

Synthesis, characterization and *in vitro* activities of aniline dithiocarbamate crystals

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One pot synthesis was used to prepare aniline dithiocarbamate from aniline, carbon(IV) sulfide and sodium hydroxide [1]. Aniline dithiocarbamate crystals (ai-dtc; $C_7H_{12}NNaO_3S_2$) which grew from solution were washed with diethyl ether, and subjected to single x-ray crystallography. The crystals were collected and mounted on a four circles diffractometer Gemini of Oxford Diffraction, using a graphite monochromated $CuK\alpha$ radiation ($\lambda = 1.54184 \text{ \AA}$). Super flip program was used to solve the crystal structure; while refinement was done using full matrix least-squares technique with the support of Jana 2006. The resulting synthetic crystalline structure (Figure 1) appeared as crystalline polymolecule (Figure 2) which has crystal data with three dimensions of $a=2.86663(4) \text{ \AA}$, $b=6.9386(3) \text{ \AA}$ and $c=11.3127(3) \text{ \AA}$. Other characterization techniques of physicochemical parameters, FT-IR, UV-Vis and NMR further confirmed ai-dtc structure. [2] For the *in vitro* antibacterial studies, ai-dtc was screened against four bacterial strains (*Staphylococcus aureus* MRSA252, *Enterococcus faecalis* ATCC 19433, *Escherichia coli* MC4100 and *Pseudomonas aeruginosa* PAO1). Result showed that ai-dtc had modest activity against *Staphylococcus aureus* [2].

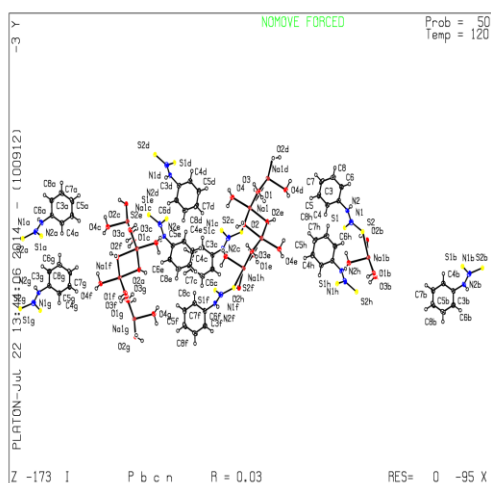


Figure 1: $C_7H_{12}NNaO_3S_2$ crystal structure

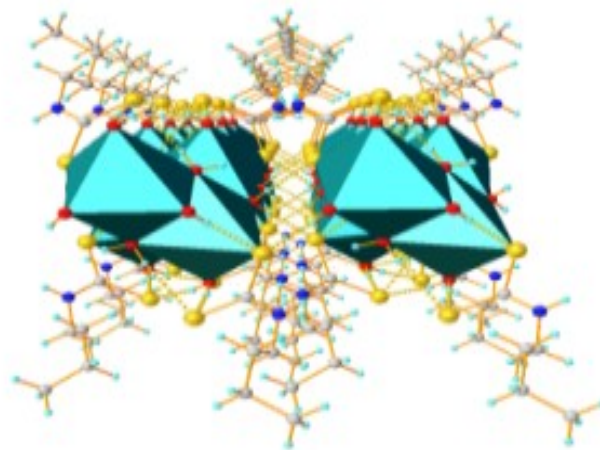


Figure 2: $C_7H_{12}NNaO_3S_2$ polymolecule.

[1] Ahamad, M. M.; SureshKumar, E. V.; Rao, R. M.; Phebe, P. Arch. Appl. Sci. Res. **2016**, *8*, 61-64.

[2] Odularu, A. T.; Ajibade, P. A. *Bioinorg. Chem. Appl.* **2019**, *2019*, 1-15.

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