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MS32-P1 Structural Characterization of Various Salts of Trospium: From Small Change of Anion to Huge Unit Cell

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Trospium chloride (TCl) is a drug used to treat urge incontinence and frequent urination. Four different salts of trospium are known. They are trospium chloride, bromide, iodide and saccharinate. A detailed structure characterization is available only for TCl. In this work, a single-crystal X-ray diffraction was used for structure characterization. The salts of trospium were prepared in two different ways. Inorganic salts were made from a mixture of TCl with hydrobromic or hydriodic acid in varied ratio. Organic salts were prepared from a mixture of TCl and sodium salt of organic acid in ratio 1:1. New structures of four forms were solved (trospium iodide, triiodide and two polymorphs of trospium saccharinate). New structures and structure of TCl were compared to each other and high similarity was found among them. There is some small trend between the anion shape and the structure, but different anions create similar structure as well. An extreme example of the structure dependent variation on the anion is trospium triiodide, which crystallized in a really huge unit cell $(V{=}19438.7~\text{\AA}^3)$ almost seventy times larger than in the other structures of the trospium salts.

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Figure 1. Primary cell of trospium triiodide

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