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Microporosity in Cage Structures Based on Zinc 3-Amino-1,2,4-Triazole (AmTAZ) Complexes. Urs Geiser, John A. Schlueter, Russell J. Funk, Jianjiang Lu, Materials Science Div., Argonne National Laboratory, 9700 South Cass Ave., Argonne, IL 60439, USA.

Motivated by the finding of microporous tubular structures in solvated ZnF(AmTAZ) and its high temperature pseudomorphosis to unusual crystal shapes of ZnO by the group of zur Loye [1], we investigated several other salts of Zn^{2+} in the presence of AmTAZ for their suitability as hosts for small molecules. Only with the addition of the counter ions NCO^- and NCS^- besides nitrate in the hydrothermal synthesis did we observe the incorporation of bridging μ_2-O^{2-} and μ_3-S^{2-} into the unusual cage structures of $[Zn_{15}(AmTAZ)_{18}(O)_6](NO_3)_4(OH)_{14}(H_2O)_4$ (*Pa-3*, $a=15.018$ Å at 150 K) and $[Zn_6(AmTAZ)_6(S)_2](NO_3)_3(OH/H_2O)_x$ (*I23*, $a=16.252$ Å at 150 K), respectively. Due to the dissymmetry of the bridging AmTAZ ligand, the resulting cages have the uncommon point groups S_6 (-3) and T (23), with 20 (3 sites) and 24 (all equivalent) Zn atoms for the O and S compounds, respectively.

1. Su, C.-Y.; Goforth, A.; Smith, M.D.; Pellechia, P.J.; zur Loye, H.-C. *J. Am. Chem. Soc.* 2004, *126*, 3576-3586.

This work was supported by the Office of Basic Energy Sciences, Division of Materials Sciences of the U. S. Department of Energy under contract W-31-109-ENG-38.