X-ray Structures and Charactrizations of Iron Complexes of Thiacalixarenetetrasulfonate

Haruo Akashi, Misato Ichikawa, Research Institute of Natural Sciences, Okayama University of Science, Ridai-cho, Okayama 700-0005, Japan. E-mail: akashi@high.ous.ac.jp

Recently, we have reported the structure of tetrasodium thiacalix[4]arenetetrasulfonate (H₄TCAS)[1]. Odo and co-workers found that some metal complexes of H4TCAS attached on ionexchangers showed peroxidase-like catalytic activity[2]. This prompted us to make single crystals of metal complexes of TCAS for the structure analyses. We succeeded in the preparation of micro crystals of Fe(III) complex of TCAS. A blue thin plate-like crystal of K₃[Fe(H₂TCAS)(H₂O)₂]8H₂O(1), selected for data collection, was mounted in the cold nitrogen stream (105 K) of RAXIS IV(Rigaku Corp.). The compound was found to crystallize in the orthorhombic space group *Pcab* with a = 18.552(1) Å, b = 18.7287(8) Å, c = 25.550(2) Å, V = 8863.1(9) Å³. The structure analysis of **1** revealed that the iron atom is located in a distorted octahedral site. The iron atom is bound to three oxygen atoms and one sulfur atom of the TCAS. This is the first example of the H₄TCAS ligand attached directly to the Fe(III) moiety. Second-sphere coordination compounds, K[Fe(H₂O)₆](H₄TCAS) and K₂[Fe(H₂O)₆](H₄TCAS), will also be reported.

[1] Akashi H., et al., *Acta Cryst.*, 2003, **E59**, m336. [2] Odo J., et al., *Anal. Sci.*, 2004, **20**, 707.

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