Reaction Kinetics of Hydrogen Atom Abstraction from C4-C6 Alkenes by the Hydrogen Atom and Methyl Radical

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Table S1 Full list of the computed high-pressure limit rate constants

		+ H			+ CH_3		
	Reaction	A	n	E_a	A	n	E_a
1-butene	R1	1.98×10^{7}	2.00	11363	5.03×10^{0}	3.33	11581
	R2	1.27×10^{7}	2.03	7817	8.07×10^{0}	3.29	9156
	R3	3.02×10^{6}	2.16	655	3.00×10^{0}	3.36	4144
	R4	3.00×10^{6}	2.19	5629	1.44×10^{0}	3.39	8560
2-butene	R5	3.97×10^{5}	2.42	2035	6.41×10^{-1}	3.55	5916
	R6	1.44×10^{7}	2.04	8551	2.29×10^{0}	3.33	9639
isobutene	R7	3.55×10^{7}	1.93	12264	5.23×10^{0}	3.28	12176
	R8	2.94×10^{5}	2.45	2092	4.91×10^{-1}	3.55	5705
1-pentene	R9	2.00×10^{7}	2.00	10973	5.53×10^{0}	3.33	11165
	R10	1.28×10^{7}	2.03	7379	5.16×10^{0}	3.29	8678
	R11	1.17×10^{7}	1.97	600	2.22×10^{0}	3.28	3869
	R12	2.21×10^{7}	1.90	2922	8.15×10^{0}	3.16	6267
	R13	3.50×10^{6}	2.15	5583	1.55×10^{0}	3.40	8754
2-pentene	R14	4.16×10^{5}	2.41	1741	6.46×10^{-1}	3.54	5514
	R15	1.36×10^{7}	2.03	8142	4.53×10^{0}	3.32	9187
	R16	1.84×10^{7}	1.98	8135	4.63×10^{0}	3.28	9091
	R17	4.87×10^{6}	2.10	304	3.19×10^{0}	3.34	3859

	R18	3.20×10^{6}	2.18	5335	4.11×10^{0}	3.38	8278
2-methyl-1-butene	R19	3.55×10^{7}	1.95	11583	1.93×10^{0}	3.32	12924
	R20	2.57×10^{5}	2.47	1743	2.65×10^{-1}	3.59	5232
	R21	7.71×10^{6}	2.04	206	2.83×10^{0}	3.32	3393
	R22	2.81×10^{6}	2.22	5837	1.78×10^{0}	3.42	8625
2-methyl-2-butene	R23	1.71×10^{7}	2.01	7963	3.45×10^{0}	3.21	9206
	R24	4.98×10^{5}	2.44	1399	5.74×10^{-1}	3.60	5213
	R25	4.74×10^{5}	2.40	1516	5.07×10^{-1}	3.62	5165
2-methyl-3-butene	R26	2.01×10^{7}	2.01	10827	4.33×10^{0}	3.33	11064
	R27	9.45×10^{6}	2.06	7504	9.50×10^{0}	3.23	8647
	R28	2.69×10^{7}	1.86	-65	1.18×10^{1}	3.17	2611
	R29	3.02×10^{6}	2.17	5139	1.19×10^{0}	3.37	7927
1-hexene	R30	1.96×10^{7}	2.00	10660	5.57×10^{-1}	3.32	10880
	R31	1.27×10^{7}	2.03	7059	4.84×10^{0}	3.32	8379
	R32	5.06×10^{6}	2.07	253	2.25×10^{0}	3.34	3491
	R33	4.38×10^{7}	1.80	3018	7.91×10^{0}	3.08	5978
	R34	3.20×10^{7}	1.85	2829	2.58×10^{1}	3.00	6368
	R35	4.13×10^{6}	2.13	5442	1.60×10^{0}	3.40	8276
2-hexene	R36	4.96×10^{5}	2.40	1418	5.34×10^{-1}	3.53	5237
	R37	1.39×10^{7}	2.03	7810	3.53×10^{0}	3.31	8910
	R38	1.64×10^{7}	1.98	7805	2.11×10^{0}	3.28	8702
	R39	4.83×10^{7}	1.78	450	1.59×10^{1}	3.06	3659
	R40	8.54×10^{6}	2.07	2516	7.25×10^{0}	3.16	5976
	R41	4.21×10^{6}	2.13	5629	2.07×10^{0}	3.39	8472
3-hexene	R42	5.83×10^{6}	2.09	5132	1.07×10^{1}	3.30	7975
	R43	1.13×10^{7}	2.00	124	5.32×10^{0}	3.27	3515
	R44	1.70×10^{7}	1.99	7628	2.97×10^{0}	3.28	8642
1-4-pentadiene	R45	2.00×10^{7}	2.00	11205	4.31×10^{0}	3.33	11356
	R46	2.08×10^{7}	1.98	7764	4.61×10^{0}	3.25	8749

R47	7.16×10^{6}	2.05	-638	7.96×10^{0}	3.29	1490

Table S2 Calculated G4 energies for the reactants and transition states at the G4 level

			+ H	+ CH_3
	G4 energy of alkenes	Reaction	TS energy	TS energy
1-butene	-157.081325	R1	-393.712654	-196.854984
		R2	-157.564684	-196.858878
		R3	-157.576667	-196.867866
		R4	-157.567754	-196.859809
2-butene	-157.085720	R5	-157.577983	-196.868988
		R6	-157.568257	-196.862484
isobutene	-157.087981	R7	-157.565624	-196.860991
		R8	-157.57986	-196.871455
1-pentene	-196.359674	R9	-196.838722	-236.134009
		R10	-196.843716	-236.137971
		R11	-196.855369	-236.146812
		R12	-196.850632	-236.142151
		R13	-196.846045	-236.137821
2-pentene	-196.363428	R14	-196.856216	-236.147357
		R15	-196.846641	-236.141032
		R16	-196.846723	-236.141226
		R17	-196.859676	-236.150478
		R18	-196.85034	-236.142384
2-methyl-1-butene	-196.365136	R19	-196.843753	-236.139055
		R20	-196.85763	-236.149311
		R21	-196.861346	-236.152899
		R22	-196.851132	-236.14337
2-methyl-2-butene	-196.367400	R23	-196.85116	-236.144971
		R24	-196.861391	-236.152227
		R25	-196.860618	-236.152027

2-methyl-3-butene	-196.362465	R26	-196.841681	-236.136943
		R27	-196.84643	-236.14092
		R28	-196.860429	-236.152135
		R29	-196.849689	-236.141984
1-hexene	-235.637979	R30	-236.117561	-275.412805
		R31	-236.122567	-275.416822
		R32	-236.134282	-275.425726
		R33	-236.12915	-275.421258
		R34	-236.129235	-275.420753
		R35	-236.124776	-275.416871
2-hexene	-235.641880	R36	-236.135259	-275.426328
		R37	-236.125658	-275.420012
		R38	-236.125737	-275.420273
		R39	-236.138427	-275.42959
		R40	-236.133065	-275.424847
		R41	-236.128415	-275.420543
3-hexene	-235.641231	R42	-236.128605	-275.420771
		R43	-236.137998	-275.428947
		R44	-236.125279	-275.419767
1-4-pentadiene	-195.146721	R45	-195.625451	-234.920831
		R46	-195.630173	-234.924855
		R47	-195.645262	-234.938513

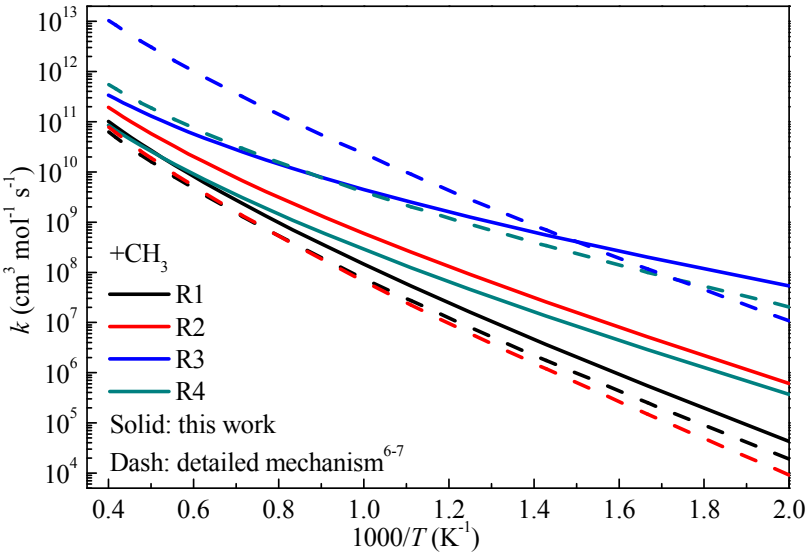

Figure S1. Comparisons of the abstraction reaction rate constants of 1-butene with the CH3 radical