Studies on bis(halogeno)dioxomolybdenum(VI)-bipyridine complexes: Synthesis and catalytic activity

Abstract:
Dioxomolybdenum(VI) complexes with the general formula [MoO(2)Cl(2)L(2)] (L(2)=3,3'-dimethyl-2,2'-bipyridine, 5,5'-dimethyl-2,2'-bipyridine, 6,6'-dimethyl-2,2'-bipyridine, 4,4'-dibromo-2,2'-bipyridine, 5,5'-dibromo-2,2'-bipyridine, 5,5'-diamino-2,2'-bipyridine; 5,5'-dinitro-2,2'-bipyridine; 5,5'-diethoxycarbonyl-2,2'-bipyridine; 6-phenyl-2,2'-bipyridine; 2,2':6',2''-terpyridine) have been prepared and characterised. [MoO(2)Cl(2)(5,5'-diethoxycarbonyl-2,2'-bipyridine)] has been examined by single crystal X-ray analysis. The complexes were applied as homogenous catalysts for the epoxidation of cyclooctene with tert-butyl hydroperoxide (TBHP) as oxidising agent. The new compounds show an overall high activity and are highly selective catalysts in the epoxidation of cyclooctene. The stability of the complexes and differences in the catalytic activity can be clearly attributed to electronic contributions of the functional groups on bipyridine ligands and to steric restrictions. DFT calculations have assisted in a better understanding of the stability of the complexes and are in agreement with experiment. The influence of the terminal oxo ligands and the Lewis base ligands on the Mo center keep the compounds on quite a stable level of electron density.
Guenyar, Alev Zhou, Ming-Dong Drees, Markus Baxter, Paul N. W. Bassioni, Ghada Herdtweck, Eberhardt Kuehn, Fritz E. Kuhn, Fritz/A-3113-2010; Drees, Markus/A-3086-2010 Graduate School NanoCat; international Graduate School for Science and Engineering (IGSSE) A. G. and F. E. K. thank the Elitenetzwerk Bayern (Graduate School NanoCat) for financial support. M. D. Z. is grateful to the international Graduate School for Science and Engineering (IGSSE) for a Ph.D. Grant. The authors thank Dr. Hugh Chaffey-Millar and Dr. Mirza Cokoja for valuable discussions and for the proofreading of the manuscript. 8 Royal soc chemistry Cambridge

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