REPORT

Experiment **MA-3313**, session 3

(beamline ID22; scheduled shifts – 9; start date and time: 21 April 2017 at 08:00; end date and time: 24 April 2017 at 08:00)

Russian Grant Proposal:

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

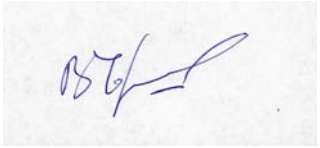
In the framework of experiment **MA-3313** in ESRF at beamline ID22, seven scientists from Moscow (Russian Federation), namely, Dr. Vladimir Chernyshev, Dr. Anna Tursina, Dr. Nadezhda Kurochkina, Dr. Sergei Nesterenko, Dr. Dmitry Albov and post-graduate student Elena Marushina delivered the powder samples of 56 compounds for the measurements. The samples were loaded into quartz and borosilicate capillaries of 0.5 – 1.0 *mm* diameter. During 9 shifts (72 *h*) all the samples were measured in the 2θ ranges 0 – 10, 0 – 20, 0 – 25 or 0 – 35°. Three MOF samples were measured in the CO_2 flow at RT and P = 10 bar. One zeolite sample (CsY) was measured in the N_2 flow at P = 10 bar and different temperatures from the range 25 – 350°C. One ternary intermetallic sample ($CePt_2Al_2$) was also measured at different temperatures in the range 25 – 350°C. Sample of $Zr(W_x, Mo_{1-x})_2O_8$ with negative thermal expansion coefficient was measured in the temperature range 25 – 500°C. In the total, 101 data sets were collected. The X-ray wavelength used was 0.399962(4) Å.

Table 1 contains the full list of the measured patterns (see Appendix).

Samples **4** – **17**, **30**, **31** – **54** and **52** – **56** are zeolites.
Samples **1** – **3** and **18** are MOFs.
Samples **19** – **29** are ternary intermetallics.
Samples **36** – **49** are β-substituted porphyrins.
Samples **32** – **35** are Covalent Organic Frameworks.
Samples **50** and **51** are biologically active organic compounds.
Sample **57** is NTE material, $Zr(W_x, Mo_{1-x})_2O_8$.

All measured patterns, excluding *amorphous* and *decomposed* (3 patterns in total), will be used in subsequent structural analysis.

In conclusion, we estimate these 9 shifts of experimental work as extremely fruitful (as usual for ID22 high-resolution station) and thank the ID22 staff for the kind and helpful assistance.



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Appendix.

Table 1. List of the patterns measured in experiment **MA-3313**, session 3.

№	User (reference) code of the sample	$2\theta_{min}$ – $2\theta_{max}$ (^{o})	Comment
	Gas-handling capillary cell		
1.1	M2 (59, D19) *MOF Isaeva*	0 – 20	RT
1.2	M2 (59, D19) *MOF Isaeva*	0 – 20	In the flow of CO_2 (*10 bar*) at RT
2.1	EC-1 (58, D18) *MOF Isaeva*	0 – 20	RT
2.2	EC-1 (58, D18) *MOF Isaeva*	0 – 20	In the flow of CO_2 (*10 bar*) at RT
3.1	#3 (29.03.2017) *MOF Isaeva*	0 – 20	RT
3.2	#3 (29.03.2017) *MOF Isaeva*	0 – 20	In the flow of CO_2 (*10 bar*) at RT
4.1	Cs-FAU_3io (fojasite)	0 – 20	RT
4.2-19	Cs-FAU_3io (fojasite)	0 – 20	In the flow of N_2 (*10 bar*) at T = RT, 50, 100, 120 …(+10)…230, 250, 300, 350^{o}C
5	NaY (B1) fojasite	0 – 25	RT
6	Na-FAU source (B2, quartz)	0 – 25	RT
7	Cs-FAU_1io (B3, quartz)	0 – 25	RT
8	Cs-FAU_3io (B4, quartz)	0 – 25	RT
9	Cs-FAU_5io (B5, quartz)	0 – 25	RT
10	SnBEA-1 (B6, SnBEA-47-13c)	0 – 25	RT
11	SnBEA-1v (B7, at 400^{o}C *in vacuo*)	0 – 25	RT
12	SnBEA-2 (B8, SnBEA-20-16c)	0 – 25	RT
13	SnBEA-2v (B9, at 400^{o}C *in vacuo*)	0 – 25	RT
14	BEC-1-svezh (B10)	0 – 25	RT
15	BEC-2 (B11, 3h at 100^{o}C)	0 – 25	RT
16	BEC-3 (B12, 10h at 100^{o}C)	0 – 25	RT
17	VP-120 (B13), *zeolite*	0 – 25	RT
18	9-5%Co MIL-53 (B14, after catalysis)	0 – 25	RT
19.1-7	CPA1 ($CePt_2Al_2$)	0 – 20	T = RT, 100, …(+50)…, 350^{o}C
19.8-18	CPA2 ($CePt_2Al_2$)	0 – 20	T = 220, …(+10)…, 320^{o}C
19.19	CPA1 ($CePt_2Al_2$)	0 – 20	RT
20	CHE25BSi (D1)	0 – 35	RT
21	CHG67-700 (D2)	0 – 35	RT
22	CDA417 (D3)	0 – 35	RT
23	CHG67-900 (D4)	0 – 35	RT
24	CHG70-900 (D5)	0 – 35	RT
25	CHG70-700 (D6)	0 – 35	RT
26	CHG78 (D7)	0 – 35	RT
27	CHG26 (D8)	0 – 35	RT
28	CDA289 (D9)	0 – 35	RT
29	CHG80 (D10)	0 – 35	RT
30	VP-30 (D11), *zeolite*	0 – 35	RT
31	VP-svezh (D12), *zeolite*	0 – 35	RT
32	V-01 (E1)	0 – 20	RT
33	V-01-02 (E2)	0 – 20	RT
34	V-03 (E3)	0 – 20	RT, *non-stable!*
35	V-04 (E4)	0 – 20	RT

36	BES36 (E5)	0 – 20	RT
37	Dina-Pd	0 – 20	RT, *non-stable!*
38	Lu-Kalinina	0 – 10	RT, *amorphous*
39	Lu-Masha	0 – 10	RT, *amorphous*
40	D148_Dina	0 – 20	RT
41	D170 (Dina)	0 – 20	RT
42	A-19-1 (EE1)	0 – 20	RT
43	D-148_new (EE2)	0 – 20	RT
44	OEPNIC (EE3)	0 – 20	RT
45	D-145 (EE4)	0 – 20	RT
46	G2S (EE5)	0 – 20	RT
47	DM-34A (EE6)	0 – 20	RT
48	A-22 (EE7)	0 – 20	RT
49	BES31 (EE8)	0 – 20	RT
50	N28 (EE9)	0 – 20	RT
51	N28_new (EE10)	0 – 20	RT, *decomposed*
52	KUZ5 (EE11, MOR_new)	0 – 30	RT
53	MOR (EE12)	0 – 30	RT
54	IPO18 (EE13)	0 – 30	RT
55	IPO8 (EE14)	0 – 30	RT
56	IPO9 (EE15)	0 – 30	RT
57.1-11	Gubanov, $[Zr(W_x, Mo_{1-x})_2O_8]$	0 – 30	T = RT, 50, …(+50)…, 500°C