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^{129}Xe NMR Analysis of Mo/Al_2O_3 Hydrodesulfurization Catalyst

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^{129}Xe NMR (nuclear magnetic resonance), a useful analytical tool for the investigation of zeolite pores, was evaluated as a novel technique for the analysis of active sites on Mo/Al_2O_3 hydrodesulfurization catalyst. ^{129}Xe NMR spectroscopy of Mo/Al_2O_3 catalyst detected a single peak attributed to xenon migrating in a few micropores on the surface of Al_2O_3. When a chemical shift δ of the peak was plotted against the amount of adsorbed xenon *N* in the NMR measurement, a nonlinear variation of δ appeared for sulfided Mo/Al_2O_3 catalyst. This result indicates that xenon strongly interacts electronically with molybdenum species on the surface. In addition, the term δ_0 was calculated which mainly depends on collisions between xenon and the catalyst surface from the fitting of the plot to a theoretical equation. As a result, δ_0 became larger with increased the molybdenum content. This result shows that migration of xenon was inhibited by molybdenum species on the surface. Increase in the sulfurization temperature also caused δ_0 to increase and almost corresponded to the sulfurization degree of molybdenum measured by XPS (X-ray photoelectron spectroscopy). This indicates that δ_0 is sensitive to formation of MoS_2 crystallites on the surface. ^{129}Xe NMR can be a powerful tool for analysis of the formation of MoS_2 crystallites on Mo/Al_2O_3 catalyst.

Keywords: ^{129}Xe NMR, Molybdenum alumina catalyst, Molybdenum sulfide crystallite, Structural analysis, Sulfurization

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