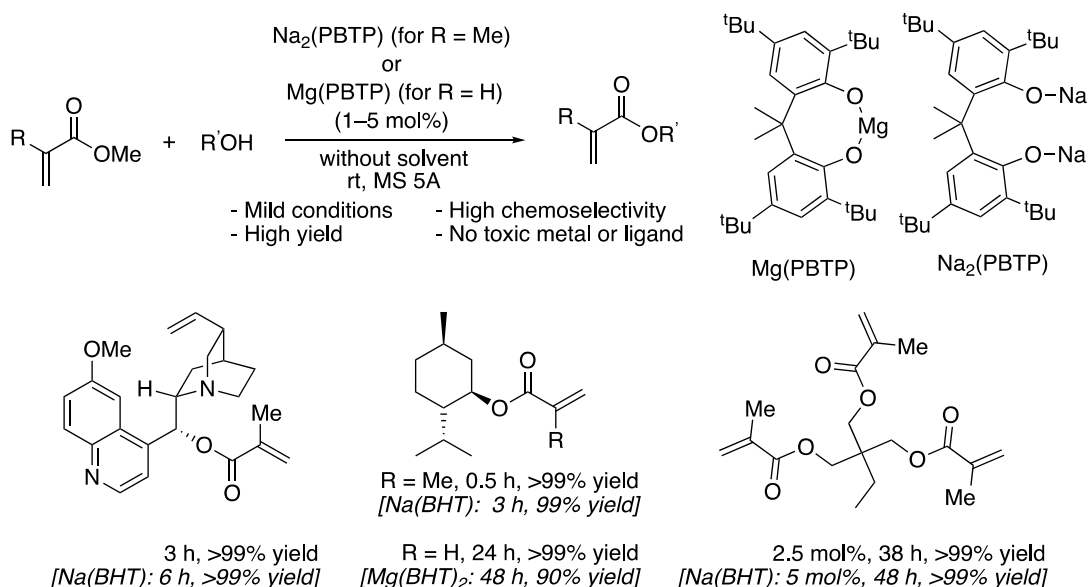


Magnesium(II) and Sodium(I) Bisphenoxide Catalysts for Transesterification of Methyl (Meth)acrylate and Their Reaction Mechanisms

(¹Venture Business Laboratory, Nagoya University, ²Graduate School of Engineering, Nagoya University, ³ Section of Theoretical Catalytic Chemistry, Institute for Catalysis, Hokkaido University) ○ Kazumasa Kon,¹Xue Zhao,² Manussada Ratanasak,³ Chie Joko,² Jun-ya Hasegawa,³ Kazuaki Ishihara²

Keywords: Transesterification; Acrylate; Methacrylate; Chemoselective; DFT Calculation

Chemoselective transesterification of methyl acrylate (MA) and methyl methacrylate (MMA) is the important synthetic method to produce (meth)acrylates because (meth)acrylates are useful for various industrial applications. Previously, we developed Mg(II) and Na(I) catalysts derived from 2,6-di-*tert*-butyl-4-methylphenol (BHT-H) for the chemoselective transesterification of MA and MMA, respectively.¹ In this presentation, we report the development of bulky Mg(II) and Na(I) bisphenoxides derived from 6,6'-(propane-2,2'-diyl)bis(2,4-di-*tert*-butyl)phenol (PBTP-H₂) as more active catalysts for chemoselective transesterification of MA and MMA.² Various primary and secondary alcohols, diols, triols and thermally unstable alcohols provided the corresponding (meth)acrylates in high yield without Michael adducts. The X-ray diffraction analyses of Mg(II) and Na(I) complexes succeeded, and DFT calculations were conducted to understand reaction mechanisms.



1) Ng, J. Q.; Arima, H.; Mochizuki, T.; Toh, K.; Matsui, K.; Ratanasak, M.; Hasegawa, J.; Hatano, M.; Ishihara, K. *ACS Catal.* **2021**, *11*, 199–207. 2) Zhao, X.; Ratanasak, M.; Kon, K.; Hasegawa, J.; Ishihara, K. *Chem. Sci.* **2022**, accepted.