

MS16-P135 - LATE | SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF NEW SALTS CONTAINING 2-AMINO-3-METHYLPYRIDINIUM CATIONS

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Ionic compounds with nitrogen containing heterocycles and organic acids are characterized by a great structural diversity, interesting physicochemical properties and potential applications, such as ferroic or nonlinear optical materials. In this context, four new salts containing 2-amino-3-methylpyridinium cations were prepared and structurally characterized.

The structure of the bis(2-amino-3-methylpyridinium) bis(hydrogen succinate) succinic acid monohydrate crystal belongs to a triclinic system with $P-1$ space group and with $a = 5.239(3)$, $b = 8.360(3)$, $c = 16.907(5)$ Å, $\alpha = 84.86(3)$, $\beta = 82.29(3)$, $\gamma = 74.43(3)^\circ$, $V = 705.8(5)$ Å³, $Z = 2$.

The structure of the bis(2-amino-3-methylpyridinium) succinate succinic acid crystal was solved in the monoclinic system in the $C2/c$ space group with $Z = 4$ and $a = 14.805(4)$, $b = 5.497(3)$, $c = 27.126(7)$ Å, $\beta = 101.60(3)^\circ$, and $V = 2162.5(14)$ Å³.

A crystal of 2-amino-3-methylpyridinium hydrogen adipate monohydrate crystallizes in the noncentrosymmetric space group $P2_1$ with $a = 5.474(3)$, $b = 17.532(5)$, $c = 7.362(3)$ Å, $\beta = 102.08(3)^\circ$, $V = 690.9(5)$ Å³, $Z = 2$.

The single crystals of the compound of 2-amino-3-methylpyridinium D,L-tartrate crystallizes in triclinic system with $P-1$ space group with $a = 7.210(3)$, $b = 9.269(3)$, $c = 10.741(4)$ Å, $\alpha = 80.87(3)$, $\beta = 78.51(3)$, $\gamma = 88.69(3)^\circ$, $V = 694.5(5)$ Å³, $Z = 2$.

Precise structural analysis of the abovementioned crystal structures, including 3D Hirshfeld surfaces and 2D fingerprint plots, will be presented at the conference.