VIII Euro-Asian Symposium «Trends in MAGnetism»

August 22–26, 2022, Kazan, Russia

Zavoisky Physical-Technical Institute FRC Kazan SC RAS

Euro-Asian Symposium «Trends in Magnetism»: EASTMAG-2022

Kazan, Russia, August 22-26, 2022

BOOK OF ABSTRACTS

VOLUME II

THE AUTOMATION OF THE SE/X-2544 EPR SPECTROMETER

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Electron paramagnetic resonance (EPR) spectrometers are used to record the EPR spectra of diverse substances in various states of aggregation: crystals, powders, liquids, and gases. The SE/X-2544 spectrometer by Radiopan (Poznan, Poland) [1] with an operating frequency of 9400 MHz (X-band) is designed to observe and record the first or second derivative of the EPR absorption signal in a wide microwave power range (up to 400 mW) at high-frequency (100 kHz) or low-frequency (80 Hz) modulation of the magnetic field, measuring the number of paramagnetic centers in the test substance, as well as performing temperature studies in a wide temperature range. The distribution geography of the SE/X-2544 EPR spectrometers in Russia is quite extensive. They are operated both in research institutes and national universities [2], such as the Institute of Organic and Physical Chemistry (Kazan), the Ufa Institute of Chemistry, the Institute of Problems of Chemical Physics (Chernogolovka), the Baltic Federal University (Kaliningrad), Institute of Physics (Krasnoyarsk).

This device is widely used in both physicochemical and biomedical research [3, 4]. To display EPR spectra, SE/X-2544 spectrometers are factory-equipped with a built-in plotter, which in practice is not exactly comfortable, especially when conducting a large amount of research. Automation of the measurement process with saving data in electronic form can significantly improve the ergonomics and productivity of scientific research.

Data exchange between an IBM-compatible computer and the spectrometer is carried out using a specialized controller (Fig. 1). The controller is connected to an LPT port operating in the Nibble Mode, in which five status lines are used to enter data into the computer: ERROR, SELECT, PAPER OUT, ACKNLG, BUSY [5]. In this case, the incoming bits occupy positions from D3 to D7 in the information word. Numeric values are calculated in several stages using shift, masking and accumulation operations.

The magnetic field is scanned using the "Field scan unit type CUP-202" block. The control code comes from the controller via a 12-bit bus. The magnetic field strength is measured with a nuclear magnetic resonance (NMR) magnetometer included in the SE/X-2544 EPR spectrometer. The induction value is reflected on the digital indicator of the NMR magnetometer block and transmitted to

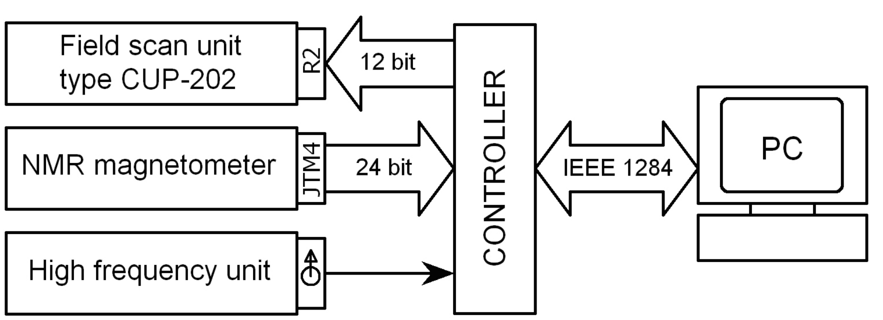

Figure 1. Scheme of data exchange between units of the SE/X-2544 EPR spectrometer and computer.

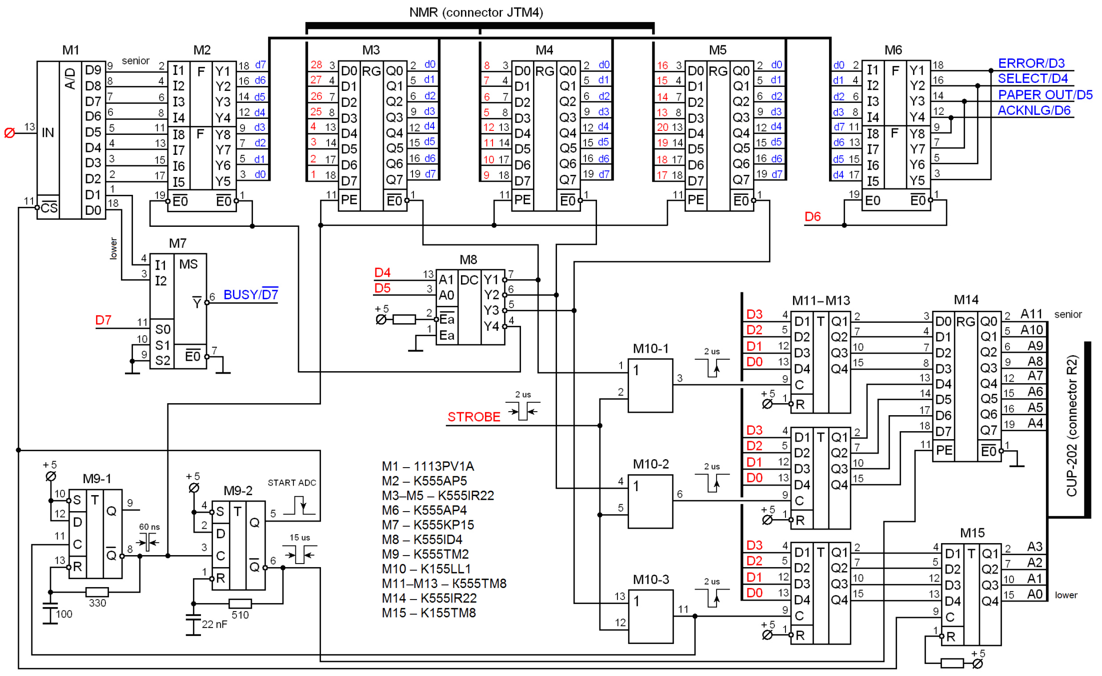

Figure 2. Schematic diagram of the controller.

the controller via a 24-bit bus. The controller also receives an analog signal from the block "High frequency unit", which carries information about the EPR spectrum. The controller is made of chips of high and medium degree of integration.

Schematic diagram of developed controller is shown in Fig. 2. The 8-bit data bus D0–D7 of the LPT port is used both to transfer the information necessary to ensure the sweep of the magnetic field, and to control the controller when data is entered into the computer. Lines D0–D3 are responsible for the transfer of nibbles of a 12-bit binary number to quad D flip-flops M11–M13. The information is recorded on the positive edge of the clock pulses, which are fed through the STROBE line and distributed in turn between D flip-flops using decoder M8 and 2-input OR gates M10-1, M10-2, M10-3.

A sync pulse from the output of M10-3 starts a single pulse generator based on the D-type flip-flop M9-1, which in turn starts the one-shot M9-2. The first single vibrator is responsible for writing the readings of a 6-digit NMR magnetic induction meter into registers M3–M5. The second one-shot provides simultaneous data transfer from D flip-flops M11–M13 to register M14 and D flip-flop M15 with subsequent fixation of information. The 12-bit binary code formed in this way is fed via the A0–A11 bus to the magnetic field scanner of the EPR spectrometer, where it controls electronic switches that switch the n-2n transformer windings in the field setter [1]. In addition, the single vibrator M9-2 puts the analog-to-digital converter (ADC) M1 into the conversion mode. The high-speed 1113PV1A-type ADC M1 converts the voltage supplied to its input into a 10-bit parallel binary code. The two least bits of the code are fed to the inputs of the multiplexer M7, and all other bits are fed to the inputs of the microchip M2, which contains two four-channel drivers.

Lines D4–D7 of the LPT-port data bus are designed to control the multiplexer M7 and decoder M8 and to activate one by one the 3-states outputs of two drivers in the M6, which are connected to the LPT-port status bus. In addition to distributing the strobe pulses, the decoder M8 switches the 3-states outputs of the microchips M2–M5 loaded on a common bus, which is connected to the inputs of the drivers of M6. The output of the multiplexer M7 is also connected to the BUSY line of the status bus. Such a circuitry solution makes it possible to transmit multi-bit numbers over buses with a limited number of lines.

The software is written in the DELPHI language. The magnetic field sweep is controlled both in one and in the opposite direction. Several different field scan speeds are available.

The work was supported by the Russian Science Foundation and the Krasnoyarsk Region Science and Technology Support Fund, grant No. 22-14-20020.

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