Optically transparent carbon film electrodes for infrared spectroelectrochemistry

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Digital Data Acquisition from a Hilger-Watts H-1200 Infrared Spectrophotometer

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OBTAINING A DIGITAL RECORD of the output of an infrared spectrophotometer can be an expensive undertaking, depending upon the construction of the instrument. The Hilger-Watts H-1200 is an inexpensive grating infrared spectrophotometer (marketed by Wilks Scientific Corp., Norwalk, Conn., for about $3500), and commercially available digital data reduction systems for such an instrument would require more capital investment than the spectrophotometer. The interface designed by Gulf General Atomic for this instrument can be built at a cost of about $450 in components and about 70 hours of labor for construction, installation, and checkout. We have employed the system to record digital spectra using a cassette magnetic tape recorder. The interface can also be used to transmit data directly to the computer memory. Data are recorded and stored as 8-bit binary characters representing the ordinate every 2.5 cm^{-1} from 4000 to 2000 cm^{-1}, and every 0.5 cm^{-1} from 2000 to 650 cm^{-1} (because of scale change at 2000 cm^{-1}). The precision of the recorded spectra is thus better than the manufacturer's specifications for the instrument (10 cm^{-1} from 4000 to 2000 cm^{-1}; 2 cm^{-1} from 2000 to 650 cm^1; 1% transmittance photometric precision). The interface can be modified to expand or compress the presentation to as many as 33,000 points per spectrum, or as few as desired. Our spectra have 3300 points from 4000 to 650 cm^{-1}. There are zero and gain controls for scale expansion of the ordinate up to 10X. An analog output is provided for a separate recorder.

INTERFACE DESCRIPTION

The electronic circuitry for the interface between the Hilger-Watts H-1200 and a Mobark 305 cassette tape recorder is shown in Figure 1. The value of the ordinate of the Hilger-Watts H-1200 (the pen position on a transmittance scale) is determined from the servopot which is already connected to the pen servomotor. Using this servopot, a 0 to −10 V analog signal is presented to an 8-bit analog-to-digital converter (Burr-Brown No. ADC30-08N-USB, no buffer amplifier). The strobe pulse to the ADC is obtained in a unique but reliable fashion. There is a small DC motor on the Hilger-Watts H-1200 which rotates the grating and drives the chart recorder. This motor operates at a maximum of about 2000 rpm, and is geared down 488:1 at the working end. The rear end of the motor shaft is flush with the rear bearing surface, and this end of the shaft rotates at from 0 to 2000 rpm. One half of the rear end of the motor shaft was painted black, and a small light is directed onto the end of the shaft, with the reflected light directed into a small PIN photodiode. The light bulb and photodiode are held in an aluminum block, which is machined to fit on the end of the motor casing. A sine wave output is obtained from the PIN photodiode as the shaft rotates, and the positive-going signal is used to obtain a 5-V pulse from a Schmidt trigger. In the present arrangement, a divide-by-ten digital logic circuit is used to present this 5-V strobe pulse to the ADC once every 10 revolutions of the chart drive motor. The strobe signal is used to initiate the digitizing step of the ADC, and a data-ready pulse from the ADC is used to strobe the tape recorder for data acquisition. The ADC has a maximum 20-μsec conversion time, yet the interface/spectrophotometer arrangement we employ has a maximum data rate of only 3 points per second. Of course, by bypassing the divide-by-ten circuit, this rate can be expanded to 30 points per second. The cassette tape recorder presently being used has a maximum incremental speed of 120 8-bit characters per second. (The tape units are made by Mobark Instruments, Sunnyvale,

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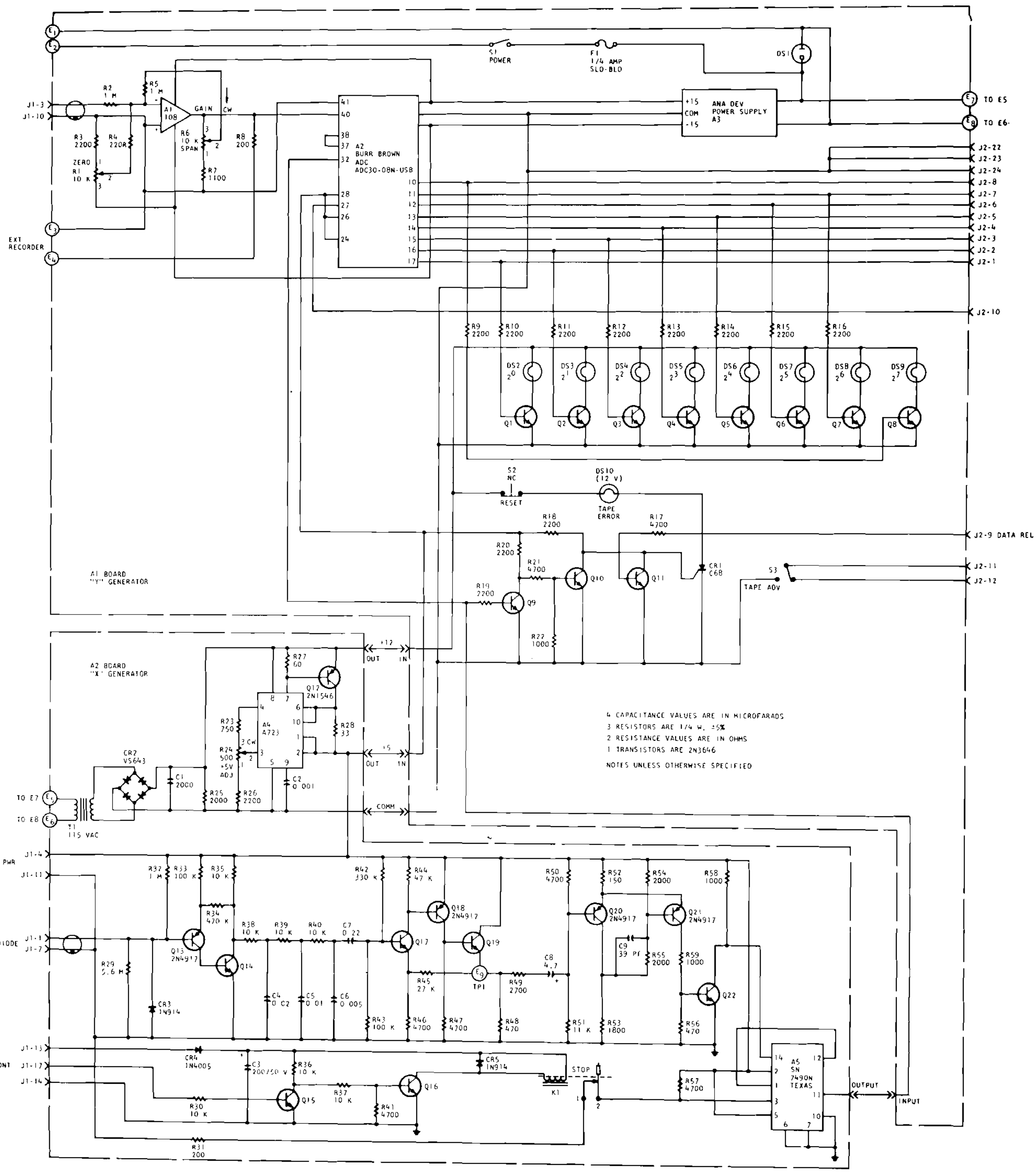

Figure 1. Schematic of digital data acquisition interface between Hilger-Watts H-1200 infrared spectrophotometer and Mobark 305 incremental cassette tape recorder

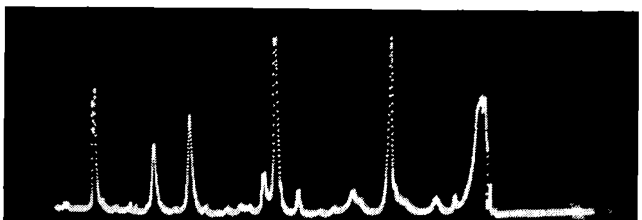

Figure 2. Photograph of visual display of last 4K core locations of XDS Sigma-2, showing digital benzene spectrum which has been inverted and converted from transmittance to absorbance

Calif.) It is possible to record up to 42 spectra on one 300-ft standard cassette tape, using 3300 characters per spectrum.

EXAMPLE OF RESULTS

The principal advantages of using such a digital data recording system are that it enables the user to smooth data, computer-average separate overlapping peaks analytically, compare spectra numerically, and generally take advantage of high-speed digital computing techniques to make the spectrophotometer a much more valuable laboratory tool. A transmission spectrum of benzene was run on the Hilger-

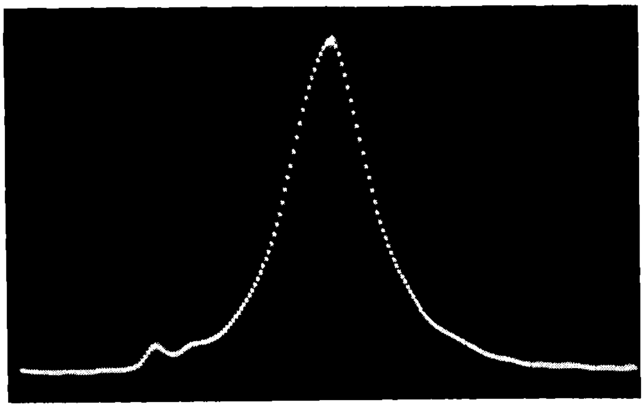

Figure 3. Portion of spectrum displayed in Figure 2, showing a single peak and illustrating the quality of the digital spectra obtained in this manner

Watts H-1200 and recorded simultaneously on the cassette tape recorder. This taped spectrum was then read directly into an XDS-Sigma 2 computer using a 300 character-per-second reproducer. The resultant spectrum, after the transmittance values had been converted to absorbance values, is shown in Figure 2. A five-point smooth, after Savitzky and Golay (*1*), was imposed on the raw data. A single peak (actually the second one from the left in Figure 2) from this smoothed spectrum is illustrated in Figure 3. Such peaks obviously can be readily integrated, either numerically or by curve-fitting approximations.

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(1) A. Savitzky and M. J. E. Golay, ANAL. CHEM., **36**, 1627 (1964)