Electronic Supplementary Information†

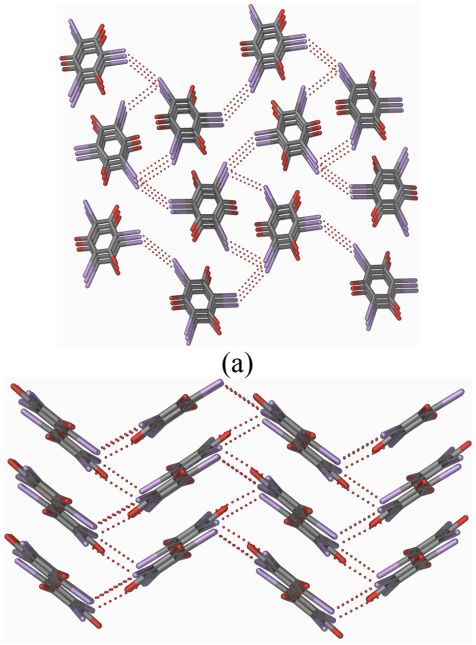


Figure S1 Solid-solution crystal structure of TIP+TIR-O. (a) Zigzag tapes mediated by I3···I2 (3.94 Å, 159.1°, 109.4°) type-II interaction along [010], (b) left-handed helix along [100] formed by I1··· I3 type-II interaction (3.96 Å, 146.3°, 82.0°), and (c) molecule make a corrugated sheet structure in (100) plane.

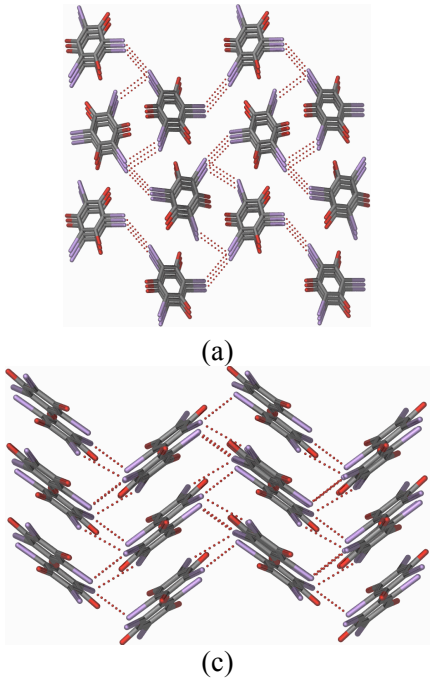
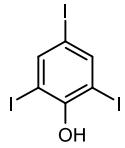
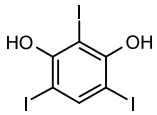
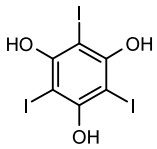
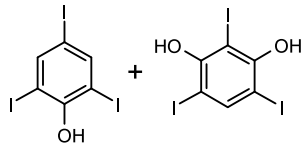
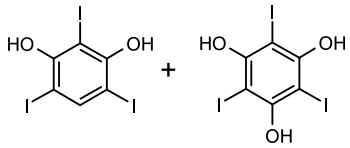
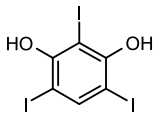
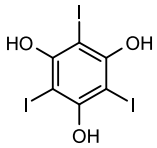
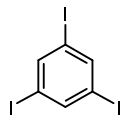
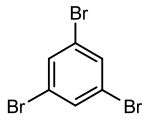
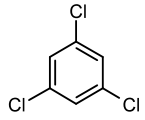
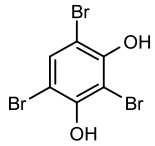
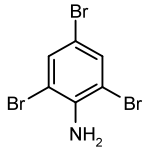
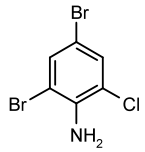
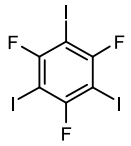


Figure S2 Packing diagram in solid-solution TIR+TIG-O. (a) Zigzag tapes mediated by I3···I2 type-II interaction (3.77 Å, 164.4°, 104.9°) along [010], (b) right-handed helix formed by I1···I3 (3.89 Å, 146.9°, 82.1°) along [100], and (c) corrugated sheet formed parallel to (100) plane.

Table S1 Space group and unit cell parameters of some halogen and hydroxyl substituted benzenes. Crystal data are taken from this paper and the Cambridge Structural Database (Version 5.29, November 2007, ConQuest 1.10, January 2008 update).

Compound/ Space group	a (Å)	b (Å)	c (Å)	β (°)	T (K)	V (Å^3)
This Paper						
 TIP ($P2_12_12_1$)	4.370	14.694	14.184	90	100	910.7
 TIR-O ($P2_12_12_1$)	4.495	13.958	15.036	90	100	943.3
 TIG-O ($P2_12_12_1$)	4.638	13.529	15.345	90	100	962.8
 TIP+TIR ($P2_12_12_1$)	4.442	14.368	14.573	90	100	930.1
 TIR+TIG ($P2_12_12_1$)	4.561	13.648	15.348	90	100	955.4
 TIR-M ($P2_1/n$)	14.882	4.332	15.585	108.49	100	952.8
 TIG ($P2_1/n$)	14.582	4.5004	15.507	107.57	100	970.2
Crystal data from CSD						
 TIB ($P2_12_12_1$)	4.329	14.224	14.515	90	161	893.7

 TBB($P2_12_12_1$)	14.23	13.55	4.08	90	298	786.7
 TCB ($P2_12_12_1$)	13.93	13.19	3.91	90	298	718.4
 TBR ($P2_12_12_1$)	4.107	12.855	15.296	90	120	807.6
 TBA ($P2_12_12_1$)	13.44	14.62	4.26	90	298	837.9
 BCA ($P2_12_12_1$)	4.178	13.24	14.86	90	298	822.2
 TIF ($P2_1/n$)	13.818	4.758	15.385	107.08	120	966.9