The crystal structures of \((\text{NH}_4)_2\text{C}_6\text{H}_5\text{O}_7\) and \((\text{NH}_4)_3\text{C}_6\text{H}_5\text{O}_7\) have been determined using a combination of powder and single crystal techniques. The structure of \((\text{NH}_4)_2\text{HC}_6\text{H}_5\text{O}_7\) has been determined previously by single crystal diffraction. All three structures were optimized using density functional techniques. The crystal structures are dominated by N-H–O hydrogen bonds, though O-H–O hydrogen bonds are also important. In \((\text{NH}_4)_2\text{HC}_6\text{H}_5\text{O}_7\), very strong centrosymmetric charge-assisted O13-H21-O13 and O14-H22-O14 hydrogen bonds link one end of the citrate into chains along the \(b\)-axis. A more-normal O12-H20–O15 links the other end of the citrate to the central ionized carboxyl group. In \((\text{NH}_4)_3\text{C}_6\text{H}_5\text{O}_7\), the very strong centrosymmetric O1-H8-O1 hydrogen bonds link the citrates into zig-zag chains along the \(b\)-axis. The citrates occupy layers parallel to the \(bc\) plane, and the ammonium ions link the layers through N-H–O hydrogen bonds. In \((\text{NH}_4)_3\text{C}_6\text{H}_5\text{O}_7\), the hydroxyl group forms a hydrogen bond to a terminal carboxylate, and there is an extensive array of N-H–O hydrogen bonds. The energies of the structures lead to a correlation between the energy of an N-H–O hydrogen bond and the Mulliken overlap population: 
\[
E(\text{N-H–O}) \ (\text{kcal/mole}) = 23.1(\text{overlap})^{0.5}
\]
Powder patterns of \((\text{NH}_4)_2\text{C}_6\text{H}_5\text{O}_7\) and \((\text{NH}_4)_3\text{C}_6\text{H}_5\text{O}_7\) have been submitted to ICDD for inclusion in the Powder Diffraction File.