Supplementary Information

Halogen and Hydrogen Bonding in Multicomponent Crystals of Tetrabromo-*1H*-Benzotriazole

Michele Baldrighi, Pierangelo Metrangolo, Tullio Pilati, Giuseppe Resnati *, and Giancarlo Terraneo

Laboratory of Nanostructured Fluorinated Materials (NFMLab), Department of Chemistry, Materials, and Chemical Engineering "Giulio Natta", Politecnico di Milano, via L. Mancinelli 7, I-20131 Milano, Italy; michele.baldrighi@polimi.it (M.B.); pierangelo.metrangolo@polimi.it (P.M.); tullio.pilati@gmail.com (T.P.); giancarlo.terraneo@polimi.it (G.T.)

* Correspondence: giuseppe.resnati@polimi.it; Tel.: +39-02-2399-3032

Table S1. Crystallographic data for **1** and **2**.

	1	**2**
	Crystal data	
Chemical formula	$C_6HBr_4N_3 \cdot CH_3OH$	$C_6H_{16}N_2 \cdot 2(C_6HBr_4N_3)$
Mr	466.78	985.68
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/c$
Temperature (K)	296	298
a, b, c (Å)	9.5254 (8), 12.4405 (10), 9.9466 (8)	9.2969 (12), 9.5812 (14), 15.468 (2)
β (°)	91.328 (10)	101.183 (12)
V (Å^3)	1178.36 (17)	1351.7 (3)
Z	4	2
Radiation type	Mo Kα	Mo Kα
μ (mm^{-1})	13.64	11.89
Crystal size (mm)	0.40 × 0.40 × 0.12	0.34 × 0.22 × 0.12
	Data collection	
T_{min}, T_{max}	0.356, 0.745	0.427, 0.778
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8790, 2340, 1720	18998, 4483, 3326
R_{int}	0.046	0.040
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.619	0.763
	Refinement	
R[$F^2 > 2\sigma(F^2)$], wR(F^2), S	0.031, 0.067, 1.01	0.032, 0.073, 1.03
No. of reflections	2340	4483
No. of parameters	145	160
No. of restraints	1	-
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
Δρmax, Δρmin (e Å−3)	0.83, −0.48	0.68, −0.86
CCDC number	1574367	1574368

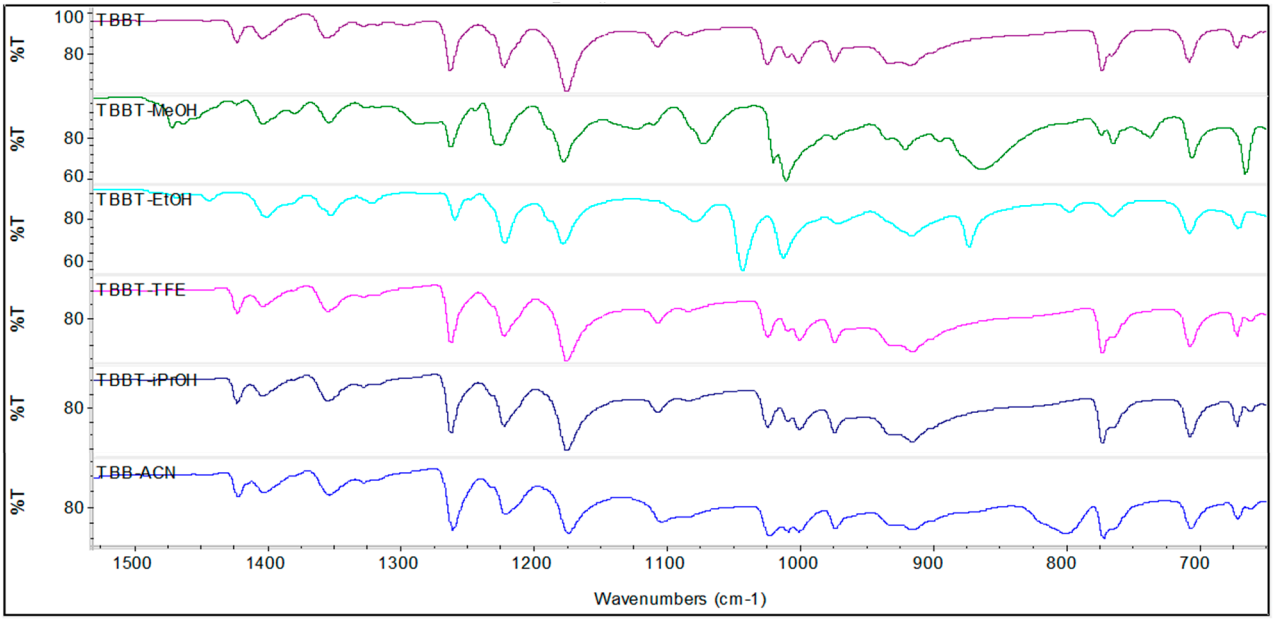

Figure S1. FTIR spectra of pure TBBT (top) and of the solids obtained on recrystallization of TBBT from methanol, ethanol, trifluoroethanol, *i*-propanol, and acetonitrile (from second to sixth spectrum in the order). Only in the case of methanol were crystals suitable for single crystal X-ray analyses obtained. It seems that pure TBBT was obtained in all cases, except that of ethanol, which might have formed a solvate, or a polymorph, of TBBT.