_i-(C_t)(C)**	-0.334	71.0	-0.223	-31.0	-0.300	71.5	-0.213	-30.9	-0.275	71.9	-0.206	-30.8	-0.256	72.2	-0.201	-30.7



		1100 K				1200 K				1300 K				1400 K			
		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)	
No.	Group	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a
	Reference:	7.826	67.0	6.642	57.0	7.900	68.6	6.733	59.0	7.967	70.2	6.818	61.0	8.030	71.8	6.896	63.0
1	**N_i-(C)(H)**	-0.374	13.1	-0.094	-17.9	-0.302	13.6	-0.055	-17.6	-0.283	13.7	-0.048	-17.5	-0.242	14.1	-0.035	-17.4
2	**$N_{i,I}$**	-0.250	37.6	-0.062	-39.7	-0.195	38.0	-0.002	-39.3	-0.181	38.1	0.011	-39.2	-0.150	38.4	0.038	-38.9
3	**N_i-(C_d)(H)**	-0.476	61.3	-0.444	-26.8	-0.335	62.2	-0.400	-26.5	-0.293	62.6	-0.385	-26.4	-0.199	63.5	-0.353	-26.1
4	**N_i-(C_t)(H)**	-0.011	66.0	-0.150	-26.0	0.038	66.3	-0.134	-25.9	0.051	66.4	-0.132	-25.8	0.079	66.7	-0.127	-25.8
5	**N_i-$(C)_2$**	-0.745	27.3	0.007	-29.5	-0.599	28.3	0.046	-29.2	-0.562	28.6	0.049	-29.2	-0.481	29.4	0.055	-29.1
6	**N_i-(C_d)(C)**	-0.632	57.3	-0.361	-30.4	-0.489	58.3	-0.349	-30.4	-0.440	58.6	-0.341	-30.3	-0.330	59.7	-0.319	-30.1
7	**N_i-$(C_d)_2$**	0.303	90.3	-0.159	-16.8	0.378	90.9	-0.140	-16.6	0.386	90.9	-0.134	-16.6	0.398	91.0	-0.122	-16.5
8	**N_i-(C_t)(C)**	-0.597	68.7	-0.308	-31.8	-0.485	69.4	-0.268	-31.5	-0.453	69.7	-0.258	-31.4	-0.382	70.4	-0.237	-31.2



		1500 K				1600 K				1700 K				1800 K			
		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)	
No.	Group	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a
	Reference:	8.087	73.4	6.969	65.0	8.140	75.0	7.037	67.0	8.190	76.5	7.100	69.0	8.236	78.1	7.158	71.0
1	**N_i-(C)(H)**	-0.139	15.9	-0.024	-17.3	-0.137	16.0	-0.024	-17.3	-0.134	16.0	-0.025	-17.3	-0.132	16.1	-0.025	-17.3
2	**$N_{i,I}$**	-0.066	39.8	0.068	-38.5	-0.063	40.0	0.068	-38.5	-0.060	40.0	0.066	-38.6	-0.058	40.1	0.066	-38.6
3	**N_i-(C_d)(H)**	0.039	67.4	-0.220	-23.7	0.042	67.5	-0.215	-23.5	0.043	67.6	-0.210	-23.4	0.043	67.6	-0.207	-23.3
4	**N_i-(C_t)(H)**	0.144	67.8	-0.116	-25.6	0.145	67.8	-0.116	-25.6	0.146	67.9	-0.116	-25.6	0.148	67.9	-0.116	-25.6
5	**N_i-$(C)_2$**	-0.290	32.6	0.015	-29.9	-0.285	32.8	0.012	-30.0	-0.281	32.9	0.008	-30.1	-0.277	33.0	0.005	-30.2
6	**N_i-(C_d)(C)**	0.054	66.3	-0.180	-27.7	0.062	66.5	-0.178	-27.6	0.068	66.7	-0.178	-27.6	0.071	66.8	-0.178	-27.6
7	**N_i-$(C_d)_2$**	0.134	85.9	-0.185	-17.9	0.115	85.3	-0.196	-18.2	0.099	84.8	-0.206	-18.6	0.085	84.3	-0.216	-18.9
8	**N_i-(C_t)(C)**	-0.208	73.3	-0.191	-30.4	-0.204	73.4	-0.190	-30.4	-0.200	73.6	-0.190	-30.4	-0.196	73.7	-0.190	-30.4

2.6. Tunneling coefficients

Table S7: Tunneling coefficients [-] for all reactions from Table S4 over the temperature range 300-1800 K.

No.	κ(T)															
	300	**400**	**500**	**600**	**700**	**800**	**900**	**1000**	**1100**	**1200**	**1300**	**1400**	**1500**	**1600**	**1700**	**1800**
1	4.3	2.1	1.6	1.4	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.0
2	8.4	3.0	2.0	1.6	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1
3	1.3	1.2	1.1	1.1	1.1	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
4	12.6	3.7	2.3	1.8	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1
5	9.4	3.2	2.1	1.6	1.4	1.3	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1
6	6.2	2.7	1.9	1.6	1.4	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.1
7	9.2	3.3	2.1	1.7	1.5	1.3	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1
8	11.9	3.5	2.2	1.7	1.5	1.4	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1
9	4.2	2.2	1.6	1.4	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.0
10	8.6	3.0	2.0	1.6	1.4	1.3	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1
11	8.5	3.0	2.0	1.6	1.4	1.3	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1
12	8.8	3.1	2.0	1.6	1.4	1.3	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1
13	1.7	1.4	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.0	1.0	1.0	1.0	1.0	1.0	1.0
14	2.4	1.6	1.4	1.3	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.0	1.0	1.0	1.0
15	9.0	3.2	2.1	1.7	1.4	1.3	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1
16	2.7	1.7	1.4	1.3	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.0	1.0	1.0	1.0
17	4.2	2.1	1.6	1.4	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.0
18	4.1	2.1	1.6	1.4	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.0
19	6.3	2.7	1.9	1.5	1.4	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.1
20	6.3	2.7	1.9	1.6	1.4	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.1
21	7.3	3.0	2.0	1.6	1.4	1.3	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1
22	25.6	5.3	2.8	2.0	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1
23	4.1	2.1	1.6	1.4	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.0
24	22.3	5.1	2.7	2.0	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1
25	8.4	3.2	2.1	1.7	1.5	1.3	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1

3. N-H-N hydrogen abstractions

3.1. Single-event Arrhenius parameters for reference reaction

Table S8: Intrinsic Arrhenius parameters over the temperature range 300-1800 K for the reference reaction of N-H-N hydrogen abstraction reactions, i.e. $^{\cdot}NH_2 + NH_3 \rightarrow NH_3 + {}^{\cdot}NH_2$. The single-event pre-exponential factor is expressed in $m^3\ mol^{-1}\ s^{-1}$ and E_a is expressed in kJ mol^{-1}.

Temperature [K]	$log\tilde{A}$	E_a
300	5.067	44.6
400	5.292	46.2
500	5.398	46.9
600	5.635	49.3
700	5.849	51.9
800	6.041	54.6
900	6.210	57.3
1000	6.361	60.0
1100	6.497	62.7
1200	6.619	65.4
1300	6.729	68.0
1400	6.830	70.6
1500	6.922	73.2
1600	7.008	75.7
1700	7.087	78.2
1800	7.161	80.6

3.2. Rate coefficients between 300 and 1800 K

Table S9: Rate coefficients [m^3 mol^{-1} s^{-1}] in the temperature range 300-1800 K for the reactions presented in Table S10. The rate coefficients do not include tunneling contributions.

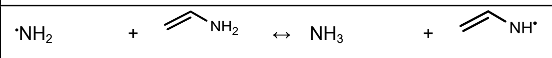
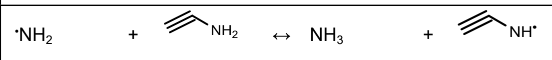
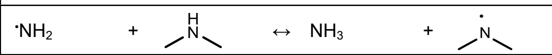
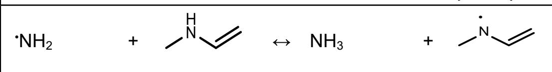
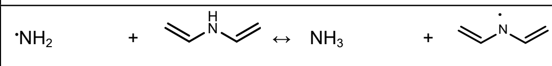
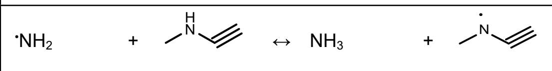
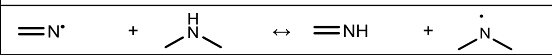
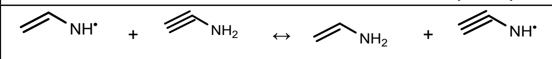
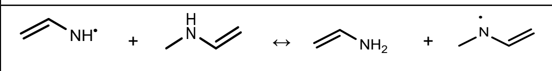
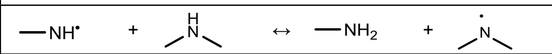
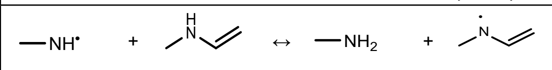
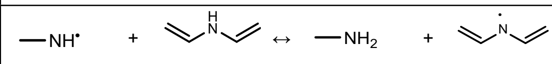
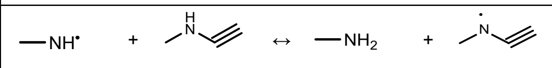
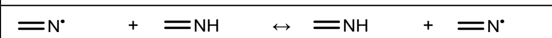
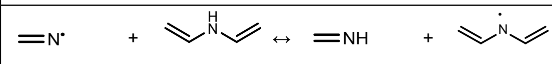
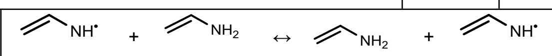
No.		300 K	400 K	500 K	600 K	700 K	800 K	900 K	1000 K	1100 K	1200 K	1300 K	1400 K	1500 K	1600 K	1700 K	1800 K
1	→	5.5E-03	5.1E-01	8.5E+00	6.1E+01	2.7E+02	8.6E+02	2.2E+03	4.9E+03	9.6E+03	1.7E+04	2.9E+04	4.6E+04	7.0E+04	1.0E+05	1.4E+05	2.0E+05
1	←	5.5E-03	5.1E-01	8.5E+00	6.1E+01	2.7E+02	8.6E+02	2.2E+03	4.9E+03	9.6E+03	1.7E+04	2.9E+04	4.6E+04	7.0E+04	1.0E+05	1.4E+05	2.0E+05
2	→	5.1E+00	9.4E+01	6.1E+02	2.3E+03	6.4E+03	1.4E+04	2.8E+04	5.0E+04	8.3E+04	1.3E+05	1.9E+05	2.7E+05	3.7E+05	5.0E+05	6.5E+05	8.3E+05
2	←	1.2E-05	5.3E-03	2.4E-01	3.3E+00	2.3E+01	1.1E+02	3.7E+02	1.0E+03	2.4E+03	5.0E+03	9.6E+03	1.7E+04	2.9E+04	4.5E+04	6.9E+04	1.0E+05
3	→	7.4E+00	9.8E+01	5.3E+02	1.8E+03	4.7E+03	1.0E+04	2.0E+04	3.5E+04	5.7E+04	8.8E+04	1.3E+05	1.9E+05	2.6E+05	3.4E+05	4.5E+05	5.8E+05
3	←	1.6E-13	7.6E-09	5.8E-06	5.4E-04	1.5E-02	1.9E-01	1.5E+00	8.1E+00	3.3E+01	1.1E+02	3.1E+02	7.6E+02	1.7E+03	3.5E+03	6.6E+03	1.2E+04
4	→	3.5E+01	3.4E+02	1.5E+03	4.3E+03	1.0E+04	2.0E+04	3.6E+04	5.9E+04	9.2E+04	1.3E+05	1.9E+05	2.6E+05	3.5E+05	4.5E+05	5.8E+05	7.3E+05
4	←	2.1E-14	1.3E-09	1.1E-06	1.2E-04	3.4E-03	4.5E-02	3.5E-01	1.9E+00	7.6E+00	2.5E+01	7.1E+01	1.7E+02	3.9E+02	7.9E+02	1.5E+03	2.6E+03
5	→	5.4E+02	2.8E+03	8.8E+03	2.0E+04	4.0E+04	7.0E+04	1.1E+05	1.7E+05	2.4E+05	3.3E+05	4.5E+05	5.9E+05	7.5E+05	9.4E+05	1.2E+06	1.4E+06
5	←	3.7E-08	5.9E-05	5.9E-03	1.4E-01	1.5E+00	9.7E+00	4.3E+01	1.5E+02	4.1E+02	1.0E+03	2.2E+03	4.3E+03	7.9E+03	1.4E+04	2.2E+04	3.5E+04
6	→	2.3E+02	1.2E+03	3.8E+03	9.2E+03	1.9E+04	3.4E+04	5.6E+04	8.8E+04	1.3E+05	1.9E+05	2.6E+05	3.4E+05	4.5E+05	5.8E+05	7.3E+05	9.0E+05
6	←	2.7E-14	2.0E-09	2.1E-06	2.4E-04	7.9E-03	1.2E-01	9.9E-01	5.8E+00	2.5E+01	8.9E+01	2.6E+02	6.8E+02	1.6E+03	3.3E+03	6.6E+03	1.2E+04
7	→	1.0E+01	1.5E+02	8.1E+02	2.7E+03	6.6E+03	1.4E+04	2.5E+04	4.2E+04	6.5E+04	9.7E+04	1.4E+05	1.9E+05	2.5E+05	3.3E+05	4.2E+05	5.3E+05
7	←	1.7E-18	3.0E-12	2.0E-08	7.4E-06	5.3E-04	1.4E-02	1.8E-01	1.4E+00	7.6E+00	3.2E+01	1.1E+02	3.2E+02	8.0E+02	1.8E+03	3.8E+03	7.4E+03
8	→	2.0E+03	6.9E+03	1.7E+04	3.3E+04	5.7E+04	9.1E+04	1.4E+05	2.0E+05	2.8E+05	3.7E+05	4.9E+05	6.3E+05	7.9E+05	9.8E+05	1.2E+06	1.4E+06
8	←	5.7E-15	5.3E-10	5.9E-07	7.2E-05	2.4E-03	3.5E-02	3.0E-01	1.7E+00	7.5E+00	2.6E+01	7.6E+01	1.9E+02	4.4E+02	9.3E+02	1.8E+03	3.3E+03
9	→	3.2E-02	1.3E+00	1.5E+01	8.3E+01	3.0E+02	8.6E+02	2.0E+03	4.2E+03	7.8E+03	1.4E+04	2.2E+04	3.4E+04	5.0E+04	7.2E+04	9.9E+04	1.3E+05
9	←	3.1E-10	1.9E-06	4.2E-04	1.7E-02	2.6E-01	2.2E+00	1.2E+01	4.8E+01	1.6E+02	4.3E+02	1.0E+03	2.2E+03	4.3E+03	7.9E+03	1.4E+04	2.3E+04
10	→	2.4E+00	3.5E+01	2.0E+02	6.9E+02	1.8E+03	4.0E+03	7.7E+03	1.3E+04	2.2E+04	3.4E+04	5.0E+04	7.0E+04	9.7E+04	1.3E+05	1.7E+05	2.2E+05
10	←	6.3E-10	2.4E-06	3.9E-04	1.3E-02	1.6E-01	1.2E+00	5.8E+00	2.1E+01	6.3E+01	1.6E+02	3.6E+02	7.4E+02	1.4E+03	2.5E+03	4.1E+03	6.5E+03
11	→	5.4E-04	7.7E-02	1.7E+00	1.5E+01	7.4E+01	2.6E+02	7.1E+02	1.7E+03	3.4E+03	6.2E+03	1.1E+04	1.7E+04	2.6E+04	3.9E+04	5.5E+04	7.6E+04
11	←	5.5E+00	5.9E+01	2.9E+02	9.7E+02	2.5E+03	5.3E+03	1.0E+04	1.7E+04	2.8E+04	4.3E+04	6.3E+04	8.9E+04	1.2E+05	1.6E+05	2.1E+05	2.7E+05
12	→	1.4E-03	1.5E-01	2.9E+00	2.3E+01	1.1E+02	3.9E+02	1.1E+03	2.5E+03	5.3E+03	1.0E+04	1.8E+04	2.9E+04	4.6E+04	6.9E+04	9.9E+04	1.4E+05
12	←	3.9E-05	7.6E-03	2.1E-01	2.1E+00	1.2E+01	4.6E+01	1.4E+02	3.5E+02	7.7E+02	1.5E+03	2.8E+03	4.7E+03	7.6E+03	1.2E+04	1.7E+04	2.5E+04
13	→	1.0E-03	1.1E-01	2.2E+00	1.7E+01	7.9E+01	2.6E+02	7.0E+02	1.6E+03	3.2E+03	5.8E+03	9.8E+03	1.6E+04	2.4E+04	3.5E+04	4.9E+04	6.7E+04
13	←	5.7E-06	2.5E-03	1.1E-01	1.5E+00	1.0E+01	4.8E+01	1.6E+02	4.5E+02	1.1E+03	2.2E+03	4.2E+03	7.5E+03	1.3E+04	2.0E+04	3.0E+04	4.4E+04
14	→	1.1E-03	1.5E-01	3.2E+00	2.8E+01	1.4E+02	5.0E+02	1.4E+03	3.3E+03	6.9E+03	1.3E+04	2.3E+04	3.7E+04	5.8E+04	8.7E+04	1.3E+05	1.8E+05

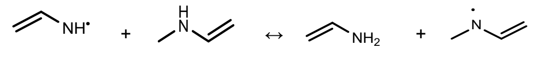
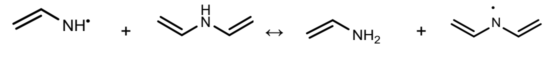
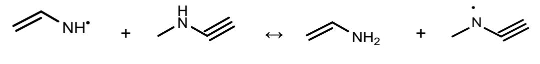
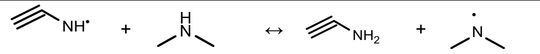
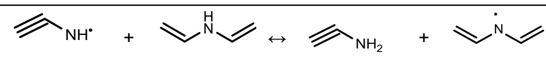
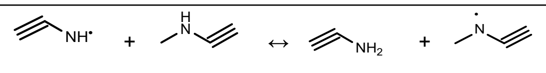
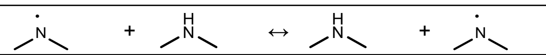
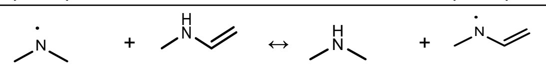
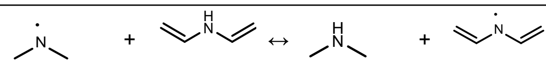
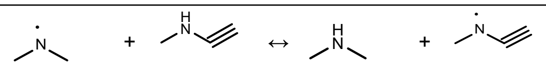
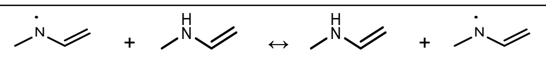
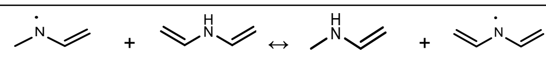
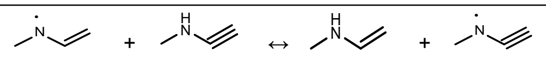
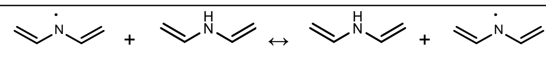
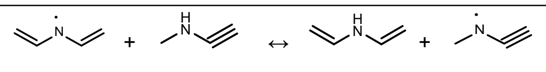
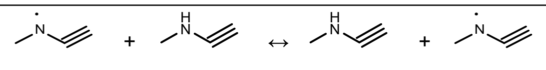
14	←	1.1E-03	1.5E-01	3.2E+00	2.8E+01	1.4E+02	5.0E+02	1.4E+03	3.3E+03	6.9E+03	1.3E+04	2.3E+04	3.7E+04	5.8E+04	8.7E+04	1.3E+05	1.8E+05
15	→	8.7E-03	6.0E-01	8.6E+00	5.6E+01	2.3E+02	6.9E+02	1.7E+03	3.6E+03	6.9E+03	1.2E+04	2.0E+04	3.1E+04	4.6E+04	6.6E+04	9.1E+04	1.2E+05
15	←	8.7E-03	6.0E-01	8.6E+00	5.6E+01	2.3E+02	6.9E+02	1.7E+03	3.6E+03	6.9E+03	1.2E+04	2.0E+04	3.1E+04	4.6E+04	6.6E+04	9.1E+04	1.2E+05
16	→	7.8E+01	5.6E+02	2.1E+03	5.6E+03	1.2E+04	2.2E+04	3.8E+04	6.1E+04	9.1E+04	1.3E+05	1.8E+05	2.4E+05	3.2E+05	4.1E+05	5.1E+05	6.4E+05
16	←	2.3E-07	2.7E-04	2.1E-02	4.2E-01	3.8E+00	2.1E+01	8.1E+01	2.5E+02	6.4E+02	1.5E+03	2.9E+03	5.5E+03	9.5E+03	1.6E+04	2.4E+04	3.7E+04
17	→	1.3E+01	1.6E+02	8.3E+02	2.8E+03	7.0E+03	1.5E+04	2.7E+04	4.7E+04	7.4E+04	1.1E+05	1.6E+05	2.2E+05	3.0E+05	4.0E+05	5.1E+05	6.4E+05
17	←	3.9E-04	5.9E-02	1.4E+00	1.3E+01	7.3E+01	2.8E+02	8.2E+02	2.0E+03	4.4E+03	8.6E+03	1.5E+04	2.6E+04	4.1E+04	6.3E+04	9.2E+04	1.3E+05
18	→	2.2E+00	2.6E+01	1.3E+02	4.3E+02	1.1E+03	2.4E+03	4.5E+03	7.9E+03	1.3E+04	2.0E+04	2.9E+04	4.1E+04	5.7E+04	7.6E+04	1.0E+05	1.3E+05
18	←	1.2E-10	7.7E-07	1.8E-04	7.9E-03	1.3E-01	1.1E+00	6.2E+00	2.6E+01	8.6E+01	2.4E+02	5.9E+02	1.3E+03	2.6E+03	4.9E+03	8.5E+03	1.4E+04
19	→	6.2E+00	5.5E+01	2.3E+02	6.7E+02	1.5E+03	3.1E+03	5.5E+03	9.0E+03	1.4E+04	2.1E+04	3.0E+04	4.1E+04	5.5E+04	7.1E+04	9.1E+04	1.2E+05
19	←	4.4E-13	2.0E-08	1.4E-05	1.3E-03	3.4E-02	4.2E-01	3.0E+00	1.5E+01	5.7E+01	1.8E+02	4.6E+02	1.1E+03	2.3E+03	4.4E+03	7.9E+03	1.3E+04
20	→	9.2E+01	6.2E+02	2.2E+03	5.7E+03	1.2E+04	2.2E+04	3.8E+04	5.9E+04	8.8E+04	1.3E+05	1.7E+05	2.3E+05	3.0E+05	3.9E+05	4.9E+05	6.1E+05
20	←	1.1E-10	8.4E-07	2.0E-04	8.7E-03	1.4E-01	1.2E+00	6.3E+00	2.6E+01	8.2E+01	2.2E+02	5.3E+02	1.1E+03	2.2E+03	4.1E+03	7.0E+03	1.1E+04
21	→	2.1E-02	1.1E+00	1.3E+01	7.7E+01	2.9E+02	8.5E+02	2.0E+03	4.2E+03	7.8E+03	1.3E+04	2.2E+04	3.3E+04	4.9E+04	6.9E+04	9.5E+04	1.3E+05
21	←	2.1E-02	1.1E+00	1.3E+01	7.7E+01	2.9E+02	8.5E+02	2.0E+03	4.2E+03	7.8E+03	1.3E+04	2.2E+04	3.3E+04	4.9E+04	6.9E+04	9.5E+04	1.3E+05
22	→	1.1E-03	1.0E-01	1.7E+00	1.3E+01	5.8E+01	1.9E+02	4.9E+02	1.1E+03	2.2E+03	3.9E+03	6.6E+03	1.1E+04	1.6E+04	2.3E+04	3.3E+04	4.5E+04
22	←	3.7E-03	2.9E-01	4.8E+00	3.5E+01	1.6E+02	5.1E+02	1.4E+03	3.1E+03	6.1E+03	1.1E+04	1.9E+04	3.0E+04	4.6E+04	6.8E+04	9.6E+04	1.3E+05
23	→	2.9E-02	1.3E+00	1.5E+01	8.5E+01	3.2E+02	9.3E+02	2.2E+03	4.7E+03	8.9E+03	1.6E+04	2.5E+04	3.9E+04	5.9E+04	8.4E+04	1.2E+05	1.6E+05
23	←	2.6E-03	1.8E-01	2.9E+00	2.1E+01	9.2E+01	3.0E+02	8.0E+02	1.8E+03	3.6E+03	6.7E+03	1.1E+04	1.8E+04	2.8E+04	4.2E+04	6.0E+04	8.2E+04
24	→	1.2E-02	5.9E-01	7.2E+00	4.2E+01	1.6E+02	4.6E+02	1.1E+03	2.3E+03	4.2E+03	7.2E+03	1.2E+04	1.8E+04	2.6E+04	3.7E+04	5.1E+04	6.8E+04
24	←	2.1E-04	3.7E-02	9.9E-01	1.0E+01	5.8E+01	2.3E+02	7.0E+02	1.8E+03	4.0E+03	7.9E+03	1.4E+04	2.5E+04	4.0E+04	6.2E+04	9.2E+04	1.3E+05
25	→	2.3E-03	1.2E-01	1.4E+00	8.3E+00	3.2E+01	9.6E+01	2.3E+02	5.0E+02	9.6E+02	1.7E+03	2.8E+03	4.4E+03	6.7E+03	9.7E+03	1.4E+04	1.9E+04
25	←	5.7E-08	8.6E-05	8.6E-03	2.1E-01	2.3E+00	1.4E+01	6.1E+01	2.0E+02	5.5E+02	1.3E+03	2.7E+03	5.2E+03	9.3E+03	1.6E+04	2.5E+04	3.8E+04
26	→	1.1E+00	1.6E+01	9.7E+01	3.6E+02	1.0E+03	2.3E+03	4.6E+03	8.2E+03	1.4E+04	2.2E+04	3.2E+04	4.7E+04	6.5E+04	8.8E+04	1.2E+05	1.5E+05
26	←	4.6E-04	4.6E-02	8.8E-01	7.3E+00	3.6E+01	1.3E+02	3.6E+02	8.6E+02	1.8E+03	3.5E+03	6.1E+03	1.0E+04	1.6E+04	2.4E+04	3.5E+04	4.9E+04
27	→	1.7E-04	1.9E-02	3.4E-01	2.5E+00	1.1E+01	3.2E+01	7.8E+01	1.6E+02	3.0E+02	5.0E+02	7.9E+02	1.2E+03	1.7E+03	2.2E+03	3.0E+03	3.8E+03
27	←	1.7E-04	1.9E-02	3.4E-01	2.5E+00	1.1E+01	3.2E+01	7.8E+01	1.6E+02	3.0E+02	5.0E+02	7.9E+02	1.2E+03	1.7E+03	2.2E+03	3.0E+03	3.8E+03
28	→	4.5E-06	2.8E-03	1.5E-01	2.4E+00	1.9E+01	9.1E+01	3.2E+02	9.2E+02	2.2E+03	4.8E+03	9.2E+03	1.7E+04	2.8E+04	4.4E+04	6.7E+04	9.9E+04
28	←	1.4E-02	7.4E-01	9.4E+00	5.7E+01	2.3E+02	6.7E+02	1.6E+03	3.5E+03	6.6E+03	1.2E+04	1.9E+04	3.0E+04	4.4E+04	6.4E+04	8.9E+04	1.2E+05
29	→	1.2E-04	1.4E-02	2.7E-01	2.1E+00	1.0E+01	3.4E+01	9.2E+01	2.1E+02	4.2E+02	7.8E+02	1.3E+03	2.1E+03	3.3E+03	4.8E+03	6.8E+03	9.4E+03
29	←	9.1E-10	3.6E-06	6.0E-04	2.0E-02	2.6E-01	1.8E+00	8.6E+00	3.0E+01	8.6E+01	2.1E+02	4.5E+02	8.7E+02	1.6E+03	2.6E+03	4.3E+03	6.5E+03
30	→	1.0E-02	6.5E-01	9.0E+00	5.8E+01	2.4E+02	7.3E+02	1.8E+03	3.9E+03	7.6E+03	1.4E+04	2.2E+04	3.5E+04	5.3E+04	7.7E+04	1.1E+05	1.5E+05

30	←	1.3E-06	6.3E-04	3.0E-02	4.3E-01	3.1E+00	1.5E+01	5.2E+01	1.5E+02	3.6E+02	7.6E+02	1.5E+03	2.7E+03	4.5E+03	7.2E+03	1.1E+04	1.6E+04
31	→	2.4E-05	7.7E-03	2.7E-01	3.2E+00	2.0E+01	8.1E+01	2.5E+02	6.5E+02	1.4E+03	2.9E+03	5.2E+03	8.9E+03	1.4E+04	2.2E+04	3.2E+04	4.5E+04
31	←	2.8E+00	4.0E+01	2.3E+02	8.5E+02	2.3E+03	5.1E+03	1.0E+04	1.8E+04	3.0E+04	4.6E+04	6.9E+04	9.8E+04	1.4E+05	1.8E+05	2.4E+05	3.1E+05
32	→	3.5E-03	2.3E-01	3.2E+00	2.0E+01	8.1E+01	2.4E+02	5.8E+02	1.2E+03	2.3E+03	4.0E+03	6.5E+03	1.0E+04	1.5E+04	2.1E+04	2.9E+04	3.9E+04
32	←	7.2E-04	1.0E-01	2.2E+00	2.0E+01	1.0E+02	3.7E+02	1.1E+03	2.5E+03	5.4E+03	1.0E+04	1.8E+04	3.0E+04	4.7E+04	7.1E+04	1.0E+05	1.4E+05
33	→	5.6E-02	1.4E+00	1.1E+01	5.0E+01	1.6E+02	4.2E+02	9.2E+02	1.8E+03	3.2E+03	5.4E+03	8.5E+03	1.3E+04	1.9E+04	2.6E+04	3.6E+04	4.7E+04
33	←	1.5E-05	7.0E-03	3.5E-01	5.3E+00	4.0E+01	1.9E+02	6.7E+02	1.9E+03	4.5E+03	9.6E+03	1.8E+04	3.2E+04	5.3E+04	8.4E+04	1.3E+05	1.8E+05
34	→	3.6E-04	6.3E-02	1.6E+00	1.5E+01	8.1E+01	3.0E+02	8.7E+02	2.1E+03	4.5E+03	8.7E+03	1.5E+04	2.5E+04	4.0E+04	6.0E+04	8.7E+04	1.2E+05
34	←	1.7E-06	1.2E-03	7.3E-02	1.2E+00	1.0E+01	5.2E+01	2.0E+02	5.8E+02	1.5E+03	3.2E+03	6.4E+03	1.2E+04	2.0E+04	3.3E+04	5.1E+04	7.7E+04
35	→	1.3E-01	2.8E+00	2.2E+01	9.7E+01	3.0E+02	7.5E+02	1.6E+03	3.1E+03	5.3E+03	8.6E+03	1.3E+04	2.0E+04	2.8E+04	3.8E+04	5.1E+04	6.7E+04
35	←	1.3E-01	2.8E+00	2.2E+01	9.7E+01	3.0E+02	7.5E+02	1.6E+03	3.1E+03	5.3E+03	8.6E+03	1.3E+04	2.0E+04	2.8E+04	3.8E+04	5.1E+04	6.7E+04
36	→	3.4E-01	7.2E+00	5.3E+01	2.3E+02	7.1E+02	1.8E+03	3.7E+03	7.1E+03	1.2E+04	2.0E+04	3.1E+04	4.6E+04	6.5E+04	9.0E+04	1.2E+05	1.6E+05
36	←	5.9E-07	5.8E-04	4.3E-02	8.5E-01	7.7E+00	4.3E+01	1.7E+02	5.3E+02	1.4E+03	3.2E+03	6.5E+03	1.2E+04	2.2E+04	3.6E+04	5.7E+04	8.6E+04
37	→	9.3E-01	1.3E+01	6.9E+01	2.4E+02	6.4E+02	1.4E+03	2.7E+03	4.8E+03	7.8E+03	1.2E+04	1.8E+04	2.5E+04	3.5E+04	4.7E+04	6.1E+04	7.8E+04
37	←	2.2E-09	1.2E-05	2.5E-03	9.5E-02	1.3E+00	1.0E+01	5.0E+01	1.8E+02	5.3E+02	1.3E+03	2.9E+03	5.7E+03	1.0E+04	1.8E+04	2.9E+04	4.5E+04
38	→	9.4E+01	4.7E+02	1.5E+03	3.5E+03	7.2E+03	1.3E+04	2.2E+04	3.4E+04	5.0E+04	7.1E+04	9.8E+04	1.3E+05	1.7E+05	2.2E+05	2.8E+05	3.4E+05
38	←	3.9E-06	1.7E-03	7.9E-02	1.1E+00	7.9E+00	3.6E+01	1.2E+02	3.4E+02	7.9E+02	1.7E+03	3.1E+03	5.5E+03	9.2E+03	1.4E+04	2.2E+04	3.2E+04
39	→	1.7E-03	1.1E-01	1.5E+00	9.5E+00	3.7E+01	1.1E+02	2.7E+02	5.6E+02	1.1E+03	1.8E+03	3.0E+03	4.6E+03	6.7E+03	9.5E+03	1.3E+04	1.7E+04
39	←	1.7E-03	1.1E-01	1.5E+00	9.5E+00	3.7E+01	1.1E+02	2.7E+02	5.6E+02	1.1E+03	1.8E+03	3.0E+03	4.6E+03	6.7E+03	9.5E+03	1.3E+04	1.7E+04
40	→	3.7E-04	3.7E-02	6.9E-01	5.4E+00	2.6E+01	8.8E+01	2.4E+02	5.5E+02	1.1E+03	2.1E+03	3.6E+03	5.8E+03	9.0E+03	1.3E+04	1.9E+04	2.6E+04
40	←	4.9E-07	4.4E-04	3.1E-02	5.8E-01	5.0E+00	2.6E+01	9.6E+01	2.8E+02	6.8E+02	1.5E+03	2.8E+03	4.9E+03	8.2E+03	1.3E+04	1.9E+04	2.8E+04
41	→	5.0E-03	4.3E-01	7.3E+00	5.2E+01	2.3E+02	7.3E+02	1.9E+03	4.2E+03	8.2E+03	1.5E+04	2.5E+04	3.9E+04	5.9E+04	8.6E+04	1.2E+05	1.7E+05
41	←	1.2E-04	2.0E-02	4.8E-01	4.4E+00	2.3E+01	8.3E+01	2.3E+02	5.5E+02	1.2E+03	2.2E+03	3.8E+03	6.1E+03	9.5E+03	1.4E+04	2.0E+04	2.8E+04
42	→	4.5E+00	4.1E+01	1.9E+02	6.2E+02	1.6E+03	3.4E+03	6.5E+03	1.1E+04	1.8E+04	2.7E+04	4.0E+04	5.5E+04	7.5E+04	9.9E+04	1.3E+05	1.6E+05
42	←	4.5E+00	4.1E+01	1.9E+02	6.2E+02	1.6E+03	3.4E+03	6.5E+03	1.1E+04	1.8E+04	2.7E+04	4.0E+04	5.5E+04	7.5E+04	9.9E+04	1.3E+05	1.6E+05
43	→	1.2E-02	1.5E+00	3.1E+01	2.5E+02	1.2E+03	3.9E+03	1.0E+04	2.2E+04	4.2E+04	7.4E+04	1.2E+05	1.8E+05	2.7E+05	3.8E+05	5.1E+05	6.8E+05
43	←	2.2E-01	5.8E+00	4.6E+01	2.0E+02	6.0E+02	1.5E+03	3.1E+03	5.7E+03	9.7E+03	1.6E+04	2.3E+04	3.4E+04	4.8E+04	6.4E+04	8.5E+04	1.1E+05
44	→	2.9E-02	1.4E+00	1.6E+01	8.9E+01	3.3E+02	9.3E+02	2.2E+03	4.4E+03	8.2E+03	1.4E+04	2.2E+04	3.4E+04	4.9E+04	6.9E+04	9.4E+04	1.3E+05
44	←	2.9E-02	1.4E+00	1.6E+01	8.9E+01	3.3E+02	9.3E+02	2.2E+03	4.4E+03	8.2E+03	1.4E+04	2.2E+04	3.4E+04	4.9E+04	6.9E+04	9.4E+04	1.3E+05
45	→	3.2E+03	1.1E+04	2.7E+04	5.2E+04	8.9E+04	1.4E+05	2.1E+05	3.0E+05	4.1E+05	5.4E+05	7.0E+05	8.9E+05	1.1E+06	1.4E+06	1.7E+06	2.0E+06
45	←	2.1E-11	3.1E-07	1.1E-04	5.7E-03	1.0E-01	9.7E-01	5.7E+00	2.5E+01	8.3E+01	2.4E+02	5.8E+02	1.3E+03	2.6E+03	4.8E+03	8.3E+03	1.4E+04

3.3. Arrhenius parameters regressed at 1000 K

Table S10: Standard reaction enthalpy [kJ mol^{-1}], pre-exponential factor [m^3 mol^{-1} s^{-1}], activation energy [kJ mol^{-1}], rate coefficient [m^3 mol^{-1} s^{-1}] and deviation factor ρ at 1000 K for all N-H-N hydrogen abstraction reactions in the training (T) and validation dataset (V). The Arrhenius parameters exclude tunneling.

No.		Reaction	ΔH_r°	Forward			Reverse			ρ (1000 K0	
				$logA$	E_a	k_{for}	$logA$	E_a	k_{rev}	*for*	*rev*
1	T	$^{\bullet}NH_2$ + NH_3 ↔ NH_3 + $^{\bullet}NH_2$	0.0	6.838	60.0	4.9E+03	6.838	60.0	4.9E+03	-	-
2	T		-33.8	6.995	43.6	5.0E+04	7.033	76.8	1.0E+03	1.1	1.1
3	T		-82.3	6.791	42.8	3.5E+04	7.513	126.2	8.1E+00	1.2	1.2
4	T		-89.7	6.765	37.9	5.9E+04	6.889	126.4	1.9E+00	1.8	1.8
5	T		-58.5	6.871	31.2	1.7E+05	7.011	92.5	1.5E+02	1.4	1.4
6	T		-93.6	6.730	33.9	8.8E+04	7.695	132.4	5.8E+00	1.2	1.2
7	T		-118.3	6.674	39.1	4.2E+04	8.228	154.7	1.4E+00	1.1	1.1
8	T		-103.5	6.770	27.9	2.0E+05	7.125	131.6	1.7E+00	1.6	1.6
9	T		-48.5	6.504	54.9	4.2E+03	7.189	105.1	4.8E+01	1.3	1.3
10	T		-55.9	6.369	42.6	1.3E+04	6.456	97.9	2.1E+01	1.4	1.4
11	T		26.4	6.540	63.4	1.7E+03	6.441	41.8	1.7E+04	1.7	1.7
12	T		-7.4	6.806	64.8	2.5E+03	6.209	69.9	3.5E+02	1.2	1.2
13	T		-11.4	6.425	61.5	1.6E+03	6.667	76.6	4.5E+02	1.1	1.1
14	T		0.0	6.931	65.1	3.3E+03	6.931	65.1	3.3E+03	2.0	2.0
15	V		0.0	6.554	57.1	3.6E+03	6.554	57.1	3.6E+03	1.8	1.8
16	V		-51.2	6.627	35.0	6.1E+04	6.829	84.6	2.5E+02	2.1	2.1
17	V		-24.8	6.791	40.4	4.7E+04	6.894	68.4	2.0E+03	1.1	1.1
18	V		-59.9	6.119	42.2	7.9E+03	7.046	107.5	2.6E+01	1.9	1.9
19	V		-84.6	5.963	38.2	9.0E+03	7.480	120.5	1.5E+01	1.0	1.0
20	V		-69.7	6.587	34.5	5.9E+04	6.905	105.0	2.6E+01	1.0	1.0
21	V		0.0	6.507	55.0	4.2E+03	6.507	55.0	4.2E+03	2.1	2.1
22	V		2.7	6.220	60.7	1.1E+03	6.703	61.3	3.1E+03	2.1	2.1
23	V		-4.7	6.616	56.0	4.7E+03	6.501	61.8	1.8E+03	1.8	1.8
24	V		-8.7	6.229	54.8	2.3E+03	6.954	70.6	1.8E+03	1.8	1.8
25	V		-33.4	5.707	57.3	5.0E+02	7.022	90.1	2.0E+02	1.1	1.1
26	V		-18.6	6.268	44.8	8.2E+03	6.384	65.7	8.6E+02	2.2	2.2
27	V		0.0	5.084	54.9	1.6E+02	5.084	54.9	1.6E+02	1.	

28	V		23.8	7.102	79.0	9.2E+02	6.520	56.8	3.5E+03	1.
29	V		-11.4	6.425	61.5	1.6E+03	6.667	76.6	4.5E+02	1.
30	V		-36.1	5.586	62.3	2.1E+02	6.418	94.4	3.0E+01	1.
31	V		-21.2	6.649	58.2	3.9E+03	6.282	78.5	1.5E+02	1.
32	V		31.1	6.538	71.1	6.5E+02	6.554	43.8	1.8E+04	1.
33	V		-4.0	6.037	56.2	1.2E+03	6.877	66.2	2.5E+03	1.
34	V		-28.7	5.933	50.9	1.8E+03	7.362	78.0	1.9E+03	1.
35	V		-13.9	6.836	66.9	2.1E+03	7.067	82.1	5.8E+02	2.
36	V		0.0	6.036	48.6	3.1E+03	6.036	48.6	3.1E+03	1.
37	V		-35.1	6.402	48.6	7.1E+03	7.226	85.9	5.3E+02	1.
38	V		-59.8	5.935	42.9	4.8E+03	7.349	97.3	1.8E+02	1.
39	V		-45.0	6.313	33.9	3.4E+04	6.527	76.3	3.4E+02	1.
40	V		0.0	5.681	55.9	5.6E+02	5.681	55.9	5.6E+02	1.
41	V		-24.7	6.058	63.2	5.5E+02	6.647	80.2	2.8E+02	1.
42	V		-9.9	6.767	60.0	4.2E+03	6.158	65.1	5.5E+02	1.
43	V		0.0	6.232	41.5	1.1E+04	6.232	41.5	1.1E+04	1.
44	V		14.8	7.422	58.9	2.2E+04	6.223	47.0	5.7E+03	2.
45	V		0.0	6.475	53.9	4.4E+03	6.475	53.9	4.4E+03	1.

3.4. Reaction path degeneracy

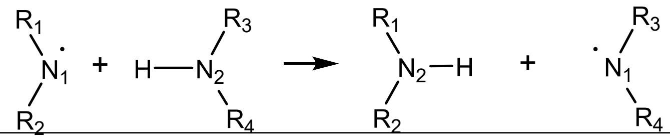
Table S11: External and internal symmetry numbers, number of optical isomers and number of single events n_e for all N-H-N hydrogen abstractions of Table S10.

No.		**Reactant 1 R·**			**Reactant 2 RH**			**Transition state**			**Reaction path degeneracy**
		σ_{ext}	σ_{int}	n_{opt}	σ_{ex}	σ_{int}	n_{opt}	σ_{ex}	σ_{int}	n_{opt}	n_e
1	→	2	1	1	3	1	1	2	1	1	3
1	←	3	1	1	2	1	1	2	1	1	3
2	←	2	1	1	1	3	1	1	3	2	4
2	→	3	1	1	3	1	1	1	3	2	6
3	←	2	1	1	1	1	1	1	1	2	4
3	→	3	1	1	1	1	1	1	1	2	6
4	←	2	1	1	1	1	1	1	1	1	2
4	→	3	1	1	1	1	1	1	1	1	3
5	←	2	1	1	1	9	1	1	9	1	2
5	→	3	1	1	2	9	1	1	9	1	6
6	←	2	1	1	1	3	2	1	3	2	2
6	→	3	1	1	1	3	1	1	3	2	6
7	←	2	1	1	1	1	1	1	1	1	2
7	→	3	1	1	1	2	1	1	1	1	6
8	←	2	1	1	1	3	2	1	3	2	2
8	→	3	1	1	1	3	1	1	3	2	6
9	←	3	1	1	1	1	1	1	3	2	2
9	→	1	3	1	1	1	1	1	3	2	2
10	←	3	1	1	1	1	1	1	3	2	2
10	→	1	3	1	1	1	1	1	3	2	2
11	←	1	2	1	1	9	1	1	9	1	2
11	→	1	1	1	2	9	1	1	9	1	2
12	←	1	1	1	1	1	1	1	1	4	4
12	→	1	1	1	1	1	1	1	1	4	4
13	←	1	1	1	1	3	2	1	3	4	2
13	→	1	1	1	1	3	1	1	3	4	4
14	←	1	1	1	1	1	1	2	1	4	2
14	→	1	1	1	1	1	1	2	1	4	2
15	←	3	1	1	1	3	1	2	9	4	2
15	→	1	3	1	3	1	1	2	9	4	2
16	←	3	1	1	1	1	1	1	3	2	2
16	→	1	3	1	1	2	1	1	3	2	4
17	←	3	1	1	1	9	1	1	27	4	4
17	→	1	3	1	2	9	1	1	27	4	8
18	←	3	1	1	1	3	2	1	9	4	2
18	→	1	3	1	1	3	1	1	9	4	4
19	←	3	1	1	1	1	1	1	3	2	2
19	→	1	3	1	1	2	1	1	3	2	4
20	←	3	1	1	1	3	2	1	9	4	2
20	→	1	3	1	1	3	1	1	9	4	4
21	←	1	2	1	1	1	1	2	1	1	1
21	→	1	1	1	1	2	1	2	1	1	1
22	←	1	2	1	1	1	1	1	1	2	4
22	→	1	1	1	1	1	1	1	1	2	2
23	←	1	2	1	1	1	1	1	1	2	4
23	→	1	1	1	1	1	1	1	1	2	2
24	→	1	2	1	1	3	2	1	3	2	2
24	←	1	1	1	1	3	1	1	3	2	2
25	→	1	2	1	1	1	1	1	1	1	2
25	←	1	1	1	1	2	1	1	1	1	2
26	→	1	2	1	1	3	2	1	3	2	2

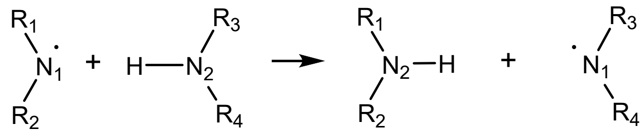
26	←	1	1	1	1	3	1	1	3	2	2
27	→	1	1	1	1	1	1	2	1	4	2
27	←	1	1	1	1	1	1	2	1	4	2
28	→	1	1	1	1	9	1	1	9	4	4
28	←	1	1	1	2	9	1	1	9	4	8
29	→	1	1	1	1	3	2	1	3	4	2
29	←	1	1	1	1	3	1	1	3	4	4
30	→	1	1	1	1	1	1	1	1	2	2
30	←	1	1	1	1	2	1	1	1	2	4
31	→	1	1	1	1	3	2	1	3	4	2
31	←	1	1	1	1	3	1	1	3	4	4
32	→	1	1	1	1	9	1	1	9	2	2
32	←	1	1	1	2	9	1	1	9	2	4
33	→	1	1	1	1	3	2	1	3	4	2
33	←	1	1	1	1	3	1	1	3	4	4
34	→	1	1	1	1	1	1	1	1	2	2
34	←	1	1	1	1	2	1	1	1	2	4
35	→	1	1	1	1	3	2	1	3	4	2
35	←	1	1	1	1	3	1	1	3	4	4
36	→	2	9	1	1	9	1	2	81	1	1
36	←	1	9	1	2	9	1	2	81	1	1
37	→	2	9	1	1	3	2	1	27	2	2
37	←	1	9	1	1	3	1	1	27	2	2
38	→	2	9	1	1	1	1	1	9	1	2
38	←	1	9	1	1	2	1	1	9	1	2
39	→	2	9	1	1	3	2	1	27	2	2
39	←	1	9	1	1	3	1	1	27	2	2
40	→	1	3	1	1	3	2	2	9	4	1
40	←	1	3	2	1	3	1	2	9	4	1
41	→	1	3	1	1	1	1	1	3	2	2
41	←	1	3	2	1	2	1	1	3	2	2
42	→	1	3	1	1	3	2	1	9	4	2
42	←	1	3	2	1	3	1	1	9	4	2
43	→	1	2	1	1	3	2	1	3	2	2
43	←	1	1	1	1	3	1	1	3	2	2
44	→	1	3	1	1	3	2	2	9	4	1
44	←	1	3	2	1	3	1	2	9	4	1
45	→	1	2	1	1	1	1	2	1	1	1
45	←	1	1	1	1	2	1	2	1	1	1

3.5. Group additivity values between 300 and 1800 K

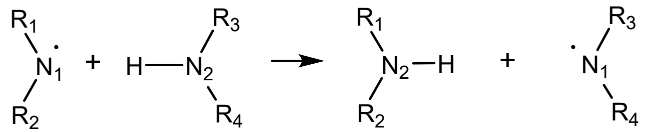
Table S12: Primary standard group additivity values ΔGAV°s between 300 and 1800 K for abstraction of a hydrogen atom from N-H by a nitrogen-centered radical, deduced from the combined training and test set. For the reference reaction, the single-event pre-exponential factor is expressed in $m^3\ mol^{-1}\ s^{-1}$ and E_a is expressed in $kJ\ mol^{-1}$.



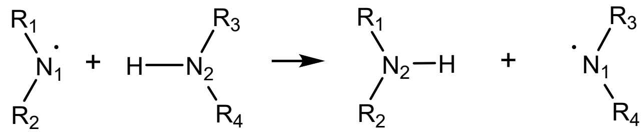
		300 K				400 K				500 K				600 K			
		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)	
No.	**Group**	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a
	Reference:	5.067	44.6	5.067	44.6	5.292	46.2	5.292	46.2	5.398	46.9	5.398	46.9	5.635	49.3	5.635	49.3
1	**N_i-(C)(H)**	-0.260	16.5	0.004	-15.4	-0.190	17.0	0.036	-15.2	-0.175	17.1	0.038	-15.2	-0.145	17.4	0.042	-15.1
2	**$N_{i,I}$**	-0.277	32.5	-0.072	-50.6	-0.221	32.9	0.000	-50.1	-0.211	32.9	0.015	-49.9	-0.190	33.2	0.045	-49.6
3	**N_i-(C_d)(H)**	-0.209	54.6	-0.553	-26.8	-0.122	55.2	-0.538	-26.7	-0.112	55.3	-0.548	-26.8	-0.093	55.5	-0.569	-27.0
4	**N_i-(C_t)(H)**	-0.387	55.5	-0.263	-32.2	-0.293	56.2	-0.189	-31.7	-0.267	56.4	-0.171	-31.6	-0.212	57.0	-0.132	-31.2
5	**N_i-$(C)_2$**	-0.703	22.9	0.054	-33.8	-0.528	24.1	0.116	-33.3	-0.487	24.4	0.116	-33.3	-0.400	25.3	0.117	-33.3
6	**N_i-(C_d)(C)**	-0.188	59.9	-0.332	-35.0	-0.049	60.9	-0.302	-34.7	-0.021	61.1	-0.306	-34.8	0.040	61.8	-0.313	-34.8
7	**N_i-$(C_d)_2$**	0.372	84.6	-0.636	-31.7	0.596	86.2	-0.590	-31.4	0.622	86.4	-0.584	-31.3	0.672	86.9	-0.568	-31.1
8	**N_i-(C_t)(C)**	-0.478	62.2	-0.151	-39.4	-0.335	63.2	-0.078	-38.9	-0.302	63.4	-0.065	-38.8	-0.230	64.2	-0.036	-38.5



		700 K				800 K				900 K				1000 K			
		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)	
No.	**Group**	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a
	Reference:	5.849	51.9	5.849	51.9	6.041	54.6	6.041	54.6	6.210	57.3	6.210	57.3	6.361	60.0	6.361	60.0
1	**N_i-(C)(H)**	-0.127	17.6	0.042	-15.1	-0.116	17.8	0.039	-15.1	-0.108	17.9	0.038	-15.2	-0.102	18.0	0.037	-15.2
2	**$N_{i,I}$**	-0.178	33.3	0.061	-49.4	-0.172	33.4	0.068	-49.3	-0.168	33.4	0.072	-49.2	-0.164	33.5	0.074	-49.2
3	**N_i-(C_d)(H)**	-0.091	55.5	-0.594	-27.3	-0.095	55.4	-0.617	-27.6	-0.100	55.3	-0.636	-27.9	-0.105	55.2	-0.652	-28.2
4	**N_i-(C_t)(H)**	-0.176	57.3	-0.107	-30.9	-0.152	57.7	-0.091	-30.6	-0.134	58.0	-0.079	-30.4	-0.122	58.2	-0.070	-30.3
5	**N_i-$(C)_2$**	-0.347	25.9	0.104	-33.5	-0.314	26.4	0.089	-33.7	-0.290	26.8	0.076	-33.9	-0.273	27.1	0.064	-34.1
6	**N_i-(C_d)(C)**	0.077	62.2	-0.325	-35.0	0.101	62.5	-0.337	-35.1	0.119	62.8	-0.346	-35.3	0.134	63.1	-0.353	-35.4
7	**N_i-$(C_d)_2$**	0.662	86.8	-0.557	-31.0	0.627	86.3	-0.547	-30.9	0.586	85.6	-0.538	-30.8	0.547	84.9	-0.530	-30.6
8	**N_i-(C_t)(C)**	-0.185	64.7	-0.019	-38.3	-0.157	65.1	-0.011	-38.2	-0.138	65.4	-0.005	-38.1	-0.123	65.7	-0.002	-38.0



No.	Group	1100 K ΔGAV°(N_1) $log\tilde{A}$	1100 K ΔGAV°(N_1) E_a	1100 K ΔGAV°(N_2) $log\tilde{A}$	1100 K ΔGAV°(N_2) E_a	1200 K ΔGAV°(N_1) $log\tilde{A}$	1200 K ΔGAV°(N_1) E_a	1200 K ΔGAV°(N_2) $log\tilde{A}$	1200 K ΔGAV°(N_2) E_a	1300 K ΔGAV°(N_1) $log\tilde{A}$	1300 K ΔGAV°(N_1) E_a	1300 K ΔGAV°(N_2) $log\tilde{A}$	1300 K ΔGAV°(N_2) E_a	1400 K ΔGAV°(N_1) $log\tilde{A}$	1400 K ΔGAV°(N_1) E_a	1400 K ΔGAV°(N_2) $log\tilde{A}$	1400 K ΔGAV°(N_2) E_a
	Reference:	6.497	62.7	6.497	62.7	6.619	65.4	6.619	65.4	6.729	68.0	6.729	68.0	6.830	70.6	6.830	70.6
1	**N_i-(C)(H)**	-0.098	18.1	0.036	-15.2	-0.093	18.2	0.035	-15.2	-0.090	18.3	0.035	-15.2	-0.087	18.4	0.034	-15.3
2	**$N_{i,I}$**	-0.162	33.6	0.074	-49.2	-0.159	33.6	0.074	-49.2	-0.157	33.6	0.074	-49.2	-0.155	33.7	0.073	-49.2
3	**N_i-(C_d)(H)**	-0.111	55.1	-0.665	-28.4	-0.117	55.0	-0.676	-28.7	-0.122	54.9	-0.685	-28.9	-0.128	54.7	-0.693	-29.1
4	**N_i-(C_t)(H)**	-0.112	58.4	-0.063	-30.1	-0.104	58.6	-0.058	-30.0	-0.096	58.8	-0.052	-29.9	-0.090	58.9	-0.047	-29.8
5	**N_i-$(C)_2$**	-0.260	27.4	0.054	-34.3	-0.249	27.6	0.046	-34.4	-0.240	27.9	0.039	-34.6	-0.233	28.0	0.033	-34.8
6	**N_i-(C_d)(C)**	0.145	63.3	-0.360	-35.5	0.155	63.5	-0.364	-35.6	0.163	63.7	-0.368	-35.7	0.170	63.9	-0.371	-35.8
7	**N_i-$(C_d)_2$**	0.511	84.2	-0.525	-30.5	0.482	83.6	-0.520	-30.4	0.457	83.1	-0.515	-30.2	0.437	82.5	-0.512	-30.2
8	**N_i-(C_t)(C)**	-0.113	65.9	0.001	-38.0	-0.105	66.1	0.002	-37.9	-0.098	66.2	0.005	-37.9	-0.093	66.3	0.005	-37.9



		1500 K				1600 K				1700 K				1800 K			
		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)	
No.	**Group**	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a
	Reference:	6.922	73.2	6.922	73.2	7.008	75.7	7.008	75.7	7.087	78.2	7.087	78.2	7.161	80.6	7.161	80.6
1	**N_i-(C)(H)**	-0.084	18.4	0.034	-15.2	-0.082	18.5	0.034	-15.3	-0.080	18.6	0.034	-15.3	-0.079	18.6	0.034	-15.3
2	**$N_{i,I}$**	-0.154	33.8	0.073	-49.3	-0.153	33.8	0.072	-49.3	-0.151	33.8	0.072	-49.3	-0.150	33.9	0.071	-49.3
3	**N_i-(C_d)(H)**	-0.133	54.6	-0.699	-29.3	-0.139	54.4	-0.705	-29.5	-0.144	54.3	-0.709	-29.6	-0.150	54.1	-0.714	-29.7
4	**N_i-(C_t)(H)**	-0.085	59.1	-0.043	-29.7	-0.080	59.2	-0.040	-29.6	-0.076	59.4	-0.036	-29.5	-0.072	59.5	-0.033	-29.4
5	**N_i-(C)$_2$**	-0.228	28.2	0.029	-34.9	-0.223	28.3	0.025	-35.0	-0.219	28.4	0.021	-35.1	-0.216	28.6	0.018	-35.2
6	**N_i-(C_d)(C)**	0.176	64.1	-0.372	-35.9	0.179	64.2	-0.374	-35.9	0.183	64.3	-0.375	-35.9	0.185	64.3	-0.377	-36.0
7	**N_i-(C_d)$_2$**	0.421	82.1	-0.509	-30.1	0.407	81.6	-0.508	-30.1	0.396	81.3	-0.507	-30.0	0.387	81.0	-0.507	-30.0
8	**N_i-(C_t)(C)**	-0.088	66.5	0.006	-37.8	-0.085	66.6	0.006	-37.9	-0.082	66.7	0.007	-37.8	-0.079	66.8	0.007	-37.8

3.6. Tunneling coefficients

Table S13: Tunneling coefficients for all reactions from Table S10 over the temperature range 300-1800 K.

No.	κ(T)															
	300	**400**	**500**	**600**	**700**	**800**	**900**	**1000**	**1100**	**1200**	**1300**	**1400**	**1500**	**1600**	**1700**	**1800**
1	19.7	4.6	2.6	1.9	1.6	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1
2	11.6	3.8	2.4	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1
3	7.4	3.0	2.0	1.6	1.4	1.3	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1
4	4.9	2.4	1.8	1.5	1.3	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.1
5	4.4	2.4	1.8	1.5	1.4	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.1
6	5.2	2.6	1.9	1.6	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1
7	9.7	3.5	2.2	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1
8	2.6	1.7	1.4	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.0	1.0	1.0	1.0
9	23.8	5.5	2.9	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
10	16.1	4.8	2.8	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
11	10.9	4.1	2.5	2.0	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
12	35.6	6.4	3.2	2.2	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
13	42.5	6.9	3.3	2.3	1.8	1.6	1.5	1.4	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
14	43.6	7.1	3.4	2.3	1.9	1.6	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1
15	25.9	5.7	3.0	2.2	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
16	8.0	3.4	2.3	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1
17	13.3	4.5	2.7	2.0	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
18	10.4	3.8	2.4	1.9	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1
19	9.5	3.8	2.4	1.9	1.6	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1
20	7.4	3.3	2.3	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1
21	25.8	5.8	3.1	2.2	1.8	1.6	1.4	1.4	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
22	28.4	6.0	3.1	2.2	1.8	1.6	1.4	1.4	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
23	24.6	5.6	3.0	2.2	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
24	27.8	5.9	3.1	2.2	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
25	50.6	8.3	3.8	2.5	2.0	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1
26	17.3	5.2	2.9	2.2	1.8	1.6	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1
27	54.5	7.6	3.5	2.3	1.9	1.6	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1
28	34.3	6.6	3.3	2.3	1.8	1.6	1.5	1.4	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
29	52.8	7.7	3.5	2.4	1.9	1.6	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1
30	36.1	6.7	3.3	2.3	1.8	1.6	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1
31	15.1	4.8	2.8	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
32	28.8	5.9	3.1	2.2	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
33	23.9	5.9	3.1	2.2	1.8	1.6	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1
34	58.4	7.7	3.5	2.3	1.9	1.6	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1
35	18.5	5.5	3.1	2.3	1.9	1.6	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.2	1.1
36	23.6	6.0	3.2	2.3	1.8	1.6	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1
37	18.5	5.6	3.1	2.3	1.9	1.6	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1
38	6.0	3.1	2.2	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1	1.1
39	31.5	6.5	3.3	2.3	1.9	1.6	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1
40	57.1	8.4	3.7	2.5	2.0	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1
41	44.7	7.5	3.5	2.4	1.9	1.6	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1
42	17.9	6.1	3.5	2.5	2.1	1.8	1.6	1.5	1.4	1.4	1.3	1.3	1.2	1.2	1.2	1.2
43	40.0	7.6	3.6	2.5	2.0	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1
44	31.4	6.8	3.5	2.4	1.9	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1
45	2.1	1.5	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.0	1.0	1.0	1.0	1.0	1.0

4. C-H-N hydrogen abstractions

4.1. Single-event Arrhenius parameters for reference reaction

Table S14: Intrinsic Arrhenius parameters over the temperature range 300-1800 K for the reference reaction of C-H-N hydrogen abstraction reactions, i.e. .e. $^{\cdot}CH_3 + CH_3NH_2 \rightarrow CH_4 + CH_3NH^{\cdot}$. The single-event pre-exponential factor is expressed in $m^3\ mol^{-1}\ s^{-1}$ and E_a is expressed in $kJ\ mol^{-1}$.

Temperature [K]	Forward		Reverse	
	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a
300	5.149	48.1	5.471	70.7
400	5.315	49.3	5.671	72.6
500	5.395	49.8	5.767	73.4
600	5.575	51.7	5.984	76.0
700	5.747	53.7	6.183	78.8
800	5.908	56.0	6.361	81.5
900	6.056	58.4	6.520	84.2
1000	6.192	60.8	6.662	86.9
1100	6.316	63.3	6.789	89.5
1200	6.430	65.8	6.904	92.1
1300	6.535	68.2	7.008	94.6
1400	6.632	70.7	7.103	97.1
1500	6.721	73.2	7.190	99.6
1600	6.803	75.6	7.271	102.0
1700	6.880	78.1	7.346	104.4
1800	6.953	80.5	7.416	106.8

4.2. Rate coefficients between 300 and 1800 K

Table S15: Rate coefficients [m^3 mol^{-1} s^{-1}] in the temperature range 300-1800 K for the reactions presented in Table S16. The rate coefficients do not include tunneling contributions.

No.		300 K	400 K	500 K	600 K	700 K	800 K	900 K	1000 K	1100 K	1200 K	1300 K	1400 K	1500 K	1600 K	1700 K	1800 K
1	→	9.1E-06	5.3E-03	2.6E-01	3.7E+00	2.6E+01	1.2E+02	4.0E+02	1.1E+03	2.5E+03	5.2E+03	9.9E+03	1.7E+04	2.8E+04	4.5E+04	6.7E+04	9.7E+04
1	←	8.3E-04	2.0E-01	5.8E+00	5.9E+01	3.4E+02	1.3E+03	3.9E+03	9.6E+03	2.1E+04	4.0E+04	7.2E+04	1.2E+05	1.9E+05	2.9E+05	4.2E+05	5.8E+05
2	→	2.2E-03	2.9E-01	5.7E+00	4.5E+01	2.1E+02	6.9E+02	1.8E+03	4.0E+03	8.0E+03	1.4E+04	2.4E+04	3.9E+04	5.9E+04	8.5E+04	1.2E+05	1.6E+05
2	←	4.6E-07	5.9E-04	4.9E-02	1.0E+00	9.7E+00	5.6E+01	2.3E+02	7.1E+02	1.9E+03	4.3E+03	9.0E+03	1.7E+04	3.0E+04	5.0E+04	7.8E+04	1.2E+05
3	→	9.8E+00	1.4E+02	7.3E+02	2.4E+03	6.0E+03	1.2E+04	2.3E+04	3.9E+04	6.1E+04	9.1E+04	1.3E+05	1.8E+05	2.4E+05	3.2E+05	4.1E+05	5.1E+05
3	←	6.0E-12	1.4E-07	6.3E-05	4.2E-03	8.9E-02	9.4E-01	6.1E+00	2.8E+01	1.0E+02	3.0E+02	7.8E+02	1.8E+03	3.7E+03	7.1E+03	1.3E+04	2.1E+04
4	→	5.8E-03	4.5E-01	6.7E+00	4.4E+01	1.8E+02	5.6E+02	1.4E+03	3.0E+03	5.8E+03	1.0E+04	1.7E+04	2.6E+04	3.9E+04	5.7E+04	7.9E+04	1.1E+05
4	←	1.2E-14	1.3E-09	1.6E-06	2.1E-04	7.5E-03	1.2E-01	1.0E+00	6.1E+00	2.7E+01	9.6E+01	2.9E+02	7.5E+02	1.7E+03	3.7E+03	7.1E+03	1.3E+04
5	→	2.5E-01	1.0E+01	1.0E+02	5.1E+02	1.7E+03	4.4E+03	9.6E+03	1.8E+04	3.2E+04	5.3E+04	8.2E+04	1.2E+05	1.7E+05	2.4E+05	3.2E+05	4.1E+05
5	←	1.4E-14	1.5E-09	1.8E-06	2.2E-04	7.3E-03	1.1E-01	9.1E-01	5.2E+00	2.2E+01	7.6E+01	2.2E+02	5.6E+02	1.3E+03	2.6E+03	5.0E+03	9.0E+03
6	→	3.4E-01	1.1E+01	1.0E+02	4.7E+02	1.5E+03	3.8E+03	8.0E+03	1.5E+04	2.6E+04	4.1E+04	6.3E+04	9.1E+04	1.3E+05	1.7E+05	2.3E+05	3.0E+05
6	←	2.1E-09	8.6E-06	1.5E-03	5.3E-02	7.5E-01	5.8E+00	3.0E+01	1.2E+02	3.6E+02	9.5E+02	2.2E+03	4.6E+03	8.9E+03	1.6E+04	2.7E+04	4.4E+04
7	→	1.1E-01	3.9E+00	3.7E+01	1.8E+02	6.2E+02	1.6E+03	3.6E+03	7.1E+03	1.3E+04	2.1E+04	3.3E+04	4.9E+04	7.0E+04	9.7E+04	1.3E+05	1.7E+05
7	←	1.2E-15	2.4E-10	4.5E-07	7.7E-05	3.4E-03	6.1E-02	6.2E-01	4.1E+00	2.0E+01	7.6E+01	2.4E+02	6.7E+02	1.6E+03	3.6E+03	7.3E+03	1.4E+04
8	→	8.3E-03	5.1E-01	6.3E+00	3.6E+01	1.3E+02	3.6E+02	8.3E+02	1.6E+03	2.9E+03	4.9E+03	7.6E+03	1.1E+04	1.6E+04	2.2E+04	3.0E+04	3.9E+04
8	←	1.2E-19	3.7E-13	3.4E-09	1.6E-06	1.4E-04	4.0E-03	5.7E-02	4.8E-01	2.8E+00	1.2E+01	4.4E+01	1.3E+02	3.4E+02	7.9E+02	1.7E+03	3.3E+03
9	→	3.8E+00	6.2E+01	3.6E+02	1.3E+03	3.3E+03	7.2E+03	1.4E+04	2.3E+04	3.7E+04	5.6E+04	8.2E+04	1.1E+05	1.5E+05	2.0E+05	2.6E+05	3.3E+05
9	←	9.8E-16	1.7E-10	2.9E-07	4.5E-05	1.8E-03	3.0E-02	2.9E-01	1.8E+00	8.2E+00	3.0E+01	9.2E+01	2.4E+02	5.7E+02	1.2E+03	2.4E+03	4.5E+03
10	→	5.5E-14	6.2E-09	7.3E-06	9.0E-04	3.0E-02	4.3E-01	3.6E+00	2.1E+01	8.8E+01	3.0E+02	8.7E+02	2.2E+03	5.0E+03	1.0E+04	2.0E+04	3.5E+04
10	←	3.1E+00	6.5E+01	4.6E+02	1.9E+03	5.4E+03	1.3E+04	2.7E+04	4.9E+04	8.4E+04	1.3E+05	2.0E+05	3.0E+05	4.2E+05	5.7E+05	7.6E+05	9.9E+05
11	→	4.9E-07	4.4E-04	2.9E-02	5.3E-01	4.5E+00	2.4E+01	9.2E+01	2.8E+02	7.1E+02	1.6E+03	3.2E+03	6.0E+03	1.1E+04	1.7E+04	2.7E+04	4.1E+04
11	←	2.9E-02	1.7E+00	2.3E+01	1.5E+02	6.3E+02	2.0E+03	5.0E+03	1.1E+04	2.2E+04	3.9E+04	6.7E+04	1.1E+05	1.6E+05	2.4E+05	3.4E+05	4.6E+05
12	→	1.7E+01	2.0E+02	1.0E+03	3.2E+03	7.7E+03	1.6E+04	2.9E+04	4.8E+04	7.5E+04	1.1E+05	1.6E+05	2.2E+05	2.9E+05	3.8E+05	4.8E+05	6.1E+05
12	←	1.2E-06	1.2E-03	9.0E-02	1.8E+00	1.6E+01	8.7E+01	3.4E+02	1.1E+03	2.7E+03	6.2E+03	1.3E+04	2.4E+04	4.1E+04	6.8E+04	1.1E+05	1.6E+05
13	→	8.5E-05	1.7E-02	4.8E-01	4.9E+00	2.7E+01	1.0E+02	3.1E+02	7.7E+02	1.7E+03	3.2E+03	5.8E+03	9.7E+03	1.5E+04	2.3E+04	3.4E+04	4.8E+04
13	←	3.1E-05	1.3E-02	5.8E-01	7.9E+00	5.5E+01	2.5E+02	8.5E+02	2.3E+03	5.5E+03	1.1E+04	2.2E+04	3.8E+04	6.3E+04	9.9E+04	1.5E+05	2.2E+05
14	→	7.0E-05	1.7E-02	5.1E-01	5.6E+00	3.3E+01	1.4E+02	4.2E+02	1.1E+03	2.4E+03	4.8E+03	8.7E+03	1.5E+04	2.4E+04	3.7E+04	5.5E+04	7.9E+04

14	←	5.2E-03	6.3E-01	1.3E+01	1.0E+02	5.0E+02	1.7E+03	4.6E+03	1.0E+04	2.1E+04	3.9E+04	6.6E+04	1.1E+05	1.6E+05	2.4E+05	3.4E+05	4.6E+05
15	→	2.7E+00	4.4E+01	2.7E+02	9.8E+02	2.6E+03	5.9E+03	1.1E+04	2.0E+04	3.3E+04	5.0E+04	7.4E+04	1.0E+05	1.4E+05	1.9E+05	2.5E+05	3.2E+05
15	←	1.4E-05	5.3E-03	2.2E-01	2.9E+00	1.9E+01	8.5E+01	2.8E+02	7.6E+02	1.7E+03	3.6E+03	6.7E+03	1.2E+04	1.9E+04	3.0E+04	4.5E+04	6.5E+04
16	→	1.4E-10	1.7E-06	5.2E-04	2.6E-02	4.6E-01	4.2E+00	2.4E+01	1.0E+02	3.4E+02	9.5E+02	2.3E+03	5.0E+03	1.0E+04	1.9E+04	3.2E+04	5.3E+04
16	←	1.8E-02	9.9E-01	1.3E+01	7.7E+01	3.1E+02	9.1E+02	2.3E+03	4.8E+03	9.3E+03	1.7E+04	2.7E+04	4.3E+04	6.5E+04	9.4E+04	1.3E+05	1.8E+05
17	→	4.2E-06	4.5E-03	3.4E-01	6.5E+00	5.8E+01	3.1E+02	1.2E+03	3.8E+03	9.7E+03	2.2E+04	4.4E+04	8.3E+04	1.4E+05	2.4E+05	3.7E+05	5.6E+05
17	←	1.4E-07	1.9E-04	1.6E-02	3.6E-01	3.5E+00	2.1E+01	8.6E+01	2.8E+02	7.7E+02	1.8E+03	3.8E+03	7.4E+03	1.3E+04	2.3E+04	3.7E+04	5.7E+04
18	→	1.5E-06	1.7E-03	1.3E-01	2.6E+00	2.3E+01	1.3E+02	5.0E+02	1.5E+03	3.9E+03	8.8E+03	1.8E+04	3.3E+04	5.8E+04	9.5E+04	1.5E+05	2.2E+05
18	←	9.9E-09	3.1E-05	4.5E-03	1.4E-01	1.8E+00	1.3E+01	6.3E+01	2.4E+02	7.2E+02	1.9E+03	4.3E+03	8.9E+03	1.7E+04	3.1E+04	5.2E+04	8.4E+04
19	→	1.1E-06	7.3E-04	4.2E-02	7.0E-01	5.6E+00	2.8E+01	1.1E+02	3.1E+02	7.8E+02	1.7E+03	3.4E+03	6.3E+03	1.1E+04	1.8E+04	2.7E+04	4.1E+04
19	←	7.0E-01	1.7E+01	1.4E+02	6.4E+02	2.1E+03	5.3E+03	1.2E+04	2.3E+04	4.0E+04	6.7E+04	1.1E+05	1.6E+05	2.3E+05	3.2E+05	4.3E+05	5.7E+05
20	→	1.9E-03	1.3E-01	2.0E+00	1.3E+01	5.7E+01	1.8E+02	4.8E+02	1.1E+03	2.2E+03	4.1E+03	7.0E+03	1.1E+04	1.8E+04	2.7E+04	3.9E+04	5.4E+04
20	←	1.2E-05	4.4E-03	1.8E-01	2.5E+00	1.8E+01	8.6E+01	3.1E+02	9.0E+02	2.3E+03	5.0E+03	1.0E+04	1.9E+04	3.2E+04	5.3E+04	8.4E+04	1.3E+05
21	→	2.5E+00	3.0E+01	1.6E+02	5.3E+02	1.4E+03	2.9E+03	5.7E+03	1.0E+04	1.7E+04	2.6E+04	3.9E+04	5.6E+04	7.9E+04	1.1E+05	1.4E+05	1.9E+05
21	←	4.1E-04	5.0E-02	1.0E+00	8.9E+00	4.5E+01	1.6E+02	4.7E+02	1.2E+03	2.5E+03	4.8E+03	8.7E+03	1.5E+04	2.4E+04	3.7E+04	5.4E+04	7.8E+04
22	→	7.7E-09	2.1E-05	2.7E-03	7.5E-02	8.7E-01	5.8E+00	2.6E+01	9.1E+01	2.6E+02	6.3E+02	1.4E+03	2.7E+03	5.0E+03	8.5E+03	1.4E+04	2.1E+04
22	←	4.4E-03	3.4E-01	5.5E+00	3.9E+01	1.7E+02	5.6E+02	1.5E+03	3.3E+03	6.7E+03	1.2E+04	2.1E+04	3.4E+04	5.2E+04	7.6E+04	1.1E+05	1.5E+05
23	→	7.7E-08	8.5E-05	6.5E-03	1.3E-01	1.2E+00	6.6E+00	2.6E+01	8.3E+01	2.2E+02	5.0E+02	1.0E+03	1.9E+03	3.4E+03	5.7E+03	9.0E+03	1.4E+04
23	←	4.3E-10	2.0E-06	3.7E-04	1.4E-02	2.0E-01	1.6E+00	8.7E+00	3.5E+01	1.1E+02	3.0E+02	7.2E+02	1.6E+03	3.1E+03	5.6E+03	9.7E+03	1.6E+04
24	→	1.6E-05	7.8E-03	3.6E-01	5.1E+00	3.6E+01	1.7E+02	5.7E+02	1.6E+03	3.7E+03	7.7E+03	1.5E+04	2.6E+04	4.3E+04	6.8E+04	1.0E+05	1.5E+05
24	←	2.4E-09	9.2E-06	1.5E-03	4.9E-02	6.5E-01	4.8E+00	2.4E+01	9.0E+01	2.8E+02	7.1E+02	1.6E+03	3.4E+03	6.5E+03	1.2E+04	1.9E+04	3.1E+04
25	→	2.3E-10	2.4E-06	7.2E-04	3.5E-02	5.9E-01	5.2E+00	2.9E+01	1.2E+02	3.9E+02	1.1E+03	2.5E+03	5.4E+03	1.0E+04	1.9E+04	3.2E+04	5.2E+04
25	←	2.0E-03	1.8E-01	3.2E+00	2.4E+01	1.1E+02	3.7E+02	9.7E+02	2.2E+03	4.4E+03	8.1E+03	1.4E+04	2.2E+04	3.4E+04	5.0E+04	7.0E+04	9.7E+04
26	→	9.4E-07	1.7E-03	1.7E-01	3.9E+00	3.9E+01	2.3E+02	9.6E+02	3.1E+03	8.1E+03	1.9E+04	3.9E+04	7.3E+04	1.3E+05	2.1E+05	3.3E+05	5.1E+05
26	←	2.1E-09	8.9E-06	1.5E-03	5.0E-02	6.7E-01	4.9E+00	2.4E+01	8.9E+01	2.7E+02	6.9E+02	1.6E+03	3.2E+03	6.0E+03	1.1E+04	1.8E+04	2.8E+04
27	→	4.5E-05	1.2E-02	4.1E-01	4.6E+00	2.8E+01	1.1E+02	3.5E+02	9.1E+02	2.0E+03	4.1E+03	7.4E+03	1.3E+04	2.0E+04	3.1E+04	4.7E+04	6.7E+04
27	←	8.8E-02	3.8E+00	4.1E+01	2.3E+02	8.1E+02	2.3E+03	5.2E+03	1.0E+04	1.9E+04	3.2E+04	5.1E+04	7.7E+04	1.1E+05	1.6E+05	2.1E+05	2.8E+05
28	→	2.2E-09	8.5E-06	1.4E-03	4.4E-02	5.7E-01	4.1E+00	2.0E+01	7.1E+01	2.1E+02	5.3E+02	1.2E+03	2.4E+03	4.5E+03	7.8E+03	1.3E+04	2.0E+04
28	←	4.9E-10	2.0E-06	3.4E-04	1.2E-02	1.7E-01	1.3E+00	6.8E+00	2.7E+01	8.3E+01	2.2E+02	5.2E+02	1.1E+03	2.1E+03	3.8E+03	6.5E+03	1.1E+04
29	→	2.6E-05	9.9E-03	3.9E-01	4.9E+00	3.2E+01	1.4E+02	4.5E+02	1.2E+03	2.7E+03	5.5E+03	1.0E+04	1.8E+04	2.9E+04	4.5E+04	6.7E+04	9.7E+04
29	←	1.1E-02	8.9E-01	1.4E+01	9.7E+01	4.2E+02	1.3E+03	3.4E+03	7.4E+03	1.4E+04	2.6E+04	4.3E+04	6.8E+04	1.0E+05	1.5E+05	2.1E+05	2.8E+05
30	→	4.2E-10	2.1E-06	4.0E-04	1.5E-02	2.1E-01	1.6E+00	8.3E+00	3.2E+01	1.0E+02	2.7E+02	6.2E+02	1.3E+03	2.5E+03	4.6E+03	7.8E+03	1.3E+04

30	←	1.1E+01	1.5E+02	8.3E+02	2.9E+03	7.8E+03	1.8E+04	3.5E+04	6.3E+04	1.1E+05	1.7E+05	2.5E+05	3.6E+05	5.1E+05	6.9E+05	9.2E+05	1.2E+06
31	→	6.2E-07	5.9E-04	4.1E-02	7.3E-01	6.2E+00	3.2E+01	1.2E+02	3.6E+02	9.1E+02	2.0E+03	4.0E+03	7.4E+03	1.3E+04	2.1E+04	3.2E+04	4.8E+04
31	←	1.5E-01	1.1E+01	1.5E+02	9.6E+02	3.9E+03	1.1E+04	2.8E+04	5.8E+04	1.1E+05	1.9E+05	3.1E+05	4.7E+05	7.0E+05	9.9E+05	1.4E+06	1.8E+06
32	→	1.9E-07	2.2E-04	1.8E-02	3.7E-01	3.5E+00	2.0E+01	7.9E+01	2.5E+02	6.7E+02	1.5E+03	3.2E+03	6.1E+03	1.1E+04	1.8E+04	2.8E+04	4.3E+04
32	←	6.1E+00	1.5E+02	1.1E+03	4.8E+03	1.4E+04	3.3E+04	6.7E+04	1.2E+05	2.0E+05	3.2E+05	4.8E+05	6.8E+05	9.4E+05	1.3E+06	1.7E+06	2.1E+06
33	→	3.7E-02	2.4E+00	3.3E+01	2.0E+02	7.9E+02	2.3E+03	5.5E+03	1.2E+04	2.2E+04	3.7E+04	6.0E+04	9.3E+04	1.4E+05	1.9E+05	2.7E+05	3.6E+05
33	←	1.1E-03	2.6E-01	7.6E+00	7.8E+01	4.4E+02	1.7E+03	5.1E+03	1.3E+04	2.7E+04	5.3E+04	9.5E+04	1.6E+05	2.5E+05	3.8E+05	5.6E+05	7.8E+05
34	→	7.6E-03	6.6E-01	1.1E+01	7.6E+01	3.3E+02	1.0E+03	2.6E+03	5.7E+03	1.1E+04	2.0E+04	3.3E+04	5.3E+04	7.9E+04	1.1E+05	1.6E+05	2.2E+05
34	←	1.7E-02	1.4E+00	2.2E+01	1.5E+02	6.5E+02	2.0E+03	5.0E+03	1.1E+04	2.1E+04	3.6E+04	6.0E+04	9.3E+04	1.4E+05	2.0E+05	2.8E+05	3.7E+05
35	→	2.1E-02	8.2E-01	8.9E+00	5.0E+01	1.9E+02	5.4E+02	1.3E+03	2.7E+03	5.1E+03	9.0E+03	1.5E+04	2.3E+04	3.4E+04	4.9E+04	6.9E+04	9.3E+04
35	←	9.0E-08	1.0E-04	8.9E-03	2.0E-01	2.1E+00	1.3E+01	5.7E+01	1.9E+02	5.4E+02	1.3E+03	2.9E+03	5.7E+03	1.0E+04	1.8E+04	2.9E+04	4.6E+04
36	→	1.1E+00	2.6E+01	1.9E+02	8.1E+02	2.4E+03	5.8E+03	1.2E+04	2.2E+04	3.7E+04	5.9E+04	9.0E+04	1.3E+05	1.8E+05	2.5E+05	3.3E+05	4.2E+05
36	←	1.5E-06	1.1E-03	7.0E-02	1.2E+00	9.9E+00	5.1E+01	1.9E+02	5.6E+02	1.4E+03	3.1E+03	6.1E+03	1.1E+04	1.9E+04	3.1E+04	4.8E+04	7.1E+04
37	→	7.1E-03	6.0E-01	9.7E+00	6.8E+01	2.9E+02	9.0E+02	2.3E+03	4.9E+03	9.5E+03	1.7E+04	2.8E+04	4.3E+04	6.4E+04	9.3E+04	1.3E+05	1.7E+05
37	←	9.4E-05	2.0E-02	5.9E-01	6.5E+00	3.9E+01	1.6E+02	5.1E+02	1.3E+03	3.0E+03	6.0E+03	1.1E+04	1.9E+04	3.1E+04	4.8E+04	7.2E+04	1.0E+05
38	→	8.0E-02	3.6E+00	4.0E+01	2.1E+02	7.4E+02	2.0E+03	4.5E+03	9.0E+03	1.6E+04	2.7E+04	4.3E+04	6.5E+04	9.4E+04	1.3E+05	1.8E+05	2.4E+05
38	←	2.7E-15	4.6E-10	7.5E-07	1.2E-04	4.9E-03	8.5E-02	8.2E-01	5.2E+00	2.5E+01	9.2E+01	2.9E+02	7.7E+02	1.8E+03	4.0E+03	8.0E+03	1.5E+04
39	→	4.7E-02	1.9E+00	2.0E+01	1.0E+02	3.7E+02	1.0E+03	2.3E+03	4.7E+03	8.5E+03	1.4E+04	2.3E+04	3.5E+04	5.0E+04	7.1E+04	9.7E+04	1.3E+05
39	←	8.1E-06	3.6E-03	1.6E-01	2.3E+00	1.6E+01	7.7E+01	2.7E+02	7.6E+02	1.8E+03	3.9E+03	7.6E+03	1.4E+04	2.3E+04	3.7E+04	5.7E+04	8.5E+04
40	→	3.4E-01	6.0E+00	3.8E+01	1.5E+02	4.1E+02	9.3E+02	1.9E+03	3.3E+03	5.6E+03	8.8E+03	1.3E+04	1.9E+04	2.7E+04	3.6E+04	4.8E+04	6.2E+04
40	←	5.2E-06	1.6E-03	6.1E-02	7.7E-01	5.1E+00	2.3E+01	7.6E+01	2.1E+02	4.9E+02	1.0E+03	2.0E+03	3.5E+03	5.9E+03	9.4E+03	1.4E+04	2.1E+04
41	→	2.1E-04	3.2E-02	7.5E-01	6.9E+00	3.6E+01	1.3E+02	3.8E+02	9.2E+02	1.9E+03	3.7E+03	6.6E+03	1.1E+04	1.7E+04	2.6E+04	3.7E+04	5.2E+04
41	←	3.6E-04	4.6E-02	1.0E+00	9.6E+00	5.3E+01	2.0E+02	6.2E+02	1.6E+03	3.5E+03	7.0E+03	1.3E+04	2.2E+04	3.6E+04	5.6E+04	8.4E+04	1.2E+05
42	→	7.4E+00	6.3E+01	2.6E+02	7.4E+02	1.7E+03	3.3E+03	5.7E+03	9.4E+03	1.4E+04	2.1E+04	3.0E+04	4.1E+04	5.4E+04	7.1E+04	9.1E+04	1.1E+05
42	←	5.4E-07	3.3E-04	1.9E-02	3.2E-01	2.7E+00	1.4E+01	5.3E+01	1.6E+02	4.1E+02	9.2E+02	1.9E+03	3.5E+03	6.1E+03	1.0E+04	1.6E+04	2.4E+04
43	→	3.1E-02	1.1E+00	1.0E+01	4.9E+01	1.6E+02	4.2E+02	9.1E+02	1.8E+03	3.1E+03	5.1E+03	7.9E+03	1.2E+04	1.7E+04	2.3E+04	3.1E+04	4.1E+04
43	←	3.2E-05	9.9E-03	3.5E-01	4.1E+00	2.5E+01	1.1E+02	3.3E+02	8.6E+02	1.9E+03	3.9E+03	7.1E+03	1.2E+04	2.0E+04	3.1E+04	4.6E+04	6.6E+04
44	→	2.7E-02	1.2E+00	1.3E+01	7.2E+01	2.6E+02	7.1E+02	1.6E+03	3.3E+03	6.1E+03	1.0E+04	1.7E+04	2.5E+04	3.7E+04	5.2E+04	7.1E+04	9.6E+04
44	←	6.5E-05	1.8E-02	5.9E-01	6.6E+00	4.0E+01	1.6E+02	5.0E+02	1.3E+03	2.9E+03	5.7E+03	1.0E+04	1.8E+04	2.9E+04	4.4E+04	6.5E+04	9.3E+04
45	→	1.8E-01	4.5E+00	3.6E+01	1.6E+02	4.8E+02	1.2E+03	2.5E+03	4.7E+03	8.1E+03	1.3E+04	2.0E+04	3.0E+04	4.2E+04	5.8E+04	7.8E+04	1.0E+05
45	←	3.8E-05	9.7E-03	3.1E-01	3.5E+00	2.1E+01	8.7E+01	2.7E+02	7.0E+02	1.6E+03	3.1E+03	5.8E+03	9.9E+03	1.6E+04	2.5E+04	3.6E+04	5.2E+04
46	→	4.7E-05	1.0E-02	3.1E-01	3.2E+00	1.8E+01	7.1E+01	2.1E+02	5.4E+02	1.2E+03	2.3E+03	4.2E+03	7.1E+03	1.1E+04	1.7E+04	2.6E+04	3.6E+04

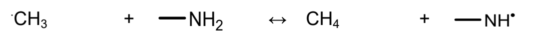
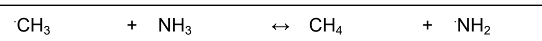
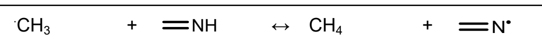
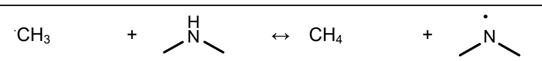
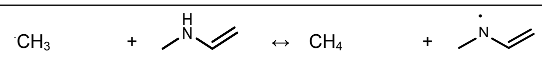
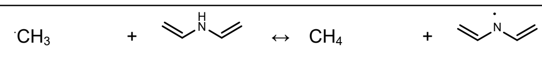
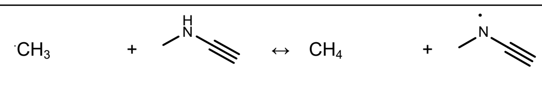
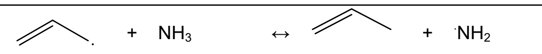
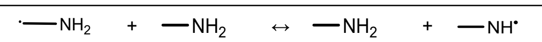
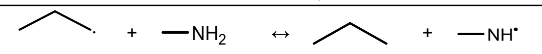
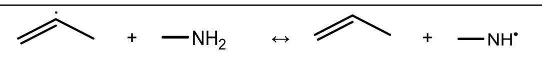
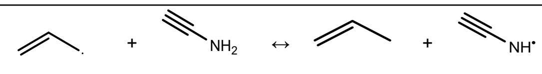
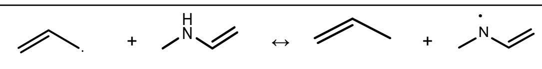
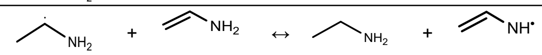
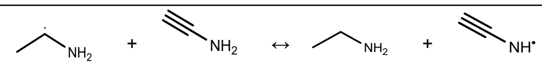
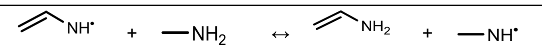
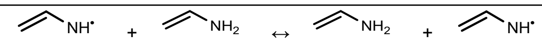
46	←	1.2E-03	1.2E-01	2.3E+00	1.9E+01	9.3E+01	3.3E+02	9.2E+02	2.2E+03	4.6E+03	8.8E+03	1.6E+04	2.6E+04	4.1E+04	6.1E+04	8.9E+04	1.3E+05
47	→	2.4E-01	3.6E+00	2.1E+01	7.5E+01	2.0E+02	4.6E+02	9.1E+02	1.6E+03	2.7E+03	4.3E+03	6.4E+03	9.2E+03	1.3E+04	1.7E+04	2.3E+04	2.9E+04
47	←	1.4E-08	4.0E-05	5.7E-03	1.8E-01	2.2E+00	1.5E+01	7.2E+01	2.5E+02	7.3E+02	1.8E+03	3.9E+03	7.6E+03	1.4E+04	2.3E+04	3.8E+04	5.8E+04
48	→	8.4E-02	3.7E+00	4.0E+01	2.2E+02	7.7E+02	2.1E+03	4.7E+03	9.4E+03	1.7E+04	2.9E+04	4.5E+04	6.8E+04	9.8E+04	1.4E+05	1.9E+05	2.5E+05
48	←	2.0E-06	1.3E-03	7.6E-02	1.3E+00	1.0E+01	5.1E+01	1.9E+02	5.6E+02	1.4E+03	3.1E+03	6.3E+03	1.2E+04	2.0E+04	3.3E+04	5.1E+04	7.7E+04
49	→	1.1E-01	3.5E+00	3.2E+01	1.5E+02	5.1E+02	1.3E+03	2.9E+03	5.7E+03	1.0E+04	1.7E+04	2.6E+04	3.8E+04	5.5E+04	7.6E+04	1.0E+05	1.3E+05
49	←	3.1E-07	2.4E-04	1.6E-02	3.1E-01	2.7E+00	1.5E+01	6.0E+01	1.9E+02	5.0E+02	1.2E+03	2.4E+03	4.6E+03	8.1E+03	1.4E+04	2.2E+04	3.3E+04
50	→	9.0E-05	2.1E-02	6.1E-01	6.4E+00	3.6E+01	1.4E+02	4.2E+02	1.0E+03	2.2E+03	4.3E+03	7.7E+03	1.3E+04	2.0E+04	3.0E+04	4.4E+04	6.1E+04
50	←	2.2E-05	5.7E-03	2.0E-01	2.4E+00	1.6E+01	7.0E+01	2.4E+02	6.5E+02	1.5E+03	3.3E+03	6.3E+03	1.1E+04	1.9E+04	3.0E+04	4.6E+04	6.8E+04
51	→	1.1E+03	4.1E+03	1.1E+04	2.1E+04	3.8E+04	6.1E+04	9.2E+04	1.3E+05	1.8E+05	2.4E+05	3.2E+05	4.1E+05	5.1E+05	6.2E+05	7.6E+05	9.1E+05
51	←	2.2E-09	9.1E-06	1.6E-03	5.8E-02	8.1E-01	6.3E+00	3.3E+01	1.3E+02	4.0E+02	1.0E+03	2.4E+03	5.1E+03	9.9E+03	1.8E+04	3.0E+04	4.9E+04
52	→	6.1E+02	2.0E+03	4.8E+03	9.4E+03	1.7E+04	2.7E+04	4.1E+04	6.0E+04	8.3E+04	1.1E+05	1.5E+05	1.9E+05	2.4E+05	3.0E+05	3.7E+05	4.5E+05
52	←	2.2E-15	3.7E-10	6.0E-07	9.5E-05	3.9E-03	6.8E-02	6.7E-01	4.3E+00	2.0E+01	7.7E+01	2.4E+02	6.6E+02	1.6E+03	3.5E+03	7.0E+03	1.3E+04
53	→	2.8E-08	6.8E-05	8.1E-03	2.1E-01	2.3E+00	1.5E+01	6.6E+01	2.2E+02	6.3E+02	1.5E+03	3.2E+03	6.4E+03	1.2E+04	2.0E+04	3.2E+04	5.0E+04
53	←	5.5E+00	1.1E+02	7.4E+02	2.9E+03	8.3E+03	1.9E+04	3.8E+04	6.9E+04	1.2E+05	1.8E+05	2.7E+05	3.8E+05	5.3E+05	7.1E+05	9.3E+05	1.2E+06
54	→	9.9E-10	4.2E-06	7.2E-04	2.5E-02	3.4E-01	2.6E+00	1.3E+01	5.1E+01	1.6E+02	4.1E+02	9.6E+02	2.0E+03	3.9E+03	6.9E+03	1.2E+04	1.9E+04
54	←	2.8E+02	1.8E+03	6.2E+03	1.6E+04	3.4E+04	6.5E+04	1.1E+05	1.8E+05	2.8E+05	4.1E+05	5.8E+05	7.9E+05	1.1E+06	1.4E+06	1.7E+06	2.2E+06
55	→	2.0E-10	1.3E-06	2.9E-04	1.2E-02	1.8E-01	1.5E+00	8.2E+00	3.3E+01	1.1E+02	3.0E+02	7.1E+02	1.5E+03	3.0E+03	5.6E+03	9.6E+03	1.6E+04
55	←	7.2E+01	7.1E+02	3.2E+03	9.9E+03	2.4E+04	5.0E+04	9.2E+04	1.6E+05	2.5E+05	3.7E+05	5.4E+05	7.6E+05	1.0E+06	1.4E+06	1.8E+06	2.2E+06
56	→	6.1E-10	3.3E-06	6.5E-04	2.4E-02	3.5E-01	2.7E+00	1.4E+01	5.3E+01	1.6E+02	4.3E+02	1.0E+03	2.1E+03	4.0E+03	7.1E+03	1.2E+04	1.9E+04
56	←	2.8E+00	5.9E+01	4.3E+02	1.8E+03	5.6E+03	1.4E+04	3.0E+04	5.6E+04	9.8E+04	1.6E+05	2.5E+05	3.7E+05	5.3E+05	7.3E+05	9.9E+05	1.3E+06
57	→	1.4E-06	1.0E-03	6.0E-02	9.7E-01	7.7E+00	3.8E+01	1.4E+02	4.0E+02	9.9E+02	2.2E+03	4.3E+03	7.7E+03	1.3E+04	2.1E+04	3.3E+04	4.9E+04
57	←	2.3E-01	1.4E+01	1.8E+02	1.1E+03	4.3E+03	1.2E+04	2.9E+04	6.1E+04	1.1E+05	2.0E+05	3.1E+05	4.8E+05	7.0E+05	9.9E+05	1.4E+06	1.8E+06
58	→	7.8E-01	1.5E+01	1.1E+02	4.3E+02	1.3E+03	3.0E+03	6.3E+03	1.2E+04	2.0E+04	3.2E+04	4.8E+04	7.0E+04	9.8E+04	1.3E+05	1.8E+05	2.3E+05
58	←	1.7E-07	2.8E-04	2.7E-02	6.0E-01	6.0E+00	3.5E+01	1.5E+02	4.7E+02	1.2E+03	2.9E+03	5.9E+03	1.1E+04	2.0E+04	3.3E+04	5.2E+04	7.8E+04
59	→	9.7E-03	4.9E-01	6.0E+00	3.6E+01	1.4E+02	4.1E+02	9.8E+02	2.0E+03	3.8E+03	6.7E+03	1.1E+04	1.7E+04	2.5E+04	3.5E+04	4.9E+04	6.5E+04
59	←	2.2E-05	6.8E-03	2.6E-01	3.3E+00	2.2E+01	9.6E+01	3.2E+02	8.6E+02	2.0E+03	4.2E+03	7.9E+03	1.4E+04	2.3E+04	3.6E+04	5.4E+04	7.8E+04
60	→	2.2E-01	6.4E+00	5.5E+01	2.6E+02	8.3E+02	2.1E+03	4.5E+03	8.7E+03	1.5E+04	2.5E+04	3.8E+04	5.7E+04	8.1E+04	1.1E+05	1.5E+05	2.0E+05
60	←	4.3E-09	1.7E-05	2.7E-03	8.8E-02	1.1E+00	7.9E+00	3.7E+01	1.3E+02	3.9E+02	9.7E+02	2.1E+03	4.2E+03	7.8E+03	1.4E+04	2.2E+04	3.5E+04
61	→	4.0E+00	4.4E+01	2.2E+02	6.9E+02	1.7E+03	3.6E+03	6.7E+03	1.1E+04	1.8E+04	2.8E+04	4.0E+04	5.6E+04	7.5E+04	9.9E+04	1.3E+05	1.6E+05
61	←	3.7E-10	2.3E-06	4.9E-04	2.0E-02	2.9E-01	2.4E+00	1.2E+01	4.8E+01	1.5E+02	4.0E+02	9.3E+02	1.9E+03	3.7E+03	6.6E+03	1.1E+04	1.8E+04
62	→	9.5E+03	2.0E+04	3.5E+04	5.7E+04	8.6E+04	1.2E+05	1.7E+05	2.3E+05	3.1E+05	4.0E+05	5.0E+05	6.2E+05	7.6E+05	9.2E+05	1.1E+06	1.3E+06

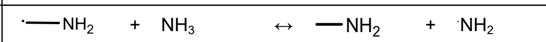
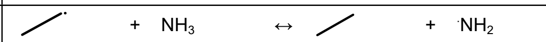
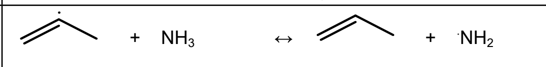
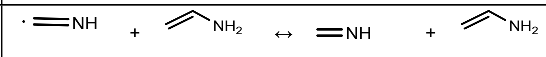
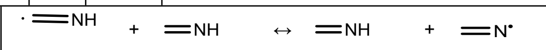
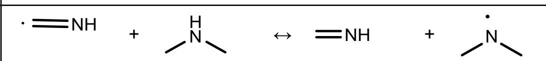
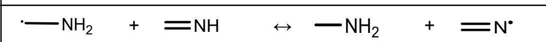
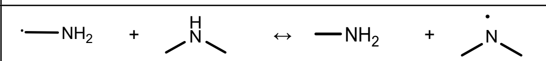
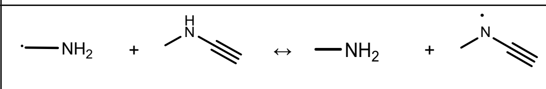
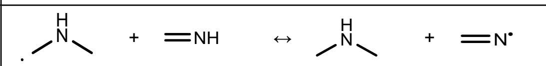
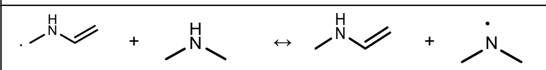
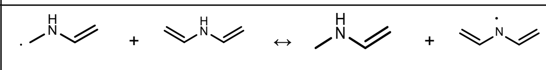
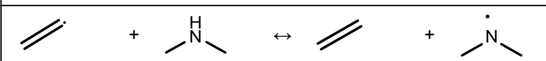
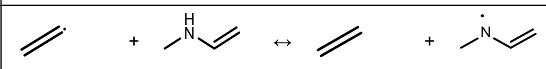
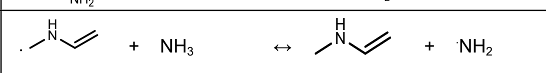
62	←	1.4E-10	1.1E-06	2.9E-04	1.3E-02	2.0E-01	1.7E+00	9.1E+00	3.6E+01	1.2E+02	3.1E+02	7.4E+02	1.6E+03	3.0E+03	5.5E+03	9.4E+03	1.5E+04
63	→	5.2E+02	2.1E+03	5.7E+03	1.2E+04	2.2E+04	3.7E+04	5.7E+04	8.3E+04	1.2E+05	1.6E+05	2.1E+05	2.7E+05	3.4E+05	4.2E+05	5.2E+05	6.2E+05
63	←	8.0E-08	9.5E-05	8.0E-03	1.7E-01	1.7E+00	1.0E+01	4.2E+01	1.4E+02	3.7E+02	8.7E+02	1.8E+03	3.5E+03	6.3E+03	1.1E+04	1.7E+04	2.6E+04
64	→	1.4E+04	2.4E+04	3.8E+04	5.6E+04	8.0E+04	1.1E+05	1.5E+05	1.9E+05	2.5E+05	3.1E+05	3.8E+05	4.7E+05	5.7E+05	6.7E+05	8.0E+05	9.3E+05
64	←	9.0E-14	3.9E-09	2.8E-06	2.5E-04	6.6E-03	8.2E-02	6.1E-01	3.1E+00	1.2E+01	3.9E+01	1.1E+02	2.6E+02	5.6E+02	1.1E+03	2.1E+03	3.6E+03
65	→	2.5E-05	1.1E-02	4.7E-01	6.6E+00	4.7E+01	2.2E+02	7.6E+02	2.1E+03	5.2E+03	1.1E+04	2.1E+04	3.8E+04	6.4E+04	1.0E+05	1.6E+05	2.3E+05
65	←	9.6E-06	3.1E-03	1.2E-01	1.5E+00	1.0E+01	4.5E+01	1.5E+02	4.2E+02	1.0E+03	2.1E+03	4.1E+03	7.3E+03	1.2E+04	2.0E+04	3.1E+04	4.5E+04
66	→	1.1E-07	2.0E-04	2.1E-02	4.8E-01	4.9E+00	3.0E+01	1.2E+02	4.0E+02	1.1E+03	2.5E+03	5.3E+03	1.0E+04	1.8E+04	3.0E+04	4.8E+04	7.3E+04
66	←	4.4E-04	4.4E-02	8.6E-01	7.0E+00	3.5E+01	1.2E+02	3.5E+02	8.3E+02	1.8E+03	3.4E+03	6.0E+03	1.0E+04	1.6E+04	2.4E+04	3.6E+04	5.0E+04
67	→	3.7E-09	1.3E-05	1.8E-03	5.5E-02	6.7E-01	4.7E+00	2.2E+01	8.1E+01	2.4E+02	6.2E+02	1.4E+03	2.9E+03	5.6E+03	9.9E+03	1.7E+04	2.7E+04
67	←	2.3E+03	1.1E+04	2.9E+04	6.1E+04	1.1E+05	1.9E+05	2.9E+05	4.4E+05	6.3E+05	8.8E+05	1.2E+06	1.6E+06	2.0E+06	2.6E+06	3.2E+06	4.0E+06
68	→	1.3E+00	2.5E+01	1.6E+02	6.2E+02	1.7E+03	3.9E+03	7.8E+03	1.4E+04	2.3E+04	3.6E+04	5.4E+04	7.6E+04	1.1E+05	1.4E+05	1.9E+05	2.4E+05
68	←	2.2E-09	1.2E-05	2.4E-03	8.9E-02	1.3E+00	9.6E+00	4.9E+01	1.9E+02	5.7E+02	1.5E+03	3.4E+03	7.0E+03	1.3E+04	2.4E+04	4.0E+04	6.3E+04
69	→	2.3E-01	8.0E+00	7.4E+01	3.5E+02	1.2E+03	2.9E+03	6.4E+03	1.2E+04	2.1E+04	3.5E+04	5.3E+04	7.8E+04	1.1E+05	1.5E+05	2.0E+05	2.7E+05
69	←	3.3E-11	5.6E-07	2.1E-04	1.2E-02	2.4E-01	2.3E+00	1.4E+01	6.2E+01	2.1E+02	6.1E+02	1.5E+03	3.3E+03	6.8E+03	1.3E+04	2.2E+04	3.7E+04
70	→	4.2E-02	1.5E+00	1.5E+01	7.6E+01	2.6E+02	7.0E+02	1.6E+03	3.1E+03	5.6E+03	9.4E+03	1.5E+04	2.2E+04	3.2E+04	4.5E+04	6.1E+04	8.0E+04
70	←	1.7E-12	6.2E-08	3.9E-05	3.2E-03	8.1E-02	9.7E-01	7.0E+00	3.5E+01	1.3E+02	4.2E+02	1.1E+03	2.6E+03	5.6E+03	1.1E+04	2.0E+04	3.5E+04
71	→	2.6E+00	3.8E+01	2.1E+02	7.2E+02	1.9E+03	4.0E+03	7.5E+03	1.3E+04	2.1E+04	3.1E+04	4.5E+04	6.3E+04	8.6E+04	1.1E+05	1.5E+05	1.9E+05
71	←	1.8E-12	5.1E-08	2.8E-05	2.1E-03	4.8E-02	5.4E-01	3.7E+00	1.8E+01	6.7E+01	2.1E+02	5.4E+02	1.3E+03	2.6E+03	5.1E+03	9.3E+03	1.6E+04
72	→	5.7E+01	3.9E+02	1.3E+03	3.3E+03	6.6E+03	1.2E+04	1.9E+04	2.9E+04	4.1E+04	5.7E+04	7.6E+04	9.8E+04	1.2E+05	1.6E+05	1.9E+05	2.3E+05
72	←	2.8E-19	8.2E-13	7.4E-09	3.5E-06	3.0E-04	8.8E-03	1.2E-01	1.1E+00	6.1E+00	2.7E+01	9.5E+01	2.8E+02	7.3E+02	1.7E+03	3.6E+03	7.1E+03
73	→	6.5E-03	2.2E-01	2.1E+00	1.0E+01	3.5E+01	9.3E+01	2.1E+02	4.3E+02	7.8E+02	1.3E+03	2.1E+03	3.3E+03	4.8E+03	6.8E+03	9.4E+03	1.3E+04
73	←	2.7E-11	3.1E-07	1.0E-04	5.7E-03	1.1E-01	1.0E+00	6.3E+00	2.8E+01	9.6E+01	2.8E+02	6.9E+02	1.5E+03	3.1E+03	5.8E+03	1.0E+04	1.7E+04
74	→	9.6E-05	3.7E-02	1.5E+00	1.9E+01	1.2E+02	5.3E+02	1.7E+03	4.6E+03	1.0E+04	2.1E+04	4.0E+04	7.0E+04	1.1E+05	1.8E+05	2.7E+05	3.8E+05
74	←	1.5E-08	3.0E-05	3.3E-03	8.4E-02	9.3E-01	6.0E+00	2.7E+01	9.4E+01	2.7E+02	6.6E+02	1.5E+03	2.9E+03	5.4E+03	9.4E+03	1.5E+04	2.4E+04
75	→	3.2E-12	8.0E-08	3.9E-05	2.6E-03	5.7E-02	6.0E-01	3.9E+00	1.8E+01	6.5E+01	1.9E+02	4.9E+02	1.1E+03	2.3E+03	4.4E+03	7.8E+03	1.3E+04
75	←	8.2E-01	2.4E+01	2.1E+02	9.6E+02	3.1E+03	7.9E+03	1.7E+04	3.3E+04	5.8E+04	9.5E+04	1.5E+05	2.2E+05	3.1E+05	4.3E+05	5.8E+05	7.6E+05
76	→	1.3E-08	3.4E-05	4.4E-03	1.2E-01	1.4E+00	9.1E+00	4.1E+01	1.4E+02	4.1E+02	9.9E+02	2.2E+03	4.3E+03	7.9E+03	1.4E+04	2.2E+04	3.5E+04
76	←	1.1E+01	1.9E+02	1.1E+03	4.1E+03	1.1E+04	2.4E+04	4.7E+04	8.1E+04	1.3E+05	2.0E+05	2.9E+05	4.1E+05	5.6E+05	7.4E+05	9.6E+05	1.2E+06
77	→	1.9E-13	1.6E-08	1.6E-05	1.7E-03	4.9E-02	6.5E-01	5.0E+00	2.7E+01	1.1E+02	3.5E+02	9.5E+02	2.3E+03	5.0E+03	1.0E+04	1.9E+04	3.2E+04
77	←	7.4E-01	2.1E+01	1.8E+02	8.0E+02	2.5E+03	6.2E+03	1.3E+04	2.4E+04	4.2E+04	6.8E+04	1.0E+05	1.5E+05	2.1E+05	2.9E+05	3.8E+05	5.0E+05
78	→	1.6E-03	1.6E-01	3.2E+00	2.6E+01	1.3E+02	4.4E+02	1.2E+03	2.9E+03	5.9E+03	1.1E+04	1.9E+04	3.2E+04	5.0E+04	7.4E+04	1.1E+05	1.5E+05

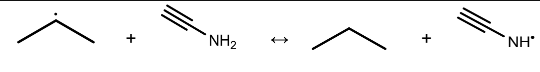
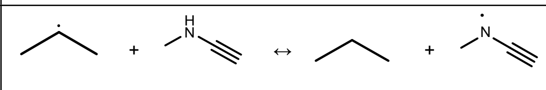
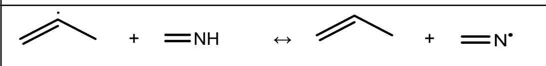
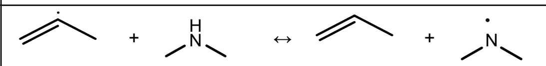
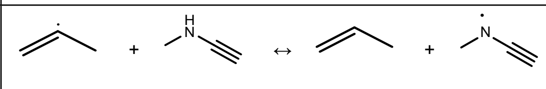
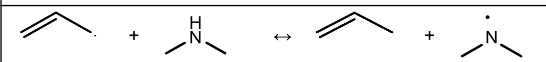
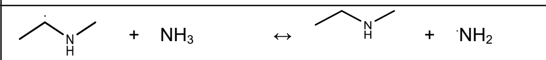
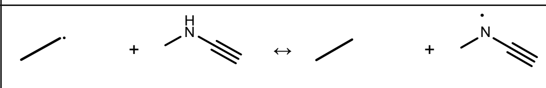
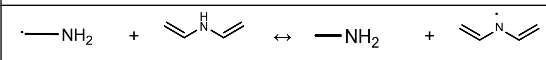
78	←	2.6E-06	1.3E-03	6.6E-02	1.0E+00	7.9E+00	3.9E+01	1.5E+02	4.3E+02	1.1E+03	2.4E+03	4.8E+03	8.9E+03	1.5E+04	2.5E+04	4.0E+04	6.0E+04
79	→	1.2E-05	4.0E-03	1.5E-01	1.8E+00	1.1E+01	4.8E+01	1.5E+02	4.0E+02	9.0E+02	1.8E+03	3.3E+03	5.7E+03	9.1E+03	1.4E+04	2.1E+04	3.0E+04
79	←	2.1E-04	2.5E-02	5.2E-01	4.6E+00	2.4E+01	8.8E+01	2.6E+02	6.3E+02	1.4E+03	2.7E+03	4.8E+03	8.1E+03	1.3E+04	2.0E+04	2.9E+04	4.2E+04
80	→	1.2E-03	1.4E-01	2.9E+00	2.4E+01	1.2E+02	4.0E+02	1.1E+03	2.5E+03	5.1E+03	9.5E+03	1.6E+04	2.6E+04	4.1E+04	6.0E+04	8.6E+04	1.2E+05
80	←	8.3E-10	3.3E-06	5.5E-04	1.9E-02	2.6E-01	2.0E+00	1.0E+01	4.0E+01	1.2E+02	3.3E+02	7.6E+02	1.6E+03	3.1E+03	5.6E+03	9.6E+03	1.6E+04
81	→	2.6E-05	1.1E-02	4.8E-01	6.8E+00	4.9E+01	2.3E+02	8.1E+02	2.3E+03	5.6E+03	1.2E+04	2.3E+04	4.2E+04	7.0E+04	1.1E+05	1.7E+05	2.5E+05
81	←	6.7E-07	3.9E-04	2.2E-02	3.6E-01	2.9E+00	1.5E+01	5.8E+01	1.8E+02	4.5E+02	1.0E+03	2.1E+03	3.9E+03	6.8E+03	1.1E+04	1.8E+04	2.7E+04
82	→	2.0E-07	3.0E-04	2.7E-02	6.0E-01	5.8E+00	3.4E+01	1.4E+02	4.3E+02	1.1E+03	2.6E+03	5.3E+03	1.0E+04	1.7E+04	2.9E+04	4.5E+04	6.7E+04
82	←	5.3E-05	8.4E-03	2.1E-01	2.1E+00	1.2E+01	4.5E+01	1.4E+02	3.5E+02	7.7E+02	1.5E+03	2.8E+03	4.8E+03	7.7E+03	1.2E+04	1.8E+04	2.5E+04
83	→	2.9E+00	4.7E+01	2.9E+02	1.1E+03	2.9E+03	6.6E+03	1.3E+04	2.3E+04	3.8E+04	5.9E+04	8.8E+04	1.3E+05	1.7E+05	2.3E+05	3.0E+05	3.9E+05
83	←	1.7E-05	7.0E-03	3.0E-01	4.0E+00	2.7E+01	1.2E+02	4.0E+02	1.1E+03	2.5E+03	5.2E+03	9.8E+03	1.7E+04	2.8E+04	4.4E+04	6.6E+04	9.5E+04
84	→	3.3E-08	1.0E-04	1.5E-02	4.4E-01	5.3E+00	3.6E+01	1.7E+02	6.0E+02	1.7E+03	4.4E+03	9.7E+03	1.9E+04	3.6E+04	6.3E+04	1.0E+05	1.7E+05
84	←	4.1E-08	8.7E-05	1.0E-02	2.7E-01	3.1E+00	2.0E+01	9.3E+01	3.3E+02	9.5E+02	2.4E+03	5.3E+03	1.1E+04	2.0E+04	3.6E+04	5.9E+04	9.4E+04
85	→	1.4E-07	2.2E-04	2.1E-02	4.7E-01	4.7E+00	2.8E+01	1.2E+02	3.7E+02	1.0E+03	2.3E+03	4.9E+03	9.3E+03	1.6E+04	2.8E+04	4.4E+04	6.6E+04
85	←	6.2E-11	4.9E-07	1.3E-04	5.9E-03	1.0E-01	9.0E-01	5.3E+00	2.2E+01	7.6E+01	2.2E+02	5.4E+02	1.2E+03	2.4E+03	4.6E+03	8.1E+03	1.4E+04
86	→	5.8E-06	3.7E-03	2.1E-01	3.3E+00	2.6E+01	1.3E+02	4.5E+02	1.3E+03	3.2E+03	6.8E+03	1.3E+04	2.4E+04	4.0E+04	6.3E+04	9.6E+04	1.4E+05
86	←	6.2E-11	3.8E-07	8.4E-05	3.5E-03	5.5E-02	4.6E-01	2.6E+00	1.0E+01	3.4E+01	9.3E+01	2.2E+02	4.8E+02	9.4E+02	1.7E+03	3.0E+03	4.9E+03
87	→	6.0E-07	3.4E-04	1.8E-02	2.7E-01	2.0E+00	9.7E+00	3.4E+01	9.8E+01	2.4E+02	5.1E+02	9.8E+02	1.8E+03	3.0E+03	4.8E+03	7.3E+03	1.1E+04
87	←	1.8E-11	1.7E-07	5.1E-05	2.6E-03	4.6E-02	4.3E-01	2.6E+00	1.2E+01	4.1E+01	1.2E+02	3.0E+02	6.8E+02	1.4E+03	2.7E+03	4.9E+03	8.3E+03

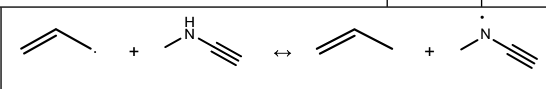
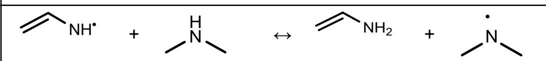
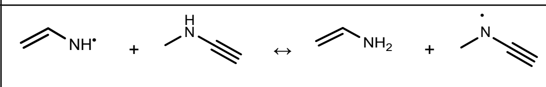
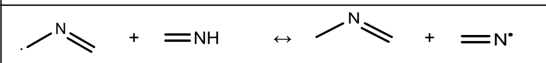
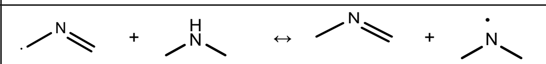
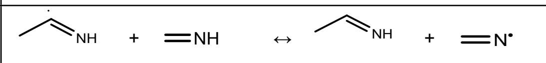
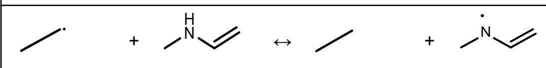
4.3. Arrhenius parameters regressed at 1000 K

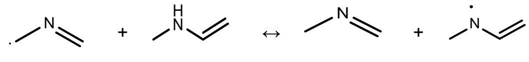
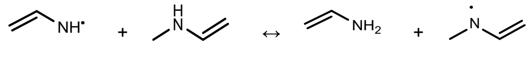
Table S16: Standard reaction enthalpy [kJ mol^{-1}], pre-exponential factor [m^3 mol^{-1} s^{-1}], activation energy [kJ mol^{-1}], rate coefficient [m^3 mol^{-1} s^{-1}] and deviation factor ρ at 1000 K for all C-H-N hydrogen abstraction reactions in the training (T) and validation dataset (V). The Arrhenius parameters exclude tunneling.

No.		Reaction	ΔH_r°	Forward			Reverse			ρ (1000 K)	
				$logA$	E_a	k_{for}	$logA$	E_a	k_{rev}	*for*	*rev*
1	T		11.8	7.231	80.5	5.2E+03	7.807	73.4	4.0E+04	-	-
2	T		-21.9	7.032	65.8	1.4E+04	7.654	92.1	4.3E+03	1.3	1.3
3	T		-73.1	6.915	44.7	9.1E+04	7.735	120.5	3.0E+02	1.7	1.6
4	T		-70.4	6.766	63.1	1.0E+04	8.077	139.8	9.6E+01	1.4	1.2
5	T		-77.8	7.106	54.5	5.3E+04	7.811	136.1	7.6E+01	1.6	1.5
6	T		-46.7	6.908	52.5	4.1E+04	7.666	107.5	9.5E+02	1.1	1.2
7	T		-81.8	6.770	56.1	2.1E+04	8.342	148.2	7.6E+01	1.1	1.1
8	T		-106.5	6.134	56.0	4.9E+03	8.188	162.9	1.2E+01	1.1	1.3
9	T		-91.7	6.768	46.1	5.6E+04	7.714	143.0	3.0E+01	1.5	1.4
10	T		85.4	8.392	135.7	3.0E+02	7.414	52.3	1.3E+05	1.1	1.0
11	T		27.9	7.105	89.4	1.6E+03	7.471	65.8	3.9E+04	1.2	1.0
12	T		-43.8	6.966	44.0	1.1E+05	7.732	90.3	6.2E+03	1.7	1.0
13	T		-6.5	6.726	73.7	3.2E+03	7.604	81.3	1.1E+04	1.8	2.0
14	T		7.1	7.019	76.5	4.8E+03	7.530	67.3	3.9E+04	1.1	1.0
15	T		-30.8	6.799	48.0	5.0E+04	7.035	79.7	3.6E+03	1.1	1.1
16	T		51.6	7.931	113.6	9.5E+02	7.001	63.7	1.7E+04	1.2	1.3
17	T		-4.2	8.260	89.9	2.2E+04	7.411	95.2	1.8E+03	1.0	1.0
18	T		-8.2	7.864	89.8	8.8E+03	7.882	105.7	1.9E+03	1.2	1.1
19	T		33.7	7.052	87.4	1.7E+03	7.290	56.4	6.7E+04	1.0	1.1
20	T		-14.8	6.611	68.7	4.1E+03	7.536	87.9	5.0E+03	1.2	1.2
21	T		-22.2	6.606	50.1	2.6E+04	6.925	74.2	4.8E+03	1.2	1.1
22	T		38.6	7.107	98.7	6.3E+02	7.024	67.2	1.2E+04	1.2	1.3
23	T		-9.9	6.698	91.7	5.0E+02	7.302	110.5	3.0E+02	1.2	1.3
24	T		-17.3	7.451	81.6	7.7E+03	7.450	105.4	7.1E+02	1.2	1.2
25	T		48.1	7.849	110.6	1.1E+03	6.836	67.0	8.1E+03	1.0	1.2
26	T		-7.8	8.298	92.3	1.9E+04	7.367	103.9	6.9E+02	1.7	1.6

27	T		19.2	6.949	76.5	4.1E+03	7.044	58.1	3.2E+04		
28	T		-0.4	7.190	102.4	5.3E+02	7.064	108.2	2.2E+02		
29	T		16.6	7.177	78.7	5.5E+03	7.230	64.5	2.6E+04		
30	V		61.6	7.133	107.9	2.7E+02	7.452	51.0	1.7E+05		
31	V		28.6	7.126	87.6	2.0E+03	7.938	60.9	1.9E+05		
32	V		40.9	7.224	92.5	1.5E+03	7.687	49.9	3.2E+05		
33	V		-10.0	7.218	60.6	3.7E+04	7.936	73.5	5.3E+04		
34	V		2.9	7.114	64.4	2.0E+04	7.303	62.8	3.6E+04		
35	V		-31.9	6.667	62.1	9.0E+03	7.408	98.3	1.3E+03		
36	V		-34.6	7.032	51.7	5.9E+04	7.282	87.0	3.1E+03	1.1	1.2
37	V		-8.2	6.985	63.2	1.7E+04	7.174	77.8	6.0E+03	1.0	1.0
38	V		-80.9	6.940	57.3	2.7E+04	8.291	145.1	9.2E+01	2.1	1.4
39	V		-23.3	6.705	58.3	1.4E+04	7.267	84.2	3.9E+03	1.2	1.1
40	V		-28.0	6.151	50.5	8.8E+03	6.599	82.1	1.0E+03	1.0	1.0
41	V		3.1	6.706	71.8	3.7E+03	7.208	77.0	7.0E+03	1.2	1.1
42	V		-41.9	6.196	42.8	2.1E+04	6.885	89.8	9.2E+02	1.3	1.2
43	V		-21.3	6.117	55.2	5.1E+03	6.960	77.2	3.9E+03	1.1	1.3
44	V		-18.2	6.587	58.9	1.0E+04	7.089	76.3	5.7E+03	1.2	1.9
45	V		-22.9	6.465	53.6	1.3E+04	6.854	76.9	3.1E+03	1.4	1.6
46	V		8.3	6.635	74.9	2.3E+03	7.076	71.7	8.8E+03	1.4	1.6
47	V		-51.5	5.826	50.2	4.3E+03	7.563	98.9	1.8E+03	1.1	1.6
48	V		-26.9	6.962	57.4	2.9E+04	7.332	87.9	3.1E+03	2.4	1.2
49	V		-31.6	6.651	55.7	1.7E+04	7.099	92.5	1.2E+03	1.1	2.2
50	V		-0.4	6.824	73.1	4.3E+03	7.132	82.9	3.3E+03	1.3	2.1
51	V		-68.5	6.814	32.6	2.4E+05	7.714	107.6	1.0E+03	1.5	1.0
52	V		-103.6	6.550	34.2	1.1E+05	8.264	146.3	7.7E+01	1.1	1.4
53	V		50.3	7.421	97.2	1.5E+03	7.427	49.7	1.8E+05	1.4	1.5
54	V		67.5	7.284	107.0	4.1E+02	7.474	42.5	4.1E+05	1.3	1.4
55	V		66.8	7.325	111.3	3.0E+02	7.584	46.0	3.7E+05	1.5	1.5
56	V		58.1	7.285	106.6	4.3E+02	7.603	54.8	1.6E+05	1.1	1.9

57	V		27.3	7.081	85.8	2.2E+03	7.911	60.0	2.0E+05	1.4	1.4
58	V		-44.1	6.783	52.2	3.2E+04	7.490	92.5	2.9E+03	1.4	1.4
59	V		-17.6	6.494	61.1	6.7E+03	7.140	80.6	4.2E+03	1.6	1.5
60	V		-48.8	6.781	54.6	2.5E+04	7.374	100.6	9.7E+02	1.2	1.2
61	V		-62.6	6.447	45.9	2.8E+04	7.280	107.3	4.0E+02	1.4	1.4
62	V		-82.0	6.837	28.3	4.0E+05	7.269	109.4	3.1E+02	1.5	1.5
63	V		-55.6	6.694	34.1	1.6E+05	7.065	94.6	8.7E+02	1.2	1.2
64	V		-100.6	6.628	25.9	3.1E+05	7.186	128.3	3.9E+01	1.0	1.1
65	V		0.5	7.692	83.7	1.1E+04	6.958	83.2	2.1E+03	1.1	1.1
66	V		26.9	7.492	93.7	2.5E+03	6.696	72.5	3.4E+03	1.0	1.1
67	V		68.5	7.339	104.1	6.2E+02	7.558	36.9	8.8E+05	1.3	1.7
68	V		-56.4	6.715	49.3	3.6E+04	7.770	105.5	1.5E+03	1.6	1.6
69	V		-61.1	6.905	54.2	3.5E+04	7.846	116.1	6.1E+02	1.2	1.2
70	V		-74.9	6.516	46.2	3.1E+04	7.697	123.5	2.1E+02	1.1	1.1
71	V		-128.3	6.325	35.9	5.7E+04	8.521	162.8	2.7E+01	2.2	1.1
72	V		-56.7	5.718	59.3	1.3E+03	7.515	116.3	2.8E+02	1.0	1.4

73	V		-18.1	7.787	79.2	2.1E+04	7.179	99.9	6.6E+02
74	V		-12.6	7.112	70.2	1.1E+04	7.225	88.1	2.4E+03
75	V		13.8	6.621	77.1	1.8E+03	6.673	74.3	2.7E+03
76	V		-31.2	6.971	68.6	9.5E+03	7.209	107.6	3.3E+02
77	V		72.4	7.515	119.9	1.9E+02	7.384	55.0	9.5E+04
78	V		52.9	7.315	99.0	9.9E+02	7.362	47.1	2.0E+05
79	V		81.8	8.195	129.8	3.5E+02	7.134	52.7	6.8E+04
80	V		-3.1	7.750	84.2	1.2E+04	6.934	90.0	1.0E+03
81	V		23.3	7.394	91.2	2.6E+03	6.516	76.3	1.5E+03
82	V		-32.0	6.921	49.1	5.9E+04	7.212	80.1	5.2E+03
83	V		-65.1	6.472	57.2	9.4E+03	8.110	125.9	4.2E+02
84	V		3.1	8.053	101.2	4.4E+03	7.810	101.6	2.4E+03

85	V		-11.8	7.451	93.6	2.3E+03	7.387	115.7	2.2E+02	
86	V		-21.7	7.511	84.3	6.8E+03	6.821	111.3	9.3E+01	
87	V		-21.3	6.378	84.2	5.1E+02	7.244	118.5	1.2E+02	

4.4. Reaction path degeneracy

Table S17: External and internal symmetry numbers, number of optical isomers and number of single events n_e for all C-H-N hydrogen abstractions of Table S16.

No.		Reactant 1 $R^{\cdot}$			Reactant 2 RH			Transition state			Reaction path degeneracy
		σ_{ext}	σ_{int}	n_{opt}	σ_{ext}	σ_{int}	n_{opt}	σ_{ext}	σ_{int}	n_{opt}	n_e
1	→	2	3	1	3	1	1	1	3	1	6
1	→	1	12	1	2	1	1	1	3	1	8
2	←	2	3	1	1	3	1	1	9	2	4
2	→	1	12	1	3	1	1	1	9	2	8
3	←	2	3	1	1	1	1	1	3	1	2
3	→	1	12	1	1	2	1	1	3	1	8
4	←	2	3	1	1	1	1	1	3	2	4
4	→	1	12	1	1	1	1	1	3	2	8
5	←	2	3	1	1	1	1	1	3	2	4
5	→	1	12	1	1	1	1	1	3	2	8
6	←	2	3	1	1	9	1	1	27	1	2
6	→	1	12	1	2	9	1	1	27	1	8
7	←	2	3	1	1	3	2	1	9	2	2
7	→	1	12	1	1	3	1	1	9	2	8
8	←	2	3	1	1	1	1	1	3	1	2
8	→	1	12	1	1	2	1	1	3	1	8
9	←	2	3	1	1	3	2	1	9	2	2
9	→	1	12	1	1	3	1	1	9	2	8
10	←	1	8	1	3	1	1	1	1	1	24
10	→	1	3	1	2	1	1	1	1	1	6
11	←	1	2	1	1	3	1	1	3	2	4
11	→	1	3	1	3	1	1	1	3	2	6
12	←	1	1	1	1	3	1	1	3	2	2
12	→	1	4	1	3	1	1	1	3	2	8
13	←	1	6	1	1	3	1	1	9	2	4
13	→	2	9	1	3	1	1	1	9	2	12
14	←	2	9	1	1	3	1	1	27	2	4
14	→	2	9	1	3	1	1	1	27	2	4
15	←	1	3	1	1	3	1	1	9	2	2
15	→	1	3	1	3	1	1	1	9	2	2
16	←	1	8	1	1	3	1	1	3	2	16
16	→	1	3	1	3	1	1	1	3	2	6
17	←	1	8	1	1	1	1	1	1	2	16
17	→	1	3	1	1	1	1	1	1	2	6
18	←	1	8	1	1	3	2	1	3	2	8
18	→	1	3	1	1	3	1	1	3	2	6
19	←	1	3	1	1	3	1	1	9	4	4
19	→	1	3	1	3	1	1	1	9	4	4
20	←	1	3	1	1	1	1	1	3	4	4
20	→	1	3	1	1	1	1	1	3	4	4
21	←	1	3	1	1	1	1	1	3	4	4
21	→	1	3	1	1	1	1	1	3	4	4
22	←	1	1	1	1	3	1	1	3	2	2
22	→	1	3	1	3	1	1	1	3	2	6
23	←	1	1	1	1	1	1	1	1	2	2
23	→	1	3	1	1	1	1	1	1	2	6
24	→	1	1	1	1	1	1	1	1	2	2
24	←	1	3	1	1	1	1	1	1	2	6
25	→	1	8	1	1	3	1	1	3	2	16
25	←	1	3	1	3	1	1	1	3	2	6
26	→	1	8	1	1	1	1	1	1	2	16

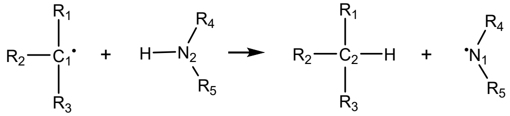
26	←	1	3	1	1	1	1	1	1	2	6
27	→	1	3	1	1	3	1	1	9	2	2
27	←	1	3	1	3	1	1	1	9	2	2
28	→	1	8	1	1	1	1	1	1	2	16
28	←	1	3	1	1	1	1	1	1	2	6
29	→	1	1	1	1	3	1	1	3	2	2
29	←	1	1	1	3	1	1	1	3	2	2
30	→	1	2	1	3	1	1	1	1	1	6
30	←	1	3	1	2	1	1	1	1	1	6
31	→	1	6	1	3	1	1	1	3	1	6
31	←	2	9	1	2	1	1	1	3	1	12
32	→	2	9	1	3	1	1	1	9	1	6
32	←	2	9	1	2	1	1	1	9	1	4
33	→	1	1	1	3	1	1	1	1	1	3
33	←	1	4	1	2	1	1	1	1	1	8
34	→	1	3	1	3	1	1	1	3	1	3
34	←	1	3	1	2	1	1	1	3	1	2
35	→	1	1	1	1	1	1	1	1	2	2
35	←	1	1	1	1	1	1	1	1	2	2
36	→	1	1	1	1	1	1	1	1	1	1
36	←	1	1	1	1	2	1	1	1	1	2
37	→	1	1	1	1	9	1	1	9	1	1
37	←	1	1	1	2	9	1	1	9	1	2
38	→	2	3	1	1	3	1	1	9	2	4
38	←	1	12	1	1	3	1	1	9	2	8
39	→	1	2	1	1	1	1	1	1	1	2
39	←	1	3	1	1	2	1	1	1	1	6
40	→	1	2	1	1	1	1	1	1	1	2
40	←	1	3	1	1	1	1	1	1	1	3
41	→	1	2	1	1	9	1	1	9	1	2
41	←	1	3	1	2	9	1	1	9	1	6
42	→	1	2	1	1	3	2	1	3	2	2
42	←	1	3	1	1	3	1	1	3	2	6
43	→	1	6	2	1	1	1	1	3	1	1
43	←	1	9	1	1	2	1	1	3	1	6
44	→	1	2	2	1	1	1	1	1	2	2
44	←	1	3	2	1	2	1	1	1	2	6
45	→	1	2	2	1	1	1	1	1	4	4
45	←	1	3	2	1	1	1	1	1	4	6
46	←	1	2	2	1	9	1	1	9	2	2
46	→	1	3	2	2	9	1	1	9	2	6
47	←	1	2	2	1	1	1	1	1	2	2
47	→	1	3	2	1	2	1	1	1	2	6
48	←	1	2	2	1	1	1	1	1	2	2
48	→	1	3	2	1	2	1	1	1	2	6
49	←	1	2	2	1	1	1	1	1	4	4
49	→	1	3	2	1	1	1	1	1	4	6
50	←	1	2	2	1	9	1	1	9	2	2
50	→	1	3	2	2	9	1	1	9	2	6
51	←	1	1	1	1	9	1	1	9	1	1
51	→	1	4	1	2	9	1	1	9	1	8
52	←	1	1	1	1	3	2	1	3	2	1
52	→	1	4	1	1	3	1	1	3	2	8
53	←	1	1	1	3	1	1	1	1	1	3
53	→	1	1	1	2	1	1	1	1	1	2
54	←	1	3	1	3	1	1	1	3	2	6
54	→	1	3	1	2	1	1	1	3	2	4
55	←	1	2	2	3	1	1	1	1	2	6
55	→	1	3	2	2	1	1	1	1	2	6
56	←	1	2	2	3	1	1	1	1	2	6
56	→	1	3	2	2	1	1	1	1	2	6

57	←	1	6	1	3	1	1	1	3	1	6
57	→	2	9	1	2	1	1	1	3	1	12
58	→	2	9	1	1	1	1	1	9	1	2
58	←	2	9	1	1	2	1	1	9	1	4
59	→	2	9	1	1	9	1	1	81	1	2
59	←	2	9	1	2	9	1	1	81	1	4
60	→	2	9	1	1	1	1	1	9	2	4
60	←	2	9	1	1	1	1	1	9	2	4
61	→	2	9	1	1	3	2	1	27	2	2
61	←	2	9	1	1	3	1	1	27	2	4
62	→	1	3	1	1	1	1	1	3	1	1
62	←	1	3	1	1	2	1	1	3	1	2
63	→	1	3	1	1	9	1	1	27	1	1
63	←	1	3	1	2	9	1	1	27	1	2
64	→	1	3	1	1	3	2	1	9	2	1
64	←	1	3	1	1	3	1	1	9	2	2
65	→	1	8	1	1	1	1	1	1	1	8
65	←	1	3	1	1	2	1	1	1	1	6
66	→	1	8	1	1	9	1	1	9	1	8
66	←	1	3	1	2	9	1	1	9	1	6
67	→	1	9	2	3	1	1	1	9	4	6
67	←	1	9	2	2	1	1	1	9	4	4
68	→	1	6	1	1	1	1	1	3	1	2
68	←	2	9	1	1	2	1	1	3	1	12
69	→	1	6	1	1	1	1	1	3	2	4
69	←	2	9	1	1	1	1	1	3	2	12
70	→	1	6	1	1	3	2	1	9	2	2
70	←	2	9	1	1	3	1	1	9	2	12
71	→	1	1	1	1	1	1	1	1	1	1
71	←	1	4	1	1	2	1	1	1	1	8
72	→	1	2	1	1	1	1	1	1	1	2
72	←	1	3	1	1	2	1	1	1	1	6
73	→	1	8	1	1	3	2	1	3	2	8
73	←	1	3	1	1	3	1	1	3	2	6
74	→	1	1	1	1	1	1	1	1	1	1
74	←	1	3	1	1	2	1	1	1	1	6
75	→	1	1	1	1	9	1	1	9	1	1
75	←	1	3	1	2	9	1	1	9	1	6
76	→	1	1	1	1	3	2	1	3	2	1
76	←	1	3	1	1	3	1	1	3	2	6
77	→	1	1	1	3	1	1	1	1	1	3
77	←	1	3	1	2	1	1	1	1	1	6
78	→	1	3	1	3	1	1	1	3	1	3
78	←	1	3	1	2	1	1	1	3	1	2
79	→	1	8	1	3	1	1	1	1	1	24
79	←	1	3	1	2	1	1	1	1	1	6
80	→	1	8	1	1	1	1	1	1	1	8
80	←	1	3	1	1	2	1	1	1	1	6
81	→	1	8	1	1	9	1	1	9	1	8
81	←	1	3	1	2	9	1	1	9	1	6
82	→	1	3	1	1	1	1	1	3	1	1
82	←	1	3	1	1	2	1	1	3	1	2
83	→	1	6	1	1	3	2	1	9	2	2
83	←	2	9	1	1	3	1	1	9	2	12
84	→	1	8	1	1	1	1	1	1	2	16
84	←	1	3	1	1	1	1	1	1	2	6
85	→	1	8	1	1	3	2	1	3	2	8
85	←	1	3	1	1	3	1	1	3	2	6
86	→	1	8	1	1	3	2	1	3	2	8
86	←	1	3	1	1	3	1	1	3	2	6
87	→	1	1	1	1	3	2	1	3	2	1

87	←	1	3	1	1	3	1	1	3	2	6

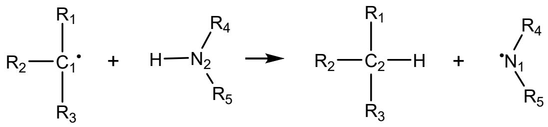
4.5. Group additivity values between 300 and 1800 K

Table S18: Primary standard group additivity values ΔGAV°s between 300 and 1800 K for abstraction of a hydrogen atom from N-H by a carbon-centered radical, deduced from the combined training and test set. For the reference reaction, the single-event pre-exponential factor is expressed in m^3 mol^{-1} s^{-1} and E_a is expressed in kJ mol^{-1}.



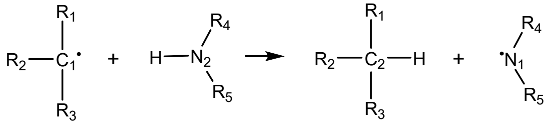
		300 K				400 K				500 K				600 K			
		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)	
No.	Group	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a
	Reference:	5.149	48.1	5.471	70.7	5.315	49.3	5.671	72.6	5.395	49.8	5.767	73.4	5.575	51.7	5.984	76.0
1	**N_i-(H)$_2$**	0.461	-12.0	0.194	19.6	0.378	-12.5	0.149	19.2	0.361	-12.7	0.143	19.2	0.325	-13.0	0.133	19.1
2	**$N_{i,I}$**	0.122	24.7	0.077	-26.6	0.102	24.5	0.109	-26.4	0.095	24.5	0.118	-26.3	0.081	24.3	0.140	-26.1
3	**N_i-(C_d)(H)**	0.062	42.2	-0.532	-8.7	0.176	43.0	-0.467	-8.3	0.211	43.3	-0.443	-8.1	0.287	44.0	-0.390	-7.6
4	**N_i-(C_t)(H)**	0.259	41.6	0.127	-14.7	0.223	41.3	0.107	-14.8	0.214	41.3	0.102	-14.8	0.197	41.1	0.093	-14.9
5	**N_i-(C)$_2$**	-0.443	11.0	0.071	-14.1	-0.345	11.7	0.092	-13.9	-0.317	11.9	0.091	-13.9	-0.258	12.5	0.090	-13.9
6	**N_i-(C)(C_d)**	0.147	48.5	-0.265	-14.7	0.259	49.2	-0.220	-14.4	0.296	49.5	-0.201	-14.3	0.375	50.3	-0.158	-13.8
7	**N_i-(C_d)$_2$**	0.886	75.2	-0.426	-8.4	0.972	75.8	-0.471	-8.7	0.970	75.8	-0.479	-8.8	0.958	75.7	-0.492	-8.9
8	**N_i-(C)(C_t)**	-0.147	45.4	-0.074	-24.7	-0.098	45.7	-0.059	-24.6	-0.086	45.8	-0.056	-24.6	-0.061	46.1	-0.049	-24.5
		ΔGAV°(C_1)		ΔGAV°(C_2)		ΔGAV°(C_1)		ΔGAV°(C_2)		ΔGAV°(C_1)		ΔGAV°(C_2)		ΔGAV°(C_1)		ΔGAV°(C_2)	
	Reference:	5.471	70.7	5.149	48.1	5.671	72.6	5.315	49.3	5.767	73.4	5.395	49.8	5.984	76.0	5.575	51.7
1	**C_i-(C)(H)$_2$**	-0.482	2.0	-0.133	-14.7	-0.381	2.7	-0.113	-14.5	-0.358	2.9	-0.117	-14.5	-0.308	3.4	-0.126	-14.6
2	**C_i-(C)$_2$(H)**	-0.700	2.8	0.059	-26.6	-0.509	4.1	0.098	-26.3	-0.461	4.5	0.093	-26.4	-0.360	5.5	0.082	-26.5
3	**$C_{i,d}$-(H)**	0.041	-23.1	0.040	-1.3	0.138	-22.4	0.093	-0.9	0.159	-22.3	0.099	-0.9	0.204	-21.8	0.113	-0.7
4	**$C_{i,d}$-(C)**	-0.170	-20.0	0.054	-11.4	-0.041	-19.1	0.106	-11.0	-0.010	-18.8	0.107	-11.0	0.056	-18.2	0.111	-10.9
5	**C_i-(C_d)(H)$_2$**	-0.160	41.0	-0.920	-35.6	-0.012	42.1	-0.840	-35.0	0.021	42.3	-0.818	-34.8	0.093	43.1	-0.770	-34.4
6	**C_i-(N)(H)$_2$**	-0.514	16.8	-0.611	-34.2	-0.390	17.6	-0.521	-33.6	-0.358	17.9	-0.497	-33.4	-0.286	18.6	-0.444	-32.8
7	**C_i-(C)(N)(H)**	-0.549	14.6	-0.428	-41.8	-0.418	15.5	-0.359	-41.3	-0.377	15.8	-0.340	-41.1	-0.286	16.8	-0.296	-40.7
8	**$C_{i,I}$-(H)**	0.008	5.6	-0.072	-33.4	0.144	6.5	0.008	-32.8	0.177	6.7	0.022	-32.7	0.246	7.5	0.054	-32.4
9	**$C_{i,I}$-(C)**	-0.093	7.5	0.008	-33.8	0.047	8.5	0.056	-33.4	0.079	8.7	0.059	-33.4	0.148	9.4	0.065	-33.4
10	**C_i-(C_I)(H)$_2$**	-0.018	27.2	-0.831	-31.0	0.151	28.4	-0.736	-30.3	0.188	28.7	-0.711	-30.1	0.268	29.5	-0.656	-29.6

11	**C_i-(C_I)(H)$_2$**	-0.127	41.0	-0.956	-29.6	0.020	42.0	-0.873	-29.0	0.050	42.3	-0.854	-28.9	0.114	42.9	-0.812	-28.4

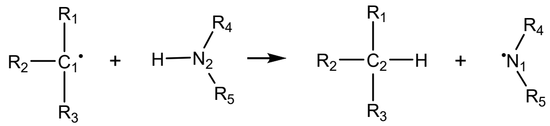


		700 K				**800 K**				**900 K**				**1000 K**			
		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)	
No.	Group	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a
	Reference:	5.747	53.7	6.183	78.8	5.908	56.0	6.361	81.5	6.056	58.4	6.520	84.2	6.192	60.8	6.662	86.9
1	**N_i-(H)$_2$**	0.307	-13.3	0.132	19.1	0.296	-13.4	0.135	19.1	0.290	-13.5	0.138	19.2	0.286	-13.6	0.141	19.2
2	**$N_{i,I}$**	0.073	24.2	0.154	-26.0	0.068	24.2	0.163	-25.8	0.066	24.1	0.169	-25.7	0.065	24.1	0.175	-25.6
3	**N_i-(C_d)(H)**	0.341	44.7	-0.351	-7.1	0.379	45.2	-0.323	-6.7	0.407	45.7	-0.303	-6.4	0.428	46.1	-0.287	-6.1
4	**N_i-(C_t)(H)**	0.188	41.0	0.089	-15.0	0.182	40.9	0.087	-15.0	0.179	40.8	0.086	-15.0	0.176	40.8	0.086	-15.0
5	**N_i-(C)$_2$**	-0.217	13.0	0.083	-14.0	-0.189	13.4	0.075	-14.1	-0.167	13.8	0.069	-14.2	-0.151	14.0	0.063	-14.3
6	**N_i-(C)(C_d)**	0.434	51.0	-0.123	-13.4	0.477	51.7	-0.098	-13.0	0.510	52.2	-0.080	-12.8	0.533	52.6	-0.068	-12.5
7	**N_i-(C_d)$_2$**	0.910	75.1	-0.496	-9.0	0.844	74.2	-0.500	-9.0	0.776	73.1	-0.506	-9.1	0.710	72.0	-0.513	-9.2
8	**N_i-(C)(C_t)**	-0.044	46.3	-0.045	-24.5	-0.033	46.4	-0.042	-24.4	-0.025	46.5	-0.040	-24.4	-0.020	46.6	-0.038	-24.4
		ΔGAV°(C_1)		ΔGAV°(C_2)		ΔGAV°(C_1)		ΔGAV°(C_2)		ΔGAV°(C_1)		ΔGAV°(C_2)		ΔGAV°(C_1)		ΔGAV°(C_2)	
	Reference:	6.183	78.8	5.747	53.7	6.361	81.5	5.908	56.0	6.520	84.2	6.056	58.4	6.662	86.9	6.192	60.8
1	**C_i-(C)(H)$_2$**	-0.278	3.8	-0.139	-14.8	-0.259	4.1	-0.151	-14.9	-0.247	4.3	-0.162	-15.1	-0.239	4.4	-0.171	-15.3
2	**C_i-(C)$_2$(H)**	-0.297	6.3	0.064	-26.7	-0.257	6.9	0.046	-26.9	-0.231	7.3	0.030	-27.2	-0.213	7.6	0.018	-27.4
3	**$C_{i,d}$-(H)**	0.230	-21.5	0.117	-0.7	0.246	-21.3	0.117	-0.7	0.255	-21.1	0.117	-0.7	0.260	-21.0	0.116	-0.7
4	**$C_{i,d}$-(C)**	0.096	-17.7	0.105	-11.0	0.122	-17.3	0.098	-11.1	0.138	-17.0	0.092	-11.2	0.148	-16.9	0.086	-11.3
5	**C_i-(C_d)(H)$_2$**	0.136	43.6	-0.731	-33.9	0.165	44.0	-0.699	-33.4	0.185	44.3	-0.671	-33.0	0.200	44.6	-0.647	-32.6
6	**C_i-(N)(H)$_2$**	-0.238	19.2	-0.405	-32.4	-0.204	19.7	-0.376	-32.0	-0.179	20.1	-0.353	-31.6	-0.161	20.4	-0.334	-31.2
7	**C_i-(C)(N)(H)**	-0.216	17.6	-0.257	-40.2	-0.160	18.4	-0.222	-39.7	-0.116	19.1	-0.190	-39.2	-0.080	19.8	-0.162	-38.7
8	**$C_{i,I}$-(H)**	0.288	8.0	0.069	-32.2	0.314	8.3	0.077	-32.1	0.331	8.6	0.081	-32.0	0.343	8.8	0.083	-32.0
9	**$C_{i,I}$-(C)**	0.191	10.0	0.062	-33.4	0.217	10.4	0.056	-33.5	0.236	10.6	0.051	-33.6	0.247	10.9	0.046	-33.6
10	**C_i-(C_I)(H)$_2$**	0.313	30.1	-0.616	-29.1	0.339	30.4	-0.586	-28.7	0.354	30.7	-0.561	-28.3	0.363	30.9	-0.541	-27.9

11	**C_i-$(C_I)(H)_2$**	0.146	43.3	-0.783	-28.1	0.162	43.5	-0.763	-27.8	0.169	43.7	-0.748	-27.5	0.170	43.7	-0.735	-27.3



		1100 K				**1200 K**				**1300 K**				**1400 K**			
		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)	
No.	Group	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a
	Reference:	6.316	63.3	6.789	89.5	6.430	65.8	6.904	92.1	6.535	68.2	7.008	94.6	6.632	70.7	7.103	97.1
1	**N_i-$(H)_2$**	0.283	-13.7	0.144	19.3	0.281	-13.7	0.146	19.3	0.279	-13.8	0.148	19.4	0.277	-13.8	0.149	19.4
2	**$N_{i,I}$**	0.065	24.1	0.179	-25.5	0.066	24.1	0.182	-25.5	0.067	24.2	0.185	-25.4	0.069	24.2	0.187	-25.4
3	**N_i-$(C_d)(H)$**	0.443	46.4	-0.274	-5.8	0.454	46.6	-0.265	-5.6	0.462	46.8	-0.257	-5.4	0.467	46.9	-0.251	-5.3
4	**N_i-$(C_t)(H)$**	0.174	40.7	0.086	-15.0	0.172	40.7	0.086	-15.0	0.171	40.7	0.086	-15.0	0.170	40.6	0.086	-15.0
5	**N_i-$(C)_2$**	-0.138	14.3	0.058	-14.4	-0.128	14.5	0.054	-14.5	-0.120	14.7	0.050	-14.6	-0.114	14.9	0.047	-14.7
6	**N_i-$(C)(C_d)$**	0.550	52.9	-0.059	-12.4	0.562	53.2	-0.054	-12.2	0.570	53.4	-0.051	-12.2	0.576	53.5	-0.050	-12.2
7	**N_i-$(C_d)_2$**	0.651	70.8	-0.522	-9.4	0.599	69.6	-0.533	-9.6	0.553	68.5	-0.544	-9.9	0.514	67.5	-0.556	-10.2
8	**N_i-$(C)(C_t)$**	-0.016	46.7	-0.037	-24.3	-0.012	46.8	-0.036	-24.3	-0.011	46.8	-0.036	-24.3	-0.008	46.9	-0.036	-24.3
		ΔGAV°(C_1)		ΔGAV°(C_2)		ΔGAV°(C_1)		ΔGAV°(C_2)		ΔGAV°(C_1)		ΔGAV°(C_2)		ΔGAV°(C_1)		ΔGAV°(C_2)	
	Reference:	6.789	89.5	6.316	63.3	6.904	92.1	6.430	65.8	7.008	94.6	6.535	68.2	7.103	97.1	6.632	70.7
1	**C_i-$(C)(H)_2$**	-0.233	4.5	-0.177	-15.4	-0.229	4.6	-0.183	-15.5	-0.226	4.7	-0.188	-15.7	-0.224	4.7	-0.192	-15.8
2	**C_i-$(C)_2(H)$**	-0.201	7.9	0.009	-27.6	-0.191	8.1	0.001	-27.8	-0.186	8.2	-0.006	-27.9	-0.181	8.3	-0.011	-28.1
3	**$C_{i,d}$-(H)**	0.264	-20.9	0.116	-0.7	0.266	-20.9	0.117	-0.7	0.268	-20.9	0.117	-0.7	0.268	-20.8	0.118	-0.7
4	**$C_{i,d}$-(C)**	0.155	-16.7	0.082	-11.4	0.160	-16.6	0.078	-11.5	0.162	-16.5	0.076	-11.5	0.164	-16.5	0.074	-11.6
5	**C_i-$(C_d)(H)_2$**	0.210	44.8	-0.625	-32.1	0.218	45.0	-0.606	-31.7	0.222	45.1	-0.590	-31.3	0.225	45.1	-0.575	-30.9
6	**C_i-$(N)(H)_2$**	-0.147	20.7	-0.319	-30.9	-0.137	20.9	-0.306	-30.7	-0.129	21.1	-0.295	-30.4	-0.122	21.3	-0.285	-30.1
7	**C_i-$(C)(N)(H)$**	-0.051	20.3	-0.136	-38.2	-0.027	20.8	-0.114	-37.7	-0.009	21.3	-0.096	-37.3	0.006	21.7	-0.080	-36.9
8	**$C_{i,I}$-(H)**	0.351	9.0	0.085	-32.0	0.357	9.1	0.087	-31.9	0.361	9.2	0.088	-31.9	0.364	9.3	0.090	-31.8
9	**$C_{i,I}$-(C)**	0.257	11.0	0.042	-33.7	0.263	11.2	0.038	-33.8	0.267	11.3	0.035	-33.9	0.269	11.4	0.033	-33.9
10	**C_i-$(C_I)(H)_2$**	0.369	31.0	-0.524	-27.6	0.371	31.0	-0.509	-27.2	0.370	31.0	-0.497	-27.0	0.368	31.0	-0.486	-26.7
11	**C_i-$(C_I)(H)_2$**	0.167	43.6	-0.726	-27.1	0.163	43.5	-0.718	-27.0	0.157	43.4	-0.712	-26.8	0.150	43.2	-0.707	-26.7



		1500 K				1600 K				1700 K				1800 K			
		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)		ΔGAV°(N_1)		ΔGAV°(N_2)	
No.	**Group**	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a	$log\tilde{A}$	E_a
	Reference:	6.721	73.2	7.190	99.6	6.803	75.6	7.271	102.0	6.880	78.1	7.346	104.4	6.953	80.5	7.416	106.8
1	**N_i-$(H)_2$**	0.276	-13.8	0.151	19.4	0.275	-13.9	0.152	19.5	0.273	-13.9	0.153	19.5	0.273	-13.9	0.153	19.5
2	**$N_{i,I}$**	0.071	24.3	0.189	-25.3	0.072	24.3	0.191	-25.2	0.074	24.4	0.193	-25.2	0.076	24.4	0.194	-25.1
3	**N_i-$(C_d)(H)$**	0.470	47.0	-0.245	-5.1	0.472	47.1	-0.240	-5.0	0.471	47.1	-0.236	-4.8	0.471	47.1	-0.233	-4.7
4	**N_i-$(C_t)(H)$**	0.169	40.6	0.086	-15.0	0.168	40.6	0.086	-15.0	0.167	40.6	0.086	-15.0	0.167	40.5	0.085	-15.1
5	**N_i-$(C)_2$**	-0.109	15.0	0.044	-14.8	-0.105	15.1	0.042	-14.8	-0.102	15.2	0.040	-14.9	-0.099	15.3	0.037	-15.0
6	**N_i-$(C)(C_d)$**	0.579	53.6	-0.050	-12.1	0.580	53.7	-0.050	-12.2	0.579	53.7	-0.052	-12.2	0.579	53.6	-0.054	-12.3
7	**N_i-$(C_d)_2$**	0.480	66.6	-0.566	-10.5	0.451	65.7	-0.576	-10.8	0.424	64.9	-0.586	-11.1	0.403	64.2	-0.595	-11.4
8	**N_i-$(C)(C_t)$**	-0.007	46.9	-0.035	-24.3	-0.006	47.0	-0.035	-24.3	-0.006	47.0	-0.035	-24.3	-0.005	47.0	-0.036	-24.3
		ΔGAV°(C_1)		ΔGAV°(C_2)		ΔGAV°(C_1)		ΔGAV°(C_2)		ΔGAV°(C_1)		ΔGAV°(C_2)		ΔGAV°(C_1)		ΔGAV°(C_2)	
	Reference:	7.190	99.6	6.721	73.2	7.271	102.0	6.803	75.6	7.346	104.4	6.880	78.1	7.416	106.8	6.953	80.5
1	**C_i-$(C)(H)_2$**	-0.222	4.8	-0.196	-15.9	-0.220	4.8	-0.198	-15.9	-0.219	4.9	-0.201	-16.0	-0.218	4.9	-0.203	-16.1
2	**C_i-$(C)_2(H)$**	-0.178	8.4	-0.016	-28.2	-0.175	8.5	-0.020	-28.3	-0.173	8.5	-0.024	-28.4	-0.172	8.6	-0.027	-28.5
3	**$C_{i,d}$-(H)**	0.269	-20.8	0.119	-0.6	0.270	-20.8	0.120	-0.6	0.270	-20.8	0.120	-0.6	0.270	-20.8	0.121	-0.6
4	**$C_{i,d}$-(C)**	0.165	-16.5	0.072	-11.6	0.166	-16.5	0.071	-11.7	0.167	-16.4	0.069	-11.7	0.166	-16.4	0.068	-11.8
5	**C_i-$(C_d)(H)_2$**	0.226	45.2	-0.562	-30.6	0.226	45.2	-0.551	-30.3	0.225	45.1	-0.542	-30.0	0.223	45.1	-0.533	-29.7
6	**C_i-$(N)(H)_2$**	-0.117	21.4	-0.277	-29.9	-0.113	21.5	-0.270	-29.7	-0.110	21.6	-0.265	-29.5	-0.108	21.7	-0.259	-29.3
7	**C_i-$(C)(N)(H)$**	0.019	22.0	-0.067	-36.5	0.030	22.3	-0.055	-36.2	0.038	22.6	-0.046	-35.9	0.044	22.8	-0.037	-35.6
8	**$C_{i,I}$-(H)**	0.367	9.4	0.091	-31.8	0.370	9.5	0.093	-31.8	0.372	9.5	0.094	-31.7	0.373	9.6	0.095	-31.7
9	**$C_{i,I}$-(C)**	0.272	11.4	0.031	-34.0	0.275	11.5	0.029	-34.1	0.276	11.5	0.027	-34.1	0.277	11.6	0.026	-34.2
10	**C_i-$(C_I)(H)_2$**	0.365	30.9	-0.477	-26.4	0.362	30.8	-0.469	-26.2	0.358	30.6	-0.463	-26.0	0.353	30.5	-0.456	-25.8
11	**C_i-$(C_I)(H)_2$**	0.143	43.0	-0.702	-26.6	0.136	42.8	-0.699	-26.5	0.128	42.6	-0.697	-26.4	0.120	42.3	-0.695	-26.3

4.6. Tunneling coefficients

Table S19: Tunneling coefficients for all reactions from Table S16 over the temperature range 300-1800 K.

No.	κ(T)															
	300	**400**	**500**	**600**	**700**	**800**	**900**	**1000**	**1100**	**1200**	**1300**	**1400**	**1500**	**1600**	**1700**	**1800**
1	36.9	5.8	2.9	2.1	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1
2	37.8	6.0	3.0	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
3	8.0	3.1	2.0	1.6	1.4	1.3	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1
4	38.5	6.3	3.1	2.2	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
5	27.8	5.6	2.9	2.1	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1	1.1
6	20.8	5.0	2.7	2.0	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1
7	29.8	5.9	3.0	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
8	50.0	7.4	3.4	2.3	1.8	1.6	1.4	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
9	14.4	4.3	2.5	1.9	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1
10	7.2	2.9	1.9	1.6	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1
11	14.3	4.0	2.4	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1
12	9.1	3.5	2.2	1.8	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1
13	42.7	6.6	3.2	2.2	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
14	33.3	6.7	3.3	2.3	1.9	1.6	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1
15	13.9	4.4	2.6	2.0	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
16	23.2	5.2	2.8	2.0	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1
17	145.3	10.5	4.0	2.5	2.0	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1
18	180.3	11.3	4.1	2.6	2.0	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1
19	10.4	3.6	2.2	1.8	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1
20	24.8	5.3	2.8	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
21	10.3	3.8	2.4	1.9	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1
22	28.1	5.6	2.9	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
23	161.9	10.8	4.0	2.5	2.0	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1
24	151.0	11.0	4.1	2.6	2.0	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1
25	268.2	13.2	4.5	2.7	2.0	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1
26	18.8	4.8	2.7	2.0	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
27	260.6	12.6	4.3	2.7	2.0	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1
28	27.0	5.5	2.9	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
29	2.8	1.8	1.4	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.0	1.0	1.0	1.0
30	22.5	4.9	2.7	2.0	1.6	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1
31	10.9	3.6	2.3	1.8	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1
32	23.1	5.0	2.7	2.0	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1	1.1
33	21.0	4.9	2.7	2.0	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1	1.1
34	25.0	5.7	3.0	2.1	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
35	18.5	4.9	2.8	2.0	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
36	34.4	6.4	3.2	2.2	1.8	1.6	1.4	1.4	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
37	37.4	6.1	3.0	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
38	27.8	5.5	2.9	2.1	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1
39	21.1	5.1	2.8	2.0	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
40	13.8	4.3	2.6	1.9	1.6	1.5	1.4	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1	1.1
41	30.1	5.8	3.0	2.1	1.8	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
42	9.4	3.8	2.4	1.9	1.6	1.5	1.4	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1	1.1
43	19.7	4.9	2.7	2.0	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
44	23.1	5.5	2.9	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
45	17.3	4.9	2.8	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
46	37.0	6.6	3.2	2.3	1.8	1.6	1.5	1.4	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
47	16.3	5.2	3.0	2.2	1.8	1.6	1.4	1.4	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
48	26.5	5.7	3.0	2.1	1.8	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
49	22.7	5.5	2.9	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
50	51.7	7.6	3.5	2.4	1.9	1.6	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1
51	3.3	2.1	1.6	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.1
52	3.1	2.0	1.6	1.4	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.0	1.0

53	6.6	2.8	1.9	1.6	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1
54	1.9	1.4	1.3	1.2	1.1	1.1	1.1	1.1	1.1	1.0	1.0	1.0	1.0	1.0	1.0	1.0
55	4.7	2.4	1.7	1.5	1.3	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.1
56	6.7	2.8	1.9	1.6	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1
57	19.6	4.7	2.6	1.9	1.6	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1
58	16.3	4.8	2.8	2.0	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
59	33.3	6.7	3.3	2.3	1.9	1.6	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1
60	28.3	6.3	3.2	2.3	1.8	1.6	1.5	1.4	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
61	12.4	4.5	2.7	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
62	1.7	1.4	1.2	1.2	1.1	1.1	1.1	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
63	4.0	2.4	1.8	1.6	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1
64	12.4	4.5	2.7	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
65	55.9	7.4	3.4	2.3	1.8	1.6	1.4	1.4	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
66	43.6	7.0	3.3	2.3	1.8	1.6	1.5	1.4	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
67	1.7	1.4	1.2	1.2	1.1	1.1	1.1	1.1	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
68	13.8	4.3	2.5	1.9	1.6	1.5	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1
69	30.6	6.2	3.1	2.2	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
70	34.7	6.8	3.3	2.3	1.8	1.6	1.5	1.4	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
71	16.3	4.9	2.8	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
72	5.6	2.8	2.0	1.6	1.4	1.3	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1
73	26.7	5.8	3.0	2.1	1.8	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
74	133.2	11.0	4.2	2.6	2.0	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1
75	10.2	3.4	2.2	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1
76	5.4	2.5	1.8	1.5	1.4	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.1
77	10.2	3.4	2.2	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1
78	37.5	6.4	3.2	2.2	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
79	36.1	6.3	3.1	2.2	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
80	78.4	9.3	3.9	2.5	2.0	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1
81	31.5	5.9	3.0	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
82	60.2	7.5	3.4	2.3	1.8	1.6	1.4	1.4	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
83	48.1	7.1	3.3	2.3	1.8	1.6	1.4	1.4	1.3	1.2	1.2	1.2	1.2	1.1	1.1	1.1
84	15.2	4.6	2.7	2.0	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
85	221.4	12.1	4.3	2.6	2.0	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1
86	259.7	12.9	4.4	2.7	2.0	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1
87	179.3	12.0	4.3	2.7	2.0	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.2	1.1	1.1

5. Temperature dependence of the group additivity values

The limited temperature dependence of the ΔGAV°s due to the use of a reference reaction enables the use of the ΔGAV°s over a large temperature range without loss of accuracy. In Figure S1, the temperature dependence of the ΔGAV°s is shown for both the pre-exponential factor as well as the activation energy with the highest temperature dependence per hydrogen abstraction reaction family.

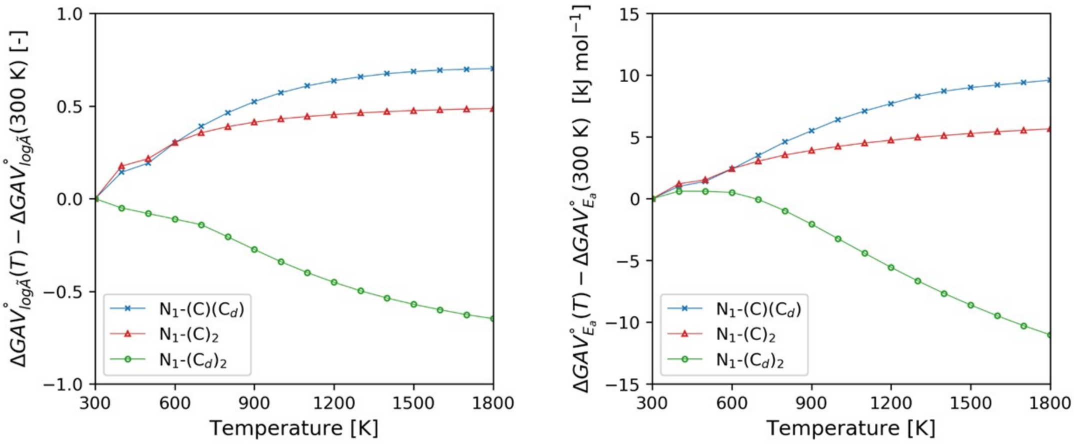


Figure S1: Temperature dependence of the standard group additivity values (ΔGAV°): Difference between ΔGAV°(T) and ΔGAV°(300 K) for $log\tilde{A}$ (left) and E_a (right) for the groups with the highest temperature dependency for the H-H-N (×), N-H-N (△) and C-H-N (○) hydrogen abstractions.

The ΔGAV° at 300 K is subtracted from the ΔGAV° at higher temperature in order to obtain the depicted temperature dependency. For hydrogen abstractions of the type H-H-N, the group with the highest temperature dependence is N_1-(C)(C_d). The difference between 300 and 1800 K for $log\tilde{A}$ amounts to +0.703, while for E_a a difference of 9.6 kJ mol^{-1} is obtained. The group N_1-$(C)_2$ has the highest temperature dependency for N-H-N hydrogen abstractions, i.e. a change of +0.487 for $log\tilde{A}$ and 5.7 kJ mol^{-1} for E_a over the temperature range 300-1800 K. For C-H-N hydrogen abstractions, the group N_1-$(C_d)_2$ displays the largest temperature dependency for $log\tilde{A}$ (-0.647) and E_a (11.0 kJ mol^{-1}). Depending on the substituents of the reactive atoms, there can be a significant temperature dependence of the ΔGAV°s.

6. Thermodynamic consistency

The equilibrium coefficient, corresponding to the ratio of the forward and reverse rate coefficient, can be calculated with equation (1) in which Δn is the change in number of moles between the products and reactants and $\Delta_r G^\circ$ the change in Gibbs free energy,

$$K_{eq} = \left(\frac{RT}{p}\right)^{-\Delta n} exp\left(-\frac{\Delta_r G^\circ}{RT}\right) \quad \textbf{(1)}$$

The forward and reverse rate coefficients are thermodynamically consistent if their ratio is equal to the equilibrium coefficient calculated from the *ab initio* thermodynamic parameters of the reactant(s) and product(s) of that reaction. When making use of a group additivity model for approximation of the kinetic parameters, this is not necessarily the case. In Table S20, the ratio of the forward and reverse rate coefficients calculated from group additivity ($\frac{k_{for,GA}}{k_{rev,GA}}$) is compared to the *ab initio* equilibrium coefficient ($K_{eq,AI}$). The mean and maximum values of the ρ parameter, obtained by dividing the highest by the lowest values for the equilibrium coefficients, are reported for 1000 K.

Table S20: Comparison of the *ab initio* calculated equilibrium coefficient ($K_{eq,AI}$) with the ratio of the forward and reverse rate coefficients calculated from group additivity ($\frac{k_{for,GA}}{k_{rev,GA}}$) and the equilibrium coefficients calculated with group additive-approximated thermodynamic data ($K_{eq,GA}$). The deviations are expressed as mean and maximum values for the ρ parameter, obtained by dividing the highest by the lowest values for the equilibrium coefficient at 1000 K for all reactions of the combined training and test set, with the final set of group additivity values.

Reaction family	$\frac{k_{for,GA}}{k_{rev,GA}}$ versus $K_{eq,AI}$		$K_{eq,AI}$ versus $K_{eq,GA}$		$\frac{k_{for,GA}}{k_{rev,GA}}$ versus $K_{eq,GA}$	
	$\langle\rho_1\rangle$	$\rho_{1,max}$	$\langle\rho_2\rangle$	$\rho_{2,max}$	$\langle\rho_3\rangle$	$\rho_{3,max}$
H-H-N	1.41	3.08	1.72	3.68	1.65	3.04
N-H-N	1.00	1.00	1.63	3.81	1.62	3.83
C-H-N	1.26	2.87	1.63	4.26	1.72	5.20

[a] $\rho_1 = max\left(\frac{k_{for,GA}}{k_{rev,GA}}, K_{eq,AI}\right)/min\left(\frac{k_{for,GA}}{k_{rev,GA}}, K_{eq,AI}\right)$, [b] $\rho_2 = max(K_{eq,AI}, K_{eq,GA})/min(K_{eq,AI}, K_{eq,GA})$, [c] $\rho_3 = max\left(\frac{k_{for,GA}}{k_{rev,GA}}, K_{eq,GA}\right)/min\left(\frac{k_{for,GA}}{k_{rev,GA}}, K_{eq,GA}\right)$

Note that for the hydrogen abstraction characterized by a N-H-N transition state, the deviations for the forward and reverse rate coefficients are of the same magnitude and thus cancel each other out when calculating the equilibrium coefficient. Overall, the ratios of the group additive-approximated forward and reverse rate coefficients are in good agreement with the *ab initio* equilibrium coefficients. For both H-H-N and C-H-N, the highest deviation is obtained for reactions for which the forward rate coefficient deviates by more than a factor of two from the *ab initio* rate coefficient. For H-H-N, this reaction includes the group N_2-(C_d)(H), while for C-H-N the highest deviation is obtained for a reaction in which the groups C_1-(N)$(H)_2$ and N_2-$(C)_2$ are present. If thermodynamic data obtained directly from *ab initio* calculations is not available for a certain species during kinetic model generation, the group additivity method is used as approximation method. This approximation influences the value of the reverse rate coefficient when it is implemented as a reverse reaction. From Table S20, it can be seen that the use of the equilibrium coefficient based on the group additive-approximated thermodynamic parameters of reactant(s) and product(s) ($K_{eq,GA}$) leads to a factor of uncertainty of around two for determination of the reverse rate coefficient based on thermodynamic consistency.

7. References

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