Inclusion Ability of Salts between Tritylthiocarboxylic Acids and Amines and Their Crystal Structures

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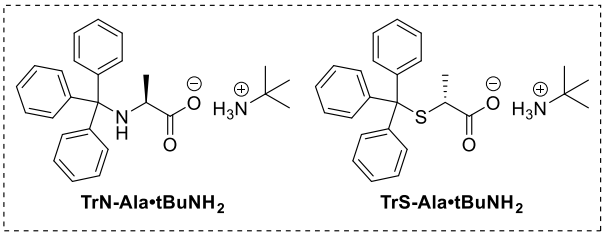
We focus on a bulky trityl group as a crystal engineering tool to provide organic salts with inclusion ability. To date, we have reported that salts between *N*-tritylamino acids and a tertiary butylamine (TrN-AA･tBuNH$_2$) included aliphatic alcohols with stereoselectivity.[1] Here, we synthesized more flexible organic salt hosts (TrS-AA ･ tBuNH$_2$) which were replaced tritylamino group with tritylthio one, because the bond length of C-S is longer than that of C-N. And we investigated its inclusion ability and crystal structures.



We reported that TrN-Ala･tBuNH$_2$ did not show inclusion ability for alcohol guests (Figure 1).[1] In this work, crystallization of TrS-Ala ･ tBuNH$_2$ from MeOH gave inclusion crystals with solvent molecule as guest, where the host-to-guest ratio was 1:1 (Figure 2). This salt showed inclusion ability by replacing N with S.

In addition, the results of PXRD suggest that TrS-Ala ･ tBuNH$_2$ demonstrates inclusion ability for various alcohol guests and can flexibly change the vacancies according to the size of the guest.

We will report these crystal structures and discuss their inclusion abilities.

1. Megumi, K.; Arif, F. N.; Matsumoto, S.; Akazome, M. *Cryst. Growth Des.* **2012**, *12*, 5680-5685.

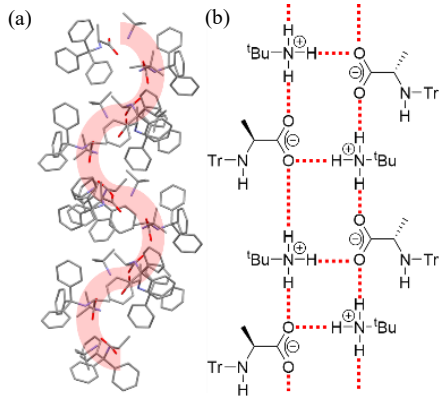


Figure 1. Crystal structure of TrN-Ala･tBuNH$_2$: (a) the curved column structure; (b) the hydrogen-bond network.

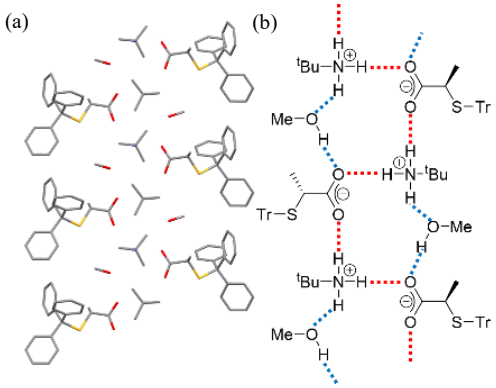


Figure 2. Crystal structure of TrS-Ala･tBuNH$_2$･MeOH: (a) packing; (b) the hydrogen-bond network.