

20 February 2018

REPORT

Experiment MA-3313

Russian Grant Proposal:

"Structural characterization of novel advanced materials on high-resolution synchrotron powder diffractometer ID22" [06/05/2016-31/12/2017].

In the framework of experiment MA-3313, **242** powder samples were measured at ID22 during four sessions.

Session 1: scheduled shifts – **6**; start date and time: 29 June 2016 at 08:00; end date and time: 01 July 2016 at 08:00. Number of measured powder samples – **57**.

Session 2: scheduled shifts – **6**; start date and time: 26 October 2016 at 08:00; end date and time: 28 October 2016 at 08:00. Number of measured powder samples – **58**.

Session 3: scheduled shifts – **9**; start date and time: 21 April 2017 at 08:00; end date and time: 24 April 2017 at 08:00. Number of measured powder samples – **56**. Three MOF samples were measured in the CO₂ flow at RT and $P = 10$ bar. One zeolite sample (CsY) was measured in the N₂ flow at $P = 10$ bar and different temperatures from the range 25 – 350°C.

Session 4: scheduled shifts – **10**; start date and time: 27 October 2017 at 24:00; end date and time: 31 October 2017 at 08:00. Number of measured powder samples – **71**.

The measured samples are representatives of the following groups of advanced materials – zeolites, MOFs, ternary intermetallics with rare-earth elements, β -substituted porphyrin-related photosensitizers, biologically active organic compounds, inorganic solid electrolytes, modulated oxides with general formula Ag_xR_yWO₄ (R = Ce, Dy, Sm).

By today, 20th February 2018, processing of approximately half of the measured synchrotron patterns has been completed. The obtained results are published in eleven papers [1-11], two papers are under review. The remaining patterns will be processed in 2018.

In conclusion, we estimate these **31** 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.

References.

[1]. Veselovsky, V.V., Lozanova, A.V., Isaeva, V.I., Lobova, A.A., Fitch, A.N., Chernyshev, V.V. "Optically active derivatives of terephthalic acid: four crystal structures from two powder patterns" (2018). *Acta Cryst.* **C74** (published online).
<https://doi.org/10.1107/S2053229618001705>

[2]. Domoroshchina, E.N., Chernyshev, V.V., Kuz'micheva, G.M., Dorokhov, A.V., Pirutko, L.V., Kravchenko, G.V., Chumakov, R.B. "Changing the characteristics and properties of zeolite Y and nano-anatase in the formation of a nano-anatase/Y composite with improved photocatalytic and adsorption properties". (2018). *Applied Nanoscience*, **8** (published online).
<https://doi.org/10.1007/s13204-018-0648-5>

[3]. Kots, P.A., Kurkin, A.V., Sushkevich, V.L., Fitch, A.N., Chernyshev, V.V., Ivanova, I.I. "Synchrotron XRD and NMR evidence of germanium redistribution during silylation of BEC-type germanosilicate." (2017). *CrysEngComm*, **19**, 5982–5988.
<https://doi.org/10.1039/c7ce01204g>

- [4]. Gavrilov, K.N., Zheglov, S.V., Chuchelkin, I.V., Maksimova, M.G., Firsin, I.D., Fitch, A.N., Chernyshev, V.V., Maximychev, A.V., Perepukhov, A.M. "Tartaric acid-derived chiral phosphite-type P,N-ligands: behavioural features in Pd-catalyzed asymmetric transformations." (2017). *Tetrahedron: Asymmetry*, **28**, 1633-1643.
<https://doi.org/10.1016/j.tetasy.2017.09.011>
- [5]. Andreev, S.V., Zverev, S.A., Zamilatskov, I.A., Kurochkina, N.M., Ponomarev, G.V., Fitch, A.N., Chernyshev, V.V. "Polymeric structure of a coproporphyrin I ruthenium(II) complex: a powder diffraction study". (2017). *Acta Cryst. C* **73**, 47-51.
<https://doi.org/10.1107/S2053229616019422>
- [6]. Pyatakov, D.A., Astakhov, A.V., Sokolov, A.N., Fakhrutdinov, A.N., Fitch, A.N., Rybakov, V.B., Chernyshev, V.V., Chernyshev, V.M. "Alkoxy base-mediated selective synthesis and new rearrangements of 1,2,4-triazolodipyrimidinones". (2017). *Tetrahedron Letters*, **58**, 748-754.
<https://doi.org/10.1016/j.tetlet.2017.01.030>
- [7]. Griбанова, V., Murashova, E., Gnida, D., Kurenbaeva, Zh., Nesterenko, S., Tursina, A., Kaczorowski, D., Griбанов, A. "Novel ternary cerium-rich intermetallic compound Ce₁₁Ru_{3.83}In₉: Crystal structure and low-temperature physical properties". (2017). *J. Alloys Compd.* **711**, 455-461.
<https://doi.org/10.1016/j.jallcom.2017.03.168>
- [8]. Veselovsky, V.V., Lozanova, A.V., Isaeva, V.I., Lobova, Chernyshev, V.V. "Optically active derivatives of terephthalic acid: synthesis and crystal structures." (2017). *Russ. Chem. Bull.* **66**, 1589-1596.
<https://doi.org/10.1007/s11172-017-1928-z>
- [9]. Lonin, I.S., Belyaev, E.S., Tsivadze, A.Y., Ponomarev, G.V., Lonina, N.N., Fitch, A.N., Chernyshev, V.V. "A Study of the Reaction between Methylpyrophosphoribide *a* and Hydrazine Hydrate". (2017). *Macrocyclics*, **10**, 474-479.
<https://doi.org/10.6060/mhc1708321>
- [10] Ponomareva, O.A., Kots, P.A., Kolyagin, Y.G., Chernyshev, V.V., Ivanova, I.I. "The position of cesium cations in the CsNaFAU(Y) structure under dehydration conditions studied by powder diffraction and magic angle spinning NMR spectroscopy". (2017). *Russ. Chem. Bull.* **66**, 2021-2027.
DOI will be assigned soon.
- [11] Avzuragova, V.A., Nesterenko, S.N., Tursina, A.I. "Ternary gallides of the Ce_{2+n}Rh_{3+3n}Ga_{1+2n} (n=0-5) structure family." (2017). *Russ. Chem. Bull.* **66**, 2015-2020.
DOI will be assigned soon.



Dr. V.V. Chernyshev
M.V.Lomonosov Moscow State University