REPORT

Experiment **MA-3313**, session 2

(beamline ID22; scheduled shifts – 6; start date and time: 26 October 2016 at 08:00; end date and time: 28 october 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. Vera Isaeva, Dr. Ivan Lonin, and post-graduate students Vera Gribanova, Victoria Avzuragova and Evgenii Belyaev delivered the powder samples of 58 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 – 10, 0 – 20, 0 – 25 or 0 – 35°. In the total, 82 data sets were collected at two temperatures, either at T = 250 K (49 patterns for organic or metal-organic compounds) or at T = 295 K (33 patterns). The X-ray wavelength used was 0.399996(3) Å.

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

Samples **1** – **3**, **51** – **54** and **80**, **81** are zeolites.
Samples **4** – **6** (and **46**, **47**) are Covalent Organic Frameworks.
Samples **7**, **26**, **27**, **33**, **35** – **38**, **45**, **48**, **55** – **60**, **71** – **79** and **82** are MOFs.
Samples **16** – **25** and **28** – **30** are ternary intermetallics.
Samples **8** – **15**, **31**, **32**, **34**, **41** – **44**, are β-substituted porphyrins.
Samples **65** – **70** are modulated oxides with general formula $Ag_xR_yWO_4$ (R = Ce, Dy, Sm).
Samples **39**, **40**, **49**, **50** , and **61** – **64** are biologically active organic compounds.

All measured patterns, excluding *fast* (D1-D10*_fast*), *poor* and *failed* (16 patterns in total), will be used in subsequent structural analysis.

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**, session 2.

№	Desk code	User (reference) code	$2\theta_{min} - 2\theta_{max}$ (°)	Comment
	Desk **B**			
1	B1	BEC-7	0 – 25	T = 250 K
2	B2	BEC-7-DMSO	0 – 25	T = 250 K
3	B3	BEC-7-calc	0 – 25	T = 250 K
4	B4	V-01-02	0 – 25	T = 250 K
5	B5	V-21	0 – 25	T = 250 K
6	B6	Acid	0 – 25	T = 250 K
7	B7	Ks-CN	0 – 25	T = 250 K
8	B8	Tomil	0 – 25	T = 250 K
9	B9	G2S	0 – 25	T = 250 K
10	B10	BES-17	0 – 25	T = 250 K
11	B11	BES-11 (= 17)	0 – 25	T = 250 K
12	B12	G4L	0 – 25	T = 250 K
13	B13	C-2	0 – 25	T = 250 K
14	B14	BES-2	0 – 25	T = 250 K
15	B15	BES-15	0 – 25	T = 250 K
	Desk **C**			
16	C16	K-238	0 – 25	RT
17	C17	K-237	0 – 25	RT
18	C18	K-198	0 – 25	RT
19	C19	K-164	0 – 25	RT
20	C20	SRN-1	0 – 25	RT
21	C21	SRN-2	0 – 25	RT
22	C22	CHA-61	0 – 25	RT
23	C23	Cere 5	0 – 25	RT
24	C24	Cha-67-831	0 – 25	RT
25	C25	CRg-14	0 – 25	RT
26	C26	M6	0 – 25	RT
27	C27	5%Rh	0 – 25	RT
28	C28	Cda-411	0 – 25	RT
29	C29	Cda-297	0 – 25	RT
30	C30	Chg-7	0 – 25	RT
	Desk **D**	*fast! (3 min)*		
31	D1_*fast*	Ru12	0 – 10	T = 250 K
32	D2_*fast*	G5L	0 – 10	T = 250 K
33	D3_*fast*	8 5%Co	0 – 10	T = 250 K *(poor)*
34	D4_*fast*	G7L	0 – 10	T = 250 K
35	D5_*fast*	9 5%Co	0 – 10	T = 250 K
36	D6_*fast*	10Ks	0 – 10	T = 250 K *(poor)*
37	D7_*fast*	11Ks	0 – 10	T = 250 K *(poor)*
38	D8_*fast*	12L	0 – 10	T = 250 K *(poor)*
39	D9_*fast*	D80s	0 – 10	T = 250 K
40	D10_*fast*	D120	0 – 10	T = 250 K *(poor)*
	Desk **D**			
41	D1	Ru12	0 – 20	T = 250 K
42	D2	G5L	0 – 20	T = 250 K

43	D3	BES-2	0 – 20	T = 250 K, re-measurement B14
44	D4	G7L	0 – 20	T = 250 K
45	D5	9 5%Co	0 – 20	T = 250 K
46	D6	V-21	0 – 20	T = 250 K, re-measurement B5
47	D7	acid	0 – 20	T = 250 K, re-measurement B6
48	D8	Ks-CN	0 – 20	T = 250 K, re-measurement B7
49	D9	D80s	0 – 20	T = 250 K
50	D10	D-100m	0 – 20	T = 250 K
51	D11	VP-calc	0 – 20	T = 250 K
52	D12	VP-50	0 – 20	T = 250 K
53	D13	VP-100	0 – 20	T = 250 K, failed (see E1)
54	D14	VP-70	0 – 20	T = 250 K, failed (see E2)
55	D15	Galkuz-4	0 – 20	T = 250 K, failed (see E3)
56	D16	Au-before	0 – 20	T = 250 K
57	D17	Au-after	0 – 20	T = 250 K
58	D18	EC-1	0 – 20	T = 250 K
59	D19	M2	0 – 20	T = 250 K
60	D20	M3	0 – 20	T = 250 K
61	D21	GPZ-HBA	0 – 20	T = 250 K
62	D22	GPZ-SA	0 – 20	T = 250 K
63	D23	Diox-8	0 – 20	T = 250 K
64	D24	T40-2 (Diox)	0 – 20	T = 250 K
65	D25	$Ce_{0,2}$ (0,6)	0 – 35	RT
66	D26	$Ce_{0,5}$	0 – 35	RT
67	D27	$Sm_{4/7}$	0 – 35	RT
68	D28	$Sm_{0,6}$	0 – 35	RT
69	D29	$Dy_{4/7}$	0 – 35	RT
70	D30	$Dy_{0,6}$	0 – 35	RT
71	D31	AG5	0 – 20	RT
72	D32	MP-28	0 – 20	RT
73	D33	AG77	0 – 20	RT
74	D34	Galkuz-1	0 – 20	RT
75	D35	Чит (4б)	0 – 20	RT
76	D36	Galkuz-2	0 – 20	RT
77	D37	AG-76	0 – 20	RT
78	D38	AG-6	0 – 20	RT
79	D39	Galkuz-3	0 – 20	RT
	Desk **E**			
80	E1	VP-100	0 – 20	re-measurement (D13)
81	E2	VP-70	0 – 35	re-measurement (D14)
82	E3	Galkuz-4	0 – 35	re-measurement (D15)