Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Reaction Kinetics of the Hydrogen Atom Abstraction from Isopentanol by H Atom and $H\dot{O}_2$ Radical

Prajakta Rajaram Parab[1], K. Alexander Heufer[1], Ravi Xavier Fernandes[2*]

[1] Physico Chemical Fundamentals of Combustion, RWTH Aachen University, Templergraben 55, 52056 Aachen, Germany

[2] Physikalich Technische Bundesanstalt (PTB) Bundesallee 100, 38116 Braunschweig, Germany

Hindered rotor analysis performed by scanning dihedral angle at b3lyp/cbsb7 for the internal rotations involved in the H-atom abstraction from isopentanol by H atom and HO_2 radical.

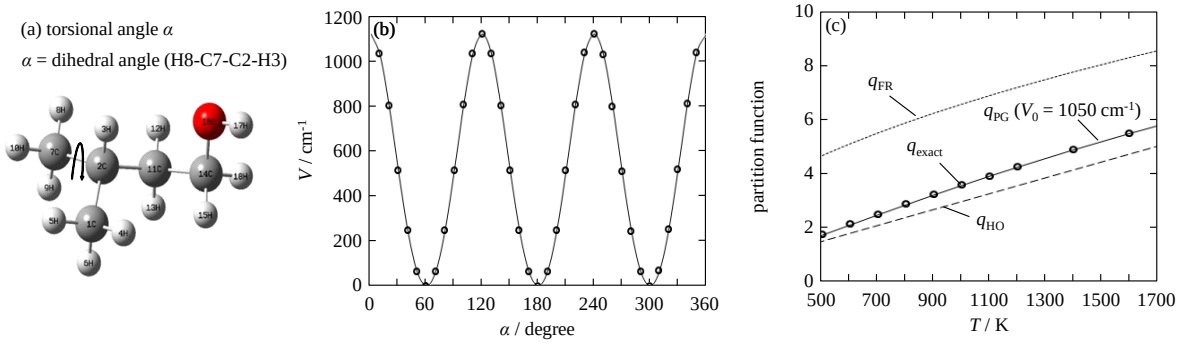

Figure S1. Hindered rotor analysis for H8-C7-C2-H3 in isopentanol.

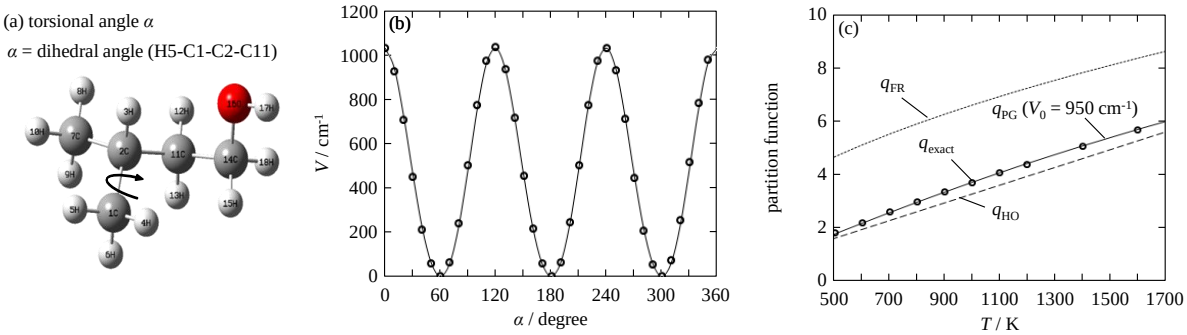

Figure S2. Hindered rotor analysis for H5-C1-C2-C11 in isopentanol.

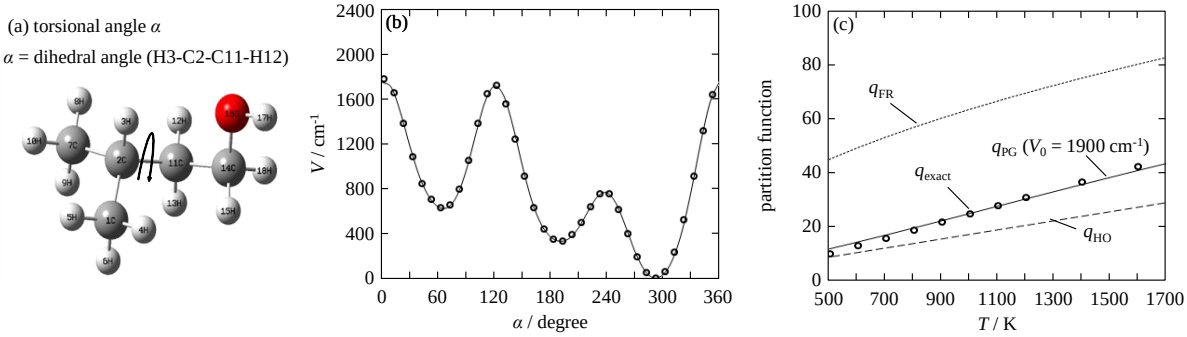

Figure S3. Hindered rotor analysis for H3-C2-C11-H12 in isopentanol.

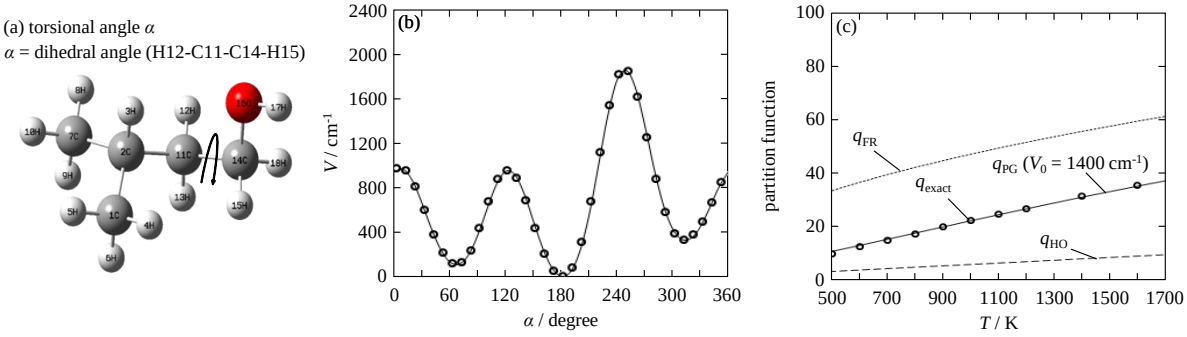

Figure S4. Hindered rotor analysis for H12-C11-C14-H15 in isopentanol.

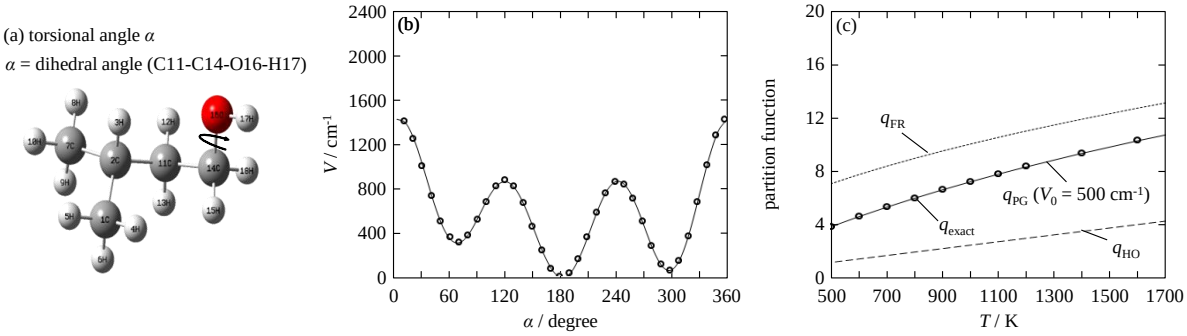

Figure S5. Hindered rotor analysis for C11-C14-O16-H17 in isopentanol.

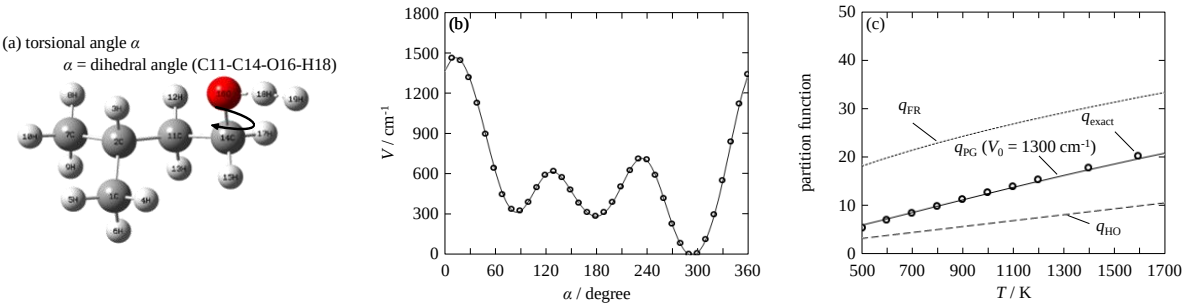

Figure S6. Hindered rotor analysis for C11-C14-O16-H18 in the TS for H-abstraction from isopentanol by H atom

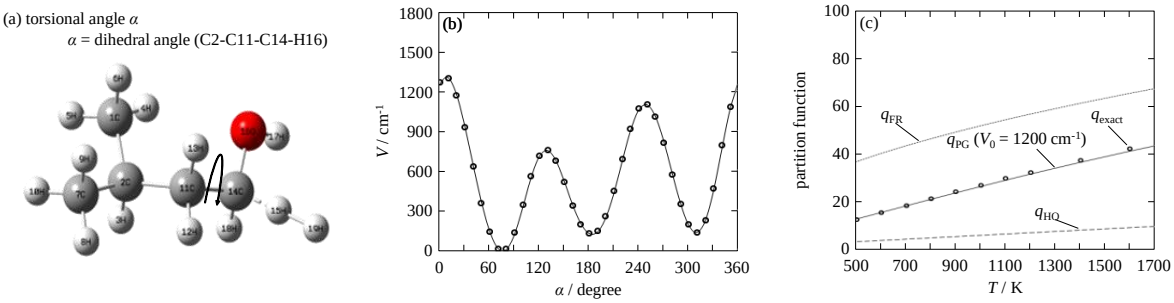

Figure S7. Hindered rotor analysis for C2-C11-C14-H16 in the TS for H-abstraction from isopentanol by H atom

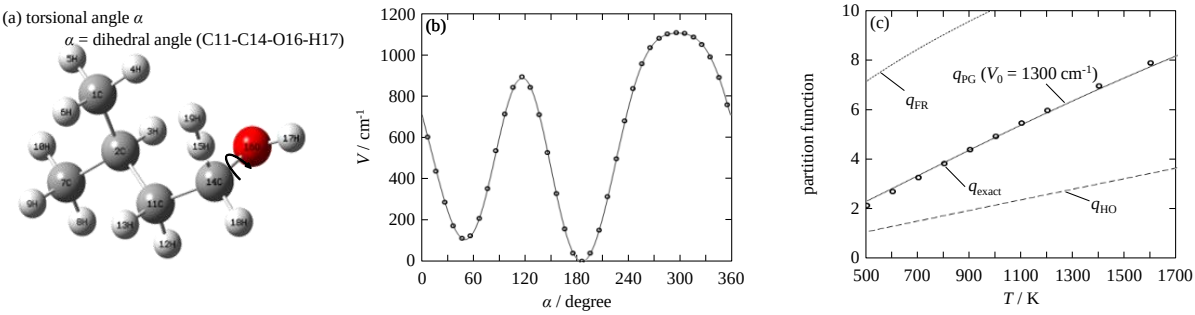

Figure S8. Hindered rotor analysis for C11-C14-O16-H17 in the TS for H-abstraction from isopentanol by H atom

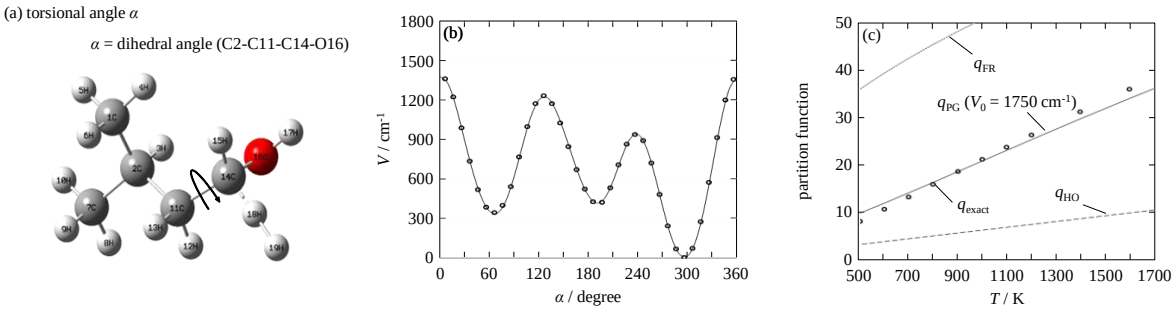

Figure S9. Hindered rotor analysis for C2-C11-C14-O16 in the TS for H-abstraction from isopentanol by H atom

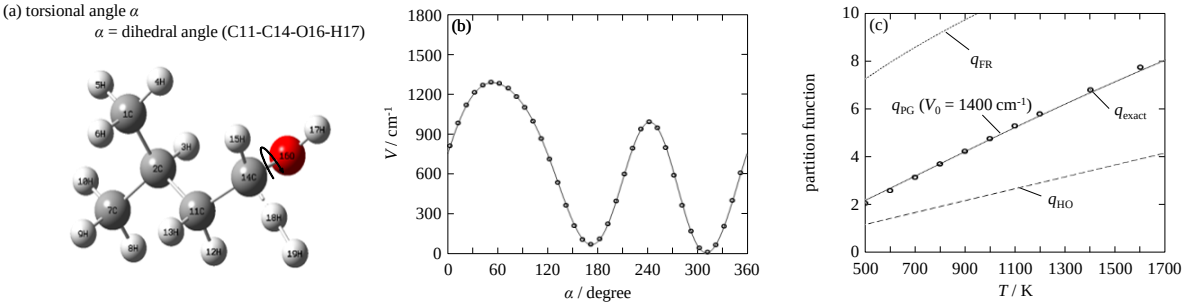

Figure S10. Hindered rotor analysis for C11-C14-O16-H17 in the TS for H-abstraction from isopentanol by H atom

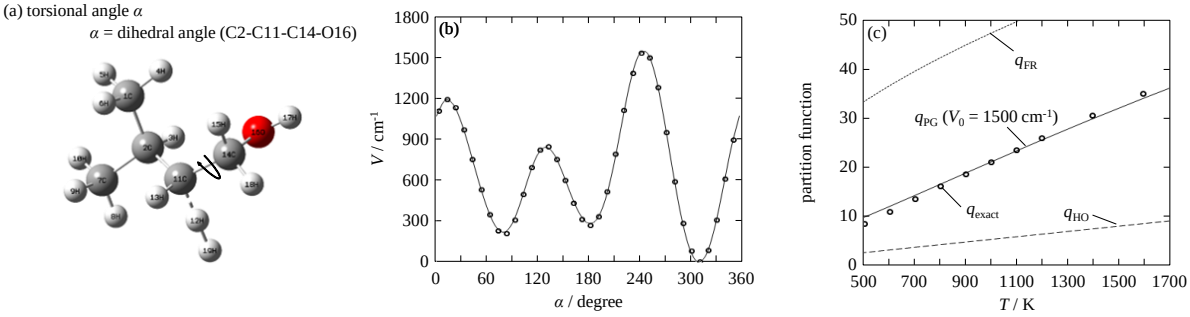

Figure S11. Hindered rotor analysis for C2-C11-C14-O16 in the TS for H-abstraction from isopentanol by H atom

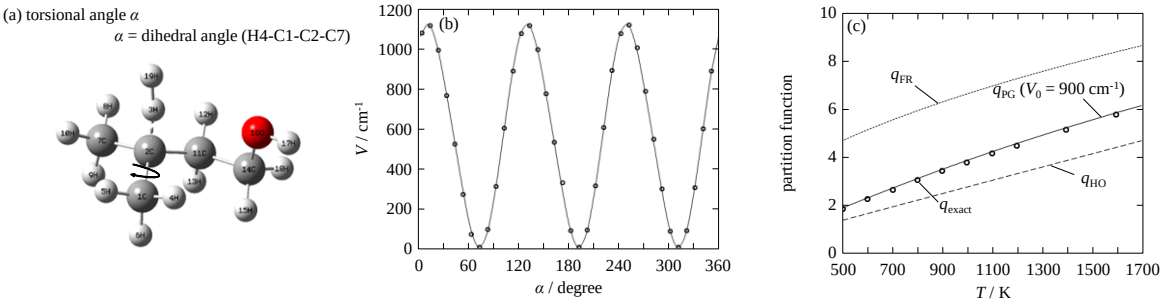

Figure S12. Hindered rotor analysis for H4-C1-C2-C7 in the TS for H-abstraction from isopentanol by H atom

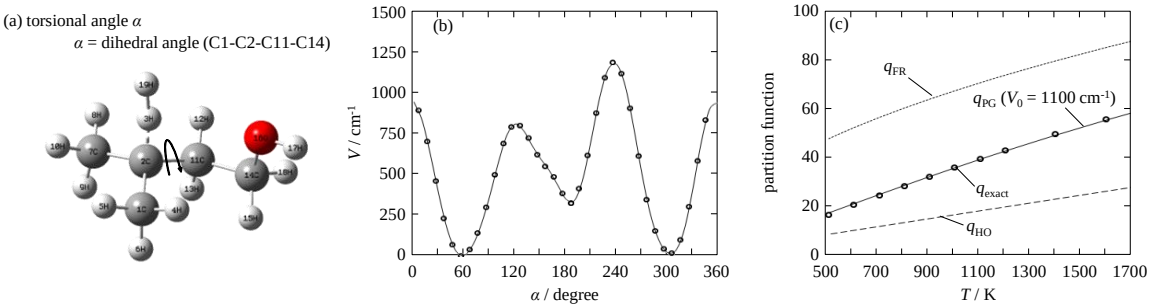

Figure S13. Hindered rotor analysis for C1-C2-C11-C14 in the TS for H-abstraction from isopentanol by H atom

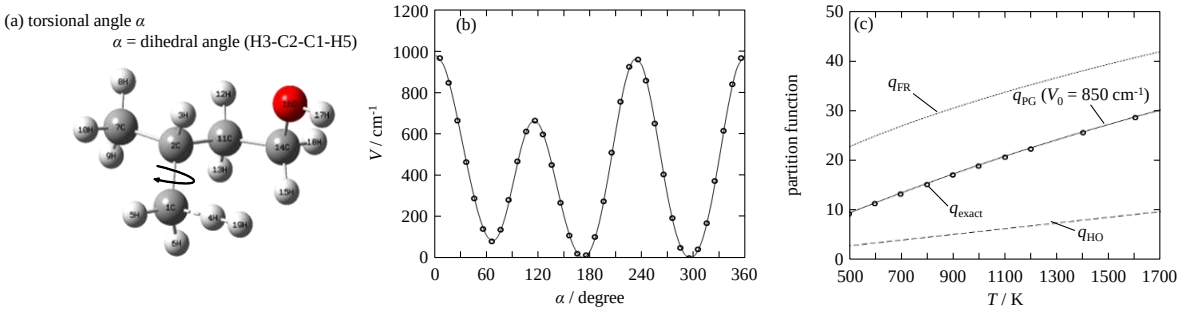

Figure S14. Hindered rotor analysis for H3-C2-C1-H5 in the TS for H-abstraction from isopentanol by H atom

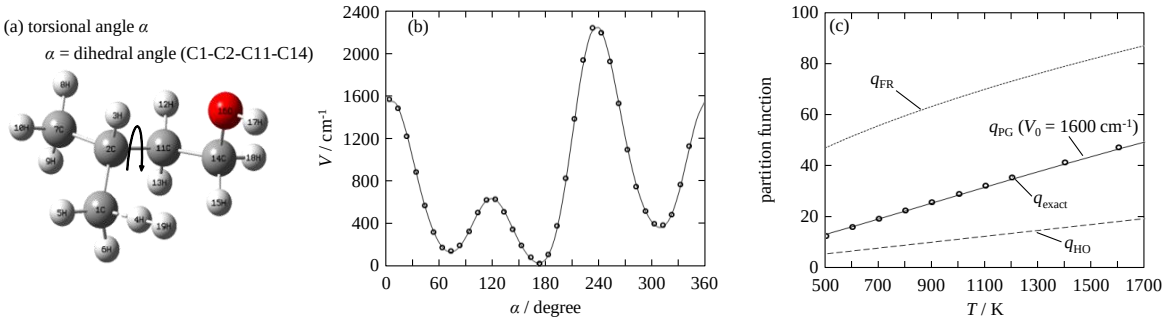

Figure S15. Hindered rotor analysis for C1-C2-C11-C14 in the TS for H-abstraction from isopentanol by H atom

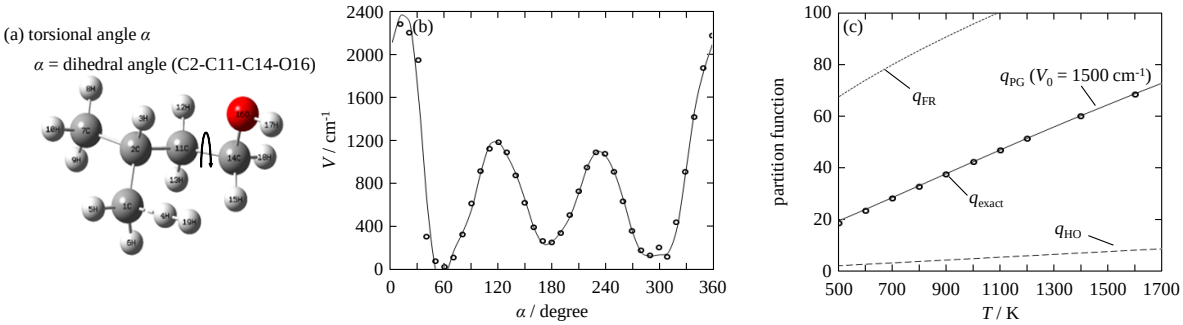

Figure S16. Hindered rotor analysis for C2-C11-C14-O16 in the TS for H-abstraction from isopentanol by H atom

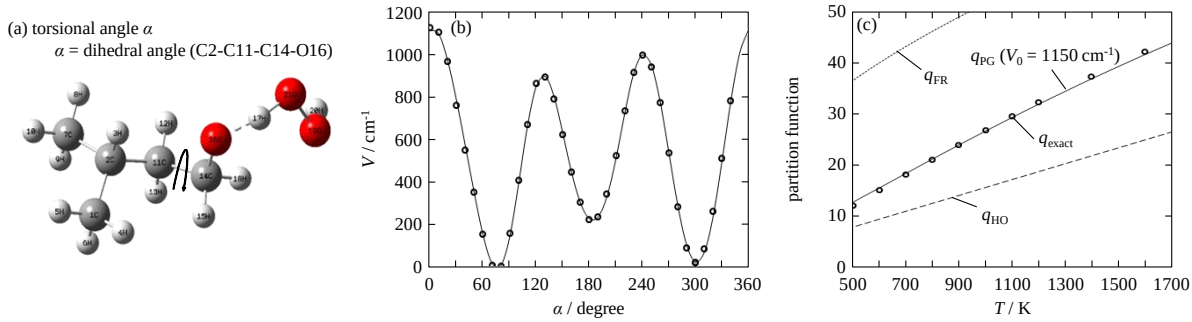

Figure S17. Hindered rotor analysis for C2-C11-C14-O16 in the TS for H-abstraction from isopentanol by HO_2 radical

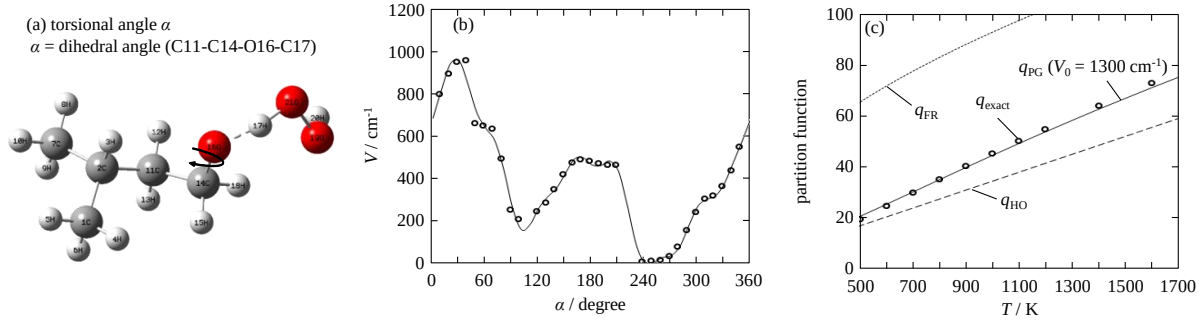

Figure S18. Hindered rotor analysis for C11-C14-O16-C17 in the TS for H-abstraction from isopentanol by HO_2 radical

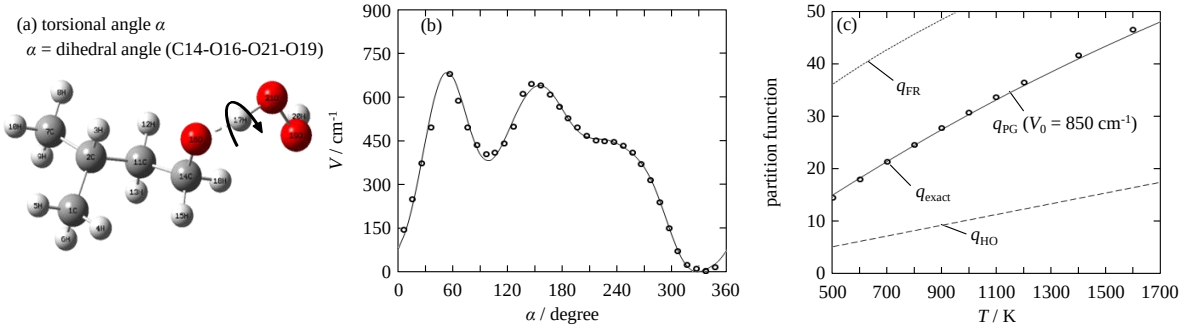

Figure S19. Hindered rotor analysis for C14-O16-O21-O19 in the TS for H-abstraction from isopentanol by HO_2 radical

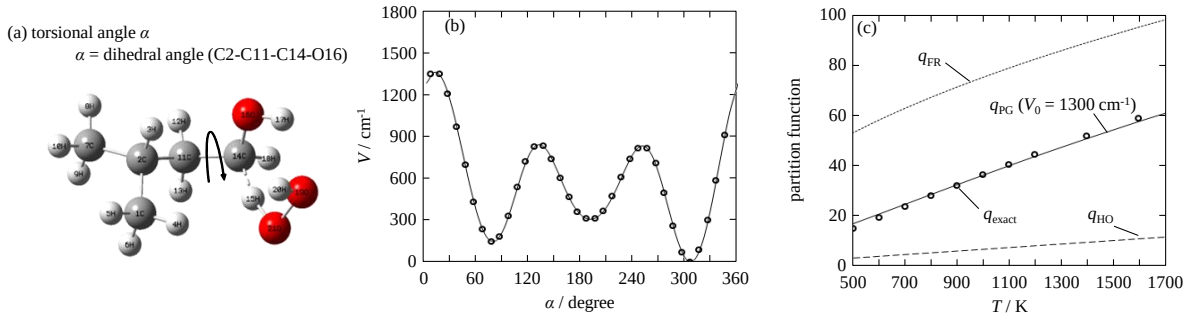

Figure S20. Hindered rotor analysis for C2-C11-C14-O16 in the TS for H-abstraction from isopentanol by HO_2 radical

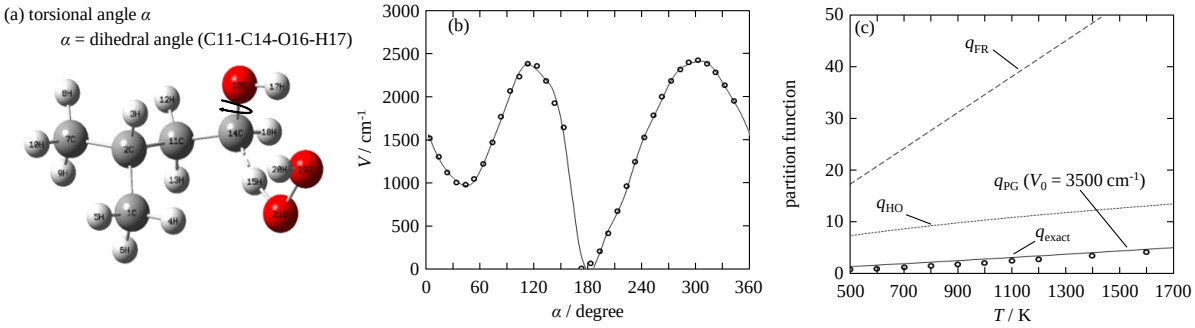

Figure S21. Hindered rotor analysis for C11-C14-O16-H17 in the TS for H-abstraction from isopentanol by HO_2 radical

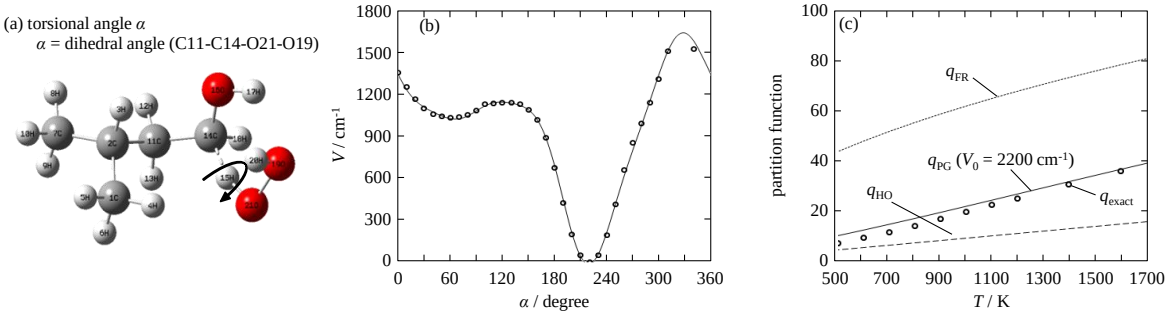

Figure S22. Hindered rotor analysis for C11-C14-O21-O19 in the TS for H-abstraction from isopentanol by HO_2 radical

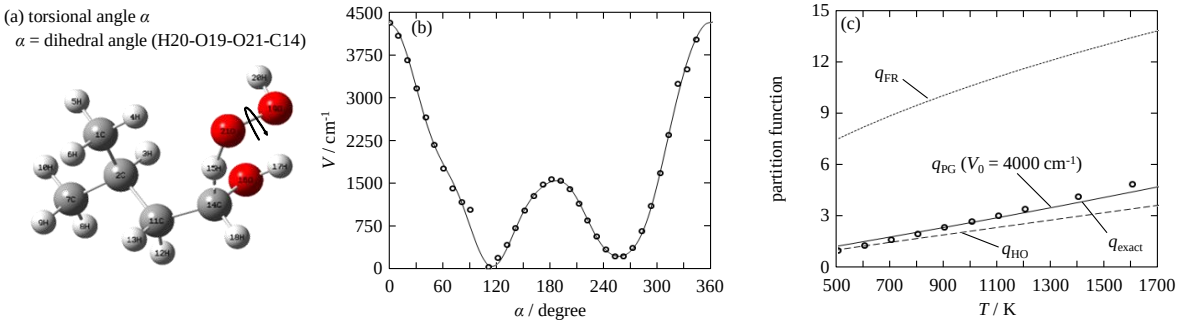

Figure S23. Hindered rotor analysis for H20-O19-O21-C14 in the TS for H-abstraction from isopentanol by HO_2 radical

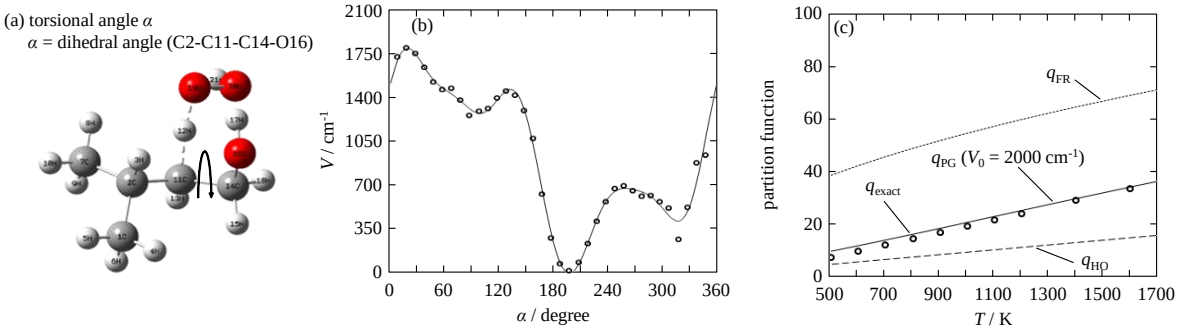

Figure S24. Hindered rotor analysis for C2-C11-C14-O16 in the TS for H-abstraction from isopentanol by HO_2 radical

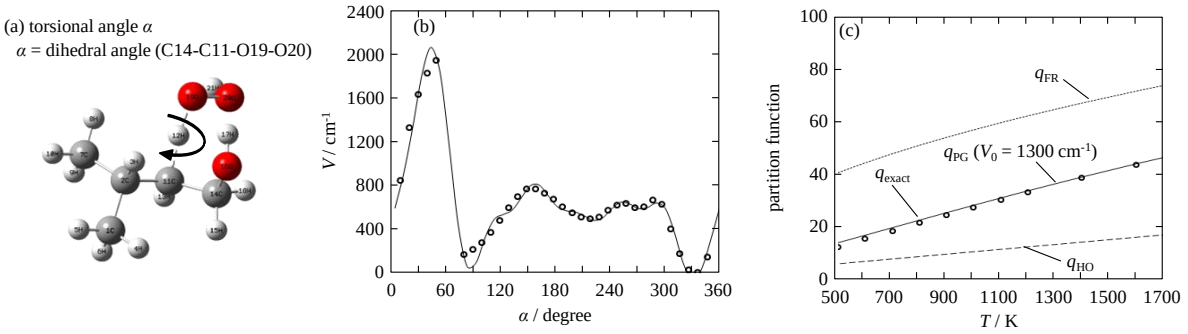

Figure S25. Hindered rotor analysis for C14-C11-O19-O20 in the TS for H-abstraction from isopentanol by HO_2 radical

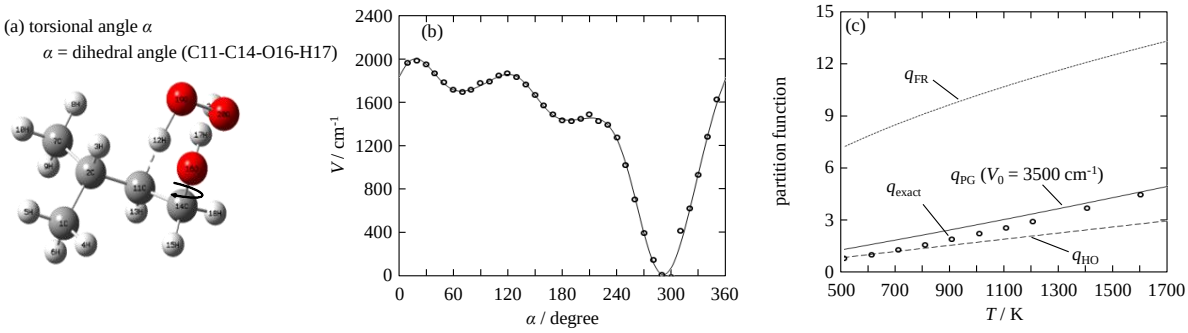

Figure S26. Hindered rotor analysis for C11-C14-O16-H17 in the TS for H-abstraction from isopentanol by HO_2 radical

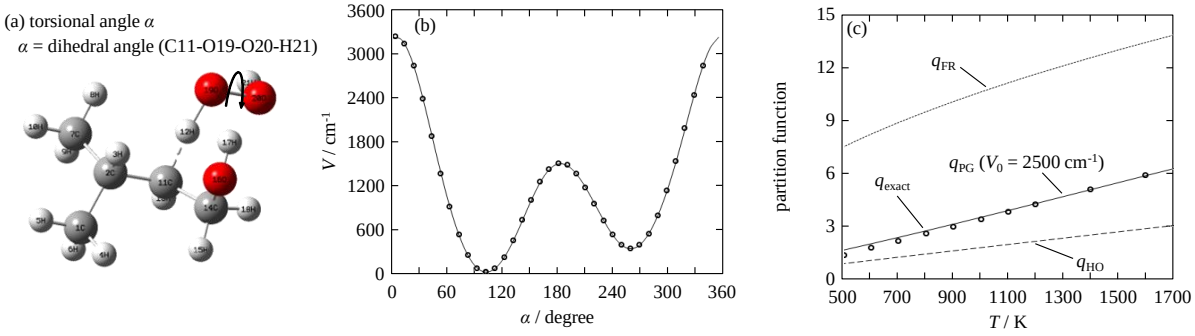

Figure S27. Hindered rotor analysis for C11-O19-O20-H21 in the TS for H-abstraction from isopentanol by HO_2 radical

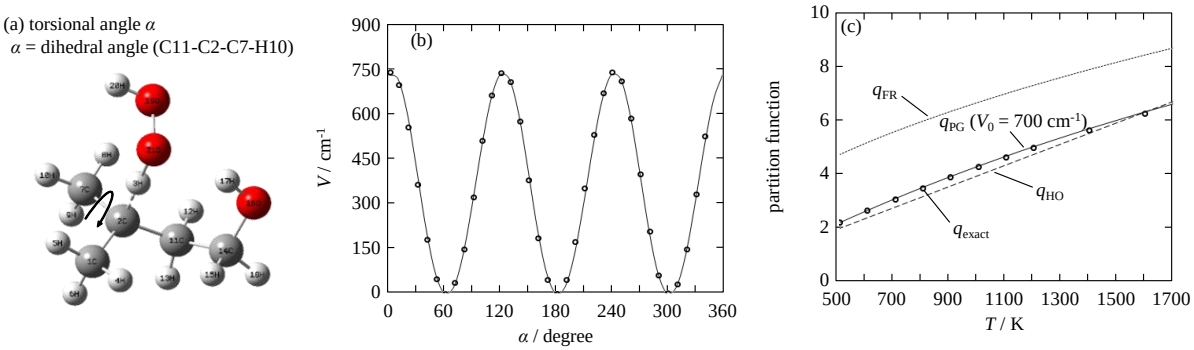

Figure S28. Hindered rotor analysis for C11-C2-C7-H10 in the TS for H-abstraction from isopentanol by HO_2 radical

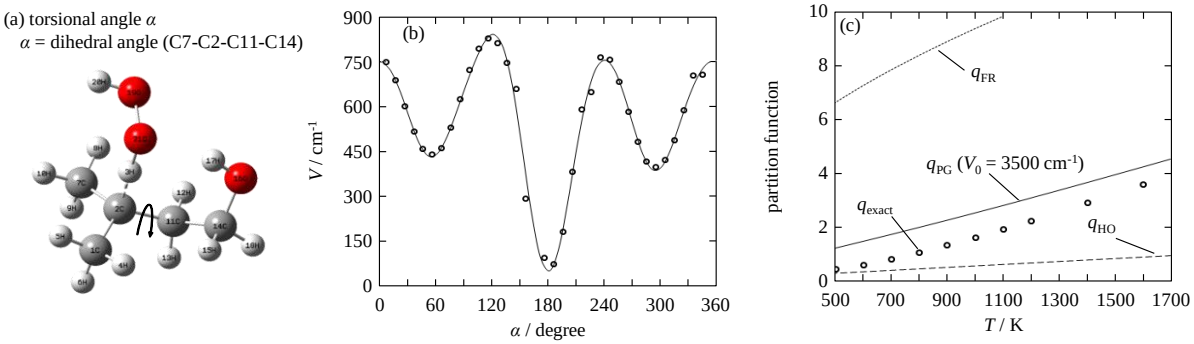

Figure S29. Hindered rotor analysis for C7-C2-C11-C14 in the TS for H-abstraction from isopentanol by HO_2 radical

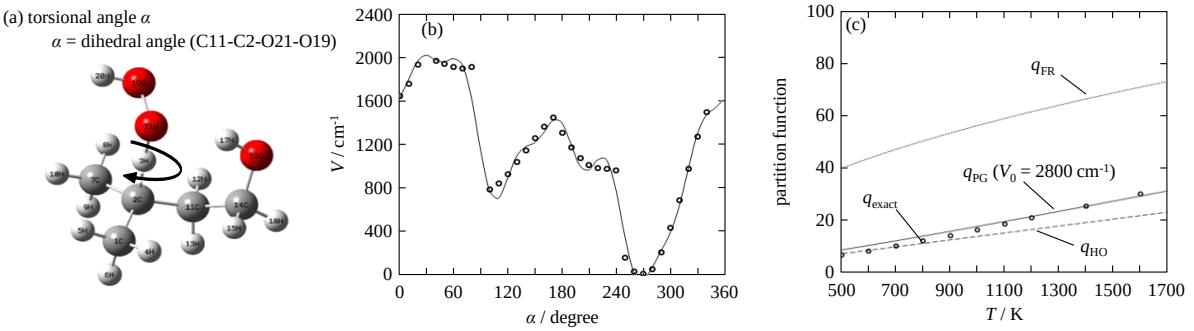

Figure S30. Hindered rotor analysis for C11-C2-O21-O19 in the TS for H-abstraction from isopentanol by HO_2 radical

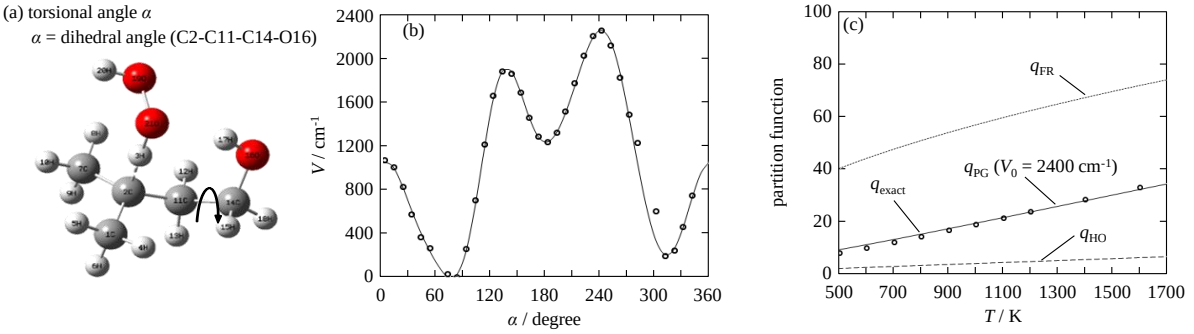

Figure S31. Hindered rotor analysis for C2-C11-O14-O16 in the TS for H-abstraction from isopentanol by HO_2 radical

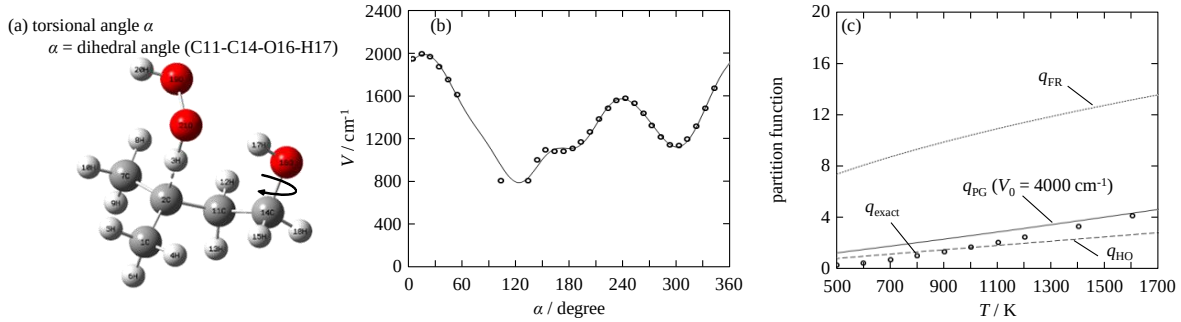

Figure S32. Hindered rotor analysis for C11-C14-O16-H17 in the TS for H-abstraction from isopentanol by HO_2 radical

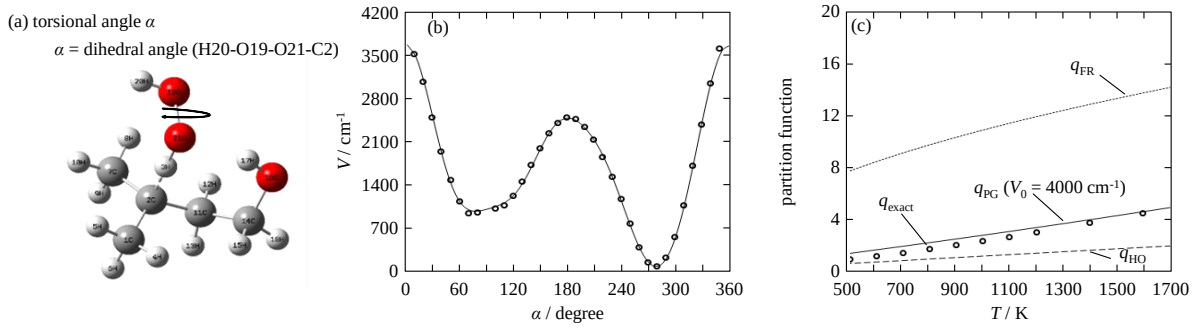

Figure S33. Hindered rotor analysis for H20-O19-O21-C2 in the TS for H-abstraction from isopentanol by HO_2 radical

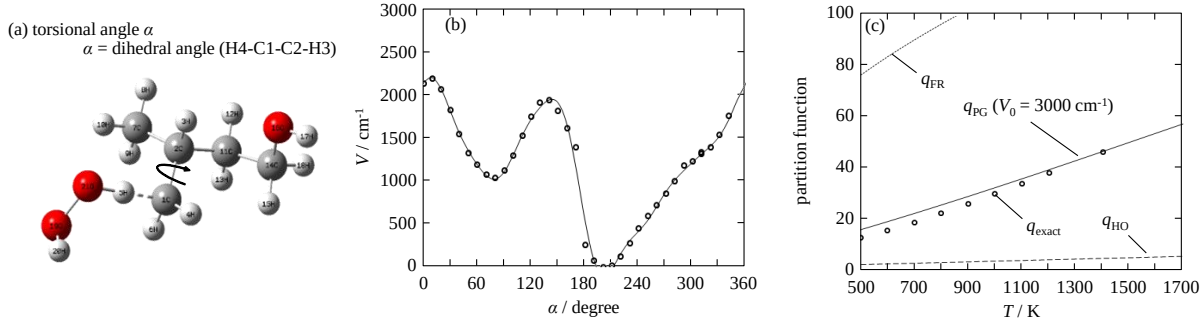

Figure S34. Hindered rotor analysis for H4-C1-C2-H3 in the TS for H-abstraction from isopentanol by HO_2 radical

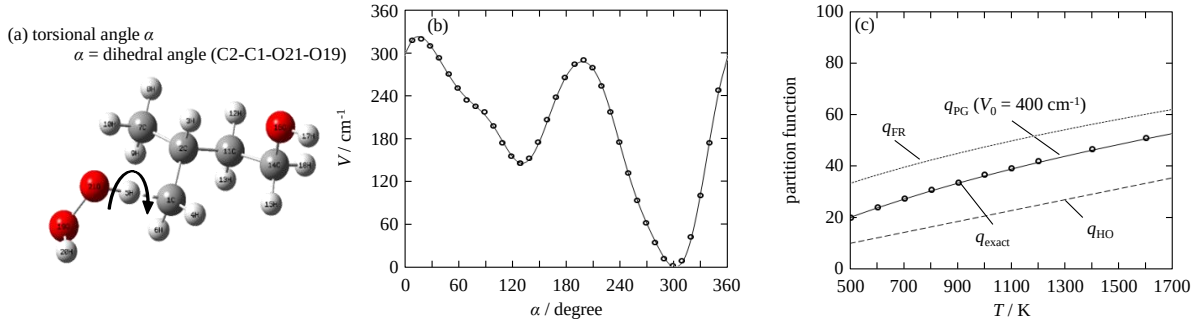

Figure S35. Hindered rotor analysis for C2-C1-O21-O19 in the TS for H-abstraction from isopentanol by HO_2 radical

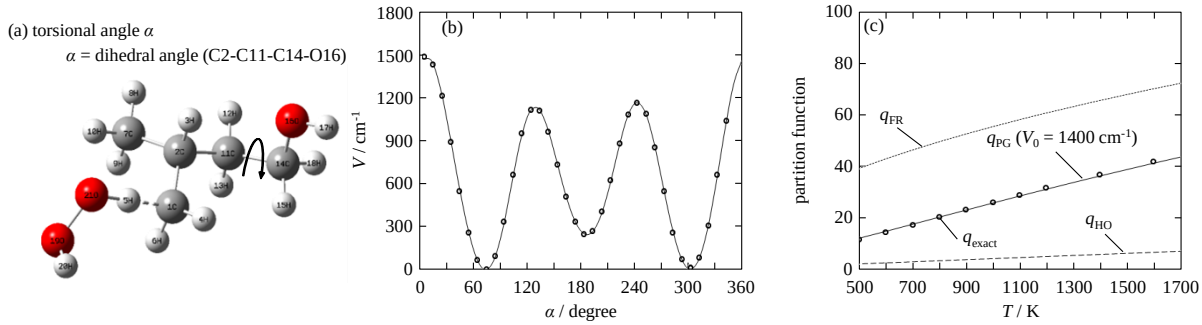

Figure S36. Hindered rotor analysis for C2-C11-C14-O16 in the TS for H-abstraction from isopentanol by HO_2 radical

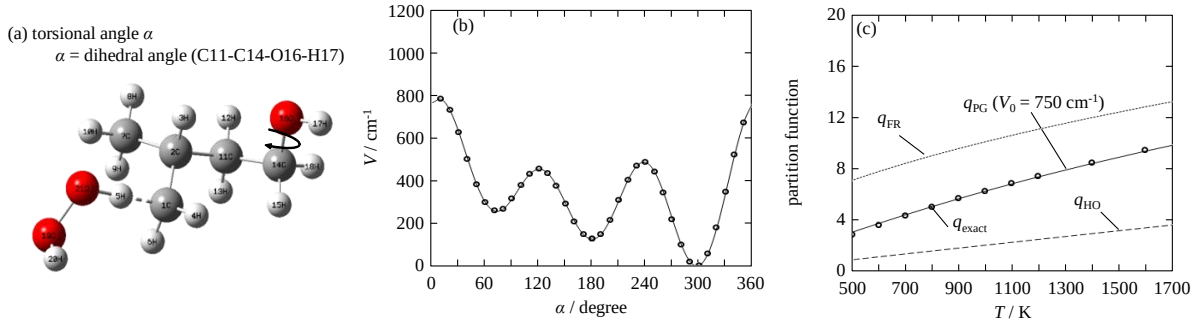

Figure S37. Hindered rotor analysis for C11-C14-O16-H17 in the TS for H-abstraction from isopentanol by HO_2 radical

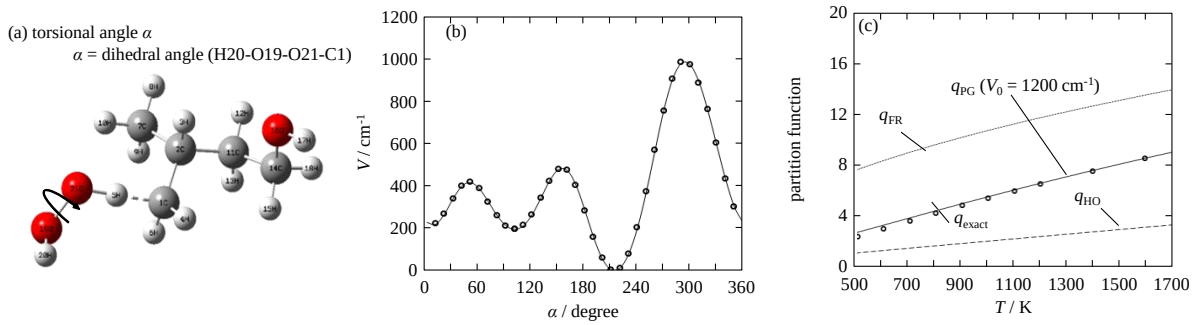

Figure S38. Hindered rotor analysis for H20-O19-O21-C1 in the TS for H-abstraction from isopentanol by HO_2 radical

Table S1. Estimated Hindered Rotor Parameters in Pitzer-Gwinn Approximation for the H-atom abstraction reaction from isopentanol by $H\dot{O}_2$ radical

bonding atom [a]	type of rotor	V_0 [b] / cm^{-1}	σ [c]
O in TS-$H\dot{O}_2$			
C_α	OHO_2H	1300	1
C_β	CH_2OHO_2H	1150	1
O	OH	850	1
$C_{\alpha 1}$ in TS-$H\dot{O}_2$			
C_α	OH	3500	1
	OOH	2200	1
C_β	CH_2OH in TS	1300	1
O	OH	4000	1
$C_{\beta 1}$ in TS-$H\dot{O}_2$			
C_α	OH	3500	1
C_β	CH_2OH	2000	1
	OOH	1300	1
O	OH	2500	1
C_γ in TS-$H\dot{O}_2$			
C_α	OH	4000	1
C_β	CH_2OH	2400	1
C_γ	$C_{\delta 2}H_3$	700	3
	CH_2CH_2OH	3500	1
	OOH	2800	1
O	OH	4000	1
$C_{\delta 2}$ in TS-$H\dot{O}_2$			
C_α	OH	750	1
C_β	CH_2OH	1400	1
C_γ	CH_3 in TS	3000	1
	CH_2CH_2OH	1600	1
$C_{\delta 1}$	OOH	400	1
O	OH	1200	1

[a]abbreviations, C_α, C_β, C_γ, and C_δ are referred in Figure 1. [b]The height of the hindrance potential. [c]The symmetry number of the internal rotation for the H-abstraction reactions by $H\dot{O}_2$ radical.