Bending the bonds: unveiling halogen interactions in the elastic polymorph of 2,5-bis(3-bromophenyl)furan

Autorzy

Konrad Dyk

Vasyl Kinzhybalo

Yuriy Horak

Serhii Butenko

Miłosz Siczek

Daniel M. Kamiński

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Streszczenie

This paper investigates the structural properties of 2, 5-bis(3-bromophenyl)furan polymorphs, focusing on the halogen interactions and their influence on crystal mechanical properties. In this study, three different polymorphic modifications were obtained which crystallize in the orthorhombic system. Two of the polymorphs possess halogen interactions but only one exhibits elastic properties. Through X-ray diffraction, crystallographic analysis and computational modelling, intricate bromine-based halogen interactions and their impact on the packing arrangement and stability were revealed. The correlation between these interactions and crystal properties, including molecular arrangement and intermolecular forces, is explored. Understanding these relationships is vital for materials design and supramolecular chemistry, enabling the rational synthesis of tailored materials.

Słowa kluczowe

2,5-bis(3-bromophenyl)furan, computational modelling, crystal packing, crystal properties, crystallographc analysis, elastic crystals, halogen interactions, supramolecular assemblies

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