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Catalytic effect of CuX (X=F, Cl, Br, I) on Nitroso−Diels−Alder reaction, a theoretical study

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In this study, Nitroso−Diels–Alder (NDA) cycloaddition reaction between the $CH_3N=O$ and cis-1,3−butadiene in the presence of the CuX (X=F,Cl, Br, I) as Lewis acid catalyst, using density functional theory calculations at the M06-2X [1] level of theory using the def2-svp basis set, has been studied. The NDA reaction is a chemical reaction for the construction of six-membered rings [2]. The copper(I)-catalyzed such as copper (I) and copper (II) complexes and copper salts have used Lewis acid catalysts in Diels-Alder reactions [3]. The aim of this work was to study various substituents of X (X=F,Cl, Br, I) on the catalytic effect of the Cu catalyst in NDA cycloaddition reaction (Fig. 1). The results showed that the largest effect on activation energies of the reaction belongs to the CuF catalyst.The activation strain model (ASM) [4], the quantum theory of atoms in molecules (QTAIM) and natural bond orbital (NBO) analysis were used to understand the nature of interactions at the TS structures.

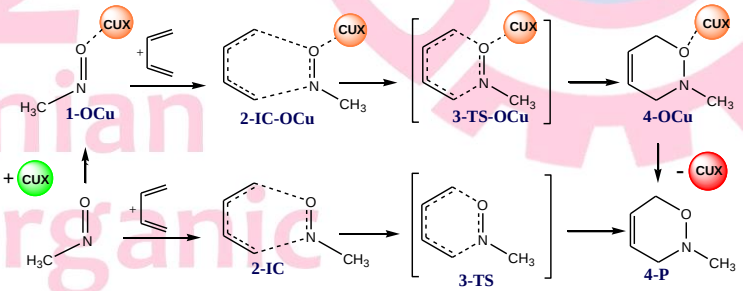


Fig. 1: Uncatalyzed NDA reaction between $CH_3N=O$ and butadiene, versus those catalyzed by a CuX compound (X=F,Cl, Br, I)via Cu···O noncovalent interactions.

Keywords: Nitroso−Diels–Alder, CuX catalyst, DFT

References

[1] Y. Zhao, D. G. Truhlar, *Theoretical chemistry accounts*, **2008**, 120, 215.
[2] O. Diels and K. Alder, *Justus Liebigs Annalen der Chemie*, **1928**, 460, 98.
[3] S. Reymond, J. Cossy, and C. Surname, *Chemical reviews*, **2008**, 108, 5359.
[4] D. H. Ess, K. Houk, *Journal of the American Chemical Society*, **2007,** 129,10646.