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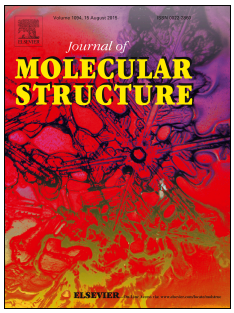

Characterization of non-classical C—Br … π interactions in (*E*)-1,3-dibromo-5-(2-(ferrocenyl)vinyl)benzene and related derivatives of ferrocene

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Characterization of non-classical C—Br···π interactions in (*E*)-1,3-dibromo-5-(2-(ferrocenyl)vinyl)benzene and related derivatives of ferrocene

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Highlights

- Crystal structure of (*E*)-1,3-dibromo-5-(2-(ferrocenyl)vinyl)benzene has been reported.
- Presence of highly directional C-Br…π interactions.
- Multiple structures reported in Cambridge Structure Database (CSD) shows presence of C-Br…π interactions
- These interactions falls in the category of "σ-hole interaction".

Abstract

Amongst the halogens, the involvement of bromine atoms in various types of intermolecular interactions is comparatively the least studied. In this manuscript, we report the formation of C—Br···π interactions, with the π-rings being the cyclopentadienyl (Cp) rings of a ferrocene molecule in a newly synthesized compound (*E*)-1,3-dibromo-5-(2-(ferrocenyl)vinyl)benzene. We have also performed a detailed quantitative analysis on C-Br…π interactions observed in the synthesized molecule and in several related molecules found in the Cambridge Structure Database (CSD) showing the presence of these interactions. A topological analysis based upon QTAIM theory and electrostatic potential ESP mapped on the Hirshfeld surface of these molecules confirm that these interactions are better described as "halogen bonds" wherein the electropositive region (σ-hole) on the Br-atom interacts with the electronegative region over the Cp-ring of the ferrocene. Further, the electronegative region on the bromine atom (perpendicular to the C-Br bond) was observed to be involved in the formation of highly directional C-H···Br interactions with the ∠C-Br···H close to 90°. Thus the bromine atom is acting as both a "halogen bond donor" and "hydrogen bond acceptor" in the crystal packing with the two interactions being mutually orthogonal.