FRANK LABORATORY OF NEUTRON PHYSICS

In 2006, the FLNP scientific program was realized under five research themes of the JINR Plan for Scientific Research and International Scientific and Technical Cooperation (PSRISTC) and was aimed at obtaining new results in condensed matter physics (theme 07-4-1031-99/2008 «Neutron Investigations of Structure and Dynamics of Condensed Matter» headed by V. L. Aksenov and A. M. Balagurov) and neutron nuclear physics (theme 06-4-1036-2001/2007 «Nuclear Physics with Neutrons — Fundamental and Applied Investigations» headed by V. N. Shvetsov and Yu. N. Kopatch). To effect scientific research, work to develop, modernize, and construct the FLNP basic facilities, IBR-2 (theme 07-4-0851-87/2007 «Upgrade of the IBR-2 Complex» headed by V. D. Ananiev and E. P. Shabalin) and IREN (theme 06-4-0993-94/2006 «IREN Project» headed by V. N. Shvetsov, I. N. Meshkov and V. G. Pyataev) as well as the IBR-2 spectrometers complex (theme 07-4-1052-2004/2008 «Development and Creation of Elements of Neutron Spectrometers for Condensed Matter Investigations» headed by A. V. Belushkin and V. I. Prikhodko) continued.

The topical problems of investigations carried out in cooperation with the leading nuclear centers were considered at the XIV International Seminar on Interaction of Neutrons with Nuclei, the V Workshop on Investigations at the IBR-2 Reactor, the International Workshop on Crystallography at High Pressures and the International Workshop on Small-Angle Neutron Scattering.

CONDENSED MATTER PHYSICS

Main Scientific Results. In addition to the complex manganese oxides (manganites), whose main peculiarity is the effect of colossal magnetoresistance [1], growing interest is being shown in the complex cobalt oxides (cobaltites) of the $Ln_{1-x}M_xCoO_3$ type, where Ln — lanthanide, M — alkaline–earth element. From the scientific point of view, cobaltites are of interest due to strong correlations between lattice, charge, spin and orbital degrees of freedom. Cobalt oxides are important in practice since they are used as electrodes in current power supplies. The peculiarities of phase transitions in cobaltites are connected with the imbalance between the intra-atomic Hund energy and the energy of crystal field corresponding to the configuration of octahedrons of CoO_6. As a result, the Co^{3+} ion may be in three different spin states: low-spin (LS, $t_{2g}^6 e_g^0$), intermediate (IS, $t_{2g}^5 e_g^1$) and high-spin (HS, $t_{2g}^4 e_g^2$) state.

At the IBR-2 reactor the investigations of atomic and magnetic structure of cobaltites were carried out (including experiments at high external pressures) [2]. At the HRFD diffractometer the composition of $Pr_{0.5}Sr_{0.5}CoO_3$ was studied, in which several magneto-structural phase transitions had been observed earlier. The diffraction spectra were measured in a wide range of temperatures (10–780 K) mainly in the mode of sample heating. In this range two phase transitions ($T_1 \approx 120$ and $T_2 \approx 300$ K) have been detected, in the course of which magnetic and crystalline structures of the sample change. On heating the symmetry sequentially varies from triclinic to rhombic and then to rhombohedral one. The transitions are greatly spread over temperature, and between 120 and 300 K the phases coexist (Fig. 1). The magnetic measurements confirm that the structural transition at 300 K coincides with the Curie ferromagnetic point. The nature of the magnetic transition at 120 K remains unknown so far [3].

At the DN-12 diffractometer the investigation of the crystalline and magnetic structure of hexagonal frustrated manganites $RMnO_3$ (R = Y, Lu) was performed at high pressures of up to 6 GPa. The obtained ex-

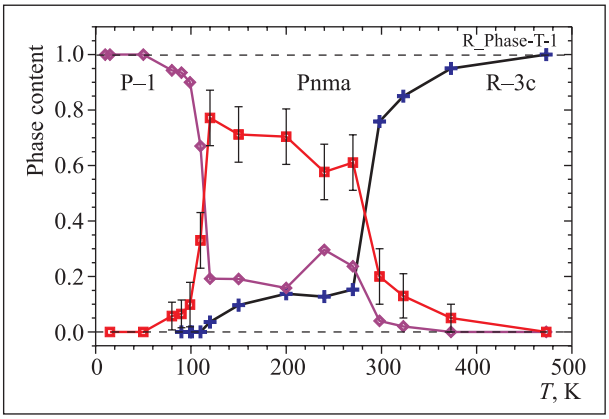

Fig. 1. Structural phase content in a sample versus temperature

perimental data, along with the results of the previous investigations of other hexagonal manganites, made it possible to relate the symmetry of triangular AFM state to the parameter of distortion of triangular lattice s formed by Mn and O atoms. The obtained generalized magnetic phase diagram allows one to explain the observed changes of the symmetry of magnetic state at chemical substitution (change in the ion radius R of the element) and on application of high pressure due to variation of s [4].

In the framework of structural investigations of the factors influencing the stabilization of ferrofluids a planned study of the effect of surfactant excess in ferrofluids on their stability started. As the first system, the classical ferrofluid based on magnetite, dispersed into benzene and covered by a single layer of oleic acid, was chosen. It is known that this system shows the most stability if the whole surfactant is adsorbed on a magnetite surface, i.e., in the absence of free surfactants in solution. In this connection, the solutions of oleic acid ($C_{17}H_{33}COOH$) in deuterated benzene (C_6D_6) were studied by small-angle neutron scattering. The aim of the study was to determine the character of interaction between molecules of the acid, and also to clarify the possibility of their clusterization. On the whole, scattering curves in the Guinier approximation point to the repulsion between the surfactant molecules. However, the value of the second virial coefficient $B = -0.02$ determined from these data is significantly larger than that for the system of hard spheres ($B = -8$). This suggests that the attraction component is essential in the pair potential of interaction between molecules. The volume of molecule of oleic acid, 657 Å^3, determined from the SANS data, differs considerably from its Van der Waals volume, 523 Å^3, and, at the same time, practically coincides with the specific volume of pure oleic acid in its liquid state. In order to clarify the given observation, the simulation of the studied system by molecular dynamics methods started [5].

At the REMUR spectrometer the investigation of the magnetic ordering and domain structure in the layers $20\times$[Fe(1.993 nm)/Cr(1.2 nm]/MgO was carried out. In this structure the magnetizations of neighboring iron layers are directed antiparallel. In the plane of layers there exist domains, which are also ordered antiferromagnetically. The type of interlayer ordering depends on the thickness of chromium layer. It was proposed to change the thickness of chromium layer by pressing and stretching it using a sound wave of megahertz range. The effects of change in diffused neutron scattering from the domain structure and of occurrence of inelastic neutron scattering due to the onset of oscillations of the magnetic moments of layers were observed in reflectometric experiments with polarized neutrons. The dependence of polarization ability on the Q_X component of momentum transfer (along the neutron beam) was determined at various values of the sound frequency $f_0 = 50$ MHz and $3f_0 = 150$ MHz. It was shown that it is possible to control the magnetic structure of the antiferromagnetic-ordered structure $20\times$[Fe(1.993 nm)/Cr(1.2 nm]/MgO by changing the level or frequency of the sound wave. This opens a new possibility to control the magnetic structure, which is characterized by a high speed of response [6].

At the DN-2 diffractometer the decay of hydrated clathrate with deuterium (composition $32D_2 : 136D_2O$) was studied at heating up to 250 K with the fixation of stages of its decomposition. Short-term (15 min) heating of the sample with the subsequent hardening down to the temperature of liquid nitrogen (95 K) made it possible to perform stepwise removal of hydrogen from clathrate pores at the same conditions of long-term exposition to study interaction of the matrix with the molecules of interstitial deuterium. It turned out that the lattice parameter under these conditions did not depend on the deuterium concentration, i.e., no signs of increase of its interaction with the lattice were shown. In order to solve the question on the nature of deuterium extraction, the intensities of individual reflexes were analyzed. Thus, the compositions of hydrides at annealing were determined graphically by imposing the column of experimental intensities on the calculated raster. The calculation of initial scattering by the Rietveld method gave the best agreement at the concentration of 32 molecules of D_2 per cell, where 16 molecules are in a large pore (8b, 2 mol. each) and 16 molecules — in a small pore (16c, 1 mol. each). After short-term (15 min) heating up to the temperature of 145 K changes in the clathrate structure are minimal. Gradual removal of hydrogen is possible up to the temperature of 195 K, when the growth of impurity phase of ice starts and the composition reaches the minimal value $x = 16_{8b} + 16 \cdot 0.7_{16c} = (27.2 \pm 0.5)D_2$. On warming up to 220 K the decomposition of clathrate along with the appearance of intensive lines of ice crystalline phases (Ih, Ic) with a noticeable portion of amorphous ice of low density are observed [7].

Complex investigations of physical properties of synthetic single-crystal quartz and quartz powder in a

temperature region of α–β transition were conducted by neutron diffraction and mechanical spectroscopy. The crystal structure of quartz powders with various average sizes of grains was determined in a temperature interval up to 620 °C and at a temperature of α–β phase transition. Temperature dependences of values of internal friction and resonance frequency in quartz samples were obtained in the vicinity of the phase transition temperature at the excitation of vibrations in the planes parallel and perpendicular to the Z axis of quartz. Different values of temperatures of the points of maximum of internal friction lying in the interval of 560–620 °C were registered. Possible reasons for the displacement of transition temperature were suggested. The maximum of internal friction, which is not associated with the structural transformations in quartz, was revealed in the vicinity of 350 °C. The aim of further studies is to find reasons for the displacement of the point of phase α–β transition in quartz and the nature of the internal friction peak at 350 °C.

At the inverted geometry spectrometer NERA the study of vibration spectra of hexane isomers was conducted accompanied by the calculations in the framework of the DFT method. Inelastic scattering spectra were measured for the isomers: 2- or 3-methyl-pentane and 2,2- or 2,3-dimethyl-butane with a general formula C_6H_{14}. Simultaneously, the diffraction spectra of these samples were measured, which allowed us to control the structure of solid phases. The DFT calculations of the structure and dynamics of molecules of the studied isomers were performed to interpret a low-frequency part of the internal vibration spectrum, which is clearly seen in the experimental spectra measured at a low temperature. Special interest in these calculations was aroused by the fact that the inelastic scattering spectra of diisopropyl measured in the glassy and crystalline phases differ from each other. The comparison of the calculated and measured spectra shows that internal vibrations in the orientation glass state correspond to the vibrations in a *gauche*-form of a molecule. This implies low potential barriers for internal rotations of molecular groups $CH(CH_3)_2$, which was also confirmed by the DFT calculations.

At the DIN-2PI spectrometer the investigation of atomic dynamics in superionic and non-superionic phases of AgCuSe was carried out for the first time using the slow neutron scattering technique. The analysis of the dynamic structural factor $S(Q,\omega)$ points to the presence of low-energy modes in the energy region of 3–4 MeV in the ordered state of AgCuSe, which presumably correspond to acoustic phonon modes. A correlation was established between the transition of AgCuSe into the superionic state and the changes in the dynamics of crystalline lattice involving an abrupt change in spectra of the dynamic structural factor, generalized density of phonon states, thermodynamic properties. An increase in thermal oscillation amplitude, a change in heat capacity at the transition into the superionic state are indicative of considerable softening of the phonon spectrum in α-AgCuSe. The phonon state density $G(\varepsilon)$ in α- and β-AgCuSe is characterized by the non-Debye behavior in the low-energy region and by two pronounced maxima at $\varepsilon \sim 10$ and 20 meV. The reason for $G(\varepsilon)$ deviation from the Debye dependence is the presence of low-energy excitation mode. At the transition from β to α phase the smearing of maxima is observed at $\varepsilon \sim 10$ and 20 meV, as a result of a change of many factors in the atomic dynamics of the studied system.

NEUTRON NUCLEAR PHYSICS

Experimental Investigations. In 2006, the FLNP investigation program in neutron nuclear physics included traditional directions of fundamental and applied research carried out on the IBR-2 and EG-5 beams and in collaboration with nuclear centers in Russia, Bulgaria, Poland, the Czech Republic, Germany, Republic of Korea, France, USA, and Japan.

In 2006, the manufacturing of the full-scale facility to measure the cross section of neutron–neutron scattering on the YAGUAR reactor was completed. The first calibration measurements on rare gases with the well-known cross sections were carried out. The cross section of thermal neutron scattering by ^{4}He measured at a constant reactor power was (0.87 ± 0.13) b (tabulated value — 0.760 b). However, during the measurements in a pulsed mode it was found that the detector was subjected to overloads due to a high level of γ-background from the reactor. The works to optimize the protection system of the detector and to modernize its electronics aimed at decreasing the recovery time in case of overloads are under way [8].

The data from the experiment carried out at the reactor in ILL (Grenoble) to observe a change in the neutron energy at passing through accelerated matter were processed. The existence of the effect follows from the validity of the equivalence principle and detailed neutron-optical calculations. A change in the neutron energy detected in the experiment was of the order of $2 \cdot 10^{-10}$ eV. The sample — a silicon plate, was moving with alternating acceleration reaching the value of 7.5 g. The corresponding change in neutron energy was detected by the UCN spectrometer with interference filters in phase with the sample motion. The obtained results undoubtedly give evidence to the existence of this effect for the first time observed in an experiment. The value of the effect corresponds to theoretical predictions with

an accuracy of the order of 15%. It has been realized that although the effect of accelerated matter had been observed only in the neutron-optical experiment so far, it is of quite universal nature and should also exist for particles of different nature [9].

The experiment aimed at checking the efficiency of control over the polarization of thermal and epithermal neutrons using a radio-frequency field was carried out on beam H8 of the KENS pulsed neutron source (KEK, Japan). The polarization of neutrons and analysis of their polarization were performed by the devices on the basis of polarized ^{3}He with optical pumping developed by the KEK–FLNP JINR collaboration in 2003–2005. The experimental results agree well with the calculations and have demonstrated high efficiency of the proposed method. The developed technique will be used to control neutron polarization in the experiment to verify T-invariance in interaction of polarized neutrons with polarized nuclei. The experiment is planned to be carried out on the JSNS source, which is under construction at present [10].

In the framework of experiments to search for neutral currents in nucleon–nucleon interactions and to determine weak π-meson coupling constant, in collaboration with PNPI, ILL and TU Munich on beam PF1B of cold polarized neutrons (ILL, Grenoble), a «zero» experiment was performed to determine the background asymmetry for a series of measurements of P-odd asymmetry in the reaction $^6\mathrm{Li}(n,\alpha)^3\mathrm{H}$. The value of $\alpha_0 = (0.0 \pm 0.5) \cdot 10^{-8}$ was obtained. The comparison of this result with the result of the main experiment $\alpha_t = -(8.6 \pm 2.0) \cdot 10^{-8}$ shows that the observed effect is determined by P-odd asymmetry of tritons from the reaction $^6\mathrm{Li}(n,\alpha)^3\mathrm{H}$. The aim of investigations is to determine the weak π-meson coupling constant f_π corresponding to the interaction of neutral currents in nucleon–nucleon processes. From the obtained data follow the limitations on the value of weak π-meson coupling constant $f_\pi = (0.4 \pm 0.4) \cdot 10^{-7}$ on the assumption that other constants are equal to theoretical «best values» and $-1.2 \cdot 10^{-7} \leqslant f_\pi \leqslant 1.6 \cdot 10^{-7}$ taking into account theoretical and experimental uncertainties of other constants [11].

Within the collaboration Jyväskylä–Darmstadt–Dubna–Gatchina in JYFL (Finland) a series of experiments to study fission using two mosaics of semiconductor detectors was carried out. In the first experiment angular, and mass–energy correlations of fission fragments in the reaction $^{238}\mathrm{U} + {}^4\mathrm{He}$ (40 MeV) were investigated. The angular resolution of the facility made possible a direct search for the ternary collinear decay events. The preliminary analysis of the obtained data has not revealed such events. A number of other effects, which could give indirect evidence to the existence of exotic fission modes, was discovered. In the second experiment, a precision measurement of energy distributions of α-particles and nuclei of ^{6}He emitted in the process of ^{252}Cf ternary spontaneous fission, was performed. A significant deviation of spectra from the Gaussian shape was observed in a low-energy region. At the same time, it was shown that consideration of precise form of energy spectrum significantly affects the determination of yields of light charged particles in ternary fission [12, 13].

In the framework of collaboration with ISR RAS the specialists from FLNP and LRB performed calculations of angular dependence of efficiency of the Lunar Exploration Neutron Detector (LEND) (one of the instruments of the NASA Lunar Reconnaissance Orbiter 2008) intended to map the flux of neutrons from the lunar surface to search for evidence of water ice and provide measurements of the space radiation environment which can be useful for future human exploration. Also, experimental calibrations of the laboratory prototype of the instrument were carried out.

Applied Investigations. In the framework of the International Program «Atmospheric Heavy Metal Deposition in Europe — Estimations Based on Moss Analysis» a series of works that involved simultaneous collection of samples in 2005–2006 in a number of regions in Central Russia, Southern Urals, Belarus, Bulgaria, Slovakia, Poland, Romania, Serbia, Macedonia, Croatia and Greece for multielement activation analysis at the IBR-2 reactor were completed. The results of the analysis on 13 elements: Al, As, Cd, Cr, Cu, Fe, Hg, Ni, Pb, Sb, Ti, V and Zn will be submitted to the European Atlas of Atmospheric Heavy Metal Deposition. Similar studies were carried out in Mongolia and Vietnam. The results of the analysis of moss-biomonitors from biosphere reserves (Prioksko-Terrasny and Voronezh biosphere reserves) obtained in collaboration with the Institute of Global Climate and ecology (Moscow) are of particular interest [14].

NEUTRON SOURCES

The IBR-2 Pulsed Reactor. In the year 2006, the IBR-2 reactor operated in accordance with the approved schedule ($\sim$ 2050 h for physical experiments).

The main results of IBR-2 modernization in 2006:

1. The main task of the year — manufacturing of fuel assemblies (FA) for the IBR-2M reactor — has been successfully fulfilled. In July the license for manufacturing FA in JINR was obtained, and on 12.07.2006 the first FA was made in the presence of a special commission. On 16.11.2006 the work was completed: 89 FA were manufactured, which provided an initial charge of the new reactor (63 FA) and burn up margin

($\sim$ 40%). The FLNP specialists have performed the work with a high quality.

2. In JINR EW: The manufacturing of rolling shielding was completed, its check assembly and tests were carried out. The control systems of the reactor were manufactured (emergency system units, compensating regulators, manual regulator).

3. Safety Control System (SCS) of IBR-2M: The prototype model of ASCS (SNIIP-SYSTEMATOM) was manufactured and tested at the IBR-2 reactor. In SNIIP-SYSTEMATOM the work on standard ASCS (including a new control panel) was started. In INEUM the work to develop CM system was continued. In JINR EW a prototype model of KO drive was manufactured, work on a prototype model of emergency shutdown system drive is in progress.

4. Moderator complex for IBR-2M: In December 2006, the following work is to be completed: manufacturing of CHF-700/15 in «Heliymash»; detail design of moderators for 3 directions: beams 2–3, beams 4–6, beams 7–11 (NIKIET); engineering design of moderators (SSDI); detail design of cryogenic pipeline and intermediate heat exchanger (Heliymash). In FLNP the calculations and experimental work on transportation of C_9H_{12} pellets were performed; design documentation on pellet generator was worked out.

5. «The program of works at the IBR-2 reactor during temporary shutdown (2007–2010)» as well as the schedule of works on modernization of IBR-2 in this period were developed, agreed upon and approved.

As of 01.12.2006 the expenses on IBR-2 modernization amounted to about 900 k$ (JINR — 550 k$, Rosatom — 350 k$).

The IREN Project. The main tasks of the Frank Laboratory of Neutron Physics and the Laboratory of Particle Physics in 2006 were the completion of disassembling of the IBR-30 reactor and assembling of the available equipment of the first stage of the LUE-200 linac.

1. Decommissioning of IBR-30. In accordance with the approved working schedule of the decommissioning the following works were carried out: «Report on Nuclear and Radiation Safety Assessment of the Research Pulsed Reactor IBR-30 in 2005» was prepared and submitted to Rostekhnadzor of RF. All the equipment from the reactor hall except for beam shutters, which would be used for the first stage of IREN, was dismantled and moved to building 117/b. All rooms of building 43 adjacent to the reactor hall were cleared. The inspection and repair of the entrance door of the reactor hall were performed. The decontamination and preparation of the reactor hall to repair were carried out.

2. Works on the LUE-200 linac. The theoretical substantiation of the possibility to obtain required parameters of an electron beam at the first stage of the linac was completed. The MK1 klystron modulator was assembled at the regular place and adjusted. The modulator and pulsed transformer for the electron gun were mounted at the regular place. Test assembling of the SHF-path of the first section was carried out. Power frame of the vacuum pump system of the LUE-200 first section was completed. The test assembling was carried out. Test assembling and certification of the buncher coil were carried out. In building 43 the focusing solenoid of the first accelerating section was mounted with geodetic tie. The electron gun was assembled at the regular place. By the end of the year, the pipeline laying-out of the water supply for the water-cooling and thermostabilization system of LUE-200 is to be completed.

DEVELOPMENT AND CREATION OF ELEMENTS OF NEUTRON SPECTROMETERS FOR CONDENSED MATTER INVESTIGATIONS

In 2006, in the framework of the theme work was focused on the following main activities: creation of gas and scintillation neutron detectors; development of sample environment systems and development of data acquisition systems and computing infrastructure.

Gas Detectors. In 2006, at the HRFD diffractometer and the REFLEX spectrometer 1-D position-sensitive detectors based on multiwire proportional chambers were put into operation. The software for acquisition and accumulation of data from these detectors is integrated into the control software package Sonix.

Two-dimensional PSD was developed with the following characteristics:

Gas mixture	2000 mbar $He^3 + 2000$ mbar CF_4
Efficiency, %	60
Sensitive area, mm	225×225
Coordinate resolution X, Y, mm	2–3
Count rate, events/s	Up to 10^6
Differential nonlinearity, %	< 10
Read-out	Delay lines, start from anode

The design and engineering documentation of the detector case, anode and cathode electrodes was worked out. All mechanical units were manufactured in JINR EW.

Electronics and software of the microstrip detector were debugged and its tests were conducted on an IBR-2 beam.

Scintillation Detectors. The 4th and 3rd sections of the FSD diffractometer were designed.

The design of the detector system for the DN-6 diffractometer was developed. It has provision for using 2 groups of detectors located in the region of scattering angle of 90 ° and scattering angle of 45 °.

In cooperation with the Institute of Metal Physics RAS (Yekaterinburg) 100-channel scintillation thermal neutron detector for the D7A spectrometer located at the IVV-2M reactor of Sverdlovsk branch of NIKIET was developed, manufactured and put into operation. The detector is constructed on the modular principle, which makes it possible to arrange channel sensitive areas on a cylindrical surface of arbitrary radius.

Development of Sample Environment Systems. In 2006, a device for placing a scatterer into a neutron beam in front of PSD of a spectrometer was included into the structure of control system of spectrometer actuators.

Controller SMC-32-CAN for control systems of spectrometer actuators was developed and tested.

On beam 9 the modernization of the chopper control system was carried out on the basis of direct-current electric drive. More stable amplifiers of the electric drive were included into the structure of the system. The control system software was renewed.

In 2006, a closed-cycle cryostat with cryocooler PT-405 with pulse tubes was manufactured for operation in a temperature range of 8–300 K. Its construction allows it to be installed in the shaft of the DN-2 spectrometer. The cryostat was used to obtain spectra of scattered neutrons from mesitylene, which is considered to be the most promising material for cold moderators of the modernized reactor IBR-2M.

Development of Data Acquisition Systems and Computing Infrastructure. A new central server *Sun Fire X4200* (AMD-64 platform) with the operating system *OS Solaris 2.10* and bulk storage device *Storage Array* (6.4 Tbyte) were put into service. The replacement of the basic server of the FLNP computer cluster (*Enterprize 3000*) by the modern system on the basis of AMD Opteron 64 and the use of bulk storage device made it possible to significantly enhance computing power of the cluster and to increase the shared disk space. At present, the former central server is used for work with applications written for the old operating system.

The first stage of work to create a new architecture of the FLNP computer cluster and to optimize network communication lines was fulfilled. A change-over of the available switches of the central network core to routing switches Cisco 3750, the installation of 1 Gbit/s interface to switch Cisco 8510 CSR and the application of high-speed communication in the main FLNP LAN links made it possible to enhance the reliability of network operation and to provide connection with the JINR network and other networks at Gigabit rates. Reorganization of the FLNP Web server was carried as well.

A large amount of work to design and manufacture electronic blocks of data acquisition systems, as well as to develop and support control software package Sonix + for IBR-2 spectrometers was carried out.

Electronic and software support was constantly provided during the IBR-2 reactor cycles.

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