

Fig. 2. The complete potential energy surface (including ZPE) accessed upon isomerization and decomposition of 2-pentanol radicals.

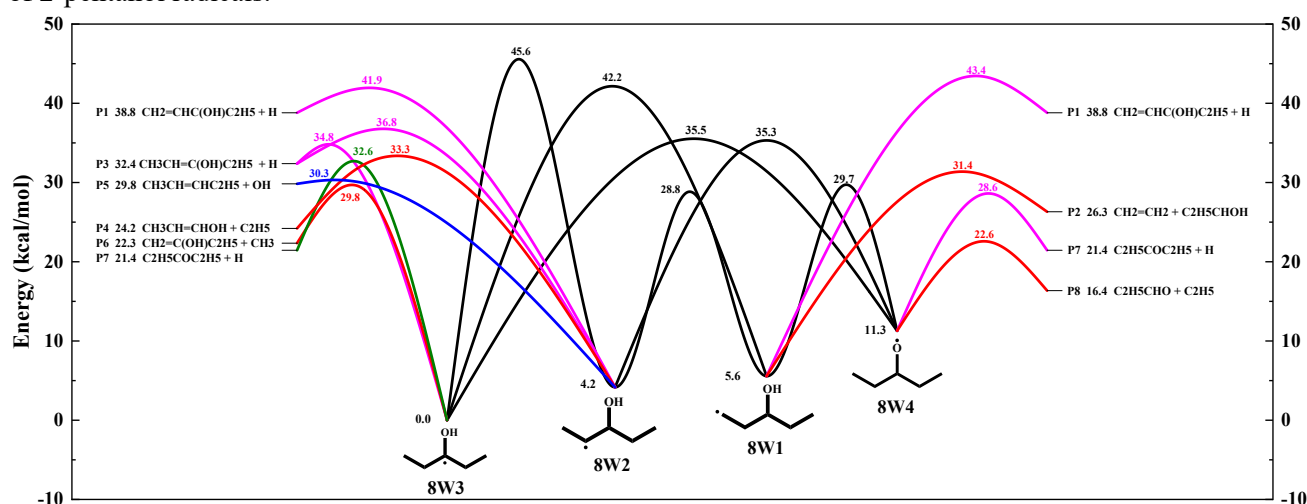


Fig. 3. The complete potential energy surface (including ZPE) accessed upon isomerization and decomposition of 3-pentanol radicals.

T1 diagnostic value

Table 1. T1 diagnostic value of all species related to important reaction channels.

Species	T1 value	Transition state of reactions	T1 value
6W1	0.0108	6W5→6W1	0.0133
6W2	0.0114	6W5→6W2	0.0130
6W3	0.0113	6W2→6W6	0.0240
6W4	0.0114	6W3→6W6	0.0253
6W5	0.0136	6W4→6W1	0.0104
6W6	0.0157	6W1→6W6	0.0226
CH ₂ =CH ₂	0.0107	6W1→CH ₂ =CH ₂ +ĊH ₂ CH ₂ CH ₂ OH	0.0207
ĊH ₂ CH ₂ CH ₂ OH	0.0108	6W2→CH ₂ =CHCH ₃ +ĊH ₂ CH ₂ OH	0.0204
CH ₂ =CHCH ₃	0.0101	6W3→CH ₂ =CHCH ₂ CH ₂ OH+ĊH ₃	0.0203
ĊH ₂ CH ₂ OH	0.0114	6W3→CH ₂ =CHC ₂ H ₅ +ĊH ₂ OH	0.0203
CH ₂ =CHCH ₂ CH ₂ OH	0.0103	6W4→CH ₂ =CHCH ₂ OH+Ċ ₂ H ₅	0.0202
CH ₂ =CHC ₂ H ₅	0.0097	6W4→CH ₂ =CHCH ₂ C ₂ H ₅ +ĊH	0.0250

$\dot{\text{C}}\text{H}_2\text{OH}$	0.0187	$6\text{W}5 \rightarrow \text{CH}_2=\text{CHOH} + \dot{\text{C}}\text{H}_2\text{C}_2\text{H}_5$	0.0213
$\text{CH}_2=\text{CHCH}_2\text{OH}$	0.0107	$6\text{W}6 \rightarrow \text{CH}_2\text{O} + \dot{\text{C}}\text{H}_2\text{CH}_2\text{C}_2\text{H}_5$	0.0190
$\dot{\text{C}}_2\text{H}_5$	0.0099	$6\text{W}6 \rightarrow \text{C}_2\text{H}_5\text{CH}_2\text{CH}_2\text{CHO} + \dot{\text{H}}$	0.0164
$\text{CH}_2=\text{CHCH}_2\text{C}_2\text{H}_5$	0.0095		
$\dot{\text{O}}\text{H}$	0.0059		
$\text{CH}_2=\text{CHOH}$	0.0126		
$\dot{\text{C}}\text{H}_2\text{C}_2\text{H}_5$	0.0099		
CH_2O	0.0158		
$\dot{\text{C}}\text{H}_2\text{CH}_2\text{C}_2\text{H}_5$	0.0099		
$\text{C}_2\text{H}_5\text{CH}_2\text{CH}_2\text{CHO}$	0.0123		
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7W1	0.0111	$7\text{W}4 \rightarrow 7\text{W}1$	0.0139
7W2	0.0111	$7\text{W}2 \rightarrow 7\text{W}5$	0.0106
7W3	0.0117	$7\text{W}2 \rightarrow 7\text{W}6$	0.0258
7W4	0.0134	$7\text{W}3 \rightarrow 7\text{W}6$	0.0186
7W5	0.0109	$7\text{W}1 \rightarrow 7\text{W}5$	0.0109
7W6	0.0175	$7\text{W}1 \rightarrow 7\text{W}6$	0.0229
$\text{CH}_2=\text{CH}_2$	0.0107	$7\text{W}1 \rightarrow \text{CH}_2=\text{CH}_2 + \dot{\text{C}}\text{H}_2\text{CH}(\text{CH}_3)\text{OH}$	0.0205
$\dot{\text{C}}\text{H}_2\text{CH}(\text{CH}_3)\text{OH}$	0.0114	$7\text{W}2 \rightarrow \text{CH}_2=\text{CHCH}_3 + \text{CH}_3\dot{\text{C}}\text{HOH}$	0.0205
$\text{CH}_2=\text{CHCH}_3$	0.0101	$7\text{W}3 \rightarrow \text{CH}_2=\text{CHCH}(\text{CH}_3)\text{OH} + \dot{\text{C}}\text{H}_3$	0.0199
$\text{CH}_3\dot{\text{C}}\text{HOH}$	0.0161	$7\text{W}3 \rightarrow \text{C}_2\text{H}_5\text{CH}=\text{CHOH} + \dot{\text{C}}\text{H}_3$	0.0214
$\text{CH}_2=\text{CHCH}(\text{CH}_3)\text{OH}$	0.0105	$7\text{W}3 \rightarrow \text{CH}_3\text{CH}=\text{CHC}_2\text{H}_5 + \dot{\text{O}}\text{H}$	0.0262
$\text{C}_2\text{H}_5\text{CH}=\text{CHOH}$	0.0113	$7\text{W}4 \rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{OH} + \dot{\text{C}}_2\text{H}_5$	0.0209
$\text{CH}_3\text{CH}=\text{CHC}_2\text{H}_5$	0.0095	$7\text{W}4 \rightarrow \text{CH}_3\text{COCH}_2\text{C}_2\text{H}_5 + \dot{\text{H}}$	0.0233
$\text{CH}_2=\text{C}(\text{CH}_3)\text{OH}$	0.0115	$7\text{W}5 \rightarrow \text{CH}_2=\text{CHOH} + \dot{\text{C}}\text{H}_2\text{C}_2\text{H}_5$	0.0219
$\dot{\text{C}}_2\text{H}_5$	0.0099	$7\text{W}5 \rightarrow \text{CH}_2=\text{CHCH}_2\text{C}_2\text{H}_5 + \dot{\text{O}}\text{H}$	0.0256
$\text{CH}_3\text{COCH}_2\text{C}_2\text{H}_5$	0.0125	$7\text{W}6 \rightarrow \text{CH}_3\text{CHO} + \dot{\text{C}}\text{H}_2\text{C}_2\text{H}_5$	0.0206
$\text{CH}_2=\text{CHOH}$	0.0126	$7\text{W}6 \rightarrow \text{C}_2\text{H}_5\text{CH}_2\text{CHO} + \dot{\text{C}}\text{H}_3$	0.0202
$\dot{\text{C}}\text{H}_2\text{C}_2\text{H}_5$	0.0098		
$\text{CH}_2=\text{CHCH}_2\text{C}_2\text{H}_5$	0.0095		
$\dot{\text{O}}\text{H}$	0.0059		
CH_3CHO	0.0147		
$\text{C}_2\text{H}_5\text{CH}_2\text{CHO}$	0.0128		
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8W1	0.0105	$8\text{W}3 \rightarrow 8\text{W}4$	0.0123
8W2	0.0113	$8\text{W}2 \rightarrow 8\text{W}1$	0.0111
8W3	0.0136	$8\text{W}2 \rightarrow 8\text{W}4$	0.0188
8W4	0.0167	$8\text{W}1 \rightarrow 8\text{W}4$	0.0243
$\text{CH}_2=\text{CH}_2$	0.0107	$8\text{W}1 \rightarrow \text{CH}_2=\text{CH}_2 + \text{C}_2\text{H}_5\dot{\text{C}}\text{HOH}$	0.0202
$\text{C}_2\text{H}_5\dot{\text{C}}\text{HOH}$	0.0151	$8\text{W}2 \rightarrow \text{CH}_3\text{CH}=\text{CHOH} + \dot{\text{C}}_2\text{H}_5$	0.0216
$\text{CH}_3\text{CH}=\text{CHOH}$	0.0118	$8\text{W}2 \rightarrow \text{CH}_3\text{CH}=\text{CHC}_2\text{H}_5 + \dot{\text{O}}\text{H}$	0.0256
$\dot{\text{C}}_2\text{H}_5$	0.0099	$8\text{W}3 \rightarrow \text{CH}_2=\text{C}(\text{OH})\text{C}_2\text{H}_5 + \dot{\text{C}}\text{H}_3$	0.0247
$\text{CH}_3\text{CH}=\text{CHC}_2\text{H}_5$	0.0094	$8\text{W}3 \rightarrow \text{C}_2\text{H}_5\text{COC}_2\text{H}_5 + \dot{\text{H}}$	0.0177
$\dot{\text{O}}\text{H}$	0.0059	$8\text{W}4 \rightarrow \text{C}_2\text{H}_5\text{CHO} + \dot{\text{C}}_2\text{H}_5$	0.0204
$\text{CH}_2=\text{C}(\text{OH})\text{C}_2\text{H}_5$	0.0110		
$\text{C}_2\text{H}_5\text{COC}_2\text{H}_5$	0.0136		

C₂H₅CHO

0.0099
