Random Interstitial Halide Accommodation in an α,ω-Alkylidene-diammonium Template

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N,N,N',N'-Tetramethylethylenediammonium diiodide $[Me_2HNCH_2]_2I_2$ (**1**) as well as a set of I/Br- (**2**) and Br/Cl-mixed-halide salts (**4** and **5**) have been prepared, and their structures determined by single crystal X-ray diffraction. The results show the $[Me_2HNCH_2]_2^{2+}$ dication to be a highly flexible template for halide inclusion, thereby tolerating the assembly of anions of different size, with phase widths of $0 \leq x \leq 2$ for a monoclinic form with $[Me_2HNCH_2]_2I_{2-x}Br_x$ and $0 \leq x \leq 1$ for a triclinic form with $[Me_2HNCH_2]_2Br_{2-x}Cl_x$. The isotypic mixed halide compounds $[Me_2HNCH_2]_2IBr$ (**2**) and $[Me_2HNCH_2]_2BrCl$ (**4**) exhibit a statistical distribution of the anions in a structure of space group $P2_1/c$ which is also found for the pure diiodide $[Me_2HNCH_2]_2I_2$ (**1**). With an excess of chloride ($x > 1$ for $Br_{2-x}Cl_x$) this structure is converted into that of the pure dichloride, $[Me_2HNCH_2]_2Cl_2$ (**6**), with space group $P1$. In all cases the halide anions are trapped in voids between the dications and fixed to the ammonium centers by strong N-H$\cdots$X and weak C-H$\cdots$X hydrogen bonding.

Key words: N,N,N',N'-Tetramethylethylenediammonium Dihalides, Mixed Halides, Hydrogen Bonding, Template, Anion Trapping