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*MEASUREMENT OF THE SURFACE AREAS OF
MINERAL POWDERS WITH A MODIFIED
PERKIN-ELMER, MODEL 212-D, SORPTOMETER
USING A NITROGEN-HELIUM GAS MIXTURE*

K. BARTELS

MINERAL SCIENCES DIVISION

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MEASUREMENT OF THE SURFACE AREAS OF MINERAL
POWDERS WITH A MODIFIED PERKIN-ELMER, MODEL 212-D,
SORPTOMETER USING A NITROGEN-HELIUM GAS MIXTURE

by

K. Bartels*

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ABSTRACT

This work compares the surface-area measurements made on four powdered materials (alumina, quartz, and two sodium carbonate powders) using the Sorptometer, employing nitrogen gas as adsorbate, with those made using the precise volumetric method (B.E.T.), employing krypton gas as adsorbate. It was found that the Sorptometer may be used successfully for rapidly comparing the surface areas of a large number of samples of a given material. However, if absolute accuracy is required, the Sorptometer must first be calibrated for each powdered material by the B.E.T. method.

The use of the Sorptometer with a pre-mixed adsorption gas (35% N₂ / 65% He, by volume) is described. The one-point method of evaluating the B.E.T. equation and the specific surface-area calculation for one of the carbonate samples are outlined. A computer program, written in FORTRAN IV language, which calculates the specific surface areas from Sorptometer data, is provided.

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LA MESURE DES SURFACES DES POUDRES MINÉRALES AVEC
UN "PERKIN-ELMER SORPTOMETER"¹ MODIFIÉ, LE MODÈLE 212-D,
UTILISANT UN MÉLANGE DE GAZ D'AZOTE-HÉLIUM

par

K. Bartels*

RÉSUMÉ

Dans ce travail, l'auteur compare les mesures de surface faites de quatre matériaux en poudre (l'alumine, le quartz et deux poudres de carbonate de sodium) utilisant le "Sorptometer" en employant le gaz d'azote comme adsorbat, pour celles faites avec la méthode volumétrique précise (B. E. T.) et en employant le gaz de krypton comme adsorbat. Il a trouvé que le "Sorptometer" peut être utilisé avec succès pour comparer rapidement les surfaces d'un grand nombre d'échantillons d'un matériel donné. Cependant, s'il est nécessaire d'avoir une précision absolue, il faut que le "Sorptometer" soit premièrement calibré pour chaque matériel en poudre par la méthode B. E. T.

L'auteur décrit l'utilisation du "Sorptometer" avec un gaz d'adsorption mélangé auparavant (35% N₂/65% He, par volume). Il présente un aperçu d'une méthode à point unique pour évaluer l'équation B. E. T. et le calcul spécifique de surface pour un des échantillons. Il présente aussi un programme machine dans le langage de FORTRAN IV qui calcule les surfaces spécifiques des données du "Sorptometer".

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1. Appareil de mesure des surfaces et des répartitions poreuses par une méthode dérivée de la chromatographie en phase gazeuse.

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INTRODUCTION

The need for measuring the surface areas of mineral powders in the Mineral Sciences Division of the Mines Branch has been discussed elsewhere^(1,2). A specially designed and constructed apparatus is already available for measuring the surface areas of mineral powders and other finely divided materials by the adsorption of krypton gas at liquid-nitrogen temperatures. This apparatus employs a volumetric method for measuring the amount of krypton before and after adsorption from a pre-calibrated gas burette. The gas pressure is measured by means of a sensitive thermistor gauge. The surface areas of the mineral powders are calculated from the adsorption results by means of the well-known B. E. T. equation⁽³⁾.

The above-mentioned apparatus, using krypton as adsorbate, now accurately measures materials with specific surface areas as low as $100 \text{ cm}^2/\text{g}$ ⁽¹⁾. However, the use of this apparatus is inherently time-consuming, (4 samples/3 days), because it is a high-vacuum system.

Because it is necessary as a routine in this laboratory to make surface-area measurements of a large number of samples in a short time, a Perkin-Elmer, Model 212-D, Sorptometer has been used for this purpose. The Sorptometer utilizes a continuous-flow method for determining the surface areas of finely divided materials. The continuous-flow method, first described in 1958 by Nelson and Eggertsen⁽⁴⁾, is similar to the volumetric method insofar as the use of the B. E. T. theory and the method of surface-area calculation are concerned. However, because the amount of adsorbed gas is determined at atmospheric pressure by concentration measurement in a continuous-flow system, the determination of the surface area is much more rapid.

The general operation of, and the modifications made in this laboratory to the Sorptometer have been described^(2,5,6,7). This work compares the surface-area measurements, made by the precise volumetric method,

using krypton gas as adsorbate, with those made using the Sorptometer, with nitrogen as adsorbate.

Included in the following sections are: a description of the modified Sorptometer; the method of measuring surface areas of samples using a pre-mixed adsorbate gas, (35% N₂/65% He by volume); the calculation of the surface area of one powdered sample using the one-point method of evaluating the B. E. T. plot; and the description of a computer program, written in FORTRAN IV language, that calculates the required information from the observed results.

Some theory and calculations which have been detailed previously (2, 5, 6, 7) have been included here for the sake of continuity.

APPARATUS

Figure 1 is a schematic diagram of the Sorptometer used in this laboratory. A detailed description of the Sorptometer is provided elsewhere (2, 5, 6, 7). The pre-mixed adsorption gas (35% N₂/65% He by volume), obtained from Union Carbide of Canada Limited, enters the instrument at A. The capillary restrictor, R, is used in the gas line in series with the pressure regulator, RG, to obtain a steady flow-rate. The adsorption gas then enters a liquid nitrogen trap, T, that freezes any condensable impurities in the gas. The purified gas then enters a constant-temperature bath, B ($t_{TC} = 26.0^{\circ}\text{C} \pm 0.2^{\circ}\text{C}$), via copper coils, C₁, and flows through the reference side of the detector, D_R. The detector is a thermal-conductivity cell containing four tungsten filaments arranged to form a Wheatstone bridge. The adsorption gas then flows through the calibration valves, V₁ and V₂, the three-valve manifold system, M, the sample tube, S, the coils, C₂, and finally through the sensing side of the detector, D_S, before venting to the atmosphere.

The two calibration valves, V_1 and V_2 , contain two loops, L_1 and L_2 , calibrated for volume. The effective volumes of the calibration gas (nitrogen, >99.999% pure) that are injected into the adsorption stream (with the valves V_1 and V_2 set at the INJECT position) from the loops L_1 , L_2 , and $(L_1 + L_2)$, are 0.2208, 0.2272, and 0.4510 ml (at STP), respectively⁽²⁾. To charge the calibration loops, the calibration gas, after entering the instrument at C, passes through the needle valve, N, and the rotameter, RT; it then flows through the calibration loops (with the valves V_1 and V_2 set at the charge position) before venting to the atmosphere. The rotameter is used only as a flow indicator.

The off-balance signal from the thermal-conductivity cell is recorded on a 0 to 5mV Bristol "Dynamaster", potentiometric, strip-chart recorder, RC. A polarity switch on the Sorptometer allows adsorption and desorption peaks to be recorded in the same direction on the recorder. The sample tubes, S, (Figure 1) are U-shaped with a space left above the sample. The saturation pressure, P_0 , of nitrogen at liquid nitrogen temperature, is measured with a liquid nitrogen barometer, MN, previously described⁽²⁾. Barometric pressure readings are obtained from a mercury barometer. Both the detector current and the zero-control knobs on the Sorptometer are of the 10-turn, lockable, digital type to assure constant base-line and detector-current settings.

MATERIALS AND METHOD

Sample Preparation

The samples of sodium carbonate, quartz, and alumina had specific surface areas between 650 and 84,000 cm^2/g , according to measurements made on the B. E. T. apparatus mentioned in the introduction. The weights for the two sodium carbonate, the alumina, and the quartz samples were, respectively, 0.3928 g, 0.5432 g, 0.8065 g, and 3.3205 g.

Prior to the Sorptometer measurements, the samples were dried in sample tubes, at between 110 and 115°C in an atmosphere of nitrogen (>99.999% pure) flowing at atmospheric pressure through the sample tubes. The sealed sample tubes were weighed after drying. Care was taken to avoid contaminating the samples with ambient air during transfer from the drying system to the Sorptometer manifold.

Calibration, Adsorption and Desorption Procedures

Both the calibration-gas and the adsorption-gas regulators on the supply cylinders were set at 20 psig. The pressure regulator, controlling the adsorption-gas pressure, was set at 30 in. water pressure for all surface-area measurements.

Before attaching the sample tube to the system, the adsorption gas was allowed to flow through the sample arm of the manifold in order to purge any air and water vapour from the sample arm. The flow of the adsorption gas through the manifold to the sample tube and to the sensing part of the detector was then established. The system was flushed with the adsorption gas for about 15 minutes prior to switching-on the detector current. This procedure is necessary because residual oxygen in the detector cell will burn out the tungsten filaments of the detector. The detector current, I_{DC} , was turned to zero (on a relative scale of ten) for all measurements. It was found that this setting provided an optimum base-line with low noise and sufficient detector sensitivity for samples that had low specific surface areas (about 600 cm²/g). The adsorption gas was passed through the sample and the detecting side of the thermal-conductivity cell until a stable base-line at the highest attenuation (x1) was attained.

Three calibration peaks were then obtained by consecutively injecting the contents of calibration loops L_1 , L_2 , and $(L_1 + L_2)$ into the adsorption-gas stream and through the sample tube, by turning the calibration valves V_1 and V_2 from the CHARGE position to the INJECT position in the corresponding order.

After each calibration peak had been recorded and the recorder pen had returned to the base-line, the next injection was made so that three consecutive calibration peaks showed on the chart paper with a common base-line.

When the calibration gas had been thoroughly flushed from the system, the sample tube and the bulb of the liquid-nitrogen manometer were immersed in a liquid-nitrogen bath to a pre-determined level, viz., 3 inches above the sample in the tube. The polarity switch was set at a position that would give a positive peak on the recorder paper. Adsorption and desorption peaks were usually obtained within 3 to 7 minutes.

When the adsorption peak reached its maximum, both mercury levels, Man_1 and Man_2 , of the liquid-nitrogen manometer, the ambient temperature, t , the barometric pressure, P_B , at temperature t_B , the Sorptometer attenuation, x_A , and the peak type (adsorption or desorption) were noted. When the pen on the recorder had returned to the base-line, the liquid-nitrogen bath was removed from the sample tube and the liquid-nitrogen manometer, and the polarity of the Sorptometer was reversed in order to accommodate the desorption peak on the chart. Similar readings of t , P_B , etc. were then noted for the desorption peak when the desorption peak reached its maximum. Further calibration peaks were recorded for each sample immediately after each pair of adsorption and desorption peaks was obtained.

Because the recorder does not have an integrator, integration of the areas under the peaks was performed by cutting out and weighing the peak areas. From this integration procedure, the calibration peak-area weight, Cal_{wt} , the adsorption peak-area weight, A_{wt} , and the desorption peak-area weight, D_{wt} , were evaluated.

From the above weights and the calibration volume, V_{cal} , the volume, $V_{ads}(STP)$ and $V_{des}(STP)$ (i. e., the volumes of nitrogen adsorbed or desorbed) were calculated. (See the One-Point Method, page 6, and Appendix Ic, page 15).

THE ONE-POINT METHOD

The B. E. T. equation for non-porous solids⁽³⁾ that is used to calculate the specific surface area, S_s , (area/g), is given by

$$\frac{P}{V \cdot (P_o - P)} = \frac{1}{V_m C} + \frac{C-1}{V_m C} \cdot \frac{P}{P_o} \quad \dots \text{(Eq. 1)}$$

- where
- V = the total volume of adsorbed (or desorbed) gas on the surface of the adsorbent at STP,
 - V_m = the volume of adsorbed gas when the entire surface is covered with a monolayer of adsorbed gas,
 - P = the equilibrium partial pressure of the adsorbate,
 - P_o = the saturation vapour pressure of the adsorbate at the temperature of the coolant (liquid nitrogen); and
 - C = constant expressing the net adsorption energy.

On the assumption that the B. E. T. plots of $P/V(P_o - P)$ against P/P_o for nitrogen adsorption have negligibly small values of intercepts, $1/V_m C$, on the ordinate, the B. E. T. equation can be written as:

$$S'_s = V \cdot \left(\frac{P_o - P}{P_o} \right) \cdot \left(\frac{S_o}{W} \right), \quad \dots \text{(Eq. 2)}$$

where

- W = the weight of the sample in grams,
- S_o = the area covered by one milliliter of the adsorbate at STP, when adsorbed as a monolayer, and
- S'_s = the specific surface area of the sample as calculated by the one-point method.

Because a mixture of nitrogen and helium of a known composition is used in the adsorption measurements, the partial pressure, P , of nitrogen, is calculated from the mole % concentration, α , of nitrogen in the mixture and from the barometric pressure, P_t , using the equation:

$$P = \frac{\alpha}{100} \cdot P_t. \quad \dots \text{(Eq. 3)}$$

Finally, by inserting the value for P into Equation 2, and using the volume of the adsorbed (or desorbed) nitrogen gas, the expression for the specific surface area, S'_s , as calculated by the one-point method, is given by

$$S'_s = \frac{V}{W} \cdot \frac{S_o}{P_o} \left(P_o - \frac{\alpha}{100} \cdot P_t \right). \quad \dots \text{(Eq. 4)}$$

Because the volume, V , of the adsorbed (or desorbed) nitrogen is proportional to the area of an adsorption or desorption peak, it is also proportional to the adsorption peak-area weight, A_{wt} , and the desorption peak-area weight, D_{wt} . Hence, V_{ads} (or V_{des}) can be calculated by relating it to the injected calibration volume of nitrogen, V_{cal} , so that, for a desorption peak,

$$V_{des} = \frac{D_{wt}}{Cal_{wt}} \cdot V_{cal}. \quad \dots \text{(Eq. 5)}$$

The value of V_{des} is then converted to STP so that

$$V_{des}(\text{STP}) = V_{des} \cdot F_{\text{STP}} \quad \dots \text{(Eq. 6)}$$

where F_{STP} is the factor that converts the desorbed volume at experimental temperature and pressure to STP (see Appendix Ic).

RESULTS AND DISCUSSION

Equations for correcting the atmospheric pressure and the tabulated pressure corrections are given in Appendix Ia. The method of calculating the saturation vapour pressure of nitrogen and the data for the corresponding monolayer areas are given in Appendix Ib. Appendix Ic gives the calculation of the factor, F_{STP} , for converting volumes at room temperature and pressure, RTP, to volume at STP. Similarly, the calculation of the factor, F_{RTP} , which converts volumes at STP to volumes at room temperature and pressure, is also given in Appendix Ic. Conversion of Beckman thermometer readings, R_{BN} , to °K, are given in Appendix Id. A typical surface-area calculation for a sodium carbonate sample, #1388-70-2-1, is given in Appendix II. Appendix III contains a discussion of the computer program SORPT1, in FORTRAN IV language, that enables a rapid calculation of surface areas from a large number of Sorptometer measurements. A listing of SORPT1 is included at the end of Appendix III.

Specific surface areas of the sodium carbonate, quartz, and alumina samples, measured using both the B. E. T. apparatus and the Sorptometer, are given in Table 1.

TABLE 1

Comparison of Surface Areas Measured by the Dynamic Flow Method (Sorptometer) and the Static Volumetric Method (B. E. T.)

Sample	Specific Surface Area (cm ² /g)		% Diff. (from B. E. T.)
	B. E. T.	Sorptometer	
Sodium Carbonate 1388-70-2-1	83700	60000	-28
Sodium Carbonate 1388-70-5A	36800	25200	-31
Quartz - 71-Cal-2	664	571	-14
Aluminum - 71-Cal-3	8870	7580	-15

From these and numerous other results obtained, the following conclusions are drawn:

1. The repeatability and speed of the Sorptometer measurements are good. For two determinations on sodium carbonate, Sample #1388-7-2-1, the twenty specific surface areas calculated from different combinations of adsorption, desorption and calibration peak-area weights, averaged $6.00 \pm 0.16 \text{ m}^2/\text{g}$. The two determinations were completed within two hours from the time of sample attachment to the shut-down of the Sorptometer.
2. The 14 to 15% error for the quartz and alumina samples, as shown in Table 1, may be due to the following:
 - (a) the assumption of the one-point method that the Y-intercept, $1/V_m C$, in the B.E.T. plot is zero, is not strictly correct.
 - (b) the B.E.T. adsorption isotherm for nitrogen is usually linear within the P/P_0 range of 0.05 to 0.35⁽¹⁾. The use of a mixture of 35% N_2 /65% He (by volume) for these determinations, resulted in P/P_0 values between 0.33 and 0.35. At P/P_0 values so close to the upper limit of linearity, the B.E.T. isotherms for the samples under investigation may not be linear.
 - (c) the large error, 28 to 32%, for the surface areas of the sodium carbonate samples, for which the degrees of hydration had not been specified, may be due to the fact that they retained surface films of water vapour. It was found, during measurement of their surface areas by the B.E.T. method, that the samples continuously gave off water vapour in vacuum. Only after evacuating the samples at 55°C for several hours was the vapour pressure sufficiently low and stable to allow the B.E.T. measurement to be made. Therefore, the degassing in a flow of high-purity nitrogen did not fully de-hydrate these samples.

The Sorptometer, with its good repeatability, may be used successfully for rapidly comparing the surface areas of a large number of samples. However, when absolute accuracy is required, the Sorptometer must first be calibrated for each powdered material using the B. E. T. method because the samples, normally handled in this laboratory, vary greatly in such physical characteristics as particle size and porosity.

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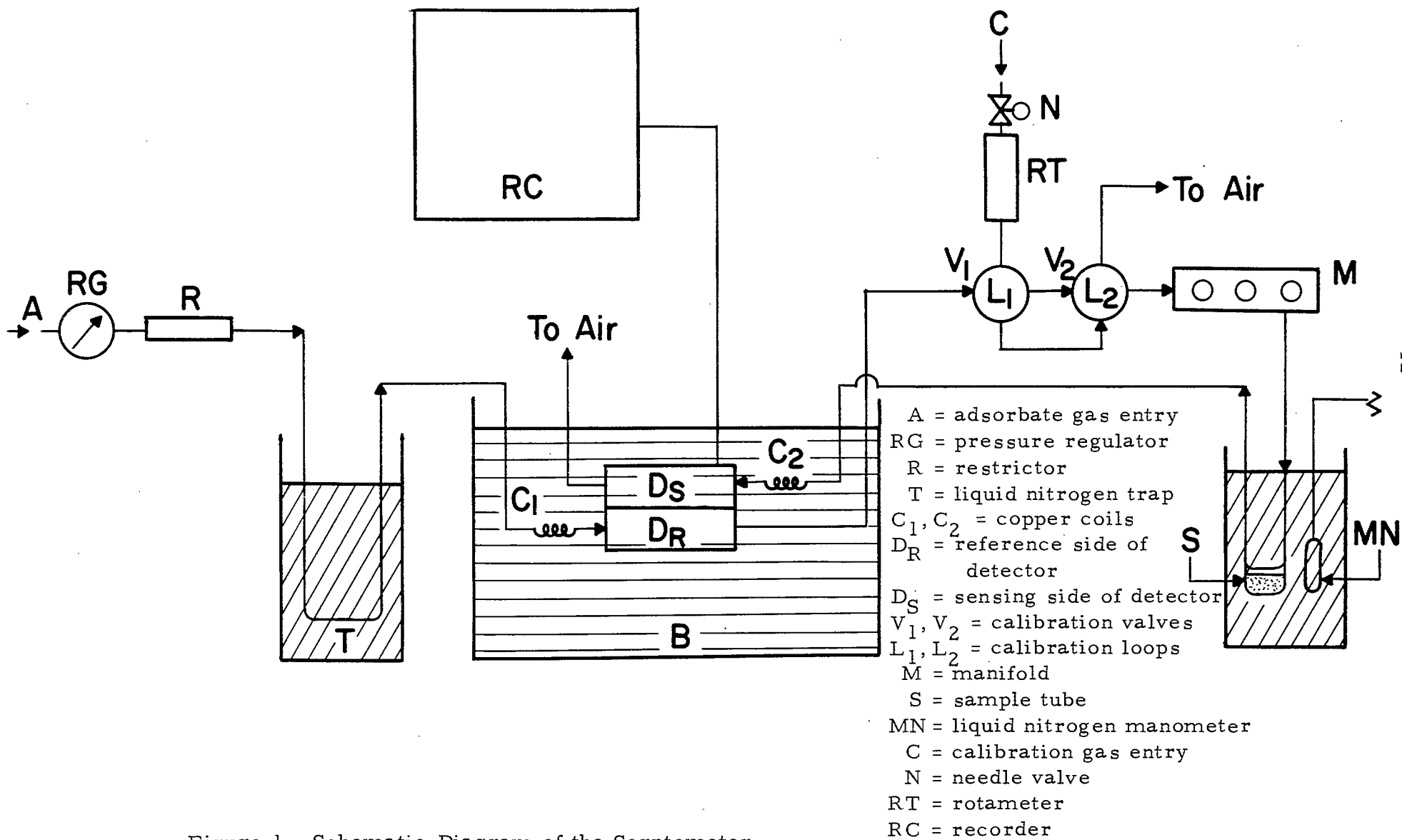


Figure 1. Schematic Diagram of the Sorptometer.

APPENDIX I

(a) Temperature Correction of the Barometric Pressure, P_B

Atmospheric pressure measurements were made with a mercury barometer. The readings were corrected to standard temperature (273.16°K) by subtracting the appropriate quantity P_{Bcorr} (in mm Hg) (see Table 2), for a given ambient temperature, t_B , (in °C), from the observed barometric pressure, P_B .

The value of the partial pressure, P , (in mm Hg), is calculated from the corrected barometric pressure, P_t , (in mm Hg), using the % mol fraction of nitrogen, α , in the adsorption gas mixture.

Hence,
$$P_t = P_B - P_{Bcorr}, \quad \dots \text{ (Eq. 7)}$$

and
$$P = P_t \cdot \alpha', \quad \dots \text{ (Eq. 8)}$$

where
$$\alpha' = \alpha / 100, \quad \dots \text{ (Eq. 9)}$$

In Equation 7, P_{Bcorr} is the barometric correction at ambient temperature, t_B , as it is found from Table 2.

TABLE 2

Temperature Correction for Barometer Readings⁽⁷⁾

Ambient Temp. (t_B) (°C)	P_{Bcorr}	(Observed mercury height in mm)					
		720	730	740	750	760	770
15	1.76	1.78	1.81	1.83	1.86	1.88	1.91
16	1.88	1.90	1.93	1.96	1.98	2.01	2.03
17	1.99	2.02	2.05	2.08	2.10	2.13	2.16
18	2.11	2.14	2.17	2.20	2.23	2.26	2.29
19	2.23	2.26	2.29	2.32	2.35	2.38	2.41
20	2.34	2.38	2.41	2.44	2.47	2.51	2.54
21	2.46	2.50	2.53	2.56	2.60	2.63	2.67
22	2.58	2.61	2.65	2.69	2.72	2.76	2.79
23	2.69	2.73	2.77	2.81	2.84	2.88	2.92
24	2.81	2.85	2.89	2.93	2.97	3.01	3.05
25	2.93	2.97	3.01	3.05	3.09	3.13	3.17
26	3.04	3.09	3.13	3.17	3.21	3.26	3.30
27	3.16	3.20	3.25	3.29	3.34	3.38	3.42
28	3.28	3.32	3.37	3.41	3.46	3.51	3.55
29	3.39	3.44	3.49	3.54	3.58	3.63	3.68
30	3.51	3.56	3.61	3.66	3.71	3.75	3.80

(b) Measurement of the Saturation Vapour Pressure of Nitrogen and the Determination of the Amount of Monolayer Coverage

P_o (mm Hg), the saturation vapour pressure of nitrogen at the temperature of liquid nitrogen, is calculated from the upper and lower levels of Hg, Man_1 and Man_2 (in mm), of the liquid nitrogen barometer.

Hence,
$$P_o = (Man_1 - Man_2) \quad \dots \text{(Eq. 10)}$$

Table 3 shows the area covered by 1 ml of nitrogen ($m^2/ml, S_o$) as a monolayer for a given value of P_o ⁽⁵⁾.

(c) Factors for Converting from Volume at Room Temperature and Pressure (RTP) to Volume at STP and Vice Versa

From the gas equation,

$$\left(\frac{PV}{T}\right)_{STP} = \left(\frac{PV}{T}\right)_{RTP} \quad \dots \text{(Eq. 11)}$$

Hence,
$$V_{RTP} = \left(\frac{P}{T}\right)_{STP} \cdot \frac{V_{STP} \cdot T_{RTP}}{P_{RTP}}, \quad \dots \text{(Eq. 12)}$$

and
$$V_{STP} = \left(\frac{T}{P}\right)_{STP} \cdot \frac{V_{RTP} \cdot P_{RTP}}{T_{RTP}}, \quad \dots \text{(Eq. 13)}$$

where
$$\left(\frac{T}{P}\right)_{STP} = F_{STP}, \quad \dots \text{(Eq. 14)}$$

and
$$\left(\frac{P}{T}\right)_{STP} = F_{RTP}. \quad \dots \text{(Eq. 15)}$$

Thus
$$F_{STP} = 0.35945^\circ K/mm \text{ Hg},$$

and
$$F_{RTP} = 2.7823 \text{ mm Hg}/^\circ K.$$

(d) Conversion of Beckman Thermometer Readings to °K

If R_{BN} is the reading of the Beckman thermometer, the ambient temperature in degrees Kelvin, T , is given by

$$T = (R_{BN} - 2.55) + 298.16, \quad \dots \text{(Eq.16)}$$

where 2.55 is the reading of the Beckman thermometer at 298.16°K.

TABLE 3

The Area, S_o , Covered by 1 ml of Nitrogen as a Monolayer for a Given Value of the Saturation Pressure of Nitrogen⁽⁵⁾

Area (S_o) Covered by 1 ml N_2 as a Monolayer [m^2/ml (STP)]	Saturation Pressure (P_o) of Nitrogen [mm Hg]
4.3685	740
4.3703	750
4.3721	760
4.3739	770
4.3756	780
4.3773	790
4.3790	800
4.3808	810
4.3826	820
4.3844	830
4.3862	840
4.3880	850
4.3898	860
4.3915	870
4.3932	880
4.3949	890
4.3966	900

APPENDIX II

Typical Calculation of the Specific Surface Area of Sodium Carbonate,
Sample #1388-70-2-1

(a) Observed Data

1. Sample weight, $W = 0.39281$ g
2. Weight of first calibration peak, $Cal_{wt} = 0.09059$ g
3. Beckman thermometer reading during calibration, $R_{BN} = 2.09$
Beckman thermometer reading during desorption, $R_{BN} = 2.07$
4. Liquid-nitrogen manometer readings:
 $Man_1 = 94.3$ mm Hg
 $Man_2 = 15.2$ mm Hg
5. Weight of first desorption-peak area, $D_{wt} = 0.32673$ g
6. Barometric pressure, $P_B = 762.9$ mm Hg
Temperature at time of barometric pressure reading, $t_B = 23.5^\circ C$
7. Constants:
 - (i) Calibration volume for first calibration peak,
 $V_{Cal_{STP}} = 0.2208$ ml.
 - (ii) Mole % of N_2 in the N_2/He mixture, $\alpha = 35\%$.

(b) Calculation of the Specific Surface Area S'_s

1. From Table 2 it is seen that, at an ambient temperature, t_B , of $23.5^\circ C$, P_{Bcorr} for a P_B of 762.9 mm Hg is 2.92 mm Hg.

Therefore,

$$P_t = P_B - P_{Bcorr}$$
$$= 762.9 - 2.92 = 759.98 \text{ mm Hg.} \quad \dots (\text{Eq. 7})$$

2. $T = (R_{BN} - 2.55) + 298.16^\circ K \quad \dots (\text{Eq. 16})$

Hence, the temperature during calibration is given by

$$T_{\text{Cal}} = (2.09-2.55) + 298.16 = 297.70^{\circ}\text{K},$$

and the temperature during desorption is given by

$$T_{\text{Des}} = (2.07-2.55) + 298.16 = 297.68^{\circ}\text{K}.$$

$$3. \quad P = \frac{\alpha}{100} \times P_t \quad \dots (\text{Eq. 3})$$

$$= \alpha' \times P_t \quad \dots (\text{Eq. 8})$$

$$= 0.350 \times 759.98 = 265.99 \text{ mm Hg.}$$

$$P_o = (\text{Man}_1 - \text{Man}_2) = 943 - 152 \quad \dots (\text{Eq. 10})$$

$$= 791 \text{ mm Hg.}$$

$$P_o - P = 791.0 - 265.99 = 525.01 \text{ mm Hg}$$

$$P/P_o = \frac{265.99}{791.0} = 0.33628$$

$$4. \quad V_{\text{Cal}_{\text{STP}}} = 0.2208 \text{ ml.}$$

$$\text{Therefore, } V_{\text{Cal}_{\text{RTP}}} = F_{\text{RTP}} \times \frac{V_{\text{Cal}_{\text{STP}}} \times T_{\text{Cal}}}{P_t} \quad \dots (\text{Eq. 12})$$

$$= \frac{2.7823 \times 0.2208 \times 297.70}{759.98}$$

$$= 0.24065.$$

$$\text{Hence, } V_{\text{Des}(\text{STP})} = \frac{D_{\text{wt}}}{\text{Cal}_{\text{wt}}} \times V_{\text{Cal}_{\text{RTP}}} \times \frac{P_t}{T_{\text{Des}}} \times F_{\text{STP}} \quad \dots (\text{Eq. 5 and 13})$$

$$= \frac{0.32673}{0.09059} \times 0.24065 \times \frac{759.98}{297.68} \times 0.35945$$

$$= 0.79649 \text{ ml.}$$

The specific surface area, S'_s , as calculated by the one-point method, is thus given by

$$\begin{aligned} S'_s &= \frac{V_{\text{Des(STP)}} \cdot S_o \cdot (P_o - P)}{W \cdot P_o}, \quad \dots \text{(Eq. 4)} \\ &= \frac{0.79649 \times 4.3775 \times 525.01}{0.39281 \times 791.0}, \\ &= 5.8914 \text{ m}^2/\text{g}. \end{aligned}$$

(c) Normalization of Peak-Area Weights Recorded at Different Sorptometer Attenuations

In rare cases, peaks for the same sample are recorded at two or more different attenuations. Thus, for the same sample, one peak may be recorded at an attenuation x_A and another may be recorded at an attenuation x_B ; A and B may have the following possible values: 1, 2, 4, 8, 16, 32, and 64 (an attenuation of x^1 resulting in the largest peak area).

Peak-area weights, Wt_{x_B} , obtained at an attenuation x_B , are normalized to peak-area weights of attenuation x_A by the equation:

$$Wt_{x_A} = Wt_{x_B} \cdot \frac{B}{A} \quad \dots \text{(Eq. 17)}$$

All the peak-area weights for a given sample must be normalized to a common attenuation in this manner, before specific surface areas can be calculated.

APPENDIX III

Computer Program for Calculating Specific Surface Areas from Sorptometer Data

(a) Description

The purpose of the program SORPT1, is to calculate the specific surface areas, S'_s , of powdered materials, whose surface areas were measured on the Perkin-Elmer, Model 212-D, Sorptometer, by the adsorption of nitrogen gas at liquid-nitrogen temperatures. The program uses the "one-point" method of evaluating the B. E. T. plot, in order to calculate the specific surface areas (see "The One-Point-Method", page 6, and Appendix II). SORPT1 was written in FORTRAN IV language. The user should provide a control-card deck compatible with his own system. The source of the data is from punched cards.

The title card, the peak cards, and the peak-index cards are read for a given sample and the array SSAREA (IK, IL) is defined from the peak-index values, KK, KL, JK, JL. With the use of this array, the specific surface areas are calculated for all possible combinations of adsorption, desorption, and calibration peak-area weights.

Readings of barometric pressure, P_B , are corrected to STP in the subroutine PBCERR. The values from Table 2, page 14, are used as data input for this subroutine. The subroutine uses a linear interpolation technique for evaluating the pressure corrections, $P_{B\text{corr}}$, from the observed barometric pressures, P_B .

The subroutine SMONO, evaluates the monolayer coverage, S_o , of 1 ml of nitrogen at the observed saturation pressure of nitrogen, P_o , using a linear interpolation technique similar to the one in the subroutine PBCERR. Table 3, page 16, is used as data for SMONO.

The input data, as well as the calculated results, are listed on the line printer. Input and output variables are given in the following sections: (b) Input Formats, and (c) Output. Details concerning the significance and the application of the variables in calculating the specific surface areas of the samples are given in the main body of the report.

(b) Input Formats

The input cards, which are described below, must be entered in the following order:

1. TITLE card.
2. PEAK cards.
3. NUMBER OF PEAKS card.
4. ADSORPTION/DESORPTION peak-index card.
5. CALIBRATION peak-index card.

1. TITLE card

FORMAT (A10, F5.3, F10.5, 2I3, 3A10, F5.1, F6.2, A5)

<u>Columns</u>	Specified punching or function of the field.
1-10	Sample identifier
11-15	Mol fraction of nitrogen in the adsorbate gas, α' .
16-25	Sample weight, W (g).
26-28	Total number of PEAK cards to be read.
29-31	End of data option; (0)/(1) continue to next statement/ go to 999 CALL EXIT.
32-41	Sample identification.
42-51	Source of original data in laboratory.
52-61	Date of completion of measurements.
62-66	Waterbath temperature, t_{TC} ($^{\circ}C$).
67-72	Detector current, I_{DC} (relative units, 0 to 10).
73-77	Attenuation xA (A=1, 2, 4, 8, 16, 32, or 64).
78-80	Blank.

2. PEAK card

<u>Columns</u>	FORMAT (A5, 3F8.5, 2I5, F5.1, F5.2, F5.1, F7.1, 5X, F8.5) Specific punching or function of the field
1-5	Peak identifier.
6-13	Calibration-peak weight, Cal_{wt} (g).
14-21	Adsorption-peak weight, A_{wt} (g).
22-29	Desorption-peak weight, D_{wt} (g).
30-34	Upper level of nitrogen manometer, Man_1 (mm Hg).
35-39	Lower level of nitrogen manometer, Man_2 (mm Hg).
40-44	Ambient temperature when using a centigrade thermometer, t ($^{\circ}C$).
45-49	Beckman thermometer reading for ambient temperature, R_{BN} .
50-54	Ambient temperature at time of barometric reading, t_B ($^{\circ}C$).
55-61	Barometric pressure, P_B (mm Hg).
62-66	Blank.
67-74	Calibration volume, $V_{Cal_{STP}}$ (ml).
75-80	Blank.

3. NUMBER OF PEAKS card

<u>Columns</u>	FORMAT (2I3) Specific function or punching of the field
1-3	Total number of adsorption and desorption peaks.
4-6	Total number of calibration peaks.
7-80	Blank.

4. ADSORPTION/DESORPTION peak index card

<u>Columns</u>	FORMAT (20I3) Indices for adsorption peaks.
1-3 to 58-60	

5. CALIBRATION peak index card

FORMAT (2013)

Columns

1-3 to
58-60 Sequential indices for calibration peaks.

(c) Output

The line-printer output lists both a summary of the input data as well as all variable values used in calculating the specific surface area of the sample. Some of the listing notation, which may not be self-evident, is given below:

RTC = the ambient temperature, $t^{\circ}\text{C}$, when measured with a Centigrade thermometer,
RBN = ambient temperature reading as measured with the Beckman thermometer,
RT = RTC or RBN after conversion to $^{\circ}\text{K}$,
TB = ambient temperature, t_{B} , at time of the barometric pressure measurement,
PRESS = the barometric pressure, P_{B} , (mm Hg),
CORR = barometric pressure correction, P_{Bcorr} , (mm Hg) necessary to bring P_{B} to STP,
PBC = corrected barometric pressure.
VCALRTP = the calibration-loop volume at ambient temperature,
STPWT = the calibration-peak area weight at STP,
VAD-DE/STP = the volume of nitrogen desorbed (or adsorbed) at STP,
SSAREA = the specific surface area.

PROGRAM SORPT1 (INPUT,OUTPUT,TAPE1=INPUT,TAPE3=OUTPUT)

C
C *****
C PROGRAM FOR CALCULATING THE SPECIFIC SURFACE AREA FROM SORPTOMETER
C DATA USING THE ONE-POINT METHOD FOR EVALUATING THE BET EQUATION
C *****

C
C DIMENSION TYPE(20),CALWGT(20),AWGT(20),DWGT(20),MAN1(20),MAN2(20),
C *RTC(20),RBN(20),TB(20),PB(20),PBCORR(20),SZERO(20),VLOOP(20),
C *RT(20),PBC(20),VCALRTP(20),PZERO(20),P(20),PDIFF(20),PDIV(20),
C *CALWGTX(20),VAISSTP(20,20),SSAREA(50,50),TYPEX(20),TYPEY(20),
C *IK(50),IL(50),STPWGT(20),JK(20),JL(20)

C
C DATA ICR/1/,LPT/3/,FRTP/2.78230/,FSTP/0.35945/,TEST/0.000001/,
C *FKELVIN/273.16/,CR/2.55/,CT/298.16/,C1/10./

C
C-----INPUT OF PARAMETERS
C 1 READ (ICR,100) SAMPLE,C,SWGT,N,KEOF,SERIES,PAGE,DATE,TC,DC,ATTN
C 100 FORMAT (A10,F5.3,F10.5,2I3,3A10,F5.1,F6.2,A5)
C IF (KEOF .EQ. 1) GO TO 999

C
C READ (ICR,120) (TYPE(K),CALWGT(K),AWGT(K),DWGT(K),MAN1(K),MAN2(K),
C *RTC(K),RBN(K),TB(K),PB(K),VLOOP(K),K=1,N)
C 120 FORMAT (A5,3F8.5,2I5,F5.1,F5.2,F5.1,F7.1,5X,F8.5)

C
C-----ARRAY DEFINITION FOR CALCULATING SPECIFIC SURFACE AREAS USING ALL
C POSSIBLE COMBINATIONS OF ADSORPTION,DESORPTION AND CALIBRATION
C PEAK-AREA WEIGHTS

C-----KK = THE TOTAL NUMBER OF ADSORPTION AND DESORPTION PEAKS

C-----KL = THE TOTAL NUMBER OF CALIBRATION PEAKS

C READ (ICR,121) KK,KL
C 121 FORMAT (2I3)

C
C-----JK ARE THE SEQUENCE NUMBERS FOR ADSORPTION AND DESORPTION PEAKS
C-----JL ARE THE SEQUENCE NUMBERS FOR CALIBRATION PEAKS

C READ (ICR,122) (JK(L),L=1,20)
C READ (ICR,122) (JL(L),L=1,20)
C 122 FORMAT (20I3)

C
C KG = KK*KL
C M = 0
C KM = 0
C DO 500 L=1,KK
C KM = KM + KL
C IF (M .GT. 1) GO TO 460
C 450 M = M + 1
C 460 IF (M - KM) 470,470,500
C 470 IK(M) = JK(L)
C GO TO 450
C 500 CONTINUE

C
C MM = 0
C DO 510 M = 1,KG
C 502 MM = MM + 1
C IF (MM - 5) 505,505,503

503 MM = 1
505 IL(M) = JL(MM)
510 CONTINUE

C

M = 0
TC1 = TEST/C1
DO 200 K = 1,N

C-----CORRECTION OF BAROMETRIC PRESSURE

CALL PBCERR (PB,TR,PBCORR,K)
PBC(K) = PB(K) - PBCORR(K)
P(K) = C*PBC(K)

C-----AMBIENT TEMPERATURE READINGS TO DEGREES KELVIN

IF (RTC(K) .GT. TEST) GO TO 125

C-----BECKMAN READINGS TO DEGREES KELVIN

RT(K) = (RRN(K) - CR) + CT
GO TO 130

C-----DEGREES CENTIGRADE TO DEGREES KELVIN

125 RT(K) = RTC(K) + FKELVIN
130 CONTINUE

C-----CALIBRATION

IF (VLOOP(K) .LT. TEST) GO TO 140

M = M + 1
PZERO(K) = TC1
PDIFF(K) = TC1
PDIV(K) = TC1
SZERO(K) = TC1
VCALRTP(M) = (VLOOP(K)*FRTP*RT(K))/PBC(K)
CALWGTX(M) = CALWGT(K)
STPWGT(M) = FSTP*CALWGT(K)*PBC(K)/RT(K)
TYPEX(M) = TYPE(K)
GO TO 150

140 CONTINUE

C

C-----EVALUATION OF MONOLAYER COVERAGE FROM PZERO

PZERO(K) = MAN1(K) - MAN2(K)
PDIFF(K) = PZERO(K) - P(K)
PDIV(K) = P(K)/PZERO(K)
CALL SMONO(PZERO,SZERO,K)

C

150 CONTINUE

200 CONTINUE

C

C

C-----CALCULATION OF SPECIFIC SURFACE AREAS

DO 350 K = 1,N
L = 1

IF (CALWGT(K) .GT. TEST) GO TO 290

TYPEY(K) = TYPE(K)

DO 300 L = 1,M

IF (AWGT(K) .GT. TEST) GO TO 260

VADSSTP(K,L) = (((DWGT(K)*VCALRTP(L))/CALWGTX(L))*FSTP*PBC(K))/RT(K)
GO TO 280

260 VADSSTP(K,L) = (((AWGT(K)*VCALRTP(L))/CALWGTX(L))*FSTP*PBC(K))/RT(K)

280 CONTINUE

SSAREA(K,L) = VADSSTP(K,L)*SZERO(K)*PDIFF(K)/(SWGT*PZERO(K))

300 CONTINUE
290 VADSSTP(K,L) = TC1
SSAREA(K,L) = TC1
350 CONTINUE

C
C-----OUTPUT
C

WRITE (LPT,800)
800 FORMAT (1H1, 43X, 49H
1***** * *****/33X, 65H **
1***** SORPTOMETER METHOD FOR SURFACE AREAS *****/
*44X,49H***** ONE POINT METHOD *****/)

C
WRITE (LPT,820) SAMPLE,SERIES,PAGE,SWGT,DATE
820 FORMAT (/2X,10H SAMPLE ,18X,10H SERIES ,20X,10H PAGES ,20X,
*10HSAMPLE WGT,20X,10H DATE , /2X,A10,18X,A10,20X,A10,20X,
*F9.5,21X,A10,/))

C
WRITE (LPT,840)C,FRTP,FSTP,CB,CT,TC,DC,ATTN
840 FORMAT (/2X,5HGAS =,F5.3,
*15H N2/HE FRTP =, F7.4,9H FSTP =,F7.5,7H CB =,F5.2,7H CT =
*,F7.2,7H TC =,F5.1,7H DC =,F6.2,9H ATTN =,A5,/))

C
WRITE (LPT,850)
850 FORMAT (1X,136HPEAK NO *** PEAK WEIGHTS *** N2 MANOME
*TER *** AMBIENT TEMP *** *** BAROMETRIC READI
*NGS *** CALIBRN,/3X,134HAND (CALWGT AWGT DWGT)
*(MAN1 MAN2) PZERO (RTC RBN RT) (TB PRES
*S CORR PRC) LOOP VOL,/ 2X,134HTYPE -G- -G-
* -G- -CM OF HG- -MM HG- -C- -B- -K-
* -C- - MM OF HG - -ML-,/)

C
WRITE (LPT,860) (TYPE(K),CALWGT(K),AWGT(K),DWGT(K),MAN1(K),MAN2(K)
*,PZERO(K),RTC(K),RBN(K),RT(K),TB(K),PB(K),PBCORR(K),PBC(K),
*VLOOP(K),K =1,N)
860 FORMAT (2X,A5,3F10.5,2I9,2F9.1,2F9.2,F9.1,3F9.2,F10.5)

C
WRITE (LPT,870)
870 FORMAT(/2X,43HTYPE P P0 - P P/P0 S0,/))

C
K = 1
880 IF(PDIFF(K) .LT. TEST) GO TO 920
WRITE (LPT,900) TYPE(K),P(K),PDIFF(K),PDIV(K),SZERO(K)
900 FORMAT (2X,A5,2F10.2,F10.5,F10.4)
920 K = K + 1
IF (K .GT. N) GO TO 921
GO TO 880
921 CONTINUE

C
WRITE (LPT,922) (TYPEX(L),L=1,M)
922 FORMAT(/25X,11A10,)

C
WRITE (LPT,925) (VCALRTP(L),L=1,M)
925 FORMAT(/10X,10HVCALRTP ,11F10.5,)

C


```
WRITE (LPT,927) (STPWGT(L),L=1,M)
927 FORMAT ( 10X,10HSTPWGT      ,11F10.5)
C
LL = 1
K = 1
930 IF (SSAREA(K,LL) .LT. TEST) GO TO 950
WRITE (LPT,940) (TYPEY(K), (VADSSTP(K,L),L=1,M))
940 FORMAT (2X,A5,3X,10HVAD-DE/STP,11F10.5)
C
WRITE (LPT,945) (SSAREA(K,L),L=1,M)
945 FORMAT (10X,10H# SSAREA #,11F10.5,)
C
950 K = K + 1
IF (K .GT. N) GO TO 960
GO TO 930
960 CONTINUE
C-----AVERAGE SURFACE AREAS
SUM = 0.
SUMADS = 0.
SUMDES = 0.
A = 0.
D = 0.
ADSAREA = 0.
DESAREA = 0.
DO 982 L=1,KG
SUM = SUM + SSAREA(IK(L),IL(L))
IF (DWGT(IK(L)) .GT. TEST) GO TO 981
SUMADS = SUMADS + SSAREA(IK(L),IL(L))
A = A + 1.
GO TO 982
981 SUMDES = SUMDES + SSAREA(IK(L),IL(L))
D = D + 1.
982 CONTINUE
G = KG
AREA = SUM/G
IF (A .LT. 1.) GO TO 971
ADSAREA = SUMADS/A
971 IF (D .LT. 1.) GO TO 975
DESAREA = SUMDES/D
975 CONTINUE
C
WRITE (LPT,983) ADSAREA,DESAREA
983 FORMAT (/,10X, 35H**** THE AVERAGE ADSORPTION AREA IS,F10.5,5H M2/
*G, /      10X,35 H**** THE AVERAGE DESORPTION AREA IS, F10.5, 5H M
*2/G, //)
C
WRITE (LPT,985) AREA
985 FORMAT (//34X,61H*****
1*****,/34X41H**** THE AVERAGE SPECIFIC SURFACE AREA IS,F10.
*5,10H M2/G ****,/34X,61H*****
1*****,)
C
WRITE (LPT,987) SAMPLE
987 FORMAT (1H1, //10X,47H***** THE SPECIFIC SURFACE AREA FOR SAMPLE NO
* ,A10,47H IS THE AVERAGE OF THE FOLLOWING SSAREAS *****,//5(7X,
```

```
*18H SSAREA (IK IL,)/)
C
WRITE (LPT,990) (SSAREA(IK(L),IL(L)),IK(L),IL(L),L=1,KG)
990 FORMAT (5(5X,F10.5,2I5))
C
GO TO 1
999 CALL EXIT
END

SUBROUTINE SMONO(PZERO,SZERO,K)
C
DIMENSION X(20),Y(20),PZERO(20),SZERO(20)
C
DATA (X(M),M=1,17)/740.,750.,760.,770.,780.,790.,800.,810.,820.,
*830.,840.,850.,860.,870.,880.,890.,900./
C
DATA (Y(M),M=1,17)/4.3685,4.3703,4.3721,4.3739,4.3756,4.3773,
*4.3790,4.3808,4.3826,4.3844,4.3862,4.3880,4.3898,4.3915,4.3932,
*4.3949,4.3966/
C
IF (PZERO(K) .LT. 740. .OR. PZERO(K) .GT. 900.) GO TO 198
C
C-----LINEAR INTERPOLATION FOR SZERO
J = 2
120 IF (PZERO(K)-X(J)) 180,160,140
140 J = J + 1
GO TO 120
160 SZERO(K) = Y(J)
GO TO 200
180 JMI = J - 1
SZERO(K) = Y(JMI) + (Y(J)-Y(JMI))/(X(J)-X(JMI))*(PZERO(K)-X(JMI))
GO TO 200
198 WRITE (LPT,199)
199 FORMAT (//10X,53H***** DATA OUT OF RANGE FOR SMONO INTERPOLATION *
1****,/)
200 RETURN
END
```

```
SUBROUTINE PBCERR (PB,TB,PBCORR,K)
DIMENSION PB(20),TB(20),PBCORR(20),X(10),Y(30,10)
```

C

```
DATA LPT/3/
DATA(X(IP),IP=1,7)/720.,730.,740.,750.,760.,770.,780./
```

C

```
DATA ((Y(IT,IP),IP=1,7),IT=15,30)/1.76,1.78,1.81,1.83,1.86,1.88,
*1.91,1.88,1.90,1.93,1.96,1.98,2.01,2.03,1.99,2.02,2.05,2.08,2.10,
*2.13,2.16,2.11,2.14,2.17,2.20,2.23,2.26,2.29,2.23,2.26,2.29,2.32,
*2.35,2.38,2.41,2.34,2.38,2.41,2.44,2.47,2.51,2.54,2.46,2.50,2.53,
*2.56,2.60,2.63,2.67,2.58,2.61,2.65,2.69,2.72,2.76,2.79,2.69,2.73,
*2.77,2.81,2.84,2.88,2.92,2.81,2.85,2.89,2.93,2.97,3.01,3.05,2.93,
*2.97,3.01,3.05,3.09,3.13,3.17,3.04,3.09,3.13,3.17,3.21,3.26,3.30,
*3.16,3.20,3.25,3.29,3.34,3.38,3.42,3.28,3.32,3.37,3.41,3.46,3.51,
*3.55,3.39,3.44,3.49,3.54,3.58,3.63,3.68,3.51,3.56,3.61,3.66,3.71,
*3.75,3.80/
```

C

```
C-----LINEAR INTERPOLATION FOR BAROMETRIC PRESSURE CORRECTION
IF(PB(K) .LT. 720. .OR. PB(K) .GT. 780. .OR. TB(K) .LT. 15. .OR.
*TB(K) .GT. 30.) GO TO 333
IT = TB(K)
J = 2
120 IF (PB(K) - X(J)) 180,160,140
140 J = J + 1
GO TO 120
160 PBCORR(K) = Y(IT,J)
GO TO 200
180 JM1 = J - 1
PBCOR1 = Y(IT,JM1)+(Y(IT,J)-Y(IT,JM1))/(X(J)-X(JM1))*(PB(K)-X(JM1)
*)
200 CONTINUE
```

C

```
ITMI = IT
IT = IT + 1
PBCOR2 = Y(IT,JM1)+(Y(IT,J)-Y(IT,JM1))/(X(J)-X(JM1))*(PB(K)-X(JM1)
*)
F = TB(K) - (ITMI)
PBCORR(K) = PBCOR1 + (PBCOR2 - PBCOR1)*F
```

C

```
GO TO 335
333 WRITE (LPT,334)
334 FORMAT (//10X, 54H***** DATA OUT OF RANGE FOR PBCORR INTERPOLATION
* *****,)
335 CONTINUE
RETURN
END
```

***** DATA DECK STRUCTURE *****

* TITLE CARD *

138870-2-1 .350 .39281 9 LAKEFIELD 14 NOV 17/71 26.0 0. X1

* PEAK CARDS *

1L1	.09059				2.09	23.5	762.9	.22080
2L2	.08956				2.05	23.5	762.9	.22720
3L12	.18187				2.07	23.5	762.9	.45100
4A		.32387		943 152	2.04	23.5	762.9	
5D			.32673	943 152	2.07	23.5	762.9	
6L12	.18228				2.07	23.5	762.9	.45100
7A		.32610		944 151	2.13	23.5	762.9	
8D			.32841	944 151	2.14	23.5	762.9	
9L12	.18134				2.14	23.5	762.9	.45100

* TOTAL NUMBER OF PEAKS CARD *

4 5

* ADSORPTION/DESORPTION PEAK INDEX CARD *

4 5 7 8

* CALIBRATION PEAK CARD *

1 2 3 4 5

* END OF FILE CARD *

***** SORPTOMETER METHOD FOR SURFACE AREAS *****
 ***** ONE POINT METHOD *****

SAMPLE 138870-2-1 SERIES LAKEFIELD PAGES 14 SAMPLE WGT .39281 DATE NOV 17/71

GAS = .350 N2/HE F RTP = 2.7823 FSTP = .35945 CB = 2.55 CT = 298.16 TC = 26.0 DC = 0.00 ATTN = X1

PEAK NO	***	PEAK WEIGHTS	***	N2 MANOMETER			***	AMBIENT TEMP			***	BAROMETRIC		READINGS	***	CALIBRN
AND	(CALWGT	AWGT	DWGT)	(MAN1	MAN2)	PZERO	(RTC	RBN	RT)	(TB	PRESS	READING	CORR	PBC)	LOOP VOL	
TYPE	-G-	-G-	-G-	-CM OF HG-	-MM HG-		-C-	-B-	-K-	-C-	- MM	OF	HG -	-	-ML-	
1L1	.09059	-0.00000	-0.00000	-0	-0	.0	-0.0	2.09	297.70	23.5	762.90	2.92	759.98	.22080		
2L2	.08956	-0.00000	-0.00000	-0	-0	.0	-0.0	2.05	297.66	23.5	762.90	2.92	759.98	.22720		
3L12	.18187	-0.00000	-0.00000	-0	-0	.0	-0.0	2.07	297.68	23.5	762.90	2.92	759.98	.45100		
4A	-0.00000	.32387	-0.00000	943	152	791.0	-0.0	2.04	297.65	23.5	762.90	2.92	759.98	-0.00000		
5D	-0.00000	-0.00000	.32673	943	152	791.0	-0.0	2.07	297.68	23.5	762.90	2.92	759.98	-0.00000		
6L12	.18228	-0.00000	-0.00000	-0	-0	.0	-0.0	2.07	297.68	23.5	762.90	2.92	759.98	.45100		
7A	-0.00000	.32610	-0.00000	944	151	793.0	-0.0	2.13	297.74	23.5	762.90	2.92	759.98	-0.00000		
8D	-0.00000	-0.00000	.32841	944	151	793.0	-0.0	2.14	297.75	23.5	762.90	2.92	759.98	-0.00000		
9L12	.18134	-0.00000	-0.00000	-0	-0	.0	-0.0	2.14	297.75	23.5	762.90	2.92	759.98	.45100		

TYPE	P	P0 - P	P/P0	S0
4A	265.99	525.01	.33628	4.3775
5D	265.99	525.01	.33628	4.3775
7A	265.99	527.01	.33543	4.3778
8D	265.99	527.01	.33543	4.3778

	1L1	2L2	3L12	6L12	9L12
VICALRTP	.24065	.24759	.49150	.49150	.49162
STPWGT	.08313	.08219	.16690	.16728	.16637
4A VAD-DE/STP	.78960	.82172	.80329	.80148	.80583
* SSAREA *	5.84027	6.07785	5.94156	5.92820	5.96033
5D VAD-DE/STP	.79649	.82889	.81030	.80848	.81286
* SSAREA *	5.89125	6.13091	5.99343	5.97995	6.01236
7A VAD-DE/STP	.79479	.82712	.80858	.80676	.81113
* SSAREA *	5.88668	6.12615	5.98877	5.97530	6.00769
8D VAD-DE/STP	.80040	.83296	.81428	.81245	.81685
* SSAREA *	5.92818	6.16934	6.03099	6.01743	6.05004

**** THE AVERAGE ADSORPTION AREA IS 5.97328 M2/G
 **** THE AVERAGE DESORPTION AREA IS 6.02039 M2/G

 **** THE AVERAGE SPECIFIC SURFACE AREA IS 5.99683 M2/G ****

***** THE SPECIFIC SURFACE AREA FOR SAMPLE NO 138870-2-1 IS THE AVERAGE OF THE FOLLOWING SSAREAS *****

SSAREA	IK	IL	SSAREA	IK	IL	SSAREA	IK	IL	SSAREA	IK	IL	SSAREA	IK	IL
5.84027	4	1	6.07785	4	2	5.94156	4	3	5.92820	4	4	5.96033	4	5
5.89125	5	1	6.13091	5	2	5.99343	5	3	5.97995	5	4	6.01236	5	5
5.88668	7	1	6.12615	7	2	5.98877	7	3	5.97530	7	4	6.00769	7	5
5.92818	8	1	6.16934	8	2	6.03099	8	3	6.01743	8	4	6.05004	8	5

