Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Material for

The Role of Intermolecular Hydrogen Bond on Dielectric Properties in Hydrogen-Bonded Material 5-Bromo-9-hydroxyphenalenone: Theoretical Investigation

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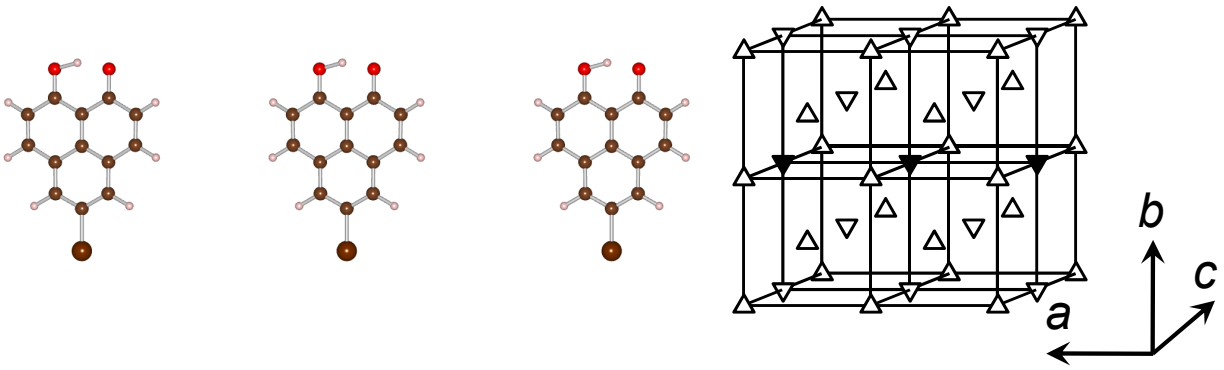

FIG. S1. Schematic structure of trimer A and its position in the crystal. Each triangle indicates a BrH-PLN molecule and inverted triangle represents an inverted one. The three solid triangles correspond to the components of the trimer.

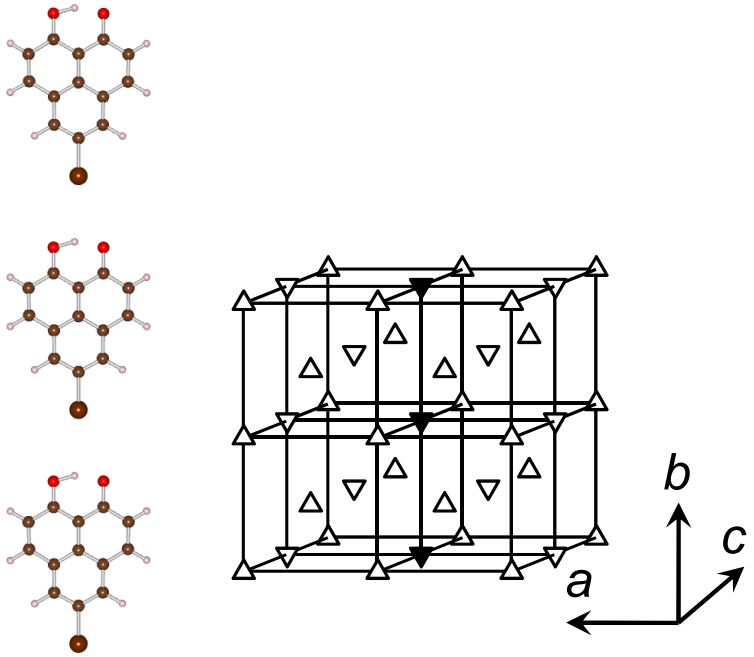

FIG. S2. Same as Fig. S1, but for trimer B.

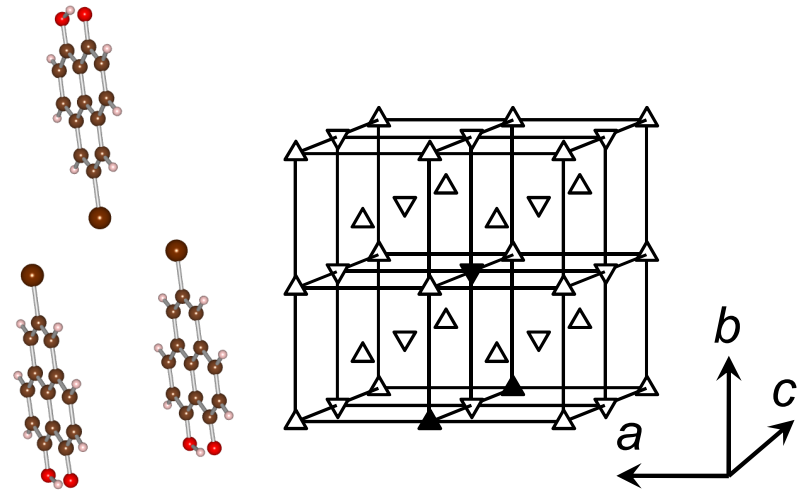

FIG. S3. Same as Fig. S1, but for trimer C.

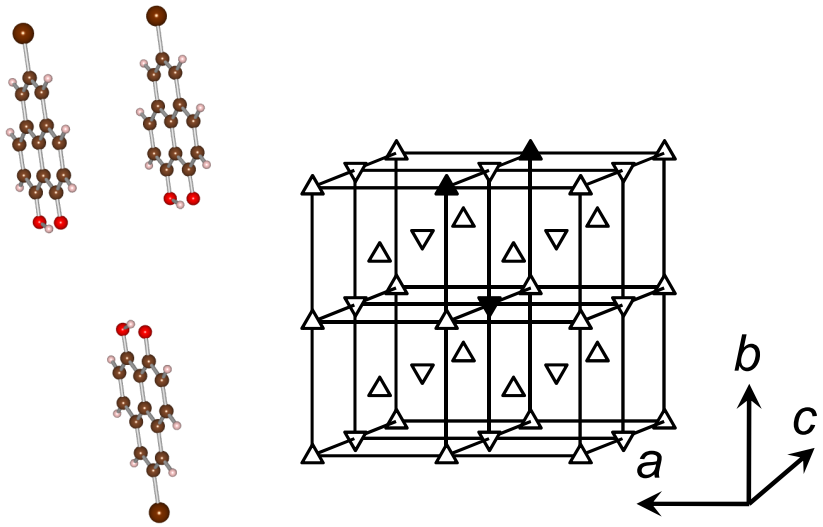

FIG. S4. Same as Fig. S1, but for trimer D.

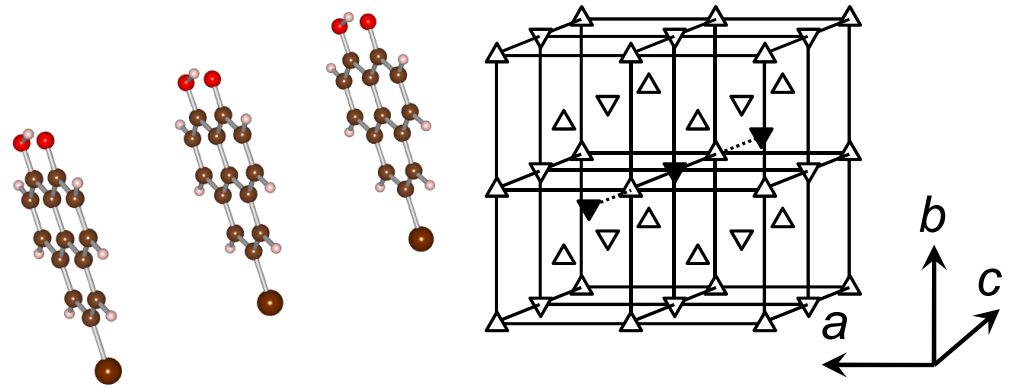

FIG. S5. Same as Fig. S1, but for trimer E.

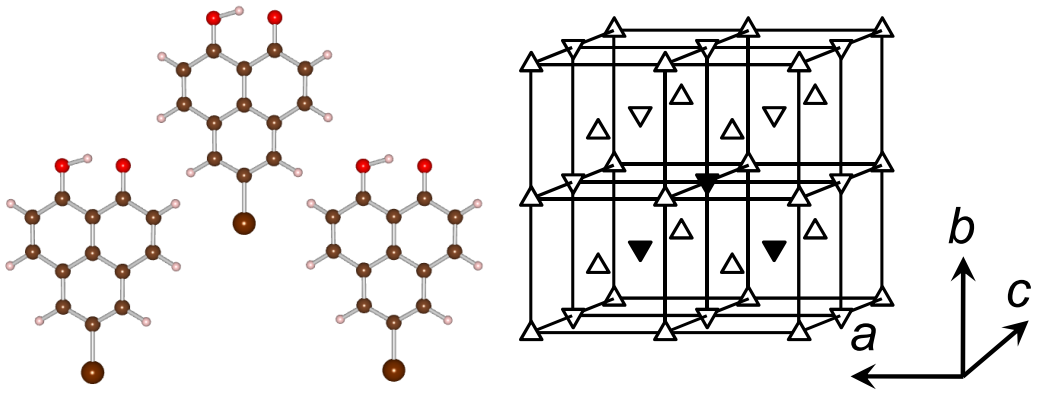

FIG. S6. Same as Fig. S1, but for trimer F.

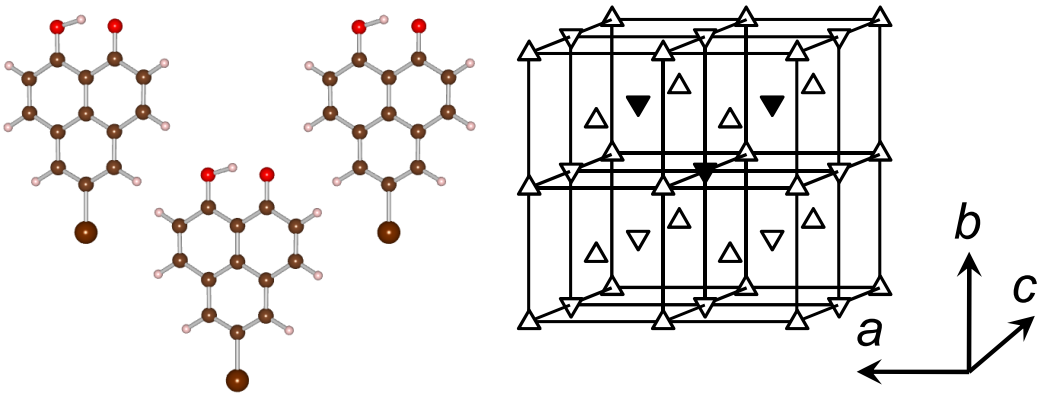

FIG. S7. Same as Fig. S1, but for trimer G.

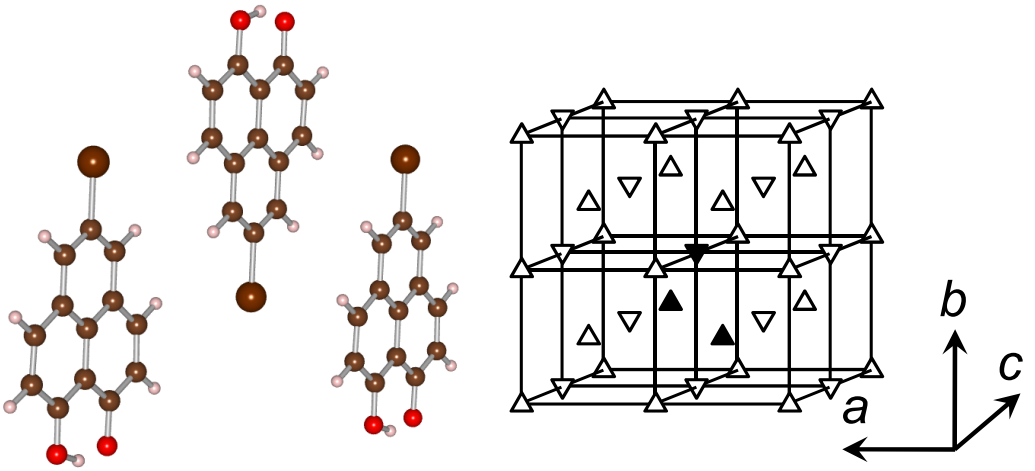

FIG. S8. Same as Fig. S1, but for trimer H.

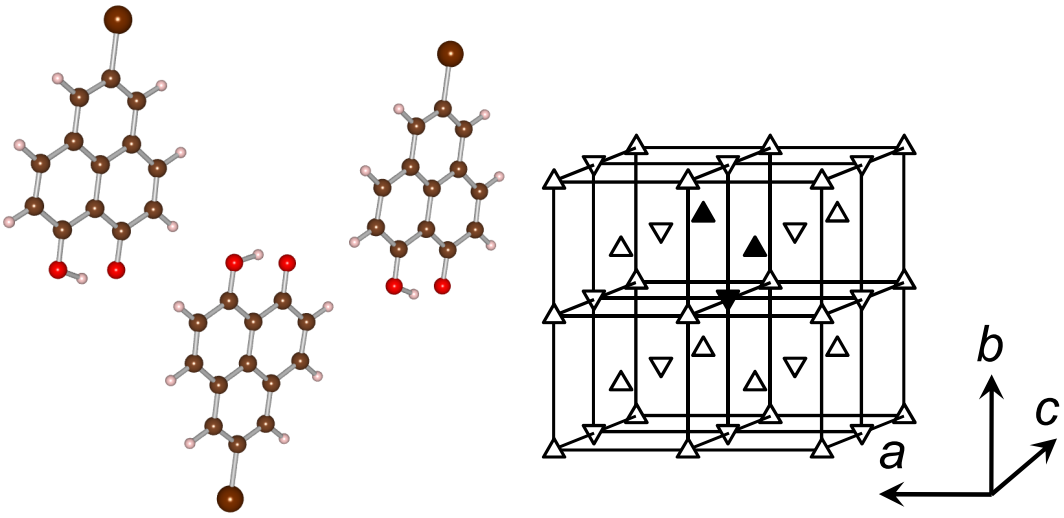

FIG. S9. Same as Fig. S1, but for trimer I.

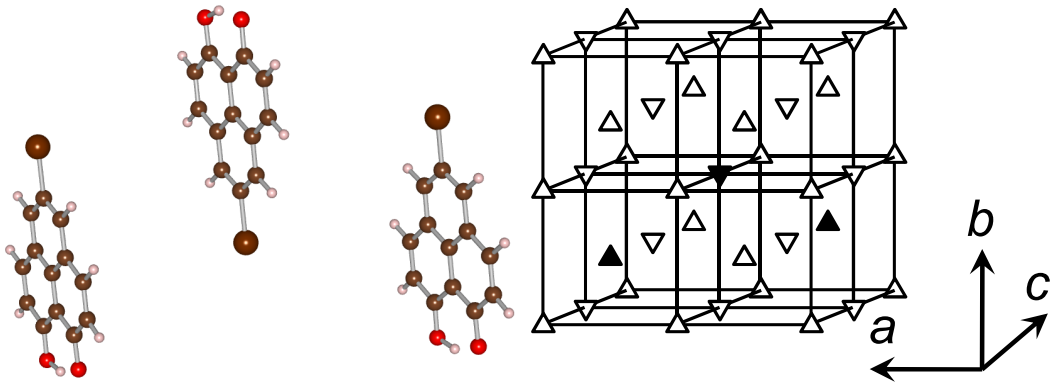

FIG. S10. Same as Fig. S1, but for trimer J.

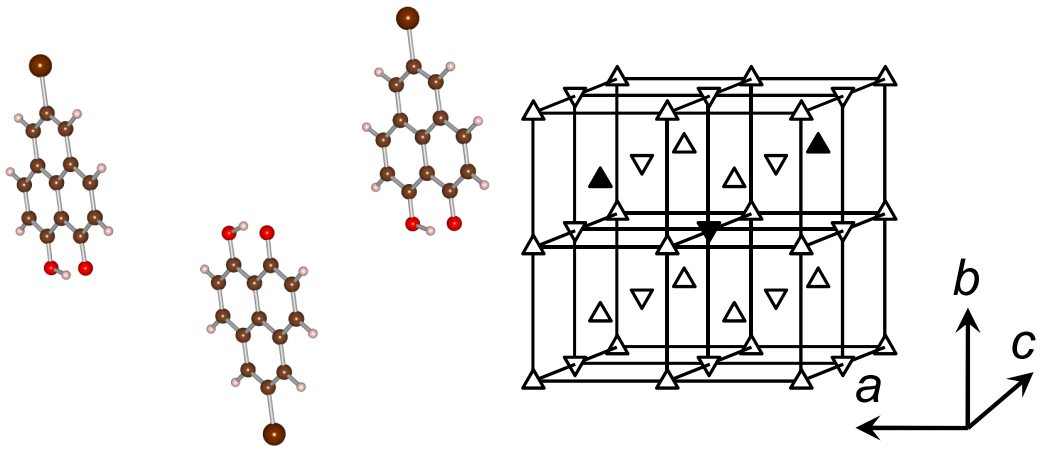

FIG. S11. Same as Fig. S1, but for trimer K.

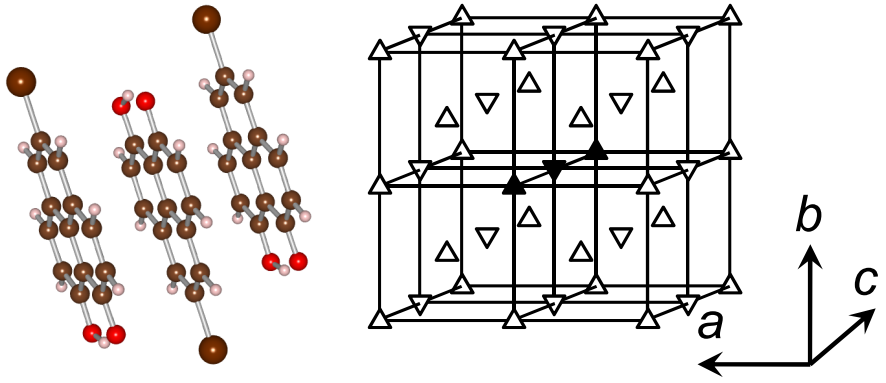

FIG. S12. Same as Fig. S1, but for trimer L.

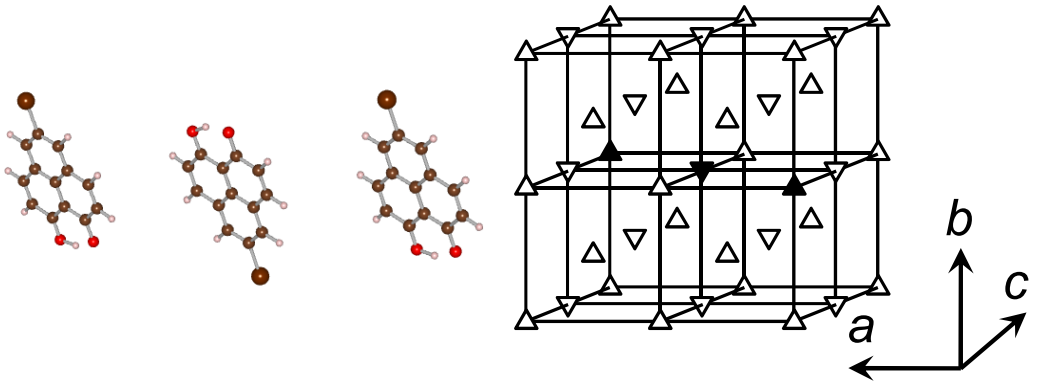

FIG. S13. Same as Fig. S1, but for trimer M.

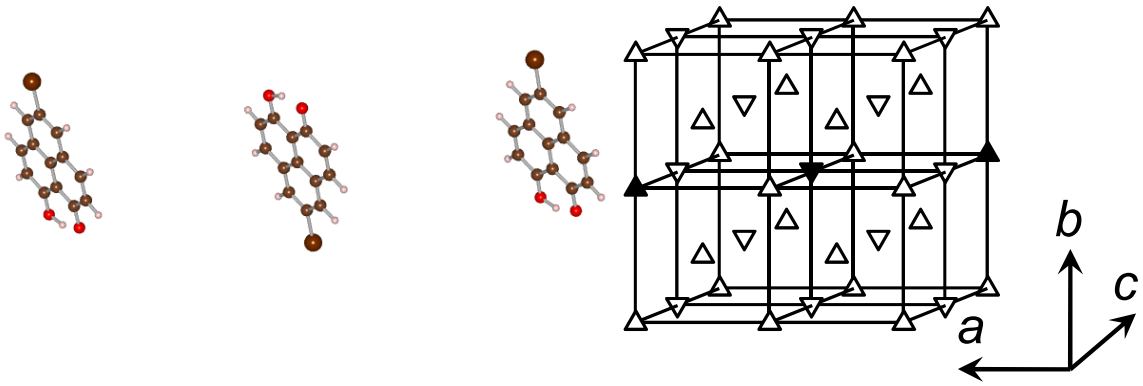

FIG. S14. Same as Fig. S1, but for trimer N.

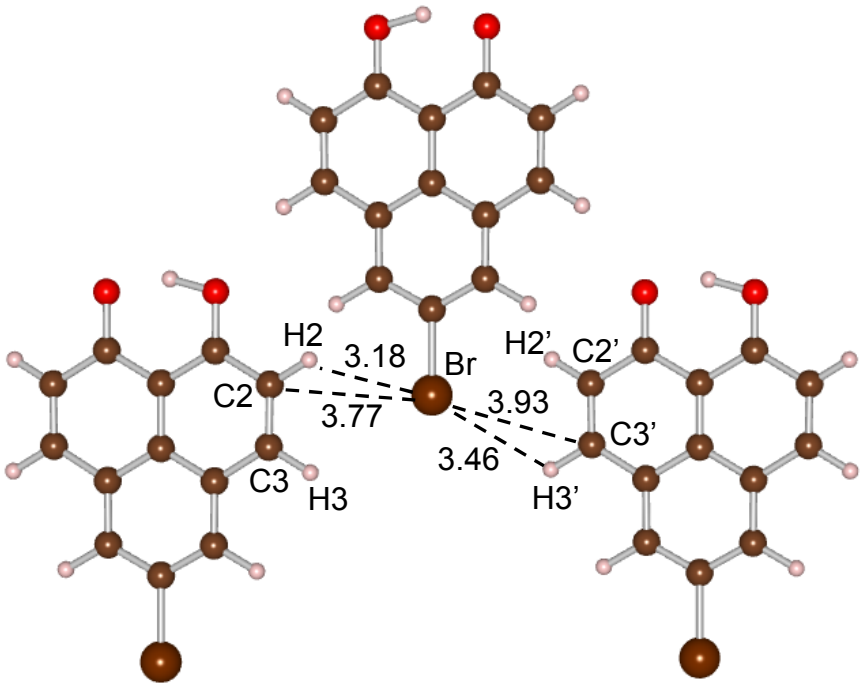

FIG. S15. Schematic structure of trimer F. The values in the figure denote the distances between atoms (in Å). Labels for atoms are given for Table S1.

TABLE S1. NPA charges for an isolated monomer and the central molecule of trimer F. The charges of the atoms around the Br atom of the central molecule are shown

	HF/3-21G(d,p)		HF/6-31G(d,p)	
Atom	Isolated	Central	Isolated	Central
Br	0.078	0.056	0.062	0.037
H2′	0.249	0.251	0.254	0.255
C2′	−0.323	−0.334	−0.317	−0.330
H3′	0.236	0.239	0.242	0.246
C3′	−0.109	−0.099	−0.112	−0.100
H2	0.249	0.253	0.254	0.256
C2	−0.334	−0.342	−0.327	−0.336
H3	0.238	0.241	0.244	0.249
C3	−0.095	−0.087	−0.099	−0.090