

# Quadrupolar Nuclei in Nanostructured Solids: Identifying Effects of Pt on Distinct <sup>23</sup>Na Sites in Pt-NaY

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## Introduction

Metal-supported zeolites play crucial roles in heterogeneous catalysis. The locations of metal particles in the zeolite framework are directly related to the catalytic activities. Therefore, understanding the chemistry of the metal dispersion is important to designing catalysts with improved performances. In this study, the locations of Pt species in zeolite NaY were inferred by analyzing the effects of catalyst preparation conditions on the distributions and relative populations of <sup>23</sup>Na cations at different cation-exchange sites, which are determined from analyses of solid-state <sup>23</sup>Na NMR spectra acquired at very high magnetic field (35.2 Tesla).

## Experimental

Calcined Pt-NaY zeolite was prepared by ion-exchanging Pt(NH<sub>3</sub>)<sub>4</sub>Cl<sub>2</sub>, followed by calcination in flowing oxygen at different temperatures (200° C, 400° C, and 600° C), according to the procedure described by Gallezot [1]. Solid-state <sup>23</sup>Na MAS NMR measurements were carried out on the 35.2 T Series-Connected-Hybrid magnet operating at 398 MHz for <sup>23</sup>Na and equipped with 2.0 mm triple-resonance MAS probehead.

# **Results and Discussion**

Different Na cation sites in zeolite NaY possess local environments that differ according to their interactions with the anionic zeolite framework, in particular the proximities and symmetry of nearby framework oxygen atoms. Such interactions give rise to a combination of different isotropic chemical shifts and different electric field gradients that are reflected by the positions and lineshapes of the <sup>23</sup>Na MAS signals. While Na in hexagonal prism has negligible quadrupolar interaction due to its symmetric octahedral coordination (Fig 1a), <sup>23</sup>Na cations located in sodalite and supercages show overlapping of quadrupolar broadened NMR lineshapes, which were resolved by MQMAS spectrum acquired at very high-field (Fig 1b). Notably, relative intensities of <sup>23</sup>Na signal from cations at different sites are found to be different in calcined 15 wt% Pt-NaY compared to the parent NaY zeolite (Fig 1c) indicating the influence of Pt on the distributions of Na cations. Detailed analyses of the <sup>23</sup>Na NMR results can be found in ref [2].

## Conclusions

The 35.2 T SCH magnet enabled the acquisition of <sup>23</sup>Na MQMAS NMR spectra with unprecedented signal sensitivity and resolution. Influence of Pt on the distribution of the distinct <sup>23</sup>Na sites are examined based on the well-resolved isotropic distributions of <sup>23</sup>Na cations in dehydrated NaY and Pt-NaY.

## Acknowledgements

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## References



[1] Gallezot, P., et al., J. Catalysis, 39, 334-349 (1975).



**Fig.1** (a) Schematic diagram of the structure of NaY zeolite and possible locations of Na cations (b) Solid-state <sup>23</sup>Na *z*-filtered MQMAS NMR spectrum of dehydrated NaY zeolite acquired at 35.2 T under MAS conditions of 24 kHz and at room temperature, (c) Single-pulse <sup>23</sup>Na MAS of dehydrated NaY (top) and 600° C calcined 15 wt% Pt-NaY.