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USE OF A BBC MICROCOMPUTER FOR THE COLLECTION AND PROCESSING OF THERMAL ANALYSIS DATA

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ABSTRACT

The use of a BBC microcomputer for the collection, processing and display of thermal analysis data is described. Details of the interface between the thermal analysis equipment and the microcomputer are given. The facilities are exemplified by TG, DTG, and DTA results obtained for samples of the zeolitic mineral analcime.

INTRODUCTION

Microcomputers in the BBC series are fitted with a four channel analog to digital converter and are ideal for the collection and processing of thermal analysis data. The simple system now described is much cheaper than the purpose-built ones currently available, and is particularly suitable for older thermal analysis equipment for which commercial data collection and analysis facilities are not available. It allows weight losses and peak temperatures to be determined more accurately than is possible from graphical output, but its most useful facility is for base-line correction. In addition it provides for the thermal traces to be plotted and to be displayed on a VDU. The programs are written in BASIC and can be readily adapted to the users' requirements. As this is not a dedicated system the computer can be used for other purposes when the thermal analysis equipment is not in use.

INSTRUMENTATION

All BBC Model B microcomputers have sufficient memory to collect and process thermal analysis data, but the model B+ (as used here) or the Master series models are desirable if a high-resolution display of the curves and sufficient memory for data are required. In addition to the computer a monitor, disk drive, and printer are required; we use a Microvitec CU6

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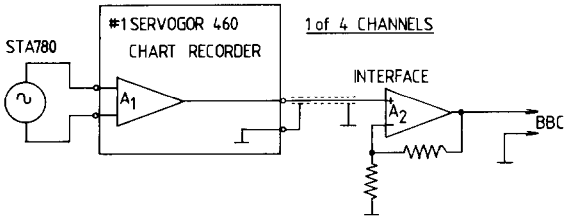

Fig. 1. General arrangement of interface. (A_1), Servogor chart recorder amplifier; this has a high impedance differential (floating) input and a ground-referenced output signal connector. (A_2), Interface amplifier and limit protection; see Fig. 2 for details.

monitor, a Cumana CD800 80 track dual double-sided disk drive and an EPSON MX80 printer. A plotter is desirable but not essential; the Linear Graphics Ltd A4M Plotmate has been found to be entirely suitable. The system should work well with most thermal analysis equipment; in our case a Stanton–Redcroft STA780 simultaneous thermal analyser is used. The problem in interfacing this and probably other thermal analysis equipment is that the output signals are not referenced to a common potential. However by using a recorder (e.g. Servogor 460) which can condition and retransmit the signals this problem can be circumvented. It is then only necessary to provide a simple interfacing circuit between the recorder outputs and the computer. The general arrangement is shown in Fig. 1 and the interfacing circuit is shown in Fig. 2.

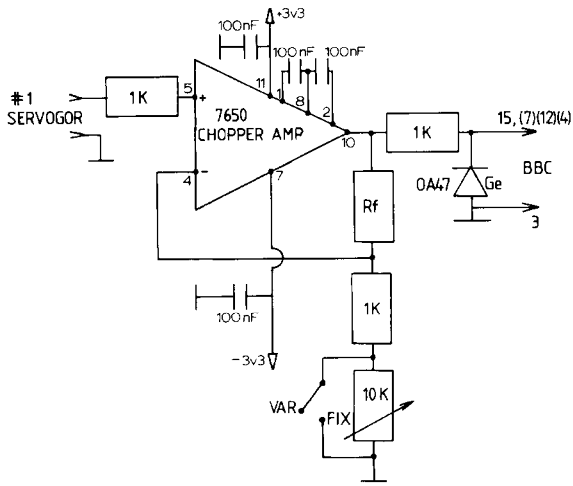

Fig. 2. Interface circuit. The ±3v3 supply and germanium diode ensure protection of BBC A/D convertor under all overload conditions. $R_f = 820R = +1v$ input = FSD on BBC A/D (@1v8 A/D reference).

SOFTWARE

With this simple system the software is used solely for data collection and subsequent processing, and not for control of the thermal analyser. The program suite is menu driven and consists of programs for data collection, base-line correction, numerical output, and graphical display.

Although the microcomputer samples all four output channels (T, TG, DTG, and DTA) ca. 60 times per second the available memory (Model B + in screen mode 135) limits the number of readings that can be recorded to 1000 per channel. The time intervals at which readings are recorded is determined by the temperature range and heating rate; for the range 0–900 °C and a heating rate of 10 °C per minute this interval is ~ 6 s. The values recorded are the average of all the readings (387) sampled over this time interval. With other temperature ranges and heating rates the time interval between readings is adjusted as appropriate.

Because the signals from the analog to digital converters drift with time, calibration facilities are provided and must be used before each run. Drifting during a run is negligible, providing the computer is permanently switched on or an adequate warm-up time is allowed. The zero values for each channel are set on the chart recorder in the normal manner, and the displayed temperature is adjusted to the actual sample temperature immediately after the calibration. Data collection is initiated when the preset starting temperature is reached, and all subsequent readings are stored. During data collection no graphical output is possible, but the current numerical value of each channel is continuously displayed.

All data processing is carried out after the run is completed. The temperatures are fitted to a polynomial in time (to allow for slight departures from the linear heating rate) and any excursions arising from thermal effects are

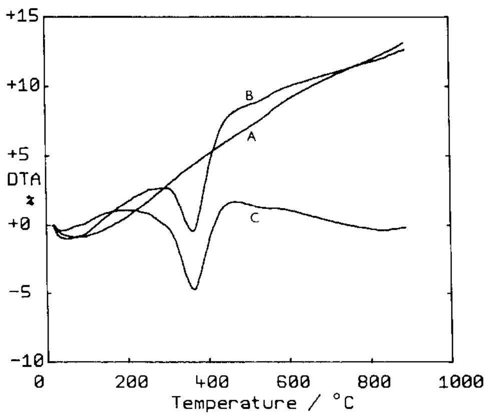

Fig. 3. Illustration of DTA baseline correction. (A), Baseline obtained with Al_2O_3; (B), uncorrected trace for analcime; (C), baseline corrected trace for analcime.

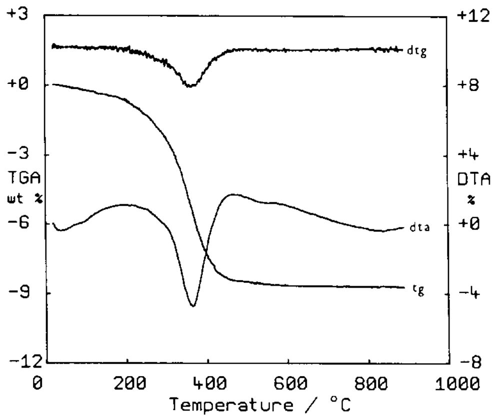

Fig. 4. Baseline corrected TG, DTG, and DTA traces obtained for a typical sample of analcime (Isle of Skye, Scotland).

eliminated. Base-line corrections are then applied to the TG, DTG and DTA signals using standard base lines obtained with thermally inert materials. New base lines are only required if changes are made to the experimental arrangements.

The base-line-corrected numerical data are stored on disk and can be listed on the printer or displayed graphically as a function of temperature either on the monitor or the plotter. The following displays are possible: (a) TG, DTG and DTA separately or together for any experimental run, (b) TG or DTG or DTA results for a series of experimental runs. Both can be shown for any chosen temperature range (abscissa) and the ordinates can be scaled as appropriate.

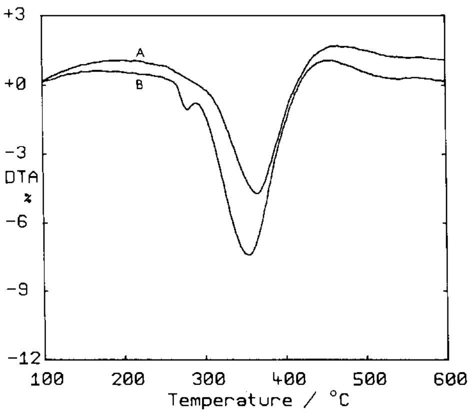

Fig. 5. DTA traces for: (A), a typical sodium rich analcime; (B), analcime from North Berwick (Scotland). The small additional endotherm in (B) indicates the presence of magnesium or calcium.

EXEMPLIFICATION

The various facilities are exemplified by typical results obtained for samples of the natural zeolite analcime. Figure 3 shows the effect of the base-line correction on the DTA trace. Figure 4 shows all three signals for a single analcime sample, and Table 1 gives numerical data in the region of

TABLE 1

Typical data collected for dehydration of analcime

Temperature (°C)	DTG (% deflection)	TGA (%wt. loss)	DTA (% deflection)
300.05	−0.69	−2.19	−0.16
310.33	−0.78	−2.58	−0.52
320.59	−1.01	−2.98	−1.14
330.82	−1.31	−3.40	−2.07
341.03	−1.67	−3.92	−3.14
351.21	−1.99	−4.53	−4.07
361.36	−2.03	−5.19	−4.65
371.49	−1.94	−5.86	−4.49
381.59	−1.61	−6.47	−3.52
391.67	−1.34	−6.98	−2.33
401.73	−1.06	−7.36	−1.17
411.77	−0.81	−7.70	−0.28
421.79	−0.42	−8.02	0.42
431.79	−0.36	−8.13	1.04
441.79	−0.21	−8.26	1.41
350.19	−1.75	−4.47	−3.99
351.21	−1.99	−4.53	−4.07
352.23	−1.91	−4.61	−4.16
353.24	−1.92	−4.65	−4.23
354.26	−1.99	−4.78	−4.30
355.28	−2.10	−4.83	−4.37
356.29	−2.07	−4.90	−4.40
357.31	−2.00	−4.95	−4.47
358.32	−1.97	−4.97	−4.53
359.34	−1.95	−5.08	−4.58
360.35	−2.03	−5.13	−4.65
361.36	−2.03	−5.19	−4.65
362.38	−2.10	−5.26	−4.67
363.39	−2.11	−5.33	−4.72
364.40	−2.07	−5.40	−4.71
365.42	−2.00	−5.43	−4.71
366.43	−1.97	−5.54	−4.71
367.44	−2.02	−5.60	−4.68
368.46	−1.97	−5.67	−4.66
369.47	−1.96	−5.72	−4.61
370.48	−2.00	−5.78	−4.57

the major dehydration event. Figure 5 shows the DTA traces for two different samples and illustrates the ease with which slight differences are detected.

The present system has been in operation for two years; no problems have been encountered, and a paper which includes data collected on the BBC microcomputer has been published [1].

Listings of the programs may be obtained from the authors.

REFERENCE

1 K.R. Franklin and B.M. Lowe, Zeolites, 7 (1987) 135.