

SPIN-DEPENDENT EFFECTS IN ETHYLENE POLYMERIZATION WITH BIS (IMINO) PYRIDINE IRON (II) COMPLEXES

Boris Minaev^{1, 2, 3}, Alina Baryshnikova³ and Wen-Hua Sun^{1, 2}

¹Key Laboratory of Engineering Plastics-ICCAS, China

²BNLMS-Peking University, China

³Bohdan Khmelnytsky National University, Ukraine

The general concept of spin-dependent polyethylene polymerization by the bis(imino) pyridine iron(II) complexes is presented. It is stressed that the driving force of ethylene polymerization in the presence of bis(imino)pyridyliron(II) is a high exothermic effect of the monomer binding to the catalyst in all three low-lying spin states. The origin of low activation barrier in termination reaction between the initial monomolecular ethylene and the growing polyethylene chain corresponds to the energy decreasing of the "ethylene-catalyst" high-spin state complex which correlates directly with the targeted low-spin products through intersystem crossing. The applicability of the spin-catalysis concept to the Brookhart-Gibson catalytic scheme is described in this work on the basis of the detailed analysis of previously published theoretical results of Ziegler's and Morokuma's groups and of recent experimental achievements. The role of the axial-equatorial isomerization in spin-catalysis of Brookhart-Gibson type is discussed in details in connection with the main mechanistic problem of ethylene catalytic polymerization e competition between chain propagation and β -hydrogen atom transfer termination. The original part of review constitutes the calculation of spin-orbit coupling matrix elements in the BrookhartGibson catalytic cycle and the discussion of external magnetic field effect on ethylene polymerization.

bfrmin@rambler.ru