

## Heat of Physisorption and the Predictions of Chi Theory

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### Abstract:

The heat of adsorption (either isosteric heat or the molar integral heat) of physisorption as a function of amount adsorbed may be calculated from the physisorption isotherm by two methods. The first utilizes the Dubinin “thermodynamic criterion” for which there exist a mapping relationship between the isotherm and the heats of physisorption which is  $q_{st} = RT \ln(P/P_s)$ . The other utilizes chi theory to determine the number of moles in a monolayer,  $n_m$ , and a defined energy value,  $E_\chi$ , for any adsorbate-adsorbent pair from the isotherm. Given  $n_m$  and  $E_\chi$ , the heat of adsorption may be calculated without any parameters. In examining the literature where both the isotherm and adsorption heat data are presented together, usually  $E_\chi$  can not be obtained from the isotherm due to the presence of background pressures which are too high.  $n_m$ , however is extractable and excellent 1-parameter fits to the heats of adsorption are possible. There are several cases where reliable values for both  $n_m$  and  $E_\chi$  are extractable. In these cases the calculation for the heats of adsorption which uses no parameters what-so-ever is in excellent agreement.