

REPORT

Experiment MA-3313

(beamline ID22; scheduled shifts – 6; start date and time: 29 June 2016 at 08:00; end date and time: 01 July 2016 at 08:00)

Russian Grant Proposal:

"Structural characterization of novel advanced materials on high-resolution synchrotron powder diffractometer ID22".

In the framework of experiment **MA-3313** in ESRF at beamline ID22, seven scientists from Moscow (Russian Federation), namely, Dr. Vladimir Chernyshev, Dr. Anna Tursina, Dr. Victor Rybakov, Dr. Ilya Zamilatskov, and post-graduate students Elena Marushina, Dina Erzina and Pavel Kots delivered 57 powder samples (of 55 compounds) for the measurements. The samples were loaded into quartz and borosilicate capillaries of 0.5 – 1.0 mm diameter. During 6 shifts (48 h) all the samples were measured in the 2θ ranges 0 – 25, 0 – 30 or 0 – 35°. The X-ray wavelength used was 0.399927(2) Å. Fifty three (53) high-resolution powder patterns were measured at room temperature. Three intermetallic compounds were measured at different high temperatures in the ranges 260 – 300 °C and 550 – 855 °C (24 patterns in 1 – 15° 2θ) with the use of hot-air blower.

Appendix (below) contains the full list of the measured samples (Table 1) and the Figures of their powder patterns in the 0.5 – 20° 2θ range.

Samples **1 – 15** and **51** are ternary intermetallics.

Samples **16 – 30**, **36 – 46**, **52** and **53** are zeolites.

Samples **31 – 35** are β -substituted porphyrins.

Samples **47 – 50** are Bi-doped (Cs, Rb, Tl, Cd)-mixed halides.

Samples **54 – 57** are organic (pharmaceutical) compounds.

All measured patterns, excluding **23**, **32** and **38** (see Figures below), will be used in subsequent structural analysis. Patterns **23**, **32** and **38** will be analyzed to find the reasons of corresponding samples degradation.

In conclusion, we estimate these 6 shifts of experimental work as extremely fruitful and thank the ID22 staff for the kind and helpful assistance.



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Appendix.

Table 1. List of the samples, measured in experiment MA-3313.

№	Desk code	User (reference) code	$2\theta_{\min} - 2\theta_{\max}$ (°)	Comment
	Desk D			
1	D1	CPA-201	0 – 30 1 – 15	Room Temperature (RT) T = 550, ... (+30) ..., 700 °C
2	D2	CPA-211	1 – 15	T = 260, 281, 300 °C
3	D3	CHA-67	1 – 15	T = 620, 640, 690, 740, 790, 810, ... (+5) ..., 855 °C
4	D4	CRA 176	0 – 35	RT
5	D5	LRA 42	0 – 35	RT
6	D6	CHG 51	0 – 35	RT
7	D7	CHG 52	0 – 35	RT
8	D8	CDA 407	0 – 35	RT
9	D9	CHA 64	0 – 35	RT
10	D10	CHA 186	0 – 35	RT
11	D11	CDA 272	0 – 35	RT
12	D12	CRG 113	0 – 35	RT
13	D13	CDA 275	0 – 35	RT
14	D14	SRA 34b	0 – 35	RT
15	D15	SRA 29a	0 – 35	RT
	Desk A			
16	A1	1CsY	0 – 30	RT
17	A2	2CsY	0 – 30	RT
18	A3	3CsY	0 – 30	RT
19	A4	4CsY	0 – 30	RT
20	A5	4CsY-b	0 – 30	RT
21	A6	BEC-5-DMSO-pH-0,01	0 – 30	RT
22	A7	BEC-7	0 – 30	RT
23	A8	BEC-5-calc	0 – 30	RT
24	A9	BEC-5	0 – 30	RT
25	A10	CBV8014-svezh	0 – 30	RT
26	A11	CBV8014 after_BBF-9	0 – 30	RT
27	A12	CBV8014 after_BBF-8	0 – 30	RT
28	A13	CBV8014 after_BBF-20	0 – 30	RT
29	A14	CBV8014 after_BBF-6	0 – 30	RT
30	A15	CBV8014 after_BBF-5	0 – 30	RT
	Desk B			
31	B1	CPIRu-verh	0 – 25	RT
32	B2	CPIPdOH	0 – 25	RT
33	B3	E-I	0 – 25	RT
34	B4	CPIRu-niz	0 – 25	RT
35	B5	DM34	0 – 25	RT
36	B6	CBV8014-tp after_BBF-21	0 – 25	RT
37	B7	CBV8014-tp	0 – 25	RT
38	B8	VIP-007 calc	0 – 25	RT
39	B9	VIP-007 180 min	0 – 25	RT
40	B10	VIP-007 120 min	0 – 25	RT
41	B11	Silicate UOP(MFI)	0 – 25	RT
42	B12	Sn-MFI Si/Sn=120	0 – 25	RT

43	B13	AG7	0 – 25	RT
44	B14	MOR	0 – 25	RT
45	B15	Y-5	0 – 25	RT
	Desk C			
46	C1	AG8	0 – 25	RT
47	C2	KUZ-1	0 – 25	RT
48	C3	KUZ-2	0 – 25	RT
49	C4	KUZ-3	0 – 25	RT
50	C5	KUZ-4	0 – 25	RT
51	C6	CDA-411	0 – 35	RT
52	C7	BEC-5-DMSO	0 – 25	RT
53	C8	BEC-5_b	0 – 25	RT
54	C9	Nilotinib	0 – 25	RT
55	C10	Ticagrelor	0 – 25	RT
56	C11	Abirateron	0 – 25	RT
57	C12	AB-413	0 – 25	RT















