CO_2 ADSORPTION ON ZEOLITE SSZ-45

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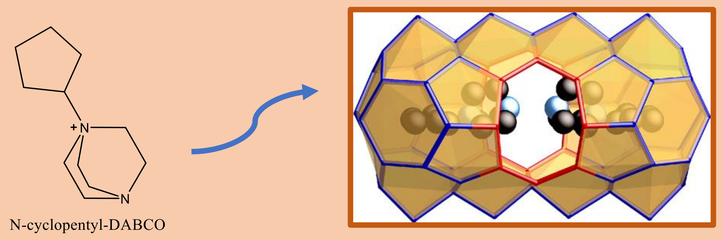
Introduction

High-silica small-pore zeolites are of particular interest for the gas separations, because they combine a fine molecular sieving and high thermal stability.[1] The high silica SSZ-45 has been recently synthesized using N-cyclopentyldiazabicicloctane as the structure direct agent (SDA).



Experimental

This material was synthetized following the procedure reported.[1]

The textural properties of SSZ-45 were determined by measurement of CO_2 and N_2 adsorption isotherms at low pressure. In addition, the CO_2 adsorption was studied at high pressure on SSZ-45 using an ISORB instrument at different temperatures (273, 283, 298, 313 and 333 K).

Surface area and pore volume

Dubinin-Astakhov (DA)

$$log_{10}V = log_{10}V_o - Dlog_{10}{}^2\left({}^{P_o}/_{P}\right)$$

Brunauer-Emmett-Teller (BET)

$$\frac{1}{V\left({}^{P_o}/_{P}-1\right)} = \frac{1}{V_m C_{BET}} + \frac{C_{BET}-1}{V_m C_{BET}}$$

Halsey equation

$$t = 3{,}54 * \left(\frac{-5}{ln\left({}^{P}/_{P_o}\right)}\right)$$

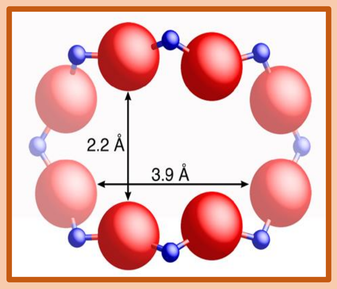
STRUCTURE

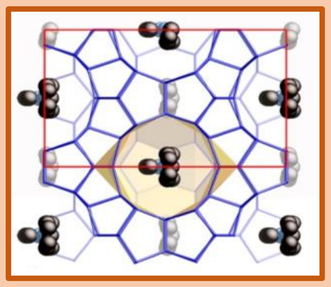
Pore system: 1D – 8R Chanels with large side pockets

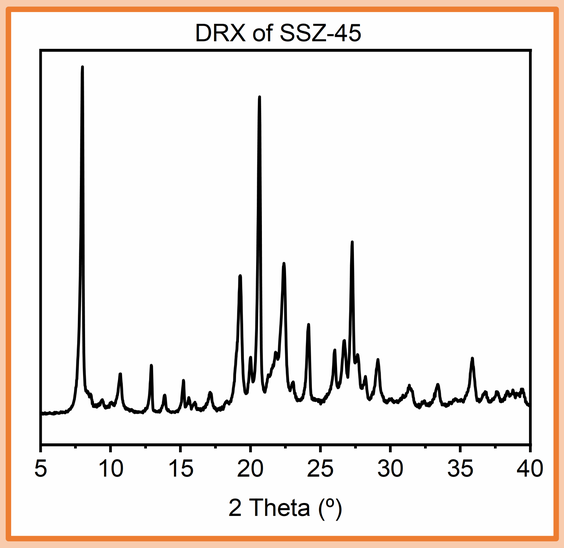
Cell parameters:

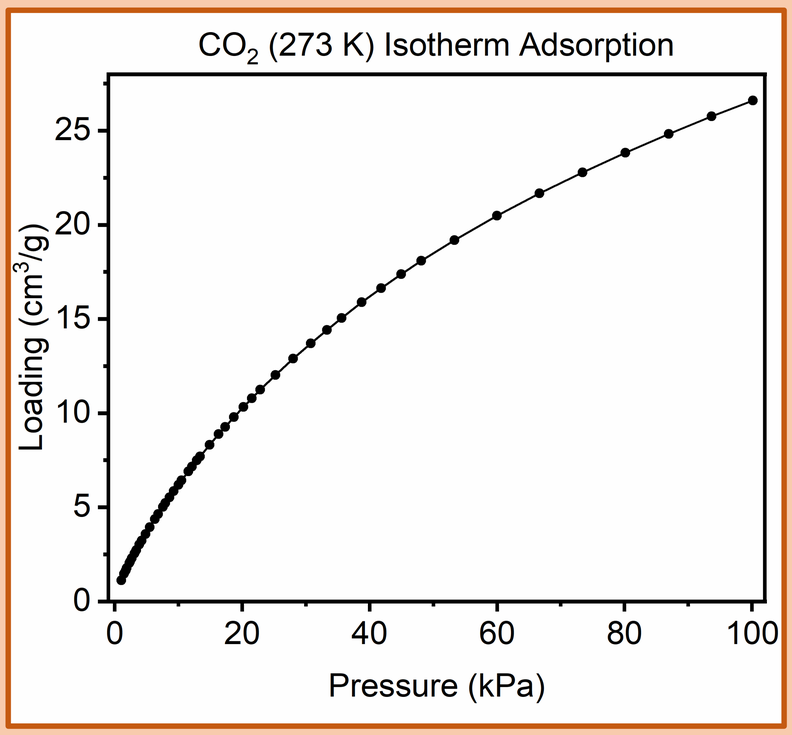
a = 13.8761 Å b = 35.7450 Å c = 22.4869 Å

α = 90.000° β = 90.000° γ = 90.000°

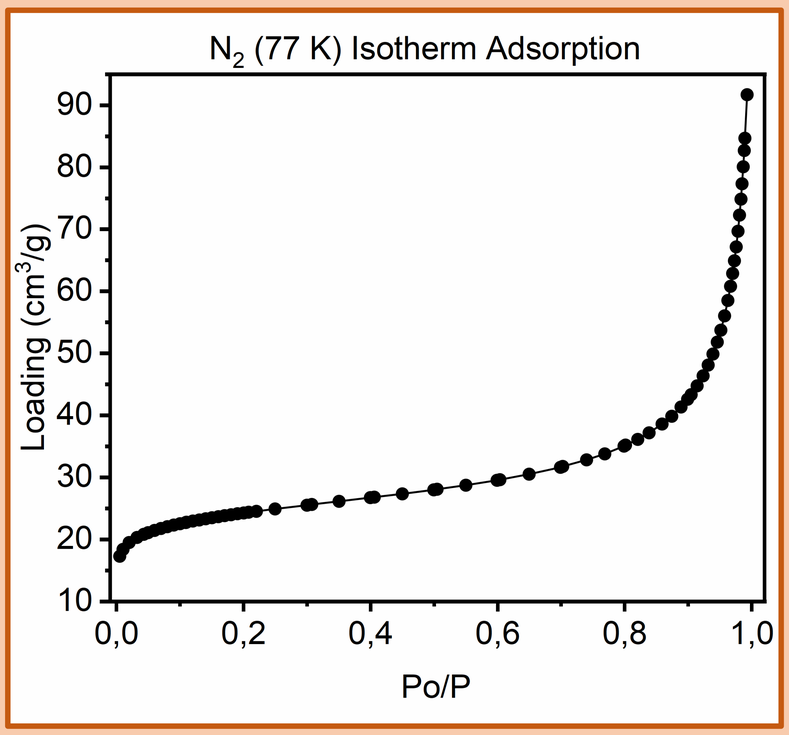




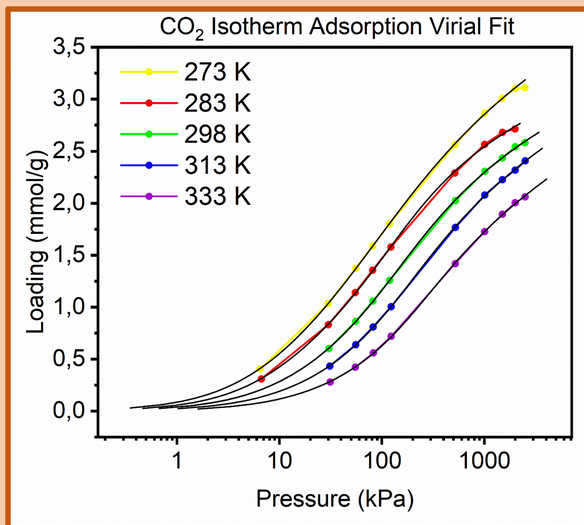


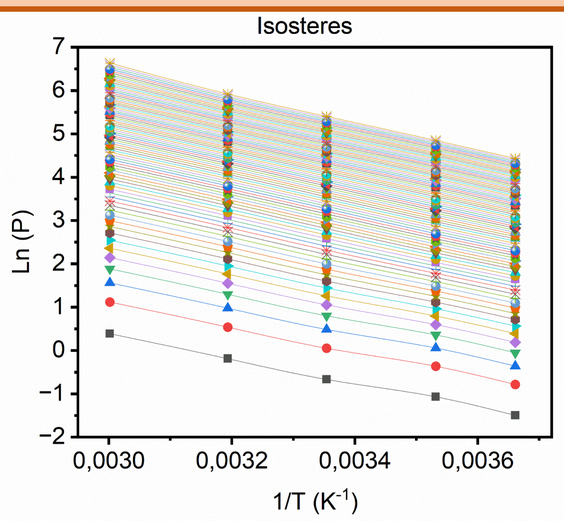


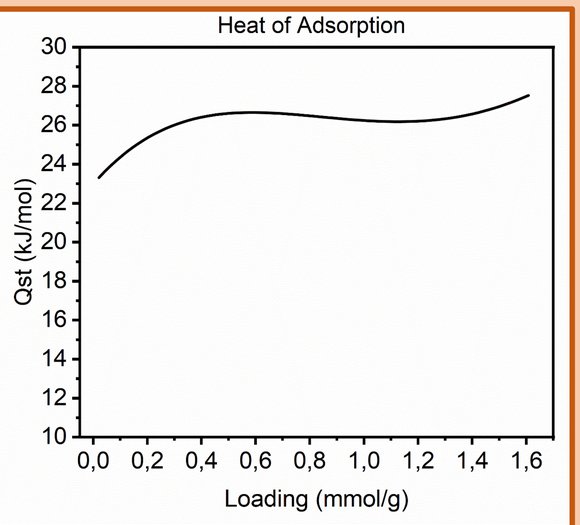
Specific Surface$_{DA}$ (m^2/g)	Micropore volume$_{DA}$ (cm^3/g)
767	0,18



Specific Surface$_{BET}$ (m^2/g)	Micropore *volume*$_{t\text{-}plot}$ (cm^3/g)
89	0,018







HEAT OF ADSORPTION

The isosteric heat of CO_2 adsorption (Q_{st}) on zeolite SSZ-45 was determined by applying the Clausius-Clapeyron's equation to the CO_2 isosteres.

The isotherms calculated using a viral type fitting to the experimental data fit them with a correlation coefficient better than 0.99. This allows the calculation of the isosteric heat in a wide range of CO_2 coverage. Results around 26 kJ/mol are obtained.

Henry constants

T (K)	273K	298K	313K	283K	333K
K_H (kPa^{-1})	0,094	0,061	0,041	0,026	0,015

Clausius-Clapeyron

$$q_{ST} = RT^2\left[\frac{\partial lnP}{\partial T}\right]_Q \equiv -R\left[\frac{\partial lnP}{\partial \frac{1}{T}}\right]_Q$$

Linearization

$$lnP = -(q_{ST}/8{,}3144) * (1/T) + C$$

By extrapolation at $Q_{st,0}$ it is possible to obtain the isosteric heat of adsorption at zero coverage **(22,7 kJ/mol)**

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References

[1] S. Smeets, D. Xie, L. B. McCusker, Chem. *Mater.* 2014, 26, 3909-3913.

CONCLUSIONS

Textural properties can not be properly determined by N_2 adsorption at 77K due to diffusional restrictions of N_2 to access the porosity, but it is possible with CO_2 adsorption at 273K. The isosteric heat of CO_2 adsorption calculated from the high pressure isotherms gives values around 26 kJ/mol, typically observed in high silica zeolites.

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