

**DETERMINATION OF POTENTIALLY CATALYTICALLY ACTIVE ZEOLITES
IN THE CONVERSION OF PIPERYLENE IN ISOPRENE**

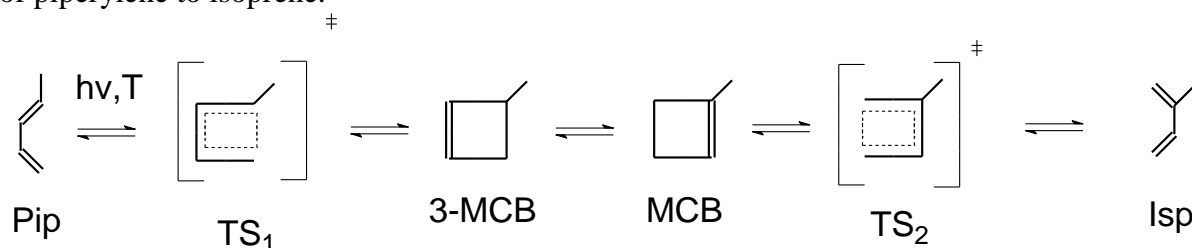
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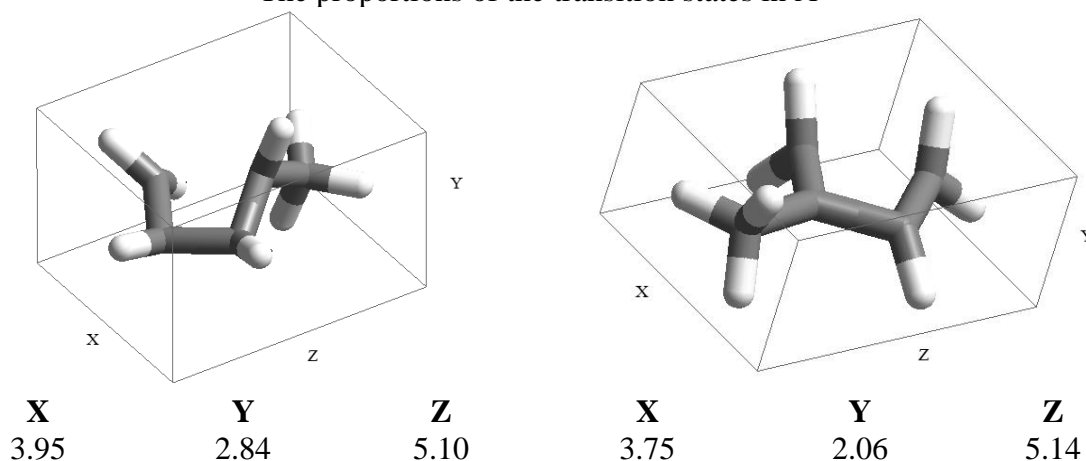
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We have considered possible ways of reducing the activation energy of the conversion of piperylene to isoprene.



In the B3LYP/6-31G (d,p) approximation, the structures of the transition states of the [2 + 2] cyclization reactions of piperylene (PS1) and the disclosure of methylcyclobutene (PS2) are determined.

The proportions of the transition states in Å



According to the principles of molecular imprinting, the activation energy can be reduced by the use of porous substances conducive to the formation of a transition state. For this purpose, cavities of such substances, for example zeolites, should have cavities complementary in shape to the transition state with cavity diameters comparable in size.

The measured PS proportions show that in our case, zeolites with a pore diameter in the range of 4.00 to 5.45 Å should be catalyzed activity, for example zeolites of the following Frame Work Type: ANA, NAT, PAR, GIS, EPI.

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