

Short Communication

Evaluation of procedures for estimation of the isosteric heat of adsorption in microporous materials



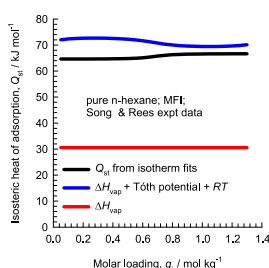
Rajamani Krishna

Van't Hoff Institute for Molecular Sciences, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands

HIGHLIGHTS

- The T -dependency of adsorption isotherms determines the isosteric heat of adsorption, Q_{st} .
- The isosteric heat of adsorption reflects both molecule–molecule and molecule–wall interactions.
- The enthalpy associated with molecule–molecule interactions is the latent heat of vaporization, ΔH_{vap} .
- The assumption $Q_{st} \approx \Delta H_{vap}$ has limited applicability.
- Generally, $Q_{st} > \Delta H_{vap}$ and can be estimated by adding the Tóth potential to ΔH_{vap} .

GRAPHICAL ABSTRACT



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ABSTRACT

The major objective of this communication is to evaluate procedures for estimation of the isosteric heat of adsorption, Q_{st} , in microporous materials such as zeolites, metal organic frameworks (MOFs), and zeolitic imidazolate frameworks (ZIFs). For this purpose we have carefully analyzed published experimental data on adsorption isotherms at different temperatures, T , for a variety of guest molecules (water, methanol, ethanol, dimethylether, cyclohexane, benzene, toluene, xylene, ethylbenzene, ethyne, propene, propane, iso-butane, 1-butene, n-hexane) in several zeolites, MOFs, and ZIFs.

Our analysis shows that when the binding energy with the structural framework is dominated by molecule–molecule interaction forces, $Q_{st} \approx \Delta H_{vap}$, the molar enthalpy of vaporization. In such cases, the molar loading q_i at any temperature T and pressure p_i , is a unique function of (p_i/P_i^{sat}) where P_i^{sat} is the saturated vapor pressure at T .

For most guest/host combinations, however, the Q_{st} values are significantly higher than ΔH_{vap} because of strong interactions of guest molecules with the material framework. For several guest/host combinations, a reasonable estimation of Q_{st} values is obtained by addition of the Tóth potential to ΔH_{vap} .

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Experimental data on the adsorption isotherms of polar compounds, such as water and alcohols, in microporous materials are commonly presented as plots of the component molar loading, q_i , as a function of (p_i/P_i^{sat}) , where p_i is the bulk pressure, and P_i^{sat} is the saturation vapor pressure at the temperature, T , at which the isotherm data are measured; see, for example, Zhang et al. (2013).

As illustration, Fig. 1a presents a plot of molar loadings, q_i , for adsorption of water in all-silica DDR zeolite as a function of (p_i/P_i^{sat}) . We note that the experimental data at various T overlap to yield a near-unique dependence of q_i on (p_i/P_i^{sat}) .

The temperature (T)-dependency of pure component adsorption isotherms in microporous materials such as zeolites, metal organic frameworks (MOFs), and zeolitic imidazolate frameworks (ZIFs) is a reflection of the binding energy between the guest molecules and the structural framework. The binding energy is

E-mail address: r.krishna@contact.uva.nl

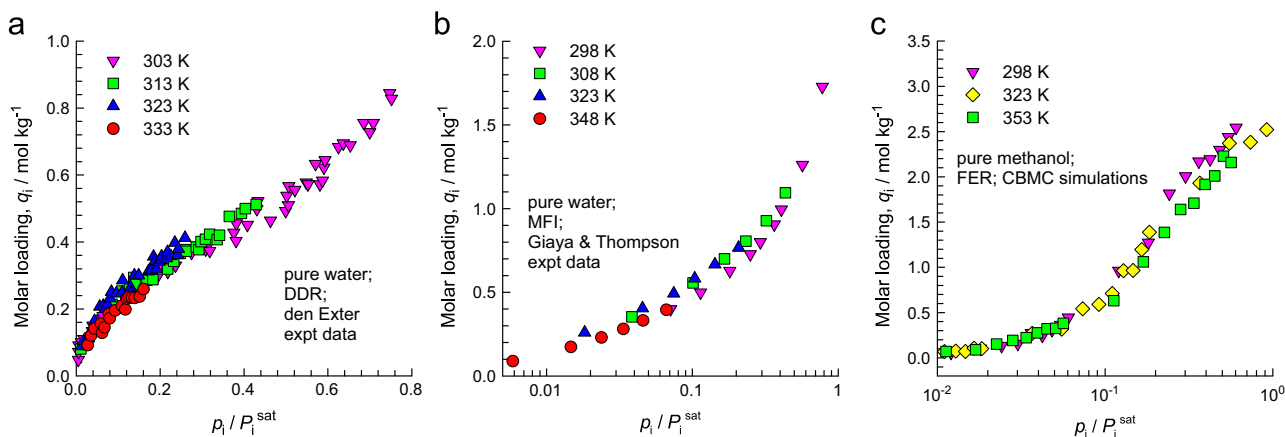


Fig. 1. Plot of component loadings vs. (p_i/P_i^{sat}) at a variety of temperatures. (a) Data of den Exter et al. (1997) for adsorption of water in DDR zeolite. (b) Data of Giaya and Thompson (2002) for adsorption of methanol in MFI zeolite. (c) Data of Hibbe et al. (2011) for adsorption of methanol in all-silica FER zeolite. Details of the calculations of the Q_{st} are available in the Supplementary material.

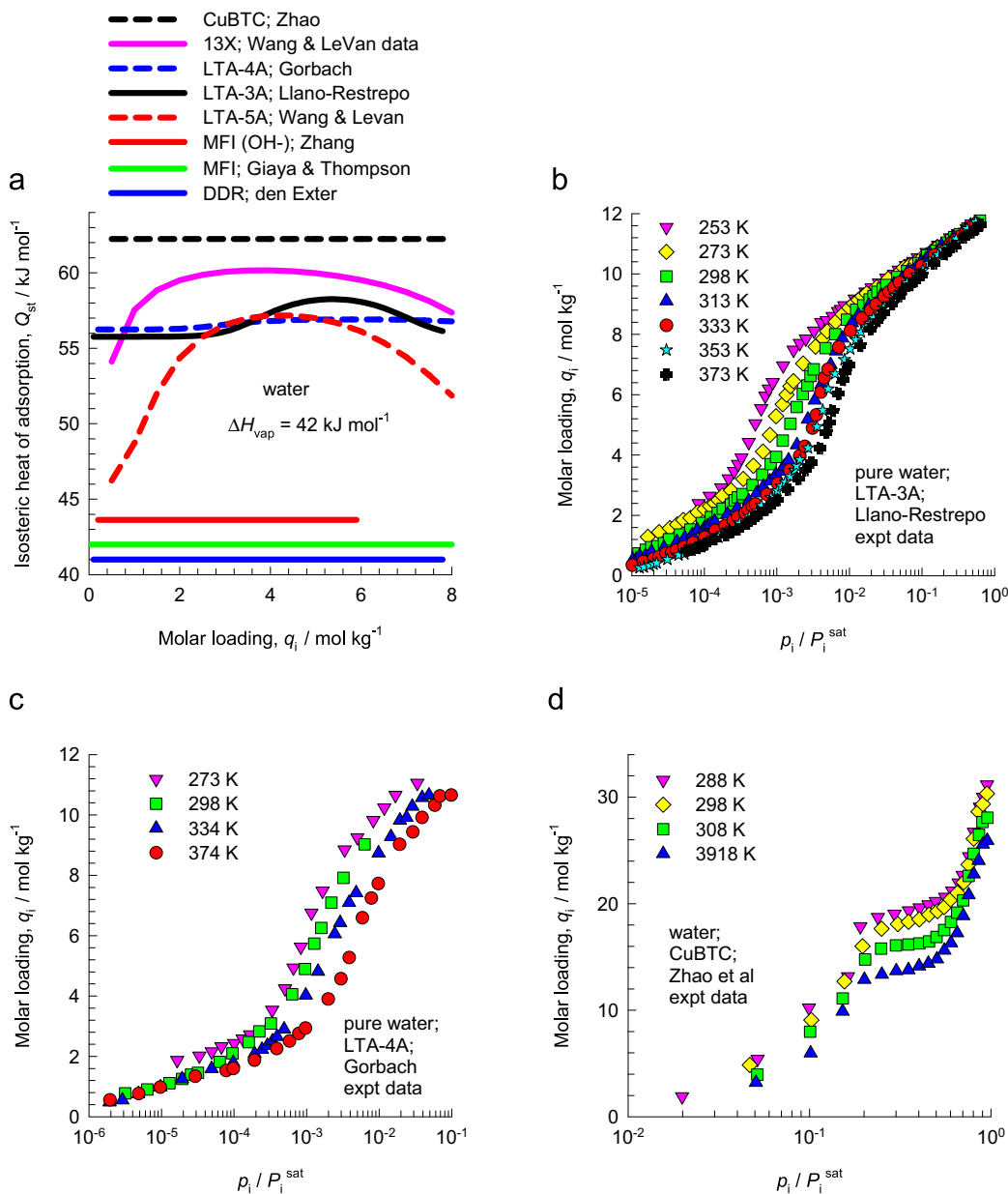


Fig. 2. (a) Comparison of the isosteric heats of adsorption, Q_{st} , of water in a variety of host materials. (b)–(d) Plot of component loadings vs. (p_i/P_i^{sat}) at a variety of temperatures. (b) Data of Llano-Restrepo and Mosquera (2009) for adsorption of water in LTA-3A. (c) Data of Gorbach et al. (2004) for adsorption of water in LTA-4A zeolite. (d) Data of Zhao et al. (2015) for adsorption of water in CuBTC. Details of the calculations of the Q_{st} are available in the Supplementary material.

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