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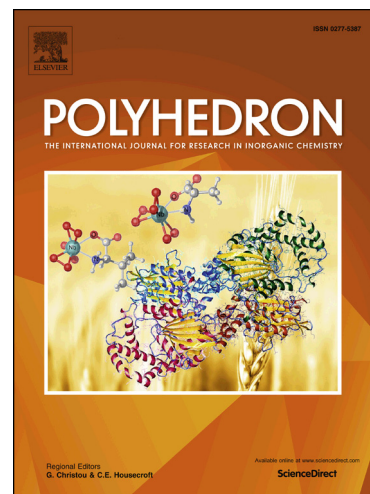
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## Bromobismuthates: cation-induced structural diversity and Hirshfeld surface analysis of cation-anion contacts

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**Abstract:** Reactions of  $[\text{BiBr}_6]^{3-}$  and bromide salts of various substituted pyridinium cations in excess of HBr result in a series of bromobismuthate anionic complexes of various geometry and nuclearity:  $[\{\text{BiBr}_4\}_n]^{n-}$ ,  $[\text{Bi}_2\text{Br}_9]^{3-}$  and  $[\text{Bi}_2\text{Br}_{10}]^{4-}$ . Hirshfeld surface analysis for 19 crystal structure was performed; impact of various X-Br contacts on the crystal structures is discussed.

**Keywords:** halometalate / halide complexes / bismuth / crystal structure / Hirshfeld surface analysis

### Introduction

Although halide complexes of late transition and p-block metals are known for over 100 years, the interest on this class of coordination compounds is persistent. Within the last decade, it is mostly focused on their numerous applications in materials science, particularly, for development of hybrid solar cells [1-7], ferroelectric and ferroelastic materials [8-10], photocatalysts [11-14] etc. From simplistic point of view the halometalates may be regarded as trivial objects for preparative chemist. Indeed, their preparation protocols are straightforward [15], and usually result in crystalline solids suitable for XRD. On the other hand, the price for the simplicity is extreme difficulty (or even impossibility) of making any reliable predictions about the structure of a particular complex forming under certain conditions. Depending on the nature of metal, p-block elements form discrete polynuclear halide complexes of different nuclearity (up to 8 for

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