

**Supplementary Info**

**“Halogen/Methyl Exchange in a Series of Isostructural 1,3-bis(*m*-Dihalophenyl)Ureas”**

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**Figure S1.** (a) Calculated powder pattern for mClPU from the single crystal structure – grown from ethanol; powder patterns for mClPU grown from (b) ethanol, (c) 1:1 (v/v) acetonitrile:ethanol, (d) chloroform, (e) acetone, (f) acetonitrile and (g) benzene.

**Figure S2.** (a) Calculated powder pattern for mBrPU from the single crystal structure – grown from benzene; powder patterns for mBrPU grown from (b) the melt, (c) 1:1 (v/v) ethanol:acetonitrile, (d) dichloromethane, (e) 1:1 (v/v) acetone:hexanes, (f) vapor diffusion of hexanes into saturated ethanol and (g) vapor diffusion of hexanes into saturated acetonitrile.

**Figure S3.** (a) Calculated powder pattern for mIPU from the single crystal structure – grown from benzene; powder patterns for mIPU grown from (b) acetonitrile, (c) acetone, (d) ethanol, and (e) benzene.

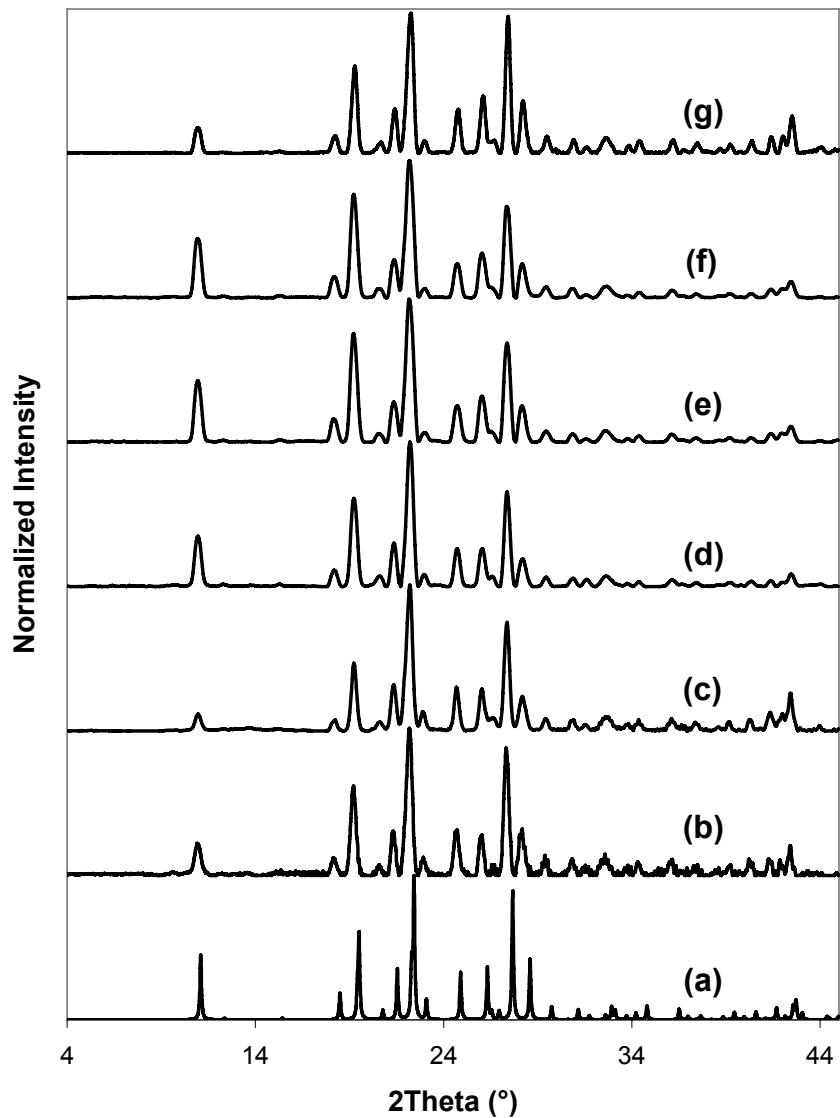
**Figure S4.** (a) Calculated powder pattern for mClMePU from the single crystal structure – grown from benzene; powder patterns for mClMePU grown from (b) benzene, (c) acetone, (d) ethyl acetate, (e) acetonitrile, (f) methylene chloride and (g) 2-propanol.

**Figure S5.** (a) Calculated powder pattern for mBrMePU from the single crystal structure – grown from acetonitrile; powder patterns for mBrMePU grown from (b) the melt, (c) acetonitrile, (d) ethanol, (e) layering of hexanes over saturated methylene chloride, (f) vapor diffusion of methylene chloride into saturated ethanol, (g) layering of benzene over saturated methylene chloride, and (h) vapor diffusion of hexanes into saturated benzene.

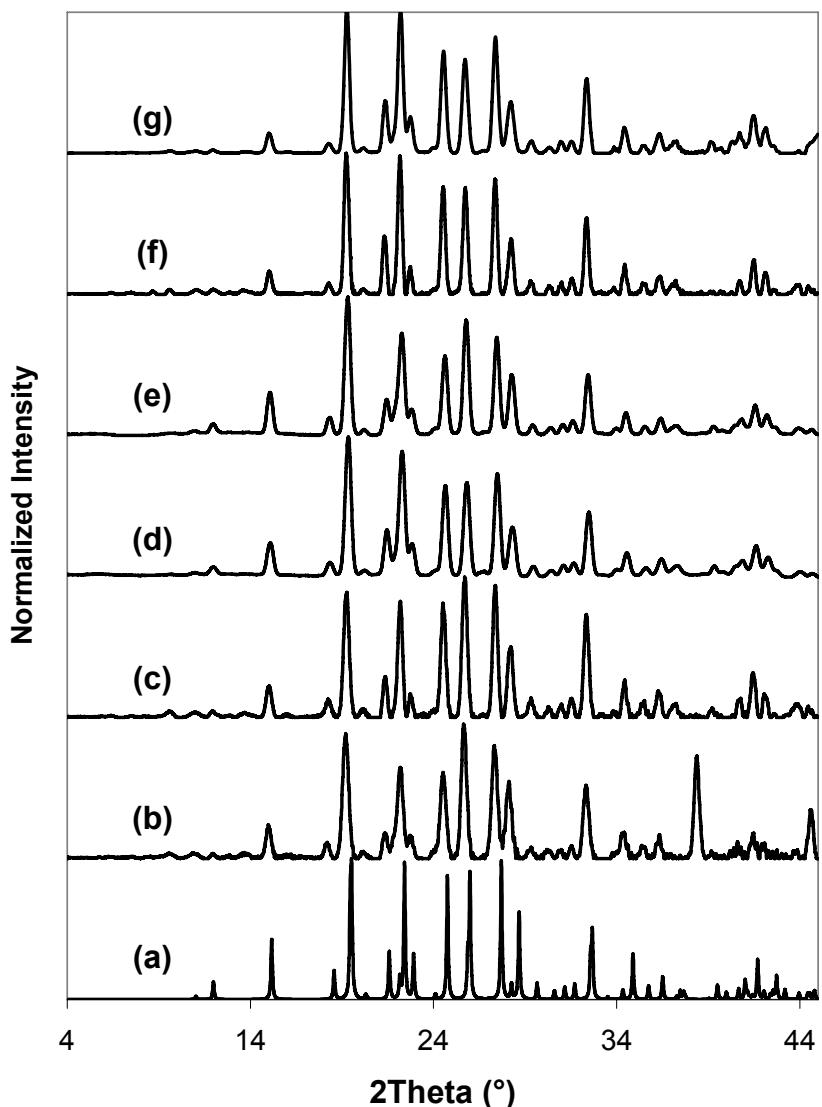
**Figure S6.** Powder patterns for mIMePU grown from (a) dichloromethane, (b) methanol, (c) 1:1 (v/v) n-heptane:propanol, (d) 1:1 (v/v) ethanol:acetonitrile, (e) benzene and (f) ethyl acetate. A single crystal structure of mIMePU could not be determined.

**Figure S7.** (a) Calculated powder pattern for mMePU from the single crystal structure – grown from 1:1 (v/v) ethanol:acetonitrile; powder patterns for mMePU grown from (b) 1:1 (v/v) acetone:acetonitrile, (c) 1:1 (v/v) acetone:benzene, (d) benzene, (e) ethyl acetate, (f) dichloromethane, (g) 1:1 (v/v) acetone:hexanes and (h) ethanol.

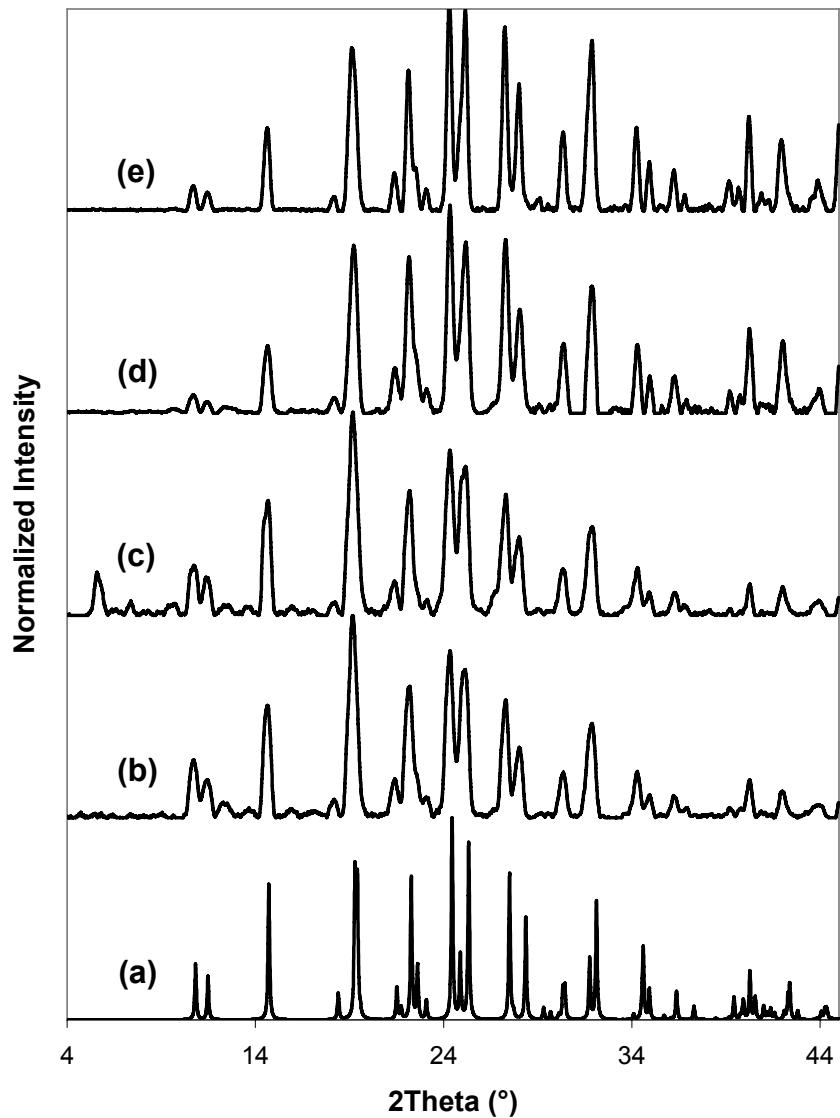
**Figure S1.** (a) Calculated powder pattern for mClPU from the single crystal structure – grown from ethanol; powder patterns for mClPU grown from (b) ethanol, (c) 1:1 (v/v) acetonitrile:ethanol, (d) chloroform, (e) acetone, (f) acetonitrile and (g) benzene.



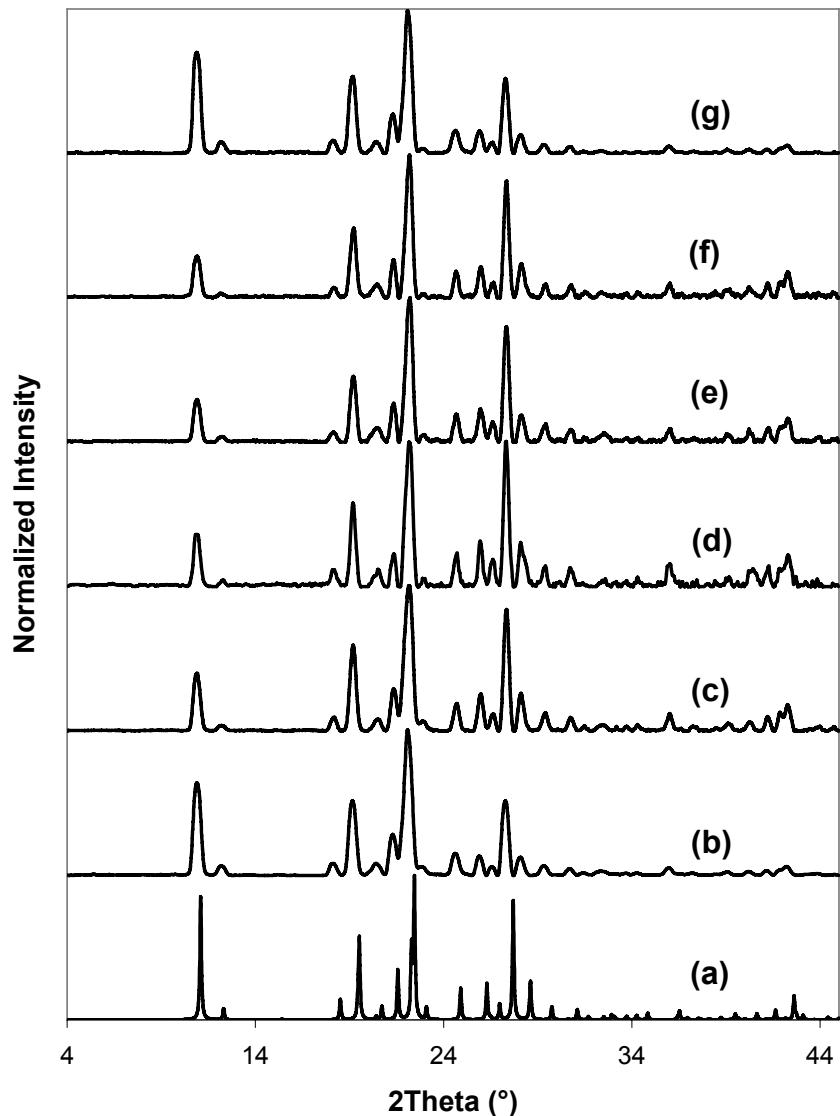
**Figure S2.** (a) Calculated powder pattern for mBrPU from the single crystal structure – grown from benzene; powder patterns for mBrPU grown from (b) the melt, (c) 1:1 (v/v) ethanol:acetonitrile, (d) dichloromethane, (e) 1:1 (v/v) acetone:hexanes, (f) vapor diffusion of hexanes into saturated ethanol and (g) vapor diffusion of hexanes into saturated acetonitrile.



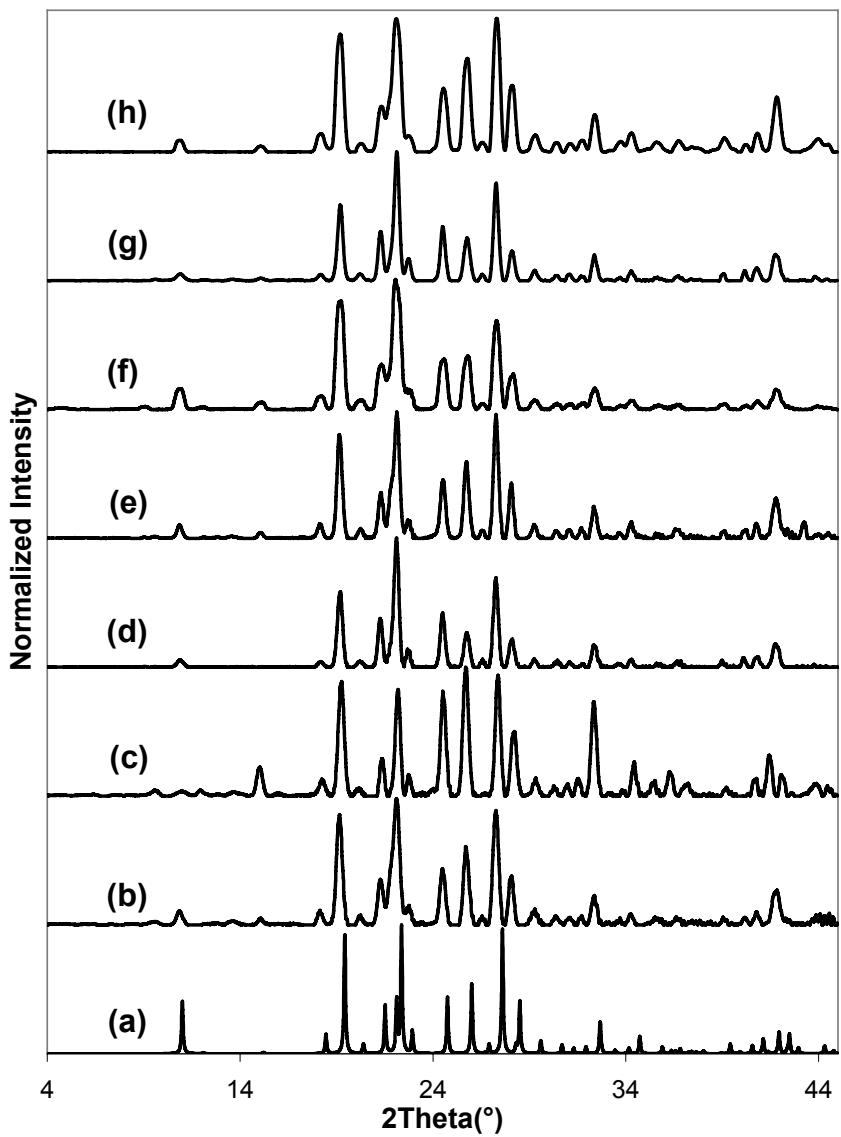
**Figure S3.** (a) Calculated powder pattern for mIPU from the single crystal structure – grown from benzene; powder patterns for mIPU grown from (b) acetonitrile, (c) acetone, (d) ethanol, and (e) benzene.



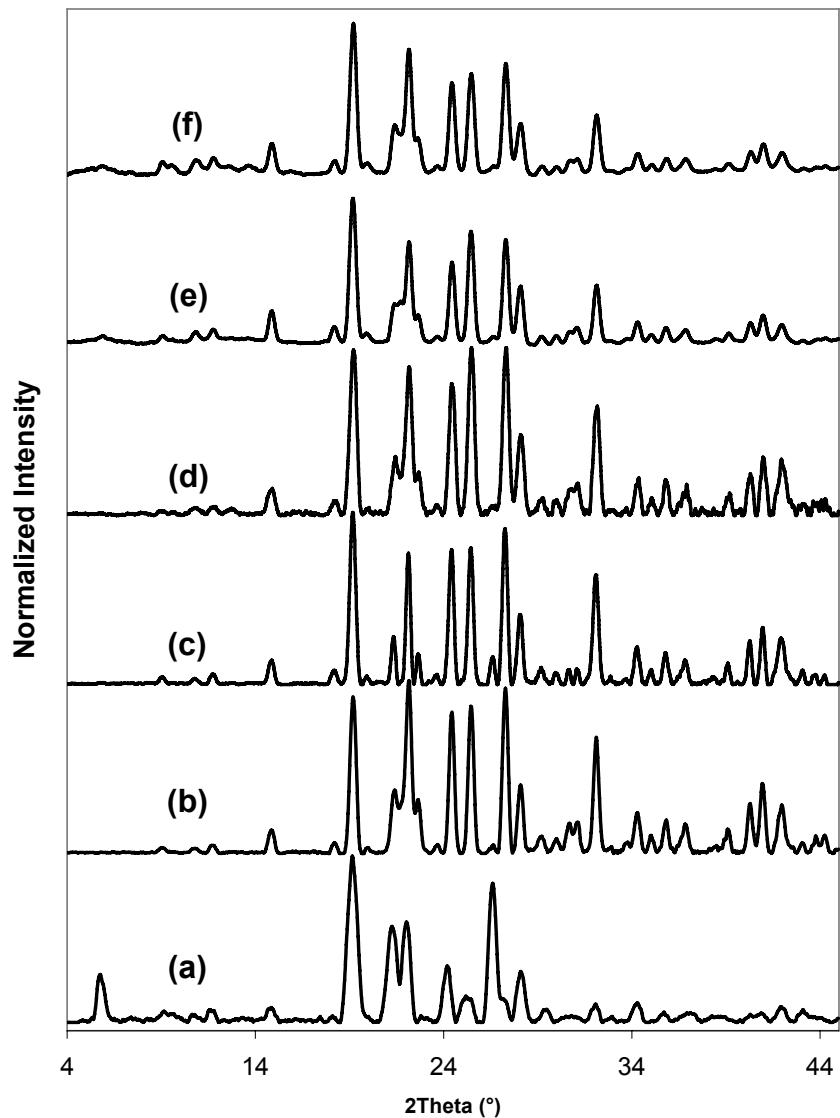
**Figure S4.** (a) Calculated powder pattern for mClMePU from the single crystal structure – grown from benzene; powder patterns for mClMePU grown from (b) benzene, (c) acetone, (d) ethyl acetate, (e) acetonitrile, (f) methylene chloride and (g) 2-propanol.



**Figure S5.** (a) Calculated powder pattern for mBrMePU from the single crystal structure – grown from acetonitrile; powder patterns for mBrMePU grown from (b) the melt, (c) acetonitrile, (d) ethanol, (e) layering of hexanes over saturated methylene chloride, (f) vapor diffusion of methylene chloride into saturated ethanol, (g) layering of benzene over saturated methylene chloride, and (h) vapor diffusion of hexanes into saturated benzene.



**Figure S6.** Powder patterns for mIMePU grown from (a) dichloromethane, (b) methanol, (c) 1:1 (v/v) n-heptane:propanol, (d) 1:1 (v/v) ethanol:acetonitrile, (e) benzene and (f) ethyl acetate. A single crystal structure of mIMePU could not been determined.



**Figure S7.** (a) Calculated powder pattern for mMePU from the single crystal structure – grown from 1:1 (v/v) ethanol:acetonitrile; powder patterns for mMePU grown from (b) 1:1 (v/v) acetone:acetonitrile, (c) 1:1 (v/v) acetone:benzene, (d) benzene, (e) ethyl acetate, (f) dichloromethane, (g) 1:1 (v/v) acetone:hexanes and (h) ethanol.

