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Applications of Synthesised Zeolite NaX and Its Modified Forms in CO2 Adsorption, Dielectric Properties, and Catalytic Activity

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Abstract:

*This study explores the multifunctional applications of synthesised zeolite NaX and its cesium-modified forms in three domains: **CO_2 adsorption**, **dielectric properties**, and **catalytic activity in Knoevenagel condensation reactions**. Sorption experiments were conducted at varying temperatures (273–363 K) using a surface area analyzer, and adsorption isotherms were analyzed using Langmuir, Freundlich, and Dubinin models. Dielectric properties were studied through DC conductivity and frequency-dependent dielectric constant measurements, while catalytic performance was evaluated in Knoevenagel condensation reactions. Results reveal that cation exchange significantly influences sorption capacity, dielectric behavior, and catalytic efficiency, highlighting the potential of modified zeolites in environmental and industrial applications.*

Keywords: Zeolite NaX, CO_2 Adsorption, Dielectric Properties, Coal Fly Ash, Knoevenagel Condensation, Cation Exchange, Mesoporous Catalysts.

Introduction:

Zeolites are crystalline aluminosilicates with unique microporous structures that enable gas adsorption, ion exchange, and catalytic activity (Breck, 1974). Their applications span environmental remediation, energy storage, and fine chemical synthesis. This research focuses on:

- **CO_2 adsorption** in NaX and Cs-modified NaX.
- **Dielectric properties** of coal fly ash-derived NaX (CFA-NaX).
- **Catalytic activity** in Knoevenagel condensation reactions.

The modification of zeolites through cation exchange alters their charge density, pore accessibility, and sorption behavior, making them versatile materials for environmental and industrial applications (Corma, 1997).

Methodology:

CO_2 Adsorption Studies:

- Conducted using NOVA-1200 analyzer at 273–363 K.
- Samples purified and activated under vacuum.
- Isotherms analyzed using Langmuir, Freundlich, and Dubinin equations.

Dielectric Properties:

- DC conductivity measured using a muffle furnace setup with brass electrodes.
- Frequency-dependent dielectric constant studied using Hewlett Packard LCR meter (75 kHz–15 MHz).

Catalytic Activity:

- Knoevenagel condensation reactions performed using mesoporous zeolites derived from coal fly ash.
- Reaction efficiency compared between parent and Cs-modified forms.

Results and Discussion:

CO_2 Adsorption:

- Isotherms approximated Langmuir type (Type I).
- Uptake decreased with increasing temperature (273–363 K).
- At 273 K and 600 Torr:
  - **NaCsX sorbed ~92 molecules/unit cell**
  - **NaX sorbed ~75 molecules/unit cell**
- Langmuir plots showed stronger sorption centers in NaX compared to NaCsX.
- Isosteric heat (qst) for NaX ~26 kJ/mol, independent of coverage, indicating homogeneous sorption sites.

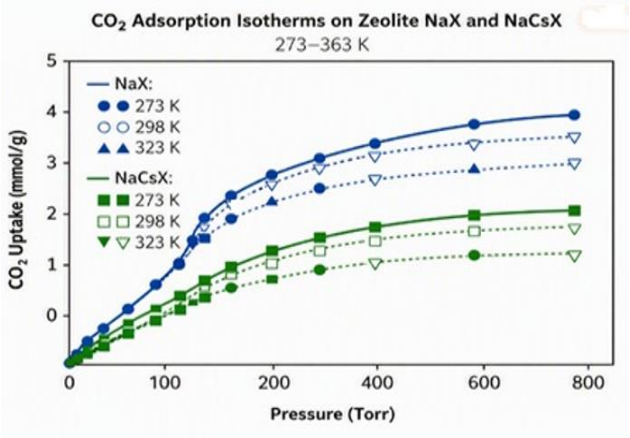
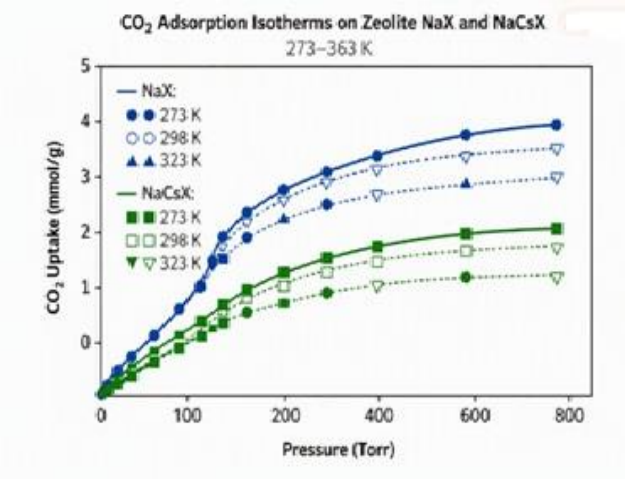


Table 1. CO_2 Uptake Comparison at 273 K, 600 Torr

Sample	Molecules per Unit Cell
NaX	75
NaCsX	92

Dielectric Properties:

- Conductivity increased with temperature, following Arrhenius law.
- Parent CFA-NaX showed higher conductivity than Cs-modified forms.
- Activation energy:
  - **NaX: 1.03 eV**
  - **NaCs(56)X: 1.37 eV**
- Dielectric constant increased beyond 150 °C, with Cs-modified samples showing abrupt rise.
- Frequency-dependent studies revealed Maxwell-Wagner effect at low frequencies and stable dielectric loss beyond 1 MHz.



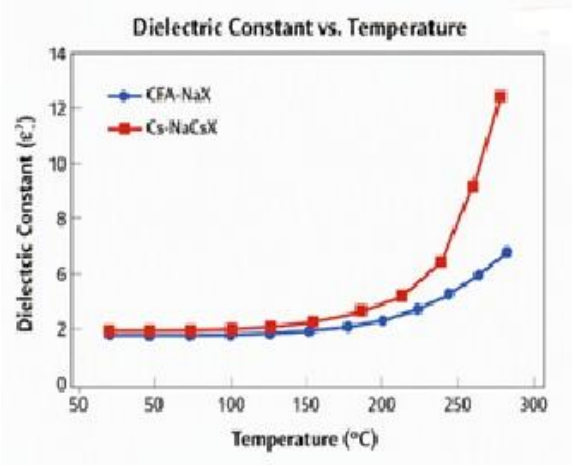


Table 2. Activation Energy of CFA-NaX and Modified Forms

Form of CFA-NaX	Activation Energy (eV)
CFA-NaX	1.03
CFA-NaCs(56)X	1.37

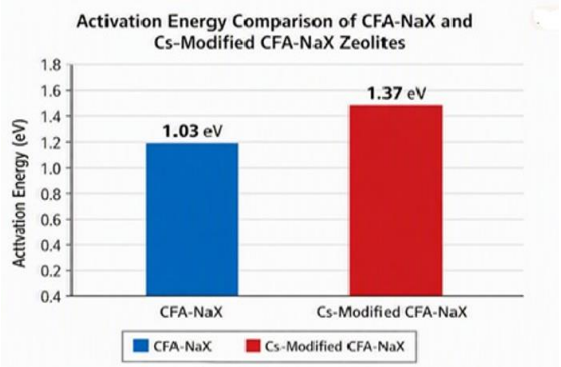


Figure 2. Activation energy comparison of CFA-NaX and Cs-Modified CFA-NaX Zeolites.

Catalytic Activity in Knoevenagel Condensation:

- Mesoporous zeolites demonstrated superior catalytic performance compared to microporous forms.
- Cs-modified zeolites enhanced proton conductivity and adsorption abilities, improving catalytic efficiency.
- The large pore size of mesoporous zeolites allowed reactions with bulky molecules, extending applicability in pharmaceuticals and fine chemicals.

Conclusion:

This study demonstrates that **cation exchange and structural modification of zeolite NaX** significantly influence its performance in adsorption, dielectric, and catalytic applications.

- **CO_2 adsorption**: NaX showed stronger sorption interactions, while Cs-modified forms exhibited higher uptake at high pressure.
- **Dielectric properties**: Parent CFA-NaX exhibited superior conductivity, while Cs-modification altered dielectric behavior.
- **Catalytic activity**: Mesoporous zeolites derived from coal fly ash proved effective in Knoevenagel

condensation, offering eco-friendly and reusable catalysts.

These findings highlight the potential of modified zeolites in **environmental CO_2 capture, energy storage, and sustainable chemical synthesis**.

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