Electronic Supplementary Material for CrystEngComm

Supplementary Information for CrystEngComm

OH – π and halogen – π interactions as driving forces in the crystal organisations of tri-bromo and tri-iodo trityl alcohols

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Table 1S. Selected geometrical parameters of molecules **1** (X=Br) and **2** (X=I) from X-ray diffraction data and calculations by DFT on the M05-2X/6-311G(d,p) level of theory.

Parameter	**1**	**1**	**2**	**2**
	Exp.	Calc.	Exp.	Calc.
C1-O20	1.434	1.430	1.432	1.429
C1-C2	1.533	1.530	1.536	1.531
C1-C8	1.544	1.529	1.544	1.531
C1-C14	1.545	1.525	1.543	1.526
C5-X1	1.905	1.901	2.099	2.113
C11-X2	1.903	1.902	2.100	2.113
C17-X3	1.903	1.903	2.097	2.114
O20-C1-C2	108.2	108.3	108.6	107.6
O20-C1-C8	109.0	109.4	110.0	109.5
O20-C1-C14	106.1	105.9	106.4	106.3
O20-C1-C2-C3	90.4	110.0	89.3	98.7
O20-C1-C8-C9	-19.2	-33.5	-17.6	-29.3
O20-C1-C14-C15	-0.3	-25.3	1.8	-8.5

Table 2S. Geometrical parameters of the additional very weak hydrogen bonds observed after the correction of X-H bond lengths. The prime (P) of secondary (S) types of contacts are indicated.

Structure	Contact	Type of the contact	Contact length (H•••X), Å	Contact angle, °
A	C3-H3•••Br1	S	2.95	161.4
	C10-H10•••Br1	P	3.01	164.5
	C19-H19•••Br3	S	3.00	137.9
	C16-H16•••Br2	P	3.05	148.5
B	C9-H9•••C3(π)	S	2.89	124.2
	C3-H3•••I1	S	3.11	156.0
	C19-H19•••I3	S	3.18	140.3
C	C10-H10•••I2	P	3.17	165.0
D	C16-H16•••C3(π)	S	2.86	130.1
	C15-H15••• Centroid of (C2-C7)	S	2.53	146.8
	C13-H13•••C15(π)	S	2.58	163.5
	C7-H7•••O20	P	2.56	143.5

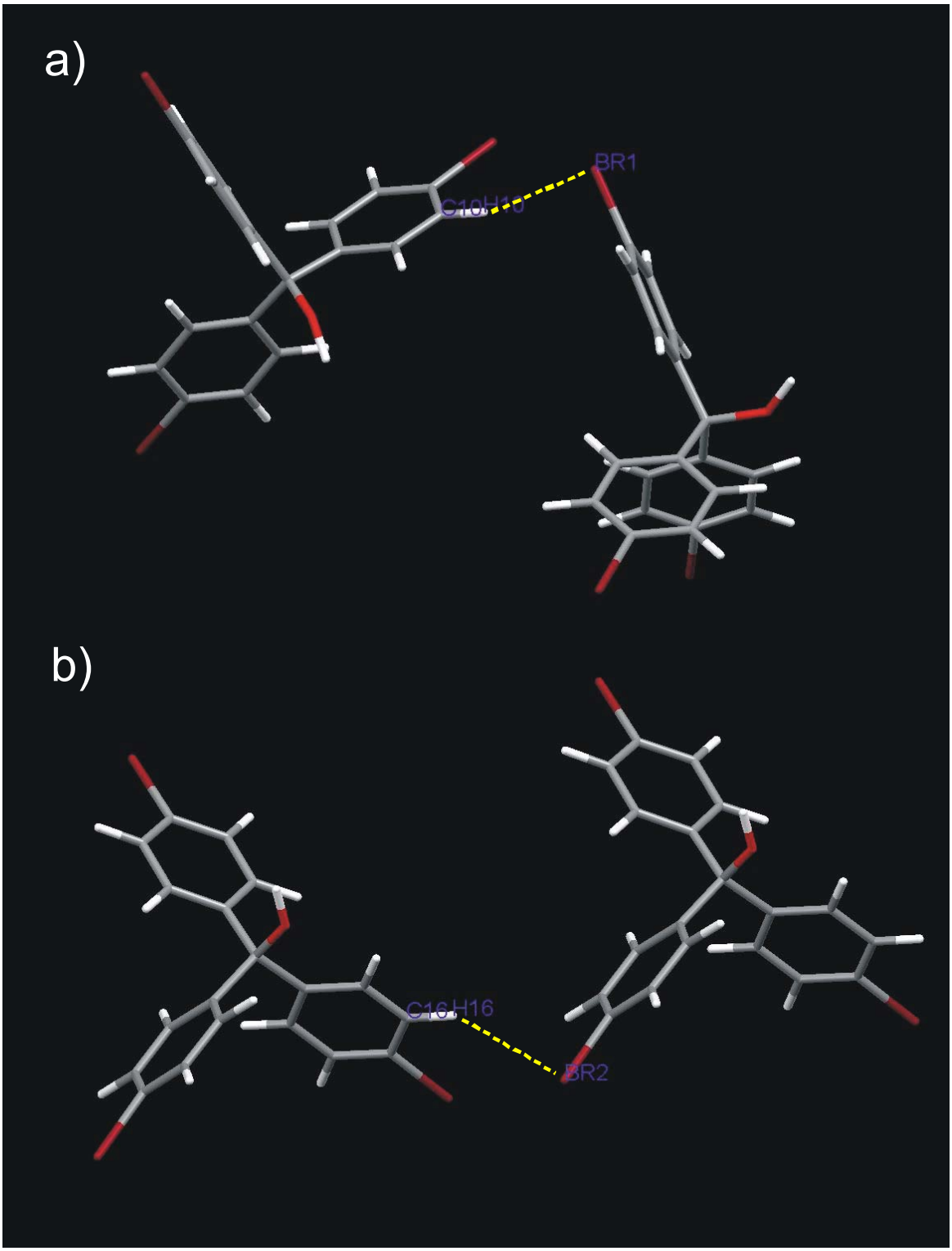

Fig. 1S. The prime contacts observed in the structure **A** after the X-H bond lengths correction: a) C10-H10•••Br1 and b) C16-H16•••Br2.

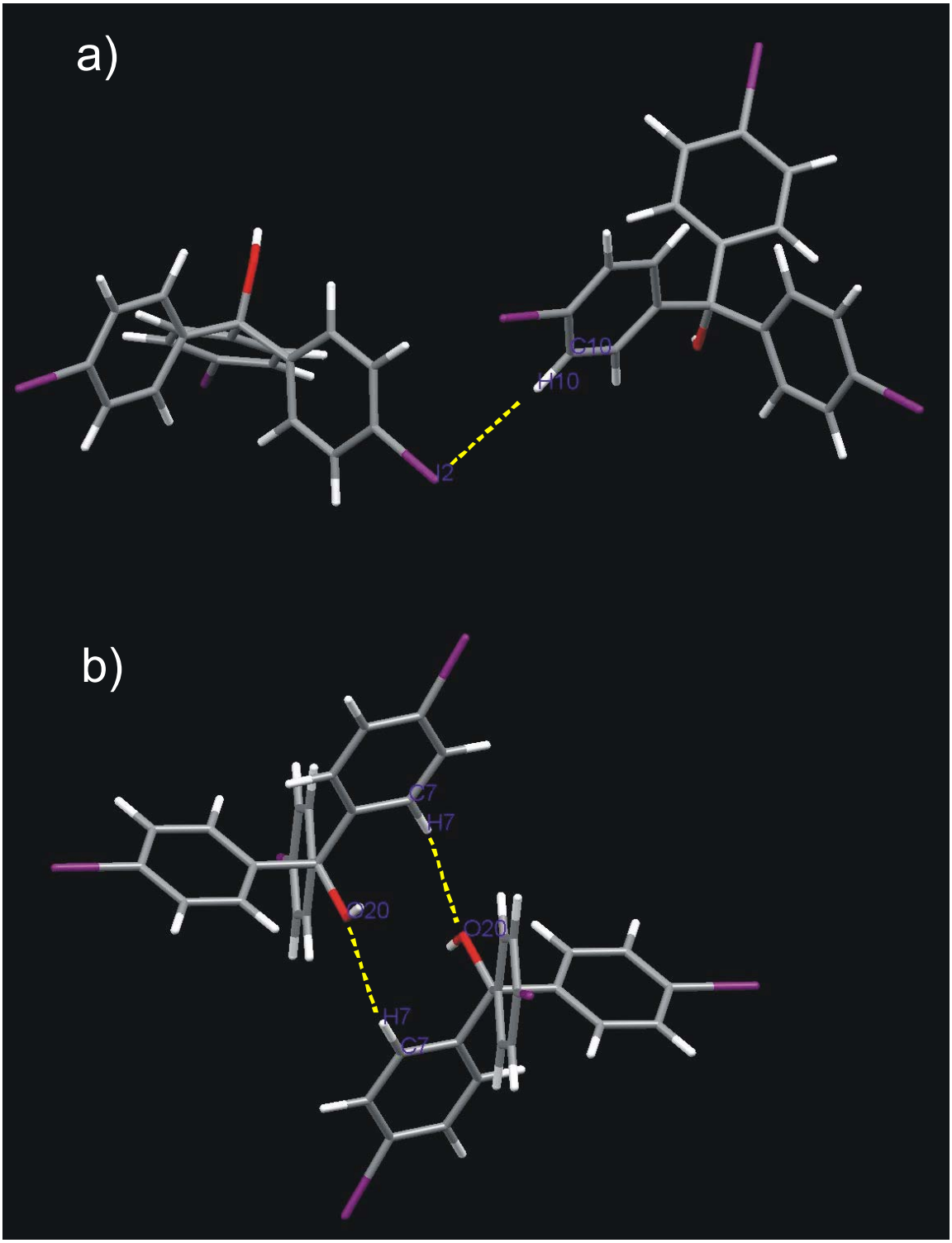

Fig. 2S. The prime contacts observed in after the X-H bond lengths correction: a) in the structure **C**, C10-H10•••I2 and b) in the structure **D**, C7-H7•••O20.