Supporting Information

Table S1. Equilibrium constants (K_{eq}, cm^3 $molecule^{-1}$ s^{-1}), rate constant of the second step (k_2, s^{-1}), tunneling corrections (κ) and reaction coordinate (s, bohr) of the variational transition state, corresponding to the abstractions from the –CHO sites.

T (K)	Conformer I				Conformer II			
	K_{eq}	k_2	κ	s	K_{eq}	k_2	κ	s
200	3.94E-21	1.01E+08	5.29	-0.43	7.31E-21	3.50E+09	3.63	-0.65
220	1.83E-21	1.92E+08	4.44	-0.43	3.11E-21	4.72E+09	3.13	-0.65
240	9.73E-22	3.24E+08	3.85	-0.43	1.54E-21	6.00E+09	2.78	-0.65
260	5.76E-22	4.99E+08	3.42	-0.43	8.55E-22	7.31E+09	2.52	-0.65
270	4.58E-22	6.04E+08	3.25	-0.43	6.61E-22	7.96E+09	2.42	-0.65
280	3.71E-22	7.18E+08	3.10	-0.43	5.21E-22	8.60E+09	2.32	-0.65
290	3.05E-22	8.43E+08	2.96	-0.43	4.19E-22	9.23E+09	2.24	-0.65
298.15	**2.63E-22**	**9.51E+08**	**2.87**	**-0.43**	**3.55E-22**	**9.74E+09**	**2.18**	**-0.65**
300	2.55E-22	9.76E+08	2.85	-0.43	3.42E-22	9.85E+09	2.17	-0.65
310	2.16E-22	1.12E+09	2.74	-0.43	2.83E-22	1.05E+10	2.10	-0.65
320	1.85E-22	1.27E+09	2.64	-0.43	2.38E-22	1.11E+10	2.04	-0.65
330	1.60E-22	1.43E+09	2.56	-0.43	2.03E-22	1.16E+10	1.99	-0.65
340	1.40E-22	1.59E+09	2.48	-0.42	1.74E-22	1.22E+10	1.94	-0.65
350	1.24E-22	1.76E+09	2.41	-0.42	1.51E-22	1.27E+10	1.90	-0.65
360	1.10E-22	1.93E+09	2.35	-0.42	1.33E-22	1.32E+10	1.85	-0.65
370	9.92E-23	2.11E+09	2.29	-0.42	1.17E-22	1.37E+10	1.82	-0.65
380	8.97E-23	2.29E+09	2.23	-0.42	1.05E-22	1.42E+10	1.78	-0.65
390	8.16E-23	2.47E+09	2.18	-0.42	9.39E-23	1.47E+10	1.75	-0.65
400	7.47E-23	2.65E+09	2.14	-0.42	8.48E-23	1.51E+10	1.72	-0.65
420	6.37E-23	3.02E+09	2.05	-0.42	7.05E-23	1.59E+10	1.67	-0.65
440	5.53E-23	3.38E+09	1.98	-0.42	5.99E-23	1.67E+10	1.62	-0.65
460	4.88E-23	3.74E+09	1.92	-0.42	5.18E-23	1.74E+10	1.58	-0.65
480	4.37E-23	4.09E+09	1.86	-0.42	4.55E-23	1.80E+10	1.55	-0.65
500	3.96E-23	4.42E+09	1.81	-0.41	4.06E-23	1.85E+10	1.52	-0.65

Table S2. Equilibrium constants (K_{eq}, cm^3 $molecule^{-1}$ s^{-1}), rate constant of the second step (k_2, s^{-1}), tunneling corrections (κ) and reaction coordinate (s, bohr) of the variational transition state, corresponding to the abstractions from the $–CH_2–$ sites.

T (K)	Conformer I				Conformer II			
	K_{eq}	k_2	κ	s	K_{eq}	k_2	κ	s
200	8.60E-20	1.72E+05	6.73	-0.30	9.64E-21	1.58E+07	7.01	-0.30
220	2.97E-20	3.38E+05	5.37	-0.26	4.19E-21	3.81E+07	5.59	-0.26
240	1.24E-20	8.22E+05	4.49	-0.26	2.12E-21	7.86E+07	4.66	-0.26
260	5.93E-21	1.73E+06	3.87	-0.26	1.20E-21	1.44E+08	4.01	-0.26
270	4.29E-21	2.39E+06	3.63	-0.26	9.33E-22	1.88E+08	3.76	-0.26
280	3.18E-21	3.23E+06	3.42	-0.26	7.41E-22	2.41E+08	3.54	-0.26
290	2.41E-21	4.25E+06	3.24	-0.26	6.00E-22	3.02E+08	3.36	-0.26
298.15	**1.96E-21**	**5.25E+06**	**3.11**	**-0.26**	**5.11E-22**	**3.60E+08**	**3.22**	**-0.26**
300	1.87E-21	5.50E+06	3.08	-0.26	4.93E-22	3.74E+08	3.19	-0.26
310	1.47E-21	6.97E+06	2.94	-0.26	4.11E-22	4.55E+08	3.05	-0.26
320	1.18E-21	8.69E+06	2.82	-0.26	3.48E-22	5.47E+08	2.92	-0.26
330	9.60E-22	1.07E+07	2.71	-0.26	2.97E-22	6.49E+08	2.81	-0.26
340	7.92E-22	1.29E+07	2.61	-0.26	2.57E-22	7.62E+08	2.70	-0.26
350	6.61E-22	1.55E+07	2.52	-0.26	2.25E-22	8.86E+08	2.61	-0.26
360	5.58E-22	1.83E+07	2.44	-0.26	1.98E-22	1.02E+09	2.53	-0.26
370	4.76E-22	2.14E+07	2.37	-0.26	1.76E-22	1.17E+09	2.45	-0.26
380	4.11E-22	2.48E+07	2.30	-0.26	1.57E-22	1.32E+09	2.38	-0.26
390	3.57E-22	2.85E+07	2.24	-0.26	1.42E-22	1.49E+09	2.32	-0.26
400	3.13E-22	3.24E+07	2.19	-0.26	1.29E-22	1.66E+09	2.26	-0.26
420	2.46E-22	4.12E+07	2.09	-0.26	1.08E-22	2.04E+09	2.16	-0.26
440	1.98E-22	5.09E+07	2.01	-0.26	9.23E-23	2.45E+09	2.07	-0.26
460	1.63E-22	6.15E+07	1.93	-0.26	8.03E-23	2.89E+09	1.99	-0.26
480	1.37E-22	7.30E+07	1.87	-0.26	7.10E-23	3.36E+09	1.93	-0.26
500	1.18E-22	8.51E+07	1.81	-0.26	6.37E-23	3.86E+09	1.87	-0.26

Table S3. Equilibrium constants (K_{eq}, cm^3 molecule^{-1} s^{-1}), rate constant of the second step (k_2, s^{-1}), tunneling corrections (κ) and reaction coordinate (s, bohr) of the variational transition state, corresponding to the abstractions from the –OH sites.

T (K)	Conformer I				Conformer II			
	K_{eq}	k_2	κ	s	K_{eq}	k_2	κ	s
200	1.25E-21	1.20E+03	8201.33	0.01	8.06E-21	9.35E+03	862.62	0.06
220	5.01E-22	8.24E+03	2294.52	0.01	3.89E-21	4.25E+04	312.60	0.06
240	2.36E-22	4.09E+04	832.27	0.01	2.15E-21	1.47E+05	139.55	0.07
260	1.26E-22	1.59E+05	365.68	0.01	1.32E-21	4.12E+05	72.82	0.07
270	9.52E-23	2.89E+05	256.52	0.01	1.06E-21	6.47E+05	55.07	0.08
280	7.37E-23	5.06E+05	185.69	0.01	8.75E-22	9.80E+05	42.73	0.08
290	5.82E-23	8.51E+05	138.24	0.01	7.32E-22	1.44E+06	33.93	0.08
298.15	**4.87E-23**	**1.27E+06**	**110.66**	**0.01**	**6.39E-22**	**1.92E+06**	**28.53**	**0.09**
300	4.68E-23	1.38E+06	105.43	0.01	6.20E-22	2.04E+06	27.46	0.09
310	3.82E-23	2.18E+06	82.21	0.01	5.33E-22	2.83E+06	22.64	0.09
320	3.16E-23	3.33E+06	65.33	0.01	4.63E-22	3.44E+06	18.96	-0.28
330	2.65E-23	4.96E+06	52.86	0.01	4.07E-22	4.25E+06	16.10	-0.28
340	2.25E-23	7.23E+06	43.43	0.01	3.61E-22	5.18E+06	13.85	-0.28
350	1.93E-23	1.03E+07	36.19	0.01	3.23E-22	6.22E+06	12.05	-0.29
360	1.68E-23	1.44E+07	30.54	0.01	2.91E-22	7.37E+06	10.59	-0.29
370	1.47E-23	1.98E+07	26.08	0.01	2.64E-22	8.65E+06	9.39	-0.29
380	1.29E-23	2.67E+07	22.51	0.01	2.42E-22	1.00E+07	8.40	-0.29
390	1.15E-23	3.55E+07	19.60	0.01	2.22E-22	1.15E+07	7.57	-0.29
400	1.03E-23	4.66E+07	17.23	0.01	2.06E-22	1.32E+07	6.87	-0.29
420	8.40E-24	7.70E+07	13.63	0.01	1.79E-22	1.67E+07	5.77	-0.30
440	7.02E-24	1.22E+08	11.06	0.01	1.58E-22	2.07E+07	4.94	-0.30
460	5.98E-24	1.85E+08	9.20	0.01	1.42E-22	2.49E+07	4.32	-0.30
480	5.18E-24	2.72E+08	7.80	0.01	1.29E-22	2.95E+07	3.83	-0.31
500	4.55E-24	3.87E+08	6.73	0.01	1.19E-22	3.43E+07	3.44	-0.31