

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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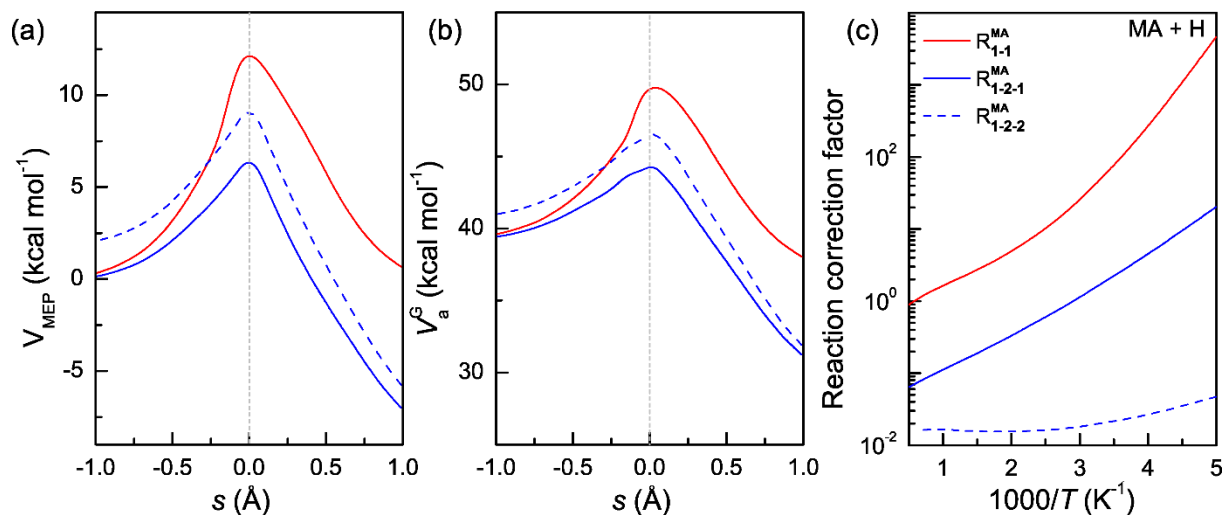


Figure S1. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from MA by H radicals. R_{1-1}^{MA} and R_{1-2}^{MA} have 1 and 2 reaction paths, respectively.

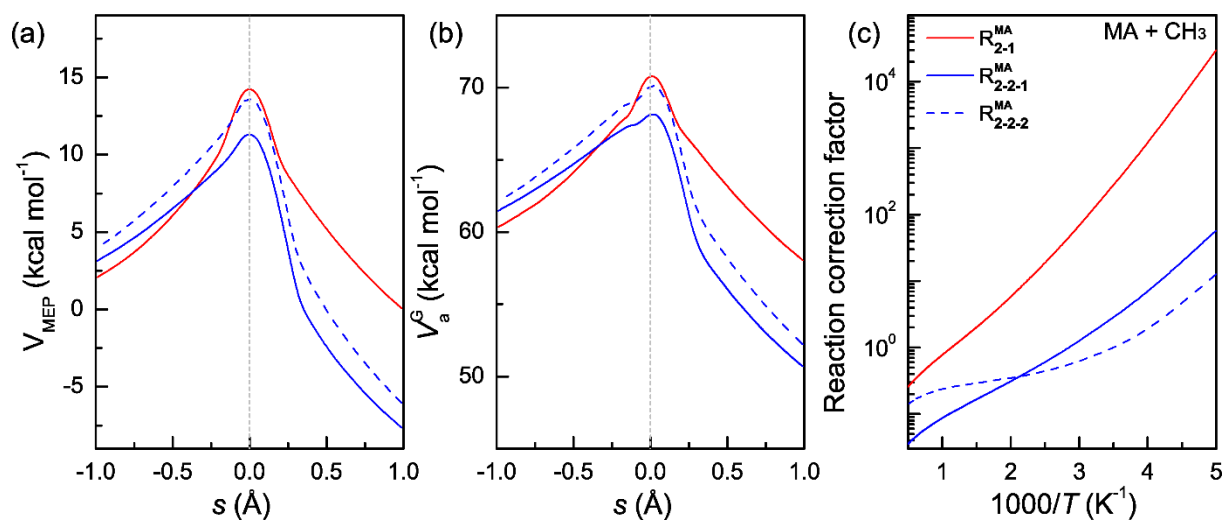


Figure S2. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from MA by CH_3 radicals. R_{2-1}^{MA} and R_{2-2}^{MA} have 1 and 2 reaction paths, respectively.

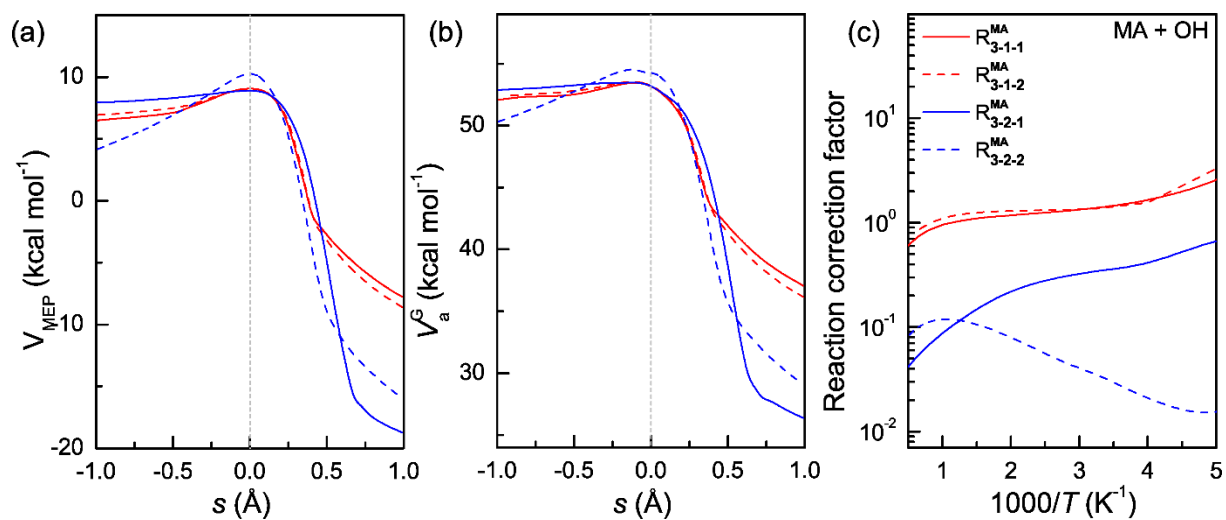


Figure S3. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from MA by OH radicals. R_{3-1}^{MA} and R_{3-2}^{MA} both have 2 reaction paths.

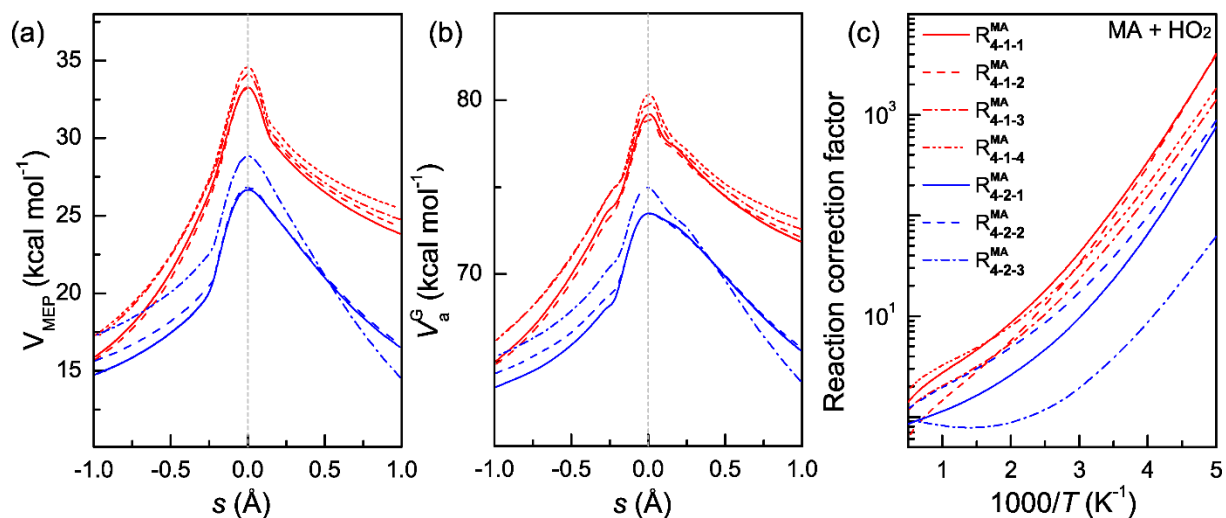


Figure S4. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from MA by HO₂ radicals. R_{4-1}^{MA} and R_{4-2}^{MA} have 4 and 3 reaction paths, respectively.

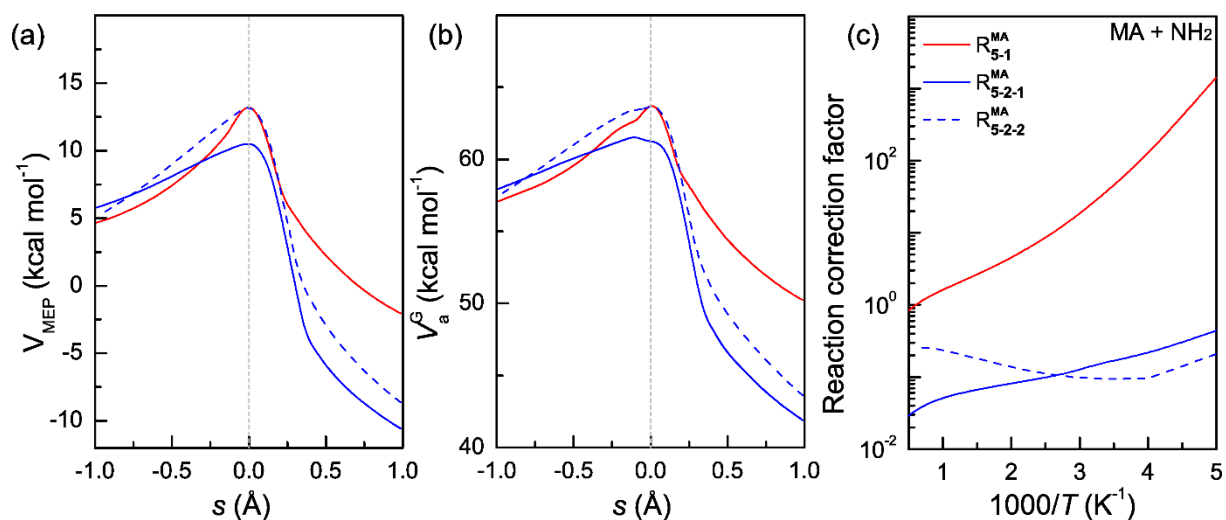


Figure S5. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from MA by NH₂ radicals. R_{5-1}^{MA} and R_{5-2}^{MA} have 1 and 2 reaction paths, respectively.

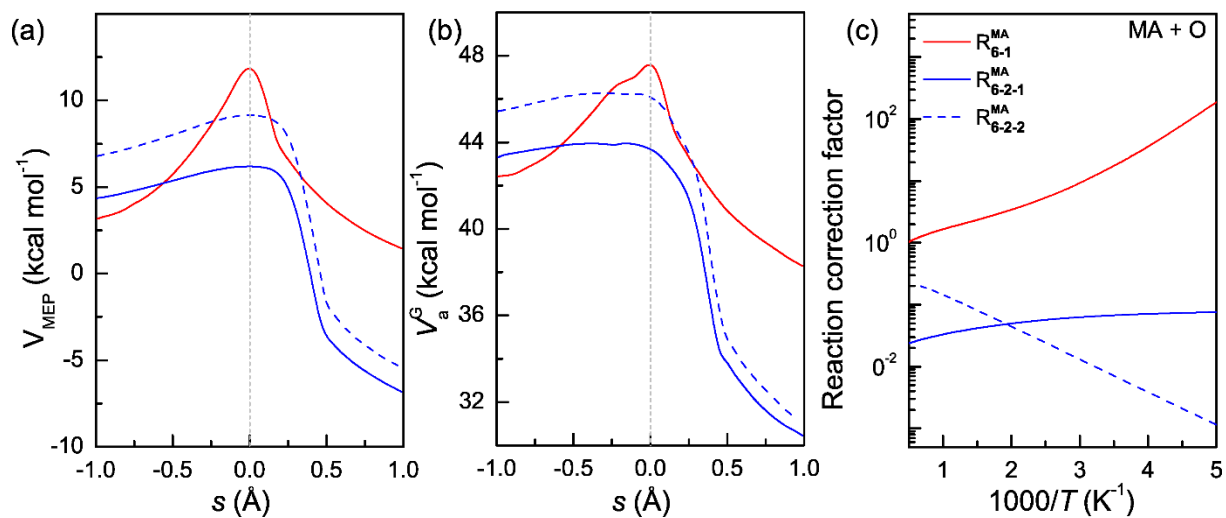


Figure S6. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from MA by O radicals. R_{6-1}^{MA} and R_{6-2}^{MA} have 1 and 2 reaction paths, respectively.

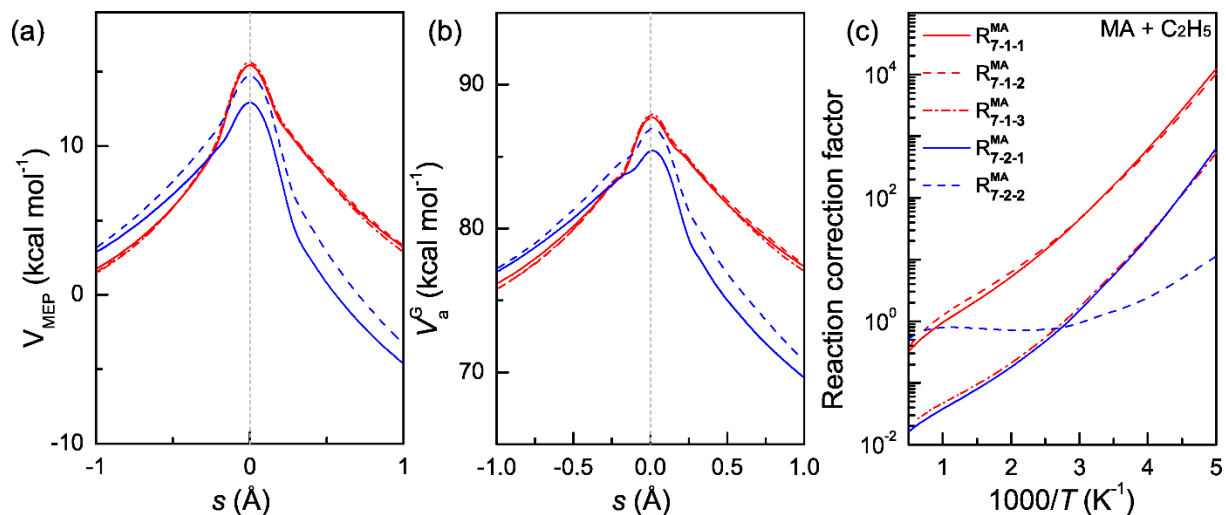


Figure S7. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from MA by C₂H₅ radicals. R_{7-1}^{MA} and R_{7-2}^{MA} have 3 and 2 reaction paths, respectively.

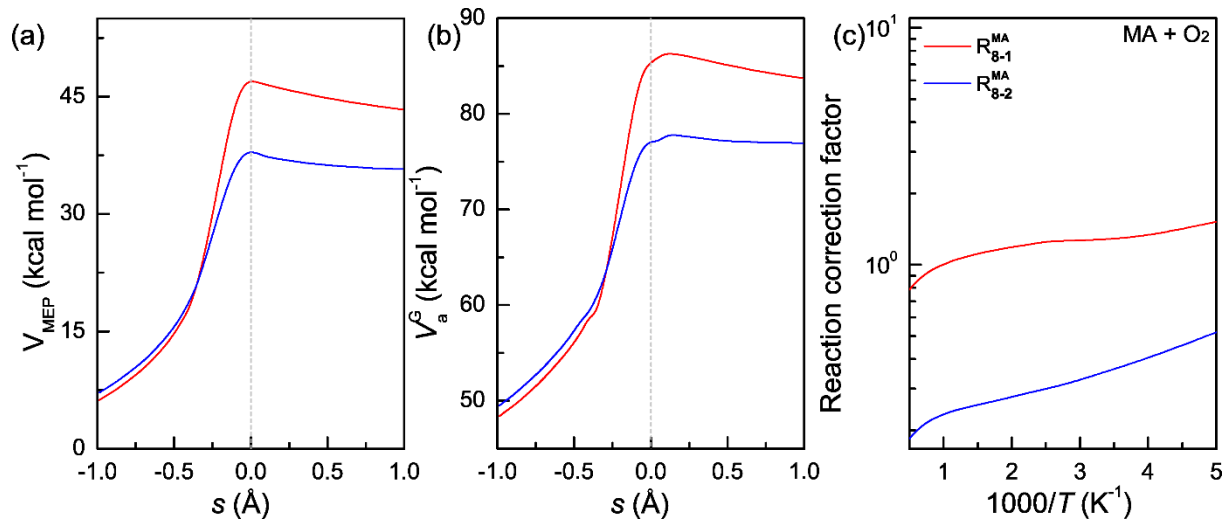


Figure S8. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from MA by O₂. R_{8-1}^{MA} and R_{8-2}^{MA} both have 1 reaction path.

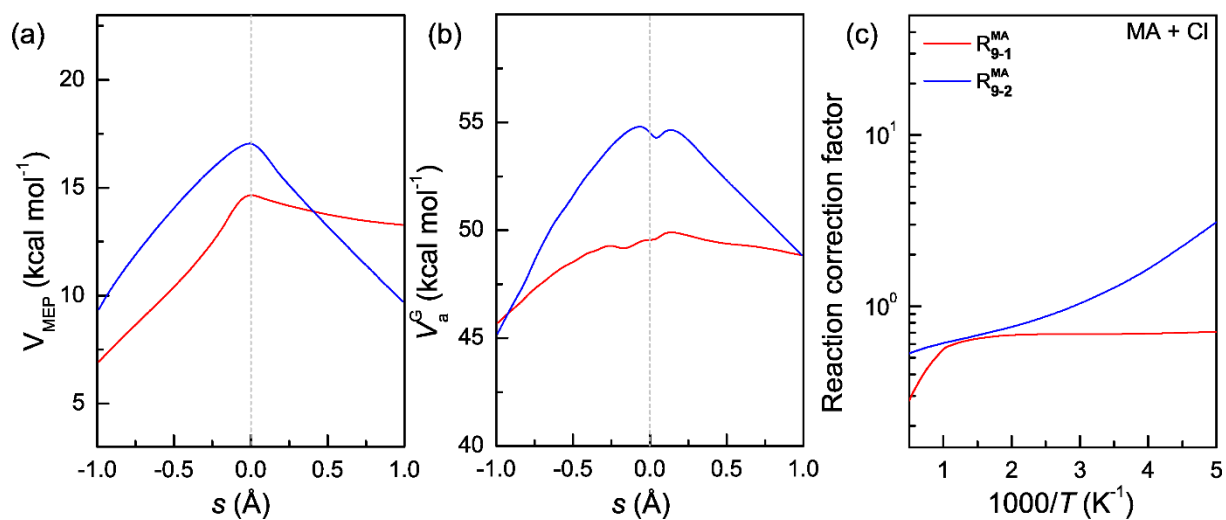


Figure S9. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from MA by Cl. R_{9-1}^{MA} and R_{9-2}^{MA} both have 1 reaction path.

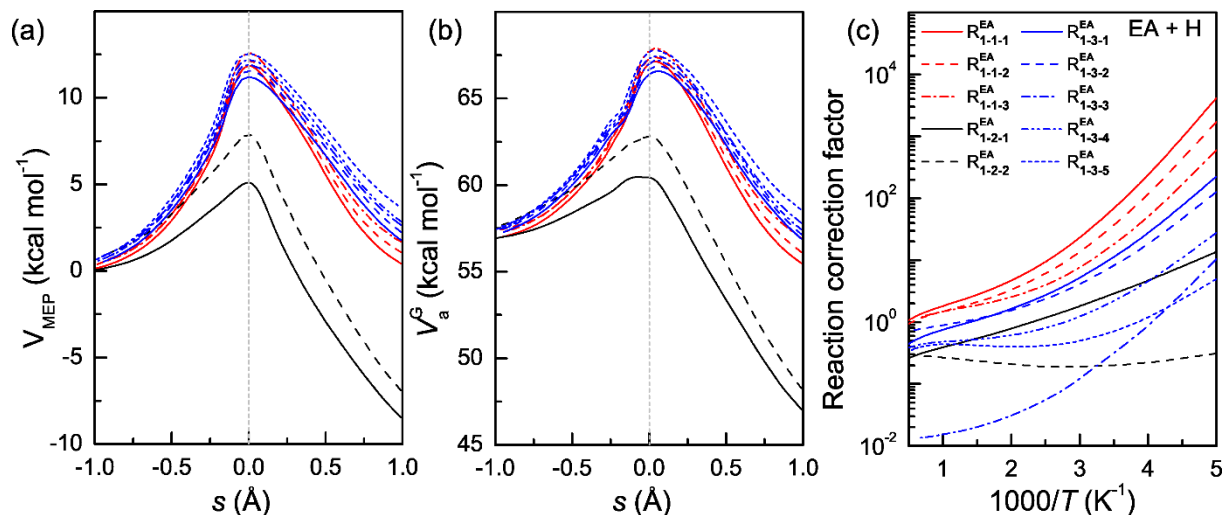


Figure S10. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from EA by H radicals. R_{1-1}^{EA} , R_{1-2}^{EA} , and R_{1-3}^{EA} have 3, 2, and 5 reaction paths, respectively.

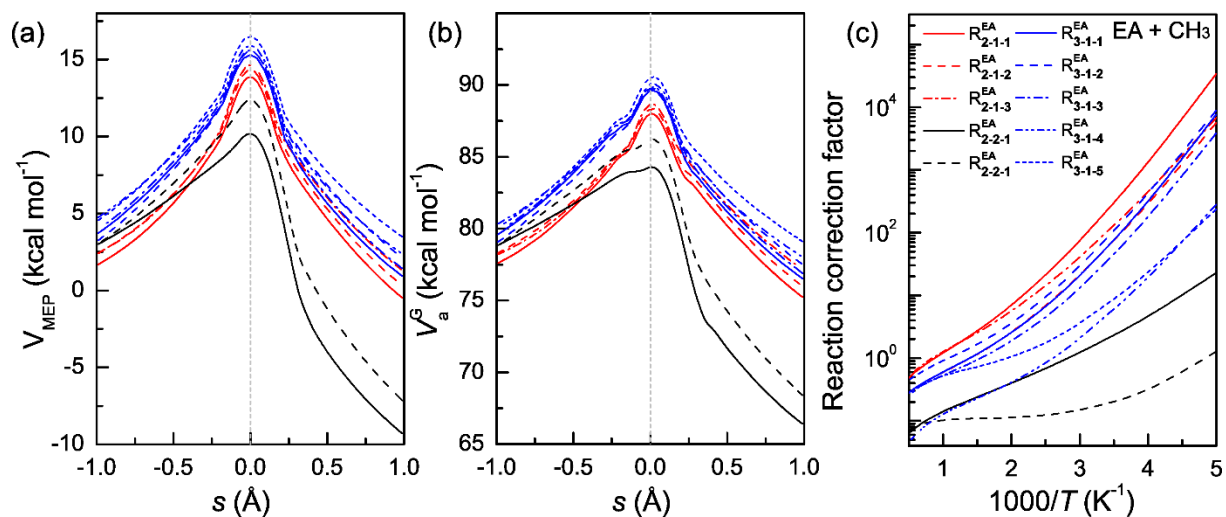


Figure S11. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from EA by CH₃ radicals. R_{2-1}^{EA} , R_{2-2}^{EA} , and R_{2-3}^{EA} have 3, 2, and 5 reaction paths, respectively.

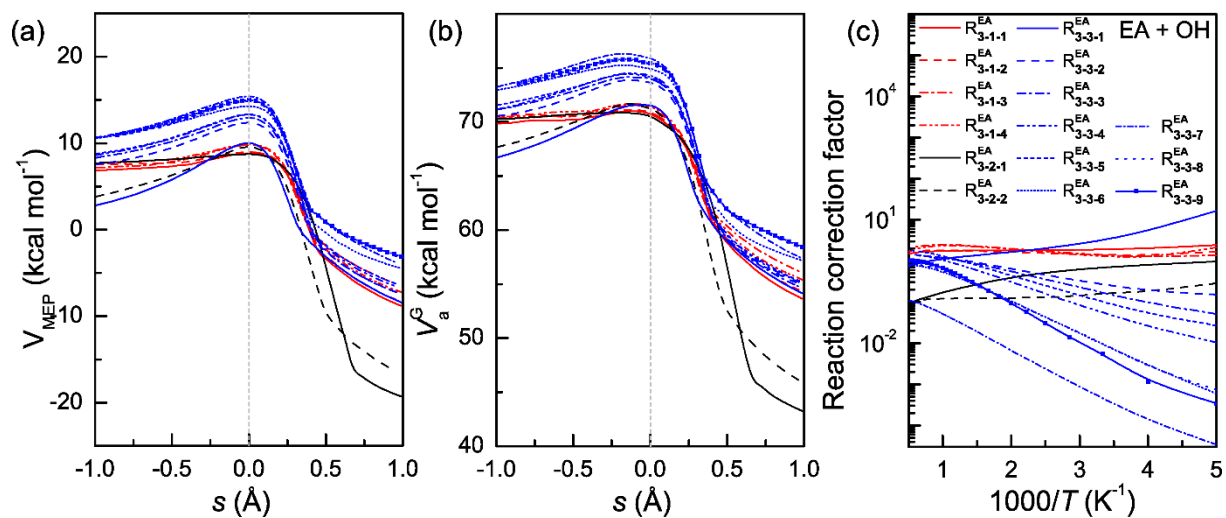


Figure S12. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from EA by OH radicals. R_{3-1}^{EA} , R_{3-2}^{EA} , and R_{3-3}^{EA} have 4, 2, and 9 reaction paths, respectively.

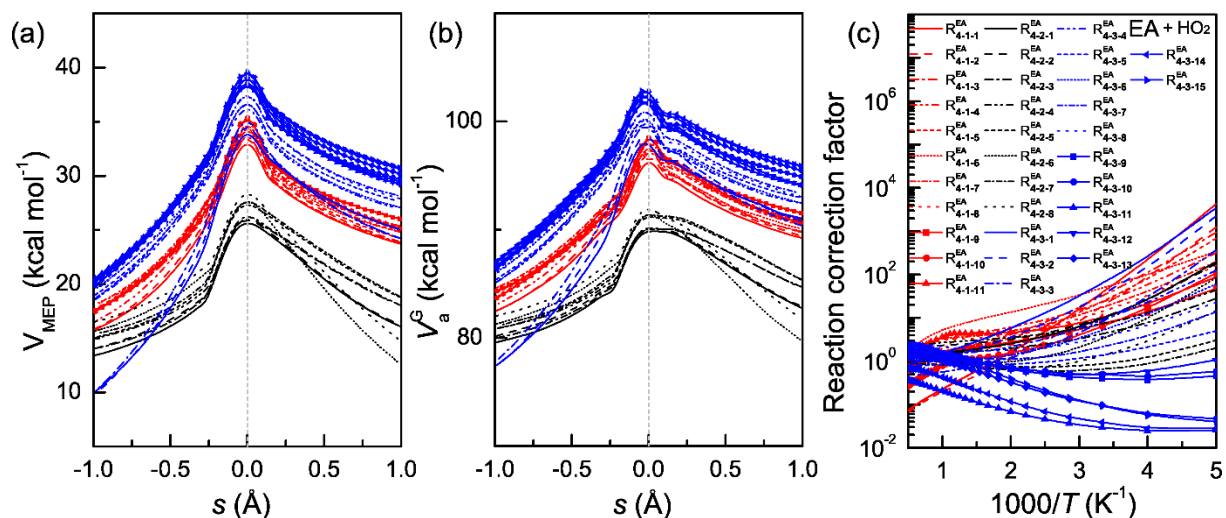


Figure S13. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from EA by HO₂ radicals. R₄₋₁^{EA}, R₄₋₂^{EA}, and R₄₋₃^{EA} have 11, 8, and 13 reaction paths, respectively.

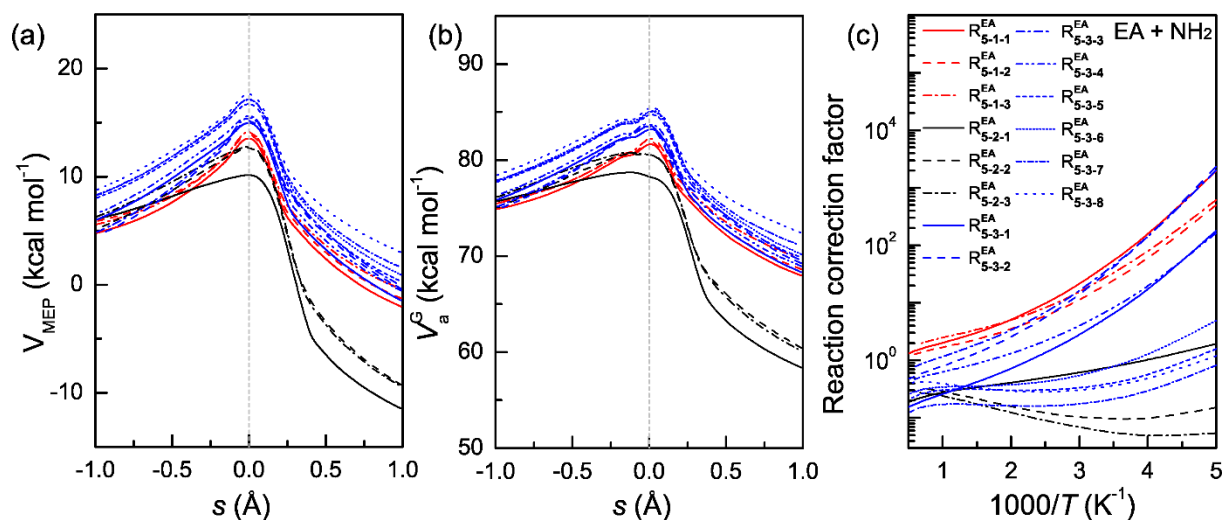


Figure S14. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from EA by NH₂ radicals. R₅₋₁^{EA}, R₅₋₂^{EA}, and R₅₋₃^{EA} have 3, 3, and 8 reaction paths, respectively.

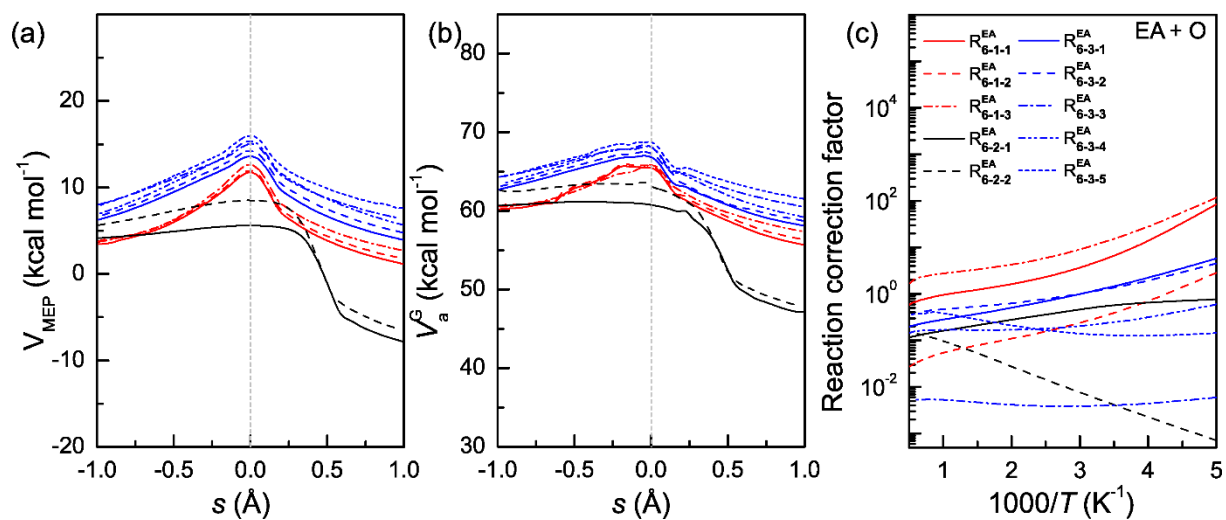


Figure S15. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from EA by O radicals. R₆₋₁^{EA}, R₆₋₂^{EA}, and R₆₋₃^{EA} have 3, 2, and 5 reaction paths, respectively.

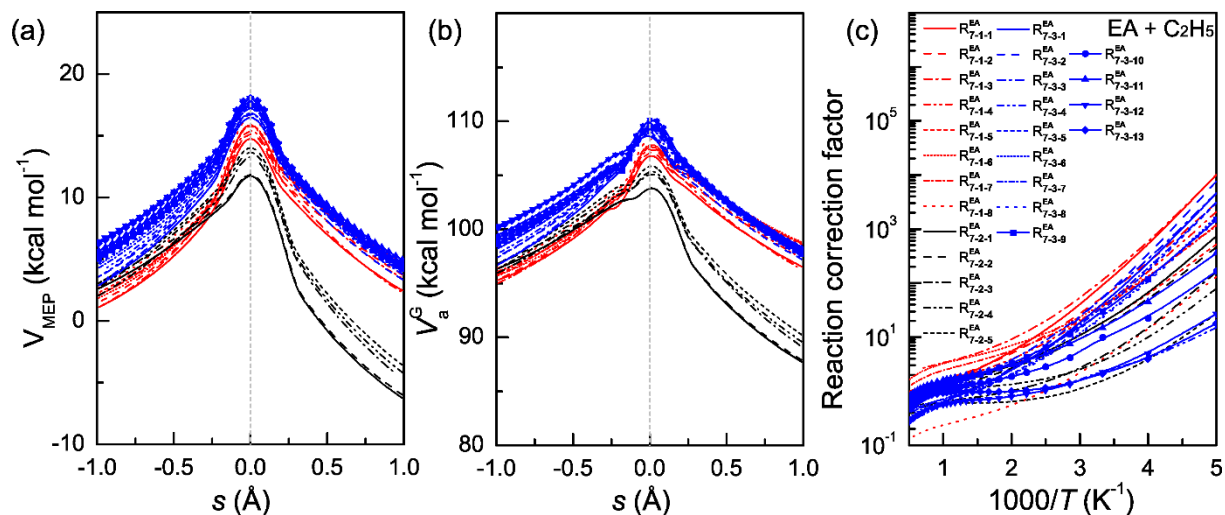


Figure S16. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from EA by C₂H₅ radicals. R₇₋₁^{EA}, R₇₋₂^{EA}, and R₇₋₃^{EA} have 8, 5, and 13 reaction paths, respectively.

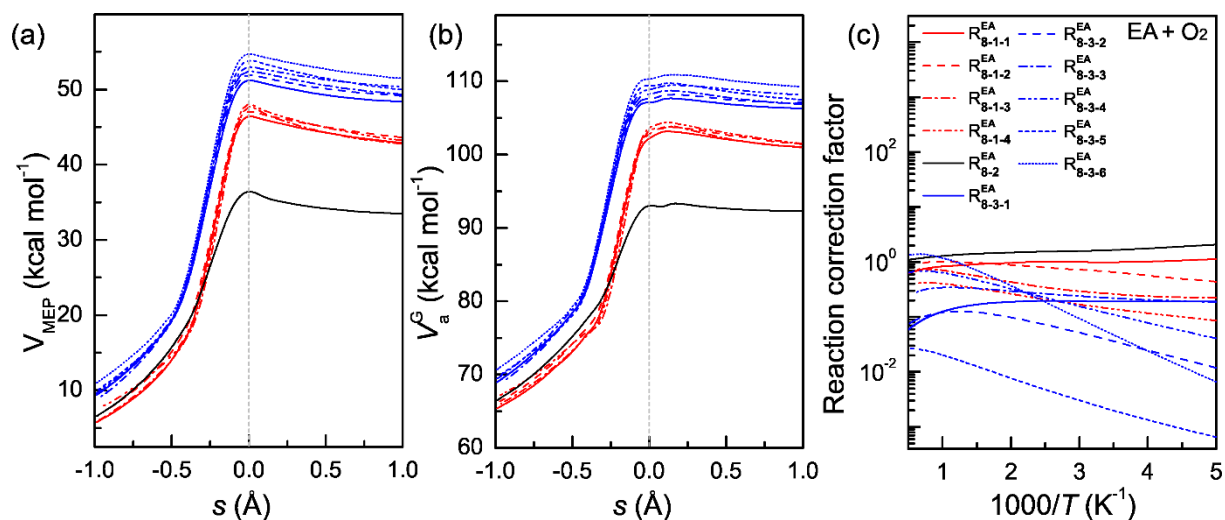


Figure S17. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from EA by C₂H₅ radicals. R₈₋₁^{EA}, R₈₋₂^{EA}, and R₈₋₃^{EA} have 4, 1, and 6 reaction paths, respectively.

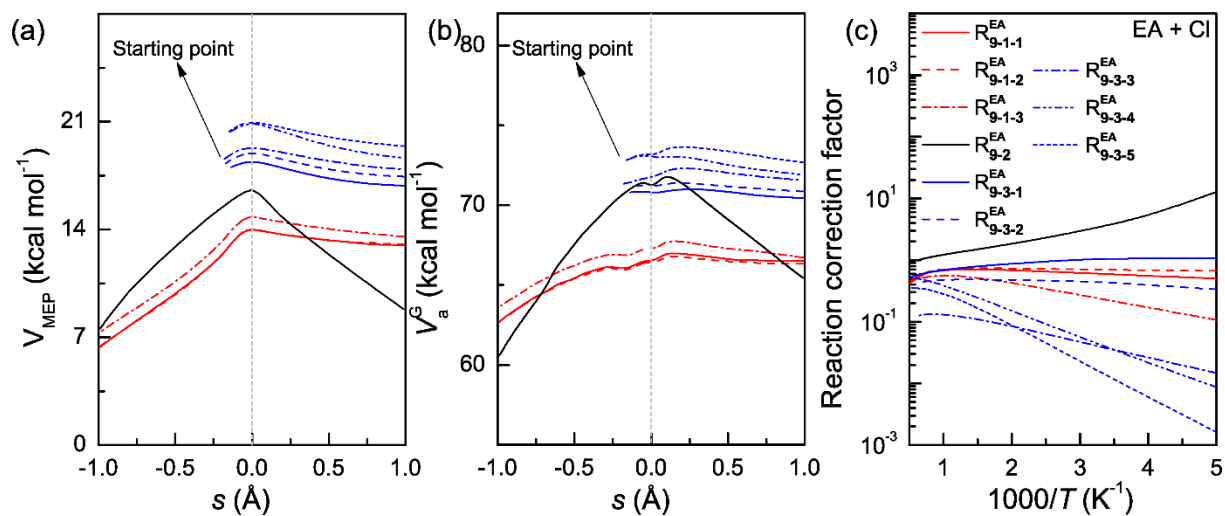


Figure S18. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from EA by Cl radicals. R₉₋₁^{EA}, R₉₋₂^{EA}, and R₉₋₃^{EA} have 3, 1, and 5 reaction paths, respectively.

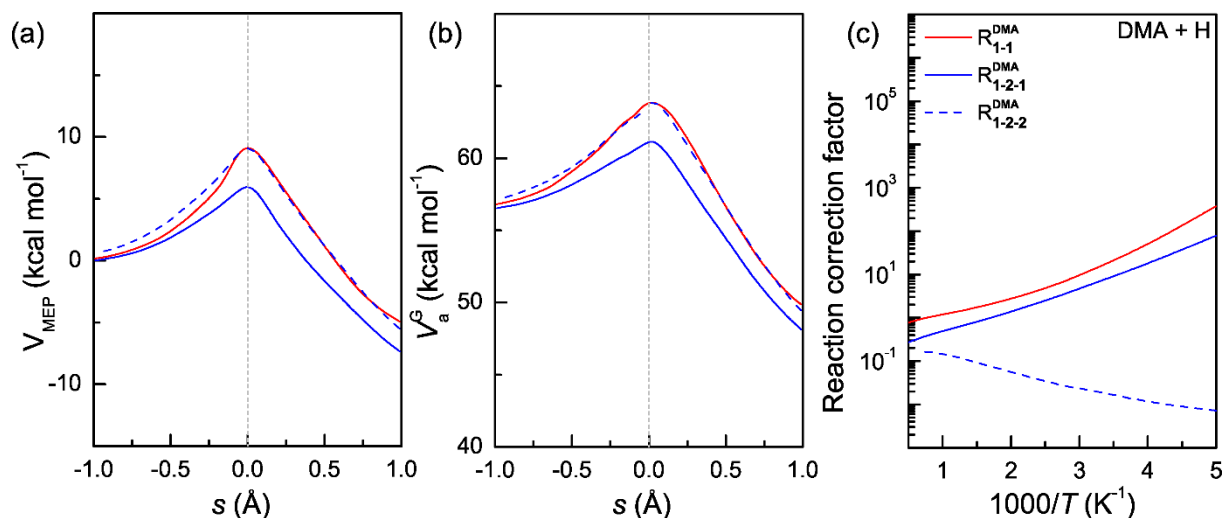


Figure S19. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from DMA by H radicals. R_{1-1}^{DMA} and R_{1-2}^{DMA} have 1 and 2 reaction paths, respectively.

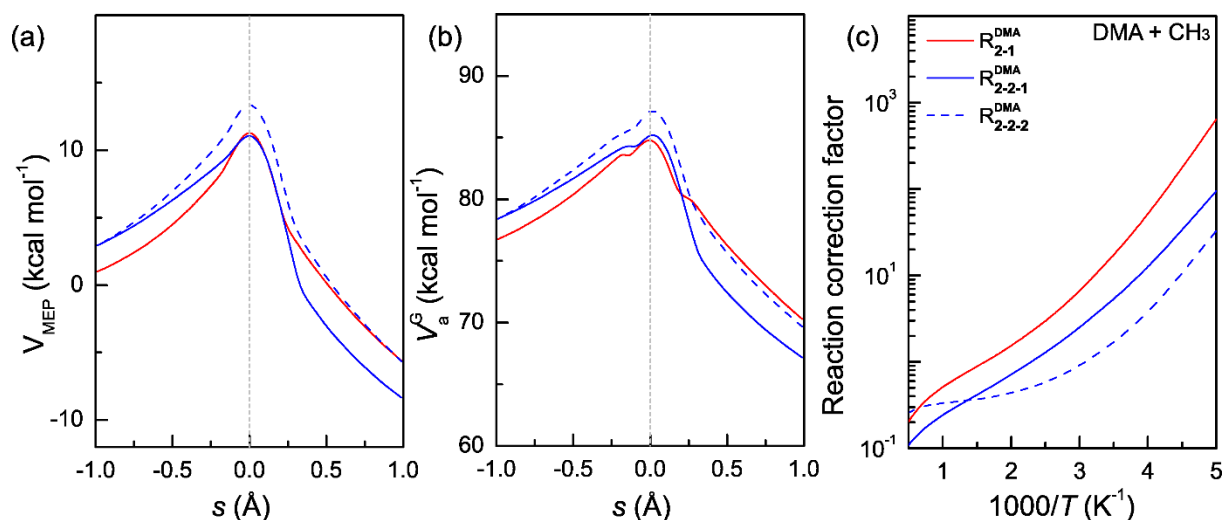


Figure S20. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from DMA by CH_3 radicals. R_{2-1}^{DMA} and R_{2-2}^{DMA} have 1 and 2 reaction paths, respectively.

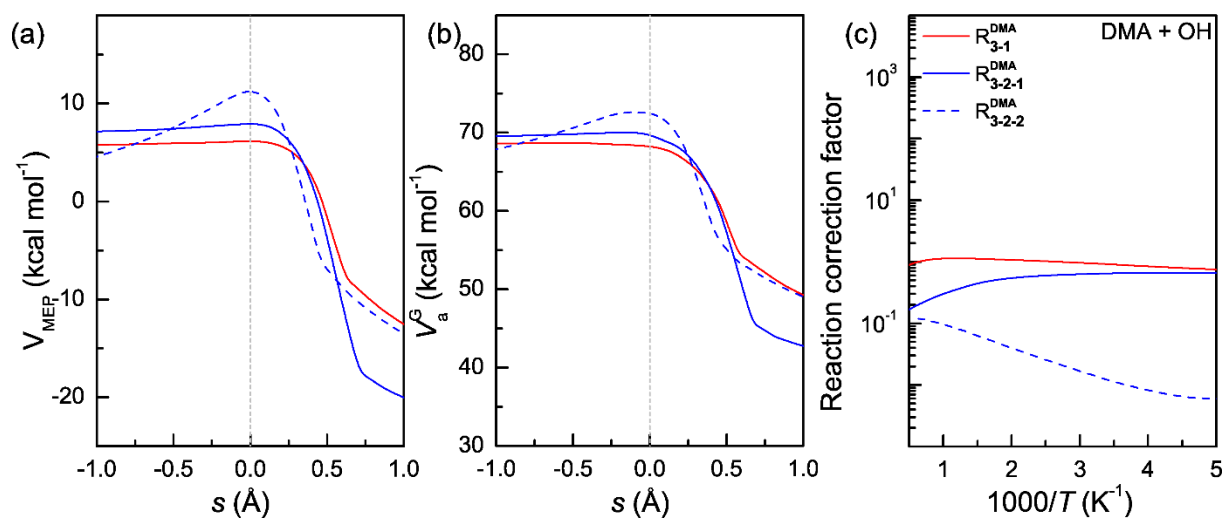


Figure S21. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from DMA by OH radicals. R_{3-1}^{DMA} and R_{3-2}^{DMA} have 1 and 2 reaction paths, respectively.

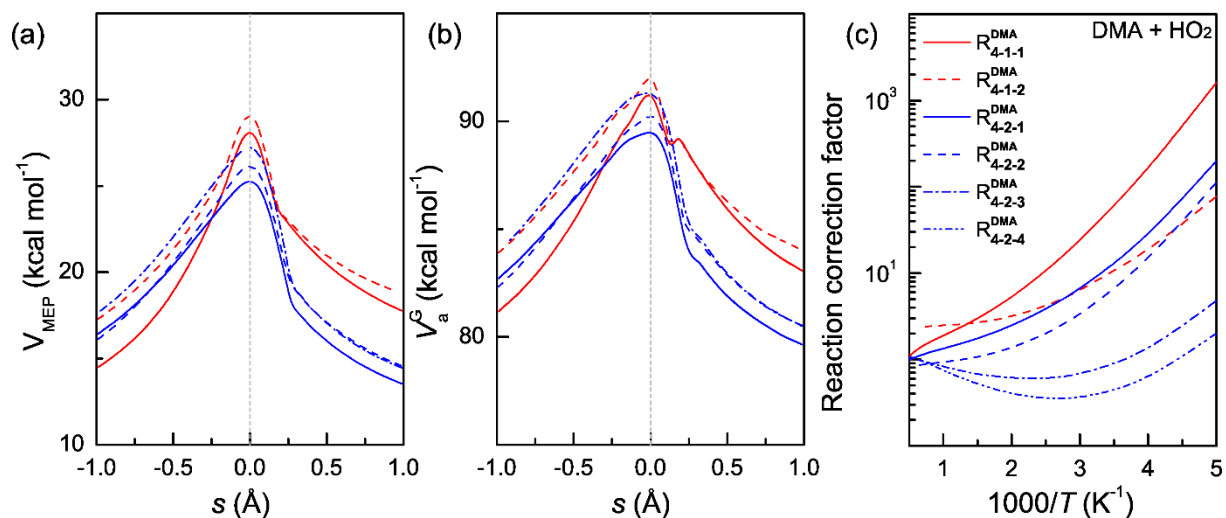


Figure S22. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from DMA by HO₂ radicals. R_{4-1}^{DMA} and R_{4-2}^{DMA} have 1 and 2 reaction paths, respectively.

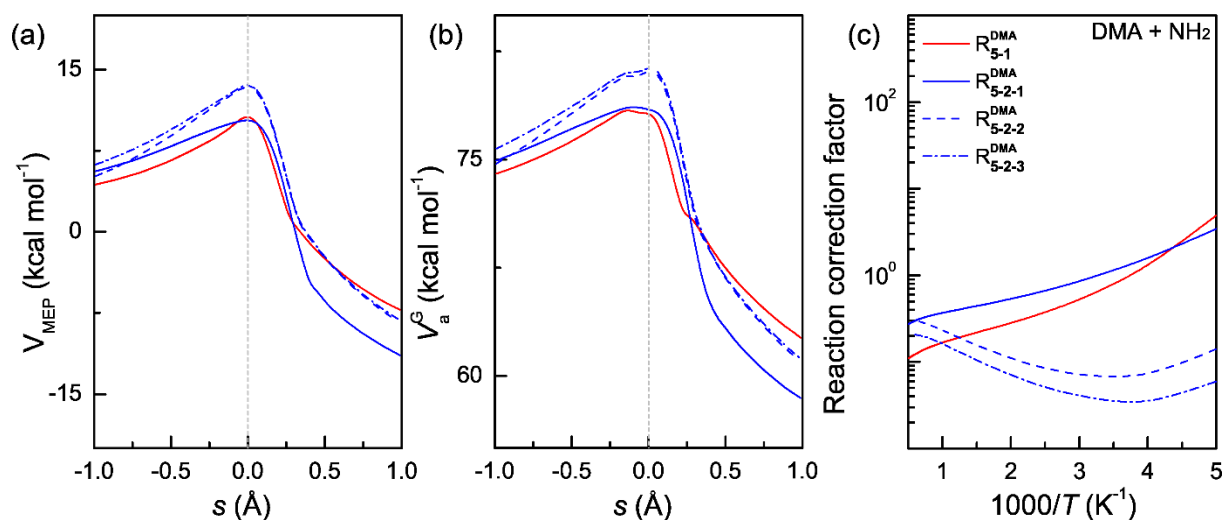


Figure S23. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from DMA by NH₂ radicals. R_{5-1}^{DMA} and R_{5-2}^{DMA} have 1 and 3 reaction paths, respectively.

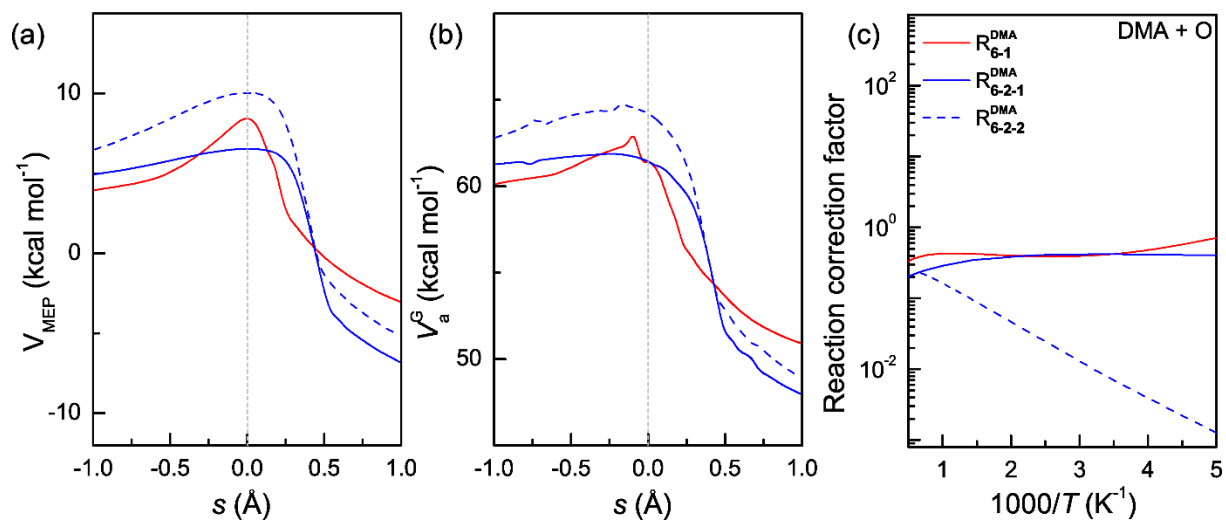


Figure S24. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from DMA by O radicals. R_{6-1}^{DMA} and R_{6-2}^{DMA} have 1 and 2 reaction paths, respectively.

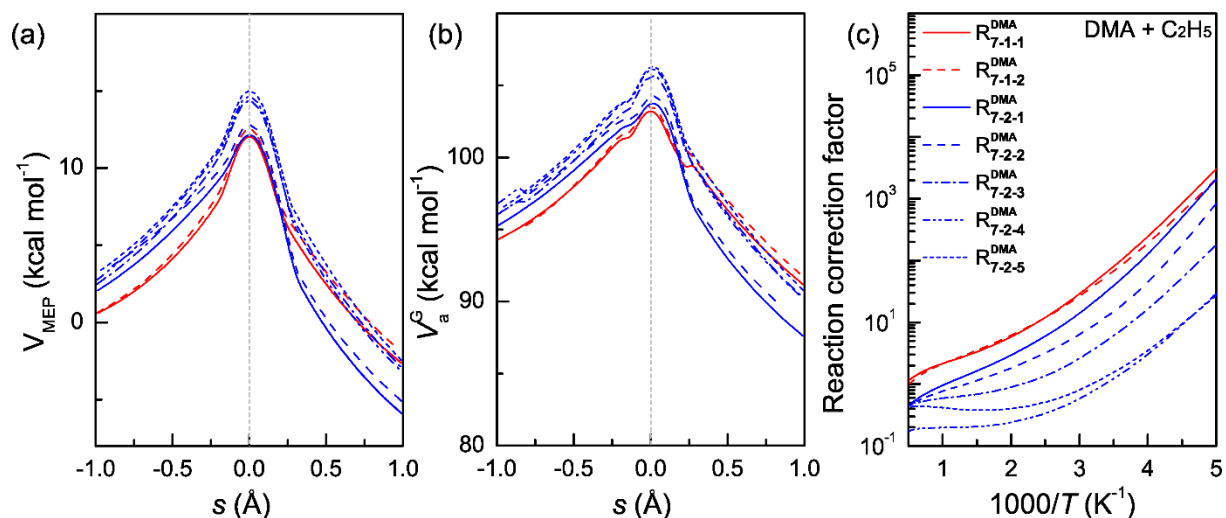


Figure S25. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from DMA by C_2H_5 radicals. $\text{R}_{7-1}^{\text{DMA}}$ and $\text{R}_{7-2}^{\text{DMA}}$ have 2 and 5 reaction paths, respectively.

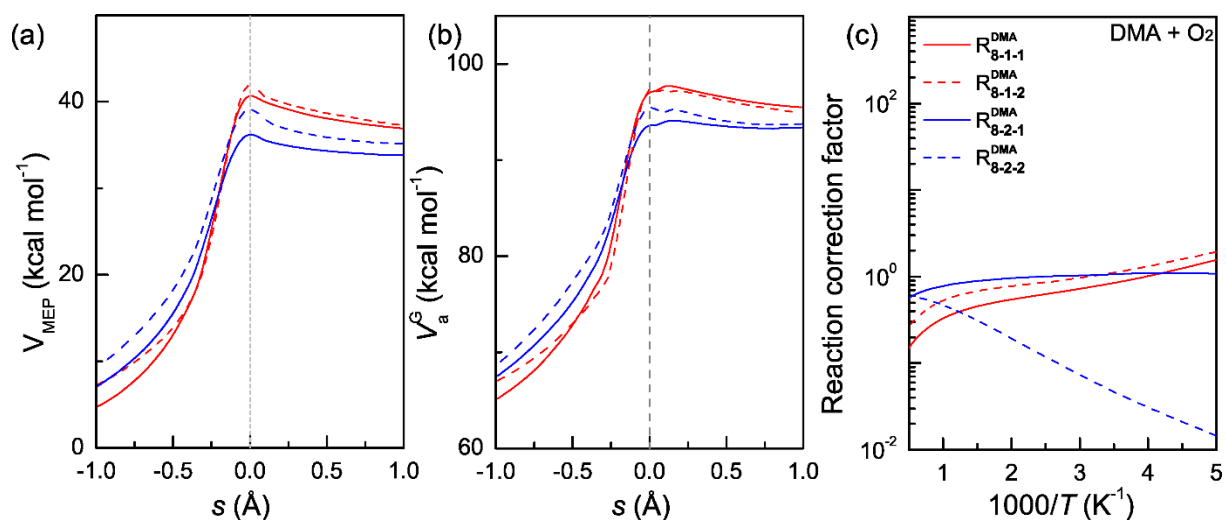


Figure S26. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from DMA by O_2 radicals. $\text{R}_{8-1}^{\text{DMA}}$ and $\text{R}_{8-2}^{\text{DMA}}$ both have 2 reaction paths.

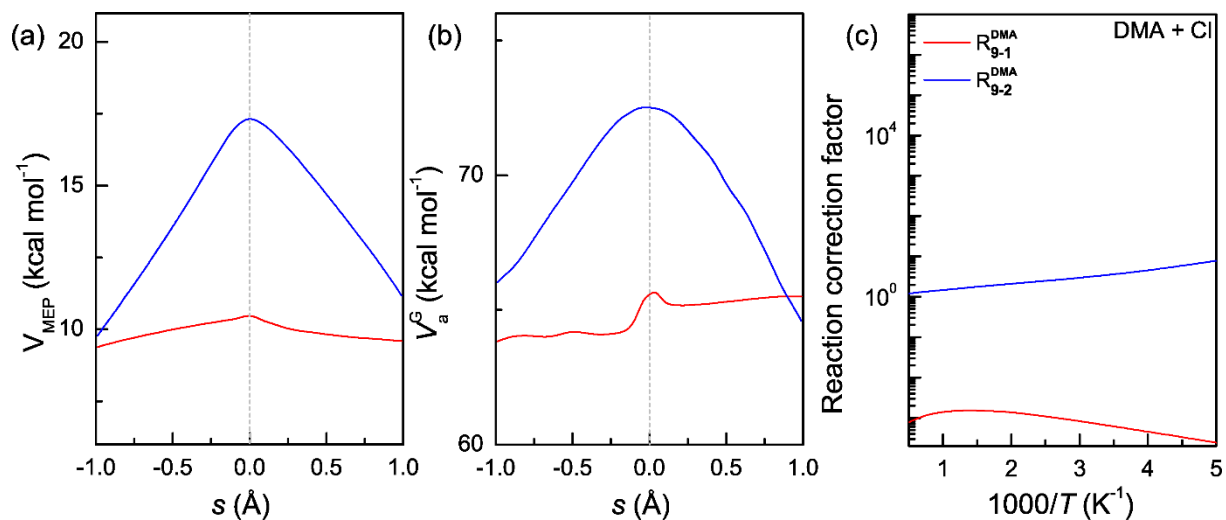


Figure S27. (a) V_{MEP} , (b) V_a^G , and reaction correction factor of each reaction path for the H-abstraction reactions from DMA by O_2 radicals. $\text{R}_{9-1}^{\text{DMA}}$ and $\text{R}_{9-2}^{\text{DMA}}$ both have 1 reaction path.

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	16.3	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}^-	
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
ωB97X-D	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
	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
MN15-L	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
	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
BH&HLYP	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
	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
PW6B95	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
	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
MP	ma-TZVP	-2.6	10.3	13.0	-6.2	13.6	19.9	-15.5	1.2	16.7	16.1	20.4	4.3	-8.2	8.7	16.8	0.9	7.0	6.2	-2.1	15.9	18.0	51.0	45.1	-5.9
	MG3S	-2.3	10.5	12.8	-6.0	13.7	19.7	-16.2	0.9	17.1	15.6	19.9	4.3	-8.1	8.8	16.8	0.4	6.7	6.4	-1.8	16.0	17.8	50.5	44.3	-6.2

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
ωB97X-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}^-
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
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	0.090095			
C	0.625379	-0.013124	-0.000067	207.03	950.52	1000.81	H	1.132497	-0.835430	-0.203942	437.39	577.29 643.32	
H	1.127113	0.958334	-0.001270	1078.09	1328.05	1387.67	C	-0.723669	0.000000	-0.072563	930.47	1252.51 1316.68	
H	0.962984	-0.583050	0.881415	1468.28	1473.71	2971.47	H	-1.242490	-0.932548	0.106299	1478.02	1652.01 3182.62	
H	0.963636	-0.586044	-0.879338	3022.81	3112.99	3436.05	H	-1.242491	0.932547	0.106300	3296.86	3594.61 3702.56	
H	-1.216320	-0.781427	0.000159				H	1.132498	0.835429	-0.203944			
R1 MA + H													
H						H ₂							
H	0.000000	0.000000	0.000000				H	0.000000	0.000000	0.372855			
							H	0.000000	0.000000	-0.372855	4417.97		
TS1-1						TS1-2							
N	0.579122	-0.382501	-0.150693				N	0.837761	0.038963	0.000015			
H	1.343416	0.612719	-0.111816	-1549.89			H	1.124554	0.545399	-0.825544			
C	-0.768830	0.131633	0.021723	182.27	372.12	704.54	C	-0.538608	-0.307822	0.000026	301.01	314.42 512.20	
H	-1.031588	0.761547	-0.832800	976.00	988.00	1067.65	H	-0.819219	-0.863850	-0.898258	752.82	973.95 1142.02	
H	-1.462106	-0.719778	0.034569	1137.83	1279.70	1387.98	H	-0.819360	-0.863265	0.898626	1171.23	1300.25 1326.40	
H	-0.928370	0.703570	0.945709	1417.74	1465.35	1491.65	H	-1.299092	0.668941	-0.000458	1384.07	1388.68 1462.53	
H	0.862811	-0.856183	0.709275	1763.02	3007.00	3070.18	H	1.124462	0.545721	0.825407	1662.58	3068.00 3148.43	
H	1.774961	1.385832	0.179580	3117.66	3472.59		H	-1.944028	1.541248	-0.000031	3572.78	3667.98	
R2 MA + CH₃													
CH ₃						CH ₄							
C	0.000000	0.000000	0.000023				C	0.000000	0.000000	0.000000			
H	0.000000	1.080901	-0.000047	536.57	1405.71	1405.71	H	0.630332	0.630332	0.630332	1325.68	1325.68 1325.68	
H	-0.936088	-0.540451	-0.000047	3143.03	3323.03	3323.25	H	-0.630332	-0.630332	0.630332	1546.14	1546.14 3034.36	
H	0.936088	-0.540451	-0.000047				H	-0.630332	0.630332	-0.630332	3160.69	3160.69 3160.69	
							H	0.630332	-0.630332	-0.630332			
TS2-1						TS2-2							
N	0.580652	0.758532	-0.149507				N	-1.545939	-0.426494	-0.000007			
H	-0.604411	0.387296	-0.186452	-1944.36			H	-1.470346	-1.006628	-0.823905			
C	1.362925	-0.453817	0.020767	69.98	139.51	163.96	C	-0.633156	0.666204	-0.000008	18.72	123.81 236.32	
H	1.268898	-1.077180	-0.873969	387.35	550.00	566.52	H	-0.736926	1.280425	-0.898525	378.78	471.75 539.71	
H	2.422385	-0.185041	0.125430	805.16	1000.20	1069.31	H	-0.736909	1.280404	0.898525	636.24	774.17 988.57	
H	1.087428	-1.060238	0.896950	1089.40	1141.55	1301.54	H	0.589605	0.302118	-0.000036	1093.47	1159.38 1166.12	
H	0.587876	1.277642	0.729674	1359.23	1414.69	1421.04	H	-1.470422	-1.006559	0.823945	1342.93	1403.89 1406.29	
C	-1.805663	-0.175675	0.014886	1431.26	1469.79	1491.05	C	1.967119	-0.177906	0.000001	1440.59	1445.29 1463.54	
H	-2.465628	0.654488	0.261327	1508.40	2990.94	3059.52	H	2.037141	-0.769324	0.910797	1658.20	3071.30 3079.15	
H	-1.678107	-0.891449	0.825722	3072.77	3107.04	3213.77	H	2.041862	-0.756491	-0.918623	3152.77	3225.39 3228.18	
H	-2.026577	-0.638285	-0.946048	3216.29	3491.67		H	2.563786	0.731732	0.007913	3562.01	3656.18	
R3 MA + OH													
OH						H ₂ O							
O	0.000000	0.000000	0.107952				H	0.765650	-0.459860	0.000000			
H	0.000000	0.000000	-0.863615	3794.45			O	0.000000	0.114973	0.000000	1610.87	3888.78 3993.46	
							H	-0.765650	-0.459927	0.000000			
RC3													

N	-0.592213	0.670378	0.000313							
H	-0.808908	1.234031	-0.813328	49.81	107.95	220.64				
C	-1.381138	-0.561838	0.000051	323.69	545.96	734.79				
H	-2.467560	-0.401278	0.000027	912.97	976.44	1082.35				
H	-1.122390	-1.155679	-0.881235	1183.76	1338.69	1447.70				
H	-1.122473	-1.155984	0.881152	1491.09	1506.31	1653.50				
H	-0.808439	1.233372	0.814535	3017.63	3098.43	3130.49				
O	2.211950	-0.122139	-0.001109	3483.86	3539.70	3619.45				
H	1.274961	0.188266	-0.000468							
TS3-1				PC3-1						
N	0.456575	0.731340	-0.136505	-655.19			N	0.781506	0.774977	0.000079
H	-0.530030	0.507524	-0.482797	88.85	128.77	178.01	H	-1.158119	0.435234	-0.005058
C	1.285155	-0.439968	0.041336	370.46	651.60	721.60	C	1.288374	-0.565646	0.004522
H	0.997429	-1.053266	0.905730	977.89	1092.55	1107.40	H	1.941304	-0.738282	0.875205
H	1.222836	-1.062110	-0.854119	1312.94	1429.42	1464.25	H	0.461590	-1.280747	0.026164
H	2.328071	-0.127919	0.174038	1488.71	1614.40	2392.60	H	1.908277	-0.754920	-0.886671
H	0.423967	1.316573	0.691098	3014.59	3080.31	3138.95	H	1.566097	1.428985	-0.016879
O	-1.671326	-0.269915	-0.062724	3581.85	3838.77		O	-1.902826	-0.182531	-0.014012
H	-1.978616	0.098946	0.775361				H	-2.697320	0.339013	0.091651
TS3-2				PC3-2						
N	1.125850	-0.592281	-0.015001	-1188.00			N	0.870912	-0.648541	-0.000227
H	1.839727	-0.736555	-0.711967	129.28	141.62	238.04	H	1.025163	-1.202099	-0.830634
C	0.583744	0.736238	0.006453	405.08	626.31	764.91	C	1.479018	0.602491	0.001047
H	0.885416	1.342053	0.868868	954.55	1031.19	1121.37	H	1.504040	1.145511	0.935661
H	0.792618	1.270898	-0.922800	1297.28	1366.89	1386.19	H	1.519284	1.139916	-0.936265
H	-0.577203	0.675071	0.070328	1460.58	1650.23	1737.65	H	-2.148552	0.984805	-0.008802
H	1.451234	-0.915718	0.883109	3048.48	3142.24	3595.87	H	1.012679	-1.197853	0.835223
O	-1.812213	-0.124051	0.006623	3690.82	3766.92		O	-2.091688	0.029663	0.000765
H	-1.277497	-0.914803	-0.174236				H	-1.149599	-0.182749	-0.005994
R4 MA + HO ₂										
HO ₂				H ₂ O ₂						
O	0.054784	0.705690	0.000000				H	-1.020957	0.638878	0.447618
O	0.054784	-0.596889	0.000000	1258.11	1468.35	3739.65	O	-0.700390	-0.116382	-0.055979
H	-0.876549	-0.870403	0.000000				O	0.700456	0.116410	-0.055915
							H	1.020426	-0.639104	0.447533
RC4										
N	-1.086606	0.670008	-0.291319							
H	-0.964258	0.618920	-1.296692	45.88	100.66	114.14				
C	-1.646498	-0.586295	0.216428	190.53	284.89	432.47				
H	-0.939491	-1.393659	0.007954	810.04	962.52	985.57				
H	-1.762237	-0.517318	1.301580	1076.46	1193.34	1292.23				
H	-2.619240	-0.845207	-0.220155	1337.49	1445.48	1491.58				
H	-1.707448	1.448125	-0.103722	1504.60	1636.13	1646.75				
O	1.653632	-0.587596	-0.326894	3026.42	3077.85	3109.84				
O	1.497741	0.431741	0.468104	3140.66	3540.40	3621.7				
H	0.550659	0.717991	0.307862							
TS4-1				PC4-1						
N	0.924749	0.598554	-0.245234	-2595.42			N	-1.253823	-0.720286	-0.236514
H	-0.102467	-0.091059	-0.372709	54.80	99.03	130.46	H	0.604475	-0.902387	0.077168
C	2.067502	-0.210287	0.094078	223.95	386.49	526.84	C	-1.751960	0.558656	0.173233
H	2.293934	-0.903889	-0.719503	701.06	994.14	1029.95	H	-0.932166	1.187054	0.528437
H	2.940619	0.438172	0.253233	1038.83	1100.28	1251.41	H	-2.262979	1.067433	-0.659821
H	1.921058	-0.783869	1.022167	1350.98	1407.12	1414.21	H	-2.503861	0.446437	0.971202
H	0.708688	1.223778	0.532418	1463.09	1484.77	1631.25	H	-2.027720	-1.288687	-0.584731
O	-1.051624	-0.704269	-0.060639	2991.16	3052.06	3126.25	O	1.525856	-0.650139	0.278834
O	-1.981210	0.294783	0.198176	3493.58	3833.46		O	1.516536	0.711733	-0.129089
H	-2.377419	0.464598	-0.663734				H	2.071633	0.687463	-0.914018
TS4-2				PC4-2						
N	-1.548801	-0.655327	0.137973	-1596.33			N	1.499855	-0.633177	-0.264095
H	-1.014599	-1.372806	-0.333085	66.93	138.15	215.91	H	0.700236	-1.228016	-0.099123
C	-1.211136	0.650284	-0.238904	332.81	449.11	569.84	C	1.491713	0.584749	0.377585

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						NH ₃							
N	0.000000	0.000000	0.140072	1526.30 3399.02 3492.45			H	-0.914521	0.236266	0.254512	1029.36 1665.46 1665.87		
H	0.000000	0.808739	-0.490253				N	-0.000022	0.000019	-0.109056	3523.40 3658.98 3659.64		
H	0.000000	-0.808739	-0.490253				H	0.661993	0.673826	0.254461			
							H	0.252683	-0.910224	0.254422			
RC5													
N	-0.888196	0.749710	0.010703	37.11 85.44 116.05									
H	-1.072117	1.142023	-0.904554	174.05 271.33 341.46									
C	-1.124808	-0.692272	0.013688	408.12 870.62 972.03									
H	-0.408719	-1.175587	-0.658140	1082.43 1176.08 1336.98									
H	-0.935065	-1.085849	1.017161	1449.77 1487.48 1505.63									
H	-2.140362	-0.990196	-0.283756	1547.79 1655.39 3014.13									
H	-1.500501	1.220622	0.664778	3095.84 3129.41 3363.03									
N	2.124478	-0.132291	-0.084360	3484.39 3543.09 3625.81									
H	1.282078	0.422550	0.125970										
H	2.869560	0.298133	0.472007										
TSS-1						PC5-1							
N	0.485232	0.740557	-0.123901	-2009.74			N	0.969561	0.786101	0.000404	92.71 124.87 127.84		
H	-0.634057	0.379882	-0.357215	94.63 111.13 162.93			H	-1.261250	0.547934	-0.002186	156.14 162.73 285.79		
C	1.336886	-0.422288	0.023491	435.39 631.87 717.18			C	1.299953	-0.609885	0.000273	351.96 957.13 1006.03		
H	1.213249	-1.074081	-0.846638	816.03 1002.88 1089.56			H	0.387205	-1.211975	0.008213	1059.66 1081.36 1327.23		
H	2.387043	-0.101237	0.049719	1091.97 1311.21 1418.42			H	1.901527	-0.872493	-0.885641	1386.07 1473.43 1475.02		
H	1.153513	-1.014026	0.933158	1421.73 1468.26 1489.56			H	1.917811	-0.870886	0.875207	1656.58 1678.49 2968.62		
H	0.462800	1.266692	0.747736	1557.47 1618.20 2990.93			H	1.840487	1.322349	-0.001785	3021.11 3120.47 3461.80		
N	-1.750412	-0.210720	-0.110519	3056.10 3111.85 3467.28			N	-2.025372	-0.122896	-0.000004	3489.58 3618.03 3651.64		
H	-2.236743	0.408218	0.539749	3526.81 3563.55			H	-2.598982	0.049941	-0.815685			
H	-1.510868	-1.040577	0.433484				H	-2.595844	0.052005	0.817437			
TSS-2						PC5-2							
N	-1.523679	-0.408341	0.000010	-1224.40			N	1.055675	-0.683935	-0.138198	79.31 117.04 146.57		
H	-1.460457	-0.991634	-0.822923	114.62 128.60 200.10			H	1.536501	-1.335830	0.460099	183.92 230.58 301.66		
C	-0.579694	0.654188	-0.000013	409.30 553.41 720.49			C	1.322326	0.653369	0.072633	513.97 631.08 741.60		
H	-0.672236	1.273268	-0.896827	786.02 833.93 997.06			H	2.324752	0.925731	0.378759	954.53 1067.56 1266.31		
H	-0.672270	1.273343	0.896745	1170.41 1227.59 1348.60			H	0.755716	1.361265	-0.521362	1334.33 1476.22 1652.78		
H	0.569955	0.229964	0.000030	1363.15 1462.95 1471.02			H	-1.452378	0.669005	0.611824	1661.80 1665.46 3163.20		
H	-1.460454	-0.991599	0.822967	1546.24 1662.87 3064.44			H	0.076455	-0.906153	-0.277438	3273.92 3506.81 3540.09		
N	1.900196	-0.319609	0.000029	3140.78 3435.78 3533.52			N	-1.931995	0.008683	0.008206	3632.65 3654.00 3681.03		
H	2.268929	0.188452	-0.808431	3568.72 3660.12			H	-2.657292	-0.441396	0.552626			
H	2.269076	0.188730	0.808247				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	72.66 88.05 195.03									
H	-0.662110	1.288464	0.796010	305.46 758.55 962.36									
C	-1.061264	-0.574775	-0.008308	1099.38 1154.15 1326.26									
H	-0.699374	-1.151768	-0.864954	1445.80 1483.22 1502.01									
H	-0.766944	-1.116414	0.895908	1648.46 3002.83 3086.78									
H	-2.160065	-0.546073	-0.051045	3123.96 3571.47 3667.92									
H	-0.601182	1.255928	-0.853178										
O	1.778708	-0.153855	0.053222										
TS6-1						PC6-1							
N	0.362755	0.711932	-0.134568	-1887.59			N	0.517970	0.541472	0.000173	27.11 54.83 202.92		
H	-0.771329	0.342157	-0.322892	143.89 148.54 443.19			H	-1.385289	0.089589	0.000165	284.79 519.20 610.74		

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	2999.39
							Cl	0.000000	0.000000	0.070853	
RC9											
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	236.80	269.76	415.31	N	-1.222103	-0.437582	-0.000046			
H	2.068818	0.196376	-0.082812	794.50	857.16	916.34	C	-0.135888	0.500190	-0.000062	214.74	313.00	415.76
C	0.049385	0.564553	0.054065	1006.99	1123.23	1151.62	H	-0.225119	1.169538	0.875373	723.81	912.93	1017.10
H	0.068131	1.131396	1.000578	1258.82	1322.02	1386.45	H	-0.225242	1.168983	-0.875810	1031.17	1095.17	1244.65
H	0.072951	1.303292	-0.756365	1422.19	1476.25	1484.38	H	-2.095396	0.096324	0.000604	1259.19	1381.44	1410.15
H	1.227359	-1.009655	0.625985	1508.80	1655.23	2965.47	C	1.211255	-0.202135	0.000030	1430.29	1475.66	1485.88
C	-1.238056	-0.238462	-0.027902	3035.53	3059.10	3112.37	H	1.305732	-0.841233	-0.883008	2944.90	2972.02	3047.86
H	-2.116266	0.407703	0.067523	3131.53	3538.96	3627.35	H	2.035026	0.518509	-0.002260	3131.31	3133.09	3453.77
H	-1.293065	-0.771301	-0.982115				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	176.42	326.01	390.74	N	1.152178	-0.319417	-0.060020	233.24	262.98	420.30
H	1.181216	-1.166620	-0.280504	558.34	671.45	941.99	H	2.001034	0.227191	-0.128318	513.01	822.91	859.44
C	0.061229	0.524117	-0.111813	990.43	1020.43	1201.67	C	-0.027425	0.537950	-0.008957	962.22	1090.25	1139.07
H	0.140927	1.573931	0.148459	1292.64	1387.99	1448.93	H	-0.006387	1.175586	-0.910911	1159.73	1314.48	1401.34
H	2.081462	0.229349	-0.116969	1459.87	1483.60	1643.88	H	-0.037007	1.238015	0.846035	1455.96	1479.10	1652.72
C	-1.242870	-0.176159	0.015456	2964.45	3031.70	3124.53	H	1.215334	-0.885662	0.777501	2949.05	2969.35	3172.22
H	-1.426665	-0.544021	1.039719	3200.39	3571.72	3682.53	C	-1.267125	-0.274791	0.003698	3284.10	3543.85	3633.32
H	-2.070310	0.485896	-0.253212				H	-1.266515	-1.247671	-0.473698			
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	-1529.95			N	1.199074	-0.407797	0.037824	-1546.75		
H	1.307411	1.128331	0.206777	166.64	242.11	359.35	H	2.075597	0.038519	-0.193962	214.59	265.68	292.07
C	-0.042484	-0.555903	0.251847	438.11	704.84	783.80	C	0.057687	0.377849	-0.296646	334.59	417.79	766.23
H	0.048922	-0.654920	1.344715	907.57	1010.21	1024.81	H	0.098413	0.674160	-1.350809	853.57	933.16	1001.56
H	-0.137423	-1.579751	-0.141801	1101.46	1151.09	1219.47	H	0.044819	1.446367	0.296191	1135.57	1173.08	1254.98
H	1.970133	-0.476776	-0.027984	1280.59	1354.75	1384.85	H	1.209361	-0.682786	1.011689	1289.61	1336.06	1384.82
H	1.422169	1.771057	0.876012	1425.02	1465.47	1475.77	H	-0.007716	2.386525	0.893142	1397.99	1431.95	1473.18
C	-1.270791	0.261590	-0.105439	1488.95	1749.55	2993.08	C	-1.240922	-0.305307	0.062885	1481.82	1654.90	3038.17
H	-1.374900	0.335277	-1.191981	3028.46	3044.16	3123.10	H	-1.273401	-0.529216	1.135993	3080.97	3113.92	3135.80
H	-2.179657	-0.186959	0.306507	3136.69	3482.56		H	-2.096172	0.335006	-0.171294			
H	-1.179385	1.277757	0.294436				H	-1.345010	-1.249250	-0.483152			
TS1-3													
N	-1.210525	0.294206	-0.227816	-1183.38									
H	-2.118559	-0.047896	0.059250	176.20	256.02	305.71							
C	-0.140180	-0.573106	0.246668	430.11	560.27	818.99							
H	-0.302081	-1.577006	-0.172928	863.17	922.45	1021.07							
H	-0.116124	-0.692975	1.343724	1125.40	1138.79	1186.40							
H	-1.099885	1.227529	0.153237	1227.53	1238.01	1320.09							
H	1.265389	1.964114	0.846545	1402.43	1441.54	1491.08							
C	1.184842	-0.041613	-0.221483	1544.45	1655.76	2969.59							
H	1.221980	0.202173	-1.284148	3024.67	3101.08	3193.70							
H	1.291067	1.132177	0.362621	3539.25	3630.37								
H	2.063911	-0.579244	0.135305										
R2 EA + CH₃													
TS2-1							TS2-2						
N	-0.057769	1.050290	-0.442588	-1946.34			N	1.066260	-1.204201	0.144392	-1765.40		
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

N	-0.425534	1.215566	-0.295042							
H	-1.020658	1.326849	-1.108395	98.47	104.82	116.97				
C	-0.914200	0.123214	0.549766	169.74	237.65	278.70				
H	-1.900275	0.334695	0.993258	330.53	395.83	452.29				
H	-0.204475	-0.002040	1.376821	800.12	882.26	917.36				
H	-0.433720	2.096816	0.204460	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							
TSS-1				PCS-1						
N	-0.173981	0.995652	-0.412578	-2012.13						
H	-1.039246	0.165889	-0.471648	91.23	122.80	155.32		38.67	92.27	126.84
C	0.903951	0.475254	0.410336	252.83	409.18	444.46		136.64	181.67	247.87
H	0.598684	0.317435	1.459293	633.82	716.75	792.83		293.59	357.92	427.21
H	1.698686	1.236403	0.440205	831.10	915.31	1027.88		727.25	913.06	1023.73
H	-0.578764	1.821768	0.025284	1102.01	1121.22	1241.36		1033.13	1068.74	1097.44
N	-1.966872	-0.598757	-0.000185	1280.54	1375.52	1401.73		1248.12	1260.42	1384.72
H	-2.766489	0.024598	0.122732	1435.29	1469.25	1475.70		1413.68	1430.83	1477.66
H	-1.663936	-0.835575	0.946192	1491.88	1552.79	1609.68		1493.79	1659.72	1684.19
C	1.436149	-0.819539	-0.180954	2965.66	3016.94	3043.31		2949.57	2978.13	3042.26
H	1.793526	-0.650111	-1.201059	3123.95	3132.89	3462.48		3124.39	3132.40	3458.78
H	2.259778	-1.218891	0.418349	3513.78	3558.47			3488.90	3618.56	3653.18
H	0.643139	-1.574071	-0.226303							
TSS-2				PCS-2						
N	-1.074518	-1.182546	-0.157742	-1028.89						
H	-0.981365	-1.183501	-1.166126	86.68	99.60	131.14		88.41	119.27	156.04
C	-0.418415	-0.065200	0.439561	231.80	306.15	407.83		157.96	177.04	212.82
H	-0.503627	-0.120198	1.531054	567.07	601.85	803.65		310.57	405.33	416.01
H	0.773086	-0.107419	0.205451	810.27	916.64	971.55		630.70	749.95	939.51
H	-0.748526	-2.069719	0.200874	1009.71	1157.90	1213.18		1000.41	1034.15	1067.45
N	2.184126	-0.113513	-0.181487	1266.51	1332.52	1385.81		1203.46	1307.91	1384.93
H	2.277789	0.887956	-0.373094	1422.18	1458.44	1473.34		1448.41	1463.01	1488.80
H	2.580555	-0.228946	0.755331	1481.08	1544.61	1657.04		1654.10	1660.51	1666.18
C	-0.918859	1.252977	-0.108633	3031.87	3068.06	3107.56		2966.52	3051.24	3120.12
H	-0.397699	2.094940	0.356677	3127.87	3431.77	3529.00		3186.18	3491.22	3535.07
H	-0.749659	1.308077	-1.190954	3555.18	3650.06			3618.60	3650.73	3669.67
H	-1.994167	1.364570	0.069821							
TSS-3				PCS-3						
N	1.166446	-0.974406	-0.275406	-1716.20						
H	1.923112	-1.531209	0.100010	100.59	130.55	161.60		45.29	71.44	106.23
C	1.107045	0.335543	0.358104	334.77	390.43	427.41		135.03	161.89	213.58
H	0.951343	0.294408	1.450264	548.53	713.57	809.01		242.90	378.85	426.32
H	2.068254	0.846105	0.196990	871.44	899.31	926.29		525.33	851.80	888.95
H	0.296592	-1.469485	-0.102746	1074.81	1132.01	1152.12		960.90	1049.69	1097.31
N	-1.980006	-0.499081	0.136727	1229.07	1317.60	1334.54		1144.06	1162.13	1334.50
H	-2.458830	-0.433015	-0.764157	1402.27	1434.02	1441.78		1398.89	1450.03	1466.49
H	-2.553586	0.047107	0.782972	1488.89	1546.57	1657.74		1651.52	1661.29	1668.81
C	-0.002075	1.139701	-0.269266	2966.37	3023.38	3092.43		2931.78	2962.29	3158.40
H	-0.221944	2.092519	0.215442	3179.93	3449.47	3531.27		3269.58	3500.62	3513.14
H	0.078499	1.222541	-1.355157	3548.26	3625.99			3619.65	3627.50	3652.79
H	-1.018345	0.393974	-0.085893							
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			N	-0.137769	-1.145830	-0.004511			
H	-1.167687	0.147984	-0.422864	94.85	145.42	251.22	H	1.631532	-0.304453	-0.002521	64.10	64.31	200.91
C	0.840072	0.511316	0.359269	401.27	481.31	685.04	C	-1.305262	-0.313392	0.004509	232.30	357.15	425.16
H	0.613351	0.459581	1.435708	781.66	913.56	1027.54	H	-1.920885	-0.565481	0.886934	516.87	629.40	724.95
H	1.634595	1.266995	0.249511	1087.65	1105.37	1237.33	H	-1.939326	-0.569508	-0.863455	915.86	1022.49	1039.87
H	-0.693281	1.815500	0.046017	1278.71	1330.30	1388.61	H	-0.421853	-2.127308	-0.003618	1099.67	1250.45	1258.92
O	-1.923651	-0.632657	0.137661	1422.39	1450.64	1477.35	O	2.451933	0.237289	0.001841	1383.70	1413.25	1431.69
C	1.303179	-0.838855	-0.156074	1484.50	1614.85	2990.84	C	-0.940943	1.160976	-0.002366	1476.50	1481.66	2956.04
H	1.540237	-0.782565	-1.222668	3024.46	3044.39	3124.30	H	-0.353322	1.406214	-0.892317	2983.43	3049.68	3132.43
H	2.191680	-1.179590	0.382664	3139.77 3504.17			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			N	0.140121	1.256618	-0.273390			
H	-0.563845	-2.089503	0.237629	63.21	103.42	236.08	H	-0.378452	1.981727	0.196536	62.51	93.66	166.97
C	-0.345126	-0.056987	0.443150	329.48	426.39	737.43	C	0.682614	0.255304	0.517368	221.58	374.12	386.59
H	-0.466794	-0.100551	1.532169	789.22	925.12	997.93	H	1.056574	0.580289	1.483230	438.24	471.39	629.05
H	0.804980	-0.006000	0.287421	1119.18	1146.81	1248.31	H	-1.308707	-0.634825	0.581146	663.42	944.70	990.67
H	-0.827697	-1.236945	-1.156650	1284.69	1383.05	1394.79	H	-0.302087	0.953601	-1.130024	1028.61	1200.52	1295.76
O	2.281461	0.053381	-0.100988	1424.78	1474.28	1480.09	O	-2.091723	-0.550730	-0.002593	1388.40	1447.71	1463.92
C	-0.922269	1.216500	-0.139305	1653.49	1739.93	3039.10	C	1.341122	-0.876856	-0.190946	1483.93	1648.92	2977.26
H	-0.455081	2.097649	0.308767	3067.34	3118.19	3134.45	H	1.638615	-1.659852	0.511485	3045.60	3125.46	3191.01
H	-0.750200	1.257551	-1.220875	3565.95 3664.40			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			N	0.828995	-1.115541	-0.338614			
H	0.359558	-1.491763	-0.166526	109.00	142.95	300.26	H	-0.150607	-1.378067	-0.348918	55.19	107.56	153.65
C	0.967102	0.375642	0.375691	412.00	444.90	575.07	C	1.016913	0.098730	0.442787	240.72	296.56	350.75
H	0.787221	0.294650	1.461341	804.34	856.59	915.10	H	0.581658	0.053148	1.458588	397.21	427.99	595.12
H	1.878836	0.981763	0.256574	987.28	1119.98	1129.64	H	2.102020	0.234356	0.597962	842.79	861.73	953.77
H	1.975801	-1.388394	0.084886	1170.20	1195.29	1250.01	H	1.349761	-1.887172	0.057085	1095.98	1140.82	1156.22
O	-2.018741	-0.564395	0.122879	1327.41	1401.26	1441.21	O	-2.235051	-0.194271	0.099310	1325.67	1396.20	1449.24
C	-0.175692	1.106423	-0.266287	1480.44	1655.91	2973.07	C	0.481490	1.284328	-0.273700	1464.65	1661.95	2942.04
H	-1.206152	0.327549	-0.094239	3017.71	3095.79	3190.99	H	-1.613647	0.539303	-0.092363	2971.96	3154.02	3265.73
H	-0.487774	2.035096	0.213095	3540.57 3633.50			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 + C₂H₅													
TS7-1				TS7-2									
N	0.715507	1.276413	-0.080272	-1939.05			N	1.481133	-1.108549	-0.440423	-1823.74		
H	-0.419514	0.852729	-0.473424	86.45	120.23	152.40	H	1.050308	-0.985117	-1.348624	41.49	98.33	128.72
C	1.331339	0.133777	0.573885	196.75	226.47	281.84	C	1.063997	-0.114046	0.496101	174.89	221.79	270.80
H	0.713470	-0.282040	1.388733	408.24	457.65	565.32	H	1.543285	-0.277072	1.467648	316.77	401.55	507.16
H	2.262906	0.481407	1.047687	758.95	799.75	859.63	H	-0.199831	-0.216512	0.749714	530.49	775.44	824.94
H	0.424618	1.948976	0.631186	875.81	914.70	1026.19	H	1.316450	-2.053070	-0.119638	834.52	906.31	939.12
C	-1.626097	0.326470	-0.629394	1041.81	1098.22	1113.96	C	-1.634922	-0.316799	0.729475	1000.90	1056.94	1133.84
C	-1.908303	-0.629019	0.499380	1147.68	1218.03	1237.01	C	-2.001655	0.210838	-0.630528	1145.46	1173.03	1213.31
H	-2.268923	1.208990	-0.655629	1277.52	1374.33	1381.91	H	-1.794328	-1.385478	0.880724	1259.98	1364.90	1389.59
H	-1.543781	-0.134812	-1.616167	1393.76	1417.86	1454.32	H	-1.967515	0.278902	1.579700	1394.27	1448.54	1452.06
H	-1.191507	-1.458084	0.516244	1465.46	1470.11	1473.87	H	-1.796249	1.283921	-0.711310	1456.91	1467.55	1470.68
H	-1.862527	-0.127144	1.472661	1482.06	1489.56	1500.28	H	-1.429726	-0.295093	-1.420113	1480.11	1485.57	1650.10
H	-2.909847	-1.071465	0.410788	2970.07	3012.39	3017.22	H	-3.064857	0.064940	-0.868286	3005.33	3019.99	3060.37
C	1.642758	-0.947462	-0.447282	3039.19	3076.64	3086.82	C	1.253253	1.286538	-0.029933	3068.67	3090.85	3095.04
H	2.286490	-0.547334	-1.236429	3104.08	3116.13	3130.56	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						PC8-1							
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	51.35	61.26	95.31
C	1.171688	0.242955	0.523374	233.86	296.95	422.17	C	-1.727136	-0.228051	0.189026	134.24	246.50	266.48
H	0.474935	-0.144155	1.301818	530.82	665.61	729.31	H	-2.034358	-0.250790	1.250415	402.32	430.77	715.43
H	2.018053	0.685605	1.070614	916.78	1007.94	1045.93	H	-2.620531	-0.557602	-0.370704	729.36	915.57	1028.59
H	0.359157	2.084589	0.356304	1115.33	1167.80	1258.57	H	-1.003785	-2.114867	0.261977	1042.53	1103.58	1256.15
O	-1.727162	0.156623	-0.457442	1294.35	1366.04	1392.63	O	1.900549	-0.291407	-0.486068	1260.41	1290.53	1384.06
O	-1.661971	-0.710479	0.472903	1400.12	1421.46	1477.27	O	1.986387	0.503853	0.541148	1410.97	1429.51	1476.58
C	1.602605	-0.909947	-0.367074	1483.10	1645.93	2873.13	C	-1.298188	1.168783	-0.221873	1490.59	1594.70	2960.23
H	2.289188	-0.562305	-1.144456	3017.79	3048.83	3131.88	H	-1.030520	1.190367	-1.283089	2988.88	3049.86	3132.36
H	2.101464	-1.687018	0.218876	3138.53 3492.19			H	-2.103593	1.890025	-0.056459	3141.11	3293.48	3490.73
H	0.729154	-1.356986	-0.852588				H	-0.421983	1.479642	0.355216			
TS8-2						PC8-2							
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	85.45	101.06	134.87
C	0.953126	0.095933	0.521835	210.73	337.49	401.98	C	1.156034	0.106353	0.507055	167.99	219.80	231.41
H	1.416585	0.176453	1.507355	425.14	574.07	699.31	H	1.697505	0.217581	1.443131	393.62	418.88	634.50
H	-0.415963	-0.245361	0.772009	856.42	941.17	993.89	H	-0.742455	-0.168004	0.858988	656.85	723.59	943.67
H	0.622142	2.113113	0.407950	1109.56	1151.76	1200.09	H	0.875123	2.126107	0.309711	991.52	1038.13	1201.91
O	-1.556751	-0.407749	0.567270	1293.43	1372.89	1388.50	O	-1.711731	-0.241148	0.632571	1289.68	1305.50	1387.50
O	-1.766766	0.088709	-0.583353	1437.61	1468.84	1479.70	O	-1.801821	0.044256	-0.630279	1447.79	1465.37	1484.63
C	1.377753	-1.069320	-0.328921	1575.47	1657.26	3020.96	C	1.320637	-1.152236	-0.279857	1550.20	1653.03	2987.26
H	1.323758	-2.004371	0.234343	3088.65	3121.55	3136.33	H	1.298468	-2.029159	0.372628	3063.24	3124.58	3133.89
H	0.718893	-1.160623	-1.201587	3568.10 3680.01			H	0.517577	-1.259103	-1.020819	3172.55	3577.59	3693.52
H	2.405546	-0.940377	-0.692933				H	2.274607	-1.165433	-0.830513			
TS8-3						PC8-3							
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	41.06	76.99	101.71
C	-1.285157	0.116544	0.495258	243.15	293.30	423.77	C	-1.400692	0.119601	0.482973	131.56	177.97	276.11
H	-2.299101	0.412713	0.814323	455.12	547.97	790.85	H	-2.437422	0.325986	0.803061	299.28	426.27	472.36
H	-0.747321	-0.161213	1.419278	871.80	910.65	979.26	H	-0.830705	-0.026051	1.419891	638.48	848.87	868.60
H	-2.043912	-1.681193	-0.126047	1037.31	1119.31	1139.18	H	-1.967067	-1.793756	0.023264	950.48	1090.13	1143.91
O	1.664354	-0.768614	0.332577	1200.90	1329.53	1390.56	O	1.733984	-0.808472	0.126296	1161.15	1283.45	1328.46
O	1.775536	0.343102	-0.273090	1418.17	1440.77	1455.77	O	2.003775	0.450694	-0.041302	1395.67	1446.32	1457.56
C	-0.632196	1.305845	-0.126472	1529.97	1663.10	2962.90	C	-0.883061	1.313266	-0.233135	1515.66	1661.71	2942.34
H	-0.464925	2.179128	0.502928	2995.81	3107.38	3212.80	H	-0.699394	2.234795	0.311630	2973.82	3147.92	3258.95
H	0.783466	0.827274	-0.274271	3547.25 3631.76			H	1.139218	0.893683	-0.209319	3412.74	3544.70	3633.09
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				N	0.602910	1.064190	-0.291808			
H	-0.758231	0.720734	-0.061896				H	-0.984658	0.512764	-0.179405	23.98	62.16	141.79
C	1.456839	0.385551	0.472369				C	1.485566	0.313106	0.549787	243.91	274.13	385.88
H	1.064661	0.220362	1.472156				H	0.920906	-0.053083	1.403996	719.40	723.52	827.37
H	2.345252	1.021157	0.548280				H	2.301049	0.947603	0.907249	924.35	1017.78	1054.84
H	0.733751	1.188670	-1.256785				H	1.132503	1.519438	-1.032144	1127.09	1257.40	1316.59
C	1.830705	-0.939169	-0.194104				C	2.070040	-0.870227	-0.234292	1393.58	1416.39	1507.15
H	2.248406	-0.768679	-1.184816				H	2.663907	-0.522166	-1.076841	1515.92	1533.47	2112.80
H	2.572744	-1.455765	0.409321				H	2.707011	-1.458902	0.420907	3065.06	3102.46	3148.16
H	0.946996	-1.564663	-0.284882				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				N	1.469942	-1.209279	-0.193418			
H	-0.184023	1.976106	0.202605				H	1.205333	-2.085748	0.221149	57.84	97.14	146.70
C	-1.089590	0.146333	0.549239				C	1.111131	-0.065881	0.491237	217.62	384.21	416.00
H	-1.610044	0.509087	1.434513				H	1.182214	-0.143450	1.566967	644.23	669.03	714.77
H	-0.155937	-0.363942	0.911735				H	-0.636707	-0.011696	0.315195	816.16	954.86	1005.37
H	-0.315189	1.009466	-1.154452				H	1.324520	-1.188611	-1.189388	1061.40	1216.51	1312.00
Cl	1.854032	-0.247272	-0.014009				Cl	-1.941771	0.006463	-0.032719	1415.57	1469.94	1496.98
C	-1.905921	-0.865686	-0.229415				C	1.416450	1.240396	-0.159356	1510.79	1666.07	1998.85
H	-1.328505	-1.234449	-1.075939				H	1.024143	1.263365	-1.176721	3057.85	3116.80	3175.66
H	-2.156060	-1.713192	0.402637				H	0.961233	2.058047	0.392348	3226.84	3597.41	3701.66
H	-2.824956	-0.416902	-0.599126				H	2.494301	1.416086	-0.210686			
TS9-3							PC9-3						
N	1.597712	-1.012586	-0.306725				N	1.548983	-1.076011	-0.324404			
H	0.694552	-1.466271	-0.327238				H	0.603017	-1.416524	-0.424273	83.93	104.64	144.80
C	1.517019	0.235658	0.432847				C	1.569786	0.151029	0.459042	274.58	342.00	436.80
H	1.165996	0.126369	1.464259				H	1.105220	0.056954	1.447936	501.57	589.20	692.28
H	2.521389	0.669681	0.485509				H	2.618842	0.414014	0.640357	846.89	877.64	964.23
H	2.253279	-1.647950	0.120932				H	2.089148	-1.800499	0.122665	1108.52	1146.72	1174.33
C	0.645829	1.207701	-0.285188				C	0.929709	1.262444	-0.284390	1336.56	1420.72	1474.94
H	-0.641232	0.586197	-0.177506				H	-0.867370	0.587008	-0.172352	1496.91	1674.00	2428.19
H	0.431413	2.149123	0.202836				H	0.716062	2.191545	0.221065	3019.73	3034.77	3201.40
H	0.737528	1.232207	-1.363410				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										
H	-0.772481	1.207820	0.000000	233.81	270.86	385.85							
C	0.026520	-0.222526	1.201868	769.52	966.23	1031.20							
H	0.966394	-0.784821	1.257905	1097.24	1186.45	1201.06							
H	-0.031534	0.416904	2.087744	1266.19	1428.58	1456.54							
H	-0.800557	-0.954905	1.242653	1464.20	1475.98	1483.69							
C	0.026520	-0.222526	-1.201868	1504.92	1506.24	2951.88							
H	-0.031534	0.416904	-2.087744	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						DMA-2							
N	0.000066	0.641663	0.000000				N	0.092419	0.479615	-0.126718			
C	0.000009	-0.165643	1.182709	102.96	164.17	436.44	H	0.117274	1.426561	0.217539	195.31	325.64	389.92
H	0.883372	-0.826696	1.207852	936.30	949.03	1010.87	C	1.243815	-0.246856	0.072780	574.29	624.27	986.04
H	0.000274	0.458901	2.079675	1028.21	1206.19	1232.09	H	1.218676	-1.291046	-0.216039	1039.37	1135.07	1254.69
H	-0.883756	-0.826156	1.208050	1385.68	1405.47	1449.32	H	2.184296	0.288091	0.054187	1314.67	1436.16	1464.69
C	0.000009	-0.165643	-1.182709	1459.71	1477.06	1479.58	C	-1.179396	-0.185722	0.032116	1472.32	1491.08	1540.57
H	0.000274	0.458901	-2.079675	2955.62	2962.83	3011.04	H	-1.989840	0.475733	-0.285365	2989.82	3075.66	3128.97
H	0.883372	-0.826696	-1.207852	3015.41	3117.42	3118.16	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				N	0.094092	-0.609281	-0.164567			
H	-0.000019	1.476067	0.023956	-1752.31			H	0.083412	-0.949797	-1.116159	-1696.20		
H	-0.000128	2.217696	0.658388	189.05	228.35	357.40	H	-1.405989	1.975547	-0.930039	186.82	213.74	297.95
C	-1.198098	-0.281331	0.087043	381.98	409.67	920.92	C	-1.144176	-0.041750	0.212389	411.27	504.30	731.77
H	-2.078645	0.303859	-0.192145	986.06	1017.01	1080.12	H	-1.996383	-0.673282	-0.048747	983.67	1040.73	1112.21
H	-1.285251	-1.273590	-0.375863	1164.98	1182.63	1227.13	H	-1.159839	0.229261	1.273306	1176.49	1230.31	1263.98
H	-1.189625	-0.424410	1.179555	1354.23	1410.98	1432.55	H	-1.335215	1.038742	-0.374141	1286.76	1363.93	1373.13
C	1.198111	-0.281302	0.087050	1454.52	1472.56	1474.52	C	1.233848	0.247093	0.091629	1436.24	1464.06	1471.41
H	2.078636	0.303960	-0.192054	1490.76	1618.54	2984.23	H	2.153490	-0.238900	-0.244616	1487.77	1512.12	2973.54
H	1.189601	-0.424462	1.179550	2985.41	3059.67	3059.98	H	1.146789	1.230179	-0.402220	3061.01	3074.31	3130.00
H	1.285350	-1.273517	-0.375933	3124.61	3124.65		H	1.317056	0.421155	1.170479	3150.71	3597.36	
R2 DMA + CH₃													
TS2-1						TS2-2							
N	0.446421	0.000002	-0.560292				N	1.118350	0.417552	-0.370453			
H	-0.762475	-0.000372	-0.451654	-1948.23			H	1.021791	0.406020	-1.376729	-1810.81		
C	-2.033407	-0.000262	0.069358	45.42	115.91	147.00	H	-2.222556	-0.430431	-0.070977	83.07	99.45	125.84
C	0.883084	-1.193203	0.132614	202.80	240.69	404.01	C	1.370144	-0.906618	0.159673	240.73	347.24	376.22
H	0.444019	-2.080586	-0.333056	530.02	542.53	560.64	H	2.192273	-1.380167	-0.383910	482.04	545.74	631.91
H	1.976000	-1.272627	0.053843	945.66	1028.59	1081.88	H	1.666264	-0.820863	1.211740	742.73	984.15	1047.17
H	0.629327	-1.190438	1.207548	1099.21	1143.66	1201.74	H	0.486031	-1.565881	0.113526	1084.82	1122.23	1176.29
C	0.882455	1.193466	0.132592	1225.71	1341.22	1405.10	C	0.039188	1.090198	0.257325	1227.31	1279.63	1395.45
H	0.443114	2.080624	-0.333251	1411.19	1422.85	1433.12	H	-0.164824	2.064632	-0.193093	1405.06	1432.22	1435.94
H	0.628457	1.190690	1.207466	1457.98	1471.92	1474.72	H	-1.043209	0.419647	0.144518	1442.65	1465.91	1471.54
H	1.975354	1.273353	0.054065	1490.31	1490.70	2960.90	H	0.196033	1.178730	1.337748	1486.78	1510.06	2970.38
H	-2.480175	-0.913120	-0.320940	2961.34	3050.89	3050.96	H	-3.032093	0.284357	-0.203490	3055.26	3066.05	3074.33
H	-2.479165	0.913860	-0.319135	3071.26	3111.46	3111.81	H	-1.974376	-0.997623	-0.966720	3125.49	3145.07	3219.08
H	-1.892189	-0.001408	1.149773	3211.50	3221.81		H	-2.297001	-1.030614	0.833459	3226.01	3594.12	
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										
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 + NH₂													
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										
TSS-1				PC5-1									
N	-0.377528	0.000386	-0.512493	-1813.87			N	-0.541657	-0.250273	-0.005527			
H	0.790800	-0.000825	-0.560377	52.18	135.82	169.16	H	1.667821	-0.619600	-0.004394	60.94	95.54	99.47
N	2.013967	-0.002019	-0.043362	210.48	232.29	394.03	N	2.605052	-0.224374	0.000952	135.30	144.29	156.99
H	2.022075	-0.801825	0.592086	533.28	630.34	747.33	H	3.097075	-0.568486	-0.813777	212.13	357.18	439.52
H	2.034339	0.818709	0.564570	955.87	1040.13	1082.39	H	3.088906	-0.571406	0.819331	949.65	952.14	1009.59
C	-0.856525	-1.200140	0.128480	1132.91	1217.71	1234.00	C	-0.456834	1.180681	0.000575	1028.59	1060.29	1211.52
H	-1.935701	-1.300950	-0.054490	1369.49	1413.17	1433.28	H	-0.965813	1.596200	0.886995	1235.46	1384.14	1403.58
H	-0.358357	-2.076048	-0.297216	1457.29	1472.38	1473.32	H	0.588798	1.499496	-0.001205	1449.31	1461.44	1477.86
H	-0.710625	-1.197445	1.222772	1491.66	1560.22	1607.18	H	-0.970905	1.603351	-0.879507	1483.31	1658.60	1678.43
C	-0.857979	1.199754	0.129558	2963.92	2964.48	3044.98	C	-1.898003	-0.707742	0.001514	2958.68	2966.85	3014.17
H	-0.708666	1.197780	1.223352	3045.54	3116.27	3116.89	H	-2.447021	-0.319062	-0.872850	3019.92	3121.78	3126.80
H	-0.363886	2.077137	-0.297856	3452.14 3547.06			H	-1.942694	-1.799693	-0.008128	3484.55	3615.81	3655.97
H	-1.938027	1.297217	-0.050081										
TSS-2				PC5-2									
N	-1.082525	0.442784	-0.360508	-1108.17			N	0.639663	0.019427	0.377194			
H	-0.986402	0.449807	-1.367034	100.07	128.29	150.33	H	-0.247093	-0.442129	0.546480	66.61	82.66	106.08
N	2.120744	-0.550620	-0.158618	241.59	375.65	396.94	N	-2.380795	-0.339096	-0.027629	157.02	189.86	233.35
H	2.406592	-0.734158	0.806945	573.22	696.52	765.72	H	-2.863115	-1.118739	-0.457381	274.32	377.32	408.05
H	2.781624	0.158518	-0.487591	827.61	989.94	1049.47	H	-3.051522	0.158647	0.544801	623.71	780.94	992.12
C	-1.383429	-0.885444	0.138275	1126.86	1215.45	1258.81	C	1.701314	-0.822557	-0.113560	1048.95	1072.34	1132.43
H	-1.668430	-0.814040	1.194384	1297.53	1369.76	1434.21	H	2.660043	-0.303531	0.000191	1256.21	1335.19	1435.40
H	-2.228781	-1.308497	-0.410900	1454.30	1467.61	1473.74	H	1.745784	-1.745829	0.470376	1470.23	1474.01	1493.34
H	-0.522654	-1.568696	0.057857	1489.84	1513.50	1548.46	H	1.584208	-1.083229	-1.178243	1565.06	1657.62	1664.88
C	0.020412	1.058497	0.277915	2987.60	3054.51	3072.83	C	0.519445	1.290337	-0.122702	2977.64	3066.40	3125.10
H	1.015115	0.364624	0.128252	3127.41	3138.65	3433.74	H	-2.077974	0.286398	-0.767579	3153.95	3266.66	3507.19
H	0.249004	2.040147	-0.145396	3531.79 3595.98			H	-0.318397	1.881221	0.229026	3559.04	3633.16	3652.49
H	-0.135501	1.128823	1.360229										
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										

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 + CI (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							
CI	-1.412256	-0.442464	-0.039784										
TS9-1													
N	0.818002	-0.000021	-0.283136				N	0.850857	-0.000118	-0.001166			
H	-0.452142	-0.000118	-0.318819	-763.61			H	-0.737188	-0.000280	-0.000708	54.40	63.37	76.52
C	1.477477	-1.218662	0.067025	27.45	62.38	74.24	C	1.624631	-1.202396	0.000143	142.25	161.50	451.69
H	1.667915	-1.245398	1.143443	138.43	368.41	492.41	H	2.268966	-1.234417	0.884211	793.22	935.14	962.92
H	0.857319	-2.062916	-0.213203	901.62	992.38	1034.31	H	0.971662	-2.068906	-0.004301	1006.55	1030.69	1044.81
H	2.442846	-1.272091	-0.441110	1046.19	1104.17	1175.05	H	2.278139	-1.231422	-0.877183	1246.93	1270.69	1419.46
C	1.477198	1.218764	0.067067	1261.98	1353.90	1424.66	C	1.623708	1.202762	0.000165	1438.21	1484.94	1491.71
H	0.855446	2.062781	-0.210328	1448.15	1480.55	1488.70	H	0.970031	2.068748	-0.002869	1512.89	1513.26	1840.07
H	1.670906	1.244227	1.142915	1505.93	1517.81	3054.91	H	2.269178	1.234649	0.883393	3038.87	3046.15	3084.54
H	2.440983	1.273837	-0.443934	3061.35	3106.61	3112.52	H	2.276018	1.232906	-0.878007	3091.47	3188.40	3189.10
CI	-1.937490	-0.000046	0.030496	3203.05	3203.55		CI	-2.102520	-0.000156	0.000104			
TS9-2													
C	0.666731	1.009101	-0.168400				C	0.766895	1.211687	0.252604			
H	0.174700	0.589997	-1.048158	-134.19			H	0.597840	2.152762	-0.247679	73.32	96.24	102.00
H	1.334425	1.806988	-0.520342	29.05	73.15	230.21	H	0.893102	1.225615	1.325803	198.93	389.55	426.28
H	-0.090125	1.457928	0.472714	271.32	379.39	761.18	H	-0.804816	0.523247	0.164212	640.25	732.43	808.75
N	1.350490	-0.051540	0.540904	965.05	1048.41	1114.70	N	1.518196	0.288403	-0.422287	872.42	991.55	1066.81
H	1.703021	0.291224	1.420968	1198.77	1202.96	1283.11	H	1.406183	0.285231	-1.421845	1159.01	1269.31	1334.45
C	2.429624	-0.624724	-0.241544	1454.15	1485.89	1490.40	C	1.736499	-1.013759	0.176566	1467.73	1493.18	1513.48
H	2.948031	-1.380212	0.342754	1509.47	1520.78	1535.37	H	2.486760	-1.553276	-0.392674	1526.07	1568.08	1753.33
H	2.010155	-1.109756	-1.121772	1539.67	3003.61	3015.29	H	2.104183	-0.873136	1.190021	3082.89	3153.65	3186.15
H	3.159208	0.120351	-0.583298	3078.38	3120.80	3134.27	H	0.816553	-1.599307	0.214003	3192.09	3295.94	3642.02
CI	-2.310057	-0.218942	-0.017031	3170.39	3592.67		CI	-1.949855	-0.198089	-0.026521			

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			

