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47,49Ti Solid State NMR and DFT Study of Ziegler-Natta Catalyst

In Ti-based Ziegler-Natta catalysts (ZNCs), disagreements exist concerning which lateral surface of the $MgCl_2$ support adsorbs Ti species so as to be an active site for the catalysis of polymerization. In the present paper, we investigated the local structure of $TiCl_4$ adsorbed onto the surface of $MgCl_2$ by ^{47,49}Ti solid-state nuclear magnetic resonance (NMR) spectra at 21.8 T along with density functional theory (DFT) calculations. The magic-angle-spinning NMR spectrum of the $TiCl_4/MgCl_2$ adduct sample prepared by 20 h of milling, which exhibited broadened and shifted peaks compared to that of the sample without milling, was simulated by a Czjzek model considering the distribution of quadrupole interaction parameters. The electric field gradient and chemical shielding tensors of ^{49}Ti were obtained via DFT calculations for model molecules of $TiCl_4$, $2TiCl_4$, and Ti_2Cl_8 adsorbed onto the (110), (104), and (104)-step defect surfaces of $MgCl_2$. By comparing the obtained NMR parameters, the ^{47,49}Ti NMR spectrum of the milled sample was assigned to $TiCl_4$ adsorbed onto the (104) surface of $MgCl_2$, which may not be a principal component of adsorption.

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