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

Reaction Rate Constants of H-Abstraction by OH from Large ketones: Measurements and Site-Specific Rate Rules

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Supplementary Material: Tables S1-S4

Table S1: Sub-mechanism for 2-hexanone.

Reaction	Pre-exponential Factor (A) (cm, mol, s)	Temperature exponent (B)	Activation energy (cal/mol)
C4H9COCH3 + OH ⇔ C2H4 + CH2CH2COCH3 + H2O	5.280E+09	0.97	1590
C4H9COCH3 + OH ⇔ C3H6 + CH3COCH2 + H2O	4.68E+07	1.61	-35
C4H9COCH3 + OH ⇔ C4H8-1 + CH3CO + H2O	4.68E+07	1.61	-35
C4H9COCH3 + OH ⇔ C3H7CHCO + CH3 + H2O	1.146E+11	0.51	63
C4H9COCH3 + OH ⇔ PC4H9 + CH2CO + H2O	5.100E+11	0.00	1192
C3H7CHCO + OH ⇔ PC4H9 + CO2	3.730E+12	0.00	-1010
C3H7CHCO + H ⇔ PC4H9 + CO	4.400E+12	0.00	1459
C3H7CHCO + O ⇔ C4H8-1 + CO2	3.200E+12	0.00	-437

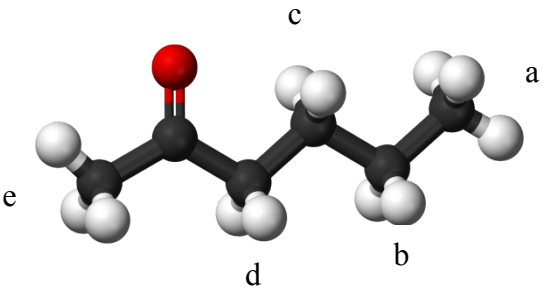

Table S2: Sub-mechanism for 3-hexanone.

Reaction	Pre-exponential Factor (A) (cm, mol, s)	Temperature exponent (B)	Activation energy (cal/mol)
C3H7COC2H5 + OH ⇔ C2H4 + C2H5COCH2 + H2O	5.280E+09	0.97	1590
C3H7COC2H5 + OH ⇔ C3H6 + C2H5CO + H2O	4.680E+7	1.61	-35
C3H7COC2H5 + OH ⇔ C2H5CHCO + C2H5 + H2O	1.146E+11	0.51	63
C3H7COC2H5 + OH ⇔ NC3H7 + CH3CHCO + H2O	5.520E+02	3.12	-1176
C3H7COC2H5 + OH ⇔ NC3H7CO + C2H4 + H2O	5.280E+09	0.97	1590

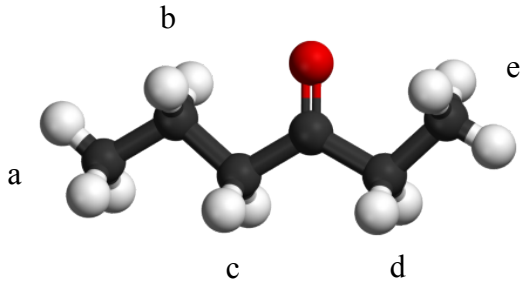

Table S3: Sub-mechanism for 3-methyl-2-pentanone.

Reaction	Pre-exponential Factor (A) (cm, mol, s)	Temperature exponent (B)	Activation energy (cal/mol)
C4H9COCH3-3 + OH ⇔ C2H4 + CH3CHCOCH2 + H2O	5.280E+09	0.97	1590
C4H9COCH3-3 + OH ⇔ C4H8 + CH3CO + H2O	4.680E+7	1.61	-35
C4H9COCH3-3 + OH ⇔ C4H8 + CH3CO + H2O	5.730e+10	0.51	63
C4H9COCH3-3 + OH ⇔ C3H7CHCO + CH3 + H2O	5.280E+09	0.97	1590
C4H9COCH3-3 + OH ⇔ PC4H9 + CH2CO + H2O	5.100E+11	0.00	1192
C3H7CHCO + OH ⇔ PC4H9 + CO2	3.730E+12	0.00	-1010
C3H7CHCO + H ⇔ PC4H9 + CO	4.400E+12	0.00	1459
C3H7CHCO + O ⇔ C4H8-1 + CO2	3.200E+12	0.00	-437

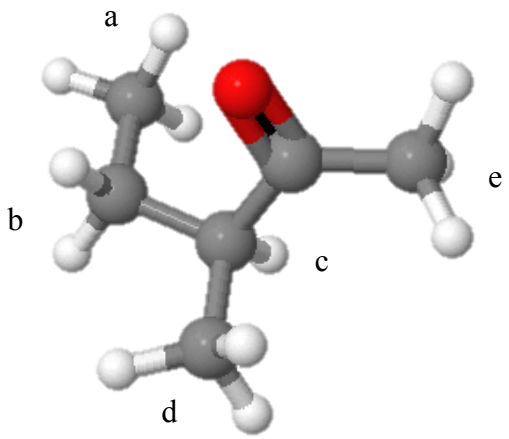

Table S4: Sub-mechanism for 4-methyl-2-pentanone.

Reaction	Pre-exponential Factor (A) (cm, mol, s)	Temperature exponent (B)	Activation energy (cal/mol)
C4H9COCH3-4 + OH ⇔ C3H6 + CH3COCH2 + H2O	1.056e+10	0.97	1590
C4H9COCH3-4 + OH ⇔ C4H8 + CH3CO + H2O	5.730E+10	0.51	63
C4H9COCH3-4 + OH ⇔ C3H7CHCO + CH3 + H2O	1.146E+11	0.51	63
C4H9COCH3-4 + OH ⇔ PC4H9 + CH2CO + H2O	5.100E+11	0.00	1192
C3H7CHCO + OH ⇔ PC4H9 + CO2	3.730E+12	0.00	-1010
C3H7CHCO + H ⇔ PC4H9 + CO	4.400E+12	0.00	1459
C3H7CHCO + O ⇔ C4H8-1 + CO2	3.200E+12	0.00	-437