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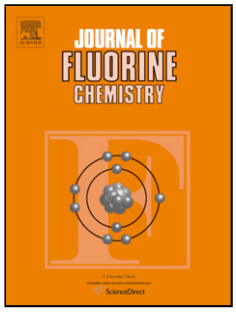

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First examples of diprotonated guanazolinium salts with fluoro-anions.

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Abstract

3,5-diamino-1,2,4-triazolium fluoride-hydrogen-difluoride $(HL)(H_2L)(HF_2)_2F$ (**I**) and heptafluorotantalate $(H_2L)TaF_7$ (**III**) have been crystallized from 66% aqueous solution of hydrogen fluoride. Fluoride-trihydrogen-tetrafluoride $(H_2L)(H_3F_4)F$ (**II**) has been crystallized from anhydrous hydrogen fluoride (L - 3,5-diamino-1,2,4-triazole). Single-crystal X-ray structure determination has shown the presence of doubly protonated H_2L^{2+} cations in each structure. In structures of **I** and **II** salts doubly protonated H_2L^{2+} units are associated with F^- anions via strong hydrogen bonds, and charge balance is provided by HF_2^- and $H_3F_4^-$ anions respectively. The N–H…F and N–H…N hydrogen bonds play an important role in the formation of 3-D structures of all compounds.

Keywords: 3,5-diamino-1,2,4-triazolium, fluoride, H-bonds, crystal structure

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