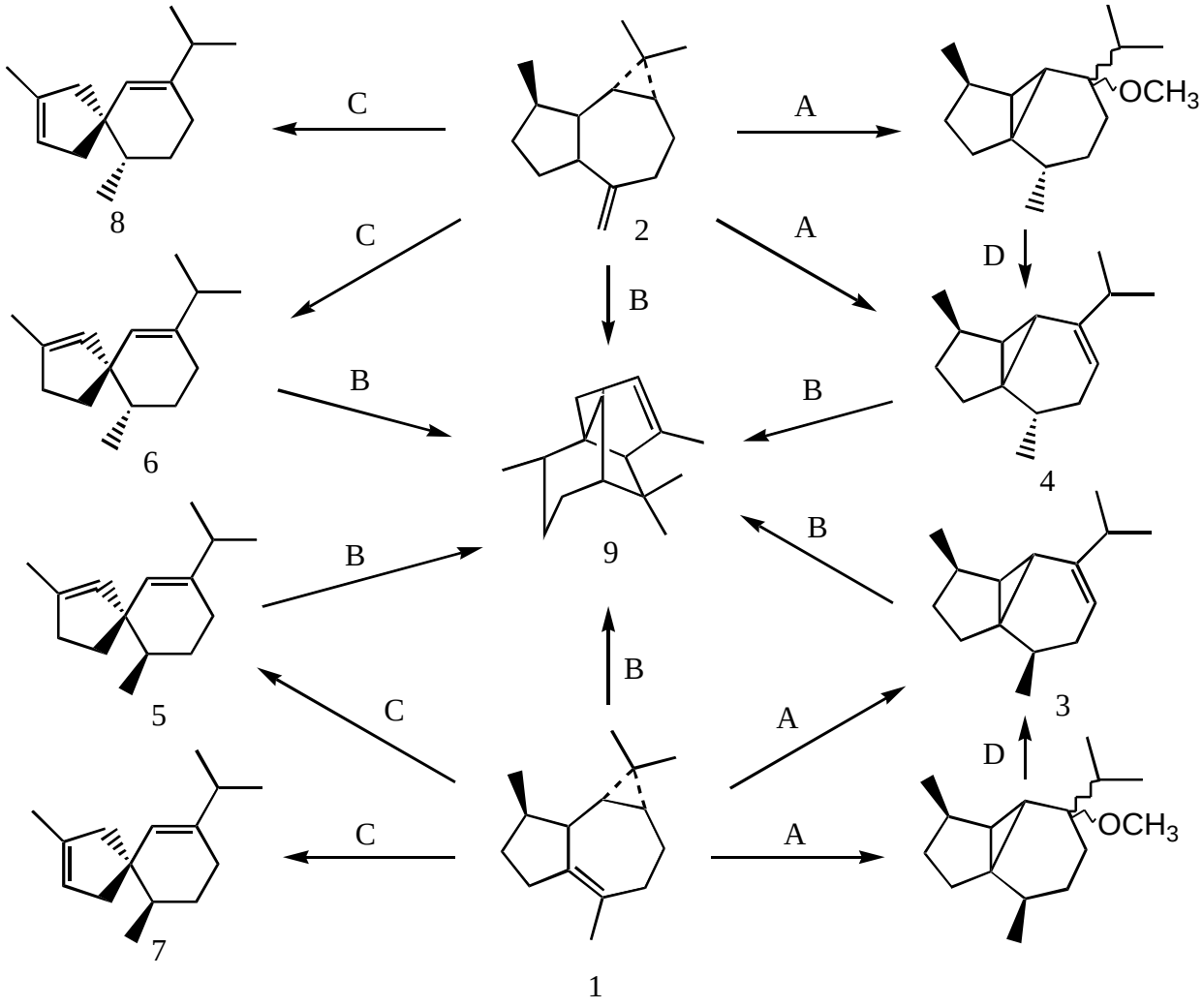
Rearrangements of Aromadendrene and Ledene in Acid Media

Marina P. Polovinka, Andrei A. Shalko, Dina V. Korchagina, Yurii V. Gatilov, and Vladimir A. Barkhash

N. N. Vorozhtsov Novosibirsk Institute of Organic Chemistry, Siberian Branch, Russian Academy of Sciences.,
9 Lavrentiev ave., 630090 Novosibirsk 90; polovina@nioch.nsc.ru

For the first time ledene 1 and aromadendrene 2 were transformed in acid-catalyzed reactions to different triciclic and spiro compounds with natural types of skeleton. Their structures were confirmed by ^{1}H and ^{13}C NMR data and the 2D spectrum of ^{13}C-^{13}C correlation. Boiling of compounds 1-6 in formic acid results in the formation of compound 9 with new type of skeleton. The mechanisms of rearrangements were theoretically analyzed using molecular mechanics and quantum chemical calculations.



A - HSO_3F-SO_2FCl;

B - HCOOH;

C - TiO_2/SO_4^{2-};

D - SiO_2