

REPORT

Experiment **MA-4527**

" Structural characterization of novel advanced materials on high-resolution synchrotron beamline ID22"

In the framework of experiment **MA-4527** granted by ESRF for 3 shifts on beam line ID22 (started on 21 September 2020 at 08:00 and ended on 22 September at 08:00) twenty high-resolution powder patterns of 18 compounds were measured. The X-ray wavelengths used were 0.354345(3) and 0.354317(3) Å. The patterns were measured in the 2θ ranges 0.5 – 38°. The Figures of all 20 patterns are shown below.

Samples **MOF46**, **MOF39a & b**, **MOF57** and **MOF137** are representatives of MOFs based on porphyrinylphosphonates. Sample **MOF46** has been measured at $T = 25, 75 \text{ \& } 150^\circ\text{C}$, three patterns are successfully indexed. Pattern for **MOF137** is also indexed. The rest patterns are under consideration.

Samples **KEP35** & **KEP290** are MOFs based on tetrakis(imidazolyl)borate and tetrakis(2-methylimidazolyl)borate with Co. The crystal structure of **KEP35** is already solved. Pattern for **KEP290** is indexed..

Samples **HZSM5**, **AHZSM1 & 2**, **TS1P** and **TS1P75** are Zeolites (structure type MFI) containing (Al, Ti) and activated with anatase. The Rietveld refinements are in progress to establish the sites of (Si, Al) and (Si, Ti) replacements and content of the pores.

Samples **CNA1 & 2**, **CCA432** and **LCA342** are ternary intermetallics with rare earth elements, La and Ce. Each sample contains several phases, including the new one, which has to be established.

Samples **GAVR48** & **GAVR49** are chiral organic diamidophosphites. Both patterns are indexed, the structure determination is in progress.

Finally, we estimate the obtained synchrotron patterns as very informative and thank the ID22 staff for their high-quality work in this remote mail-in experiment.

Dr. V.V. Chernyshev

M.V.Lomonosov Moscow State University







