MS27-2-13 Crystal Structure of High-Pressure Modification of Gold(III) Trifluoride
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Abstract
Gold(III) trifluoride is a binary compond of gold and fluorine. At standard conditions the compound crystallizes in the hexagonal space group $P6_122$ (or $P6_522$) [1]. A few phase transitions at higher pressures were predicted and observed in the Raman spectra of AuF_3 by Kurzydowski and coworkers [2]. To the best of our knowledge, no crystal structure of any of the high pressure modifications of AuF_3 was so far determined experimentally.
Here we will present our latest data on the first experimental determination of the crystal structure of gold(III) trifluoride at higher pressure. The crystals of AuF_3 were synthesized in a fluorine oven by interaction of gold metal powder with fluorine-argon mixture at increased temperatures. The crystals grown in the colder part of the fluorine oven were transferred and stored in a glove box and were used for single crystal X-ray diffraction later.
The diffraction experiment was carried out using a One20DAC diamond anvil cell by Almax easyLab. The pressure in the DAC was controlled using the ruby fluorescence method and was set to be equal to approximately 2 GPa. At the conditions of the experiment we observed the phase transition predicted and observed in the Raman spectra of AuF_3 by Kurzydowski and coworkers [1]. We confirm that the high pressure polymorph modification of gold trifluoride crystallizes in the hexagonal space group $P6_1$ (or $P6_5$). The following unit cell parameters were determined from the diffraction data: a = 4.9195(4), c = 16.3956(13) Å, V = 343.64(6) Å^3, Z = 6 at 293 K and ca. 2 GPa.

References
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