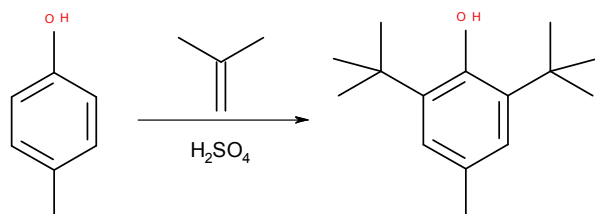




Sample: Organic Chemistry - Friedel - Crafts Reaction Mechanism

Friedel-Crafts Alkylation

Friedel - Crafts reaction in its many variations is the most important method for introducing alkyl groups into the aromatic ring. As the alkylating agents used are alkyl halides, alcohols, or particularly in industry, alkenes.

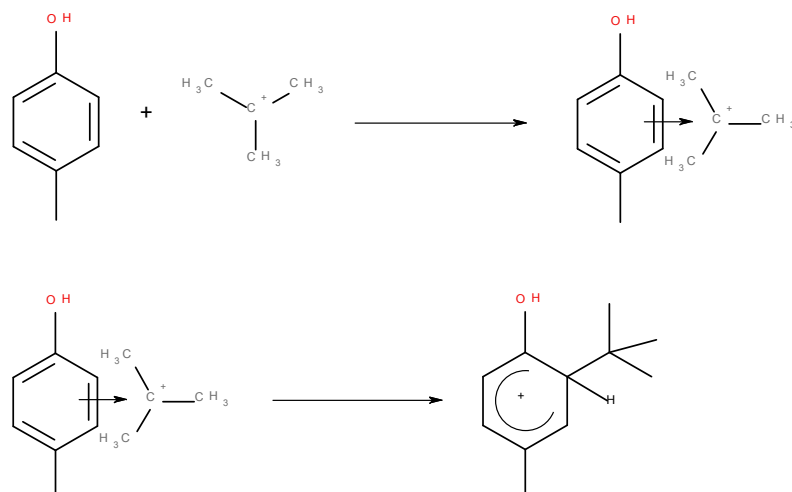


Catalysts for the reaction are Lewis acids as aluminum chloride, boron fluoride, or sometimes mineral acids as sulfuric or phosphoric acid. The mechanism of this reaction - bimolecular electrophilic substitution (S_E2) (Groves, J. K., 1972).

The role of the catalyst is to increase the electrophilicity of alkylating agent due to its transfer to strongly polarized complex or an ion pair :

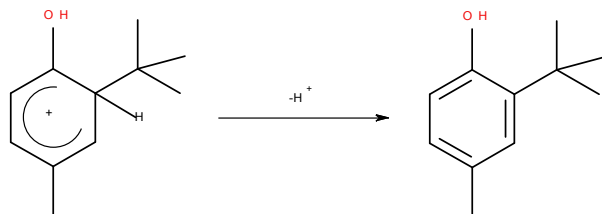


Highly polarized complex mineral acid reagent is reacted with an aromatic compound to form π-Complex, which becomes stronger σ-complex (W. E. Truce and C. W. Vriesen, 1953).



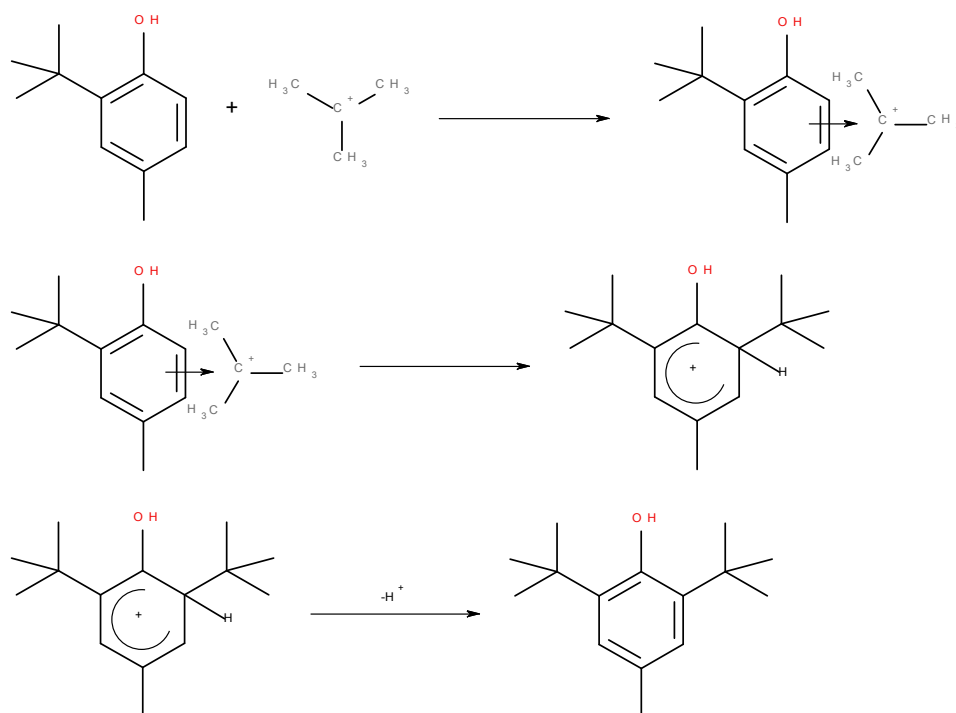
π-Complex formation occurs at a rapid preliminary stage, its role is small and the speed of the overall process is practically not affected (Smith, Michael B.; March, Jerry, 2007).

Further cleavage occurs proton action formed from the action bases, which can be a solvent molecule.



Formation and decay of σ - complex with elimination of a proton is the main direction of the reaction. In some cases, the σ - complexes one can but select, if disintegration is difficult, for example for steric reasons or because of the absence of a strong base (Groves, J. K., 1972).

The input of second t-butyl group occurs in the same way:



References:

1. Smith, Michael B.; March, Jerry (2007), *Advanced Organic Chemistry: Reactions, Mechanisms, and Structure* (6th ed.), New York: Wiley-Interscience, ISBN 0-471-72091-7
2. Groves, J. K. (1972). "The Friedel–Crafts acylation of alkenes". *Chem. Soc. Rev.* 1: 73. doi:10.1039/cs9720100073.
3. W. E. Truce and C. W. Vriesen (1953). "Friedel—Crafts Reactions of Methanesulfonyl Chloride with Benzene and Certain Substituted Benzenes". *J. Am. Chem. Soc.* 75: 5032–5036.