METHODS TO MEASURE STRAIN IN ALKENES

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Alkenes are organic compounds that have a carbon-carbon double bond functional group. Usually this functional group has planar structure that determines geometry of alkene molecules. However, if the double bond is situated at a bridgehead position, where the double bond carbon atoms belong to two different cycles, or if there are very bulky substituents at the double bond, the planar geometry of the double bond can be distorted. The strain effect, rising from this distortion, changes energy of the molecule and will also change its reactivity. It has been shown that strain effect may play a significant role in certain reactions [1-4].

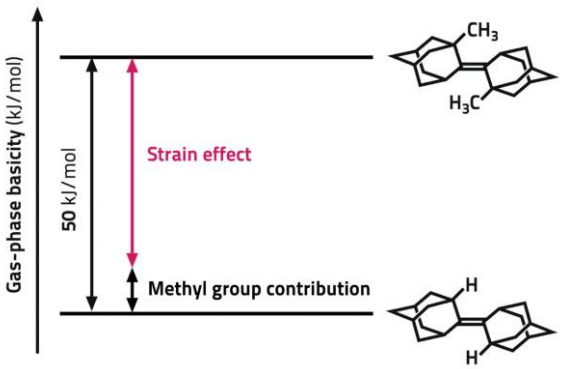

Fig.1 Gas-phase basicity difference for (E)-1-methyl-2-(1-methyl-2-adamantylidene)adamantane and adamantylideneadamantane [1].

We propose a novel method for estimation of the strain effect [5]. This method is based on measurement of alkane gas-phase basicity (GB) that can be done by using FT-ICR method, which is available in our Institute. The theoretical and experimental evaluation of the results revealed that GB values correlate well with experimental results and are in agreement with the general understanding of the strain phenomenon.

References

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