Cooperative Halogen Bonding and π – π Stacking Interactions as Drivers of Polymorphism

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Understanding the mechanisms underlying the formation of different polymorphic forms of a given compound is a fundamental issue in modern physical chemistry, with significant implications for the design of functional materials, including those with pharmaceutical relevance. In the present study, the formation of two polymorphic forms of a polyyne compound is elucidated, as confirmed by X-ray crystallographic analysis. The emergence of these polymorphs results from a delicate interplay between halogen bonding and a network of noncovalent π–π stacking interactions. A combination of experimental techniques, single-crystal X-ray diffraction, and theoretical studies allows us to construct a coherent model that rationalizes the formation of both polymorphic modifications of the investigated system.

Słowa kluczowe

1-haloalkynes, halogen bonds, noncovalent interactions, polymorphs, solid states

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