Theoretical Studies on the Influence of Metallic Cations on Ring Opening of Propylene Oxide Catalyzed by Metal Salen Complexes

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Abstract

We studied the ring opening of propylene oxide (PO) by salen-M coordinated OH- group [M = Al(III), Sc(III), Cr(III), Mn(III), Fe(III), Co(II), Co(III), Ni(II), Cu(II), Zn(II), Ru(III) and Rh(III)]. The results show that the ring opening energy barriers for M(II) complexes are much lower than those with M(III) complexes in the gas phase, and the barriers correlate linearly with the negative charges on the OH- group, the Fukui function condensed on the OH- group. The nucleophilicity ordering in gas phase can be rationalized by the ratio of formal positive charges/radius of M cations. Solvent effect greatly increases the barriers of M(II) complexes, but slightly changes the results of M(III) ones, making the barriers similar. Analysis indicates that the reaction heats are linearly proportional to the reverse reaction barriers. The relationships established here can be used to estimate the ring opening barriers and to screen epoxide ring opening catalysts.

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