**Layered Ammonia Polyuranates: Structural Peculiarities**

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One of the crucial steps of nuclear fuel cycle is a fabrication of fuel pellets. In case of UO2 fuel, enriched UF6 is hydrolyzed and subsequently reacted with ammonia, forming the ammonia polyuranates xUO3·yNH3·zH2O. Though properties of ammonium polyuranates have been actively investigated previously [1,2], neither the chemical composition, nor structure of such compounds have not been uniquely determined. It is still debated, whether xUO3·yNH3·zH2O are compounds of individual phases with certain stoichiometry or a homogeneous system in which ratio of UO3/NH3/H2O can be varied continuously. The advancement of the characterization techniques, including synchrotron-based methods of X-ray diffraction (XRD) and neutron diffraction makes it possible to investigate structure of ammonium uranates even though only polycrystalline samples can be synthetically obtained. Technical achievements unsurprisingly resumed scientific interest to this problem[3,4].

Here we showed the results of structural characterization of ammonia uranate system. All samples were synthesized by adding ammonia aqueous solution to solid UO3 with various ratio of UO3/NH3. The precipitates were washed and investigated with a bunch of methods, including XRD, TEM, elemental analysis, infrared, Raman and EXAFS spectroscopies.

Table 1. Results of the structure solution for ammonium polyuranates.

|  |  |  |
| --- | --- | --- |
|  | 3UO3·NH3·5H2O | 2UO3·NH3·3H2O |
| Space group | Pnnn | I212121 |
| Formula units | 6 | 6 |
| a, Å | 12.229(1) | 12.175(1) |
| b, Å | 15.012(1) | 14.421(1) |
| c, Å | 7.1327(8) | 7.0691(7) |
| Rwp | 0.0366 | 0.0498 |

It was found, that stoichiometry and synthesis time have a significant effect on the product properties, resulting in monophasic or polyphasic samples. The chemical composition of monophasic samples have been revealed and found to be 3UO3·NH3·5H2O and 2UO3·NH3·3H2O. All samples possess a layer structure similar to uranium oxohydroxide (schoepite), with interlayer water partially substituted with NH4+. Diffraction data was used for structure solution, additional crystallographic information was obtained (Table 1).

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