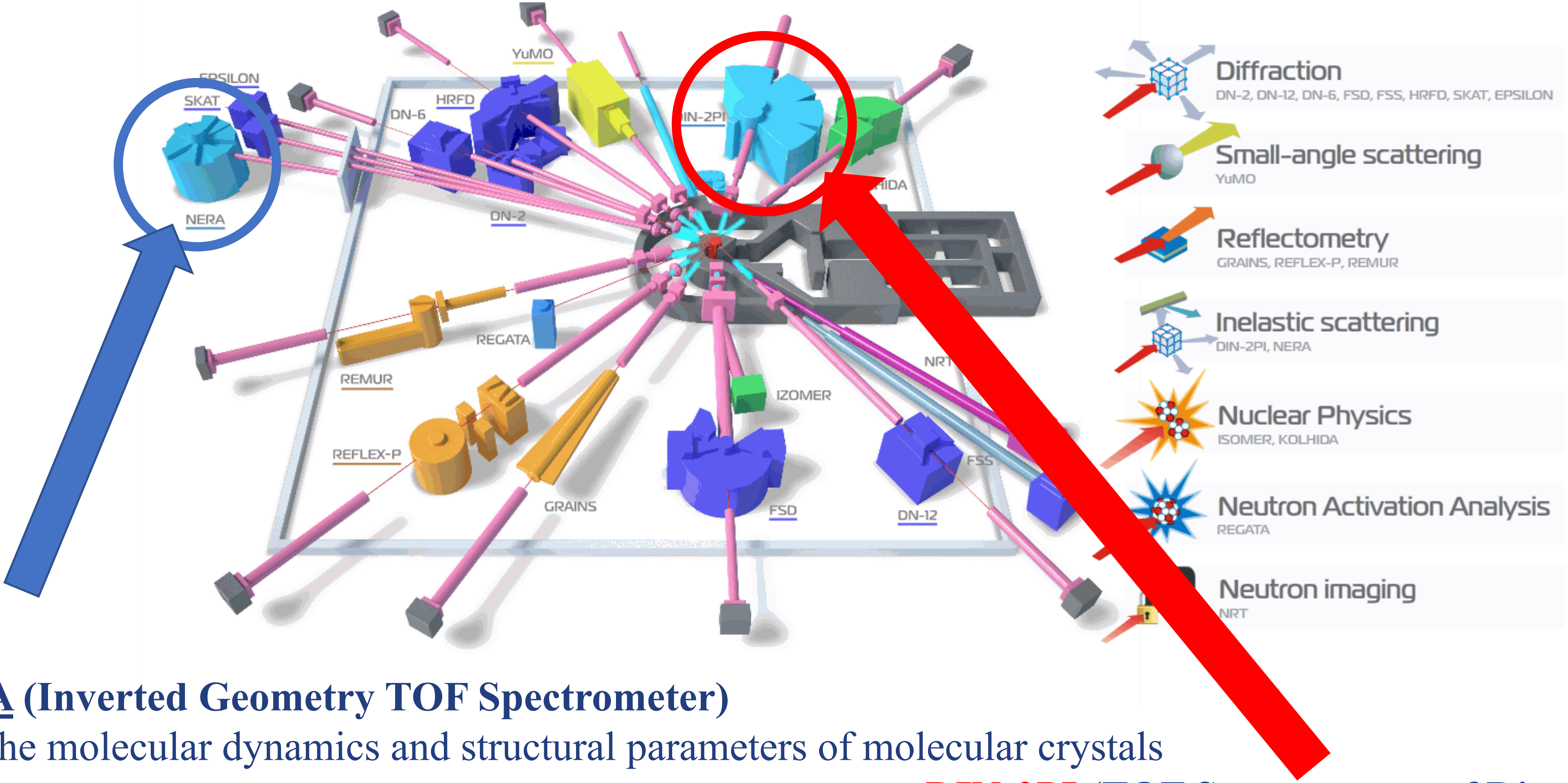
Inelastic neutron scattering at IBR-2 reactor: current state and further prospects

D.M. Chudoba

PAC CM, Dubna 17-18.06.2019



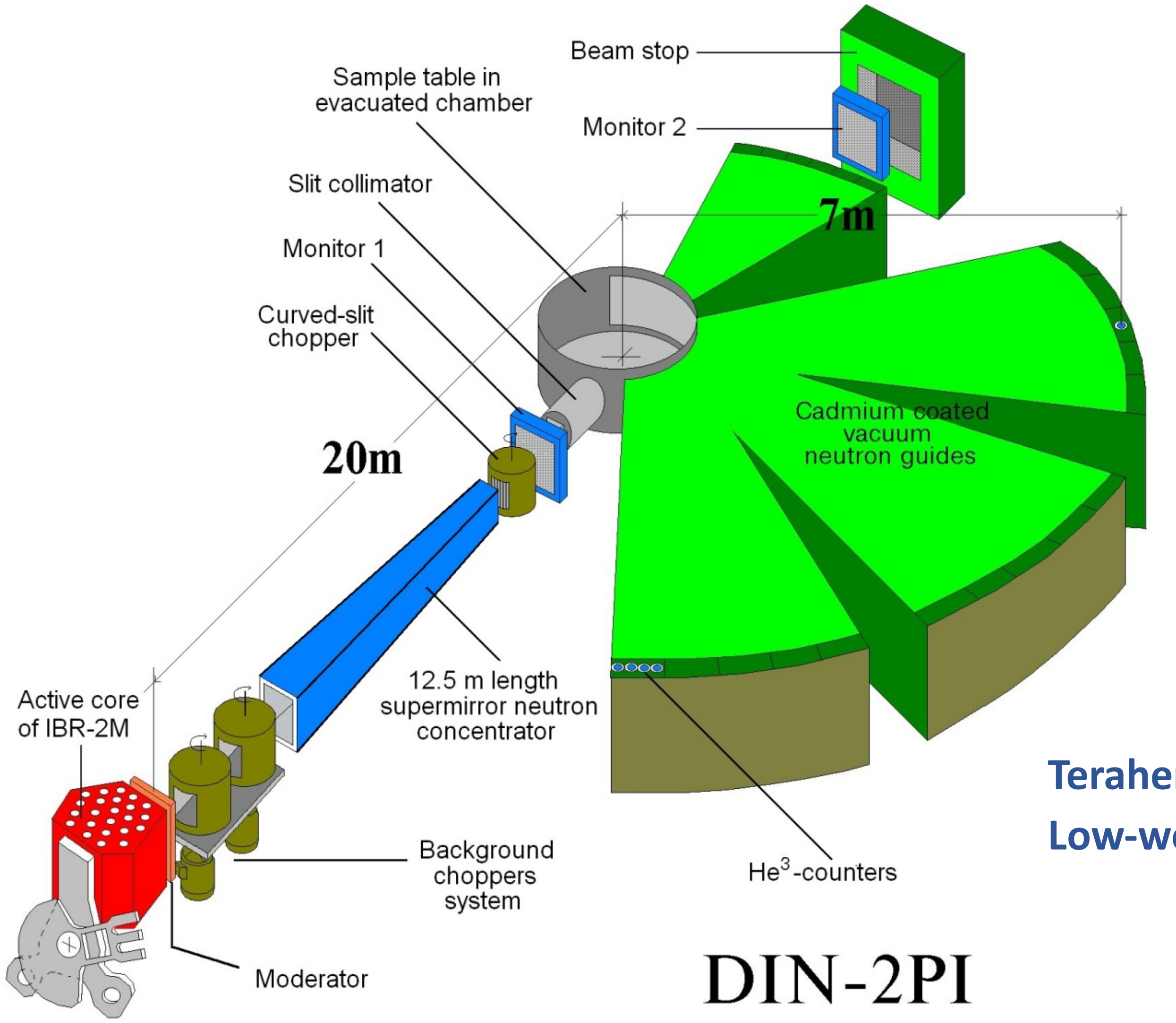
- **NERA (Inverted Geometry TOF Spectrometer)**

study of the molecular dynamics and structural parameters of molecular crystals

- **DIN-2PI (TOF Spectrometer of Direct Geometry)**

study of the lattice and atomic dynamics of liquids and amorphous materials

Time-of-flight spectrometer of direct geometry



DIN-2PI

Scattering angles	5° – 135°
Dimensions of the beam on the sample, mm^2	160 × 120
Neutron flux at the sample for E_0 = 10 meV, n/cm^2s	$1.5 \cdot 10^3$
The range of primary energies (meV)	1 – 30
The energy resolution $\Delta E_0/E_0$, %	4 – 10

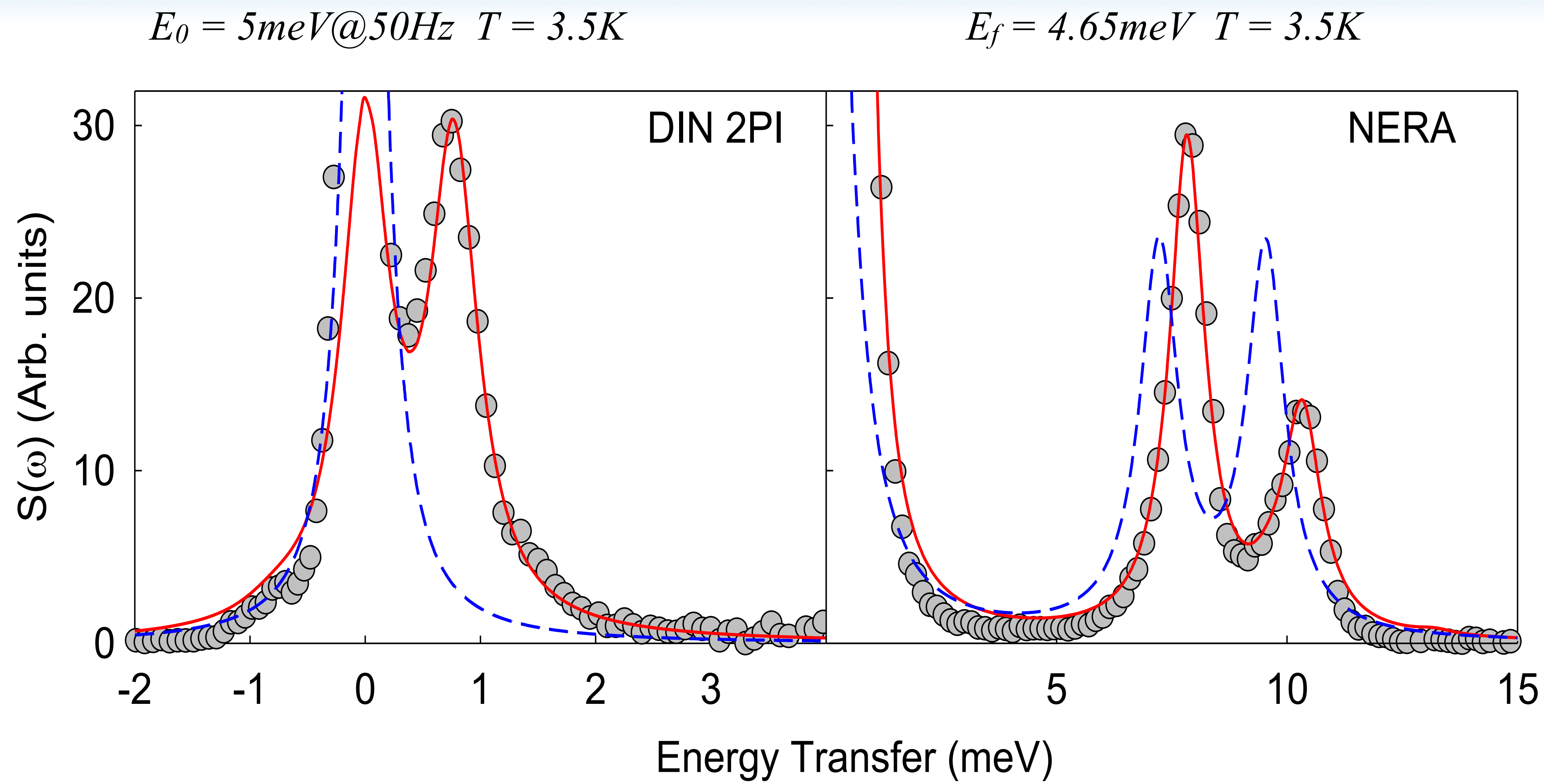
The investigation of lattice dynamics Ag2Te and Ag2S by inelastic neutron scattering

Superatoms in lattice dynamics of RAl_2 intermetallic systems.

Terahertz Neutron Spectroscopy of Molecular Crystals with DIN-2PI: Low-weight Hydrogen-Bonded Solids

И.В. Калинин, В.М. Морозов, А.Г. Новиков, А.В. Пучков, В.В. Савостин, В.В. Сударев, А.П. Булкин, С.И. Калинин, В.М. Пусенков, В.А. Ульянов
"Характеристики спектрометра ДИН-2ПИ с нейтронным концентратором"
Журнал технической физики, ***2014***, *том 84, вып. 2*

Crystal field effects in $Ho^{11}B_{12}$

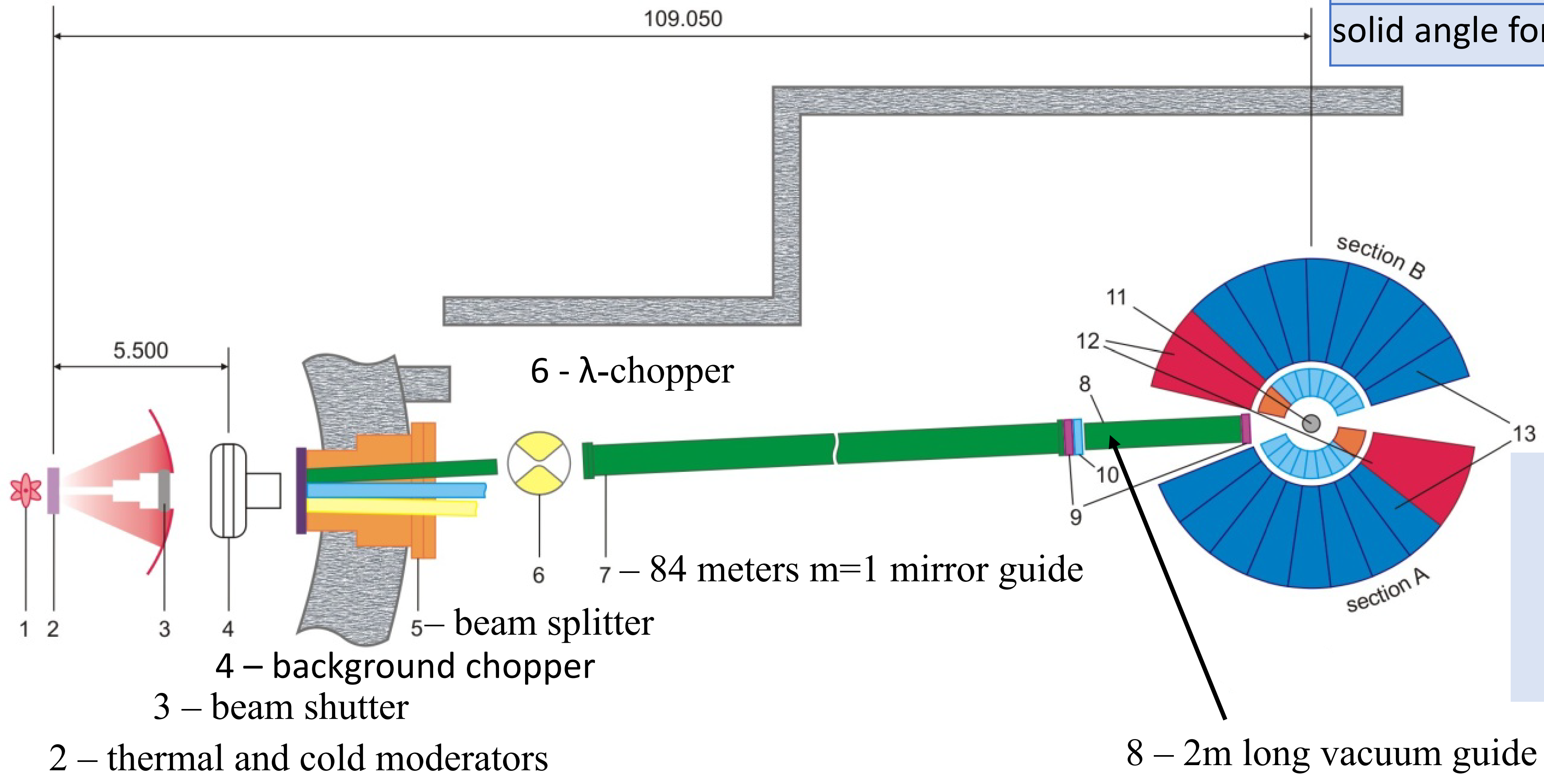


$Ho^{11}B_{12}$ scattering law (grey circles) measured at DIN 2PI and NERA spectrometers at 3.5K.
The initial energy at DIN 2PI spectrometer was 5meV and final energy at NERA 4.85meV.
Solid red line is the S(ω) calculated with the crystal field model including mean field and blue dashed line is expected spectrum without magnetic order *i.e.* crystal field only.

NERA - Time-of-flight spectrometer of direct geometry:

primary spectrometer

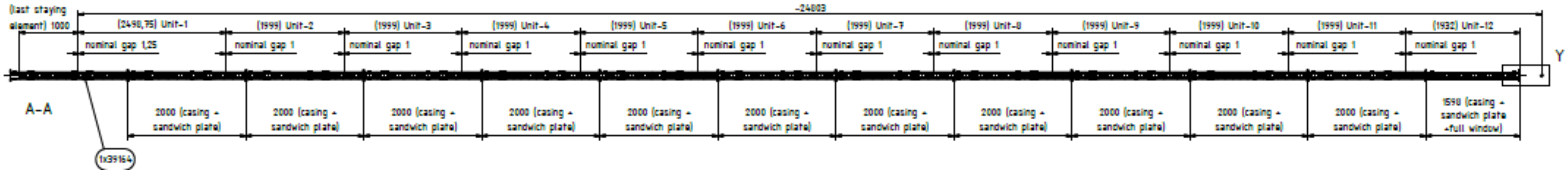
Energy transfer range (INS)	1-130 meV
solid angle for INS	~ 0.2 sr



Average neutron flux:
- at splitter
5.8×10^7 n/cm^{2}s
- at sample position
$3{,}5 \cdot 10^6$ n/cm^{2}s

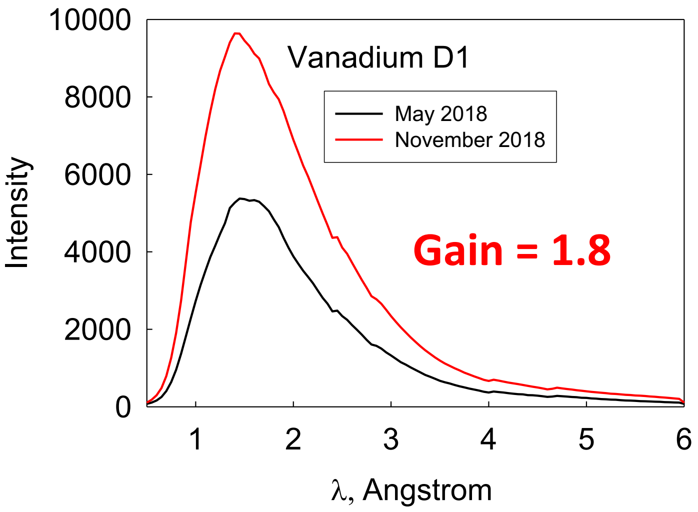
NERA primary spectrometer upgrade

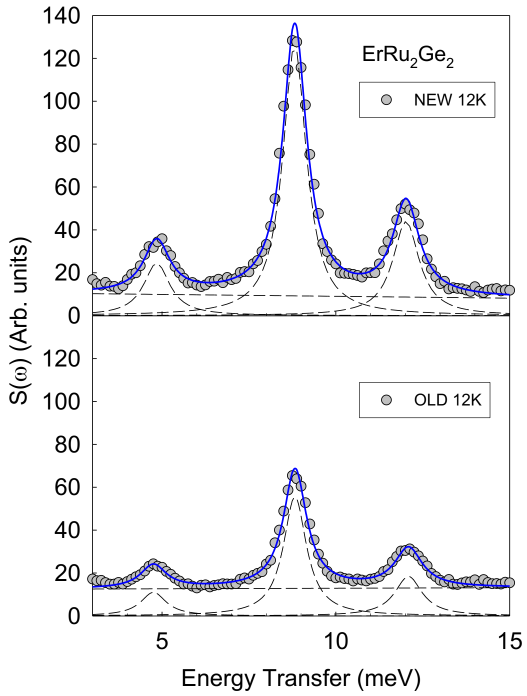
autumn 2018



24.8 m of the old m=1 neutron guide was replaced with parabolic vertically tapered supermirror guide
entrance beam size – 160x50mm: exit beam size 50x50mm

Units 1–7 m = 2
Units 8–10 m = 3 $m_{effective} = 5$
Units 11–12 m = 5





MAY / JUNE: **NEW DETECTORS**
TEST: 10.2019

slightly oversubscribed

2016	2017	2018
20	13	18
PL/RU/RO	PL/RU/DE	PL/BU/RU/DE

Hydrogen bonded molecular complexes formed by maleic acid with methyl-derivatives of pyrazine in solid state.

The inelastic neutron scattering study of variation of the ground-state multiplet of Tm3+ ions in Tm2Fe17 induced by the spin reorientation phase tran

IINS study of glass-forming single-phenyl alcohols 2TFP, 3TFP, 4TFP

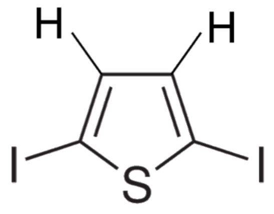
Vibrational dynamics studies of glass-forming in soft matter compounds with one phenyl ring

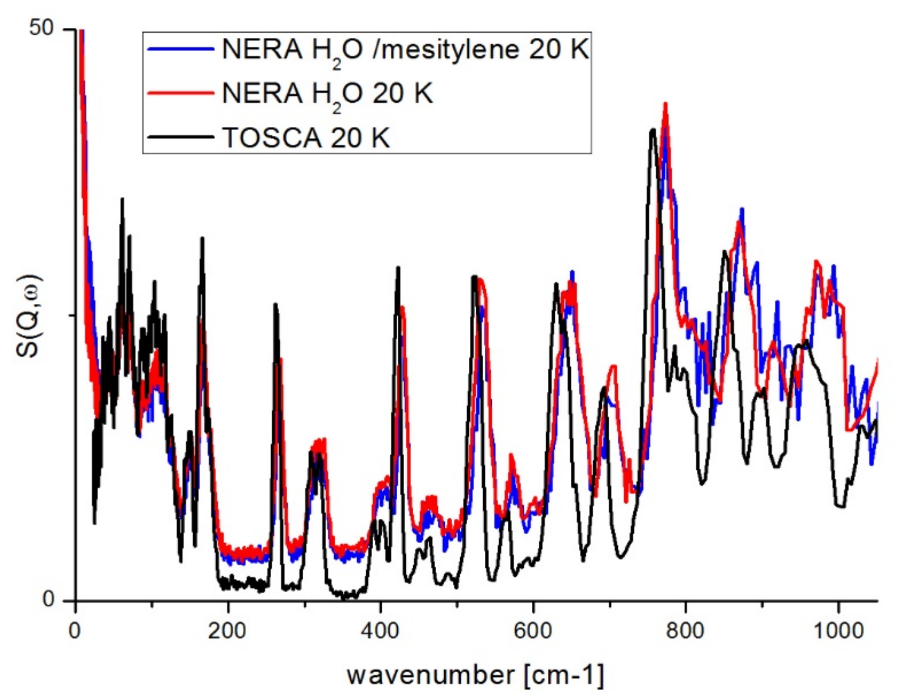
Neutron scattering study of pyridinium chlorochromate under pressure

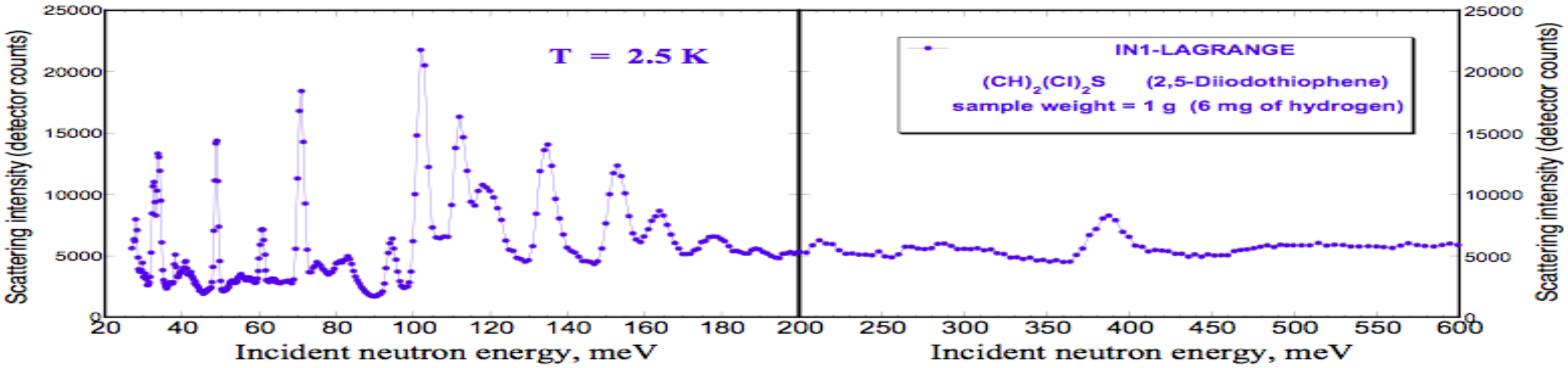
Local Structure of Ionic Liquids Explored with Incoherent Inelastic Neutron Scattering

Microscopic picture of Li - ion transportation in plastic crystals – rotation-translation coupling

2,5 diiodothiophene
$(CH)_2(CI)_2S$







m_H = 6mg,

4 hours (2+2 each panel) for raw scans

courtesy of A.Ivanov

SUMMARY

	DIN-2PI	NERA
pros	- relatively good resolution ~4% at E_i<5 meV - good angular coverage range 5º – 135º	- wide energy transfer range - reasonable energy resolution - simultaneous ND and INS measurements
cons	- low luminosity due to lack of cold moderator - obsolete detector system	- low luminosity and therefore need for large samples or long counting time - high background, highly likely due to delayed neutrons

Possible improvements in inelastic scattering experiments with direct geometry INS instruments at IBR 2:

- Cold moderator (bispectral)
- 100m supermirror neutron guide (will extend E_i range up to 150 meV)
- New secondary spectrometer (chopper system + large solid angle PSD)

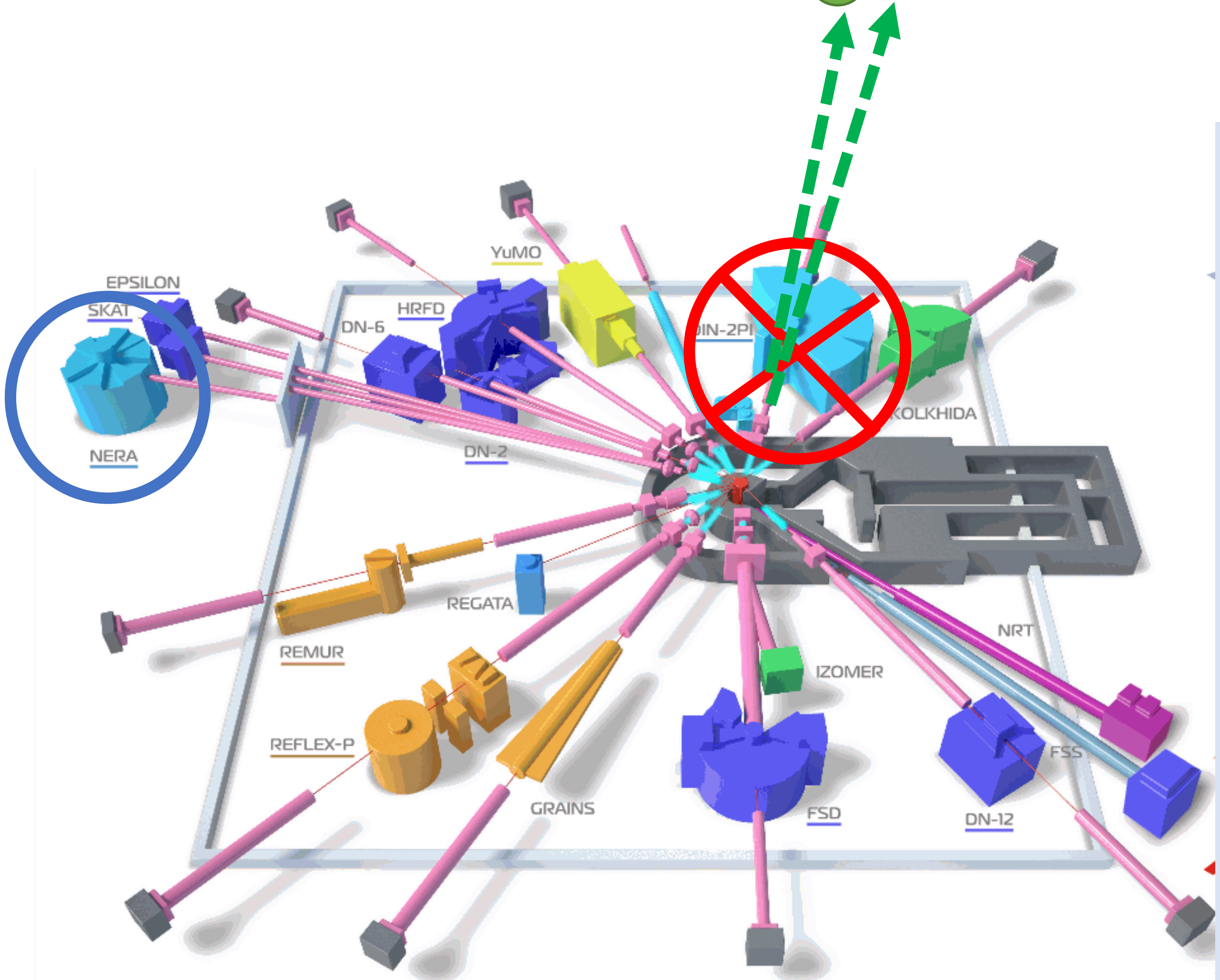
Possible improvements in inelastic scattering experiments with inverse geometry INS instruments at IBR 2:

- New beam splitter + new supermirror neutron guide from the beginning + new cascade of choppers
- New secondary spectrometer with large solid angle (current one is nearly 30 years old with solid angle ~ 0.2 sr)

MODERNIZATION OF SPECTROMETER OR CONSTRUCTION OF A NEW ONE(S) FROM SCRATCH

- Most of the above mentioned issues, and the increase of luminosity / acceptance of the instrument in particular **requires a complete redesign of the machine**, meaning, in practice, **building a new one** within the given boundary conditions.
- Building of new instruments at a new neutron guide tube - cheaper and easier.
- Modernization of NERA means a long-term disruption to the operation of SKAT and EPSILON instruments that share the same housing and the guide tube.

1) inverse geometry INS instrument 1 2 **2) direct geometry INS instrument**



A workhorse, high throughput inverse geometry instrument of large acceptance analyser matrix, with as broad dynamic range as possible.

MC simulations and conceptual design work now underway.

Research areas – inverse geometry

BROAD ENERGY TRANSFER RANGE SPECTROSCOPY

Efficient hydrogen storage requires intensive work on metal hydrides and like materials. The study of AlH_3 needs both high resolution low-energy transfer spectroscopy and that far beyond upper limit currently available on NERA.

Hydrogen bonds in molecular matter (vibrational analysis). This requires access to higher wavenumbers than currently achievable on NERA.

Complex rare earth – transition metal oxides (polymorphism, involving geometrically frustrated magnetism, order – disorder transitions). Require INS spectroscopy beyond the range that NERA can offer.

REAL TIME INS SPECTROSCOPY

New materials for high-efficiency batteries.
Neutron scattering on a high-luminosity INS spectrometer can sched light on the changes to this material as the battery is being discharged in real time.

Research areas – direct geometry

Excitations in unconventional superconductors

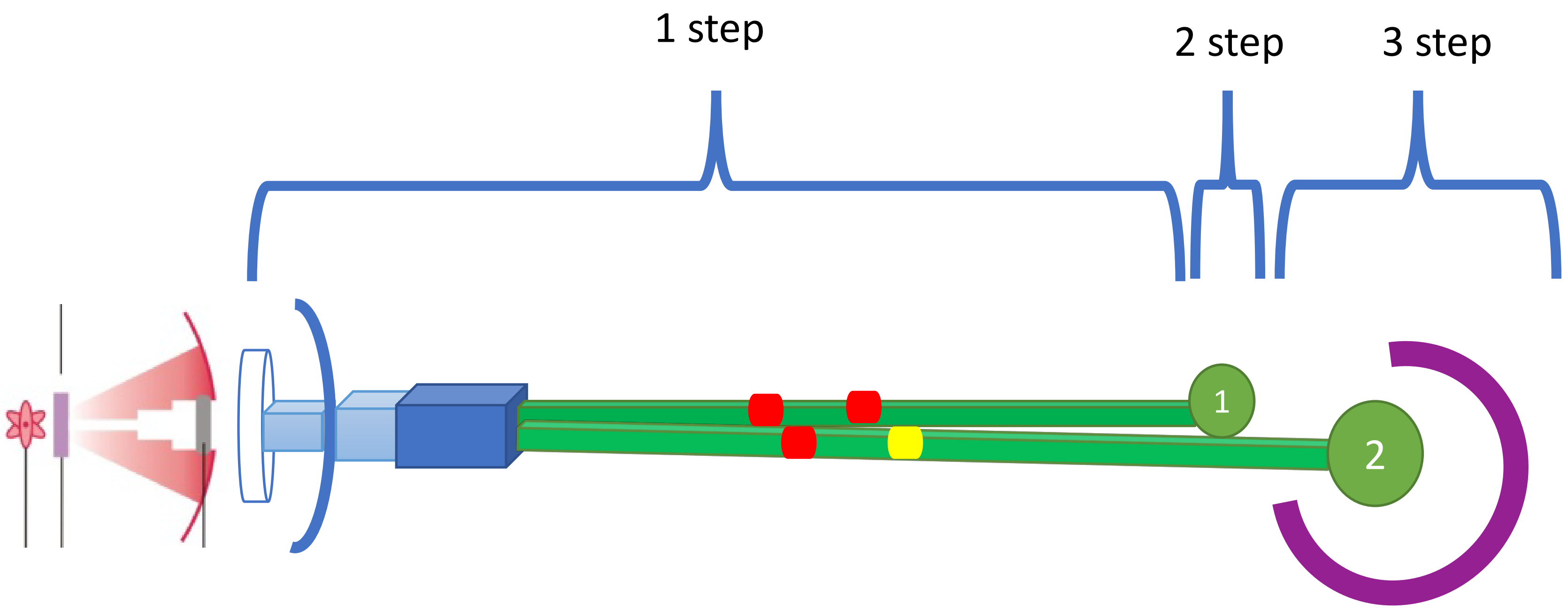
Excitations in frustrated magnets

Spin dynamics of low dimensional magnets/quantum magnets

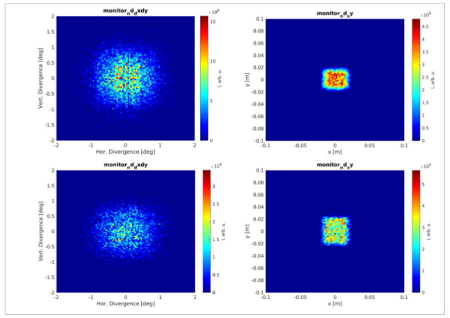
Spin dynamics of strongly correlated electron systems (heavy fermions, mixed valence etc)

Atomic and magnetic dynamics of functional materials, including catalysis metals, ion-transport materials, fuel cell membranes, nanomaterials, thermo-electric and magneto-caloric materials

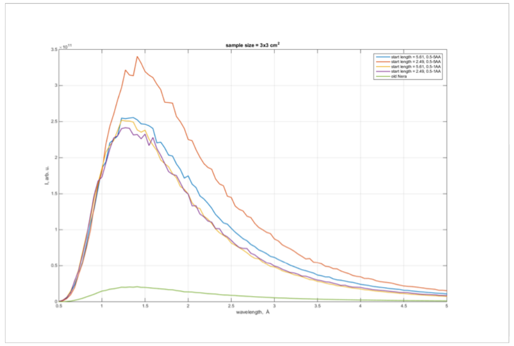
Neutron guides/splitter/choppers/ → Inverse geometry INS instrument → Direct geometry INS instrument



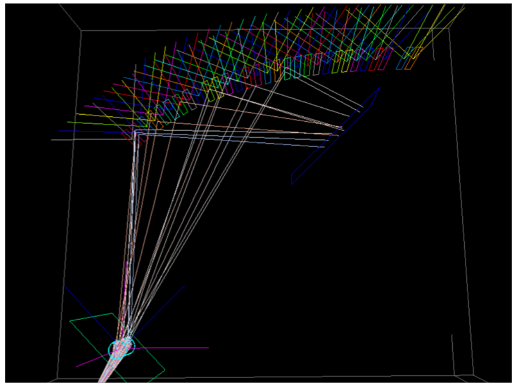
Inverse geometry INS instrument



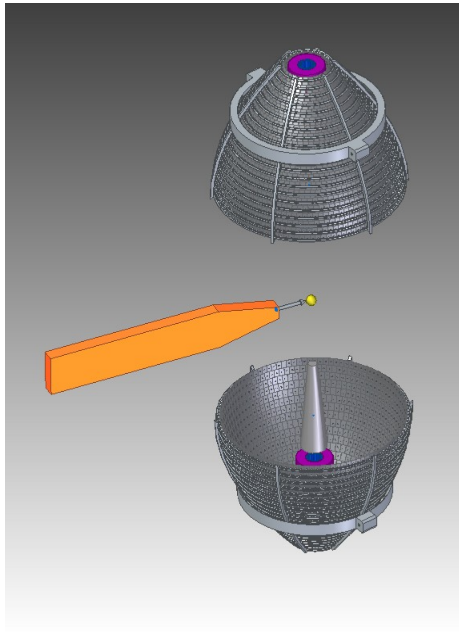
MC simulations (MacStas) of optics



MC simulations (MacStas) of secondary spectrometer



Conceptual design



	<u>Proposed</u> Project Schedule for inverse geometry INS instrument	**2019**	**2020**	**2021**	**2022**	**2023**
1	Neutronguides – simulations/tender/contract					
	Neutronguides – construction work/installation					
2	Science case					
	Conceptual design					
	Preparations of technical specifications					
	The documents for opening a new project in the frame of FLNP theme within the topical plan of JINR submitted to PAC for CM					
	Construction works					
	Installation					
	Testing					
	Commissioning					

Neutronguides – simulations/tender/contract	FLNP PNPI NRC «KI» SWISSNEUTRONICS
Neutronguides – construction work/installation	SWISSNEUTRONICS FLNP
Science case	Institute of Nuclear Physics PAN FLNP AMU
Conceptual design	FLNP Institute of Nuclear Physics PAN AMU PNPI NRC «KI» SPbU ILL ISIS
Preparations of technical specifications	FLNP PNPI NRC «KI» SPbU Institute of Nuclear Physics PAN FRAKOTERM
The documents for opening a new theme within the topical plan of JINR submitted to PAC for CM	FLNP
Construction works	FLNP Institute of Nuclear Physics PAN FRAKOTERM
Installation	FLNP Institute of Nuclear Physics PAN FRAKOTERM
Testing	FLNP
Commissioning	FLNP

FLNP

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A. PETROVA
Y. KIRIENKO

Thanks for your kind attention !

Example of hydrogen (molecular) dynamics

diiodothiophene

5K 17h 18g