

Electronic Supplementary Information for:

**Insights into the H-abstraction reaction kinetics from amines in their
degeneration fates under the atmospheric and combustion conditions**

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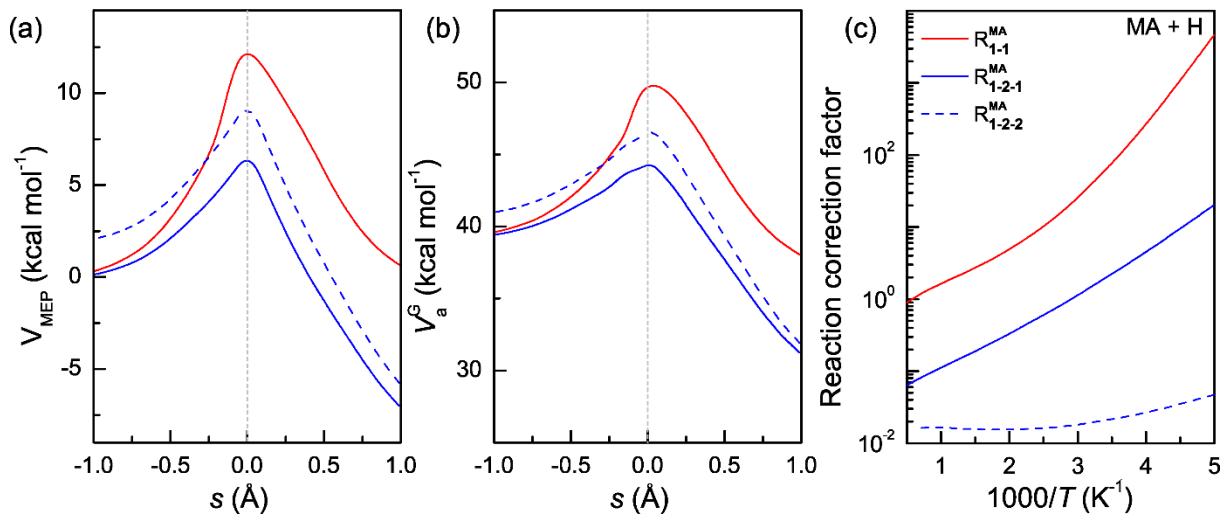


Figure S1. (a) V_{MEP} , (b) V_a^{G} , and reaction correction factor of each reaction path for the H-abstraction reactions from MA by H radicals. R_{1-1}^{MA} and R_{1-2}^{MA} have 1 and 2 reaction paths, respectively.

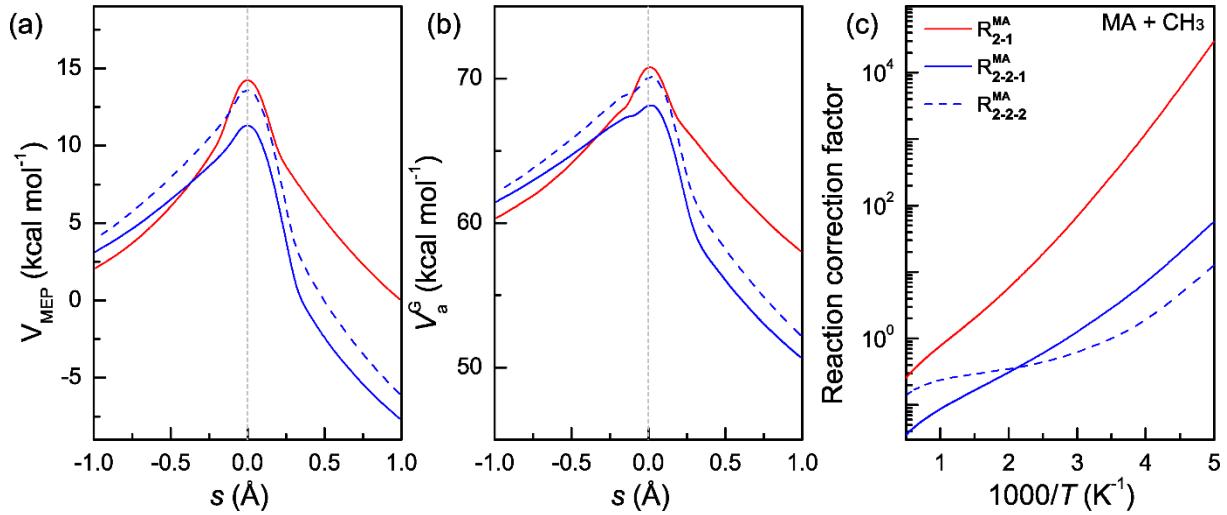


Figure S2. (a) V_{MEP} , (b) V_a^{G} , and reaction correction factor of each reaction path for the H-abstraction reactions from MA by CH₃ radicals. R_{2-1}^{MA} and R_{2-2}^{MA} have 1 and 2 reaction paths, respectively.

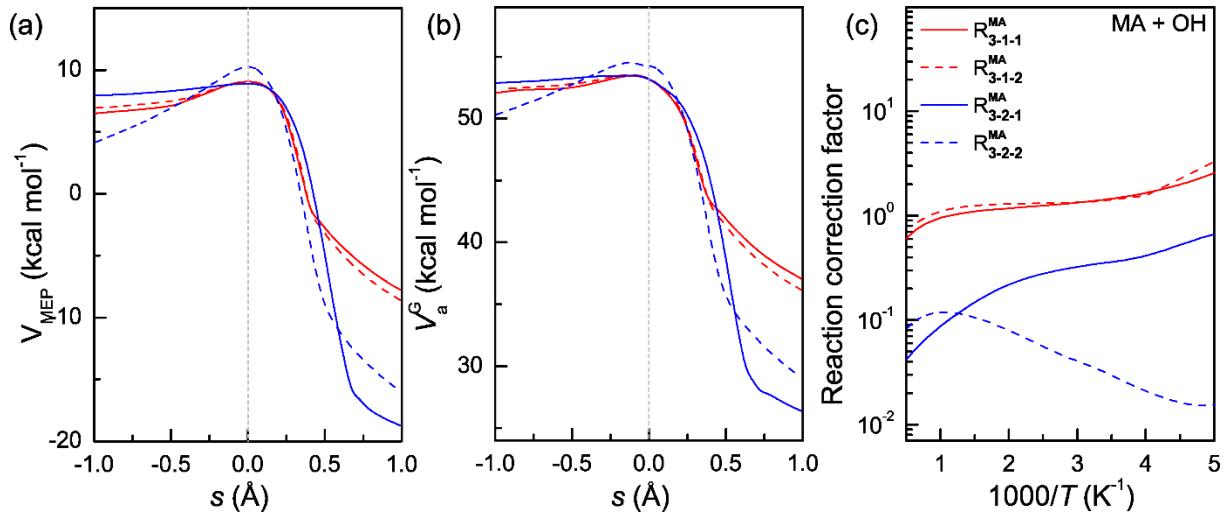


Figure S3. (a) V_{MEP} , (b) V_a^{G} , and reaction correction factor of each reaction path for the H-abstraction reactions from MA by OH radicals. R_{3-1}^{MA} and R_{3-2}^{MA} both have 2 reaction paths.

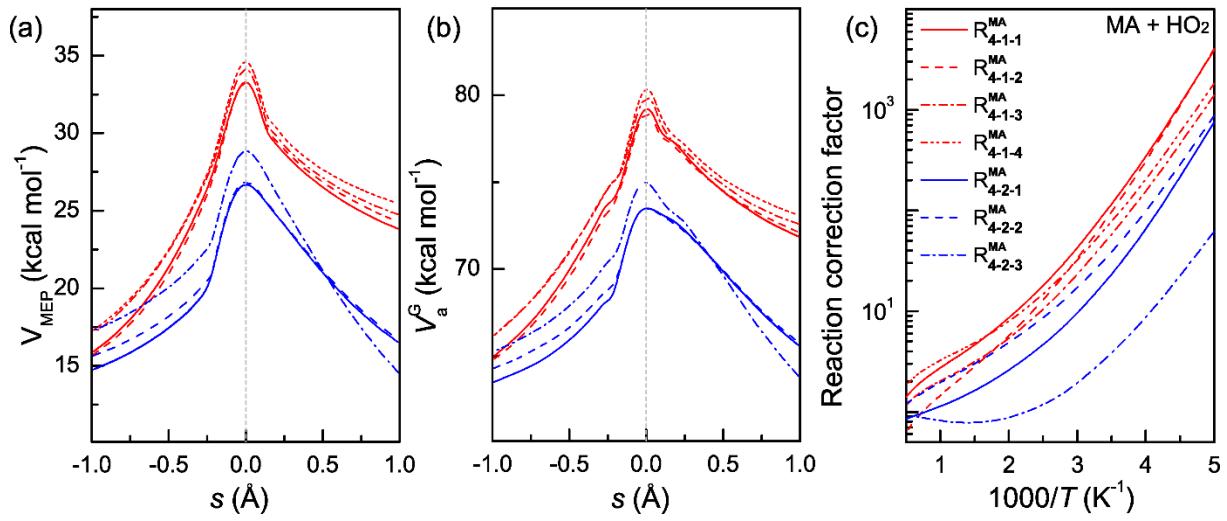


Figure S4. (a) V_{MEP} , (b) V_a^{G} , and reaction correction factor of each reaction path for the H-abstraction reactions from MA by HO₂ radicals. R_{4-1}^{MA} and R_{4-2}^{MA} have 4 and 3 reaction paths, respectively.

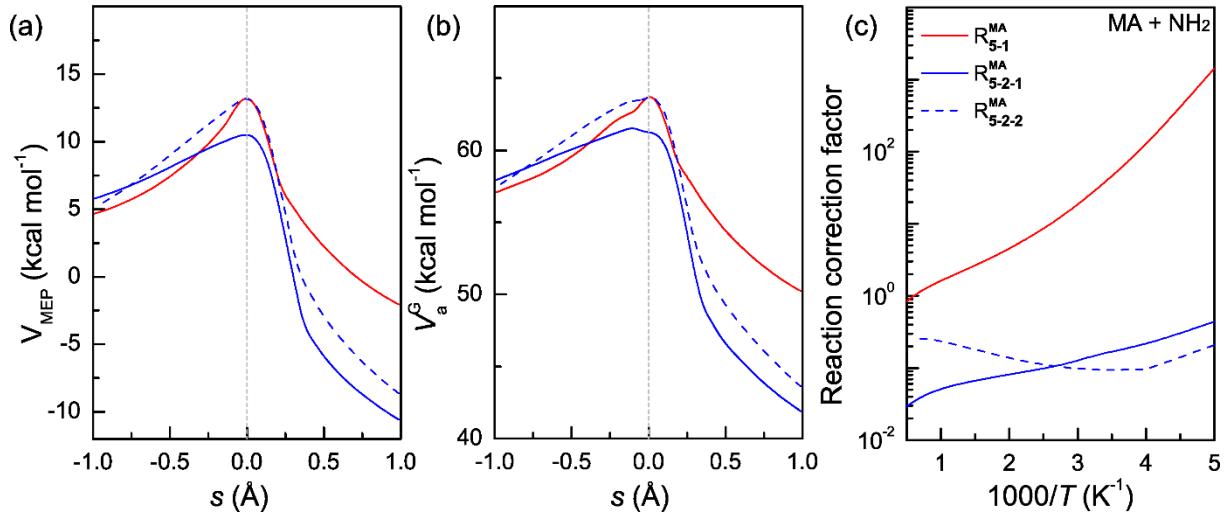


Figure S5. (a) V_{MEP} , (b) V_a^{G} , and reaction correction factor of each reaction path for the H-abstraction reactions from MA by NH₂ radicals. R_{5-1}^{MA} and R_{5-2}^{MA} have 1 and 2 reaction paths, respectively.

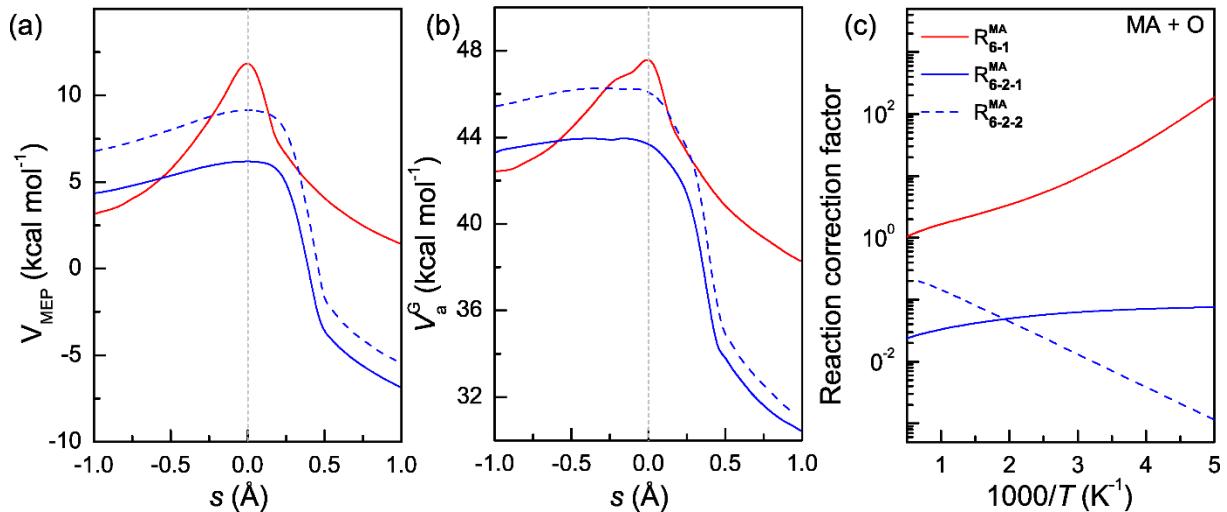


Figure S6. (a) V_{MEP} , (b) V_a^{G} , and reaction correction factor of each reaction path for the H-abstraction reactions from MA by O radicals. R_{6-1}^{MA} and R_{6-2}^{MA} have 1 and 2 reaction paths, respectively.

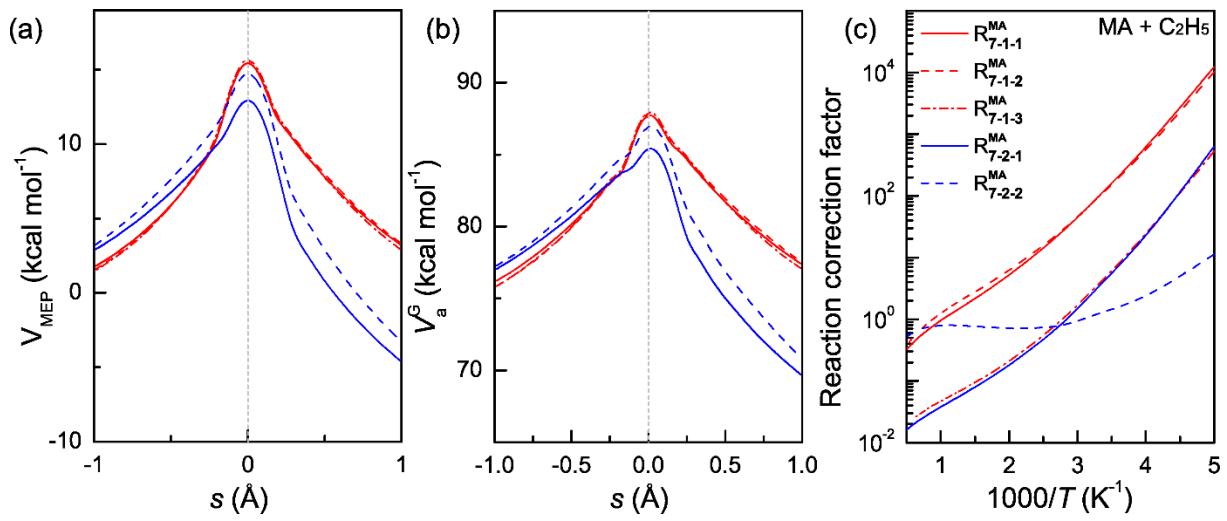


Figure S7. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from MA by C₂H₅ radicals. R_{7-1}^{MA} and R_{7-2}^{MA} have 3 and 2 reaction paths, respectively.

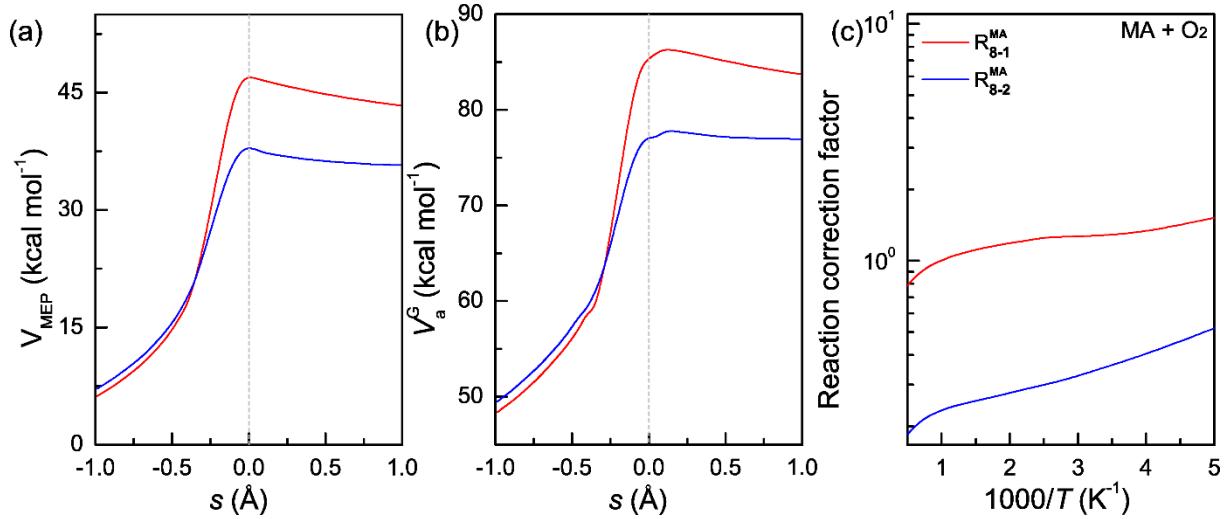


Figure S8. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from MA by O₂. R_{8-1}^{MA} and R_{8-2}^{MA} both have 1 reaction path.

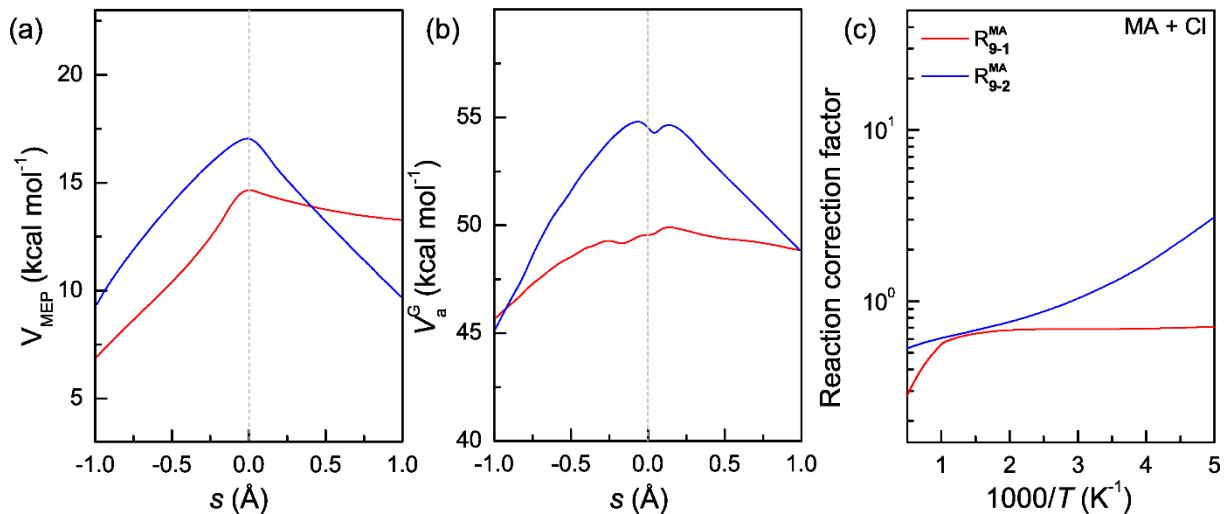


Figure S9. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from MA by Cl. R_{9-1}^{MA} and R_{9-2}^{MA} both have 1 reaction path.

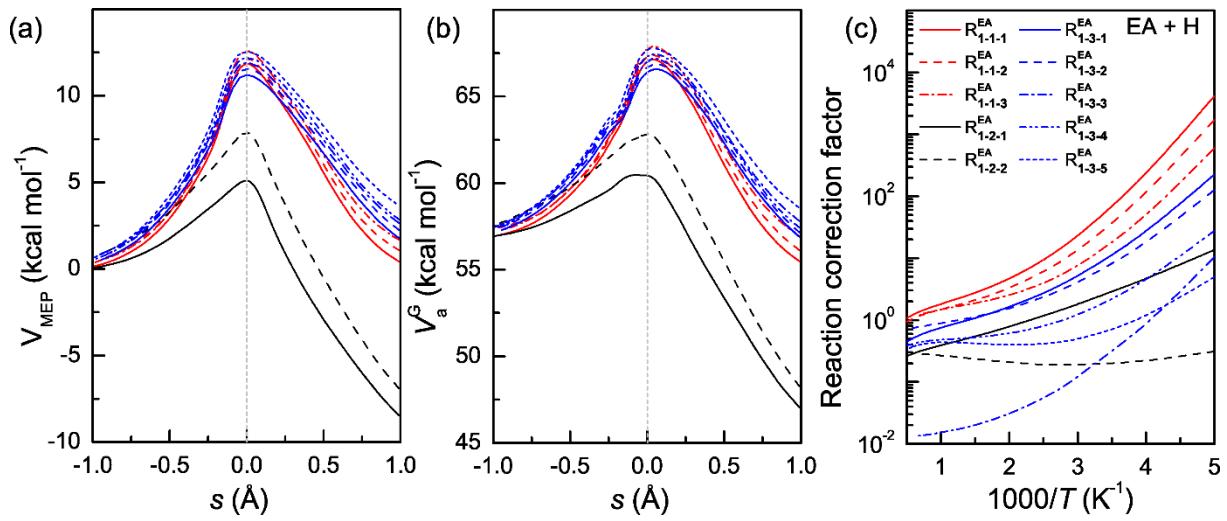


Figure S10. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from EA by H radicals. R_{1-1}^{EA} , R_{1-2}^{EA} , and R_{1-3}^{EA} have 3, 2, and 5 reaction paths, respectively.

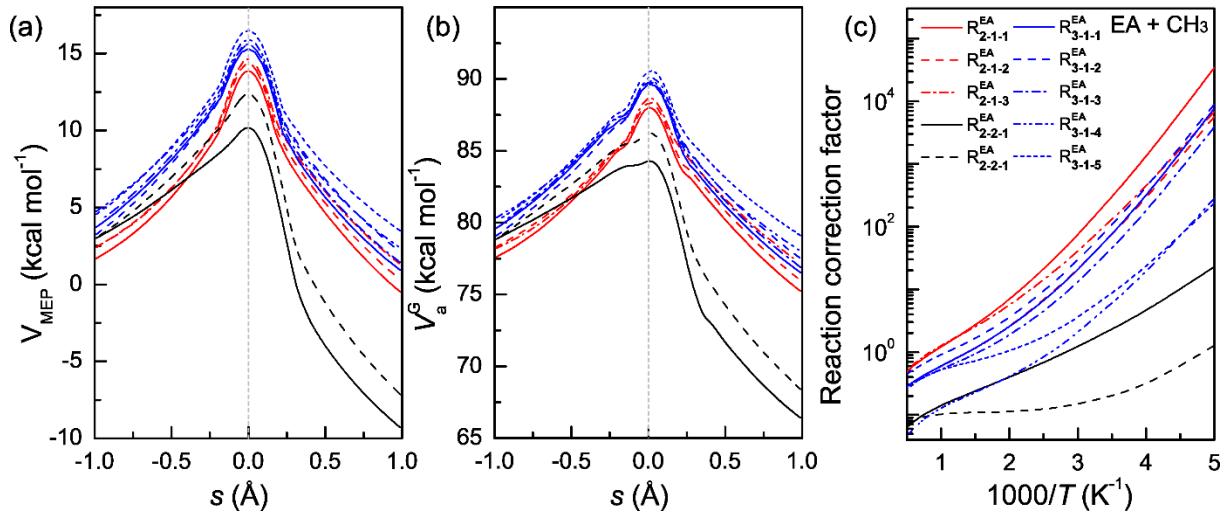


Figure S11. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from EA by CH₃ radicals. R_{2-1}^{EA} , R_{2-2}^{EA} , and R_{2-3}^{EA} have 3, 2, and 5 reaction paths, respectively.

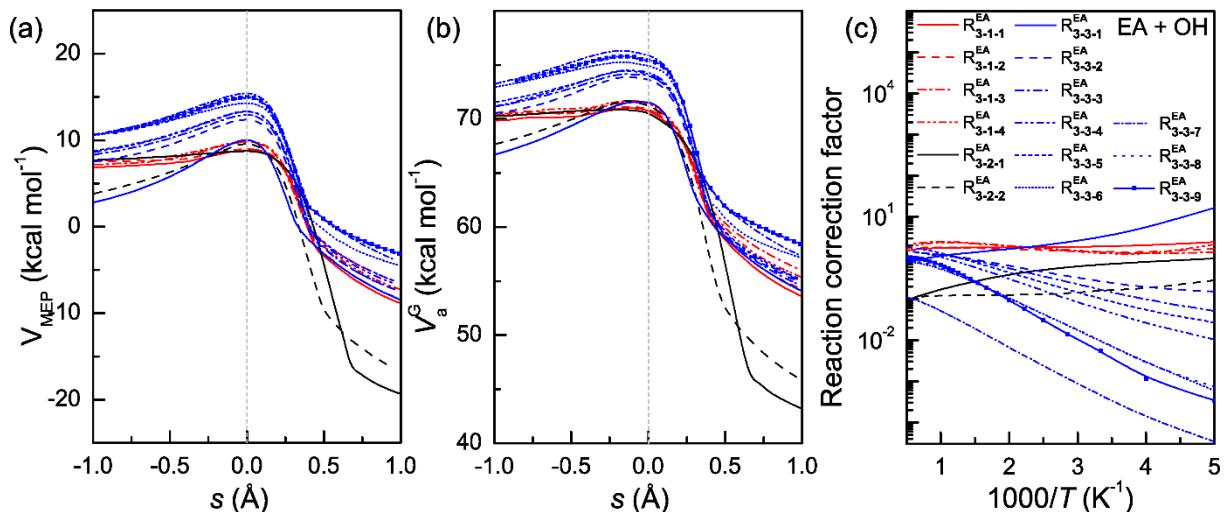


Figure S12. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from EA by OH radicals. R_{3-1}^{EA} , R_{3-2}^{EA} , and R_{3-3}^{EA} have 4, 2, and 9 reaction paths, respectively.

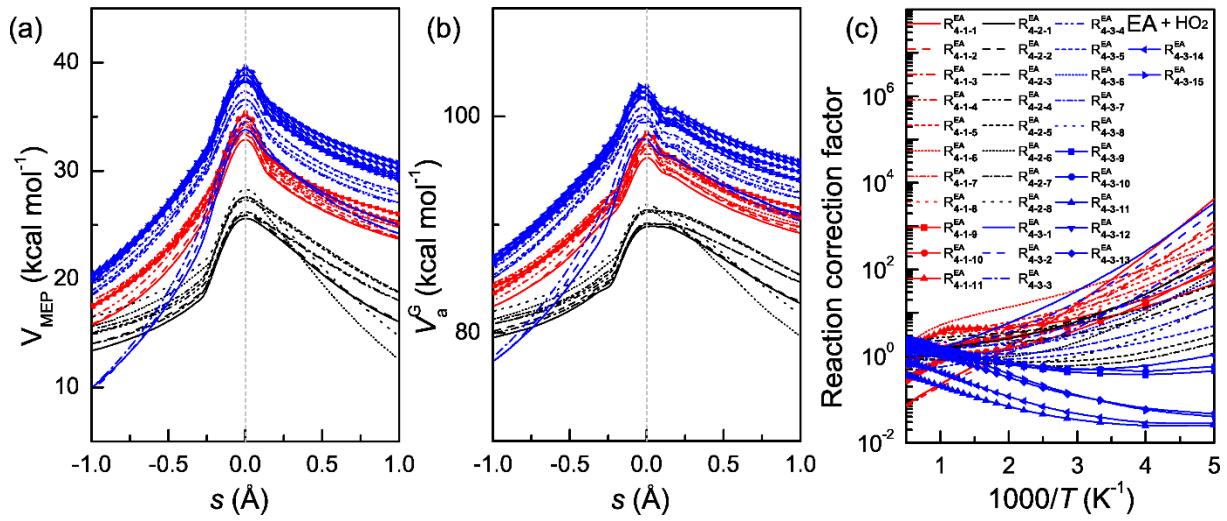


Figure S13. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from EA by HO₂ radicals. R_{4-1}^{EA} , R_{4-2}^{EA} , and R_{4-3}^{EA} have 11, 8, and 13 reaction paths, respectively.

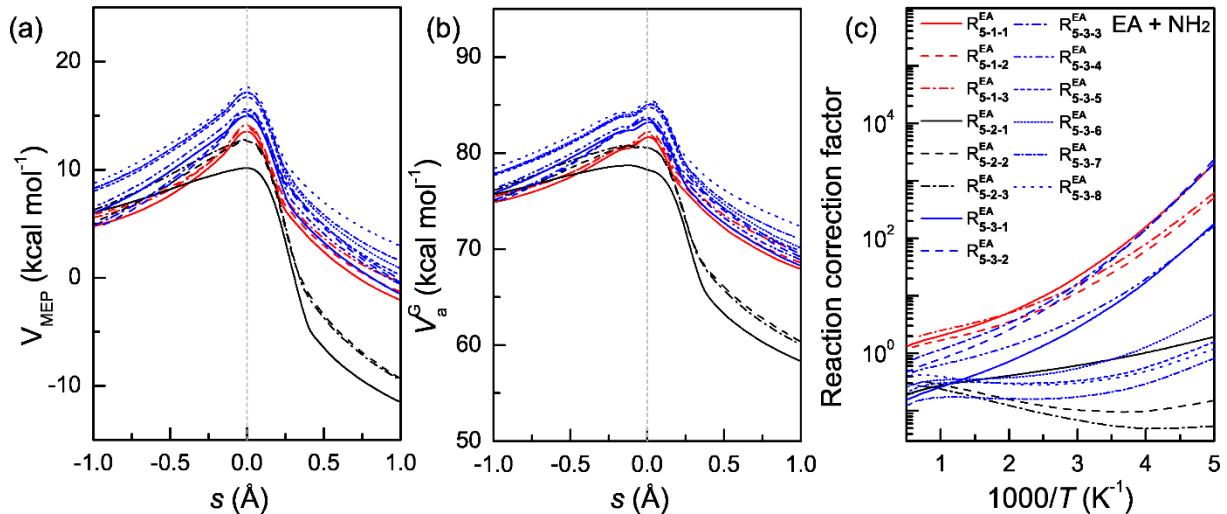


Figure S14. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from EA by NH₂ radicals. R_{5-1}^{EA} , R_{5-2}^{EA} , and R_{5-3}^{EA} have 3, 3, and 8 reaction paths, respectively.

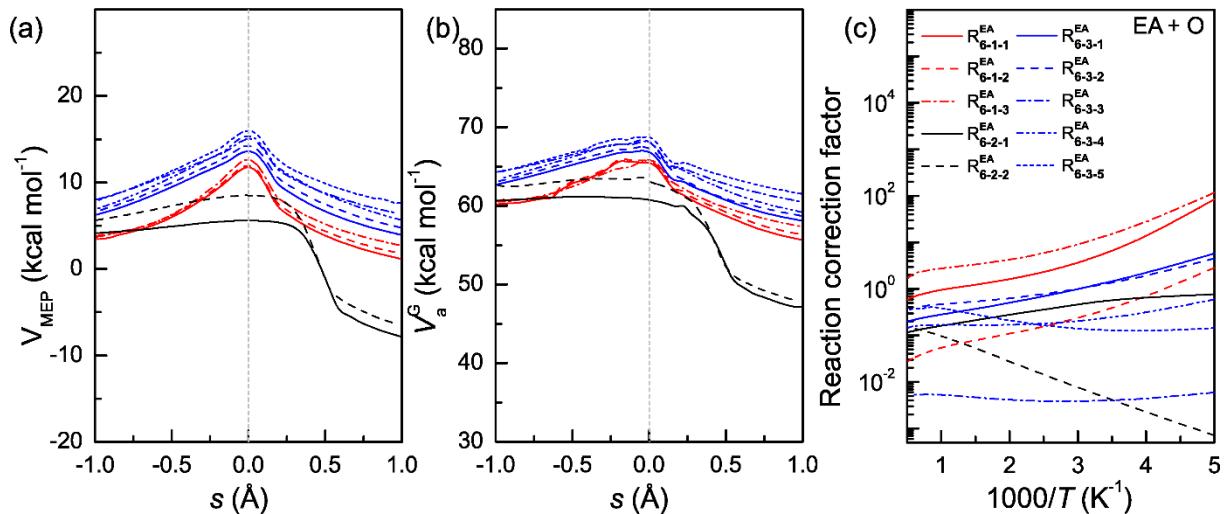


Figure S15. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from EA by O radicals. R_{6-1}^{EA} , R_{6-2}^{EA} , and R_{6-3}^{EA} have 3, 2, and 5 reaction paths, respectively.

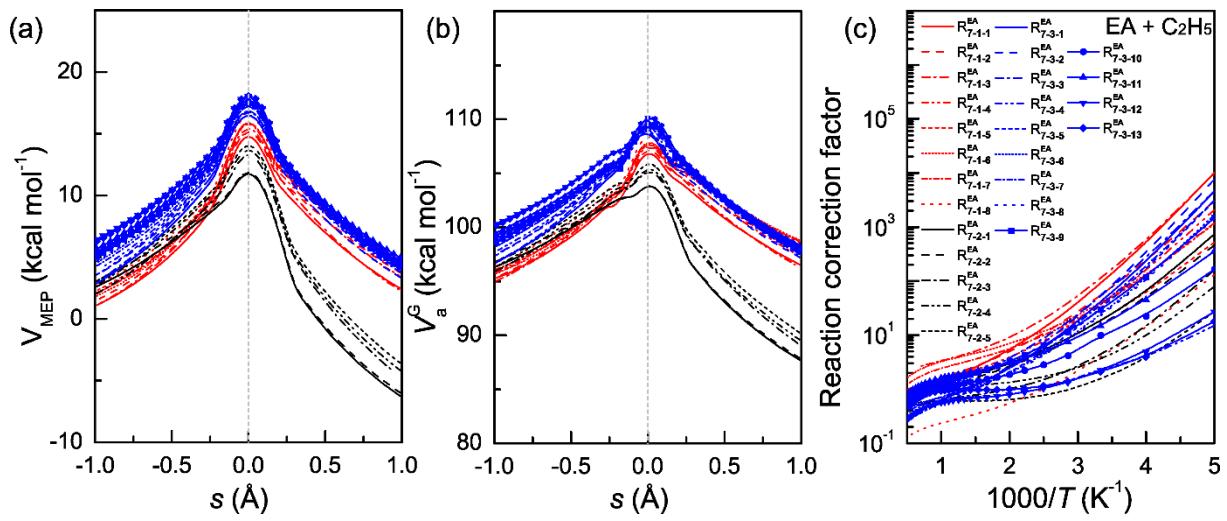


Figure S16. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from EA by C₂H₅ radicals. R_{8-1}^{EA} , R_{8-2}^{EA} , and R_{8-3}^{EA} have 8, 5, and 13 reaction paths, respectively.

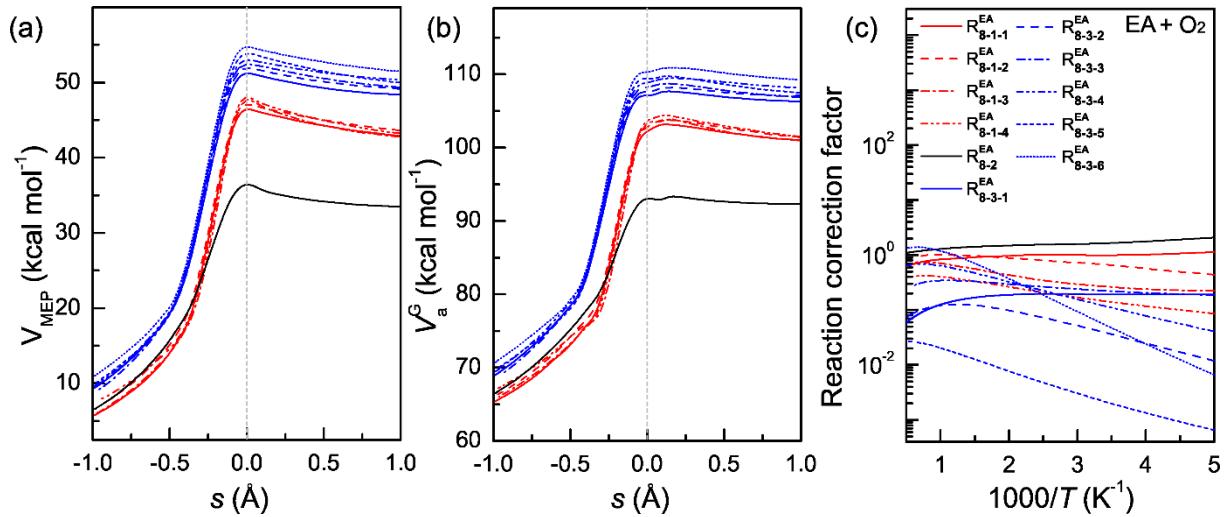


Figure S17. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from EA by C₂H₅ radicals. R_{8-1}^{EA} , R_{8-2}^{EA} , and R_{8-3}^{EA} have 4, 1, and 6 reaction paths, respectively.

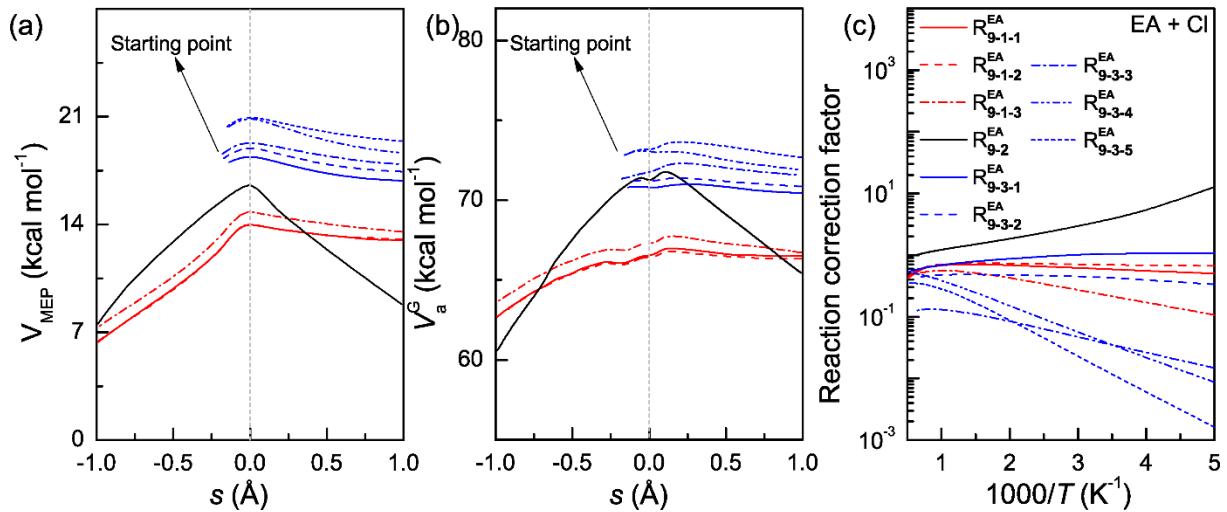


Figure S18. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from EA by Cl radicals. R_{9-1}^{EA} , R_{9-2}^{EA} , and R_{9-3}^{EA} have 3, 1, and 5 reaction paths, respectively.

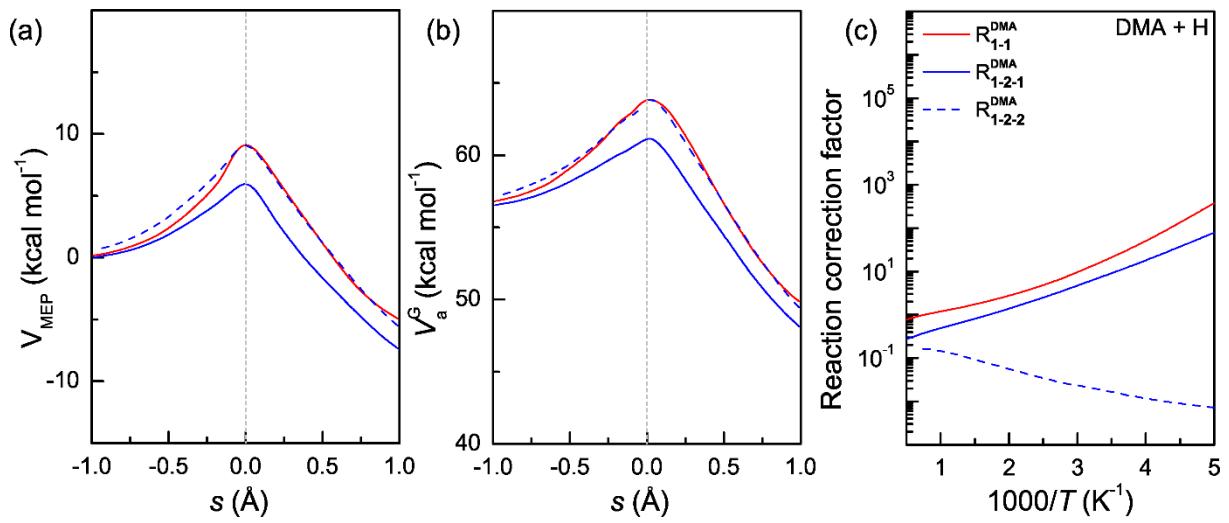


Figure S19. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from DMA by H radicals. R_{1-1}^{DMA} and R_{1-2}^{DMA} have 1 and 2 reaction paths, respectively.

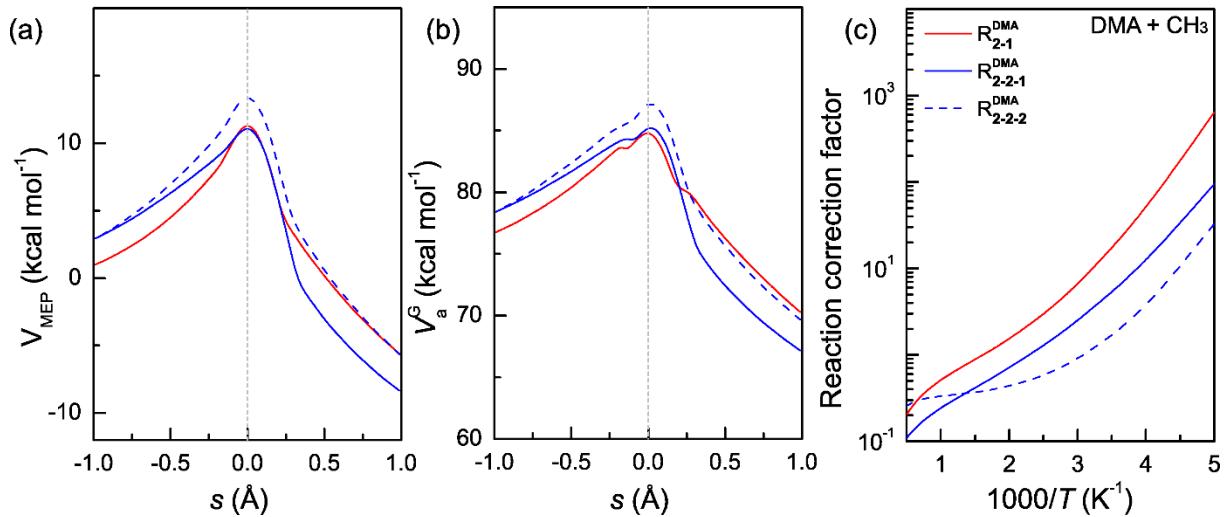


Figure S20. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from DMA by CH₃ radicals. R_{2-1}^{DMA} and R_{2-2}^{DMA} have 1 and 2 reaction paths, respectively.

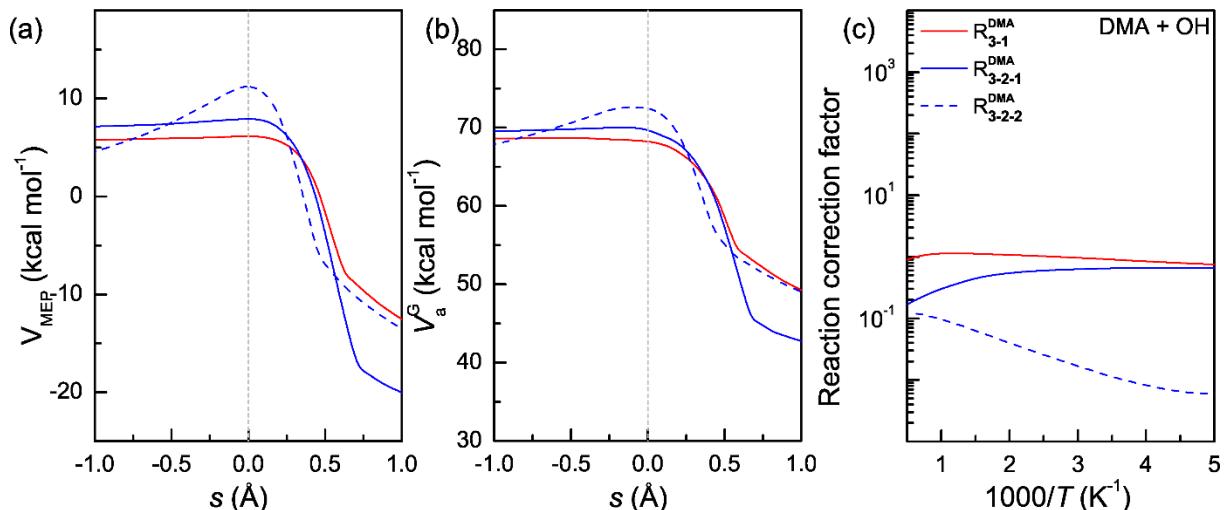


Figure S21. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from DMA by OH radicals. R_{3-1}^{DMA} and R_{3-2}^{DMA} have 1 and 2 reaction paths, respectively.

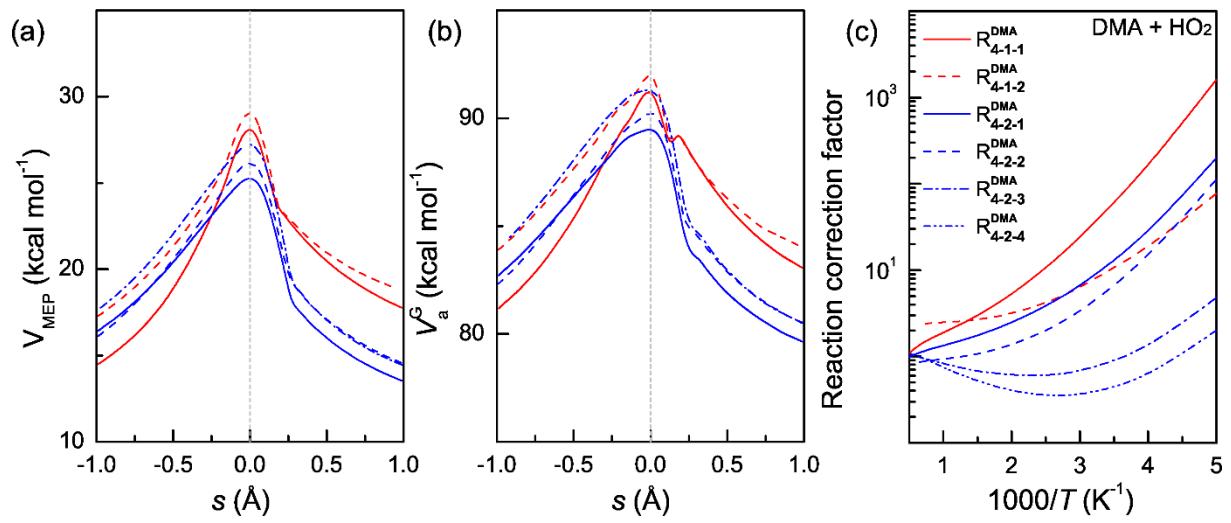


Figure S22. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from DMA by HO₂ radicals. R_{4-1}^{DMA} and R_{4-2}^{DMA} have 1 and 2 reaction paths, respectively.

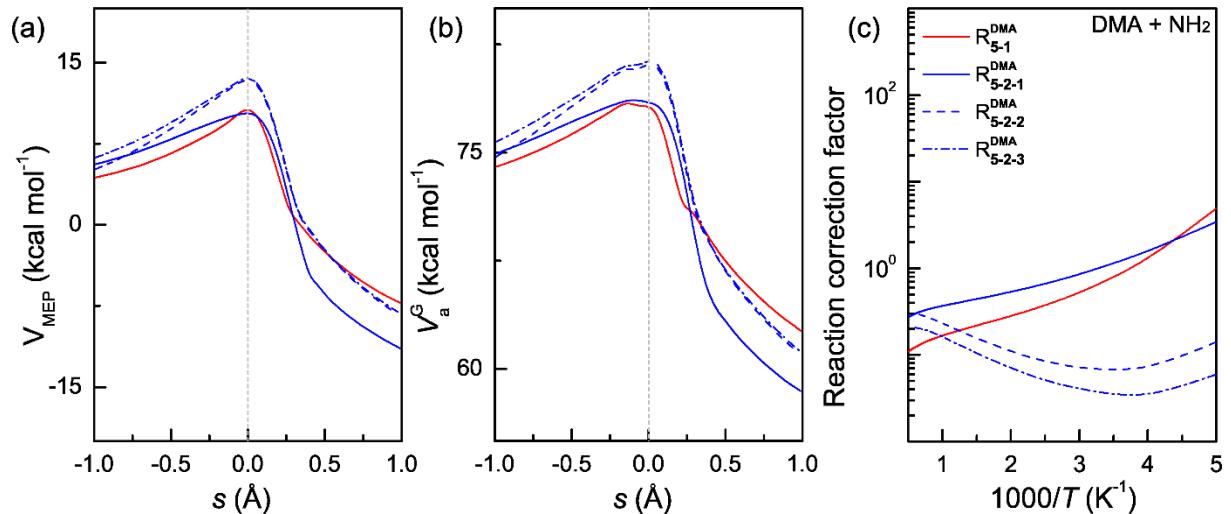


Figure S23. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from DMA by NH₂ radicals. R_{5-1}^{DMA} and R_{5-2}^{DMA} have 1 and 3 reaction paths, respectively.

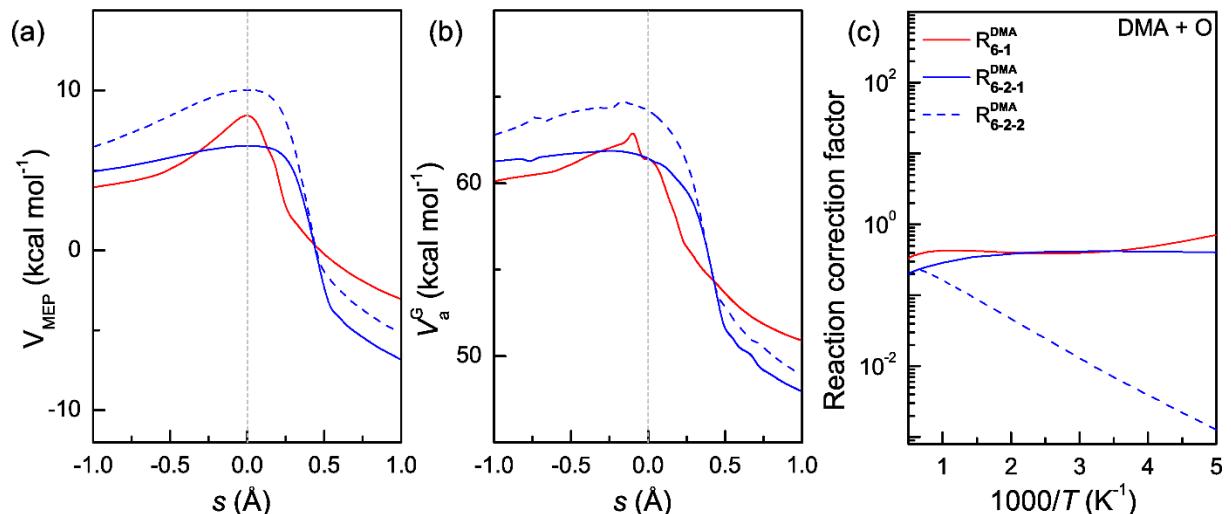


Figure S24. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from DMA by O radicals. R_{6-1}^{DMA} and R_{6-2}^{DMA} have 1 and 2 reaction paths, respectively.

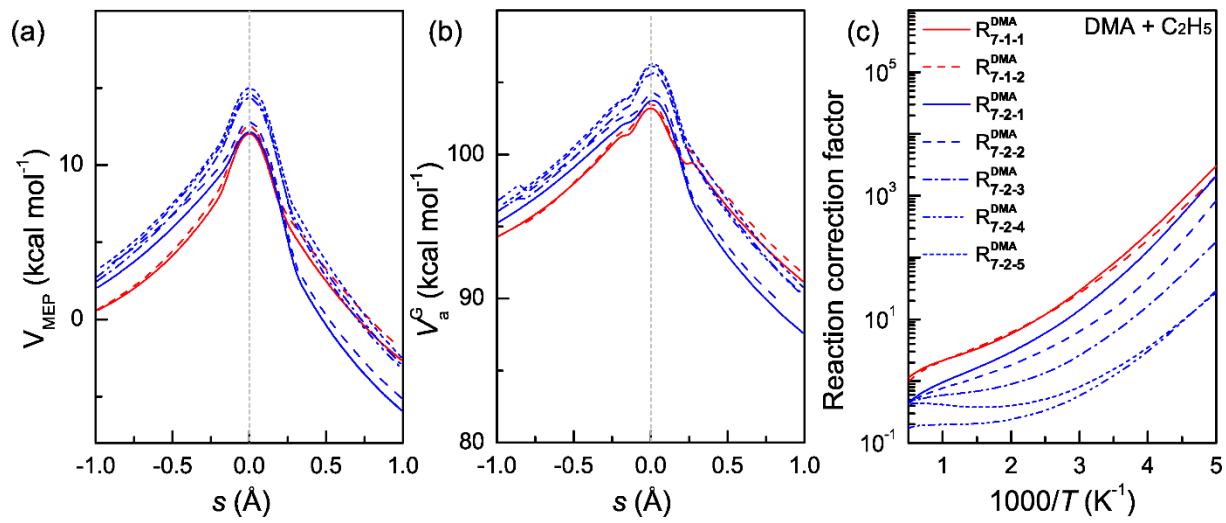


Figure S25. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from DMA by C₂H₅ radicals. R_{7-1}^{DMA} and R_{7-2}^{DMA} have 2 and 5 reaction paths, respectively.

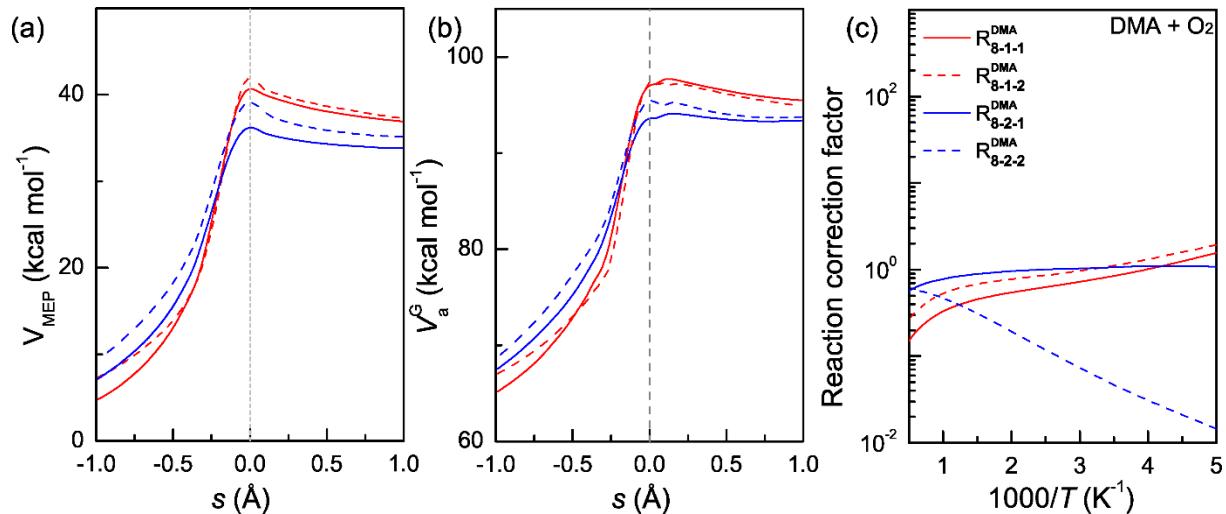


Figure S26. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from DMA by O₂ radicals. R_{8-1}^{DMA} and R_{8-2}^{DMA} both have 2 reaction paths.

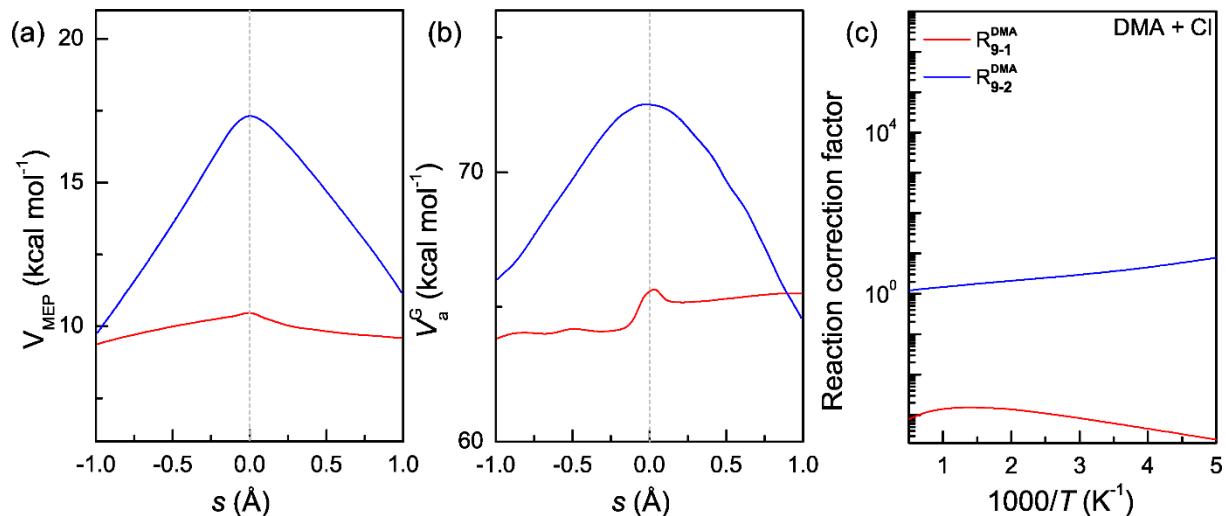


Figure S27. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from DMA by O₂ radicals. R_{9-1}^{DMA} and R_{9-2}^{DMA} both have 1 reaction path.

Table S1.

Reaction energies (ΔH), and forward and reverse barrier heights (ΔE^+ and ΔE^-) for the H-abstraction reactions from MA by H, CH₃, OH, HO₂, NH₂, O, C₂H₅, and O₂ at the N site, obtained with different methods on the basis of the M08-HX/ma-TZVP geometries. Units are in kcal mol⁻¹.

Methods		R1-1 (MA+H)			R2-1 (MA+CH ₃)			R3-1 (MA+OH)			R4-1 (MA+HO ₂)			R5-1 (MA+NH ₂)			R6-1 (MA+O)			R7-1 (MA+C ₂ H ₅)			R8-1 (MA+O ₂)		
		ΔH_{1-1}	ΔE_{1-1}^+	ΔE_{1-1}^-	ΔH_{2-1}	ΔE_{2-1}^+	ΔE_{2-1}^-	ΔH_{3-1}	ΔE_{3-1}^+	ΔE_{3-1}^-	ΔH_{4-1}	ΔE_{4-1}^+	ΔE_{4-1}^-	ΔH_{5-1}	ΔE_{5-1}^+	ΔE_{5-1}^-	ΔH_{6-1}	ΔE_{6-1}^+	ΔE_{6-1}^-	ΔH_{7-1}	ΔE_{7-1}^+	ΔE_{7-1}^-	ΔH_{8-1}	ΔE_{8-1}^+	ΔE_{8-1}^-
CCSD(T)/CBS		-1.8	11.6	13.4	-4.7	13.5	18.2	-18.0	-0.4	17.7	13.8	18.7	5.0	-7.6	7.9	15.5	0.5	7.4	6.9	-1.1	14.4	15.5	52.8	46.4	-6.3
M08-HX	ma-TZVP	0.0	12.2	12.2	-4.2	14.3	18.6	-16.2	0.2	16.5	163	20.9	4.5	-8.2	8.5	16.7	1.8	7.9	6.1	-0.3	15.6	15.9	53.7	47.0	-6.7
	MG3S	-0.1	12.2	12.3	-4.0	14.3	18.2	-16.9	-0.5	16.4	15.7	20.0	4.3	-8.2	8.3	16.5	1.3	7.3	6.1	0.0	15.4	15.4	53.1	45.7	-7.4
	jun-TZ	-0.3	12.1	12.4	-4.1	14.5	18.5	-17.3	-0.4	16.9	15.3	20.1	4.9	-8.2	8.7	16.8	0.9	7.4	6.5	-0.2	15.7	15.9	52.8	46.2	-6.6
	jul-TZ	-0.3	12.1	12.4	-4.1	14.4	18.5	-17.3	-0.4	16.8	15.2	20.1	4.9	-8.2	8.7	16.9	0.9	7.4	6.5	-0.2	15.7	15.9	52.7	46.2	-6.6
	maug-TZ	-0.2	12.2	12.4	-3.9	14.5	18.5	-17.1	-0.3	16.8	15.3	20.1	4.8	-8.2	8.7	16.9	1.2	7.6	6.4	-0.1	15.8	15.8	53.0	46.4	-6.6
	TZ	-0.5	11.6	12.1	-4.6	13.7	18.2	-16.5	-0.9	15.6	15.6	19.5	3.9	-8.0	7.8	15.8	1.8	7.3	5.5	-0.7	14.9	15.6	53.1	45.4	-7.7
M06-2X	ma-TZVP	-1.4	12.1	13.4	-5.1	12.2	17.3	-16.6	-1.1	15.5	15.4	17.6	2.3	-8.1	6.2	14.3	1.2	5.1	3.9	-1.0	13.5	14.6	54.6	45.5	-9.1
	MG3S	-1.4	11.9	13.3	-5.0	12.0	17.1	-17.1	-1.3	15.8	14.9	17.1	2.2	-7.9	6.2	14.1	0.8	4.9	4.1	-0.9	13.4	14.3	54.1	44.7	-9.4
	jun-TZ	-1.5	11.9	13.4	-5.1	12.2	17.3	-17.5	-1.4	16.1	14.4	17.0	2.6	-8.0	6.5	14.4	0.3	4.7	4.4	-1.0	13.6	14.6	53.5	44.6	-8.9
	jul-TZ	-1.5	11.9	13.4	-5.1	12.2	17.3	-17.5	-1.4	16.1	14.3	17.0	2.6	-8.0	6.5	14.4	0.3	4.7	4.3	-1.0	13.6	14.5	53.4	44.5	-8.9
	maug-TZ	-1.4	12.0	13.4	-5.0	12.3	17.2	-17.4	-1.3	16.0	14.4	17.0	2.6	-8.0	6.4	14.4	0.5	4.8	4.3	-0.9	13.6	14.5	53.6	44.7	-8.9
	TZ	-1.6	11.4	13.1	-5.4	11.5	16.9	-16.7	-1.9	14.8	14.7	16.4	1.7	-7.8	5.6	13.4	1.2	4.6	3.4	-1.3	12.9	14.2	53.8	43.7	-10.0
M05-2X	ma-TZVP	-1.0	12.9	13.9	-5.5	12.5	18.0	-17.1	-0.9	16.2	15.9	18.3	2.4	-8.6	6.9	15.6	1.2	5.3	4.1	-1.3	14.1	15.4	54.7	46.4	-8.3
	MG3S	-0.9	13.0	14.0	-5.4	12.6	18.0	-17.7	-1.0	16.7	15.3	18.0	2.7	-8.5	7.1	15.7	0.5	5.0	4.5	-1.1	14.2	15.3	53.9	45.6	-8.3
	jun-TZ	-1.1	13.0	14.0	-5.4	12.7	18.1	-18.1	-1.2	16.9	14.8	17.7	2.9	-8.5	7.4	15.8	0.1	4.8	4.7	-1.2	14.3	15.5	53.2	45.3	-7.9
	jul-TZ	-1.0	13.0	14.0	-5.4	12.7	18.0	-18.1	-1.3	16.8	14.7	17.7	3.0	-8.5	7.3	15.8	0.1	4.8	4.7	-1.1	14.3	15.4	53.1	45.2	-7.8
	maug-TZ	-1.0	13.0	14.0	-5.3	12.7	18.0	-17.9	-1.2	16.8	14.8	17.7	2.9	-8.5	7.3	15.8	0.2	4.9	4.6	-1.1	14.3	15.4	53.3	45.4	-7.9
	TZ	-1.2	12.4	13.6	-5.7	12.0	17.7	-17.3	-1.7	15.7	15.0	17.2	2.1	-8.3	6.5	14.8	0.8	4.6	3.8	-1.5	13.7	15.2	53.3	44.4	-8.9
B3LYP	ma-TZVP	-6.3	4.9	11.2	-7.0	10.6	17.6	-17.6	-7.0	10.6	15.6	14.2	-1.3	-9.0	3.4	12.5	-3.1	-2.0	1.2	-2.4	13.4	15.8	50.7	38.7	-12.0
	MG3S	-6.0	5.2	11.1	-6.8	10.8	17.6	-18.3	-7.1	11.2	15.1	14.1	-1.0	-8.9	3.7	12.6	-3.7	-2.0	1.6	-2.1	13.7	15.8	50.1	38.3	-11.8
	jun-TZ	-6.1	5.0	11.2	-6.9	10.7	17.6	-18.4	-7.1	11.4	14.8	14.1	-0.7	-8.9	3.9	12.8	-3.9	-2.0	1.9	-2.2	13.7	15.9	49.9	38.4	-11.4
	jul-TZ	-6.1	5.0	11.1	-6.9	10.7	17.6	-18.4	-7.1	11.3	14.8	14.1	-0.7	-8.9	3.9	12.8	-3.9	-2.1	1.8	-2.2	13.7	15.8	49.8	38.4	-11.4

Methods	R1-1 (MA+H)			R2-1 (MA+CH ₃)			R3-1 (MA+OH)			R4-1 (MA+HO ₂)			R5-1 (MA+NH ₂)			R6-1 (MA+O)			R7-1 (MA+C ₂ H ₅)			R8-1 (MA+O ₂)			
	ΔH_{1-1}	ΔE_{1-1}^+	ΔE_{1-1}^-	ΔH_{2-1}	ΔE_{2-1}^+	ΔE_{2-1}^-	ΔH_{3-1}	ΔE_{3-1}^+	ΔE_{3-1}^-	ΔH_{4-1}	ΔE_{4-1}^+	ΔE_{4-1}^-	ΔH_{5-1}	ΔE_{5-1}^+	ΔE_{5-1}^-	ΔH_{6-1}	ΔE_{6-1}^+	ΔE_{6-1}^-	ΔH_{7-1}	ΔE_{7-1}^+	ΔE_{7-1}^-	ΔH_{8-1}	ΔE_{8-1}^+	ΔE_{8-1}^-	
^o B97X-D	maug-TZ	-6.1	5.0	11.1	-6.8	10.7	17.6	-18.3	-7.1	11.2	14.9	14.1	-0.8	-8.9	3.8	12.7	-3.7	-2.0	1.7	-2.2	13.6	15.8	50.0	38.5	-11.5
	TZ	-6.3	4.3	10.6	-7.4	9.7	17.1	-17.5	-7.9	9.6	15.4	13.2	-2.2	-8.7	2.6	11.3	-2.8	-2.3	0.5	-2.7	12.7	15.4	50.3	37.1	-13.1
	ma-TZVP	-2.1	9.9	12.0	-6.5	10.5	17.0	-16.9	-3.9	13.1	17.0	17.8	0.8	-8.7	4.9	13.7	-0.3	2.8	3.0	-2.2	12.0	14.2	53.6	43.5	-10.1
	MG3S	-1.8	10.1	11.9	-6.2	10.6	16.8	-17.9	-4.4	13.5	16.3	17.1	0.8	-8.6	5.0	13.6	-1.0	2.2	3.2	-1.8	12.1	13.9	52.8	42.4	-10.4
	jun-TZ	-2.1	9.9	11.9	-6.4	10.5	16.9	-17.9	-4.1	13.7	16.3	17.4	1.2	-8.6	5.2	13.8	-1.1	2.4	3.5	-2.0	12.1	14.2	52.7	42.9	-9.8
	jul-TZ	-2.1	9.9	11.9	-6.4	10.5	16.9	-17.8	-4.2	13.7	16.2	17.4	1.2	-8.6	5.2	13.8	-1.1	2.4	3.5	-2.0	12.1	14.1	52.7	42.8	-9.8
MN15-L	maug-TZ	-2.0	9.9	11.9	-6.4	10.5	16.9	-17.7	-4.1	13.6	16.3	17.4	1.1	-8.6	5.1	13.8	-0.9	2.5	3.4	-2.0	12.1	14.1	52.9	42.9	-9.9
	TZ	-2.2	9.3	11.5	-6.9	9.7	16.6	-17.0	-4.7	12.3	16.7	16.8	0.1	-8.4	4.3	12.7	-0.2	2.3	2.5	-2.5	11.4	13.8	53.0	41.9	-11.1
	ma-TZVP	-6.7	7.5	14.2	-6.9	13.0	19.9	-17.6	-2.9	14.7	13.0	14.4	1.4	-8.4	6.1	14.5	-1.0	3.4	4.4	-2.5	13.6	16.1	51.0	39.8	-11.2
	MG3S	-6.1	8.1	14.2	-6.3	13.5	19.8	-18.6	-3.1	15.5	12.7	14.5	1.7	-8.6	6.5	15.1	-1.7	3.3	5.0	-1.9	14.0	15.9	50.7	39.6	-11.1
	jun-TZ	-6.0	7.9	13.9	-6.1	13.4	19.5	-18.5	-3.2	15.3	12.5	14.3	1.8	-8.3	6.4	14.8	-1.5	3.3	4.9	-1.9	13.9	15.8	50.7	39.7	-11.0
	jul-TZ	-6.0	7.9	13.9	-6.2	13.3	19.5	-18.6	-3.3	15.2	12.6	14.2	1.7	-8.4	6.3	14.7	-1.7	3.1	4.7	-1.9	13.7	15.6	50.6	39.5	-11.1
BH&HLYP	maug-TZ	-5.9	8.0	13.9	-6.4	13.4	19.5	-18.4	-3.2	15.2	12.6	14.3	1.7	-8.4	6.3	14.7	-1.3	3.4	4.8	-1.8	13.9	15.7	50.8	39.8	-11.1
	TZ	-6.1	7.3	13.4	-6.7	12.4	19.1	-17.6	-3.8	13.8	13.1	13.6	0.5	-8.2	5.2	13.4	-0.5	3.2	3.7	-2.4	12.9	15.4	51.2	38.7	-12.5
	ma-TZVP	-6.5	9.1	15.6	-7.1	15.7	22.8	-14.6	3.4	18.0	15.1	22.1	7.0	-7.9	11.6	19.5	1.0	9.3	8.3	-3.2	17.9	21.1	49.1	45.8	-3.3
	MG3S	-6.2	9.3	15.5	-6.8	15.9	22.7	-15.3	3.2	18.5	14.6	21.8	7.2	-7.8	11.8	19.6	0.4	9.2	8.7	-2.9	18.1	21.0	48.6	45.3	-3.3
	jun-TZ	-6.3	9.2	15.5	-6.9	15.8	22.7	-15.4	3.3	18.7	14.4	21.9	7.5	-7.8	12.0	19.8	0.2	9.1	8.9	-3.0	18.1	21.0	48.4	45.5	-2.9
	jul-TZ	-6.3	9.2	15.5	-6.9	15.8	22.7	-15.4	3.3	18.7	14.4	21.9	7.5	-7.8	11.9	19.7	0.2	9.1	8.9	-2.9	18.1	21.0	48.6	45.4	-2.9
PW6B95	maug-TZ	-6.2	9.2	15.4	-6.9	15.8	22.7	-15.3	3.3	18.6	14.5	21.9	7.4	-7.8	11.9	19.7	0.4	9.2	8.8	-2.9	18.0	21.0	48.5	45.5	-3.0
	TZ	-6.5	8.6	15.1	-7.4	15.0	22.4	-14.6	2.6	17.2	14.7	21.4	6.6	-7.6	11.0	18.7	1.1	9.0	8.0	-3.4	17.3	20.7	48.5	44.5	-4.0
	ma-TZVP	-3.3	8.3	11.6	-7.4	10.2	17.6	-17.3	-5.4	11.9	16.7	16.7	0.0	-9.1	4.1	13.3	-0.4	1.6	2.0	-2.7	12.6	15.2	52.9	42.0	-11.0
	MG3S	-3.0	8.5	11.5	-7.1	10.4	17.5	-18.0	-5.6	12.4	16.2	16.4	0.2	-9.0	4.4	13.4	-1.0	1.4	2.4	-2.3	12.7	15.1	52.4	41.3	-11.1
	jun-TZ	-3.1	8.4	11.5	-7.3	10.4	17.6	-18.1	-5.5	12.6	16.0	16.5	0.5	-9.0	4.6	13.5	-1.2	1.5	2.7	-2.5	12.8	15.3	42.1	41.6	-10.5
	jul-TZ	-3.1	8.4	11.5	-7.2	10.3	17.6	-18.1	-5.5	12.5	16.0	16.5	0.5	-9.0	4.6	13.5	-1.2	1.5	2.6	-2.5	12.8	15.2	52.0	41.5	-10.5
MP	maug-TZ	-3.1	8.4	11.5	-7.2	10.4	17.6	-18.0	-5.5	12.5	16.1	16.5	0.4	-9.0	4.5	13.5	-1.0	1.5	2.5	-2.5	12.8	15.2	52.2	41.6	-10.6
	TZ	-3.3	7.7	11.0	-7.8	9.4	17.2	-17.2	-6.3	10.9	16.5	15.7	-0.8	-8.8	3.3	12.1	-0.1	1.2	1.4	-3.0	1.8	14.8	52.5	40.4	-12.1

Methods	R1-1 (MA+H)			R2-1 (MA+CH ₃)			R3-1 (MA+OH)			R4-1 (MA+HO ₂)			R5-1 (MA+NH ₂)			R6-1 (MA+O)			R7-1 (MA+C ₂ H ₅)			R8-1 (MA+O ₂)			
	ΔH_{1-1}	ΔE_{1-1}^+	ΔE_{1-1}^-	ΔH_{2-1}	ΔE_{2-1}^+	ΔE_{2-1}^-	ΔH_{3-1}	ΔE_{3-1}^+	ΔE_{3-1}^-	ΔH_{4-1}	ΔE_{4-1}^+	ΔE_{4-1}^-	ΔH_{5-1}	ΔE_{5-1}^+	ΔE_{5-1}^-	ΔH_{6-1}	ΔE_{6-1}^+	ΔE_{6-1}^-	ΔH_{7-1}	ΔE_{7-1}^+	ΔE_{7-1}^-	ΔH_{8-1}	ΔE_{8-1}^+	ΔE_{8-1}^-	
jun-TZ	-2.5	10.4	12.8	-6.1	13.7	19.8	-16.4	1.0	17.4	15.4	20.1	4.7	-8.0	8.9	17.0	0.1	6.8	6.7	-1.9	46.0	17.9	50.2	44.6	-5.6	
jul-TZ	-2.5	10.3	12.8	-6.1	13.7	19.8	16.3	1.0	17.4	15.4	20.1	4.7	-8.0	8.9	17.0	0.1	6.7	6.6	-1.9	16.0	17.9	50.1	44.5	-5.6	
maug-TZ	-2.4	10.4	12.8	-6.1	13.7	19.7	-16.2	1.1	17.3	15.4	20.0	4.6	-8.3	8.9	17.1	0.3	6.9	6.6	-1.9	16.0	17.9	50.3	44.6	-5.7	
TZ	-2.6	9.8	12.5	-6.5	13.0	19.5	-15.6	0.5	16.1	15.7	19.5	3.9	-7.9	8.1	16.0	0.9	6.7	5.8	-2.3	15.3	17.7	50.4	43.7	-6.7	
SOGGA11-X	ma-TZVP	-2.0	10.5	12.5	-8.2	11.4	19.6	-16.1	-1.1	15.0	16.7	19.9	3.2	-8.6	7.0	15.7	-0.4	4.6	5.0	-3.8	13.7	17.6	52.6	45.1	-7.4
	MG3S	-1.4	10.8	12.3	-7.6	11.5	19.1	-17.1	-1.8	15.3	16.1	19.1	3.1	-8.7	6.9	15.6	-0.9	4.2	5.1	-3.2	13.7	16.9	51.8	44.0	-7.8
	jun-TZ	-1.8	10.5	12.4	-7.8	11.6	19.4	-16.9	-1.3	15.5	16.0	19.5	3.5	-8.4	7.3	15.8	-0.8	4.6	5.4	-3.4	13.9	17.3	51.9	44.6	-7.3
	jul-TZ	-1.8	10.5	12.3	-7.8	11.6	19.4	-16.9	-1.4	15.5	16.0	19.4	3.4	-8.5	7.3	15.7	-0.8	4.6	5.4	-3.4	13.9	17.3	51.8	44.5	-7.3
	maug-TZ	-1.8	10.6	12.3	-7.7	11.7	19.4	-16.7	-1.3	15.4	16.1	19.5	3.4	-8.7	7.3	15.9	-0.6	4.7	5.3	-3.4	13.9	17.3	52.0	44.7	-7.4
	TZ	-2.0	10.0	12.0	-8.3	10.8	19.1	-16.1	-1.9	14.2	16.4	18.9	2.5	-8.3	6.4	14.7	0.0	4.5	4.5	-3.9	13.1	17.0	52.1	43.7	-8.4

Table S2.

Reaction energies (ΔH), and forward and reverse barrier heights (ΔE^+ and ΔE^-) for the H-abstraction reactions from MA by H, CH₃, OH, HO₂, NH₂, O, C₂H₅, and O₂ at the C site, obtained with different methods on the basis of the M08-HX/ma-TZVP geometries. Units are in kcal mol⁻¹.

Methods		R1-2 (MA+H)			R2-2 (MA+CH ₃)			R3-2 (MA+OH)			R4-2 (MA+HO ₂)			R5-2 (MA+NH ₂)			R6-2 (MA+O)			R7-2 (MA+C ₂ H ₅)			R8-2 (MA+O ₂)		
		ΔH_{1-2}	ΔE_{1-2}^+	ΔE_{1-2}^-	ΔH_{2-2}	ΔE_{2-2}^+	ΔE_{2-2}^-	ΔH_{3-2}	ΔE_{3-2}^+	ΔE_{3-2}^-	ΔH_{4-2}	ΔE_{4-2}^+	ΔE_{4-2}^-	ΔH_{5-2}	ΔE_{5-2}^+	ΔE_{5-2}^-	ΔH_{6-2}	ΔE_{6-2}^+	ΔE_{6-2}^-	ΔH_{7-2}	ΔE_{7-2}^+	ΔE_{7-2}^-	ΔH_{8-2}	ΔE_{8-2}^+	ΔE_{8-2}^-
CCSD(T)/CBS		-9.2	6.8	16.1	-12.1	12.0	24.1	-25.5	1.2	26.7	6.3	14.1	7.7	-15.1	6.6	21.6	-6.9	4.6	11.5	-8.6	13.3	21.8	45.3	39.4	-5.9
M08-HX	ma-TZVP	-9.1	6.4	15.5	-13.3	11.4	24.7	-25.3	1.5	26.7	7.3	13.3	6.0	-17.3	5.7	23.0	-7.2	2.2	9.4	-9.4	13.0	22.4	44.6	38.0	-6.7
	MG3S	-9.4	6.6	16.0	-13.2	11.3	24.5	-26.2	0.9	27.1	6.4	12.2	5.8	-17.5	5.5	22.9	-8.0	1.6	9.6	-9.3	12.8	22.1	43.8	36.6	-7.2
	jun-TZ	-9.3	6.6	15.8	-13.0	11.6	24.6	-26.2	1.2	27.4	6.3	12.6	6.3	-17.2	5.8	23.0	-8.1	1.8	9.8	-9.1	13.2	22.3	43.9	37.3	-6.6
	jul-TZ	-9.2	6.6	15.8	-13.1	11.6	24.6	-26.2	1.1	27.3	6.3	12.6	6.3	-17.2	5.8	22.9	-8.0	1.7	9.8	-9.1	13.2	22.3	43.8	37.3	-6.5
	maug-TZ	-9.3	6.6	15.9	-13.0	11.6	24.7	-26.2	1.1	27.3	6.3	12.6	6.3	-17.3	5.7	23.0	-7.9	1.8	9.7	-9.1	13.3	22.4	43.9	37.4	-6.5
	TZ	-9.0	6.6	15.6	-13.0	11.4	24.5	-25.0	0.6	25.6	7.1	12.3	5.1	-16.5	5.6	22.1	-6.7	2.1	8.8	-9.1	12.7	21.8	44.6	36.9	-7.7
M06-2X	ma-TZVP	-9.2	7.1	16.2	-12.8	10.7	23.6	-24.3	0.5	24.9	7.6	11.8	4.3	-15.9	5.0	20.9	-6.6	1.3	7.9	-8.8	12.3	21.1	46.8	37.5	-9.4
	MG3S	-9.2	7.2	16.5	-12.9	10.6	23.5	-24.9	0.5	25.4	7.0	11.4	4.3	-15.8	5.0	20.8	-7.1	1.1	8.1	-8.8	12.1	20.9	46.3	36.7	-9.6
	jun-TZ	-9.1	7.2	16.3	-12.7	10.8	23.5	-25.1	0.4	25.5	6.8	11.3	4.6	-15.5	5.2	20.7	-7.3	0.9	8.2	-8.6	12.4	21.0	45.9	36.7	-9.2
	jul-TZ	-9.1	7.2	16.3	-12.7	10.8	23.5	-25.1	0.4	25.5	6.7	11.3	4.6	-15.6	5.2	20.7	-7.3	0.9	8.2	-8.6	12.4	21.0	45.8	36.6	-9.1
	maug-TZ	-9.2	7.2	16.4	-12.7	10.8	23.6	-25.1	0.3	25.5	6.6	11.3	4.6	-15.7	5.1	20.8	-7.3	0.9	8.2	-8.7	12.4	21.1	45.9	36.7	-9.1
	TZ	-9.0	7.1	16.1	-12.8	10.6	23.4	-24.1	0.0	24.0	7.3	11.0	3.6	-15.1	4.9	20.1	-6.2	1.2	7.4	-8.7	11.9	20.6	46.4	36.2	-10.2
M05-2X	ma-TZVP	-9.3	7.9	17.1	-13.7	10.7	24.4	-25.4	0.5	25.9	7.7	11.9	4.3	-16.9	5.0	22.0	-7.0	1.2	8.3	-9.6	12.6	22.2	46.4	37.6	-8.9
	MG3S	-9.3	8.1	17.5	-13.8	10.6	24.4	-26.1	0.5	26.6	6.9	11.5	4.6	-16.9	5.1	22.0	-7.9	0.9	8.8	-9.5	12.6	22.2	45.5	36.7	-8.8
	jun-TZ	-9.2	8.1	17.3	-13.5	10.9	24.4	-26.2	0.4	26.6	6.6	11.4	4.8	-16.6	5.3	21.9	-8.1	0.8	8.9	-9.3	12.9	22.2	45.0	36.6	-8.4
	jul-TZ	-9.2	8.1	17.3	-13.5	10.9	24.4	-26.2	0.3	26.6	6.6	11.3	4.8	-16.7	5.3	21.9	-8.1	0.8	8.8	-9.3	12.9	22.2	44.9	36.5	-8.4
	maug-TZ	-9.3	8.1	17.4	-13.6	10.9	24.4	-26.2	0.3	26.5	6.5	11.3	4.8	-16.8	5.2	22.0	-8.0	0.8	8.8	-9.4	12.9	22.3	45.0	36.6	-8.4
	TZ	-9.2	8.0	17.1	-13.7	10.7	24.3	-25.3	0.0	25.3	7.1	11.0	4.0	-16.3	5.1	21.4	-7.2	1.0	8.2	-9.5	12.4	21.9	45.3	36.1	-9.3
B3LYP	ma-TZVP	-13.7	0.7	14.3	-14.4	9.0	23.3	-24.9	-3.0	21.9	8.2	10.0	1.7	-16.4	2.1	18.5	-10.5	-5.4	5.1	-9.8	12.4	22.2	43.4	33.1	-10.3
	MG3S	-13.6	0.9	14.5	-14.4	9.0	23.4	-25.9	-3.1	22.8	7.5	9.7	2.2	-16.5	2.2	18.7	-11.3	-5.6	5.7	-9.7	12.5	22.2	42.6	32.6	-10.0
	jun-TZ	-13.5	0.8	14.3	-14.3	9.0	23.3	-25.9	-3.0	22.9	7.4	9.9	2.5	-16.3	2.4	18.7	-11.3	-5.5	5.9	-9.6	12.6	22.2	42.4	32.8	-9.7
	jul-TZ	-13.5	0.7	14.3	-14.3	9.0	23.3	-25.8	-3.0	22.9	7.4	9.9	2.5	-16.3	2.4	18.6	-11.3	-5.5	5.8	-9.6	12.6	22.2	42.3	32.7	-9.6

Methods	R1-2 (MA+H)			R2-2 (MA+CH ₃)			R3-2 (MA+OH)			R4-2 (MA+HO ₂)			R5-2 (MA+NH ₂)			R6-2 (MA+O)			R7-2 (MA+C ₂ H ₅)			R8-2 (MA+O ₂)			
	ΔH_{1-2}	ΔE_{1-2}^+	ΔE_{1-2}^-	ΔH_{2-2}	ΔE_{2-2}^+	ΔE_{2-2}^-	ΔH_{3-2}	ΔE_{3-2}^+	ΔE_{3-2}^-	ΔH_{4-2}	ΔE_{4-2}^+	ΔE_{4-2}^-	ΔH_{5-2}	ΔE_{5-2}^+	ΔE_{5-2}^-	ΔH_{6-2}	ΔE_{6-2}^+	ΔE_{6-2}^-	ΔH_{7-2}	ΔE_{7-2}^+	ΔE_{7-2}^-	ΔH_{8-2}	ΔE_{8-2}^+	ΔE_{8-2}^-	
maug-TZ	-13.6	0.7	14.3	-14.3	9.0	23..3	-25.8	-3.1	22.8	7.4	9.8	2.4	-16.4	2.3	18.7	-11.2	-5.5	5.7	-9.7	12.5	22.2	42.5	32.7	-9.7	
TZ	-13.4	0.5	13.9	-14.5	8.6	23.1	-24.6	-3.6	21.0	8.3	9.3	1.0	-15.8	1.9	17.6	-9.9	-5.1	4.8	-9.8	11.8	21.6	43.2	31.9	-11.2	
^o B97X-D	ma-TZVP	-9.7	5.2	14.9	-14.1	8.6	22.6	-24.5	-1.5	23.0	9.5	12.2	2.8	-16.3	3.3	19.6	-7.8	-1.0	6.8	-9.7	10.5	20.2	46.0	36.0	-10.0
	MG3S	-9.7	5.4	15.1	-14.0	8.6	22.6	-25.7	-2.0	23.7	8.5	11.4	3.0	-16.5	3.3	19.7	-8.8	-1.6	7.2	-9.6	10.5	20.1	44.9	34.9	-10.0
	jun-TZ	-9.6	5.3	14.9	-14.0	8.6	22.6	-25.4	-1.6	23.8	8.7	12.0	3.2	-16.1	3.5	19.6	-8.6	-1.2	7.4	-9.6	10.6	20.2	45.2	35.5	-9.7
	jul-TZ	-9.6	5.3	14.9	-14.0	8.6	22.6	-25.4	-1.6	23.8	8.7	11.9	3.3	-16.2	3.5	19.6	-8.6	-1.2	7.4	-9.6	10.6	20.2	45.1	35.4	-9.6
	maug-TZ	-9.7	5.2	14.9	-14.0	8.6	22.6	-25.4	-1.6	23.7	8.6	11.9	3.2	-16.3	3.4	19.7	-8.5	-1.2	7.4	-9.6	10.6	20.2	45.2	35.5	-9.7
	TZ	-9.5	5.1	14.7	-14.2	8.3	22.5	-24.3	-2.0	22.3	9.4	11.6	2.2	-15.7	3.2	18.9	-7.5	-0.9	6.6	-9.8	10.0	19.7	45.7	34.9	-10.8
MN15-L	ma-TZVP	-11.2	3.7	14.9	-11.3	12.7	24.0	-22.1	1.2	23.3	8.5	10.1	1.5	-12.8	5.8	18.7	-5.4	-0.2	5.2	-7.0	13.7	20.7	46.6	35.4	-11.2
	MG3S	-11.2	3.8	15.1	-11.4	12.5	24.0	-23.7	0.8	24.5	7.6	9.5	1.9	-13.7	5.7	19.4	-6.8	-0.9	5.9	-7.1	13.5	20.6	45.6	24.5	-11.0
	jun-TZ	-11.0	3.6	14.7	-11.2	12.5	23.7	-23.6	0.9	24.5	7.4	9.6	2.1	-13.4	5.7	19.1	-6.6	-0.7	6.0	-7.0	13.5	20.4	45.6	34.7	-10.8
	jul-TZ	-11.1	3.6	14.7	-11.3	12.4	23.7	-23.7	0.8	24.4	7.5	9.5	2.0	-13.4	5.6	19.1	-6.7	-0.8	5.9	-7.0	13.3	20.3	45.6	34.7	-10.9
	maug-TZ	-11.0	3.6	14.7	-11.2	12.5	23.7	-23.5	0.9	24.4	7.4	9.5	2.1	-13.5	5.6	19.1	-6.5	-0.7	5.8	-7.0	13.4	20.4	45.7	34.8	-10.9
	TZ	-10.5	3.5	14.0	-11.2	12.1	23.3	-22.1	0.5	22.6	8.7	9.3	0.6	-12.7	5.2	17.8	-5.0	-0.2	4.8	-6.9	12.7	19.6	46.8	34.3	-12.4
BH&HLYP	ma-TZVP	-12.0	4.5	16.5	-12.6	13.9	26.5	-20.1	3.8	23.9	9.5	18.2	8.7	-13.5	9.1	22.6	-4.6	4.5	9.1	-8.7	16.7	25.4	43.6	40.4	-3.2
	MG3S	-12.0	4.6	16.6	-12.7	13.9	26.5	-21.1	3.7	24.8	8.8	17.9	9.1	-13.7	9.1	22.8	-5.4	4.3	9.7	-8.7	16.8	25.5	42.8	39.8	-3.0
	jun-TZ	-11.9	4.5	16.5	-12.6	13.9	26.5	-21.1	3.9	25.0	8.8	18.1	9.3	-13.5	9.3	22.7	-5.5	4.4	9.9	-8.6	16.8	25.4	42.7	40.0	-2.7
	jul-TZ	-11.9	4.5	16.5	-12.6	13.9	26.5	-21.1	3.9	24.9	8.7	18.1	9.3	-13.5	9.3	22.7	-5.5	4.4	9.8	-8.6	16.8	25.4	42.6	40.0	-2.6
	maug-TZ	-12.0	4.5	16.5	-12.6	13.8	26.4	-21.1	3.8	24.8	8.7	18.0	9.2	-13.6	9.2	22.7	-5.4	4.4	9.8	-8.7	16.8	25.4	42.7	40.0	-2.7
	TZ	-11.8	4.4	16.2	-12.7	13.6	26.3	-20.0	3.3	23.2	9.4	17.6	8.2	-13.0	8.9	21.9	-4.3	4.6	8.9	-8.7	16.2	25.0	43.2	39.4	-3.8
PW6B95	ma-TZVP	-10.9	3.5	14.4	-15.0	8.4	23.4	-24.9	-2.5	22.4	9.1	11.4	2.3	-16.7	2.5	19.2	-8.0	-2.8	5.3	-10.3	11.4	21.6	45.3	35.2	-10.1
	MG3S	-10.8	3.7	14.5	-15.0	8.4	23.4	-25.8	-2.7	23.2	8.4	10.9	2.5	-16.9	2.5	19.4	-8.8	-3.0	5.8	-10.2	11.4	21.6	44.5	34.5	-10.1
	jun-TZ	-10.8	3.6	14.4	-14.9	8.4	23.4	-25.7	-2.4	23.3	8.4	11.2	2.9	-16.6	2.7	19.3	-8.8	-2.9	5.9	-10.1	11.5	21.6	44.4	34.8	-9.6
	jul-TZ	-10.8	3.6	14.4	-14.9	8.4	23.4	-25.7	-2.5	23.3	8.3	11.2	2.9	-16.6	2.7	19.3	-8.8	-2.9	5.9	-10.1	11.5	21.6	44.3	34.8	-9.6
	maug-TZ	-10.8	3.6	14.4	-14.9	8.4	23.7	-25.7	-2.5	23.2	8.3	11.2	2.8	-16.7	2.6	19.3	-8.7	-2.9	5.8	-10.2	11.4	21.6	44.5	34.8	-9.6
	TZ	-10.6	3.4	14.1	-15.1	8.1	23.1	-24.5	-3.0	21.5	9.2	10.8	1.5	-16.1	2.2	18.3	-7.4	-2.5	4.9	-10.3	10.7	21.0	45.2	34.1	-11.0
MP	ma-TZVP	-9.2	4.9	14.1	-12.8	11.4	24.2	-22.1	2.1	24.2	9.5	15.8	6.4	-14.7	6.5	21.2	-5.7	2.9	8.6	-8.7	14.2	22.9	44.4	38.5	-5.8
	MG3S	-9.1	5.1	14.2	-12.9	11.3	24.2	-23.1	1.8	24.9	8.8	15.2	6.5	-14.9	6.4	21.3	-6.5	2.5	9.0	-8.7	14.1	22.8	43.7	37.7	-6.0

Methods	R1-2 (MA+H)			R2-2 (MA+CH ₃)			R3-2 (MA+OH)			R4-2 (MA+HO ₂)			R5-2 (MA+NH ₂)			R6-2 (MA+O)			R7-2 (MA+C ₂ H ₅)			R8-2 (MA+O ₂)			
	ΔH_{1-2}	ΔE_{1-2}^+	ΔE_{1-2}^-	ΔH_{2-2}	ΔE_{2-2}^+	ΔE_{2-2}^-	ΔH_{3-2}	ΔE_{3-2}^+	ΔE_{3-2}^-	ΔH_{4-2}	ΔE_{4-2}^+	ΔE_{4-2}^-	ΔH_{5-2}	ΔE_{5-2}^+	ΔE_{5-2}^-	ΔH_{6-2}	ΔE_{6-2}^+	ΔE_{6-2}^-	ΔH_{7-2}	ΔE_{7-2}^+	ΔE_{7-2}^-	ΔH_{8-2}	ΔE_{8-2}^+	ΔE_{8-2}^-	
SOGGA11-X	jun-TZ	-9.1	4.9	14.1	-12.8	11.3	24.2	-23.0	2.1	25.1	8.7	15.6	6.9	-14.7	6.6	21.3	-6.6	2.7	9.2	-8.6	14.2	22.8	43.5	38.0	-5.5
	jul-TZ	-9.1	4.9	14.1	-12.8	11.4	24.2	-23.0	2.1	25.1	8.7	15.6	6.9	-14.7	6.6	21.3	-6.6	2.7	9.2	-8.6	14.2	22.8	43.4	38.0	-5.5
	maug-TZ	-9.2	4.9	14.1	-12.8	11.3	24.1	-23.0	2.0	25.0	8.7	15.5	6.8	-15.0	6.5	21.5	-6.5	2.7	9.1	-8.6	14.2	22.8	43.6	38.0	-5.5
	TZ	-9.0	4.9	13.9	-12.9	11.1	24.0	-22.0	1.6	23.6	9.3	15.2	5.9	-14.3	6.3	20.6	-5.5	2.9	8.3	-8.7	13.7	22.4	44.0	37.5	-6.5
	ma-TZVP	-7.6	5.7	13.3	-13.8	10.2	24.0	-21.7	0.7	22.4	11.1	15.3	4.2	-14.2	5.4	19.6	-6.0	0.6	6.6	-9.4	13.1	22.5	47.0	39.1	-7.9
	MG3S	-7.6	5.9	13.5	-13.7	10.0	23.7	-23.3	0.1	23.3	10.0	14.3	4.3	-14.8	5.0	19.8	-7.0	0.0	7.0	-9.3	12.8	22.1	45.7	37.7	-8.1
SOGGA11-X	jun-TZ	-7.5	5.8	13.3	-13.5	10.3	23.8	-22.6	0.7	23.3	10.3	14.8	4.5	-14.2	5.5	19.7	-6.5	0.6	7.1	-9.2	13.1	22.3	46.2	38.5	-7.7
	jul-TZ	-7.6	5.7	13.3	-13.5	10.3	23.8	-22.6	0.6	23.2	10.2	14.8	4.6	-14.2	5.5	19.7	-6.6	0.6	7.1	-9.2	13.1	22.3	46.1	38.4	-7.7
	maug-TZ	-7.6	5.7	13.3	-13.5	10.3	23.8	-22.5	0.6	23.1	10.3	14.8	4.5	-14.5	5.4	19.9	-6.4	0.6	7.1	-9.2	13.1	22.3	46.2	38.5	-7.7
	TZ	-7.4	5.6	13.0	-13.7	10.0	23.7	-21.5	0.2	21.7	11.0	14.5	3.5	-13.7	5.2	18.8	-5.4	0.9	6.2	-9.3	12.6	21.9	46.7	38.0	-8.7

Table S3.

Optimized geometries and frequencies of the involved species for the H-abstraction systems MA + H/CH₃/OH /HO₂/NH₂/O/C₂H₅/O₂/Cl using the M08-HX/ma-TZVP method.

Geometry			Frequency	Geometry			Frequency
Reactants							
MA							
N	-0.746306	-0.000001	-0.118898				
H	-1.152529	-0.814739	0.322787	291.16	827.36	967.80	
C	0.703922	-0.000010	0.017732	1092.44	1166.39	1338.14	
H	1.115090	-0.879849	-0.486977	1445.90	1487.78	1506.81	
H	1.115096	0.879937	-0.486817	1662.01	2991.73	3079.76	
H	1.075497	-0.000034	1.054202	3118.31	3551.48	3636.31	
H	-1.152543	0.814754	0.322705				
DMA-1				DMA-2			
N	-0.798527	0.152991	-0.000080		N	0.651714	0.000000
C	0.625379	-0.013124	-0.000067	207.03	950.52	1000.81	0.090095
H	1.127113	0.958334	-0.001270	1078.09	1328.05	1387.67	H
H	0.962984	-0.583050	0.881415	1468.28	1473.71	2971.47	C
H	0.963636	-0.586044	-0.879338	3022.81	3112.99	3436.05	H
H	-1.216320	-0.781427	0.000159		H	-1.242490	-0.932548
					H	-1.242491	0.932547
					H	1.132498	0.835429
					H		-0.203944
R1 MA + H							
H				H ₂			
H	0.000000	0.000000	0.000000		H	0.000000	0.000000
					H	0.000000	-0.372855
TS1-1				TS1-2			
N	0.579122	-0.382501	-0.150693		N	0.837761	0.038963
H	1.343416	0.612719	-0.111816	-1549.89	H	1.124554	0.545399
C	-0.768830	0.131633	0.021723	182.27	372.12	704.54	C
H	-1.031588	0.761547	-0.832800	976.00	988.00	1067.65	H
H	-1.462106	-0.719778	0.034569	1137.83	1279.70	1387.98	H
H	-0.928370	0.703570	0.945709	1417.74	1465.35	1491.65	H
H	0.862811	-0.856183	0.709275	1763.02	3007.00	3070.18	H
H	1.774961	1.385832	0.179580	3117.66	3472.59		H
					H	1.124462	0.545721
					H	-1.944028	1.541248
					H		-0.000031
R2 MA + CH ₃							
CH ₃				CH ₄			
C	0.000000	0.000000	0.000023		C	0.000000	0.000000
H	0.000000	1.080901	-0.000047	536.57	1405.71	1405.71	H
H	-0.936088	-0.540451	-0.000047	3143.03	3323.03	3323.25	H
H	0.936088	-0.540451	-0.000047		H	-0.630332	-0.630332
					H	-0.630332	0.630332
					H	-0.630332	-0.630332
					H	0.630332	-0.630332
TS2-1				TS2-2			
N	0.580652	0.758532	-0.149507		N	-1.545939	-0.426494
H	-0.604411	0.387296	-0.186452	-1944.36	H	-1.470346	-1.006628
C	1.362925	-0.453817	0.020767	69.98	139.51	163.96	C
H	1.268898	-1.077180	-0.873969	387.35	550.00	566.52	H
H	2.422385	-0.185041	0.125430	805.16	1000.20	1069.31	H
H	1.087428	-1.060238	0.896950	1089.40	1141.55	1301.54	H
H	0.587876	1.277642	0.729674	1359.23	1414.69	1421.04	H
C	-1.805663	-0.175675	0.014886	1431.26	1469.79	1491.05	H
H	-2.465628	0.654488	0.261327	1508.40	2990.94	3059.52	C
H	-1.678107	-0.891449	0.825722	3072.77	3107.04	3213.77	H
H	-2.026577	-0.638285	-0.946048	3216.29	3491.67		H
					H	2.041862	-0.756491
					H	2.563786	0.731732
					H		0.007913
R3 MA + OH							
OH				H ₂ O			
O	0.000000	0.000000	0.107952		H	0.765650	-0.459860
H	0.000000	0.000000	-0.863615	3794.45	O	0.000000	0.114973
					H	-0.765650	-0.459927
RC3							

H	-1.272976	0.809258	-1.318571	595.04	744.89	975.63	H	1.106485	0.592903	1.391684	730.86	946.52	1029.38	
H	-1.757445	1.410710	0.322874	1071.39	1160.89	1223.06	H	2.270548	1.290418	0.115247	1274.98	1321.76	1380.19	
H	0.022352	0.852710	0.031019	1291.53	1351.06	1403.85	H	-0.511888	0.938352	-0.302584	1475.13	1515.70	1650.93	
H	-1.550093	-0.814872	1.135202	1460.39	1515.47	1664.08	H	1.819346	-0.646921	-1.219077	3156.34	3271.08	3583.34	
O	1.268919	0.679973	0.294015	3072.09	3161.13	3577.38	O	-1.412744	0.607531	-0.479039	3618.66	3699.36	3866.53	
O	1.455913	-0.635345	-0.095724		3675.26	3832.59	O	-1.434900	-0.569018	0.314592				
H	1.882530	-0.556446	-0.956159				H	-2.052838	-0.331094	1.012586				
R5 MA + NH₂														
NH ₂														
N	0.000000	0.000000	0.140072				H	-0.914521	0.236266	0.254512				
H	0.000000	0.808739	-0.490253	1526.30	3399.02	3492.45	N	-0.000022	0.000019	-0.109056	1029.36	1665.46	1665.87	
H	0.000000	-0.808739	-0.490253				H	0.661993	0.673826	0.254461	3523.40	3658.98	3659.64	
RC5														
N	-0.888196	0.749710	0.010703											
H	-1.072117	1.142023	-0.904554	37.11	85.44	116.05								
C	-1.124808	-0.692272	0.013688	174.05	271.33	341.46								
H	-0.408719	-1.175587	-0.658140	408.12	870.62	972.03								
H	-0.935065	-1.085849	1.017161	1082.43	1176.08	1336.98								
H	-2.140362	-0.990196	-0.283756	1449.77	1487.48	1505.63								
H	-1.500501	1.220622	0.664778	1547.79	1655.39	3014.13								
N	2.124478	-0.132291	-0.084360	3095.84	3129.41	3363.03								
H	1.282078	0.422550	0.125970	3484.39	3543.09	3625.81								
H	2.869560	0.298133	0.472007											
TS5-1														
N	0.485232	0.740557	-0.123901				N	0.969561	0.786101	0.000404				
H	-0.634057	0.379882	-0.357215	-2009.74			H	-1.261250	0.547934	-0.002186	92.71	124.87	127.84	
C	1.336886	-0.422288	0.023491	94.63	111.13	162.93	C	1.299953	-0.609885	0.000273	156.14	162.73	285.79	
H	1.213249	-1.074081	-0.846638	435.39	631.87	717.18	H	0.387205	-1.211975	0.008213	351.96	957.13	1006.03	
H	2.387043	-0.101237	0.049719	816.03	1002.88	1089.56	H	1.901527	-0.872493	-0.885641	1059.66	1081.36	1327.23	
H	1.153513	-1.014026	0.933158	1091.97	1311.21	1418.42	H	1.917811	-0.870886	0.875207	1386.07	1473.43	1475.02	
H	0.462800	1.266692	0.747736	1421.73	1468.26	1489.56	H	1.840487	1.322349	-0.001785	1656.58	1678.49	2968.62	
N	-1.750412	-0.210720	-0.110519	1557.47	1618.20	2990.93	N	-2.025372	-0.122896	-0.000004	3021.11	3120.47	3461.80	
H	-2.236743	0.408218	0.539749	3056.10	3111.85	3467.28	H	-2.598982	0.049941	-0.815685	3489.58	3618.03	3651.64	
H	-1.510868	-1.040577	0.433484	3526.81	3563.55		H	-2.595844	0.052005	0.817437				
TS5-2														
N	-1.523679	-0.408341	0.000010				N	1.055675	-0.683935	-0.138198				
H	-1.460457	-0.991634	-0.822923	-1224.40			H	1.536501	-1.335830	0.460099	79.31	117.04	146.57	
C	-0.579694	0.654188	-0.000013	114.62	128.60	200.10	C	1.322326	0.653369	0.072633	183.92	230.58	301.66	
H	-0.672236	1.273268	-0.896827	409.30	553.41	720.49	H	2.324752	0.925731	0.378759	513.97	631.08	741.60	
H	-0.672270	1.273343	0.896745	786.02	833.93	997.06	H	0.755716	1.361265	-0.521362	954.53	1067.56	1266.31	
H	0.569955	0.229964	0.000030	1170.41	1227.59	1348.60	H	-1.452378	0.669005	0.611824	1334.33	1476.22	1652.78	
H	-1.460454	-0.991599	0.822967	1363.15	1462.95	1471.02	H	0.076455	-0.906153	-0.277438	1661.80	1665.46	3163.20	
N	1.900196	-0.319609	0.000029	1546.24	1662.87	3064.44	N	-1.931995	0.008683	0.008206	3273.92	3506.81	3540.09	
H	2.268929	0.188452	-0.808431	3140.78	3435.78	3533.52	H	-2.657292	-0.441396	0.552626	3632.65	3654.00	3681.03	
H	2.269076	0.188730	0.808247	3568.72	3660.12		H	-2.383472	0.533927	-0.730361				
R6 MA + O														
O														
O	0.000000	0.000000	0.000000											
RC6														
N	-0.422899	0.728693	-0.010153											
H	-0.662110	1.288464	0.796010	72.66	88.05	195.03								
C	-1.061264	-0.574775	-0.008308	305.46	758.55	962.36								
H	-0.699374	-1.151768	-0.864954	1099.38	1154.15	1326.26								
H	-0.766944	-1.116414	0.895908	1445.80	1483.22	1502.01								
H	-2.160065	-0.546073	-0.051045	1648.46	3002.83	3086.78								
H	-0.601182	1.255928	-0.853178	3123.96	3571.47	3667.92								
O	1.778708	-0.153855	0.053222											
TS6-1														
PC6-1														
N	0.362755	0.711932	-0.134568				N	0.517970	0.541472	0.000173	27.11	54.83	202.92	
H	-0.771329	0.342157	-0.322892	-1887.59			H	-1.385289	0.089589	0.000165	284.79	519.20	610.74	

C	1.254213	-0.413978	0.018602	700.91	965.92	1051.41	C	1.623786	-0.367943	-0.000010	959.11	1008.35	1094.25							
H	1.201372	-1.052804	-0.866222	1070.83	1253.09	1309.17	H	1.273910	-1.402985	0.001369	1328.18	1388.76	1463.74							
H	2.282877	-0.041319	0.116843	1410.00	1436.16	1462.14	H	2.264965	-0.208106	-0.881613	1475.09	2978.44	3031.14							
H	1.036780	-1.017233	0.911161	1490.21	3006.20	3068.91	H	2.266982	-0.206327	0.879782	3127.09	3469.18	3580.90							
H	0.356756	1.264617	0.722786	3131.61 3512.43			H	0.878224	1.497911	-0.000518										
O	-1.771377	-0.249385	0.033586				O	-2.333412	-0.169091	-0.000042										
TS6-2							PC6-2													
N	-1.441074	-0.395577	-0.000039	-344.76			N	-0.882143	0.712090	0.000013										
H	-1.431509	-0.972209	0.828480	113.96	210.15	437.36	H	-0.523617	1.138340	-0.839945	89.53	108.45	187.73							
C	-0.469575	0.635269	-0.000127	706.50	962.50	1091.29	C	-1.024712	-0.660650	-0.000002	460.39	517.67	618.46							
H	-0.545569	1.258418	-0.895859	1166.30	1278.26	1321.52	H	-1.330184	-1.121130	0.931733	708.47	726.34	952.44							
H	-0.545946	1.258893	0.895248	1406.19	1453.98	1597.14	H	-1.330290	-1.121098	-0.931718	1263.87	1321.22	1477.10							
H	0.640221	0.242320	0.000255	1660.30	3067.78	3141.45	H	1.196244	-0.761518	-0.000019	1657.65	3166.81	3281.56							
H	-1.431262	-0.972606	-0.828278	3579.93 3675.84			H	-0.523479	1.138308	0.839929	3602.31	3639.57	3709.05							
O	2.027379	-0.232174	0.000149				O	1.854325	-0.036704	-0.000008										
R7 MA + C ₂ H ₅																				
C ₂ H ₅							C ₂ H ₆													
C	-0.792028	0.000000	-0.018049				H	-1.160561	-0.816689	-0.610583										
C	0.691536	0.000000	-0.001477	112.32	475.18	807.41	C	-0.762086	0.000003	-0.000057	303.24	815.46	818.67							
H	-1.347917	0.927558	0.039950	975.23	1083.42	1189.82	C	0.762028	0.000011	0.000009	1021.22	1212.55	1213.45							
H	-1.347918	-0.927557	0.039950	1393.05	1458.89	1472.77	H	-1.160660	0.937270	-0.401599	1394.99	1414.41	1490.75							
H	1.103840	-0.887124	-0.494557	1476.07	2978.26	3063.54	H	-1.160752	-0.120592	1.012442	1491.09	1492.57	1493.09							
H	1.103840	0.887099	-0.494603	3110.96	3172.42	3274.56	H	1.160744	-0.935037	0.406637	3039.59	3041.37	3103.24							
H	1.091109	0.000027	1.026416				H	1.160698	0.115435	-1.013066	3106.21	3125.87	3128.89							
TS7-1							TS7-2													
N	-1.299369	-0.669965	-0.375677	-1916.87			N	1.781337	-0.640136	-0.145929										
H	-0.045264	-0.782363	-0.181865	50.53	130.51	152.36	H	1.686714	-0.824887	-1.135032	46.34	100.48	144.87							
C	-1.639236	0.637194	0.158695	218.98	238.81	464.47	C	1.325412	0.657032	0.227048	211.83	285.57	423.19							
H	-1.237029	1.416908	-0.496165	558.13	750.57	836.42	H	1.440209	0.834909	1.299433	500.64	617.36	761.12							
H	-2.731620	0.751525	0.174903	912.44	997.80	1055.98	H	1.817388	1.443592	-0.350817	831.98	871.33	989.32							
H	-1.274911	0.822464	1.182106	1070.84	1088.66	1165.71	H	0.054132	0.820189	-0.001893	1054.71	1131.23	1156.43							
H	-1.634022	-1.381104	0.276704	1219.32	1306.16	1375.11	H	1.334120	-1.381362	0.376033	1163.28	1216.38	1344.11							
C	1.209838	-0.730788	0.217773	1391.56	1419.84	1453.51	C	-1.354434	0.740373	-0.216093	1389.57	1435.40	1443.76							
C	1.704585	0.647071	-0.137768	1467.86	1476.18	1480.54	C	-1.681556	-0.683443	0.142240	1454.15	1465.87	1474.62							
H	1.186612	-0.950195	1.287220	1491.35	1495.62	2979.46	H	-1.751740	1.500166	0.458116	1479.86	1657.27	3005.72							
H	1.663122	-1.545044	-0.351397	3019.48	3053.12	3080.26	H	-1.483197	1.008240	-1.265483	3065.45	3066.44	3090.57							
H	1.570383	0.854307	-1.204906	3090.25	3103.69	3110.91	H	-1.194114	-1.389054	-0.540724	3096.88	3150.12	3181.17							
H	1.173065	1.421834	0.425485	3167.15 3481.73			H	-1.349420	-0.922696	1.160501										
H	2.774128	0.760555	0.085449				H	-2.759988	-0.891911	0.102198										
R8 MA + O ₂																				
O ₂																				
O	0.000000	0.000000	0.592038	1774.51																
TS8-1							PC8-1													
N	-1.099620	-0.781057	-0.003279	-1924.53			N	1.133104	0.735755	-0.000206										
H	0.264934	-0.789913	-0.183146	96.39	172.91	198.20	H	-0.665850	0.822567	-0.000199	25.09	75.84	108.95							
C	-1.520035	0.581426	-0.073877	299.49	505.97	665.26	C	1.777215	-0.542810	0.000137	191.59	274.17	313.48							
H	-1.635768	0.891686	-1.117332	989.47	996.57	1110.63	H	1.032701	-1.340890	0.000032	697.96	964.72	1008.43							
H	-2.436055	0.787128	0.491234	1198.96	1340.38	1364.51	H	2.431608	-0.648841	-0.879979	1100.29	1288.45	1325.80							
H	-0.708309	1.216888	0.346982	1396.03	1446.03	1479.97	H	2.430924	-0.648570	0.880814	1385.21	1467.38	1470.10							
H	-1.333957	-1.169950	0.910851	1651.68	2882.04	3054.52	H	1.837901	1.474569	-0.000420	1612.13	2986.05	3038.69							
O	1.345888	-0.552650	-0.135164	3116.50 3497.26			O	-1.619318	0.553972	0.000280	3151.50	3351.08	3484.05							
O	1.487450	0.683026	0.137367				O	-1.588470	-0.748005	-0.000234										
TS8-2							PC8-2													
N	1.430844	-0.676408	-0.000099	-1819.03			N	1.489186	-0.651605	-0.158612										
H	1.155934	-1.172536	0.834642	22.78	159.27	251.96	H	0.799700	-1.299450	0.193723										
C	1.222834	0.691519	0.000206	339.05	556.98	558.90	C	1.374400	0.655898	0.249772										
H	1.532589	1.192303	0.917268	683.91	958.73	1081.66	H	1.087424	0.809781	1.285652										
H	1.533775	1.192915	-0.916123	1168.16	1256.99	1333.93	H	2.046325	1.373882	-0.206473										
H	-0.224131	0.838513	-0.000472	1381.34	1469.88	1583.36	H	-0.519951	0.845763	-0.285448										

H	1.156853	-1.172047	-0.835439	1661.54 3095.52 3196.03	H	1.764455	-0.824058	-1.111647	
O	-1.354370	0.614885	-0.000250	3591.57 3692.32	O	-1.467647	0.546177	-0.337100	
O	-1.459122	-0.651560	0.000198		O	-1.513509	-0.581187	0.304081	
R9 MA + Cl									
Cl					HCl				
Cl	-1.717103	-0.078219	0.000074		H	0.000000	0.000000	-1.204502	
RC9					Cl	0.000000	0.000000	0.070853	2999.39
N	1.284752	0.680101	0.037704						
H	0.957687	1.129904	-0.800264	149.76 160.02 358.31					
C	1.342783	-0.767032	0.014807	441.48 717.41 949.71					
H	1.910652	-1.076458	-0.856217	1092.92 1157.75 1320.00					
H	1.868310	-1.106101	0.901273	1474.18 1516.04 1521.43					
H	0.350091	-1.218082	-0.017029	1652.03 3086.47 3173.15					
H	0.916671	1.100810	0.873870	3208.25 3606.73 3709.81					
Cl	3.509631	1.451821	0.107810						
TS9-1					PC9-1				
N	-1.065101	0.700042	-0.124106		N	1.242333	0.684404	-0.000840	
H	0.195978	0.456382	-0.309373	-1109.37	H	-0.480374	0.395802	-0.000567	55.66 87.13 147.40
C	-1.885485	-0.466784	0.017531	112.89 120.49 355.26	C	2.051634	-0.494677	-0.000164	295.23 692.04 726.56
H	-1.632212	-1.187069	-0.752295	594.73 949.57 1001.77	H	1.422413	-1.379183	-0.011596	978.56 1019.82 1107.04
H	-1.745682	-0.922426	1.000872	1061.13 1131.76 1223.26	H	2.715400	-0.505981	-0.870240	1332.65 1416.13 1499.37
H	-2.936438	-0.181651	-0.064241	1372.64 1429.38 1492.71	H	2.695032	-0.516045	0.885156	1508.80 2251.23 3040.72
H	-1.240483	1.377199	0.612576	1514.62 3062.59 3111.33	H	1.832147	1.512367	0.002858	3081.96 3181.08 3507.08
Cl	1.536909	-0.096590	0.016236	3202.00 3530.06	Cl	-1.717103	-0.078219	0.000074	
TS9-2					PC9-2				
N	1.425186	0.750137	0.000023		N	1.918959	-0.560757	0.000026	
H	1.038080	1.165385	-0.831969	-1772.82	H	1.793732	-1.100456	0.838246	82.59 174.87 175.04
C	1.483002	-0.667592	0.000021	139.16 148.21 374.94	C	1.408910	0.715986	0.000007	528.98 629.60 677.75
H	1.987888	-1.029625	-0.890946	561.66 812.67 953.80	H	1.486776	1.264631	0.924696	722.38 852.71 961.11
H	1.987811	-1.029626	0.891031	1144.19 1332.09 1405.62	H	1.487168	1.264772	-0.924572	1276.15 1337.17 1506.07
H	0.448082	-1.099366	-0.000025	1470.73 1498.62 1656.94	H	-0.400586	0.410560	0.000156	1672.68 2185.64 3205.43
H	1.038061	1.165382	0.832006	2052.20 3135.60 3195.55	H	1.794280	-1.100194	-0.838407	3314.86 3613.63 3714.38
Cl	-1.492602	-0.024562	-0.000022	3573.18 3687.04	Cl	-1.649855	-0.065290	-0.000020	

Table S4.

Optimized geometries and frequencies of the involved species for the H-abstraction systems EA + H/CH₃/OH /HO₂/NH₂/O/C₂H₅/O₂/Cl using the M08-HX/ma-TZVP method.

Geometry			Frequency			Geometry			Frequency								
Reactants																	
EA						EA-1											
N	1.198049	-0.318741	-0.115106				N	-1.222103	-0.437582	-0.000046							
H	2.068818	0.196376	-0.082812	236.80	269.76	415.31	C	-0.135888	0.500190	-0.000062	214.74	313.00	415.76				
C	0.049385	0.564553	0.054065	794.50	857.16	916.34	H	-0.225119	1.169538	0.875373	723.81	912.93	1017.10				
H	0.068131	1.131396	1.000578	1006.99	1123.23	1151.62	H	-0.225242	1.168983	-0.875810	1031.17	1095.17	1244.65				
H	0.072951	1.303292	-0.756365	1258.82	1322.02	1386.45	H	-2.095396	0.096324	0.000604	1259.19	1381.44	1410.15				
H	1.227359	-1.009655	0.625985	1422.19	1476.25	1484.38	C	1.211255	-0.202135	0.000030	1430.29	1475.66	1485.88				
C	-1.238056	-0.238462	-0.027902	1508.80	1655.23	2965.47	H	1.305732	-0.841233	-0.883008	2944.90	2972.02	3047.86				
H	-2.116266	0.407703	0.067523	3035.53	3059.10	3112.37	H	2.035026	0.518509	-0.002260	3131.31	3133.09	3453.77				
H	-1.293065	-0.771301	-0.982115	3131.53	3538.96	3627.35	H	1.307520	-0.837373	0.885622							
H	-1.282249	-0.983168	0.775969														
EA-2						EA-3											
N	1.210490	-0.230656	0.098359				N	1.152178	-0.319417	-0.060020							
H	1.181216	-1.166620	-0.280504	176.42	326.01	390.74	H	2.001034	0.227191	-0.128318	233.24	262.98	420.30				
C	0.061229	0.524117	-0.111813	558.34	671.45	941.99	C	-0.027425	0.537950	-0.008957	513.01	822.91	859.44				
H	0.140927	1.573931	0.148459	990.43	1020.43	1201.67	H	-0.006387	1.175586	-0.910911	962.22	1090.25	1139.07				
H	2.081462	0.229349	-0.116969	1292.64	1387.99	1448.93	H	-0.037007	1.238015	0.846035	1159.73	1314.48	1401.34				
C	-1.242870	-0.176159	0.015456	1459.87	1483.60	1643.88	H	1.215334	-0.885662	0.777501	1455.96	1479.10	1652.72				
H	-1.426665	-0.544021	1.039719	2964.45	3031.70	3124.53	C	-1.267125	-0.274791	0.003698	2949.05	2969.35	3172.22				
H	-2.070310	0.485896	-0.253212	3200.39	3571.72	3682.53	H	-1.266515	-1.247671	-0.473698	3284.10	3543.85	3633.32				
H	-1.290215	-1.051689	-0.647861							H	-2.204404	0.149511	0.341086				
R1 EA + H																	
TS1-1						TS1-2											
N	1.143198	0.021695	-0.363590				N	1.199074	-0.407797	0.037824							
H	1.307411	1.128331	0.206777	-1529.95				H	2.075597	0.038519	-0.193962	214.59	265.68	292.07			
C	-0.042484	-0.555903	0.251847	166.64	242.11	359.35	C	0.057687	0.377849	-0.296646	334.59	417.79	766.23				
H	0.048922	-0.654920	1.344715	438.11	704.84	783.80	H	0.098413	0.674160	-1.350809	853.57	933.16	1001.56				
H	-0.137423	-1.579751	-0.141801	907.57	1010.21	1024.81	H	0.044819	1.446367	0.296191	1135.57	1173.08	1254.98				
H	1.970133	-0.476776	-0.027984	1101.46	1151.09	1219.47	H	1.209361	-0.682786	1.011689	1289.61	1336.06	1384.82				
H	1.422169	1.771057	0.876012	1280.59	1354.75	1384.85	H	-0.007716	2.386525	0.893142	1397.99	1431.95	1473.18				
C	-1.270791	0.261590	-0.105439	1425.02	1465.47	1475.77	C	-1.240922	-0.305307	0.062885	1481.82	1654.90	3038.17				
H	-1.374900	0.335277	-1.191981	1488.95	1749.55	2993.08	H	-1.273401	-0.529216	1.135993	3080.97	3113.92	3135.80				
H	-2.179657	-0.186959	0.306507	3028.46	3044.16	3123.10	H	-2.096172	0.335006	-0.171294			3553.33 3649.67				
H	-1.179385	1.277757	0.294436														
TS1-3																	
N	-1.210525	0.294206	-0.227816				N										
H	-2.118559	-0.047896	0.059250	-1183.38													
C	-0.140180	-0.573106	0.246668	176.20	256.02	305.71	N										
H	-0.302081	-1.577006	-0.172928	430.11	560.27	818.99	H										
H	-0.116124	-0.692975	1.343724	863.17	922.45	1021.07	C										
H	-1.099885	1.227529	0.153237	1125.40	1138.79	1186.40	H										
H	1.265389	1.964114	0.846545	1227.53	1238.01	1320.09	C										
C	1.184842	-0.041613	-0.221483	1402.43	1441.54	1491.08	H										
H	1.221980	0.202173	-1.284148	1544.45	1655.76	2969.59	C										
H	1.291067	1.132177	0.362621	3024.67	3101.08	3193.70	H										
H	2.063911	-0.579244	0.135305														
R2 EA + CH ₃																	
TS2-1						TS2-2											
N	-0.057769	1.050290	-0.442588				N	1.066260	-1.204201	0.144392							
H	-1.053732	0.314937	-0.338162	74.71	112.55	155.72	H	0.974765	-1.209553	1.152705	31.38	92.87	129.39				
C	0.949925	0.442639	0.413815	255.71	385.19	409.57	C	0.457560	-0.056790	-0.449131	222.07	297.52	386.76				
H	0.599838	0.297616	1.450233	557.14	574.32	774.21	H	0.552069	-0.098744	-1.539933	483.60	500.37	539.91				
H	1.799488	1.139932	0.472526	820.01	912.72	1026.65	H	-0.793783	-0.036613	-0.255020	783.67	878.04	932.48				
H	-0.401482	1.902217	0.003257	1094.98	1114.16	1141.63	H	0.713961	-2.076876	-0.224705	1002.60	1092.62	1146.20				

C	-2.063914	-0.466665	0.087631	1234.68 1278.56 1339.67	C	-2.228760	0.005755	0.078205	1175.15 1261.99 1356.83
H	-2.177244	-1.189404	-0.719138	1383.50 1411.01 1420.80	H	-2.558064	-1.015959	-0.098407	1388.82 1407.28 1417.50
H	-2.921044	0.194179	0.205830	1432.49 1469.11 1474.74	H	-2.241684	0.311482	1.122376	1445.14 1452.38 1470.26
H	-1.715186	-0.903488	1.023235	1489.83 1509.93 2972.25	H	-2.638765	0.739274	-0.612257	1481.93 1651.16 3024.89
C	1.403667	-0.883495	-0.172048	3021.03 3040.69 3071.26	C	0.973728	1.236204	0.133196	3071.13 3082.12 3097.95
H	1.776878	-0.738727	-1.190368	3118.51 3133.21 3209.90	H	0.472435	2.096393	-0.320490	3124.41 3228.88 3231.70
H	2.194501	-1.337175	0.433162	3217.63 3491.78	H	0.785756	1.272490	1.213890	3551.40 3648.66
H	0.564293	-1.586992	-0.218847		H	2.054316	1.336498	-0.022523	
TS2-3									
N	-1.253058	-0.950279	-0.296675	-1686.79					
H	-0.379569	-1.465103	-0.280543	81.52 108.82 119.04					
C	-1.100315	0.323090	0.398405	288.53 352.26 406.58					
H	-2.067993	0.844907	0.363938	506.36 544.18 686.71					
H	-0.841785	0.214826	1.467054	832.51 880.54 923.36					
H	-1.957815	-1.529403	0.141704	1037.82 1127.78 1142.33					
C	2.130168	-0.392484	0.094332	1154.00 1218.54 1319.00					
H	1.857097	-0.929038	1.002659	1370.15 1377.51 1403.71					
H	2.197946	-1.022973	-0.790851	1436.70 1440.53 1443.35					
H	2.977809	0.278117	0.220930	1493.00 1653.64 2956.04					
C	-0.042658	1.148261	-0.282557	3022.80 3069.80 3092.91					
H	0.181610	2.100778	0.200315	3181.52 3207.94 3221.59					
H	1.062999	0.447188	-0.148093	3541.47 3630.20					
H	-0.182058	1.239448	-1.361461						
R3 EA + OH									
RC3									
N	-0.085028	1.126778	0.266572						
H	-0.037425	2.056939	-0.133185	49.95 85.00 215.70					
C	-1.065195	0.294313	-0.439484	259.59 301.57 416.10					
H	-2.067474	0.748942	-0.457800	620.44 705.65 804.52					
H	-0.734217	0.203502	-1.480787	908.29 937.38 1009.15					
H	-0.352486	1.236077	1.239265	1112.63 1167.69 1257.86					
O	2.352343	-0.411246	-0.094583	1325.02 1392.55 1425.14					
H	1.580282	0.182646	0.070346	1480.98 1486.03 1509.99					
C	-1.130048	-1.082374	0.199219	1647.64 2998.66 3035.04					
H	-1.449194	-1.010763	1.245923	3067.86 3114.58 3134.32					
H	-1.844989	-1.723577	-0.324356	3469.61 3532.14 3615.39					
H	-0.146585	-1.562882	0.172842						
TS3-1									
N	-0.215318	0.990317	-0.418379	-647.72					
H	-0.947728	0.251099	-0.655428	100.39 139.92 180.24	N	-0.357686	-1.206280	0.000206	
C	0.863064	0.488485	0.410309	253.36 373.77 415.81	H	1.472274	-0.434859	0.000370	37.26 75.16 107.02
H	1.649522	1.256736	0.430329	651.40 723.70 796.32	C	-1.379661	-0.198821	-0.000282	185.23 238.26 318.47
H	0.539636	0.339694	1.452266	917.66 1004.60 1110.89	H	-2.036114	-0.352351	-0.876159	380.36 440.45 601.89
H	-0.651889	1.825593	-0.043568	1130.47 1242.97 1288.06	H	-2.037362	-0.352342	0.874624	717.97 913.05 1022.39
O	-1.851594	-0.641023	0.060494	1380.95 1416.98 1470.66	H	-0.798454	-2.128239	0.000695	1036.44 1096.66 1251.66
H	-2.404267	-0.094826	0.633904	1477.89 1493.50 1606.02	O	2.223936	0.175861	0.000298	1256.42 1384.69 1412.69
C	1.396422	-0.814103	-0.156387	2442.28 2994.94 3035.18	H	3.014151	-0.363175	-0.002735	1430.21 1475.42 1479.23
H	1.750246	-0.670877	-1.182079	3046.49 3132.04 3133.74	C	-0.788958	1.200437	0.000087	1642.69 2952.77 2979.31
H	2.225887	-1.190779	0.448843	3584.97 3836.25	H	-0.156004	1.350171	-0.879818	3050.32 3133.71 3136.96
H	0.601654	-1.566969	-0.163103		H	-1.577996	1.958333	-0.000001	3469.99 3726.43 3951.33
TS3-2									
N	-1.269064	-1.041245	-0.184351	-486.23					
H	-1.064067	-1.097584	-1.174453	44.22 65.86 114.17	N	0.516543	1.265357	-0.286462	98.35 124.79 164.38
C	-0.461050	-0.051918	0.471922	238.41 306.02 422.06	H	-0.165224	1.059131	-1.005740	183.17 216.95 312.33
H	-0.703724	-0.041890	1.541811	539.46 761.22 786.92	C	0.877570	0.185679	0.504727	382.27 397.61 478.25
H	0.647159	-0.308455	0.415600	919.40 1001.69 1120.52	H	1.448565	0.432972	1.394478	652.69 718.67 943.40
H	-1.164196	-1.961557	0.221019	1159.38 1258.33 1305.86	H	-1.346401	-0.206230	0.585924	999.32 1032.10 1203.60
O	2.206855	-0.317859	-0.094966	1385.27 1415.56 1428.49	H	0.296355	2.119124	0.202265	1304.13 1386.14 1448.79
H	2.350659	0.635304	0.010855	1473.98 1485.33 1656.57	O	-2.100812	-0.191862	-0.017210	1465.60 1485.19 1614.18
C	-0.657739	1.319242	-0.145648	2067.42 3035.18 3058.04	H	-2.703388	-0.873738	0.279347	1653.97 2974.75 3050.14
H	-0.051491	2.073132	0.366885	3114.93 3125.51 3555.20	C	1.133194	-1.104135	-0.196224	3123.10 3190.63 3567.12
H					H	1.277793	-1.918921	0.518699	3681.96 3759.85 3953.61

H	-0.364059	1.309801	-1.201940	3649.45	3802.74	H	0.288422	-1.368233	-0.846894				
H	-1.708942	1.618902	-0.087234			H	2.029981	-1.055975	-0.836189				
R4 EA + HO₂													
RC4													
N	-0.638635	1.223306	-0.110450										
H	-1.158969	1.536860	-0.923944	43.68	100.73	117.03							
C	-1.348535	0.113775	0.547170	167.70	255.19	275.86							
H	-2.351770	0.413686	0.883782	369.73	440.05	802.50							
H	-0.767368	-0.165830	1.431650	841.02	910.39	971.15							
H	-0.560305	2.019354	0.513178	1020.61	1106.81	1176.31							
O	1.833839	-0.572247	0.555903	1259.89	1289.59	1332.01							
O	1.854507	0.178396	-0.508636	1394.03	1427.90	1477.96							
H	0.969467	0.649329	-0.496892	1482.69	1503.17	1642.62							
C	-1.444516	-1.070991	-0.397013	1645.96	3012.00	3037.11							
H	-0.445362	-1.415766	-0.681562	3066.69	3095.38	3120.07							
H	-1.972305	-1.903283	0.077083	3139.13	3526.65	3609.62							
H	-1.991403	-0.803387	-1.309223										
TS4-1													
N	0.513990	0.513990	-0.159377				N	0.840282	1.208893	0.014834			
H	-0.588435	-0.588435	-0.529652	-2525.30			H	-0.910779	0.711012	-0.515013	26.36	70.22	103.24
C	1.230367	1.230367	0.538308	61.60	121.05	163.39	C	1.790609	0.152099	0.208149	128.89	221.27	250.93
H	0.611186	0.611186	1.371286	228.57	301.48	351.91	H	2.088611	0.136039	1.272474	262.89	381.87	434.60
H	2.122877	2.122877	1.009392	429.80	506.66	696.08	H	2.718785	0.392431	-0.341085	719.46	743.24	915.02
H	0.342669	0.342669	0.462100	750.87	917.35	1000.40	H	1.262369	2.098384	0.287302	1025.36	1029.41	1043.08
O	-1.660652	-1.660652	-0.502117	1037.98	1071.30	1109.59	O	-1.776083	0.281219	-0.660852	1099.73	1254.15	1257.35
O	-1.578204	-1.578204	0.350267	1216.80	1269.84	1340.04	O	-1.943444	-0.413355	0.567588	1382.69	1386.20	1412.16
H	-2.163381	-2.163381	1.074440	1385.09	1403.76	1421.30	H	-2.647477	0.090675	0.986289	1428.93	1476.69	1488.70
C	1.594135	1.594135	-0.397344	1428.74	1477.18	1486.72	C	1.229071	-1.192819	-0.218105	1553.33	2954.71	2981.72
H	2.220875	2.220875	-1.217426	1594.32	2934.27	3008.09	H	0.963233	-1.175982	-1.279704	3050.47	3132.81	3141.11
H	2.135357	2.135357	0.136692	3046.30	3131.39	3134.06	H	1.959930	-1.990658	-0.056418	3481.75	3606.24	3867.17
H	0.684757	0.684757	-0.822182	3497.98	3848.43		H	0.321503	-1.422748	0.348168			
TS4-2													
N	-1.020749	1.280414	-0.243743				N	-0.959161	1.241140	-0.376362			
H	-0.780434	2.114996	0.272160	-1489.09			H	-0.793647	2.136565	0.055966	59.30	101.15	136.38
C	-0.970742	0.097410	0.514532	81.14	131.73	140.53	C	-1.283159	0.198881	0.475462	151.15	190.17	213.13
H	-1.489097	0.209464	1.472326	211.05	327.88	379.17	H	-1.875025	0.476538	1.342848	245.11	388.52	410.88
H	0.242373	-0.105002	0.831349	426.08	443.08	594.66	H	0.771468	-0.031007	0.953819	549.23	670.97	707.17
H	-0.474100	1.224798	-1.095236	762.09	884.75	941.26	H	-0.264538	1.022512	-1.079275	942.27	995.17	1027.68
O	1.536370	-0.201663	0.741516	999.66	1080.75	1148.11	O	1.731421	-0.018322	0.775067	1034.21	1203.61	1305.85
O	1.737476	0.069176	-0.600932	1198.34	1241.81	1284.20	O	1.753529	-0.125322	-0.641780	1371.58	1385.10	1448.56
H	1.880016	-0.801927	-0.987847	1380.64	1402.46	1429.24	H	2.184795	-0.976191	-0.768349	1463.85	1483.08	1522.06
C	-1.367261	-1.132583	-0.264070	1469.86	1478.27	1523.67	C	-1.481834	-1.143303	-0.142143	1654.13	2977.28	3054.79
H	-0.744857	-1.228767	-1.162825	1658.91	3027.29	3082.79	H	-0.629052	-1.409975	-0.780508	3122.05	3187.59	3567.51
H	-1.238969	-2.035638	0.338343	3099.49	3135.81	3554.92	H	-1.588713	-1.916381	0.623625	3593.42	3683.35	3866.88
H	-2.412436	-1.069893	-0.589515	3658.33	3830.10		H	-2.380798	-1.174363	-0.779797			
TS4-3													
N	1.055770	-1.073119	-0.434463				N	0.896314	-1.103852	-0.257636			
H	1.308064	-0.822349	-1.384001	-2391.75			H	0.978781	-1.099134	-1.269040	29.63	79.72	107.84
C	1.306768	0.043643	0.481670	111.02	175.83	206.61	C	1.788189	-0.092471	0.321041	124.72	193.20	232.72
H	2.384236	0.206945	0.670810	273.68	323.38	423.40	H	2.851546	-0.283172	0.100581	273.19	345.34	461.78
H	0.851134	-0.201612	1.449804	443.79	580.65	668.23	H	1.692251	-0.165757	1.418573	525.52	773.82	861.97
H	1.606500	-1.883873	-0.179281	822.32	887.32	930.28	H	1.149326	-2.032700	0.059942	927.38	978.37	1030.23
O	-1.623430	0.443801	-0.413148	1006.93	1059.16	1079.99	O	-2.005775	0.722712	-0.143555	1100.80	1129.79	1175.96
O	-1.594776	-0.623775	0.468418	1109.38	1156.75	1256.61	O	-1.910312	-0.663636	0.161776	1314.70	1379.44	1402.47
H	-0.941963	-1.212982	0.048492	1281.64	1408.54	1449.46	H	-0.947084	-0.816410	0.061574	1462.86	1482.18	1591.26
C	0.709078	1.313196	-0.042804	1480.61	1485.31	1520.59	C	1.407643	1.263611	-0.140835	1643.98	2963.71	2992.28
H	0.997380	1.591559	-1.058984	1647.42	2942.33	3057.94	H	0.373578	1.465797	-0.399082	3166.34	3283.24	3516.70
H	-0.631580	0.980952	-0.232238	3094.26	3195.11	3539.56	H	-2.335842	1.079675	0.686067	3533.59	3616.61	3869.17
H	0.686407	2.151954	0.651284	3626.12	3665.67		H	2.116947	2.079214	-0.082172			
R5 EA + NH ₂													
RC5													

N	-0.425534	1.215566	-0.295042	98.47	104.82	116.97			
H	-1.020658	1.326849	-1.108395	169.74	237.65	278.70			
C	-0.914200	0.123214	0.549766	330.53	395.83	452.29			
H	-1.900275	0.334695	0.993258	800.12	882.26	917.36			
H	-0.204475	-0.002040	1.376821	1007.32	1115.73	1163.80			
N	2.302063	-0.276195	0.114725	1256.57	1321.17	1390.39			
H	3.162823	-0.071964	-0.402234	1425.87	1478.11	1480.17			
H	1.602579	0.380328	-0.262882	1508.01	1549.14	1647.03			
C	-0.977733	-1.163712	-0.254152	2996.80	3037.48	3074.83			
H	0.016033	-1.426682	-0.630909	3117.11	3136.43	3356.49			
H	-1.341602	-1.992041	0.360796	3483.98	3528.76	3614.36			
H	-1.656038	-1.056487	-1.109658						
TS5-1							PC5-1		
N	-0.173981	0.995652	-0.412578	-2012.13			N	-0.500618	-1.205525
H	-1.039246	0.165889	-0.471648	91.23	122.80	155.32	H	1.638072	-0.456066
C	0.903951	0.475254	0.410336	252.83	409.18	444.46	C	-1.425240	-0.186706
H	0.598684	0.317435	1.459293	633.82	716.75	792.83	H	-1.636831	-0.318043
H	1.698686	1.236403	0.440205	831.10	915.31	1027.88	H	-2.398877	-0.340874
H	-0.578764	1.821768	0.025284	1102.01	1121.22	1241.36	H	-0.940525	-2.116852
N	-1.966872	-0.598757	-0.000185	1280.54	1375.52	1401.73	N	2.425642	0.124451
H	-2.766489	0.024598	0.122732	1435.29	1469.25	1475.70	H	2.876496	0.464814
H	-1.663936	-0.835575	0.946192	1491.88	1552.79	1609.68	H	3.091960	-0.460850
C	1.436149	-0.819539	-0.180954	2965.66	3016.94	3043.31	C	-0.886040	1.207439
H	1.793526	-0.650111	-1.201059	3123.95	3132.89	3462.48	H	-0.731242	1.350415
H	2.259778	-1.218891	0.418349	3513.78 3558.47			H	-1.584469	1.973540
H	0.643139	-1.574071	-0.226303				H	0.077930	0.347038
TS5-2							PC5-2		
N	-1.074518	-1.182546	-0.157742	-1028.89			N	0.580046	1.239724
H	-0.981365	-1.183501	-1.166126	86.68	99.60	131.14	H	-0.292158	1.027740
C	-0.418415	-0.065200	0.439561	231.80	306.15	407.83	C	1.062561	0.200144
H	-0.503627	-0.120198	1.531054	567.07	601.85	803.65	H	1.834607	0.470345
H	0.773086	-0.107419	0.205451	810.27	916.64	971.55	H	-1.513665	-0.257817
H	-0.748526	-2.069719	0.200874	1009.71	1157.90	1213.18	H	0.553541	2.143283
N	2.184126	-0.113513	-0.181487	1266.51	1332.52	1385.81	N	-2.193822	-0.161178
H	2.277789	0.887956	-0.373094	1422.18	1458.44	1473.34	H	-2.551977	-1.083218
H	2.580555	-0.228946	0.755331	1481.08	1544.61	1657.04	H	-2.966611	0.391199
C	-0.918859	1.252977	-0.108633	3031.87	3068.06	3107.56	C	1.093501	-1.151085
H	-0.397699	2.094940	0.356677	3127.87	3431.77	3529.00	H	1.319569	-1.925641
H	-0.749659	1.308077	-1.190954	3555.18 3650.06			H	0.127083	-1.389251
H	-1.994167	1.364570	0.069821				H	1.849669	-1.220812
TS5-3							PC5-3		
N	1.166446	-0.974406	-0.275406	-1716.20			N	0.688823	-1.173043
H	1.923112	-1.531209	0.100010	100.59	130.55	161.60	H	1.024852	-2.047931
C	1.107045	0.335543	0.358104	334.77	390.43	427.41	C	1.188813	-0.044629
H	0.951343	0.294408	1.450264	548.53	713.57	809.01	H	0.797305	-0.002542
H	2.068254	0.846105	0.196990	871.44	899.31	926.29	H	2.282060	-0.164157
H	0.296592	-1.469485	-0.102746	1074.81	1132.01	1152.12	H	-0.327283	-1.180609
N	-1.980006	-0.499081	0.136727	1229.07	1317.60	1334.54	N	-2.227249	0.012304
H	-2.458830	-0.433015	-0.764157	1402.27	1434.02	1441.78	H	-2.869776	-0.003305
H	-2.553586	0.047107	0.782972	1488.89	1546.57	1657.74	H	-2.775100	0.052175
C	-0.002075	1.139701	-0.269266	2966.37	3023.38	3092.43	C	0.900866	1.240456
H	-0.221944	2.092519	0.215442	3179.93	3449.47	3531.27	H	0.985133	2.181454
H	0.078499	1.222541	-1.355157	3548.26 3625.99			H	0.795805	1.248874
H	-1.018345	0.393974	-0.085893				H	-1.682090	0.866253
R6 EA + O									
RC6									
N	0.313655	0.958754	0.296186	63.22	139.95	184.30			
H	0.704522	1.806231	-0.091965	259.61	297.26	422.81			
C	-0.830119	0.452350	-0.447729	759.42	818.48	917.40			

H	-0.492652	0.240321	-1.469260	995.39 1123.97 1146.99							
H	-1.648379	1.187587	-0.522409	1252.85 1312.71 1390.43							
H	0.106365	1.105313	1.275971	1419.36 1479.61 1490.02							
O	1.973737	-0.707652	-0.103270	1511.52 1641.43 2979.65							
C	-1.340134	-0.824734	0.196492	3037.90 3068.83 3116.88							
H	-1.680257	-0.634655	1.221705	3140.59 3557.34 3655.18							
H	-2.183821	-1.238100	-0.363865								
H	-0.538878	-1.568962	0.232407								
TS6-1				PC6-1							
N	-0.300487	0.983658	-0.395631	-1846.41 94.85 145.42 251.22 401.27 481.31 685.04 781.66 913.56 1027.54 1087.65 1105.37 1237.33 1278.71 1330.30 1388.61 1422.39 1450.64 1477.35 1484.50 1614.85 2990.84 3024.46 3044.39 3124.30 3139.77 3504.17	N	-0.137769	-1.145830	-0.004511			
H	-1.167687	0.147984	-0.422864		H	1.631532	-0.304453	-0.002521	64.10	64.31	200.91
C	0.840072	0.511316	0.359269		C	-1.305262	-0.313392	0.004509	232.30	357.15	425.16
H	0.613351	0.459581	1.435708		H	-1.920885	-0.565481	0.886934	516.87	629.40	724.95
H	1.634595	1.266995	0.249511		H	-1.939326	-0.569508	-0.863455	915.86	1022.49	1039.87
H	-0.693281	1.815500	0.046017		H	-0.421853	-2.127308	-0.003618	1099.67	1250.45	1258.92
O	-1.923651	-0.632657	0.137661		O	2.451933	0.237289	0.001841	1383.70	1413.25	1431.69
C	1.303179	-0.838855	-0.156074		C	-0.940943	1.160976	-0.002366	1476.50	1481.66	2956.04
H	1.540237	-0.782565	-1.222668		H	-0.353322	1.406214	-0.892317	2983.43	3049.68	3132.43
H	2.191680	-1.179590	0.382664		H	-1.837314	1.787936	0.006381	3136.25	3481.68	3574.01
H	0.514220	-1.587015	-0.019412		H	-0.332685	1.409592	0.872588			
TS6-2				PC6-2							
N	-0.912367	-1.223720	-0.148696	-334.02 63.21 103.42 236.08 329.48 426.39 737.43 789.22 925.12 997.93 1119.18 1146.81 1248.31 1284.69 1383.05 1394.79 1424.78 1474.28 1480.09 1653.49 1739.93 3039.10 3067.34 3118.19 3134.45 3565.95 3664.40	N	0.140121	1.256618	-0.273390			
H	-0.563845	-2.089503	0.237629		H	-0.378452	1.981727	0.196536	62.51	93.66	166.97
C	-0.345126	-0.056987	0.443150		C	0.682614	0.255304	0.517368	221.58	374.12	386.59
H	-0.466794	-0.100551	1.532169		H	1.056574	0.580289	1.483230	438.24	471.39	629.05
H	0.804980	-0.006000	0.287421		H	-1.308707	-0.634825	0.581146	663.42	944.70	990.67
H	-0.827697	-1.236945	-1.156650		H	-0.302087	0.953601	-1.130024	1028.61	1200.52	1295.76
O	2.281461	0.053381	-0.100988		O	-2.091723	-0.550730	-0.002593	1388.40	1447.71	1463.92
C	-0.922269	1.216500	-0.139305		C	1.341122	-0.876856	-0.190946	1483.93	1648.92	2977.26
H	-0.455081	2.097649	0.308767		H	1.638615	-1.659852	0.511485	3045.60	3125.46	3191.01
H	-0.750200	1.257551	-1.220875		H	0.661499	-1.326252	-0.928498	3580.68	3609.86	3693.37
H	-2.002110	1.259721	0.037248		H	2.243068	-0.555868	-0.737933			
TS6-3											
N	1.173968	-0.899720	-0.291322	-1593.91 109.00 142.95 300.26 412.00 444.90 575.07 804.34 856.59 915.10 987.28 1119.98 1129.64 1170.20 1195.29 1250.01 1327.41 1401.26 1441.21 1480.44 1655.91 2973.07 3017.71 3095.79 3190.99 3540.57 3633.50	N	0.828995	-1.115541	-0.338614			
H	0.359558	-1.491763	-0.166526		H	-0.150607	-1.378067	-0.348918	55.19	107.56	153.65
C	0.967102	0.375642	0.375691		C	1.016913	0.098730	0.442787	240.72	296.56	350.75
H	0.787221	0.294650	1.461341		H	0.581658	0.053148	1.458588	397.21	427.99	595.12
H	1.878836	0.981763	0.256574		H	2.102020	0.234356	0.597962	842.79	861.73	953.77
H	1.975801	-1.388394	0.084886		H	1.349761	-1.887172	0.057085	1095.98	1140.82	1156.22
O	-2.018741	-0.564395	0.122879		O	-2.235051	-0.194271	0.099310	1325.67	1396.20	1449.24
C	-0.175692	1.106423	-0.266287		C	0.481490	1.284328	-0.273700	1464.65	1661.95	2942.04
H	-1.206152	0.327549	-0.094239		H	-1.613647	0.539303	-0.092363	2971.96	3154.02	3265.73
H	-0.487774	2.035096	0.213095		H	0.346728	2.225895	0.247741	3544.42	3615.70	3635.01
H	-0.123795	1.161908	-1.355338		H	0.471113	1.277137	-1.358808			
R7 EA + C ₂ H ₅											
TS7-1				TS7-2							
N	0.715507	1.276413	-0.080272	-1939.05 86.45 120.23 152.40 196.75 226.47 281.84 408.24 457.65 565.32 758.95 799.75 859.63 875.81 914.70 1026.19 1041.81 1098.22 1113.96 1147.68 1218.03 1237.01 1277.52 1374.33 1381.91 1393.76 1417.86 1454.32 1465.46 1470.11 1473.87 1482.06 1489.56 1500.28 2970.07 3012.39 3017.22 3039.19 3076.64 3086.82 3104.08 3116.13 3130.56	N	1.481133	-1.108549	-0.440423			
H	-0.419514	0.852729	-0.473424		H	1.050308	-0.985117	-1.348624	41.49	98.33	128.72
C	1.331339	0.133777	0.573885		C	1.063997	-0.114046	0.496101	174.89	221.79	270.80
H	0.713470	-0.282040	1.388733		H	1.543285	-0.277072	1.467648	316.77	401.55	507.16
H	2.262906	0.481407	1.047687		H	-0.199831	-0.216512	0.749714	530.49	775.44	824.94
H	0.424618	1.948976	0.631186		H	1.316450	-2.053070	-0.119638	834.52	906.31	939.12
C	-1.626097	0.326470	-0.629394		C	-1.634922	-0.316799	0.729475	1000.90	1056.94	1133.84
C	-1.908303	-0.629019	0.499380		C	-2.001655	0.210838	-0.630528	1145.46	1173.03	1213.31
H	-2.268923	1.208990	-0.655629		H	-1.794328	-1.385478	0.880724	1259.98	1364.90	1389.59
H	-1.543781	-0.134812	-1.616167		H	-1.967515	0.278902	1.579700	1394.27	1448.54	1452.06
H	-1.191507	-1.458084	0.516244		H	-1.796249	1.283921	-0.711310	1456.91	1467.55	1470.68
H	-1.862527	-0.127144	1.472661		H	-1.429726	-0.295093	-1.420113	1480.11	1485.57	1650.10
H	-2.909847	-1.071465	0.410788		H	-3.064857	0.064940	-0.868286	3005.33	3019.99	3060.37
C	1.642758	-0.947462	-0.447282		C	1.253253	1.286538	-0.029933	3068.67	3090.85	3095.04
H	2.286490	-0.547334	-1.236429		H	0.711719	1.415729	-0.976179	3101.77	3120.23	3181.97

H	2.142094	-1.803863	0.016379	3163.47	3478.10	H	0.866989	2.026149	0.678371	3548.70	3646.79
H	0.719796	-1.304852	-0.919657			H	2.311788	1.503350	-0.219727		
TS7-3											
N	-1.372288	-1.000965	0.524340		-1651.09						
H	-1.835729	-1.858033	0.249274		67.36	115.08	137.96				
C	-1.412116	-0.009301	-0.547444		186.08	222.63	256.17				
H	-2.434058	0.175593	-0.929205		407.46	416.57	508.60				
H	-0.833445	-0.403080	-1.394531		663.45	806.02	835.11				
H	-1.850402	-0.650991	1.346856		860.70	915.06	928.05				
C	1.664267	0.432880	0.572418		1020.75	1055.03	1112.30				
C	1.913006	-0.630665	-0.464612		1139.51	1175.25	1219.78				
H	2.330774	1.297086	0.527454		1253.58	1293.78	1384.46				
H	1.544987	0.058619	1.590317		1389.47	1404.69	1417.33				
H	1.161381	-1.423208	-0.382984		1446.75	1450.09	1474.58				
H	1.871521	-0.217695	-1.479680		1483.86	1501.81	1650.64				
H	2.901569	-1.094481	-0.345954		2935.37	3015.00	3039.60				
C	-0.798070	1.281731	-0.081191		3075.82	3082.12	3086.66				
H	0.463700	0.941943	0.298465		3109.36	3170.30	3171.49				
H	-0.674055	2.040517	-0.854760		3538.35	3625.66					
H	-1.242748	1.692614	0.829343								
R8 EA + O ₂											
TS8-1											
N	0.465254	1.244342	-0.214282		-1991.77			N	-0.675133	-1.183346	0.002943
H	-0.761421	0.702678	-0.512078		94.37	98.22	152.67	H	0.997154	-0.697321	-0.421516
C	1.171688	0.242955	0.523374		233.86	296.95	422.17	C	-1.727136	-0.228051	0.189026
H	0.474935	-0.144155	1.301818		530.82	665.61	729.31	H	-2.034358	-0.250790	1.250415
H	2.018053	0.685605	1.070614		916.78	1007.94	1045.93	H	-2.620531	-0.557602	-0.370704
H	0.359157	2.084589	0.356304		1115.33	1167.80	1258.57	H	-1.003785	-2.114867	0.261977
O	-1.727162	0.156623	-0.457442		1294.35	1366.04	1392.63	O	1.900549	-0.291407	-0.486068
O	-1.661971	-0.710479	0.472903		1400.12	1421.46	1477.27	O	1.986387	0.503853	0.541148
C	1.602605	-0.909947	-0.367074		1483.10	1645.93	2873.13	C	-1.298188	1.168783	-0.221873
H	2.289188	-0.562305	-1.144456		3017.79	3048.83	3131.88	H	-1.030520	1.190367	-1.283089
H	2.101464	-1.687018	0.218876		3138.53	3492.19		H	-2.103593	1.890025	-0.056459
H	0.729154	-1.356986	-0.852588					H	-0.421983	1.479642	0.355216
TS8-2											
N	0.879135	1.310819	-0.147099		-1900.06			N	0.993152	1.273852	-0.214521
H	0.377950	1.278081	-1.026259		76.98	147.42	156.96	H	0.375497	1.211475	-1.013003
C	0.953126	0.095933	0.521835		210.73	337.49	401.98	C	1.156034	0.106353	0.507055
H	1.416585	0.176453	1.507355		425.14	574.07	699.31	H	1.697505	0.217581	1.443131
H	-0.415963	-0.245361	0.772009		856.42	941.17	993.89	H	-0.742455	-0.168004	0.858988
H	0.622142	2.113113	0.407950		1109.56	1151.76	1200.09	H	0.875123	2.126107	0.309711
O	-1.556751	-0.407749	0.567270		1293.43	1372.89	1388.50	O	-1.711731	-0.241148	0.632571
O	-1.766766	0.088709	-0.583353		1437.61	1468.84	1479.70	O	-1.801821	0.044256	-0.630279
C	1.377753	-1.069320	-0.328921		1575.47	1657.26	3020.96	C	1.320637	-1.152236	-0.279857
H	1.323758	-2.004371	0.234343		3088.65	3121.55	3136.33	H	1.298468	-2.029159	0.372628
H	0.718893	-1.160623	-1.201587		3568.10	3680.01		H	0.517577	-1.259103	-1.020819
H	2.405546	-0.940377	-0.692933					H	2.274607	-1.165433	-0.830513
TS8-3											
N	-1.408420	-0.970539	-0.464899		-1662.32			N	-1.420470	-1.047241	-0.385698
H	-0.507510	-1.415782	-0.600651		43.89	119.74	143.23	H	-0.476588	-1.395150	-0.514274
C	-1.285157	0.116544	0.495258		243.15	293.30	423.77	C	-1.400692	0.119601	0.482973
H	-2.299101	0.412713	0.814323		455.12	547.97	790.85	H	-2.437422	0.325986	0.803061
H	-0.747321	-0.161213	1.419278		871.80	910.65	979.26	H	-0.830705	-0.026051	1.419891
H	-2.043912	-1.681193	-0.126047		1037.31	1119.31	1139.18	H	-1.967067	-1.793756	0.023264
O	1.664354	-0.768614	0.332577		1200.90	1329.53	1390.56	O	1.733984	-0.808472	0.126296
O	1.775536	0.343102	-0.273090		1418.17	1440.77	1455.77	O	2.003775	0.450694	-0.041302
C	-0.632196	1.305845	-0.126472		1529.97	1663.10	2962.90	C	-0.883061	1.313266	-0.233135
H	-0.464925	2.179128	0.502928		2995.81	3107.38	3212.80	H	-0.699394	2.234795	0.311630
H	0.783466	0.827274	-0.274271		3547.25	3631.76		H	1.139218	0.893683	-0.209319
H	-0.876757	1.502607	-1.169880					H	-0.984310	1.356203	-1.313342
R9 EA + Cl (M05-2X/ma-TZVP)											

RC9														
N	0.206868	-0.697881	0.000076											
H	0.207132	-1.256936	-0.837389	73.31	114.18	256.82								
C	1.089479	0.454591	0.000163	275.23	434.28	465.48								
H	0.838092	1.049280	-0.873898	736.16	791.28	915.84								
H	0.838316	1.048962	0.874503	980.31	1084.15	1148.83								
H	0.206978	-1.256949	0.837529	1259.99	1383.25	1395.04								
C	2.564692	0.076115	-0.000104	1428.37	1511.00	1512.84								
H	2.814792	-0.508967	-0.883174	1531.44	1648.31	3094.02								
H	3.181031	0.972762	-0.000038	3135.64	3154.89	3168.01								
H	2.815042	-0.509284	0.882683	3185.32	3591.85	3695.69								
Cl	-2.005185	0.109395	0.000176											
TS9-1							PC9-1							
N	0.473313	1.113225	-0.276228	-1019.47			N	0.602910	1.064190	-0.291808				
H	-0.758231	0.720734	-0.061896	73.62	114.22	254.64	H	-0.984658	0.512764	-0.179405	23.98	62.16	141.79	
C	1.456839	0.385551	0.472369	322.92	407.34	591.71	C	1.485566	0.313106	0.549787	243.91	274.13	385.88	
H	1.064661	0.220362	1.472156	798.19	916.25	978.26	H	0.920906	-0.053083	1.403996	719.40	723.52	827.37	
H	2.345252	1.021157	0.548280	1042.40	1085.69	1101.58	H	2.301049	0.947603	0.907249	924.35	1017.78	1054.84	
H	0.733751	1.188670	-1.256785	1219.14	1271.67	1333.24	H	1.132503	1.519438	-1.032144	1127.09	1257.40	1316.59	
C	1.830705	-0.939169	-0.194104	1417.55	1424.02	1496.03	C	2.070040	-0.870227	-0.234292	1393.58	1416.39	1507.15	
H	2.248406	-0.768679	-1.184816	1510.73	1524.63	3052.03	H	2.663907	-0.522166	-1.076841	1515.92	1533.47	2112.80	
H	2.572744	-1.455765	0.409321	3100.39	3158.15	3177.10	H	2.707011	-1.458902	0.420907	3065.06	3102.46	3148.16	
H	0.946996	-1.564663	-0.284882	3190.12	3505.84		H	1.268205	-1.502878	-0.605113	3176.77	3185.94	3494.30	
Cl	-1.893649	-0.225452	0.036625								Cl	-2.091937	-0.208787	0.018297
TS9-2							PC9-2							
N	-0.710110	1.250509	-0.257537	-2358.20			N	1.469942	-1.209279	-0.193418				
H	-0.184023	1.976106	0.202605	49.09	151.67	238.59	H	1.205333	-2.085748	0.221149	57.84	97.14	146.70	
C	-1.089590	0.146333	0.549239	306.76	419.23	539.33	C	1.111131	-0.065881	0.491237	217.62	384.21	416.00	
H	-1.610044	0.509087	1.434513	722.69	902.41	952.48	H	1.182214	-0.143450	1.566967	644.23	669.03	714.77	
H	-0.155937	-0.363942	0.911735	995.60	1133.53	1252.38	H	-0.636707	-0.011696	0.315195	816.16	954.86	1005.37	
H	-0.315189	1.009466	-1.154452	1260.05	1407.28	1432.20	H	1.324520	-1.188611	-1.189388	1061.40	1216.51	1312.00	
Cl	1.854032	-0.247272	-0.014009	1439.25	1512.17	1515.87	Cl	-1.941771	0.006463	-0.032719	1415.57	1469.94	1496.98	
C	-1.905921	-0.865686	-0.229415	1639.96	1916.98	3099.40	C	1.416450	1.240396	-0.159356	1510.79	1666.07	1998.85	
H	-1.328505	-1.234449	-1.075939	3124.59	3167.46	3183.22	H	1.024143	1.263365	-1.176721	3057.85	3116.80	3175.66	
H	-2.156060	-1.713192	0.402637	3555.87	3677.52		H	0.961233	2.058047	0.392348	3226.84	3597.41	3701.66	
H	-2.824956	-0.416902	-0.599126								2.494301	1.416086	-0.210686	
TS9-3							PC9-3							
N	1.597712	-1.012586	-0.306725	-724.92			N	1.548983	-1.076011	-0.324404				
H	0.694552	-1.466271	-0.327238	94.62	132.28	268.47	H	0.603017	-1.416524	-0.424273	83.93	104.64	144.80	
C	1.517019	0.235658	0.432847	401.35	427.76	570.87	C	1.569786	0.151029	0.459042	274.58	342.00	436.80	
H	1.165996	0.126369	1.464259	770.34	842.75	877.76	H	1.105220	0.056954	1.447936	501.57	589.20	692.28	
H	2.521389	0.669681	0.485509	899.31	929.29	1088.32	H	2.618842	0.414014	0.640357	846.89	877.64	964.23	
H	2.253279	-1.647950	0.120932	1142.53	1154.77	1224.34	H	2.089148	-1.800499	0.122665	1108.52	1146.72	1174.33	
C	0.645829	1.207701	-0.285188	1340.95	1423.63	1473.49	C	0.929709	1.262444	-0.284390	1336.56	1420.72	1474.94	
H	-0.641232	0.586197	-0.177506	1498.55	1670.98	3037.64	H	-0.867370	0.587008	-0.172352	1496.91	1674.00	2428.19	
H	0.431413	2.149123	0.202836	3059.59	3173.78	3274.41	H	0.716062	2.191545	0.221065	3019.73	3034.77	3201.40	
H	0.737528	1.232207	-1.363410	3555.92	3640.07		H	0.988227	1.260884	-1.362067	3310.17	3560.99	3642.37	
Cl	-1.842588	-0.189494	0.050338								Cl	-1.946647	-0.131891	0.044093

Table S5.

Optimized geometries and frequencies of the involved species for the H-abstraction systems DMA + H/CH₃/OH/HO₂/NH₂/O/C₂H₅/O₂/Cl using the M08-HX/ma-TZVP method.

Geometry			Frequency			Geometry			Frequency											
Reactants																				
DMA																				
N	0.026520	0.586877	0.000000	233.81	270.86	385.85														
H	-0.772481	1.207820	0.000000	769.52	966.23	1031.20														
C	0.026520	-0.222526	1.201868	1097.24	1186.45	1201.06														
H	0.966394	-0.784821	1.257905	1266.19	1428.58	1456.54														
H	-0.031534	0.416904	2.087744	1464.20	1475.98	1483.69														
H	-0.800557	-0.954905	1.242653	1504.92	1506.24	2951.88														
C	0.026520	-0.222526	-1.201868	2953.11	3059.12	3061.99														
H	0.966394	-0.784821	-1.257905	3116.99	3117.07	3572.07														
H	-0.800557	-0.954905	-1.242653																	
DMA-1																				
N	0.000066	0.641663	0.000000	102.96	164.17	436.44	N	0.092419	0.479615	-0.126718										
C	0.000009	-0.165643	1.182709	936.30	949.03	1010.87	H	0.117274	1.426561	0.217539	195.31	325.64	389.92							
H	0.883372	-0.826696	1.207852	1028.21	1206.19	1232.09	C	1.243815	-0.246856	0.072780	574.29	624.27	986.04							
H	0.000274	0.458901	2.079675	1385.68	1405.47	1449.32	H	1.218676	-1.291046	-0.216039	1039.37	1135.07	1254.69							
H	-0.883756	-0.826156	1.208050	1459.71	1477.06	1479.58	H	2.184296	0.288091	0.054187	1314.67	1436.16	1464.69							
C	0.000009	-0.165643	-1.182709	2955.62	2962.83	3011.04	C	-1.179396	-0.185722	0.032116	1472.32	1491.08	1540.57							
H	0.000274	0.458901	-2.079675	3015.41	3117.42	3118.16	H	-1.989840	0.475733	-0.285365	2989.82	3075.66	3128.97							
H	0.883372	-0.826696	-1.207852				H	-1.198118	-1.074371	-0.608451	3171.62	3290.01	3634.08							
H	-0.883756	-0.826156	-1.208050				H	-1.367570	-0.510489	1.067384										
R1 DMA + H																				
TS1-1						TS1-2														
N	0.000001	0.352885	-0.421430	-1752.31			N	0.094092	-0.609281	-0.164567	-1696.20									
H	-0.000019	1.476067	0.023956	189.05	228.35	357.40	H	0.083412	-0.949797	-1.116159	186.82	213.74	297.95							
H	-0.000128	2.217696	0.658388	381.98	409.67	920.92	H	-1.405989	1.975547	-0.930039	411.27	504.30	731.77							
C	-1.198098	-0.281331	0.087043	986.06	1017.01	1080.12	C	-1.144176	-0.041750	0.212389	983.67	1040.73	1112.21							
H	-2.078645	0.303859	-0.192145	1164.98	1182.63	1227.13	H	-1.996383	-0.673282	-0.048747	1176.49	1230.31	1263.98							
H	-1.285251	-1.273590	-0.375863	1354.23	1410.98	1432.55	H	-1.159839	0.229261	1.273306	1286.76	1363.93	1373.13							
H	-1.189625	-0.424410	1.179555	1454.52	1472.56	1474.52	H	-1.335215	1.038742	-0.374141	1436.24	1464.06	1471.41							
C	1.198111	-0.281302	0.087050	1490.76	1618.54	2984.23	C	1.233848	0.247093	0.091629	1487.77	1512.12	2973.54							
H	2.078636	0.303960	-0.192054	2985.41	3059.67	3059.98	H	2.153490	-0.238900	-0.244616	3061.01	3074.31	3130.00							
H	1.189601	-0.424462	1.179550	3124.61			H	1.146789	1.230179	-0.402220	3150.71		3597.36							
H	1.285350	-1.273517	-0.375933				H	1.317056	0.421155	1.170479										
R2 DMA + CH ₃																				
TS2-1						TS2-2														
N	0.446421	0.000002	-0.560292	-1948.23			N	1.118350	0.417552	-0.370453	-1810.81									
H	-0.762475	-0.000372	-0.451654	45.42	115.91	147.00	H	1.021791	0.406020	-1.376729	83.07	99.45	125.84							
C	-2.033407	-0.000262	0.069358	202.80	240.69	404.01	C	-2.222556	-0.430431	-0.070977	240.73	347.24	376.22							
C	0.883084	-1.193203	0.132614	530.02	542.53	560.64	C	1.370144	-0.906618	0.159673	482.04	545.74	631.91							
H	0.444019	-2.080586	-0.333056	945.66	1028.59	1081.88	H	2.192273	-1.380167	-0.383910	742.73	984.15	1047.17							
H	1.976000	-1.272627	0.053843	1099.21	1143.66	1201.74	H	1.666264	-0.820863	1.211740	1084.82	1122.23	1176.29							
H	0.629327	-1.190438	1.207548	1225.71	1341.22	1405.10	H	0.486031	-1.565881	0.113526	1227.31	1279.63	1395.45							
C	0.882455	1.193466	0.132592	1411.19	1422.85	1433.12	C	0.039188	1.090198	0.257325	1405.06	1432.22	1435.94							
H	0.443114	2.080624	-0.333251	1457.98	1471.92	1474.72	H	-0.164824	2.064632	-0.193093	1442.65	1465.91	1471.54							
H	0.628457	1.190690	1.207466	1490.31	1490.70	2960.90	H	-1.043209	0.419647	0.144518	1486.78	1510.06	2970.38							
H	1.975354	1.273353	0.054065	2961.34	3050.89	3050.96	H	0.196033	1.178730	1.337748	3055.26	3066.05	3074.33							
H	-2.480175	-0.913120	-0.320940	3071.26	3111.46	3111.81	H	-3.032093	0.284357	-0.203490	3125.49	3145.07	3219.08							
H	-2.479165	0.913860	-0.319135	3211.50			H	-1.974376	-0.997623	-0.966720	3226.01		3594.12							
H	-1.892189	-0.001408	1.149773				H	-2.297001	-1.030614	0.833459										
R3 DMA + OH																				
RC3																				
N	-0.390048	0.000032	0.431628	36.31	70.32	190.42														
H	-0.564013	-0.000007	1.430111	211.35	277.81	391.81														

C	-0.950356	-1.207320	-0.159589	576.63 712.38 875.73					
H	-0.664047	-1.255139	-1.216085	960.01 1030.26 1095.83					
H	-0.543841	-2.091843	0.338281	1187.34 1205.04 1264.44					
H	-2.050608	-1.241883	-0.106069	1429.51 1456.63 1461.22					
C	-0.951033	1.207052	-0.159622	1474.62 1485.68 1503.56					
H	-0.545043	2.091816	0.338246	1505.86 2986.63 2986.90					
H	-0.664720	1.255022	-1.216110	3078.77 3081.72 3129.27					
H	-2.051307	1.240982	-0.106129	3129.31 3443.41 3567.39					
O	2.465414	0.000269	-0.086211						
H	1.498940	0.000286	0.121316						
TS3-1				TS3-2					
N	-0.390301	0.016511	-0.514086	-375.05	N	1.135391	0.366048	-0.350319	-465.41
H	0.569295	-0.026432	-0.888422	108.44 119.16 179.31	H	1.074696	0.366328	-1.359706	87.69 95.44 146.82
C	-0.855993	-1.185669	0.123515	198.96 212.17 322.03	C	0.086027	1.132454	0.234121	247.87 303.65 393.73
H	-1.952329	-1.222531	0.081217	463.08 606.03 961.70	H	0.237219	1.222439	1.316405	562.83 732.32 970.29
H	-0.462058	-2.062610	-0.396008	1046.25 1096.55 1140.20	H	0.023603	2.130260	-0.209531	1029.96 1053.79 1129.24
H	-0.569649	-1.239767	1.188204	1217.82 1253.45 1424.74	H	-0.929858	0.636458	0.081677	1215.80 1264.98 1393.73
C	-0.720313	1.246579	0.157724	1441.87 1455.31 1467.15	C	1.222134	-0.981846	0.173149	1433.49 1441.56 1451.13
H	-0.224950	2.082564	-0.339255	1471.14 1496.21 1504.99	H	2.008636	-1.536874	-0.345168	1471.96 1492.35 1511.38
H	-1.806451	1.402656	0.117827	2964.32 2991.25 3051.41	H	1.484390	-0.938516	1.236825	2090.22 2974.74 3053.15
H	-0.413028	1.239800	1.215112	3059.75 3120.59 3137.89	H	0.268915	-1.529846	0.077916	3069.34 3123.92 3128.35
O	1.905875	0.007665	0.033328	3151.14 3824.29	O	-2.177575	-0.427472	-0.187428	3597.05 3803.13
H	1.802115	-0.716035	0.665868		H	-2.543707	-0.396458	0.709620	
R4 DMA + HO ₂									
RC4									
N	0.920743	0.000202	0.540745						
H	1.479722	0.000506	1.386544	64.28 84.53 125.26					
O	-1.863203	-0.000939	-0.684879	184.60 211.52 241.58					
O	-1.774378	0.001146	0.614929	306.23 402.25 858.92					
H	-0.783376	0.001085	0.790135	890.67 953.96 1033.19					
C	1.201131	1.207773	-0.232133	1095.43 1179.19 1214.94					
H	0.519087	1.239085	-1.087851	1267.26 1290.56 1427.79					
H	1.020811	2.094970	0.381167	1455.29 1455.63 1477.63					
H	2.235561	1.237559	-0.607358	1488.83 1500.13 1501.55					
C	1.200580	-1.208214	-0.230962	1651.13 2973.57 2999.42					
H	2.234934	-1.238745	-0.606348	3012.24 3090.85 3093.59					
H	1.020052	-2.094749	0.383231	3131.94 3132.17 3558.06					
H	0.518403	-1.240136	-1.086559						
TS4-1				PC4-1					
N	0.908972	-0.014593	-0.574596	-2165.95	N	-0.899895	-0.172590	-0.041470	
H	-0.273855	-0.042806	-0.872940	68.75 131.18 168.95	H	0.862663	-0.770313	-0.294404	26.12 71.39 81.25
O	-1.471323	-0.075019	-0.723324	183.15 213.02 353.95	O	1.835066	-0.789015	-0.396486	99.26 125.62 181.72
O	-1.698264	-0.047035	0.648139	396.52 422.35 626.95	O	2.195609	0.389306	0.312971	221.77 293.50 445.61
H	-2.012739	0.850585	0.800524	957.93 1023.92 1026.90	H	2.627223	0.027586	1.092463	734.69 957.82 970.17
C	1.156074	1.202473	0.147179	1042.21 1062.72 1190.31	C	-2.183685	-0.758594	0.193759	1009.98 1027.90 1030.06
H	2.215081	1.256700	0.435311	1231.19 1349.19 1394.34	H	-2.874028	-0.523851	-0.633321	1217.27 1241.03 1384.54
H	0.906285	2.070494	-0.467957	1402.20 1411.99 1447.38	H	-2.106002	-1.843463	0.295562	1385.32 1405.46 1448.45
H	0.564865	1.232621	1.081510	1461.82 1471.78 1488.86	H	-2.638361	-0.342304	1.107791	1457.76 1475.63 1482.84
C	1.161832	-1.177959	0.233060	1572.73 2949.54 2965.53	C	-0.958102	1.251871	-0.184264	1568.11 2967.03 2974.15
H	0.505799	-1.179457	1.122295	3047.26 3056.20 3129.41	H	-1.426629	1.713310	0.700627	3023.38 3029.07 3130.49
H	0.979131	-2.087632	-0.343143	3137.44 3837.96	H	0.045279	1.662184	-0.317636	3138.18 3583.32 3869.96
H	2.201890	-1.169006	0.586625		H	-1.585555	1.522988	-1.049641	
TS4-2				PC4-2					
N	1.219121	0.135016	0.553986	-1440.95	N	-1.110855	0.179771	-0.537201	57.07 88.13 142.86
H	0.777994	-0.179485	1.407449	103.69 128.09 151.86	H	-0.384691	-0.031628	-1.207910	146.73 210.87 225.24
O	-1.606224	0.222155	-0.650354	198.16 320.34 393.25	O	1.611940	-0.295635	0.779910	268.67 406.14 409.28
O	-1.587008	-0.646346	0.430377	445.32 505.95 603.19	O	1.851395	-0.157754	-0.612534	610.37 698.67 731.68
H	-2.226442	-0.261602	1.039545	699.80 988.76 1049.94	H	2.699681	0.296108	-0.628114	990.18 1028.41 1047.21
C	0.622078	1.271153	0.008572	1065.22 1121.92 1180.32	C	-0.886061	1.303039	0.214163	1136.39 1256.55 1330.79
H	1.151430	1.636642	-0.876511	1250.04 1293.74 1316.68	H	-1.606587	1.519979	0.996234	1382.92 1435.59 1466.61
H	-0.523868	0.924987	-0.425123	1392.93 1435.38 1459.84	H	0.884526	0.343222	0.913345	1474.72 1488.63 1513.43

H	0.440607	2.058211	0.743911	1472.83 1485.69 1518.05	H	-0.383380	2.129101	-0.277037	1555.42 2996.68 3084.83
C	1.490533	-0.947174	-0.369446	1526.59 3008.65 3067.82	C	-1.702373	-0.978031	0.094064	3132.96 3151.84 3266.54
H	2.004943	-1.759124	0.150273	3088.57 3136.10 3159.61	H	-1.987080	-1.710895	-0.664886	3587.57 3614.68 3866.01
H	0.567344	-1.335820	-0.824934	3610.68 3834.86	H	-1.016653	-1.457018	0.809799	
H	2.144338	-0.579270	-1.167456		H	-2.605911	-0.670200	0.630607	
R5 DMA + NH ₂									
RC5									
N	0.677443	0.000004	0.577226						
H	1.367020	0.000037	1.318154	39.38 88.48 129.23					
N	-2.302576	0.000004	-0.129956	180.66 237.83 282.05					
H	-3.135117	-0.000364	0.466899	317.54 366.96 396.04					
H	-1.503700	-0.000038	0.521411	811.91 960.63 1035.05					
C	0.808017	1.202110	-0.229465	1098.31 1188.43 1196.80					
H	-0.027918	1.244276	-0.938431	1267.84 1428.20 1456.55					
H	0.757298	2.090594	0.407008	1460.43 1477.61 1485.21					
H	1.745793	1.237393	-0.810379	1507.23 1507.76 1540.83					
C	0.808135	-1.202076	-0.229483	2976.79 2977.52 3073.53					
H	1.745743	-1.237085	-0.810688	3076.54 3125.50 3125.59					
H	0.757894	-2.090557	0.407031	3358.55 3487.09 3567.83					
H	-0.027994	-1.244514	-0.938207						
TS5-1					PC5-1				
N	-0.377528	0.000386	-0.512493		N	-0.541657	-0.250273	-0.005527	
H	0.790800	-0.000825	-0.560377	-1813.87	H	1.667821	-0.619600	-0.004394	60.94 95.54 99.47
N	2.013967	-0.002019	-0.043362	52.18 135.82 169.16	N	2.605052	-0.224374	0.000952	135.30 144.29 156.99
H	2.022075	-0.801825	0.592086	210.48 232.29 394.03	H	3.097075	-0.568486	-0.813777	212.13 357.18 439.52
H	2.034339	0.818709	0.564570	533.28 630.34 747.33	H	3.088906	-0.571406	0.819331	949.65 952.14 1009.59
C	-0.856525	-1.200140	0.128480	955.87 1040.13 1082.39	C	-0.456834	1.180681	0.000575	1028.59 1060.29 1211.52
H	-1.935701	-1.300950	-0.054490	1132.91 1217.71 1234.00	H	-0.965813	1.596200	0.886995	1235.46 1384.14 1403.58
H	-0.358357	-2.076048	-0.297216	1369.49 1413.17 1433.28	H	0.588798	1.499496	-0.001205	1449.31 1461.44 1477.86
H	-0.710625	-1.197445	1.222772	1457.29 1472.38 1473.32	H	-0.970905	1.603351	-0.879507	1483.31 1658.60 1678.43
C	-0.857979	1.199754	0.129558	1491.66 1560.22 1607.18	C	-1.898003	-0.707742	0.001514	2958.68 2966.85 3014.17
H	-0.708666	1.197780	1.223352	2963.92 2964.48 3044.98	H	-2.447021	-0.319062	-0.872850	3019.92 3121.78 3126.80
H	-0.363886	2.077137	-0.297856	3045.54 3116.27 3116.89	H	-1.942694	-1.799693	-0.008128	3484.55 3615.81 3655.97
H	-1.938027	1.297217	-0.050081	3452.14 3547.06	H	-2.430912	-0.335910	0.893035	
TS5-2					PC5-2				
N	-1.082525	0.442784	-0.360508		N	0.639663	0.019427	0.377194	
H	-0.986402	0.449807	-1.367034	-1108.17	H	-0.247093	-0.442129	0.546480	66.61 82.66 106.08
N	2.120744	-0.550620	-0.158618	100.07 128.29 150.33	N	-2.380795	-0.339096	-0.027629	157.02 189.86 233.35
H	2.406592	-0.734158	0.806945	241.59 375.65 396.94	H	-2.863115	-1.118739	-0.457381	274.32 377.32 408.05
H	2.781624	0.158518	-0.487591	573.22 696.52 765.72	H	-3.051522	0.158647	0.544801	623.71 780.94 992.12
C	-1.383429	-0.885444	0.138275	827.61 989.94 1049.47	C	1.701314	-0.822557	-0.113560	1048.95 1072.34 1132.43
H	-1.668430	-0.814040	1.194384	1126.86 1215.45 1258.81	H	2.660043	-0.303531	0.000191	1256.21 1335.19 1435.40
H	-2.228781	-1.308497	-0.410900	1297.53 1369.76 1434.21	H	1.745784	-1.745829	0.470376	1470.23 1474.01 1493.34
H	-0.522654	-1.568696	0.057857	1454.30 1467.61 1473.74	H	1.584208	-1.083229	-1.178243	1565.06 1657.62 1664.88
C	0.020412	1.058497	0.277915	1489.84 1513.50 1548.46	C	0.519445	1.290337	-0.122702	2977.64 3066.40 3125.10
H	1.015115	0.364624	0.128252	2987.60 3054.51 3072.83	H	-2.077974	0.286398	-0.767579	3153.95 3266.66 3507.19
H	0.249004	2.040147	-0.145396	3127.41 3138.65 3433.74	H	-0.318397	1.881221	0.229026	3559.04 3633.16 3652.49
H	-0.135501	1.128823	1.360229	3531.79 3595.98	H	1.431432	1.798198	-0.417056	
R6 DMA + O									
RC6									
N	0.268292	0.020425	-0.478200						
H	0.435904	0.057972	-1.473363	87.06 120.81 185.02					
C	0.968924	-1.058217	0.176614	207.04 276.60 379.46					
H	0.549966	-1.189843	1.180518	690.74 963.73 1036.98					
H	0.822090	-1.990446	-0.375121	1094.30 1176.11 1214.11					
H	2.051933	-0.870943	0.275785	1264.23 1427.03 1450.96					
C	0.410878	1.303861	0.166275	1459.79 1472.63 1479.32					
H	-0.139106	2.065714	-0.392529	1497.67 1503.42 2971.24					
H	-0.021683	1.242393	1.171993	2973.64 3068.83 3077.82					
H	1.462293	1.623337	0.265419	3125.71 3129.96 3616.27					
O	-1.914781	-0.319378	0.079670						

TS6-1							PC6-1						
N	0.500534	0.276759	0.000000		-1488.08		N	-0.282051	0.000015	0.000015			
H	0.520546	-0.883374	0.000000	118.39	145.05	159.61	H	1.654240	0.000036	0.000036	49.23	77.69	85.40
C	-0.118415	0.776489	-1.202505	219.77	396.54	545.82	C	-1.078616	-1.189751	-1.189751	171.21	174.81	444.52
H	0.060148	1.858451	-1.268068	951.14	1019.41	1064.85	H	-1.737194	-1.215655	-1.215655	560.31	632.70	957.21
H	0.319673	0.294828	-2.079703	1096.46	1168.19	1231.99	H	-0.447566	-2.081494	-2.081494	964.28	1012.22	1029.55
H	-1.207809	0.617163	-1.205849	1316.30	1408.61	1425.29	H	-1.737840	-1.215502	-1.215502	1216.13	1237.71	1386.19
C	-0.118415	0.776489	1.202505	1443.97	1448.79	1466.15	C	-1.078719	1.189711	1.189711	1406.80	1451.63	1456.14
H	0.319673	0.294828	2.079703	1469.02	1493.83	2991.35	H	-0.447746	2.081508	2.081508	1476.86	1481.19	2968.08
H	0.060148	1.858451	1.268068	2994.13	3063.07	3064.37	H	-1.737424	1.215491	1.215491	2974.22	3025.42	3030.36
H	-1.207809	0.617163	1.205849	3133.53	3133.87		H	-1.737820	1.215473	1.215473	3126.16	3126.79	3544.85
O	-0.118415	-1.989086	0.000000				O	2.638715	0.000035	0.000035			
TS6-2							PC6-2						
N	0.993578	0.441456	-0.357216		-351.74		N	0.674124	0.199845	-0.507907			
H	0.952487	0.461219	-1.366498	83.05	122.22	234.28	H	0.167971	0.035983	-1.364702	77.85	109.00	144.01
C	-0.128221	1.050480	0.246494	365.25	398.70	699.67	C	0.308547	1.309530	0.210965	207.34	357.80	399.62
H	0.009174	1.147462	1.329795	977.28	1038.79	1053.39	H	0.835036	1.475442	1.144850	457.46	617.07	694.77
H	-0.358909	2.022480	-0.197241	1128.99	1224.10	1263.76	H	-0.049717	2.165261	-0.349394	985.10	1040.32	1098.18
H	-1.094930	0.396082	0.131594	1352.26	1395.11	1436.65	H	-1.646811	0.323757	0.488537	1234.32	1270.72	1349.84
C	1.317267	-0.872120	0.157788	1450.55	1470.70	1488.25	C	1.128475	-0.984100	0.185666	1445.54	1469.69	1486.57
H	2.187171	-1.276857	-0.365577	1511.38	1668.31	2980.12	H	1.540639	-1.697866	-0.531636	1547.22	1822.16	3010.98
H	1.567946	-0.789700	1.221346	3055.09	3077.39	3133.97	H	1.924362	-0.703413	0.883715	3090.57	3136.01	3156.36
H	0.476105	-1.578634	0.059883	3139.53	3610.43		H	0.322382	-1.473628	0.751225	3273.71	3607.01	3639.15
O	-2.228546	-0.567800	-0.092310				O	-2.054358	-0.434629	0.019120			
R7 DMA + C ₂ H ₅													
TS7-1							TS7-2						
N	-1.045426	-0.068633	-0.574375		-1959.35		N	-1.404526	0.083241	-0.572447			
H	0.166096	-0.255514	-0.791081	68.39	129.30	165.60	H	-0.945815	-0.303038	-1.386981			
C	1.497936	-0.435271	-0.666291	205.26	222.13	240.18	C	1.705414	0.324964	0.664830	85.75	110.17	126.47
C	1.951516	0.249855	0.593449	296.10	416.69	544.72	C	1.903538	-0.607986	-0.498261	184.93	212.33	272.58
H	1.575581	-1.524703	-0.653705	561.60	833.65	869.30	H	2.369478	1.189813	0.694969	381.25	418.64	510.56
H	1.882190	-0.011277	-1.595883	944.88	1029.32	1043.96	H	1.594070	-0.147259	1.641696	624.62	724.78	834.65
H	1.822907	1.335775	0.530382	1084.01	1109.62	1153.51	H	1.168436	-1.422454	-0.487959	871.71	982.97	1042.94
H	1.388933	-0.102935	1.466956	1204.16	1220.05	1226.20	H	1.799991	-0.077009	-1.453506	1056.96	1116.13	1133.37
H	3.013606	0.059448	0.800762	1370.99	1390.51	1408.80	H	2.897641	-1.076374	-0.501331	1169.90	1215.07	1227.43
C	-1.397718	-1.064412	0.412084	1431.91	1452.57	1456.37	C	-1.627196	-0.922618	0.444905	1278.73	1389.94	1420.19
H	-1.205896	-2.067958	0.019995	1466.84	1469.56	1480.38	H	-2.103726	-1.803645	0.006081	1433.32	1446.34	1454.31
H	-0.856028	-0.943826	1.368240	1481.07	1490.35	1494.58	H	-0.699239	-1.237200	0.954947	1467.43	1470.79	1474.53
H	-2.471215	-0.987256	0.636438	2952.94	2959.53	3014.15	H	-2.302660	-0.517953	1.207663	1481.82	1488.32	1511.02
C	-1.131567	1.265237	-0.024640	3038.27	3042.03	3074.51	C	-0.740336	1.243057	-0.096022	2966.32	3003.85	3058.41
H	-0.688538	1.987416	-0.718088	3087.94	3102.35	3106.99	H	-0.545174	1.969343	-0.888558	3061.79	3067.10	3087.21
H	-2.190045	1.531699	0.109041	3108.06	3170.62		H	-1.276631	1.700364	0.741847	3094.27	3121.19	3148.81
H	-0.640618	1.367108	0.959966				H	0.426788	0.918216	0.385547			
R8 DMA + O ₂													
TS8-1							PC8-1						
C	-1.143235	1.189255	0.169121		-2272.01		C	0.976070	1.297510	-0.000113			
N	-0.854509	0.000149	-0.578020	67.73	131.43	161.05	N	0.803021	-0.125098	-0.000756	29.46	81.54	98.72
C	-1.143975	-1.189022	0.168706	178.90	211.47	348.11	C	2.042997	-0.839570	0.000312	102.16	141.22	187.82
H	-0.980757	2.080188	-0.442082	418.37	661.48	948.94	H	0.006341	1.798423	-0.000733	247.52	453.13	693.80
H	-0.471741	1.234990	1.048834	1005.06	1018.16	1037.70	H	1.555951	1.613070	-0.882920	961.99	977.70	1010.88
H	-2.174987	1.177233	0.546368	1170.94	1225.90	1303.66	H	1.554370	1.612406	0.883986	1029.32	1222.50	1240.52
H	0.454505	-0.000078	-0.813013	1339.63	1383.24	1406.34	H	-0.866786	-0.728435	-0.000496	1289.53	1384.43	1405.05
H	-2.175512	-1.176233	0.546524	1448.93	1454.99	1473.71	H	2.641418	-0.570972	0.886059	1450.17	1456.97	1478.93
H	-0.982612	-2.079833	-0.442969	1485.00	1652.96	2937.48	H	1.874250	-1.918697	-0.002997	1481.17	1628.56	2972.81
H	-0.472077	-1.235773	1.048057	2941.87	3046.35	3052.16	H	2.646578	-0.565977	-0.880346	2978.71	3029.57	3035.00
O	1.572177	0.000287	-0.598321	3131.64	3132.75		O	-1.857625	-0.809736	-0.000291	3131.56	3146.13	3252.82
O	1.741323	-0.000654	0.664254				O	-2.285833	0.420764	0.000485			
TS8-2							PC8-2						
C	1.538558	-0.899631	-0.353234		-1863.11		C	1.473768	-1.012069	-0.343135	50.24	90.65	122.63
N	1.120528	0.164412	0.532794	95.08	120.13	142.60	N	1.167691	0.100063	0.528339	153.09	216.13	229.57
C	0.543365	1.287228	-0.021363	201.12	335.64	416.95	C	0.830902	1.308138	-0.022711	399.60	423.94	658.69

H	2.089840	-1.656025	0.210031	489.95	566.12	686.30	H	1.918104	-1.826094	0.234328	704.98	794.01	990.54
H	2.201653	-0.485966	-1.119773	989.61	1049.63	1057.89	H	2.198429	-0.686185	-1.095928	1048.54	1135.31	1256.82
H	0.683084	-1.380289	-0.849801	1135.00	1176.91	1263.68	H	0.579657	-1.392556	-0.859689	1290.03	1332.63	1435.86
H	0.687607	-0.154033	1.388887	1312.95	1368.92	1435.92	H	0.650932	-0.151966	1.358863	1467.60	1474.63	1485.17
H	-0.760152	0.821433	-0.426495	1463.46	1474.79	1486.81	H	-0.945449	0.734050	-0.538518	1549.56	1556.65	3003.03
H	0.302366	2.072405	0.695458	1543.94	1584.37	3010.82	H	0.574380	2.102950	0.670759	3055.77	3091.31	3135.73
H	1.032688	1.632231	-0.933671	3091.07	3094.37	3138.26	H	1.349834	1.576616	-0.939064	3139.31	3249.65	3621.65
O	-1.728269	0.168992	-0.482813		3193.28	3620.34	O	-1.792326	0.200325	-0.548151			
O	-1.593271	-0.709770	0.426986				O	-1.748643	-0.554533	0.506395			

R9 DMA + Cl (M05-2X/ma-ZTVP)

R9													
C	0.950272	1.502196	-0.246888										
H	0.726230	1.401154	-1.305263	152.11 171.50 201.59									
H	1.965073	1.890144	-0.126730	222.28 369.15 396.30									
H	0.236332	2.188705	0.194512	706.50 952.96 1059.37									
N	0.809446	0.204498	0.372872	1095.08 1185.16 1213.24									
H	0.736143	0.221308	1.376742	1283.19 1457.48 1476.32									
C	1.622637	-0.865612	-0.157905	1480.75 1503.99 1515.88									
H	1.366447	-1.792086	0.343942	1521.52 1522.72 3065.76									
H	1.400033	-0.970846	-1.216165	3068.10 3160.77 3162.44									
H	2.687430	-0.653869	-0.030812	3208.36 3208.77 3636.32									
Cl	-1.412256	-0.442464	-0.039784										

TS9-1							PC9-1						
N	0.818002	-0.000021	-0.283136	-763.61							N	0.850857	-0.000118
H	-0.452142	-0.000118	-0.318819	27.45 62.38 74.24							H	-0.737188	-0.000280
C	1.477477	-1.218662	0.067025	138.43 368.41 492.41							C	1.624631	-1.202396
H	1.667915	-1.245398	1.143443	901.62 992.38 1034.31							H	2.268966	-1.234417
H	0.857319	-2.062916	-0.213203	1046.19 1104.17 1175.05							H	0.971662	-2.068906
H	2.442846	-1.272091	-0.441110	1261.98 1353.90 1424.66							H	2.278139	-1.231422
C	1.477198	1.218764	0.067067	1448.15 1480.55 1488.70							C	1.623708	1.202762
H	0.855446	2.062781	-0.210328	1505.93 1517.81 3054.91							H	0.970031	2.068748
H	1.670906	1.244227	1.142915	3061.35 3106.61 3112.52							H	2.269178	1.234649
H	2.440983	1.273837	-0.443934	3203.05 3203.55							H	2.276018	1.232906
Cl	-1.937490	-0.000046	0.030496								Cl	-2.102520	-0.000156

TS9-2							PC9-2						
C	0.666731	1.009101	-0.168400	-134.19							C	0.766895	1.211687
H	0.174700	0.589997	-1.048158	29.05 73.15 230.21							H	0.597840	2.152762
H	1.334425	1.806988	-0.520342	271.32 379.39 761.18							H	0.893102	1.225615
H	-0.090125	1.457928	0.472714	965.05 1048.41 1114.70							H	-0.804816	0.523247
N	1.350490	-0.051540	0.540904	1198.77 1202.96 1283.11							N	1.518196	0.288403
H	1.703021	0.291224	1.420968	1454.15 1485.89 1490.40							H	1.406183	0.285231
C	2.429624	-0.624724	-0.241544	1509.47 1520.78 1535.37							C	1.736499	-1.013759
H	2.948031	-1.380212	0.342754	1539.67 3003.61 3015.29							H	2.486760	-1.553276
H	2.010155	-1.109756	-1.121772	3078.38 3120.80 3134.27							H	2.104183	-0.873136
H	3.159208	0.120351	-0.583298	3170.39 3592.67							H	0.816553	-1.599307
Cl	-2.310057	-0.218942	-0.017031								Cl	-1.949855	-0.198089

Table S6.

Calculated MP-CVT/SCT rate constants for the H-abstraction reactions from MA by H/CH₃/OH/HO₂/NH₂/O/C₂H₅/O₂/Cl radicals. Units are in cm³ mol⁻¹ s⁻¹.

T / K	k_{1-1}^{MA}	k_{1-2}^{MA}	k_{2-1}^{MA}	k_{2-2}^{MA}	k_{3-1}^{MA}	k_{3-2}^{MA}	k_{4-1}^{MA}	k_{4-2}^{MA}	k_{5-1}^{MA}	k_{5-2}^{MA}
200	1.008E07	4.403E10	2.781E+02	9.491E+02	5.504E+12	1.594E+13	1.075E-06	6.663E+00	2.199E+07	6.371E+06
250	4.414E07	4.852E10	5.334E+03	1.347E+04	3.030E+12	1.508E+13	1.040E-03	2.035E+02	4.287E+07	3.078E+07
300	1.575E08	5.653E10	4.574E+04	1.106E+05	2.323E+12	1.090E+13	1.060E-01	2.387E+03	9.141E+07	1.159E+08
350	5.403E08	7.128E10	2.873E+05	6.957E+05	2.304E+12	8.443E+12	5.633E+00	2.554E+04	2.169E+08	3.539E+08
400	1.464E09	8.713E10	1.169E+06	2.904E+06	2.271E+12	6.527E+12	1.018E+02	1.465E+05	4.370E+08	8.849E+08
450	3.432E09	1.056E11	3.734E+06	9.538E+06	2.313E+12	5.287E+12	1.055E+03	6.236E+05	8.109E+08	1.930E+09
500	7.150E09	1.272E11	1.000E+07	2.619E+07	2.410E+12	4.474E+12	7.329E+03	2.125E+06	1.406E+09	3.797E+09
550	1.349E10	1.517E11	2.336E+07	6.244E+07	2.541E+12	3.925E+12	3.764E+04	6.089E+06	2.295E+09	6.872E+09
600	2.352E10	1.795E11	4.906E+07	1.333E+08	2.699E+12	3.542E+12	1.534E+05	1.525E+07	3.570E+09	1.165E+10
650	3.837E10	2.104E11	9.449E+07	2.600E+08	2.877E+12	3.279E+12	5.200E+05	3.423E+07	5.325E+09	1.867E+10
700	5.934E10	2.450E11	1.701E+08	4.716E+08	3.077E+12	3.106E+12	1.523E+06	7.044E+07	7.671E+09	2.864E+10
750	8.761E10	2.829E11	2.889E+08	8.039E+08	3.290E+12	2.983E+12	3.951E+06	1.346E+08	1.072E+10	4.224E+10
800	1.247E11	3.247E11	4.668E+08	1.303E+09	3.520E+12	2.916E+12	9.279E+06	2.422E+08	1.459E+10	6.033E+10
850	1.716E11	3.699E11	7.230E+08	2.019E+09	3.761E+12	2.881E+12	2.002E+07	4.134E+08	1.942E+10	8.369E+10
900	2.297E11	4.191E11	1.081E+09	3.014E+09	4.016E+12	2.873E+12	4.022E+07	6.752E+08	2.534E+10	1.133E+11
950	3.002E11	4.723E11	1.566E+09	4.359E+09	4.289E+12	2.886E+12	7.602E+07	1.062E+09	3.250E+10	1.501E+11
1000	3.843E11	5.292E11	2.208E+09	6.123E+09	4.570E+12	2.915E+12	1.362E+08	1.614E+09	4.099E+10	1.951E+11
1100	5.965E11	6.545E11	4.091E+09	1.124E+10	5.156E+12	3.010E+12	3.822E+08	3.424E+09	6.260E+10	3.133E+11
1200	8.740E11	7.953E11	7.014E+09	1.906E+10	5.786E+12	3.146E+12	9.283E+08	6.617E+09	9.144E+10	4.761E+11
1300	1.221E12	9.514E11	1.130E+10	3.036E+10	6.456E+12	3.314E+12	2.010E+09	1.185E+10	1.285E+11	6.914E+11
1400	1.645E12	1.122E12	1.733E+10	4.579E+10	7.165E+12	3.507E+12	3.966E+09	1.997E+10	1.747E+11	9.663E+11
1500	2.148E12	1.309E12	2.543E+10	6.638E+10	7.916E+12	3.724E+12	7.254E+09	3.198E+10	2.313E+11	1.310E+12
1600	2.731E12	1.510E12	3.606E+10	9.287E+10	8.710E+12	3.961E+12	1.246E+10	4.904E+10	2.995E+11	1.728E+12
1700	3.394E12	1.723E12	4.950E+10	1.258E+11	9.531E+12	4.211E+12	2.023E+10	7.237E+10	3.792E+11	2.225E+12
1800	4.143E12	1.952E12	6.633E+10	1.665E+11	1.040E+13	4.483E+12	3.147E+10	1.035E+11	4.727E+11	2.812E+12
1900	4.971E12	2.194E12	8.696E+10	2.152E+11	1.131E+13	4.769E+12	4.697E+10	1.440E+11	5.794E+11	3.490E+12
2000	5.877E12	2.457E12	1.115E+11	2.725E+11	1.225E+13	5.067E+12	6.777E+10	1.953E+11	7.012E+11	4.263E+12
T / K	k_{6-1}^{MA}	k_{6-2}^{MA}	k_{7-1}^{MA}	k_{7-2}^{MA}	k_{8-1}^{MA}	k_{8-2}^{MA}	k_{9-1}^{MA}	k_{9-2}^{MA}		
200	5.346E+10	1.722E+11	1.898E+04	1.508E+05	6.106E-37	1.453E-27	1.687E+14	1.687E+14		
250	6.381E+10	1.873E+11	7.672E+04	1.470E+05	1.720E-27	5.362E-20	1.301E+14	1.298E+14		
300	8.668E+10	2.004E+11	2.405E+05	2.780E+05	2.364E-21	4.399E-15	1.097E+14	1.084E+14		
350	1.368E+11	2.410E+11	7.284E+05	5.893E+05	1.442E-16	3.024E-11	9.852E+13	9.560E+13		
400	2.006E+11	2.848E+11	1.747E+06	1.390E+06	4.042E-13	1.811E-08	9.259E+13	8.684E+13		
450	2.858E+11	3.418E+11	3.701E+06	3.167E+06	1.961E-10	2.737E-06	8.977E+13	8.028E+13		
500	3.955E+11	4.138E+11	7.096E+06	6.724E+06	2.886E-08	1.578E-04	8.893E+13	7.504E+13		
550	5.316E+11	4.991E+11	1.254E+07	1.320E+07	1.758E-06	4.500E-03	8.935E+13	7.070E+13		
600	6.971E+11	6.020E+11	2.076E+07	2.410E+07	5.532E-05	7.545E-02	9.058E+13	6.705E+13		
650	8.930E+11	7.210E+11	3.246E+07	4.113E+07	1.040E-03	8.398E-01	9.240E+13	6.390E+13		
700	1.122E+12	8.580E+11	4.845E+07	6.633E+07	1.322E-02	6.768E+00	9.465E+13	6.139E+13		
750	1.386E+12	1.012E+12	6.946E+07	1.017E+08	1.210E-01	4.197E+01	9.717E+13	5.936E+13		
800	1.686E+12	1.184E+12	9.619E+07	1.494E+08	8.531E-01	2.107E+02	9.990E+13	5.776E+13		
850	2.022E+12	1.374E+12	1.293E+08	2.112E+08	4.831E+00	8.835E+02	1.027E+14	5.647E+13		
900	2.396E+12	1.582E+12	1.696E+08	2.898E+08	2.284E+01	3.204E+03	1.057E+14	5.554E+13		
950	2.808E+12	1.810E+12	2.173E+08	3.860E+08	9.259E+01	1.023E+04	1.087E+14	5.485E+13		
1000	3.261E+12	2.056E+12	2.727E+08	5.013E+08	3.294E+02	2.938E+04	1.118E+14	5.444E+13		
1100	4.278E+12	2.602E+12	4.089E+08	7.952E+08	3.013E+03	1.851E+05	1.180E+14	5.419E+13		
1200	5.450E+12	3.221E+12	5.793E+08	1.177E+09	1.954E+04	8.801E+05	1.242E+14	5.462E+13		
1300	6.774E+12	3.911E+12	7.861E+08	1.654E+09	9.698E+04	3.354E+06	1.303E+14	5.560E+13		
1400	8.250E+12	4.671E+12	1.026E+09	2.218E+09	3.894E+05	1.074E+07	1.365E+14	5.702E+13		
1500	9.883E+12	5.499E+12	1.299E+09	2.872E+09	1.319E+06	2.985E+07	1.426E+14	5.885E+13		
1600	1.165E+13	6.394E+12	1.606E+09	3.613E+09	3.884E+06	7.392E+07	1.485E+14	6.093E+13		
1700	1.355E+13	7.341E+12	1.936E+09	4.418E+09	1.017E+07	1.656E+08	1.542E+14	6.330E+13		
1800	1.559E+13	8.357E+12	2.300E+09	5.306E+09	2.417E+07	3.431E+08	1.599E+14	6.590E+13		
1900	1.776E+13	9.424E+12	2.686E+09	6.255E+09	5.286E+07	6.642E+08	1.653E+14	6.872E+13		
2000	2.004E+13	1.054E+13	3.091E+09	7.250E+09	1.076E+08	1.208E+09	1.704E+14	7.175E+13		

Table S7.

Calculated MP-CVT/SCT rate constants for the H-abstraction reactions from EA by H/CH₃/OH/HO₂/NH₂/O/C₂H₅/O₂/Cl radicals. Units are in cm³ mol⁻¹ s⁻¹.

T / K	k_{1-1}^{EA}	k_{1-2}^{EA}	k_{1-3}^{EA}	k_{2-1}^{EA}	k_{2-2}^{EA}	k_{2-3}^{EA}	k_{3-1}^{EA}	k_{3-2}^{EA}	k_{3-3}^{EA}	k_{4-1}^{EA}
200	2.324E+05	1.099E+10	7.288E+04	8.293E+02	9.248E+03	1.132E+01	8.364E+12	1.896E+13	1.261E+12	7.165E-07
250	1.839E+06	1.901E+10	9.204E+05	9.730E+03	1.031E+05	2.973E+02	4.219E+12	1.471E+13	3.330E+11	4.823E-04
300	1.013E+07	3.045E+10	6.577E+06	6.393E+04	6.354E+05	3.325E+03	2.979E+12	1.187E+13	1.746E+11	4.691E-02
350	4.871E+07	4.858E+10	3.695E+07	3.427E+05	3.110E+06	2.815E+04	2.751E+12	1.009E+13	1.559E+11	2.492E+00
400	1.735E+08	7.228E+10	1.431E+08	1.274E+06	1.056E+07	1.493E+05	2.610E+12	8.787E+12	1.540E+11	4.709E+01
450	5.107E+08	1.036E+11	4.427E+08	3.865E+06	2.936E+07	6.109E+05	2.604E+12	7.806E+12	1.680E+11	5.128E+02
500	1.288E+09	1.423E+11	1.154E+09	1.004E+07	7.033E+07	2.037E+06	2.679E+12	7.043E+12	1.930E+11	3.728E+03
550	2.869E+09	1.927E+11	2.630E+09	2.313E+07	1.502E+08	5.819E+06	2.807E+12	6.453E+12	2.273E+11	1.998E+04
600	5.776E+09	2.549E+11	5.389E+09	4.838E+07	2.931E+08	1.463E+07	2.975E+12	6.012E+12	2.707E+11	8.460E+04
650	1.070E+10	3.303E+11	1.013E+10	9.350E+07	5.317E+08	3.312E+07	3.174E+12	5.697E+12	3.233E+11	2.972E+05
700	1.852E+10	4.203E+11	1.777E+10	1.693E+08	9.084E+08	6.874E+07	3.401E+12	5.479E+12	3.855E+11	8.986E+05
750	3.028E+10	5.265E+11	2.938E+10	2.900E+08	1.476E+09	1.327E+08	3.656E+12	5.354E+12	4.577E+11	2.402E+06
800	4.719E+10	6.500E+11	4.623E+10	4.740E+08	2.298E+09	2.408E+08	3.937E+12	5.300E+12	5.406E+11	5.799E+06
850	7.056E+10	7.921E+11	6.977E+10	7.437E+08	3.450E+09	4.145E+08	4.243E+12	5.304E+12	6.345E+11	1.284E+07
900	1.018E+11	9.535E+11	1.015E+11	1.126E+09	5.015E+09	6.815E+08	4.573E+12	5.355E+12	7.394E+11	2.475E+07
950	1.426E+11	1.136E+12	1.433E+11	1.654E+09	7.092E+09	1.077E+09	4.931E+12	5.450E+12	8.571E+11	4.661E+07
1000	1.944E+11	1.340E+12	1.969E+11	2.365E+09	9.791E+09	1.644E+09	5.317E+12	5.585E+12	9.878E+11	8.339E+07
1100	3.376E+11	1.816E+12	3.467E+11	4.505E+09	1.751E+10	3.504E+09	6.171E+12	5.950E+12	1.289E+12	2.340E+08
1200	5.447E+11	2.394E+12	5.664E+11	7.939E+09	2.921E+10	6.776E+09	7.144E+12	6.431E+12	1.648E+12	5.414E+08
1300	8.281E+11	3.062E+12	8.712E+11	1.313E+10	4.602E+10	1.212E+10	8.242E+12	7.016E+12	2.068E+12	1.159E+09
1400	1.200E+12	3.829E+12	1.276E+12	2.057E+10	6.919E+10	2.032E+10	9.470E+12	7.698E+12	2.554E+12	2.268E+09
1500	1.672E+12	4.696E+12	1.795E+12	3.091E+10	1.000E+11	3.233E+10	1.083E+13	8.472E+12	3.109E+12	4.097E+09
1600	2.252E+12	5.660E+12	2.441E+12	4.474E+10	1.398E+11	4.916E+10	1.232E+13	9.327E+12	3.729E+12	6.962E+09
1700	2.949E+12	6.718E+12	3.223E+12	6.272E+10	1.898E+11	7.197E+10	1.392E+13	1.026E+13	4.427E+12	1.124E+10
1800	3.768E+12	7.870E+12	4.153E+12	8.552E+10	2.514E+11	1.020E+11	1.564E+13	1.127E+13	5.200E+12	1.735E+10
1900	4.718E+12	9.116E+12	5.240E+12	1.139E+11	3.262E+11	1.405E+11	1.748E+13	1.236E+13	6.052E+12	2.580E+10
2000	5.798E+12	1.049E+13	6.494E+12	1.484E+11	4.148E+11	1.889E+11	1.942E+13	1.352E+13	6.978E+12	3.711E+10
T / K	k_{4-2}^{EA}	k_{4-3}^{EA}	k_{5-1}^{EA}	k_{5-2}^{EA}	k_{5-3}^{EA}	k_{6-1}^{EA}	k_{6-2}^{EA}	k_{6-3}^{EA}	k_{7-1}^{EA}	k_{7-2}^{EA}
200	2.256E+01	2.256E+01	1.162E+07	1.382E+07	2.346E+04	1.437E+10	1.210E+12	1.067E+06	2.275E-02	4.254E+00
250	4.630E+02	4.630E+02	2.153E+07	4.669E+07	1.175E+05	1.733E+10	1.275E+12	9.766E+06	1.157E+00	8.867E+01
300	4.618E+03	4.618E+03	4.582E+07	1.201E+08	4.816E+05	2.526E+10	1.188E+12	4.763E+07	2.115E+01	1.028E+03
350	4.492E+04	4.492E+04	1.108E+08	3.042E+08	1.973E+06	4.352E+10	1.108E+12	1.939E+08	2.523E+02	8.772E+03
400	2.420E+05	2.420E+05	2.283E+08	6.327E+08	6.134E+06	6.845E+10	1.053E+12	5.637E+08	1.744E+03	4.752E+04
450	9.882E+05	9.882E+05	4.356E+08	1.200E+09	1.643E+07	1.039E+11	1.042E+12	1.376E+09	8.747E+03	1.962E+05
500	3.271E+06	3.271E+06	7.778E+08	2.122E+09	3.894E+07	1.521E+11	1.064E+12	2.952E+09	3.437E+04	6.575E+05
550	9.200E+06	9.200E+06	1.312E+09	3.539E+09	8.357E+07	2.152E+11	1.114E+12	5.733E+09	1.120E+05	1.876E+06
600	2.275E+07	2.275E+07	2.110E+09	5.626E+09	1.651E+08	2.953E+11	1.187E+12	1.030E+10	3.147E+05	4.706E+06
650	5.073E+07	5.073E+07	3.257E+09	8.587E+09	3.047E+08	3.945E+11	1.283E+12	1.735E+10	7.838E+05	1.064E+07
700	1.039E+08	1.039E+08	4.854E+09	1.266E+10	5.306E+08	5.148E+11	1.400E+12	2.774E+10	1.768E+06	2.207E+07
750	1.983E+08	1.983E+08	7.019E+09	1.811E+10	8.798E+08	6.582E+11	1.536E+12	4.244E+10	3.675E+06	4.263E+07
800	3.556E+08	3.556E+08	9.885E+09	2.523E+10	1.399E+09	8.264E+11	1.693E+12	6.254E+10	7.121E+06	7.744E+07
850	6.079E+08	6.079E+08	1.360E+10	3.436E+10	2.145E+09	1.021E+12	1.868E+12	8.921E+10	1.301E+07	1.335E+08
900	9.946E+08	9.946E+08	1.832E+10	4.583E+10	3.184E+09	1.242E+12	2.061E+12	1.237E+11	2.262E+07	2.205E+08
950	1.567E+09	1.567E+09	2.423E+10	6.003E+10	4.597E+09	1.492E+12	2.272E+12	1.673E+11	3.757E+07	3.496E+08
1000	2.387E+09	2.387E+09	3.153E+10	7.738E+10	6.475E+09	1.772E+12	2.501E+12	2.215E+11	6.004E+07	5.354E+08
1100	5.088E+09	5.088E+09	5.108E+10	1.231E+11	1.204E+10	2.418E+12	3.009E+12	3.665E+11	1.392E+08	1.152E+09
1200	9.868E+09	9.868E+09	7.872E+10	1.864E+11	2.083E+10	3.181E+12	3.582E+12	5.694E+11	2.895E+08	2.249E+09
1300	1.772E+10	1.772E+10	1.164E+11	2.710E+11	3.398E+10	4.058E+12	4.218E+12	8.108E+11	5.531E+08	4.065E+09
1400	2.989E+10	2.989E+10	1.659E+11	3.806E+11	5.277E+10	5.049E+12	4.916E+12	1.138E+12	9.822E+08	6.875E+09
1500	4.780E+10	4.780E+10	2.297E+11	5.189E+11	7.865E+10	6.148E+12	5.676E+12	1.544E+12	1.646E+09	1.103E+10
1600	7.306E+10	7.306E+10	3.097E+11	6.896E+11	1.130E+11	7.351E+12	6.492E+12	2.031E+12	2.627E+09	1.693E+10
1700	1.074E+11	1.074E+11	4.079E+11	8.962E+11	1.577E+11	8.652E+12	7.364E+12	2.605E+12	4.009E+09	2.494E+10
1800	1.526E+11	1.526E+11	5.266E+11	1.142E+12	2.143E+11	9.584E+12	8.290E+12	3.267E+12	5.914E+09	3.561E+10
1900	2.106E+11	2.106E+11	6.680E+11	1.432E+12	2.847E+11	1.062E+13	9.273E+12	4.021E+12	8.455E+09	4.941E+10
2000	2.831E+11	2.831E+11	8.336E+11	1.767E+12	3.705E+11	1.170E+13	1.030E+13	4.865E+12	1.175E+10	6.679E+10

T / K	k_{7-3}^{EA}	k_{8-1}^{EA}	k_{8-2}^{EA}	k_{8-3}^{EA}	k_{9-1}^{EA}	k_{9-2}^{EA}	k_{9-3}^{EA}			
200	2.887E-04	2.466E-37	1.055E-26	2.912E-42	3.009E+13	3.009E+13	3.009E+13			
250	3.609E-02	7.298E-28	1.972E-19	8.561E-32	2.119E+13	2.119E+13	2.117E+13			
300	1.179E+00	1.083E-21	1.070E-14	5.657E-25	1.700E+13	1.700E+13	1.694E+13			
350	2.205E+01	6.784E-17	5.479E-11	1.229E-19	1.497E+13	1.496E+13	1.485E+13			
400	2.143E+02	2.009E-13	2.684E-08	9.040E-16	1.397E+13	1.397E+13	1.377E+13			
450	1.423E+03	1.055E-10	3.470E-06	9.892E-13	1.350E+13	1.349E+13	1.319E+13			
500	7.094E+03	1.629E-08	1.768E-04	2.825E-10	1.329E+13	1.328E+13	1.287E+13			
550	2.837E+04	1.053E-06	4.562E-03	3.015E-08	1.325E+13	1.323E+13	1.270E+13			
600	9.516E+04	3.503E-05	7.047E-02	1.530E-06	1.329E+13	1.325E+13	1.263E+13			
650	2.767E+05	6.977E-04	7.319E-01	4.366E-05	1.340E+13	1.335E+13	1.263E+13			
700	7.145E+05	9.269E-03	5.561E+00	7.899E-04	1.356E+13	1.348E+13	1.270E+13			
750	1.673E+06	8.893E-02	3.283E+01	9.907E-03	1.377E+13	1.366E+13	1.282E+13			
800	3.600E+06	6.541E-01	1.578E+02	9.207E-02	1.401E+13	1.387E+13	1.299E+13			
850	7.214E+06	3.860E+00	6.401E+02	6.674E-01	1.429E+13	1.412E+13	1.320E+13			
900	1.362E+07	1.894E+01	2.250E+03	3.928E+00	1.459E+13	1.438E+13	1.344E+13			
950	2.433E+07	7.946E+01	7.009E+03	1.938E+01	1.493E+13	1.467E+13	1.372E+13			
1000	4.151E+07	2.919E+02	1.970E+04	8.228E+01	1.528E+13	1.498E+13	1.403E+13			
1100	1.075E+08	2.829E+03	1.205E+05	1.021E+03	1.607E+13	1.566E+13	1.473E+13			
1200	2.448E+08	1.929E+04	5.609E+05	8.526E+03	1.694E+13	1.642E+13	1.553E+13			
1300	5.037E+08	1.000E+05	2.112E+06	5.232E+04	1.792E+13	1.728E+13	1.644E+13			
1400	9.513E+08	4.174E+05	6.722E+06	2.515E+05	1.900E+13	1.823E+13	1.746E+13			
1500	1.680E+09	1.462E+06	1.867E+07	9.937E+05	2.020E+13	1.929E+13	1.859E+13			
1600	2.801E+09	4.433E+06	4.633E+07	3.340E+06	2.152E+13	2.046E+13	1.984E+13			
1700	4.440E+09	1.192E+07	1.047E+08	9.819E+06	2.295E+13	2.174E+13	2.121E+13			
1800	6.769E+09	2.899E+07	2.186E+08	2.581E+07	2.450E+13	2.312E+13	2.268E+13			
1900	9.958E+09	6.472E+07	4.267E+08	6.169E+07	2.616E+13	2.461E+13	2.428E+13			
2000	1.419E+10	1.342E+08	7.863E+08	1.359E+08	2.794E+13	2.621E+13	2.599E+13			

Table S8.

Calculated MP-CVT/SCT rate constants for the H-abstraction reactions from DMA by H/CH₃/OH/HO₂/NH₂/O/C₂H₅/O₂/Cl radicals. Units are in cm³ mol⁻¹ s⁻¹.

T / K	k_{1-1}^{DMA}	k_{1-2}^{DMA}	k_{2-1}^{DMA}	k_{2-2}^{DMA}	k_{3-1}^{DMA}	k_{3-2}^{DMA}	k_{4-1}^{DMA}	k_{4-2}^{DMA}	k_{5-1}^{DMA}	k_{5-2}^{DMA}
200	5.019E+07	9.876E+09	8.379E+04	3.716E+03	4.061E+13	4.141E+13	9.253E-04	1.196E+01	1.625E+07	1.040E+07
250	2.041E+08	1.839E+10	4.362E+05	3.759E+04	3.577E+13	3.691E+13	1.575E-01	2.412E+02	2.903E+07	3.978E+07
300	6.498E+08	3.051E+10	1.789E+06	2.454E+05	3.041E+13	3.164E+13	5.521E+00	2.228E+03	5.746E+07	1.097E+08
350	1.859E+09	4.916E+10	6.912E+06	1.304E+06	2.604E+13	2.587E+13	1.268E+02	1.999E+04	1.218E+08	2.894E+08
400	4.278E+09	7.246E+10	2.040E+07	4.781E+06	2.165E+13	2.008E+13	1.284E+03	1.013E+05	2.194E+08	6.119E+08
450	8.647E+09	1.020E+11	5.145E+07	1.416E+07	1.948E+13	1.685E+13	8.567E+03	3.943E+05	3.654E+08	1.167E+09
500	1.580E+10	1.387E+11	1.142E+08	3.568E+07	1.724E+13	1.351E+13	4.200E+04	1.254E+06	5.725E+08	1.849E+09
550	2.666E+10	1.835E+11	2.288E+08	7.934E+07	1.631E+13	1.181E+13	1.630E+05	3.403E+06	8.540E+08	3.070E+09
600	4.224E+10	2.375E+11	4.219E+08	1.599E+08	1.525E+13	1.015E+13	5.276E+05	8.179E+06	1.224E+09	4.850E+09
650	6.357E+10	3.020E+11	7.264E+08	2.976E+08	1.489E+13	9.184E+12	1.478E+06	1.780E+07	1.691E+09	7.357E+09
700	9.173E+10	3.776E+11	1.180E+09	5.190E+08	1.450E+13	8.252E+12	3.679E+06	3.567E+07	2.271E+09	1.077E+10
750	1.277E+11	4.655E+11	1.825E+09	8.573E+08	1.452E+13	7.709E+12	8.311E+06	6.679E+07	2.980E+09	1.532E+10
800	1.728E+11	5.666E+11	2.718E+09	1.353E+09	1.444E+13	7.182E+12	1.731E+07	1.181E+08	3.851E+09	2.123E+10
850	2.278E+11	6.818E+11	3.904E+09	2.055E+09	1.457E+13	6.895E+12	3.369E+07	1.988E+08	4.875E+09	2.876E+10
900	2.936E+11	8.113E+11	5.435E+09	3.017E+09	1.477E+13	6.665E+12	6.183E+07	3.209E+08	6.079E+09	3.818E+10
950	3.715E+11	9.562E+11	7.380E+09	4.304E+09	1.510E+13	6.631E+12	1.079E+08	4.995E+08	7.487E+09	4.982E+10
1000	4.625E+11	1.117E+12	9.808E+09	5.984E+09	1.535E+13	6.470E+12	1.802E+08	7.527E+08	9.115E+09	6.397E+10
1100	6.858E+11	1.485E+12	1.630E+10	1.084E+10	1.626E+13	6.559E+12	4.503E+08	1.576E+09	1.312E+10	1.012E+11
1200	9.703E+11	1.920E+12	2.546E+10	1.830E+10	1.699E+13	6.623E+12	9.982E+08	3.019E+09	1.828E+10	1.528E+11
1300	1.322E+12	2.412E+12	3.784E+10	2.915E+10	1.801E+13	6.895E+12	2.009E+09	5.376E+09	2.478E+10	2.217E+11
1400	1.746E+12	2.979E+12	5.394E+10	4.430E+10	1.908E+13	7.211E+12	3.744E+09	9.028E+09	3.273E+10	3.114E+11
1500	2.246E+12	3.617E+12	7.419E+10	6.469E+10	2.033E+13	7.709E+12	6.540E+09	1.442E+10	4.252E+10	4.252E+11
1600	2.826E+12	4.322E+12	9.912E+10	9.141E+10	2.156E+13	8.090E+12	1.083E+10	2.210E+10	5.404E+10	5.661E+11
1700	3.488E+12	5.100E+12	1.296E+11	1.255E+11	2.298E+13	8.716E+12	1.712E+10	3.268E+10	6.796E+10	7.387E+11
1800	4.242E+12	5.930E+12	1.660E+11	1.682E+11	2.443E+13	9.209E+12	2.602E+10	4.685E+10	8.392E+10	9.468E+11
1900	5.076E+12	6.818E+12	2.087E+11	2.205E+11	2.625E+13	9.855E+12	3.821E+10	6.535E+10	1.028E+11	1.193E+12
2000	6.008E+12	7.773E+12	2.575E+11	2.840E+11	2.772E+13	1.055E+13	5.454E+10	8.910E+10	1.248E+11	1.484E+12
T / K	k_{6-1}^{DMA}	k_{6-2}^{DMA}	k_{7-1}^{DMA}	k_{7-2}^{DMA}	k_{8-1}^{DMA}	k_{8-2}^{DMA}	k_{9-1}^{DMA}	k_{9-2}^{DMA}		
200	2.549E+12	1.670E+12	1.960E+05	4.577E+04	8.042E-31	8.210E-27	4.558E+13	4.558E+13		
250	1.995E+12	1.758E+12	5.080E+05	1.073E+05	1.008E-22	1.795E-19	6.998E+13	6.998E+13		
300	1.937E+12	1.873E+12	1.226E+06	3.056E+05	1.899E-17	9.514E-15	9.254E+13	9.254E+13		
350	2.056E+12	2.017E+12	3.072E+06	9.370E+05	2.521E-13	4.898E-11	1.112E+14	1.112E+14		
400	2.263E+12	2.183E+12	6.436E+06	2.336E+06	2.417E-10	2.357E-08	1.255E+14	1.255E+14		
450	2.530E+12	2.359E+12	1.234E+07	5.173E+06	5.269E-08	3.017E-06	1.358E+14	1.356E+14		
500	2.840E+12	2.557E+12	2.189E+07	1.035E+07	4.045E-06	1.523E-04	1.430E+14	1.424E+14		
550	3.184E+12	2.746E+12	3.640E+07	1.905E+07	1.447E-04	3.900E-03	1.481E+14	1.470E+14		
600	3.560E+12	2.995E+12	5.733E+07	3.273E+07	2.910E-03	5.978E-02	1.519E+14	1.498E+14		
650	3.966E+12	3.273E+12	8.628E+07	5.313E+07	3.758E-02	6.171E-01	1.552E+14	1.518E+14		
700	4.393E+12	3.572E+12	1.248E+08	8.214E+07	3.412E-01	4.656E+00	1.584E+14	1.533E+14		
750	4.843E+12	3.858E+12	1.745E+08	1.219E+08	2.337E+00	2.730E+01	1.617E+14	1.545E+14		
800	5.320E+12	4.171E+12	2.372E+08	1.748E+08	1.272E+01	1.303E+02	1.651E+14	1.555E+14		
850	5.817E+12	4.514E+12	3.143E+08	2.433E+08	5.722E+01	5.243E+02	1.688E+14	1.566E+14		
900	6.336E+12	4.882E+12	4.073E+08	3.297E+08	2.196E+02	1.828E+03	1.727E+14	1.577E+14		
950	6.872E+12	5.276E+12	5.178E+08	4.369E+08	7.366E+02	5.648E+03	1.767E+14	1.589E+14		
1000	7.433E+12	5.694E+12	6.470E+08	5.672E+08	2.203E+03	1.573E+04	1.809E+14	1.603E+14		
1100	8.610E+12	6.603E+12	9.668E+08	9.084E+08	1.486E+04	9.445E+04	1.886E+14	1.630E+14		
1200	9.875E+12	7.610E+12	1.376E+09	1.375E+09	7.423E+04	4.320E+05	1.951E+14	1.663E+14		
1300	1.121E+13	8.704E+12	1.881E+09	1.986E+09	2.939E+05	1.597E+06	1.994E+14	1.700E+14		
1400	1.264E+13	9.896E+12	2.490E+09	2.763E+09	9.688E+05	4.998E+06	2.014E+14	1.742E+14		
1500	1.417E+13	1.118E+13	3.206E+09	3.723E+09	2.754E+06	1.364E+07	2.003E+14	1.788E+14		
1600	1.577E+13	1.255E+13	4.034E+09	4.884E+09	6.942E+06	3.334E+07	1.962E+14	1.837E+14		
1700	1.748E+13	1.402E+13	4.976E+09	6.255E+09	1.582E+07	7.422E+07	1.909E+14	1.892E+14		
1800	1.927E+13	1.559E+13	6.032E+09	7.860E+09	3.318E+07	1.530E+08	1.837E+14	1.951E+14		
1900	2.118E+13	1.724E+13	7.205E+09	9.703E+09	6.479E+07	2.949E+08	1.771E+14	2.014E+14		
2000	2.318E+13	1.901E+13	8.499E+09	1.181E+10	1.192E+08	5.376E+08	1.678E+14	2.082E+14		