

**Alternativeness of ester synthesis reaction mechanism: a case study
of propyl acetate**

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Starting point configuration

1

MatStudio 3D 0

20 18 0 0 0 0 0 0 0 0999 V2000

```
-8.5978  0.3013  0.1497 C  0 0 0 0 0 0 0 0 0 0 0 0
-7.1020  0.3107  0.2348 C  0 0 0 0 0 0 0 0 0 0 0 0
-6.5371  1.5026  0.5393 O  0 0 0 0 0 0 0 0 0 0 0 0
-6.3878 -0.6526  0.0595 O  0 0 0 0 0 0 0 0 0 0 0 0
-8.9572 -0.7030 -0.0573 H  0 0 0 0 0 0 0 0 0 0 0 0
-8.9387  0.9814 -0.6327 H  0 0 0 0 0 0 0 0 0 0 0 0
-9.0287  0.6491  1.0913 H  0 0 0 0 0 0 0 0 0 0 0 0
-7.2196  2.1777  0.6625 H  0 0 0 0 0 0 0 0 0 0 0 0
-3.5454  0.1847 -0.0845 C  0 0 0 0 0 0 0 0 0 0 0 0
-4.3607  1.1439  0.7781 C  0 0 0 0 0 0 0 0 0 0 0 0
-5.7582  1.3758  0.2337 C  0 0 0 0 0 0 0 0 0 0 0 0
-6.5438  2.2519  1.0547 O  0 0 0 0 0 0 0 0 0 0 0 0
-4.0220 -0.7961 -0.1467 H  0 0 0 0 0 0 0 0 0 0 0 0
-2.5444  0.0460  0.3271 H  0 0 0 0 0 0 0 0 0 0 0 0
-3.4358  0.5682 -1.1018 H  0 0 0 0 0 0 0 0 0 0 0 0
-3.8433  2.1063  0.8458 H  0 0 0 0 0 0 0 0 0 0 0 0
-4.4387  0.7576  1.7980 H  0 0 0 0 0 0 0 0 0 0 0 0
-6.3123  0.4377  0.1922 H  0 0 0 0 0 0 0 0 0 0 0 0
-5.7053  1.7718 -0.7861 H  0 0 0 0 0 0 0 0 0 0 0 0
-6.0926  3.1048  1.0841 H  0 0 0 0 0 0 0 0 0 0 0 0
```

```
1 2 1 0 0 0
2 3 1 0 0 0
2 4 2 0 0 0
1 5 1 0 0 0
1 6 1 0 0 0
1 7 1 0 0 0
3 8 1 0 0 0
9 10 1 0 0 0
10 11 1 0 0 0
11 12 1 0 0 0
9 13 1 0 0 0
9 14 1 0 0 0
9 15 1 0 0 0
10 16 1 0 0 0
10 17 1 0 0 0
11 18 1 0 0 0
11 19 1 0 0 0
12 20 1 0 0 0
M $3D 1
M $3D -9 9 O_OH_aceticacid-C
M $3D 3 11 0.8462 0.8462
M END
```