

Supporting Information

A self-assembled nanotube supported by halogen bonding interactions

Information included:

- Details of the Hirshfeld analysis of compound **2**.
- Figure S1: Additional figure regarding self-inclusion in XIGLAA.
- Figure S2: Additional figure regarding Hirshfeld analysis of QEVBEZ.

Hirshfeld Analysis, Compound 2

General Surface Information

Type Hirshfeld
Resolution High (Standard)
Isovalue 0.5

Volume 745.49 Å³
Area 554.22 Å²
Globularity 0.717
Asphericity 0.005

Surface Property Information

7 Properties

Name Min Mean Max Units

d i 1.050 1.808 3.011 Å
d e 1.051 1.806 2.886 Å
d norm -0.115 0.610 2.219
Shape Index -0.997 0.168 0.998
Curvedness -3.792 -0.999 0.356

Fingerprint Breakdown

Filtering fingerprint by element type.
Surface area included (as percentage of the total surface area)
for close contacts between atoms inside and outside the surface.

Inside Outside Atom

Atom	BR	O	H	C
BR	0.4	0.2	8.0	4.9 13.5
C	4.8	.	9.6	2.4 16.8
H	4.9	1.0	53.9	8.8 68.5
O	0.2 .	1.0	.	1.2
	10.3 1.2	72.4	16.0	

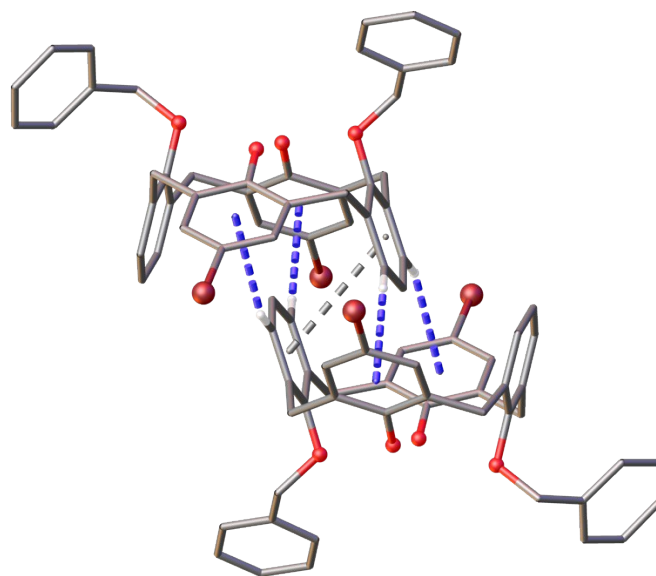


Figure S1. Symmetry expanded structure of XIGLAA.

The asymmetric unit in XIGLAA comprises one calixarene and a chloroform of crystallisation. Symmetry expansion reveals that s.e. C[4]_s self-include and that this occurs with a total of one π -stacking and four CH... π interactions, with two of the latter being crystallographically unique; the two unique CH...aromatic centroid distances were found to be 2.997 Å and 3.018 Å, whilst the π -stacking aromatic centroid...centroid distance was 3.865 Å.

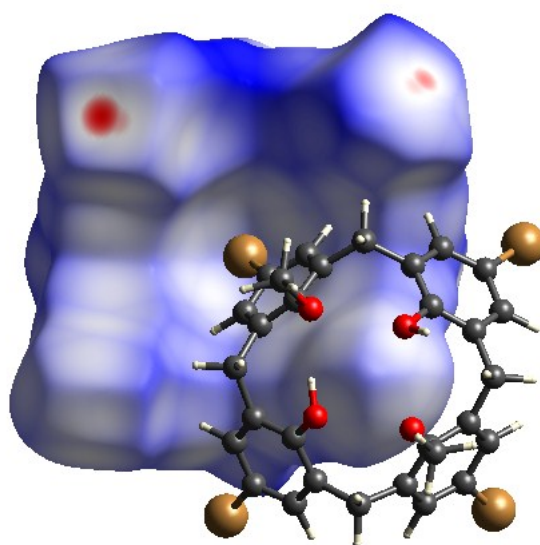


Figure S2. Diagram from the Hirshfeld analysis of QEVBEZ showing a lack of Br... π interactions during self-inclusion.