Supporting Information

Theoretical studies on isomerization and decomposition reactions of 2-methyl-1-butanol radicals

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Table S1. Modified Arrhenius parameters for the rate coefficients of isomerization and decomposition reactions of 2M1B radcials[a].

Reactions	A_1	n_1	E_1	A_2	n_2	E_2
RC1→RC5	5.91E+33	-6.4639	20968	2.42E+15	-1.6	12380
RC2→RC6	1.39E+12	-0.83703	14233	9.74E-06	-1.824	-3352.3
RC3→RC5	2.58E+37	-7.5639	20816	9.31E+17	-2.4039	11891
RC3→RC6	1.09E+19	-3.0626	11187	1.11E+52	-15.21	12576
RC4→RC6	-3.83E+25	-5.6776	11146	9.97E+10	-0.81428	9236.2
RC5→RC6	4.30E+21	-3.7323	7458.2	7.18E+09	-0.47246	4236
RC1→$CH_3CHCHOH+C_2H_5$	4.47E+33	-5.7258	22756	4.34E+20	-2.3081	16288
RC3→$CH_3CH_2CHCH_2+CH_2OH$	3.41E+33	-5.7083	21417	3.77E+19	-2.0457	14852
RC4→$CH_3CHCH_3+CH_2OH$	2.58E+24	-3.2755	19889	5.73E+16	-1.3959	15206
RC5→$CH_3CHCH_2OH+C_2H_4$	-1.95E+28	-4.4468	16415	1.87E+24	-3.1195	15812
RC6→$CH_3CH_2CHCH_3+CH_2O$	1.05E+36	-7.0472	10424	2.52E+19	-2.0112	6724
RC2→2M1Butene+OH	1.62E+31	-5.1405	20312	1.76E+21	-2.5724	14347

[a] The units of A and E are s^{-1}, cm^3 and kcal/mol.

Table S2: A list species discussed in this work, along with their formulas, nomenclatures and structures in the present kinetic model.

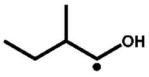
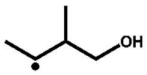
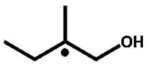
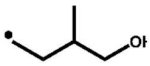
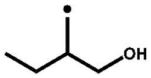
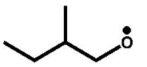
Formula	Nomenclature	Structure	Formula	Nomenclature	Structure
$CH_3CH_2CH(CH_3)CHOH$	RC1		$CH_3CHCH(CH_3)CH_2OH$	RC4	
$CH_3CH_2C(CH_3)CH_2OH$	RC2		$CH_2CH_2CH(CH_3)CH_2OH$	RC5	
$CH_3CH_2CH(CH_2)CH_2OH$	RC3		$CH_3CH_2CH(CH_3)CHOH$	RC6	

Fig.S1. Detailed isomerization channels of (a) RC1 and (b) RC2. Energies were calculated at CBS-QB3 level. All energies are relative to this of RC1 with the unit of kcal/mol.

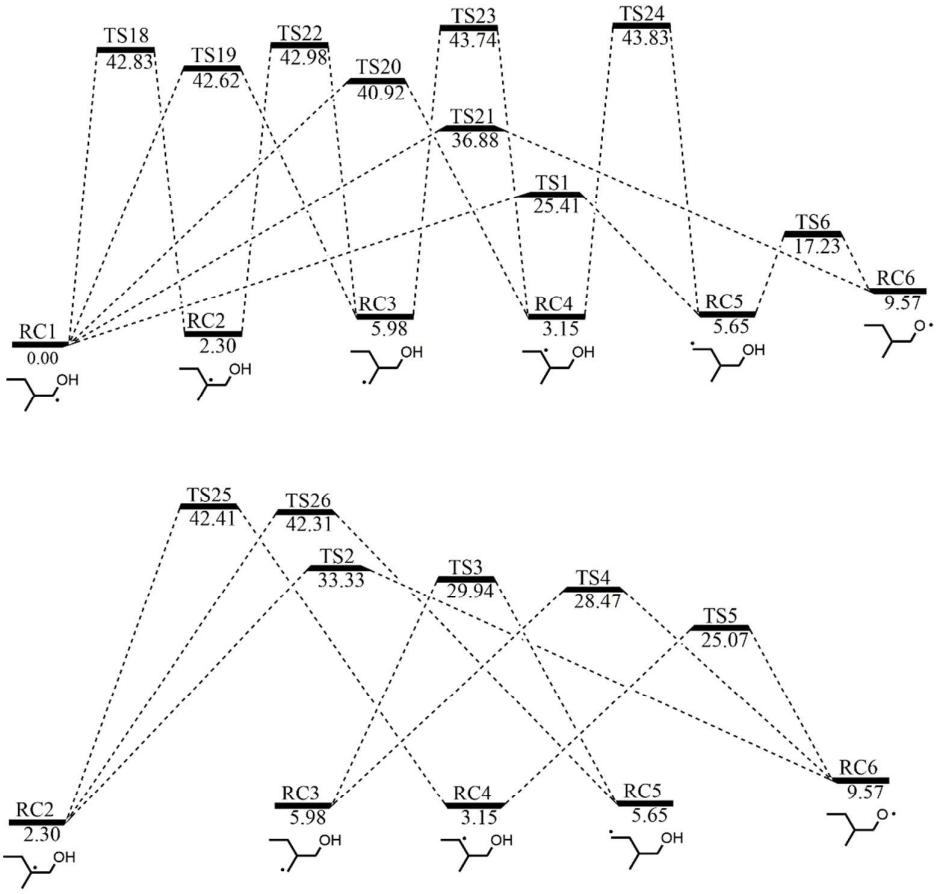


Fig.S2. Detailed decomposition channels of RC1. Energies were calculated at CBS-QB3 level. All energies are relative to this of RC1 with the unit of kcal/mol.

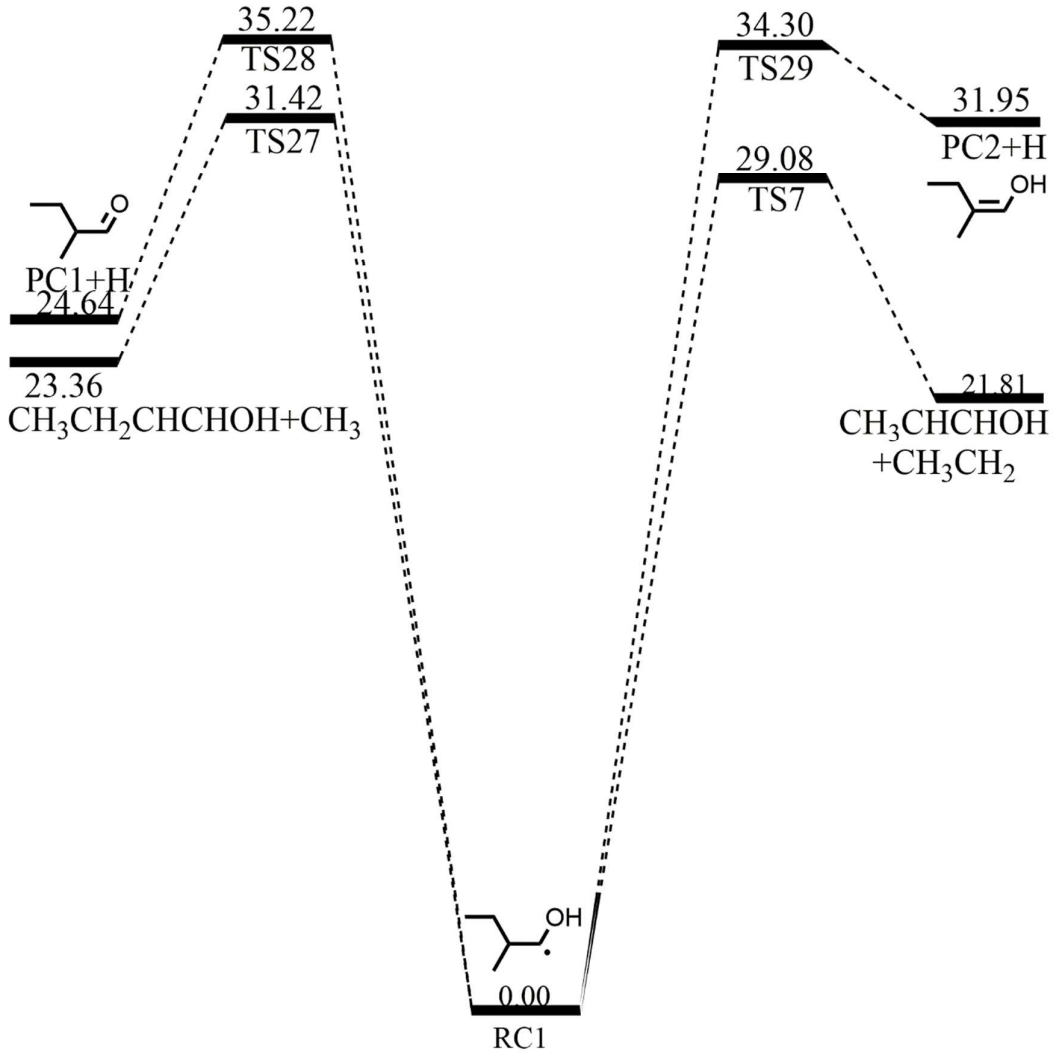


Fig.S3. Detailed reaction channels of RC2. Energies were calculated at CBS-QB3 level. All energies are relative to this of RC1 with the unit of kcal/mol.

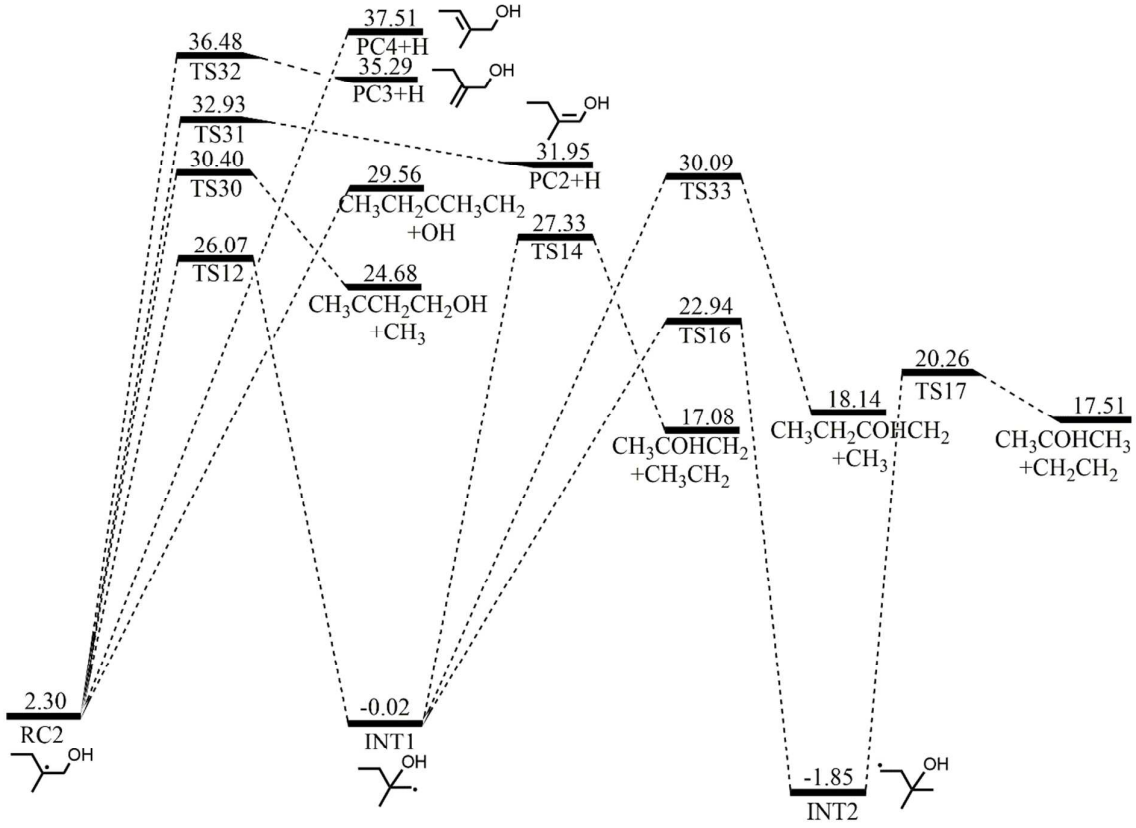


Fig.S4. Detailed decomposition channels of RC3 and RC4. Energies were calculated at CBS-QB3 level. All energies are relative to this of RC1 with the unit of kcal/mol.

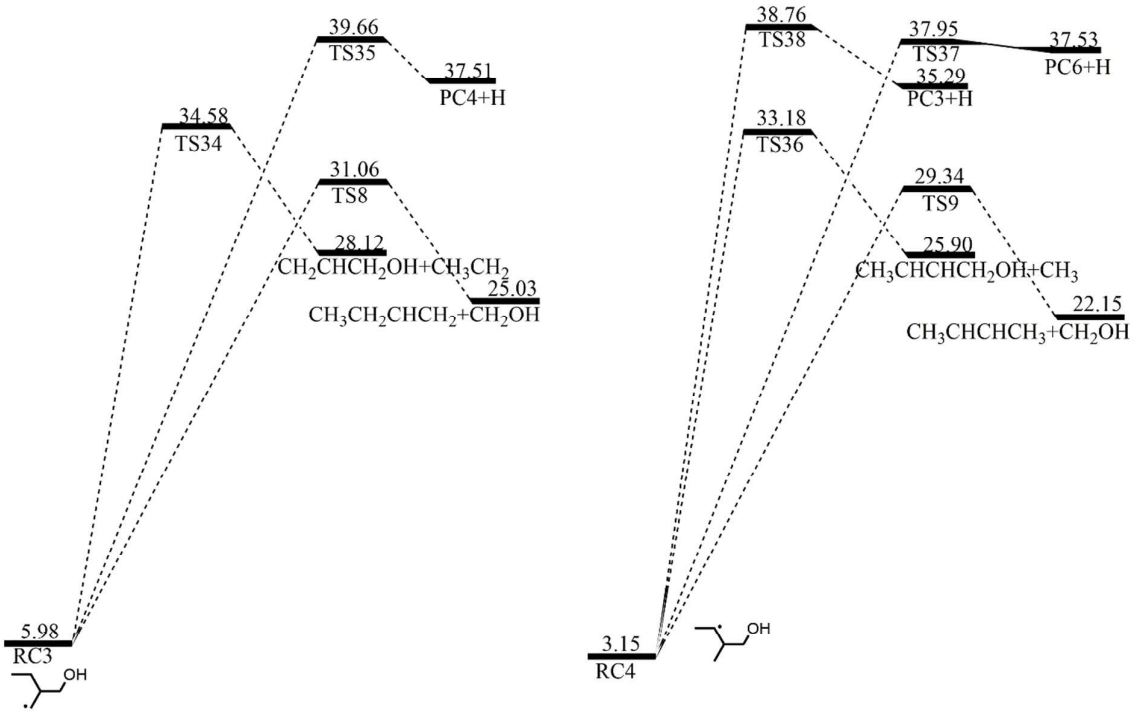


Fig.S5. Detailed reaction channels of RC4. Energies were calculated at CBS-QB3 level. All energies are relative to this of RC1 with the unit of kcal/mol.

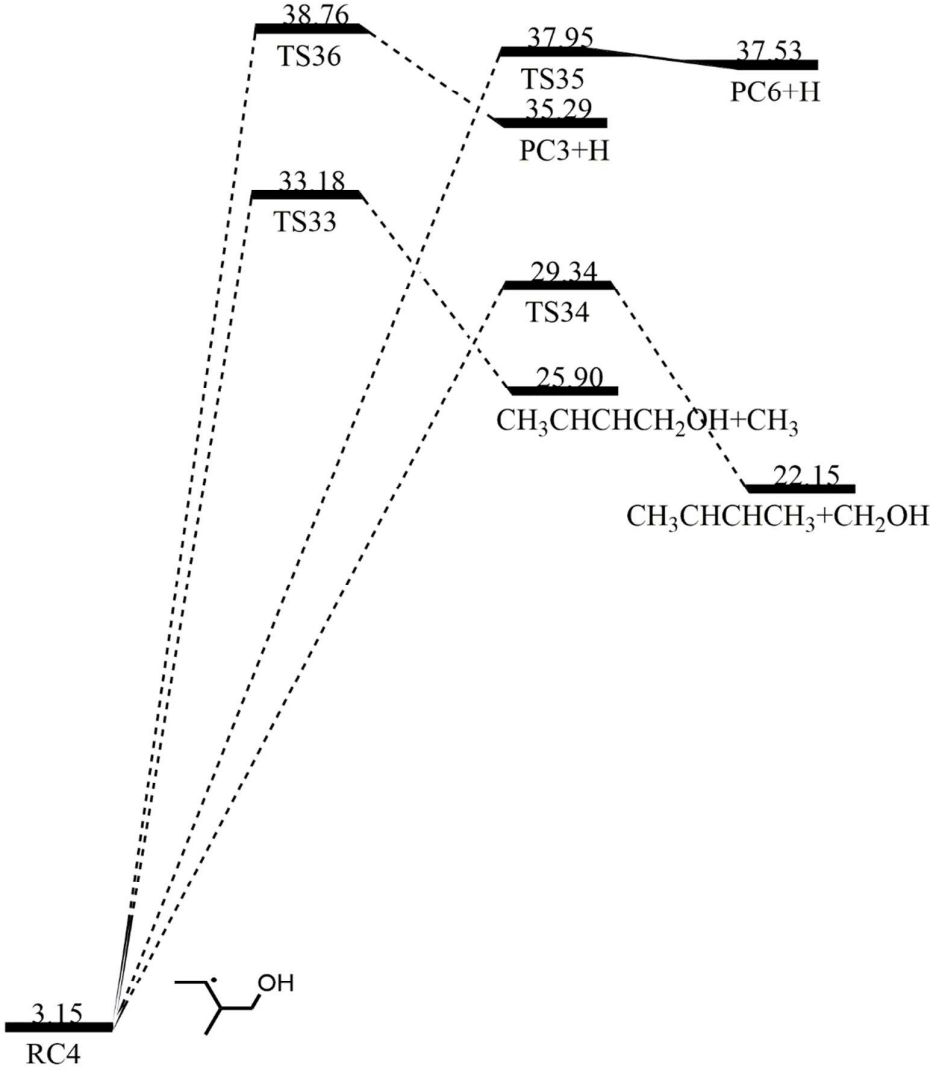


Fig.S6. Detailed decomposition channels of (a) RC5 and (b) RC6. Energies were calculated at CBS-QB3 level. All energies are relative to this of RC1 with the unit of kcal/mol.

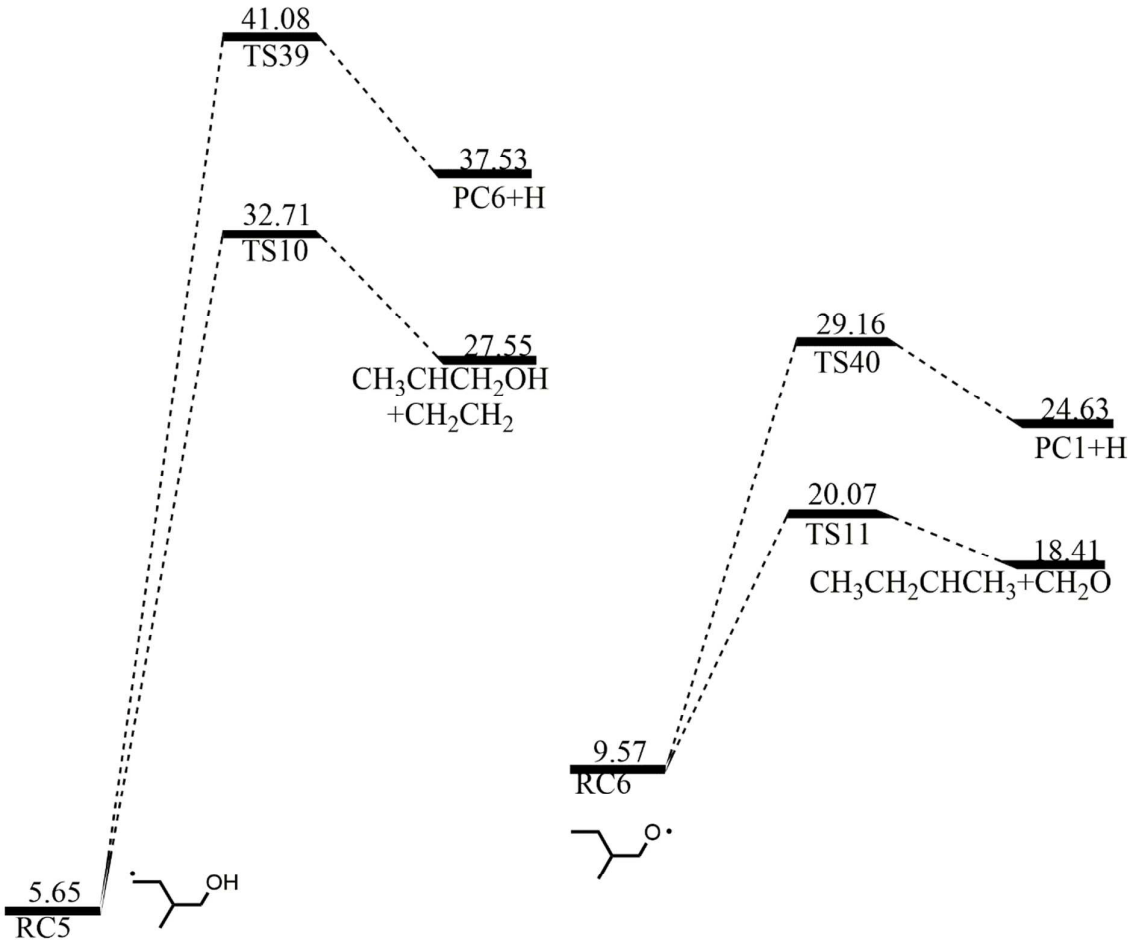


Fig.S7. Detailed isomerization channels of RC6. Energies were calculated at CBS-QB3 level.

All energies are relative to this of RC1 with the unit of kcal/mol.

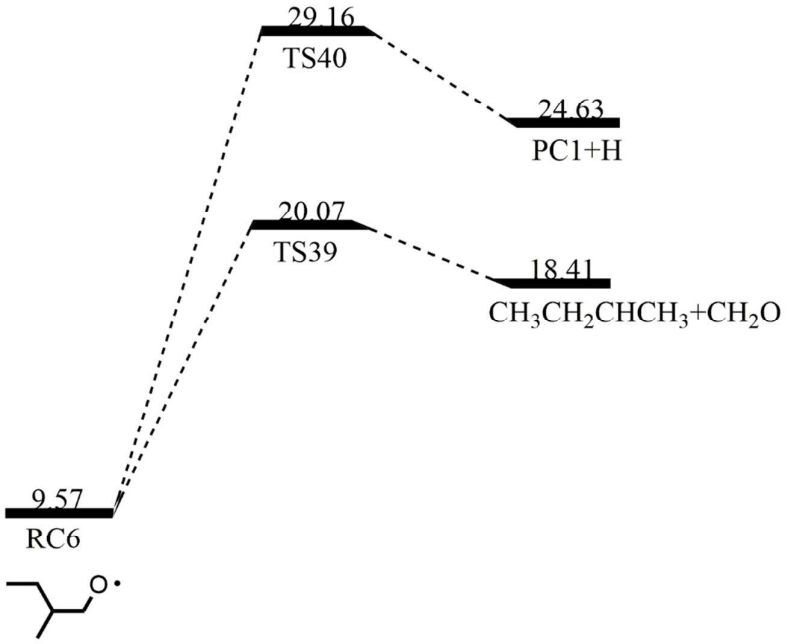


Fig.S8. The lowest energy conformers of RC1-RC6 calculated at the QCISD(T)/CBS//M062x/cc-pVTZ level.

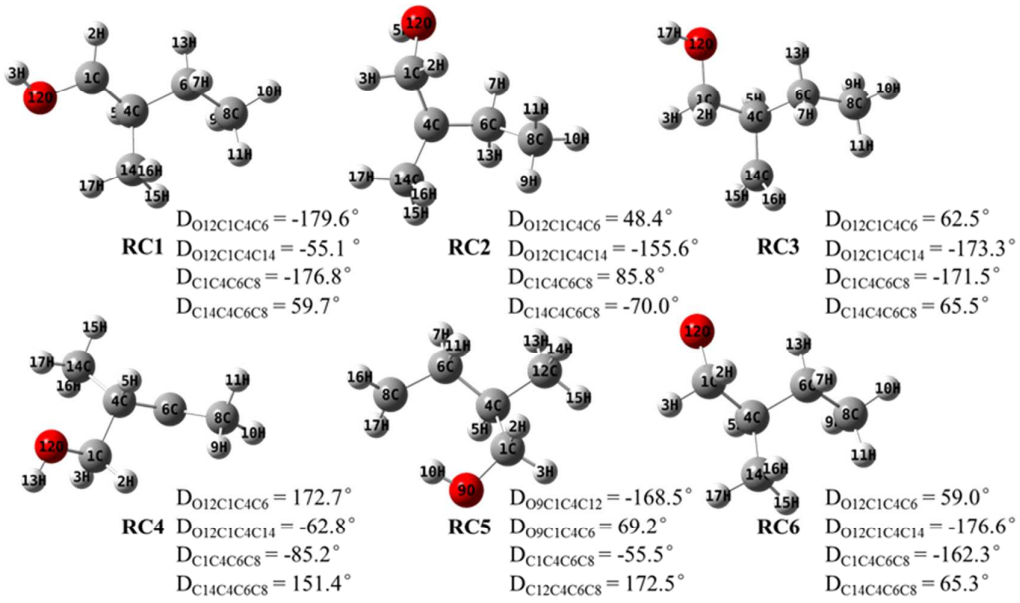


Fig.S9. Sensitivity analysis of C_2H_4 under pyrolytic conditions in a flow reactor at 30 Torr, 1300 K and 760 Torr, 1100K.