

PCTPro-2000

Direct Van't Hoff measurement

**Introduction:** The thermodynamic stability (heats of formation and decomposition) of hydrogen storage materials is a critical parameter for practical applications. It is vital to measure this accurately under true equilibrium conditions. Unfortunately, many of today's materials are kinetically hindered, requiring unreasonably long measurements times using the classic PCT isotherm method. The "direct van't Hoff measurement" approach enables rapid determination of reaction enthalpies using the PCTPro-2000.

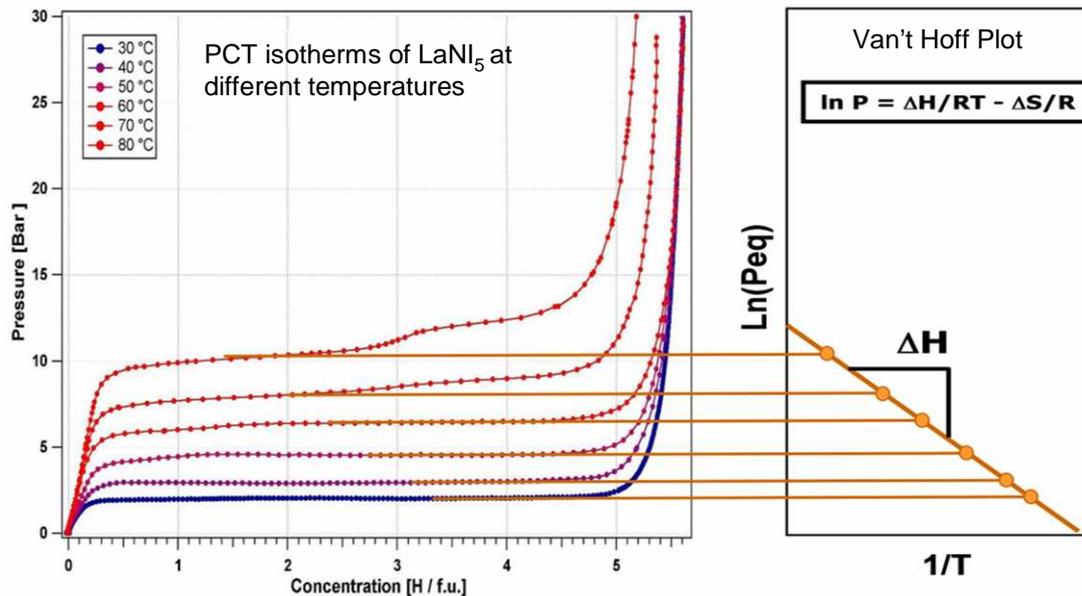


Fig. 1: Classic van't Hoff measurement

**Experimental**

A sample of LaNi<sub>5</sub> was analyzed using two different approaches:

- The classical one, where a PCT measurement is carried out for each temperature (fig. 1).
- The "direct van't Hoff measurement", where the advanced features of the PCTPro-2000 is employed (fig. 2 and fig. 3).

**Classical Methods of determination (fig. 1)**

Thermodynamics data are typically derived from a series of isotherms. These are collected by a precise process of dosing small quantities of gas to the sample and waiting for equilibrium at each dose. The enthalpy is obtained from the equilibrium pressure at one concentration from each isotherm. It is time consuming to obtain a reliable value of enthalpy of formation



**Instrument**  
**PCTPro-2000**  
 -260°C / 500°C

[www.setaram.com](http://www.setaram.com) – [sales@setaram.com](mailto:sales@setaram.com)



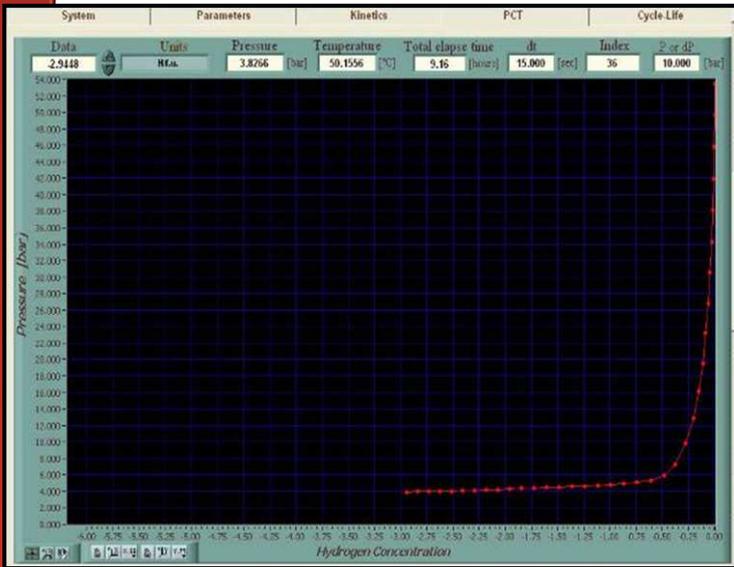
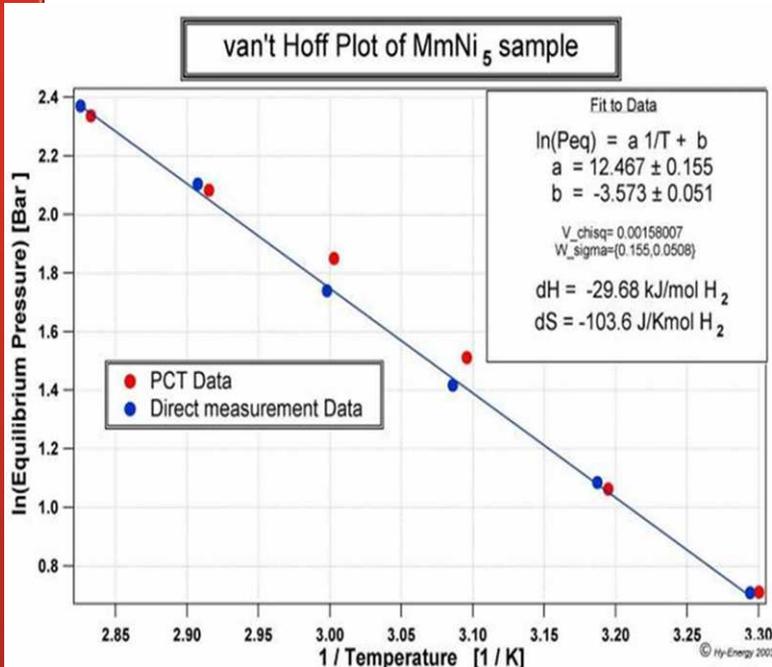


Fig. 2: Partial PCT stopped at a defined concentration • Fig. 3: Pressure vs. Time Profile



• Fig. 4: Comparison of van't Hoff plots obtained by the classical and the direct method

### Direct van't Hoff measurement (fig. 3, and fig. 4)

This method is accessible thanks to the unique features of the PCTPro 2000.

A PCT measurement is started and stopped to a specific (mid) composition on the plateau.

Then the time for aliquot is changed to a very large value.

and then the temperature is increased in steps.

The equilibrium pressure for each temperature is determined after reaching the steady state.

The “direct van't Hoff” plot is then constructed from the equilibrium pressures and temperatures of this single measurement.

### Conclusion

The enthalpy of formation is classically derived from series of PCT measurements. However, this process is very time consuming.

The specially designed PCTPro-2000 instrument can determine thermodynamics in a quick single direct measurement. The time saving is significant (orders of magnitude) and also offers improved accuracy in the measurement compared to the classical method (fig. 4).

***This feature provides the ability to obtain much faster results in your exploratory research and the discovery of new materials.***