

## Supplementary Materials

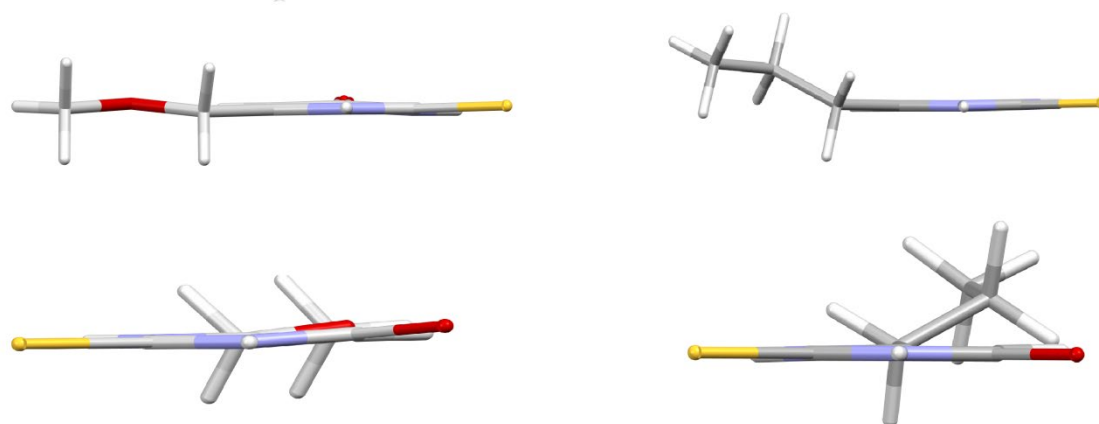


Figure S1 The view of MMTU (left) and PTU(right) from the aromatic ring perspective

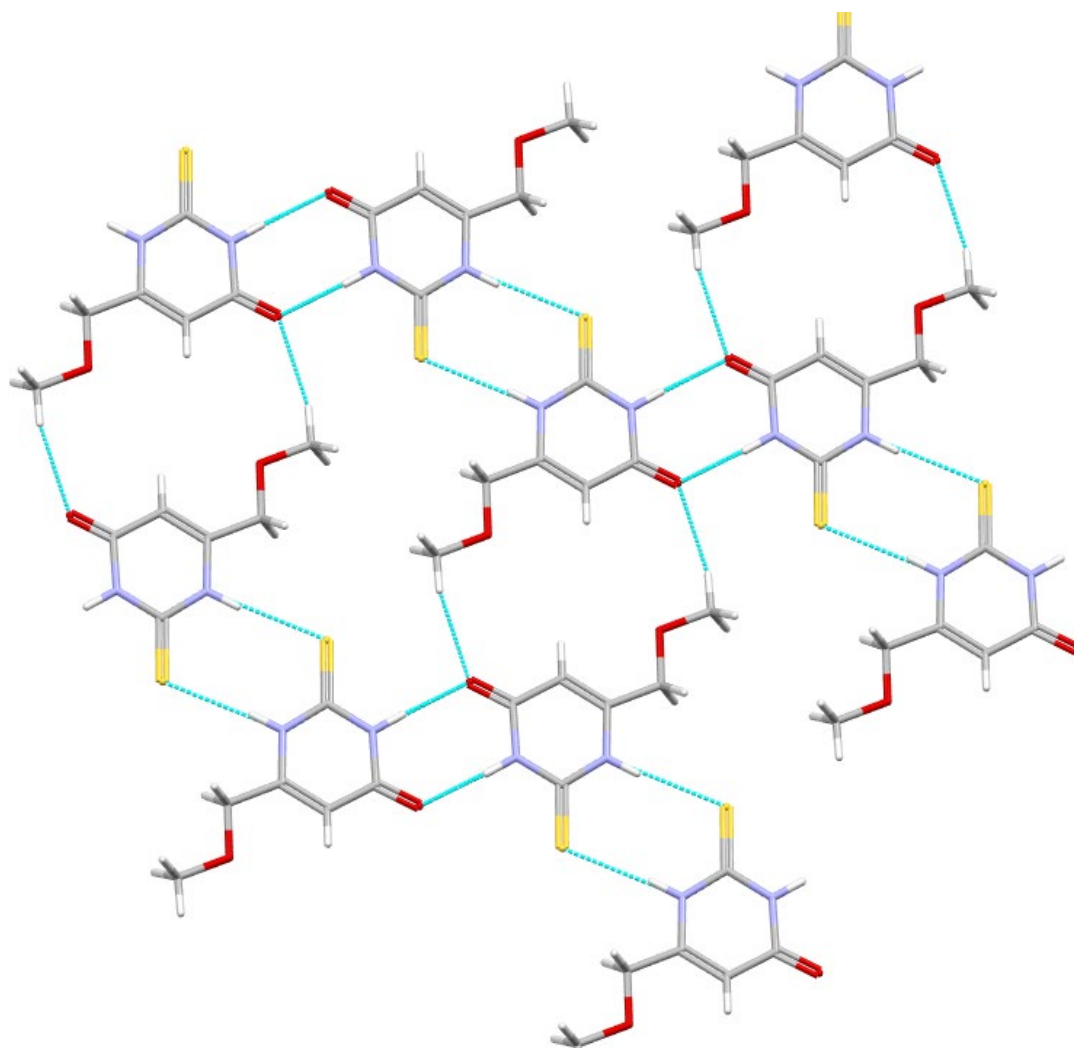


Figure S2 Two dimensional hydrogen bond layer in the crystal structure of MMTU

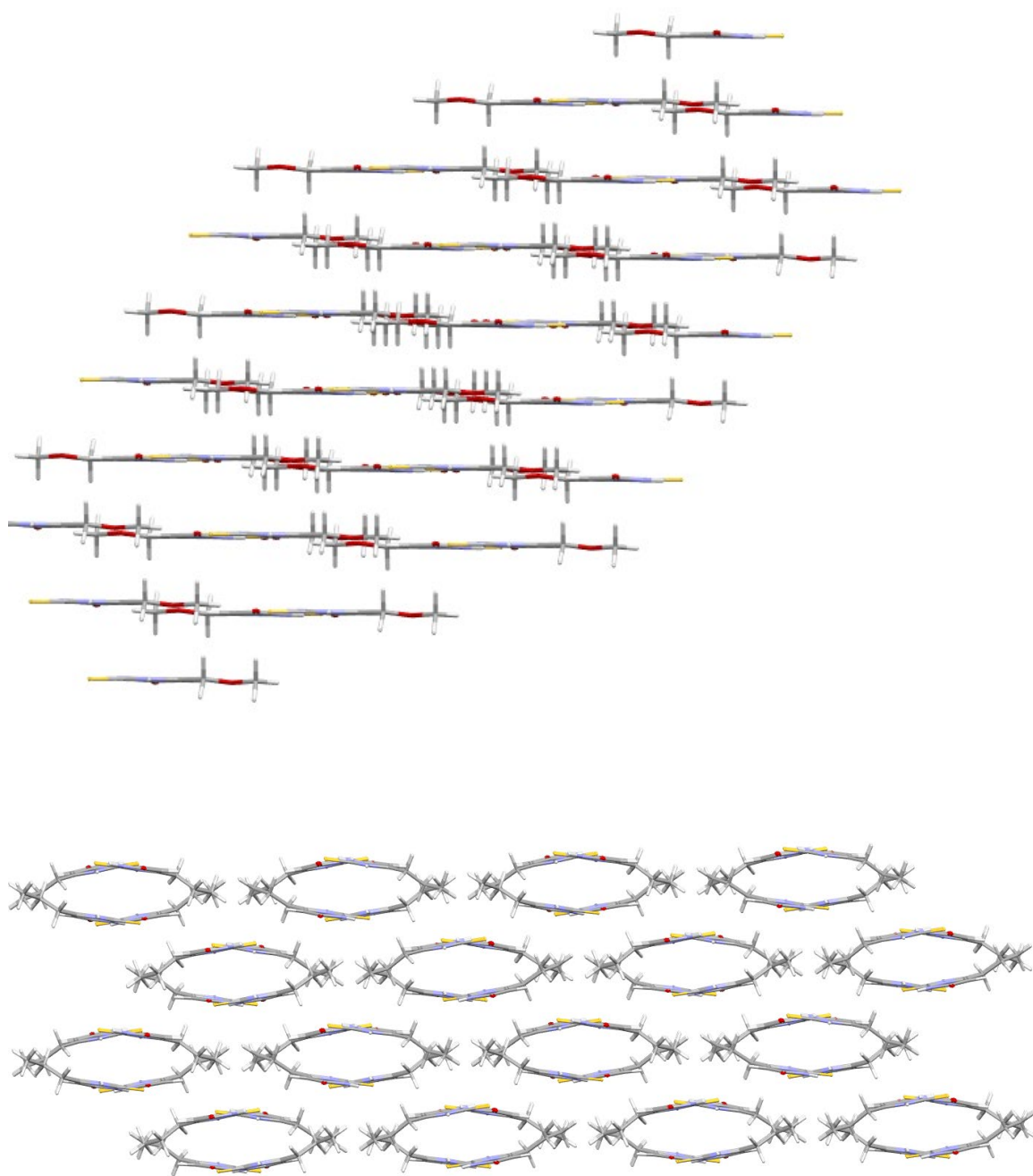


Figure S3 The crystal packing of MMTU (top) and PTU (bottom) along the NH...S, NH...O hydrogen bonded chains

**Table S1.** Crystallographic data and refinement details.

MMTU		
Crystal data		
Chemical formula	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> S	
<i>M</i> <sub>r</sub>	172.20	
Crystal system, space group	Triclinic, <i>P</i> <sup>−</sup> 1	
Temperature (K)	130	
<i>a</i> , <i>b</i> , <i>c</i> (Å)	4.4995 (1), 9.2328 (3), 9.9558 (3)	
α, β, γ (°)	112.581 (3), 91.546 (2), 97.313 (2)	
<i>V</i> (Å <sup>3</sup> )	377.48 (2)	
<i>Z</i>	2	
Radiation type	Cu <i>K</i> α	
μ (mm <sup>−1</sup> )	3.43	
Crystal size (mm)	0.38 × 0.26 × 0.24	
Data collection		
Absorption correction	Multi-scan	
<i>T</i> <sub>min</sub> , <i>T</i> <sub>max</sub>	0.492, 1.000	
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	13348, 1526, 1507	
<i>R</i> <sub>int</sub>	0.027	
(sin θ/λ) <sub>max</sub> (Å <sup>−1</sup> )	0.625	
Refinement		
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>Goof</i>	0.031, 0.087, 1.07	
No. of reflections	1526	
No. of parameters	132	
Δ <sub>max</sub> , Δ <sub>min</sub> (e Å <sup>−3</sup> )	0.35, −0.29	
CCDS deposition number	2387155	