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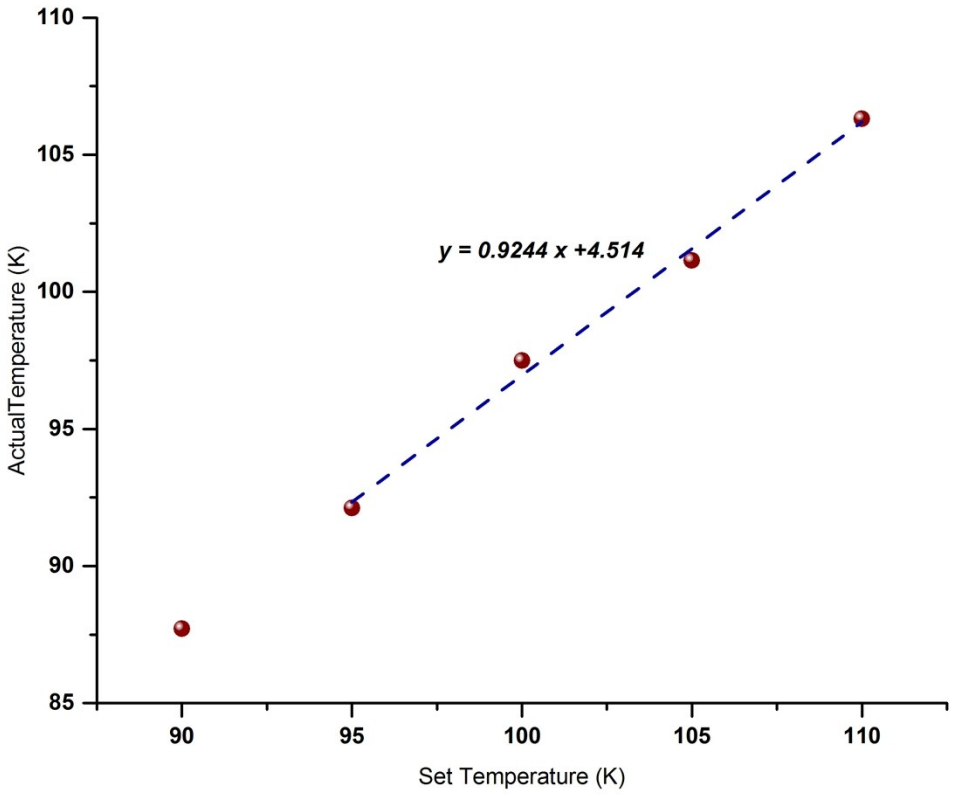
Thermodynamic Evidence of a Transition in ZIF-8 upon CH_4 sorption

Dinuka H. Gallaba, Aldo D. Migone

Department of Physics, Southern Illinois University Carbondale IL 62901

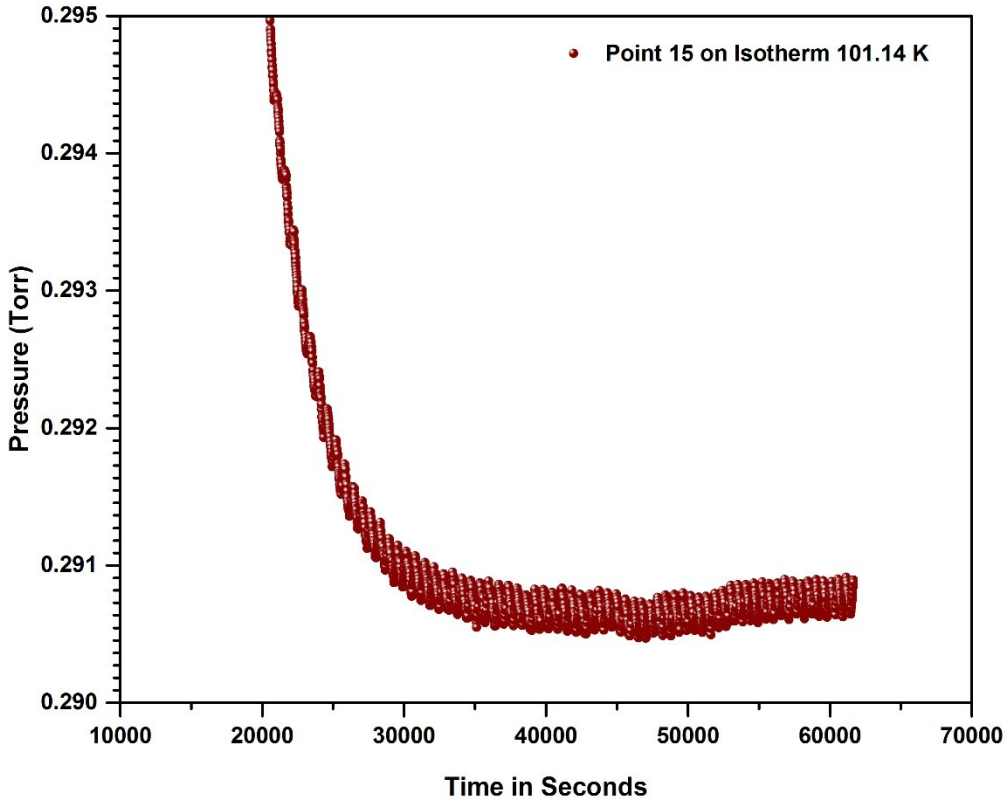
Supplementary Information:

S1. Sensor (set) temperature and the temperature obtained from the saturated vapor pressure[1] (Actual temperature) for liquid methane.



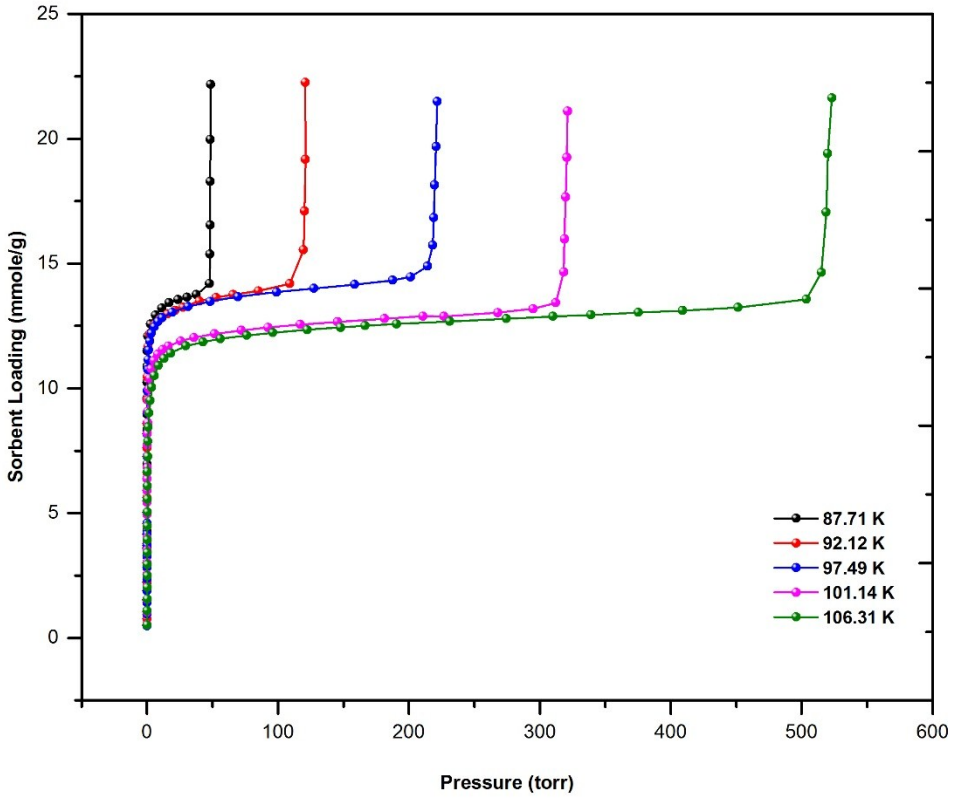
S2. Pressure change with time in seconds, for the data point no 15 on the 101.14 K isotherm

Measuring the pressure beyond the time needed for equilibrium (typically the period was on the order of hours after equilibrium was reached). Which allowed us to ensure that the data was measured at equilibrium.



S3: Methane Isotherms: Linear plot of Sorbent loading as a function pressure.

The subs-step feature is not visible in the isotherms, (compared to Fig 1)



S4 We determined the dose from a calibrated volume (V_{dose}) and the difference between the initial and final pressure ($P_i - P_f$). The amount (A_{vap}) in the vapor phase inside the cell was determined from the final value of the pressure when equilibrium was reached and the effective value of the cell at the measured temperature. The amount adsorbed was the value of the sum total of gas added to the cell, minus the amount present in the vapor phase

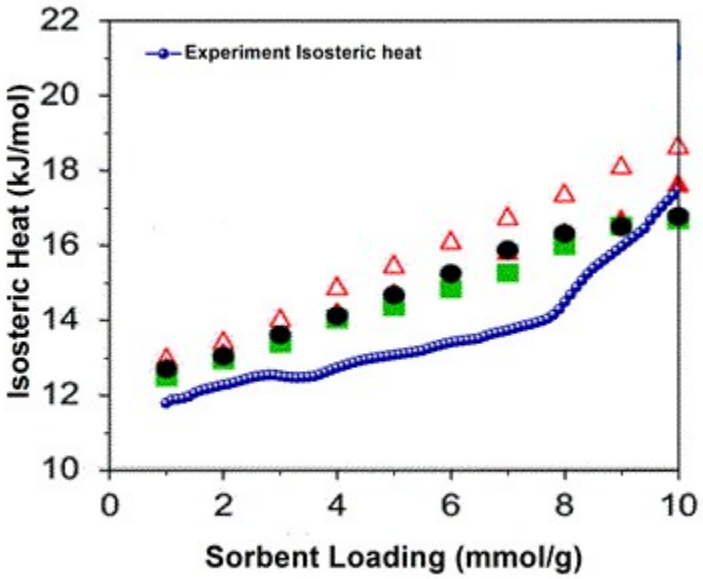
$$A_{in} = (P_i - P_f)V_{dose} \times \frac{273}{T_{room}}$$

$$A_{vap} = P_f \times V_{cell} \times \frac{273}{T_{cell}}$$

$$A_{sum} = \sum A_{in}$$

$A_{ads} = (A_{sum} - A_{vap})$

S5 Comparison of our experimental isosteric heat results with the results from simulations and experiment of Jimenez et al.[2]



△ UFF(+) ZIF-8HP (open red triangles)

▲ UFF(+) ZIF-8AP (closed red triangles)

■ UFF(*) on ZIF-8AP (green squares)

● The experimental (black circles)

*This image is adapted from the work of Jimenez et al[2]

Reference

1. Mallard, P. J. L. a. W. G., Nist Chemistry Webbook, Nist Standard Reference Database Number 69. National Institute of Standards and Technology, Gaithersburg MD, 20899.

2. Fairen-Jimenez, D., Galvelis, R., Torrisi, A., Gellan, A. D., Wharmby, M. T., Wright, P. A., & Dueren, T. (2012). Flexibility and swing effect on the adsorption of energy-related gases on ZIF-8: combined experimental and simulation study. Dalton Transactions, 41(35), 10752-10762.