APPLICATION NOTE 006

Calculating Isosteric Heats of Adsorption from HPVA Data Using MicroActive

An update in version 3.0 of Micromeritics' MicroActive software allows for pasting HPVA II data into MicroActive sample files. This feature is extremely useful for fitting data to various isotherm models and for calculating isosteric heats of adsorption from isotherms measured at differing temperatures. The following instructions explain how to paste HPVA II data into MicroActive and use the sample files to calculate heats of adsorption:

1. Version 22.0.9 of the HPVA II Excel macro automatically prints columns of data with appropriate headers for pasting into MicroActive. Activate this function by selecting "Edit" from the "HPVA Options" menu. Check the "Print MicroActive Data" box and click OK.

Print M	licroActiv	/e Data?)
	OK	

- 2. When an isotherm report is generated the MicroActive data is located at the bottom of the spreadsheet. Copy the two columns of data, including the two column headers labeled "Absolute Pressure (mbar)" and either "Quantity Adsorbed (cm3/g STP)" or "Quantity Adsorbed (mmol/g)"
- 3. Open MicroActive. Create a new sample file by choosing "Open" from the "File" menu. Enter a unique file name with the extension ".SMP" and click "Open." Click "Yes" when asked to create the file.
- 4. Select "Advanced" from the drop down menu located at the bottom of the SMP file window. Select the "Sample Description" tab. Locate "Type of Data" and select "Manually entered.



5. New options will appear in the drop down menu located at the bottom of the SMP file window. Select "Isotherm" and a blank graph will appear.



6. Click "p° and T..." and enter the analysis temperature. Saturation pressure for condensable adsorbates can be entered if plotting isotherms as a function of relative pressure is desired. If the adsorbate is in the supercritical state ignore the saturation pressure and isotherm data should only be viewed as a function of absolute pressure. Click "OK" to save changes.



- 7. Select "Absolute Pressure" or "Relative Pressure" to reflect how the data should be plotted.
- Click "Paste." The isotherm data will be automatically plotted on an absolute scale and a logarithmic scale.





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- 9. Click "Save" in the bottom left corner of the SMP file window to update progress.
- 10. Repeat steps 2-9 for additional isotherms at different temperatures. At least two temperature isotherms are needed for isosteric heats of adsorption calculations.



- 11. From the "Reports" menu select "Heats of Adsorption..."
- 12. Click "Add Samples..." and select the sample files previously created.

13. Heat of Adsorption will be plotted as a function of Quantity Adsorbed per gram. Click "Edit Quantities..." to insert a range of quantities adsorbed. For best results, the entered adsorption range should be covered by every isotherm.





