Universität Basel

Publication

1,4-Dibromo-2,5-bis(phenylalkoxy)benzene Derivatives: C-Br...π(arene) Versus C-H...Br and Br...Br Interactions in the Solid State

JournalArticle (Originalarbeit in einer wissenschaftlichen Zeitschrift)

ID 4618097
Author(s) Manfroni, Giacomo; Prescimone, Alessandro; Constable, Edwin C.; Housecroft, Catherine E.
Author(s) at UniBasel Housecroft, Catherine ; Constable, Edwin Charles ; Manfroni, Giacomo ; Prescimone, Alessandro ;
Year 2021
Title 1,4-Dibromo-2,5-bis(phenylalkoxy)benzene Derivatives: C-Br...π(arene) Versus C-H...Br and Br...Br Interactions in the Solid State
Journal Crystals
Volume 11
Number 4
Pages / **Article-Number** 325
Keywords bromine; crystal structure; intermolecular interactions; packing interactions
We have prepared and characterized 1,4-dibromo-2,5-bis(2-phenylethoxy)benzene (1) and 1,4-dibromo-2,5-bis(3-phenylpropoxy)benzene (2). Their single-crystal structures confirm that, at the molecular level, they are similar with the phenylalkoxy chains in extended conformations. However, there are significant differences in packing interactions. The packing in 1 is dominated by C-Br...π(arene) interactions, with each Br located over one C-C bond of the central arene ring of an adjacent molecule. In contrast, the packing of molecules of 2 involves a combination of C-H...Br hydrogen bonds, Br...Br interactions, and arene-arene π-stacking. The single-crystal structures of both orthorhombic and triclinic polymorphs of 1 have been determined and the packing interactions are shown to be essentially identical.
Publisher MDPI
ISSN/ISBN 2073-4352
URL https://www.mdpi.com/2073-4352/11/4/325
edoc-URL https://edoc.unibas.ch/82460/
Full Text on edoc Available;
Digital Object Identifier DOI 10.3390/cryst11040325