Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

Assemblies of Salts of Urea and Thiourea Derivatives and Release of Host from Composites with Calcium oxide

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Figure S16. Fluorescence spectroscopic titration (λ_{ex} = 258 nm) of *Hnaphurea.*$ClO_4.H_2O$ (10 μM) in water upon addition of $NaHAsO_4.7H_2O$ (As in +5 oxidation state) (10 μM in 10 μL aliquots) showing enhancement of emission.

Figure S17. Fluorescence spectroscopic titration (λ_{ex} = 258 nm) of *Hnaphurea.*$ClO_4.H_2O$ (10 μM) in water upon addition of NaOH (10 μM in 10 μL aliquots) showing enhancement of emission.

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Figure S34. Intensity versus time curve of different ratios of *Hnaphurea*@CaO pellets in water (λ_{ex} = 258 nm, λ_{em} = 385 nm).

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Table 1Sa. Crystallographic parameters of the urea/thiourea derivatives and their salts

Parameters	*Hphenurea.ClO$_4$*	*phenthiourea*	*Hphenthiourea.ClO$_4$*	*Hphenthiourea.NO$_3$*
Formula	$C_{13}H_{14}ClN_3O_5$	$C_{13}H_{13}N_3S$	$C_{13}H_{14}ClN_3O_4S$	$C_{13}H_{14}N_4O_3S$
CCDC	2171843	2171848	2172477	2171845
Mol.wt.	327.72	243.334	343.78	306.34
Space group	Pbca	P2$_1$/c	I2/a	P2$_1$/c
a(Å)	10.6033(11)	5.9160(4)	18.620(3)	11.5055(9)
b(Å)	9.1856(9)	22.1005(16)	5.4988(8)	8.4091(7)
c (Å)	30.910(3)	9.9693(5)	30.636(4)	14.4045(13)
α (°)	90	90	90	90
β (°)	90	100.216(6)	96.337(8)	92.059(3)
γ (°)	90	90	90	90
V (Å^3)	3010.5(5)	1282.79(14)	3117.6(8)	1392.7(2)
Density, g cm^{-3}	1.446	1.260	1.465	1.461
Abs. coeff., mm^{-1}	0.281	0.233	0.400	0.249
F (000)	1360	512.756	1424	640
Total no. of reflections	2666	2256	2750	2460
Reflections, I > 2σ(I)	1762	1630	2062	1890
Max. θ/°	25.047	25.04	24.998	25.046
Ranges (h, k, l)	$-11\leq h \leq 12$	$-7\leq h \leq 7$	$-22\leq h \leq 22$	$-13\leq h \leq 13$
	$10\leq k \leq 10$	$-29\leq k \leq 27$	$-6\leq k \leq 6$	$-10\leq k \leq 10$
	$-36\leq l \leq 36$	$-6\leq l \leq 12$	$-36\leq l \leq 36$	$-17\leq l \leq 17$
Complete to 2θ (%)	99.7	99.9	99.9	99.8
Data/restraints/parameters	2666/6/ 220	2256/0/162	2750/ 0/ 199	2460/1/190
GooF (F^2)	1.046	1.0614	1.038	1.031
R indices [I > 2σ(I)]	0.0650	0.0410	0.0810	0.0443
wR$_2$ [I > 2σ(I)]	0.1792	0.0834	0.1397	0.1023
R indices (all data)	0.0997	0.0645	0.1098	0.0610
wR$_2$ (all data)	0.2044	0.0949	0.1649	0.1121

Table 1Sb. Crystallographic parameters of the urea/thiourea derivatives and their salts

Parameters	*naphurea.H_2O*	*Hnaphurea.ClO_4.H_2O*	*Hnaphurea.NO_3*	*Naphthiourea*	*Hnapthiourea.ClO_4*
Formula	$C_{17}H_{17}N_3O_2$	$C_{17}H_{18}ClN_3O_6$	$C_{17}H_{16}N_4O_4$	$C_{17}H_{15}N_3S$	$C_{17}H_{16}ClN_3O_4S$
CCDC	2171849	2171846	2171847	2173492	2171850
Mol.wt.	295.33	395.79	340.34	293.38	393.84
Space group	$Pca2_1$	$P2_1/c$	Pbca	$P\bar{1}$	Pbca
a(Å)	43.205(6)	10.886(3)	15.1546(10)	9.4256(6)	8.241(2)
b(Å)	7.7050(11)	8.2613(18)	13.0529(9)	9.7491(6)	17.685(5)
c (Å)	4.5617(6)	20.140(5)	16.4184(11)	17.9657(12)	25.201(7)
α (°)	90	90	90	85.658(2)	90
β (°)	90	98.990(6)	90	85.018(2)	90
γ (°)	90	90	90	69.168(2)	90
V ($Å^3$)	1518.6(4)	1789.0(7)	3247.7(4)	1535.35(17)	3672.9(18)
Density, g cm^{-3}	1.292	1.470	1.392	1.269	1.424
Abs. coeff., mm^{-1}	0.087	0.255	0.102	0.207	0.349
F (000)	624	824	1424	616	1632
Total no. of reflections	2570	3124	2397	5374	3225
Reflections, I > 2σ(I)	1986	2554	1862	4443	2744
Max. θ/°	24.684	25.046	23.490	25.000	24.998
Ranges (h, k, l)	$-50\leq h\leq 50$	$-12\leq h\leq 12$	$-16\leq h\leq 16$	$-11\leq h\leq 11$	$-9\leq h\leq 9$
	$-9\leq k\leq 9$	$-9\leq k\leq 9$	$-14\leq k\leq 14$	$-11\leq k\leq 11$	$-21\leq k\leq 21$
	$-5\leq l\leq 5$	$-23\leq l\leq 23$	$-18\leq l\leq 18$	$-21\leq l\leq 21$	$-29\leq l\leq 29$
Complete to 2θ (%)	99.7	99.0	99.8	99.4	99.8
Data/restraints/parameters	2570/1/215	3124/0/260	2397/0/238	5374/1/ 395	3225/0/248
GooF (F^2)	1.133	1.053	1.258	1.095	1.087
R indices [I > 2σ(I)]	0.0890	0.0629	0.0669	0.0486	0.0640
wR_2 [I > 2σ(I)]	0.2066	0.1658	0.1166	0.0965	0.1600
R indices (all data)	0.1236	0.0773	0.0895	0.0617	0.0753
wR_2 (all data)	0.2288	0.1860	0.1314	0.1055	0.1666

Table S2. Hydrogen-bond parameters in the urea/thiourea derivatives and corresponding perchlorate and nitrate salts

Salts	D-H···A	d_{D-H} (Å)	$d_{H\cdots A}$ (Å)	$d_{D\cdots A}$ (Å)	∠D-H···A (°)
Hphenurea.ClO_4	N(1) -H(1) ···O(1) [3/2-x, -1/2+y, z]	0.85 (2)	2.00 (2)	2.833 (3)	166 (3)
	N(2) -H(2) ···O(1) [3/2-x, -1/2+y, z]	0.849 (19)	2.30 (2)	3.034 (3)	145 (3)
	N(3) -H(3) ···O(5A) [1-x,1-y,-z]	0.86	1.88	2.675 (10)	153
	N(3) -H(3) ···O(3A^B) [1-x,1-y,-z]	0.86	2.31	3.051 (19)	144
	N(3) -H(3) ···O(5A^B) [1-x,1-y,-z]	0.86	2.23	3.05 (3)	160
	C(8) -H(8B) ···O(4A) [x,y,z]	0.97	2.40	3.314 (8)	157
	C(8) -H(8B) ···O(2A^B) [x,y,z]	0.97	2.36	3.24 (3)	151
	C(11) -H(11) ···O(2A) [1/2+x,1/2-y,-z]	0.93	2.49	3.367 (8)	157
Phenthiourea	N(1) -H(1) ···S(1) [-x, -y, 1-z]	0.85 (2)	2.50 (2)	3.340 (2)	168.6 (19)
	N(2) -H(2) ···N(3) [x, 1/2-y, -1/2+z]	0.91(2)	2.21 (2)	3.005 (3)	144.7(18)
Hphenthiourea.ClO_4	N(1) –H(1A)···S(1) [1/2-x, 5/2-y, 1/2-z]	0.86	2.53	3.355 (4)	162
	N(2) -H(2A) ···O(3) [x, y, z]	0.86	2.17	2.940 (8)	150
	N(3) -H(3A) ···O(4) [1/2+x, 1-y, z]	0.86	1.91	2.750 (10)	167
Hphenthiourea .NO_3	N(1) -H(1) ···O(2) [1-x, 1/2+y, 1/2-z]	0.86	2.21	3.052 (3)	167
	N(3) -H(3) ···O(1) [x, 1/2-y, 1/2+z]	0.86	1.95	2.803 (3)	173
naphurea.H_2O	N(1) -H(1A) ··· O(1) [x, y, -1+z]	0.77 (9)	2.15 (9)	2.858 (9)	153 (8)
	N(2) -H(2A) ···O(1) [x, y, -1+z]	0.83 (9)	2.12(9)	2.873 (9)	151 (7)
	O(2) -H(2C) ···O(2) [1/2-x, y, -1/2+z]	0.82 (12)	1.94 (12)	2.750 (11)	172 (9)
	O(2) -H(2D) ···N(3) [x, 1+y, -1+z]	0.86 (9)	2.03 (10)	2.873 (11)	170 (8)
Hnaphurea.ClO_4.H_2O	O(6) -H(6A) ···O(1) [x, 1+y, z]	0.85	2.04	2.892 (4)	177
	N(1) -H(1) ···O(1) [1-x, 1/2+y, 1/2-z]	0.86	2.22	3.010 (3)	153
	O(6) -H(6B) ···O(2) [x, 1+y, z]	0.85	2.40	3.183 (7)	154
	N(2) -H(2) ···O(1) [1-x, 1/2+y, 1/2-z]	0.86	2.17	2.975 (3)	156
	N(3) -H(3) ···O(6) [-x, -1/2+y, 1/2-z]	0.86	1.89	2.723 (5)	164

	C(4) -H(4) ···O(2A^B) [1-x, -y, -z]	0.93	2.58	3.50 (4)	169
	C(14) -H(14) ···O(2) [x, y, z]	0.93	2.51	3.377 (7)	156
	C(15) -H(15) ···O(5A^B) [x, y, z]	0.93	2.33	3.10 (2)	141
	C(16) -H(16) ···O(4A^B) [x, 1/2-y, 1/2+z]	0.93	2.56	3.349 (7)	143
Hnaphurea.NO_3	N(1) -H(1) ···O(2) [x, 1/2-y, -1/2+z]	0.86 (3)	2.01 (3)	2.860 (4)	170 (4)
	N(2) -H(2) ···O(3) [x, 1/2-y, -1/2+z]	0.87 (4)	2.05 (4)	2.903 (4)	169 (3)
	N(3) -H(3) ···O(1) [-1/2+x, y, 1/2-z]	1.04 (5)	1.63 (5)	2.663 (4)	170 (4)
	C(15) -H(15) ···O(4) [-1/2+x, y, 1/2-z]	0.93	2.58	3.506 (4)	171
naphthiourea	N(1) -H(1) ···S(1) [1-x, -y, 1-z]	0.82 (3)	2.60 (3)	3.391(2)	164 (3)
	N(2) -H(2) ···N(6) [-x, 1-y, 1-z]	0.84 (2)	2.145 (19)	2.888 (3)	147.1 (17)
	N(4) -H(4A) ···S(2) [1-x, -y, -z]	0.82 (3)	2.61 (3)	3.415 (2)	169 (2)
	N(5) -H(5) ···N(3) [1-x, 1-y, 1-z]	0.80 (3)	2.13 (3)	2.888 (4)	158 (2)
Hnapthiourea.ClO_4	N(1) -H(1) ···S(1) [-1/2+x, y, 1/2-z]	0.86	2.46	3.264 (3)	157
	N(2) -H(2) ···O(3A) [x, y, z]	0.86	2.26	3.053 (10)	152
	N(2) -H(2) ···O(3A^B) [x, y, z]	0.86	2.31	3.02 (4)	140
	N(3) -H(3) ···O(3A) [1/2-x, 1/2+y, z]	0.86	2.01	2.847 (10)	164
	N(3) -H(3) ···O(3A^B) [1/2-x, 1/2+y, z]	0.86	2.06	2.83 (4)	148
	N(3) -H(3) ···O(4A^B) [1/2-x, 1/2+y, z]	0.86	2.40	3.122 (19)	142
	C(15) -H(15) ···O(4A^B) [-x, 1-y, -z]	0.93	2.47	3.279 (18)	145

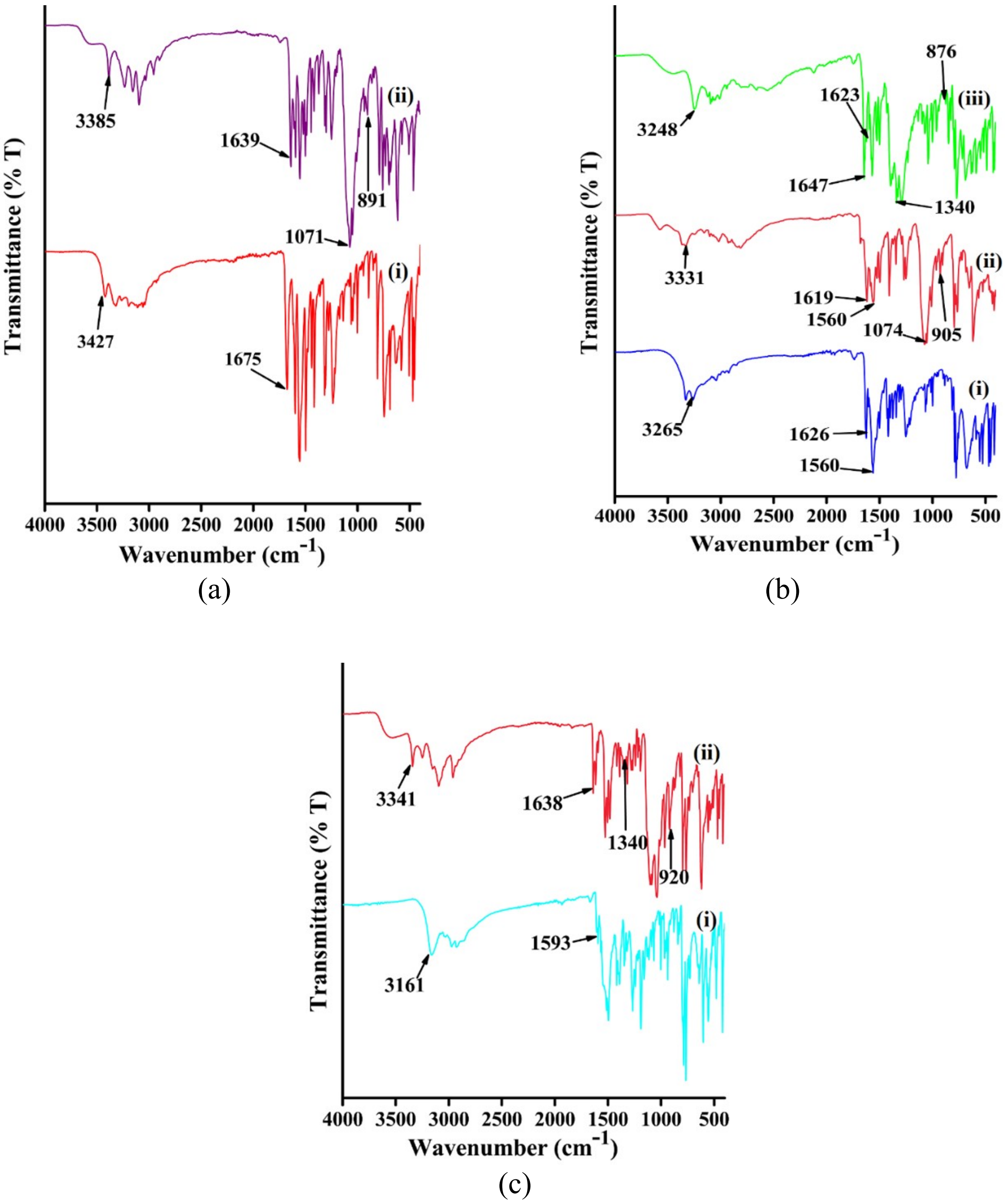
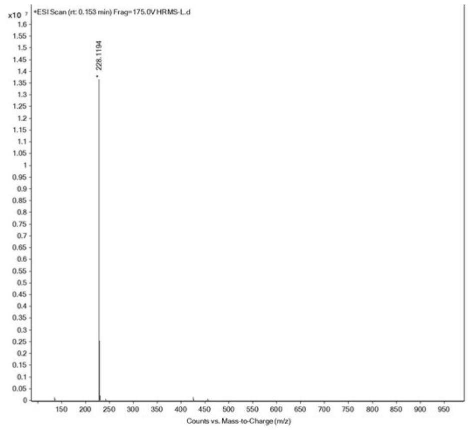


Figure S1. IR-spectra of the solid samples of (a) (i) *phenurea.H_2O*, (ii) *Hphenurea.ClO_4,* (b) (i) *naphurea.H_2O*, (ii) *Hnaphurea.ClO_4.H_2O*, (iii) *Hnaphurea.NO_3*; (c) (i) *naphthiourea*, (ii) *Hnaphthiourea ClO_4*.



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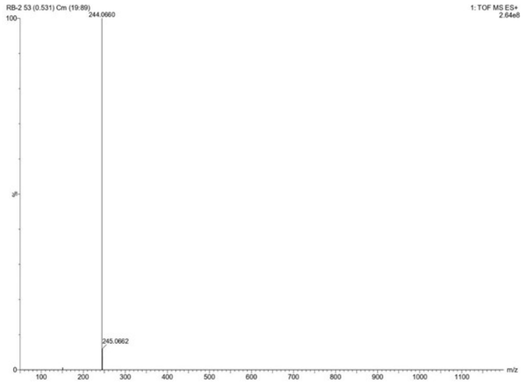

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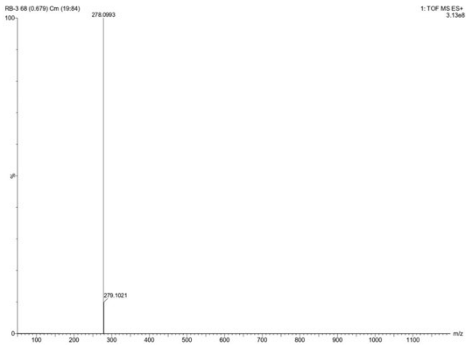

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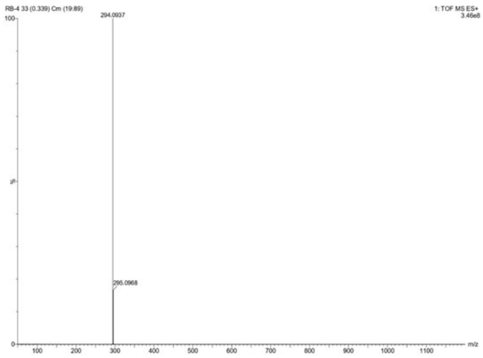
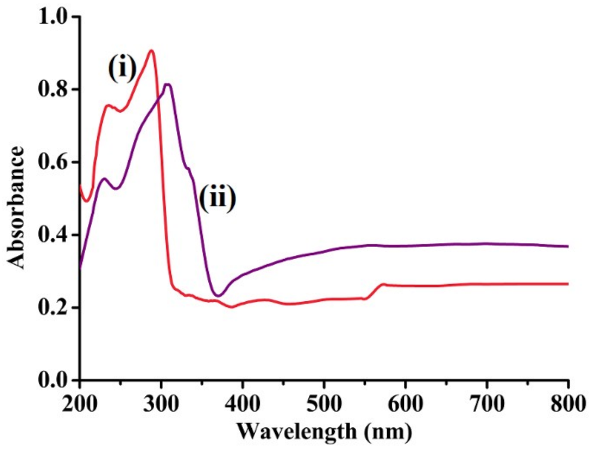


(d)

Figure S2. ESI mass of the (a) *phenurea*, (b) *phenthiourea*, (c) *naphurea* and (d) *naphthiourea*.



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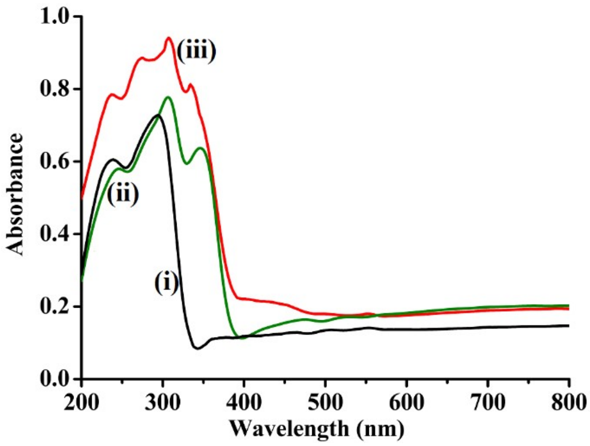

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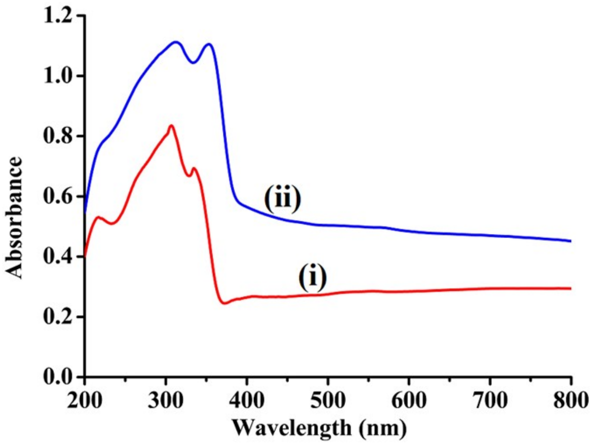
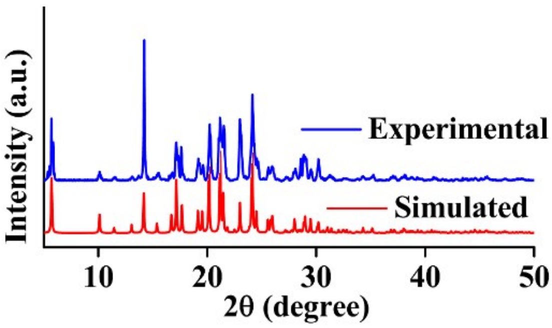
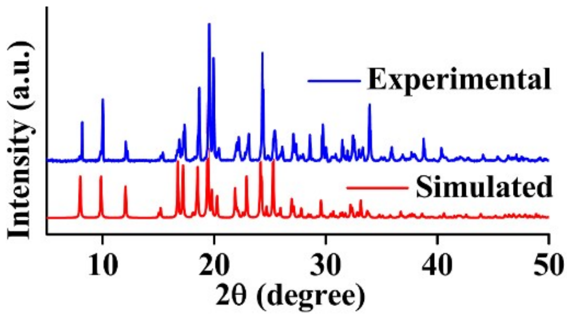


(c)

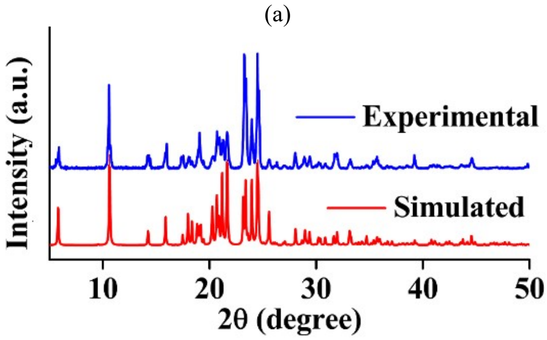
Figure S3. UV-vis spectra of solid samples of (a) *phenurea.H_2O* (λ_{max} = 291 nm), *Hphenurea.ClO_4* (λ_{max} = 309 nm), (b) (i) *phenthiourea* (λ_{max} = 295 nm), (ii) *Hphenthiourea.ClO_4* (λ_{max} = 307 nm), (iii) *Hphenthiourea.NO_3* (λ_{max} = 307 nm), (c) (i) *naphthiourea* (λ_{max} = 306 nm), (ii) *Hnaphthiourea.ClO_4* (λ_{max} = 312 nm, 353 nm).



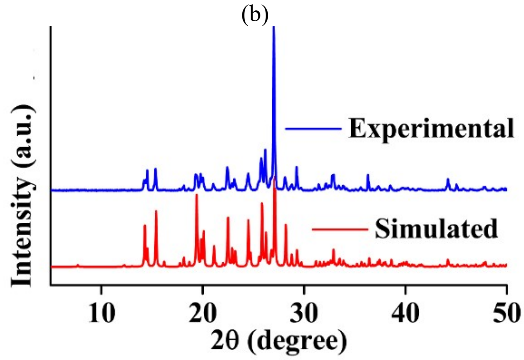
(a)



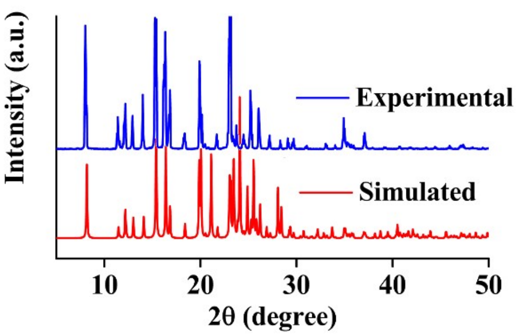
(b)



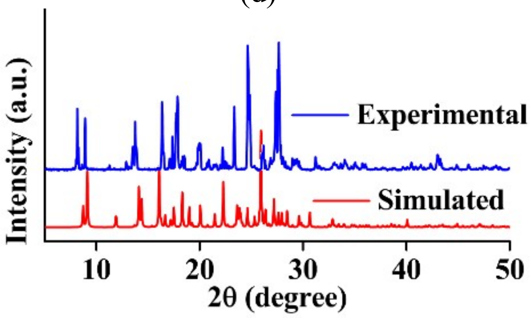
(c)



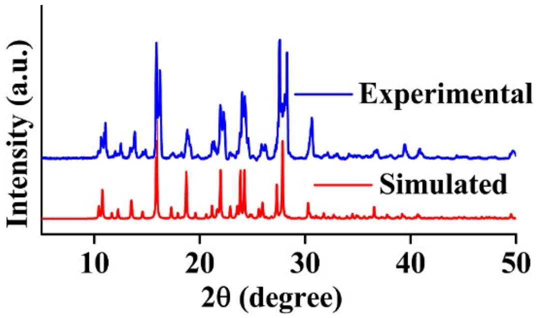
(d)



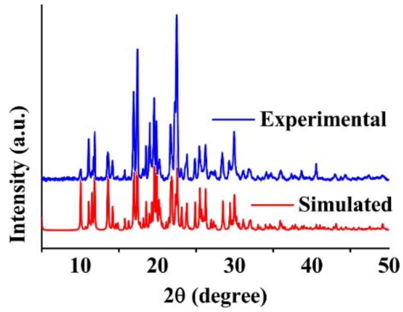
(e)



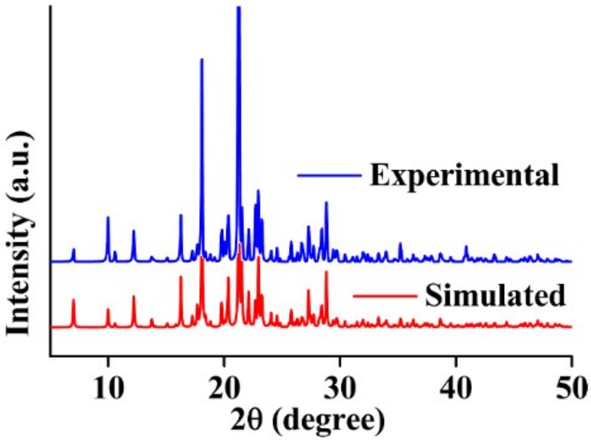
(f)



(g)

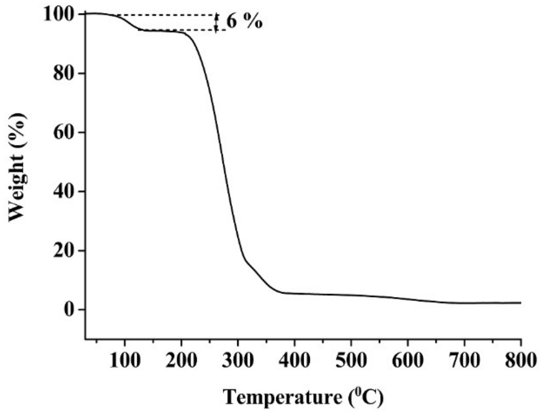


(h)

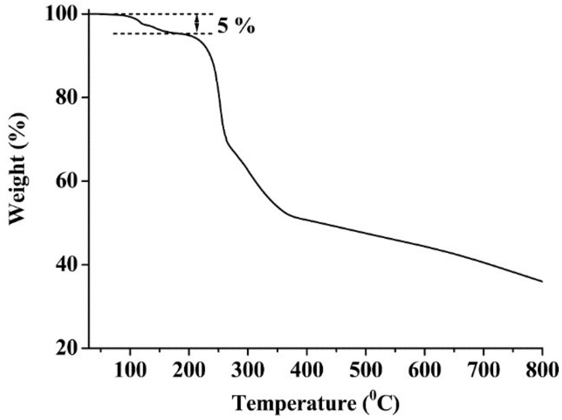


(i)

Figure S4. Powder X-ray diffraction patterns of (a) *Hphenurea.ClO$_4$,* (b) *phenthiourea,* (c) *Hphenthiourea.ClO$_4$*, (d) *Hphenthiourea*.NO$_3$, (e) *naphurea.H$_2$O*, (f) *Hnaphurea.ClO$_4$.H$_2$O*, (g) *Hnaphurea.NO$_3$*, (h) *naphthiourea*, (i) H*naphthiourea*.*ClO$_4$*.



(a)



(b)

Figure S5. Thermogram of (a) *naphurea.H$_2$O*, (b) *Hnaphurea.ClO$_4$.H$_2$O* (heating rate 10˚C/min).

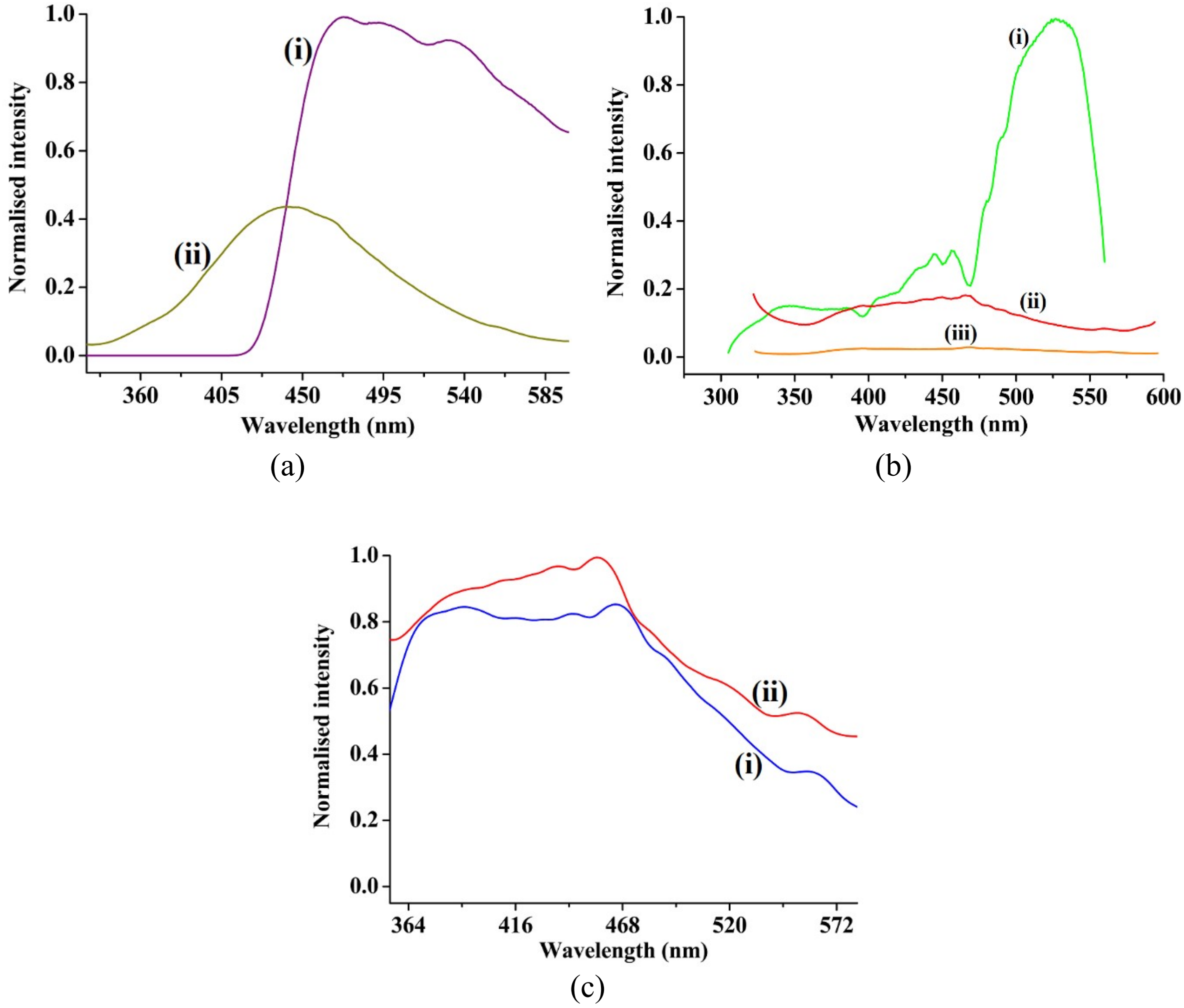


Figure S6. Solid-state photoluminescence spectra of (a) (i) *phenurea.H$_2$O* (λ_{ex} = 330 nm, λ_{em} = 473 nm, 492 nm, 530 nm), (ii) *Hphenurea*.ClO$_4$ (λ_{ex} = 309 nm, λ_{em} = 440 nm); (b) (i) *phenthiourea* (λ_{ex} = 295 nm, λ_{em} = 530 nm), (ii) *Hphenthiourea.ClO$_4$* (λ_{ex} = 307 nm, λ_{em} = 468 nm), (iii) *Hphenthiourea*.NO$_3$ (λ_{ex} = 307 nm, λ_{em} = 468 nm); (c) (i) *naphththiourea* (λ_{ex} = 306 nm, λ_{em} = 468 nm), (ii) *Hnaphththiourea.ClO$_4$* (λ_{ex} = 321 nm, λ_{em} = 468 nm).

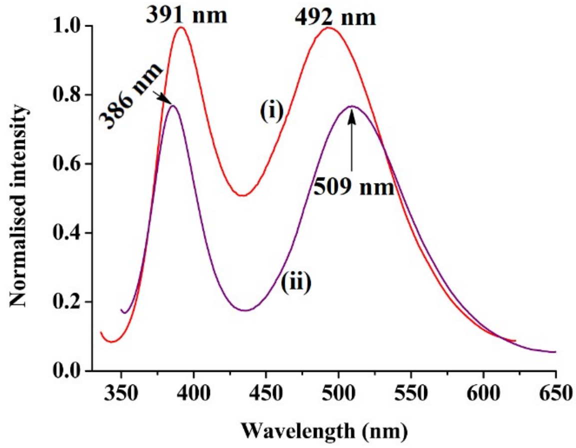
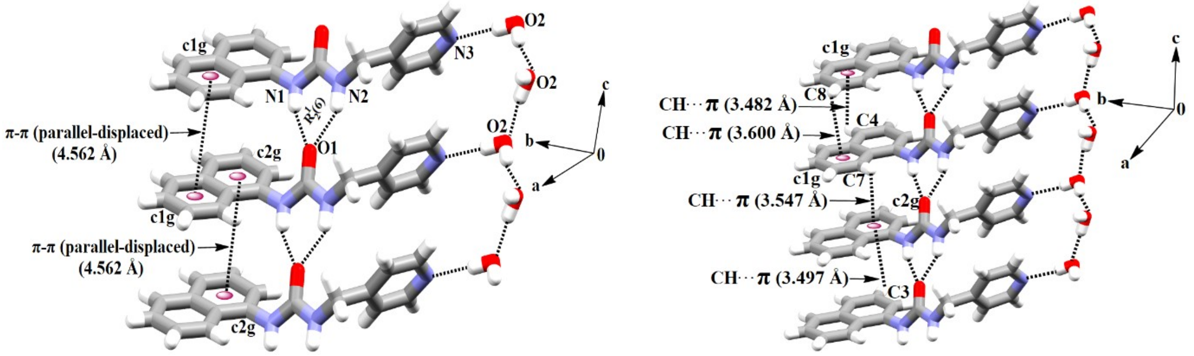


Figure S7. Solid-state photoluminescence spectra of *Hnaphurea.NO$_3$* (i) λ_{ex} = 321 nm, λ_{em} = 391 nm, 492 nm and (ii) λ_{ex} = 335 nm, λ_{em} = 386 nm, 509 nm.



(a) (b)

Figure S8. (a) Arrangements of the naphthalene rings and (b) the C-H···π interactions in *naphurea.H_2O*.

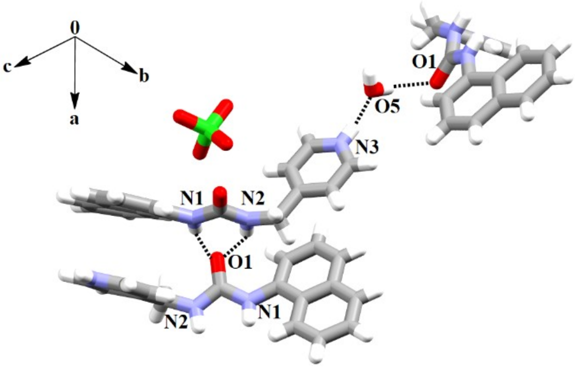


Figure S9. Free perchlorate anion and the urea tapes showing the projections of the carbonyls in the *Hnaphurea.ClO_4.H_2O*.

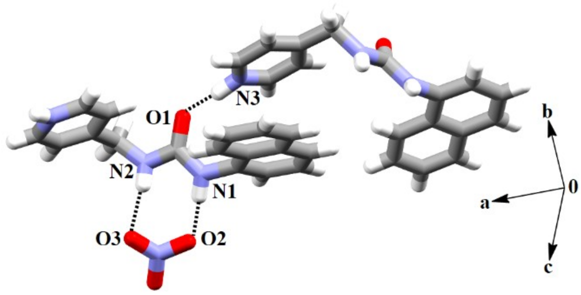


Figure S10. Hydrogen bond environment of nitrate ion in the *Hnaphurea.NO_3*.

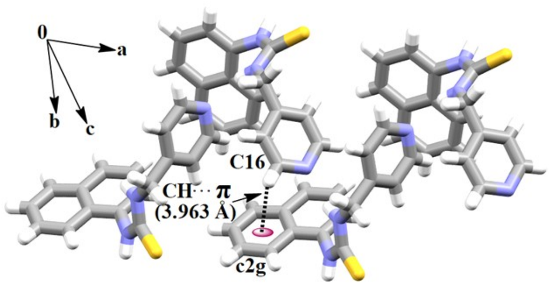
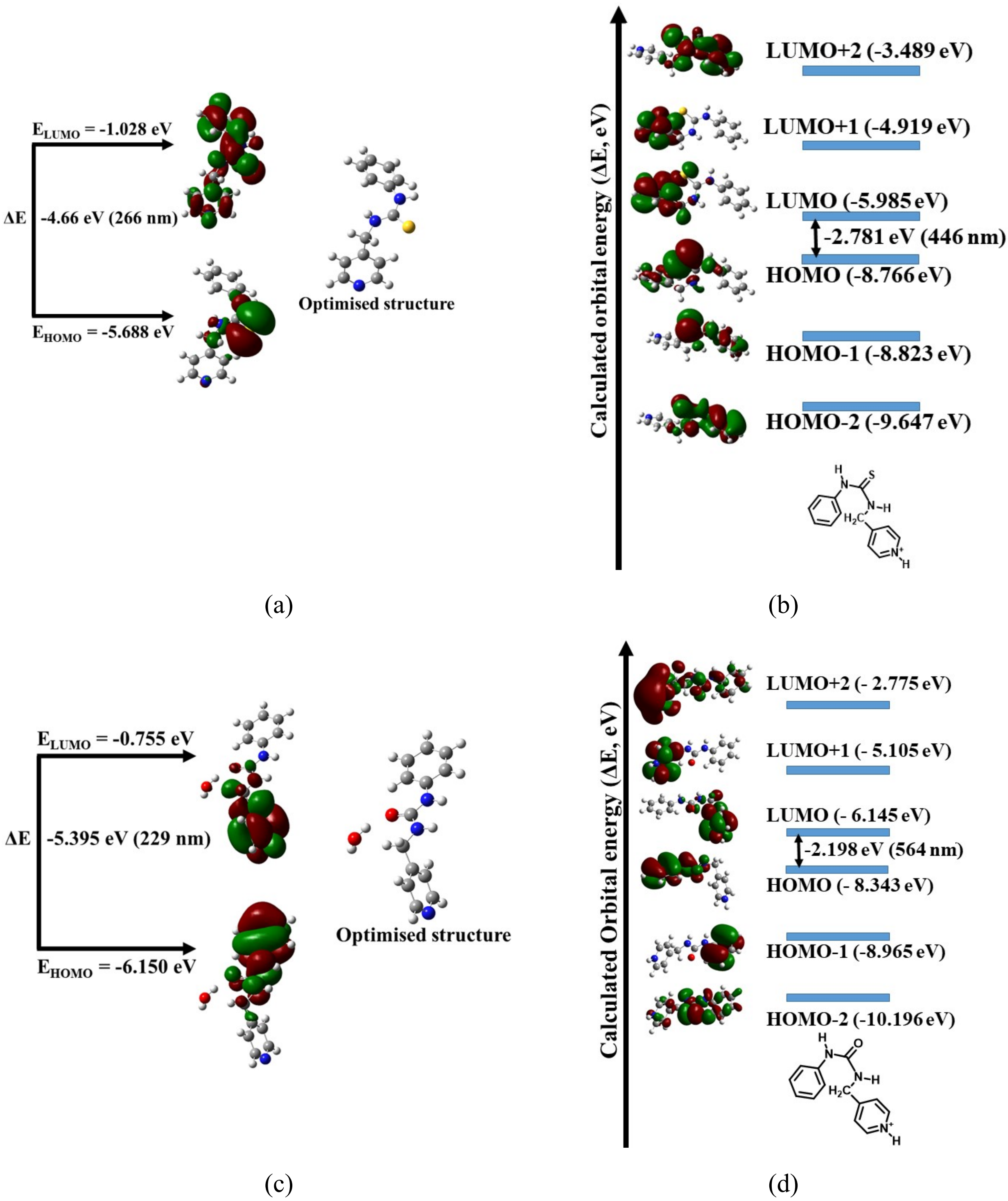
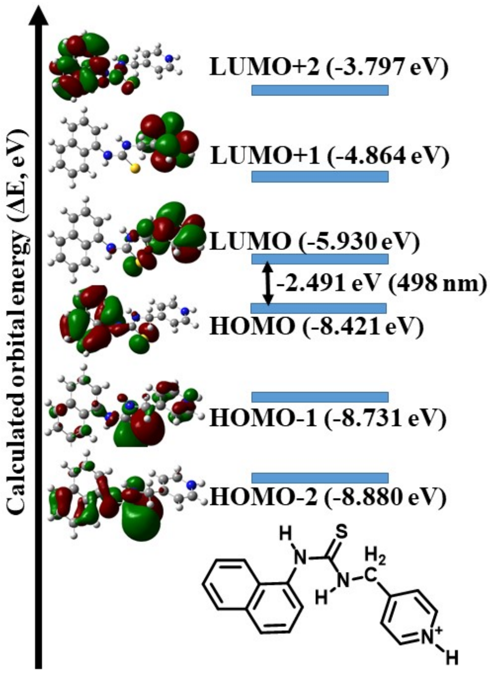


Figure S11. C-H···π interaction in the self-assembly of *Hnaphthiourea*.

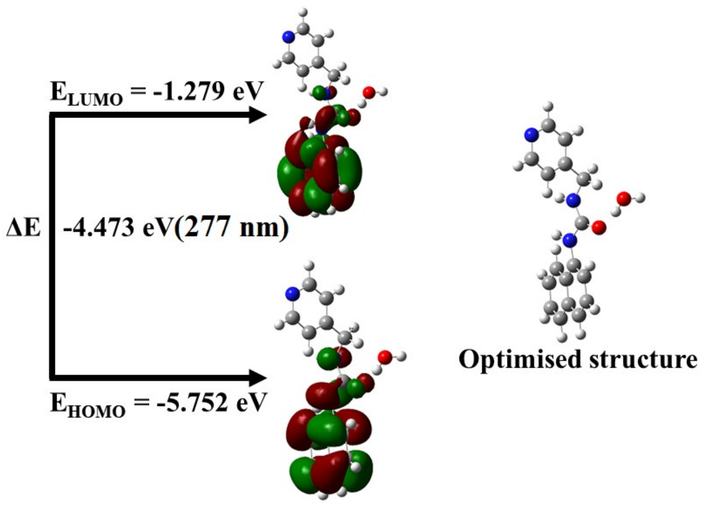


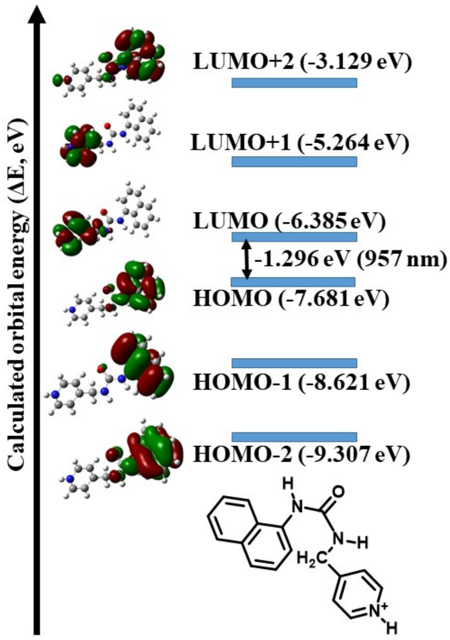
E_LUMO = -1.028 eV
ΔE
-4.66 eV (266 nm)
E_HOMO = -5.688 eV
Optimised structure
Calculated orbital energy (ΔE, eV)
LUMO+2 (-3.489 eV)
LUMO+1 (-4.919 eV)
LUMO (-5.985 eV)
-2.781 eV (446 nm)
HOMO (-8.766 eV)
HOMO-1 (-8.823 eV)
HOMO-2 (-9.647 eV)
(a)
(b)
E_LUMO = -0.755 eV
ΔE
-5.395 eV (229 nm)
E_HOMO = -6.150 eV
Optimised structure
Calculated Orbital energy (ΔE, eV)
LUMO+2 (- 2.775 eV)
LUMO+1 (- 5.105 eV)
LUMO (- 6.145 eV)
-2.198 eV (564 nm)
HOMO (- 8.343 eV)
HOMO-1 (-8.965 eV)
HOMO-2 (-10.196 eV)
(c)
(d)


Calculated orbital energy (ΔE, eV)
LUMO+2 (-3.797 eV)
LUMO+1 (-4.864 eV)
LUMO (-5.930 eV)
-2.491 eV (498 nm)
HOMO (-8.421 eV)
HOMO-1 (-8.731 eV)
HOMO-2 (-8.880 eV)

(e)

(f)


E_{LUMO} = -1.279 eV
ΔE
-4.473 eV(277 nm)
E_{HOMO} = -5.752 eV
Optimised structure


Calculated orbital energy (ΔE, eV)
LUMO+2 (-3.129 eV)
LUMO+1 (-5.264 eV)
LUMO (-6.385 eV)
-1.296 eV (957 nm)
HOMO (-7.681 eV)
HOMO-1 (-8.621 eV)
HOMO-2 (-9.307 eV)

(g)

(h)

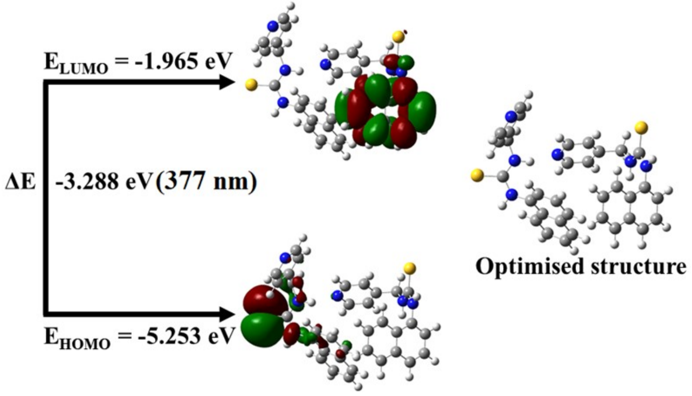


Figure S12. Electronic energy levels calculated by DFT showing the HOMO-LUMO gap in *(a) phenthiourea,* (b) *Hphenthiourea cation,* (c) *phenurea.H_2O*, (d) *Hphenurea cation,* (e) *naphthiourea,* (f) *Hnaphthiourea cation,* (g) *naphurea.H_2O,* (h) *Hnaphurea cation.*

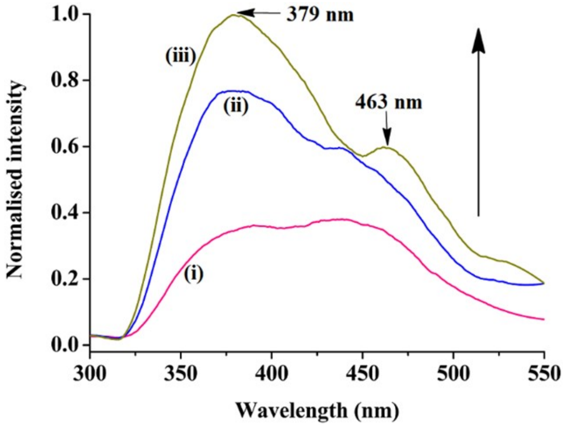


Figure S13. The changes in emission spectra of *Hnaphurea.NO_3* in water upon addition of water (10 μL aliquots) (λ_{ex} = 258 nm).

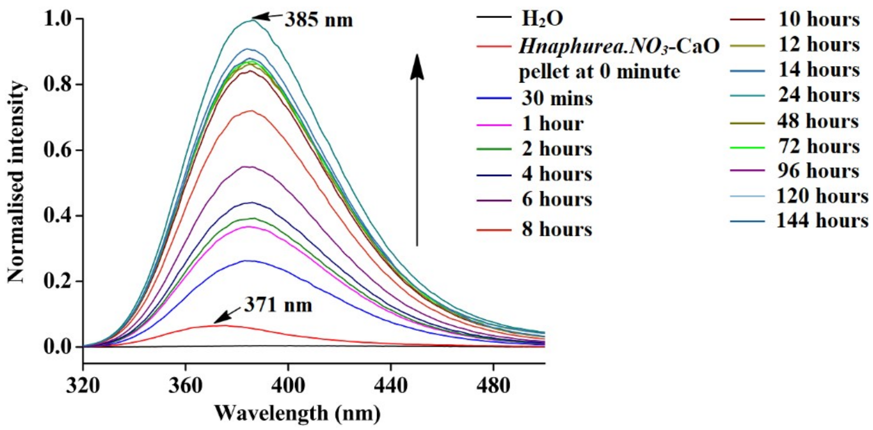


Figure S14. Changes in the emission spectra of supernatant water upon release of *naphurea* from *Hnaphurea.NO_3*@CaO pellet in water (λ_{ex} = 258 nm).

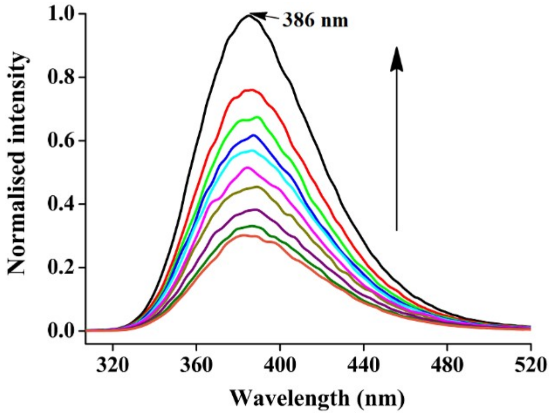


Figure S15. Fluorescence spectroscopic titration (λ_{ex} = 258 nm) of *Hnaphurea.ClO$_4$.H$_2$O* (10 μM) in water upon addition of $NaAsO_2$ (As in +3 oxidation state) (10 μM in 10 μL aliquots) showing enhancement of emission.

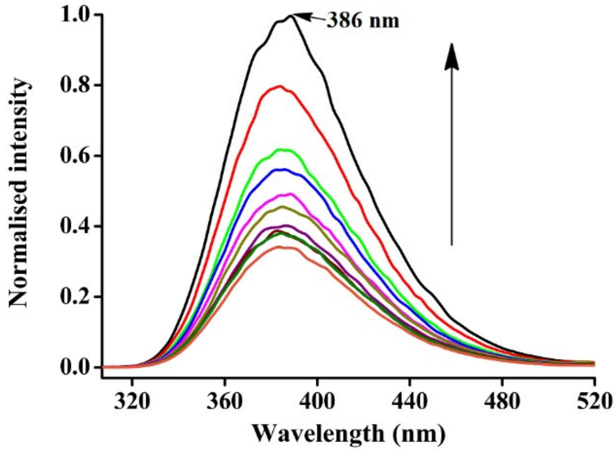


Figure S16. Fluorescence spectroscopic titration (λ_{ex} = 258 nm) of *Hnaphurea.ClO$_4$.H$_2$O* (10 μM) in water upon addition of $NaHAsO_4.7H_2O$ (As in +5 oxidation state) (10 μM in 10 μL aliquots) showing enhancement of emission.

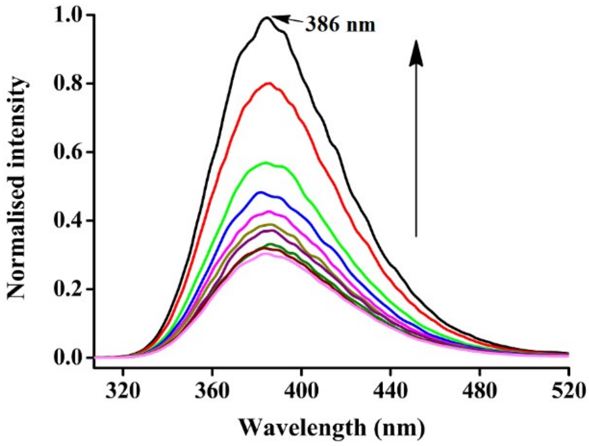
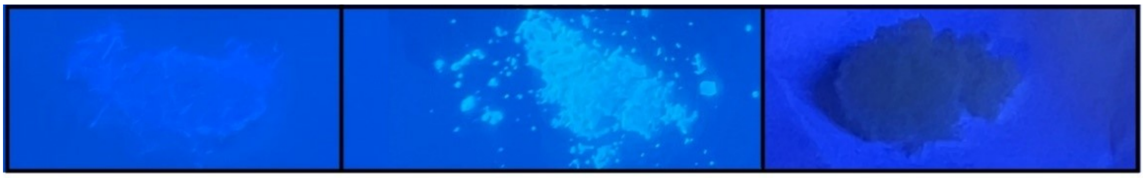
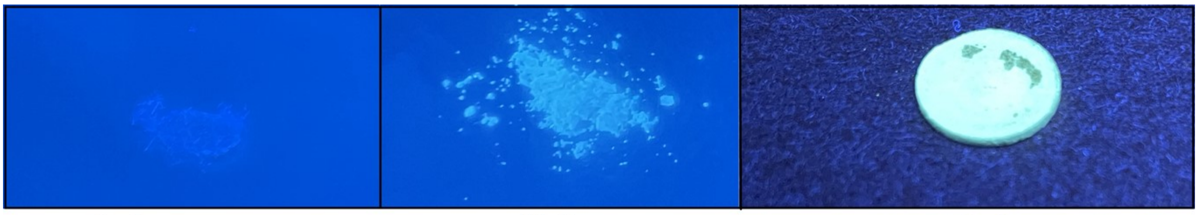


Figure S17. Fluorescence spectroscopic titration (λ_{ex} = 258 nm) of *Hnaphurea.ClO$_4$.H$_2$O* (10 μM) in water upon addition of NaOH (10 μM in 10 μL aliquots) showing enhancement of emission.



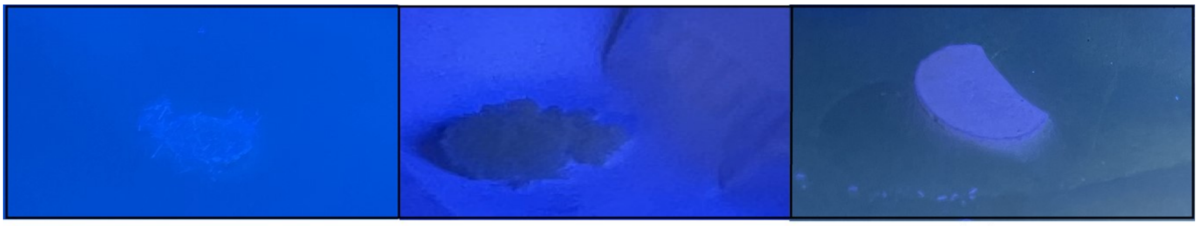
(a) (b) (c)

Figure S18. Photograph of solid samples of (a) *naphurea.H$_2$O*, (b) *Hnaphurea.ClO$_4$.H$_2$O*, (c) *Hnaphurea.NO$_3$* under UV lamp at 365 nm.



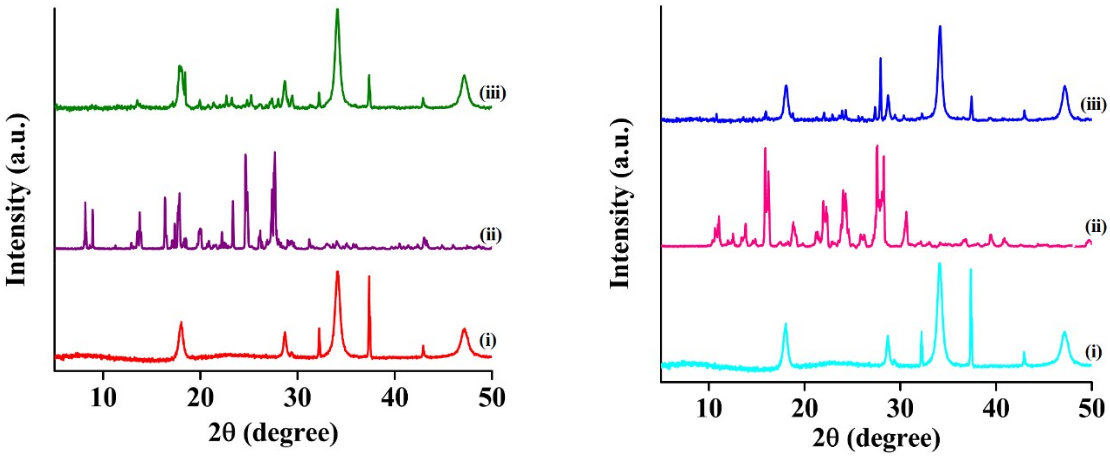
(a) (b) (c)

Figure S19. Photograph of solid samples of (a) *naphurea.H$_2$O*, (b) *Hnaphurea.ClO$_4$.H$_2$O*, (c) *Hnaphurea.ClO$_4$.H$_2$O*@CaO pellet (1:1 ratio) under UV-lamp at 365 nm.



(a) (b) (c)

Figure S20. Photograph of solid samples of (a) *naphurea.H$_2$O*, (b) *Hnaphurea.NO$_3$*, (c) *Hnaphurea.NO$_3$*@CaO (1:1 ratio) pellet under UV-lamp at 365 nm.



(a) (b)

Figure S21. Powder X-ray diffraction patterns of (a) (i) CaO, (ii) *Hnaphurea.ClO$_4$.H$_2$O*, (iii) CaO@*Hnaphurea.ClO$_4$.H$_2$O* (1:1 ratio); (b) (i) CaO, (ii) *Hnaphurea.NO$_3$*, (iii) CaO@*Hnaphurea.NO$_3$* (1:1 ratio).

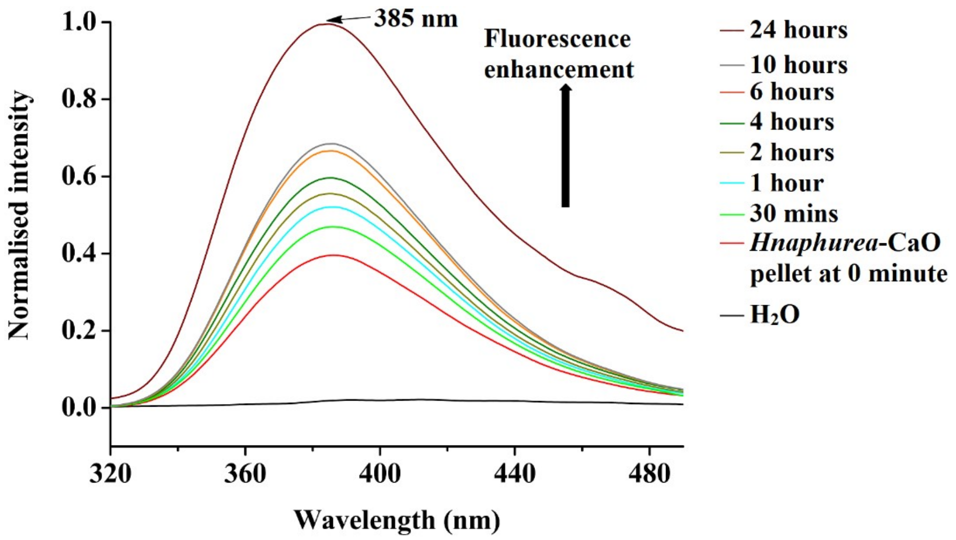


Figure S22. Changes in the fluorescence emission during the release of *naphurea* from *Hnaphurea*@CaO pellet (1:1 ratio) in water (λ_{ex} = 258 nm).

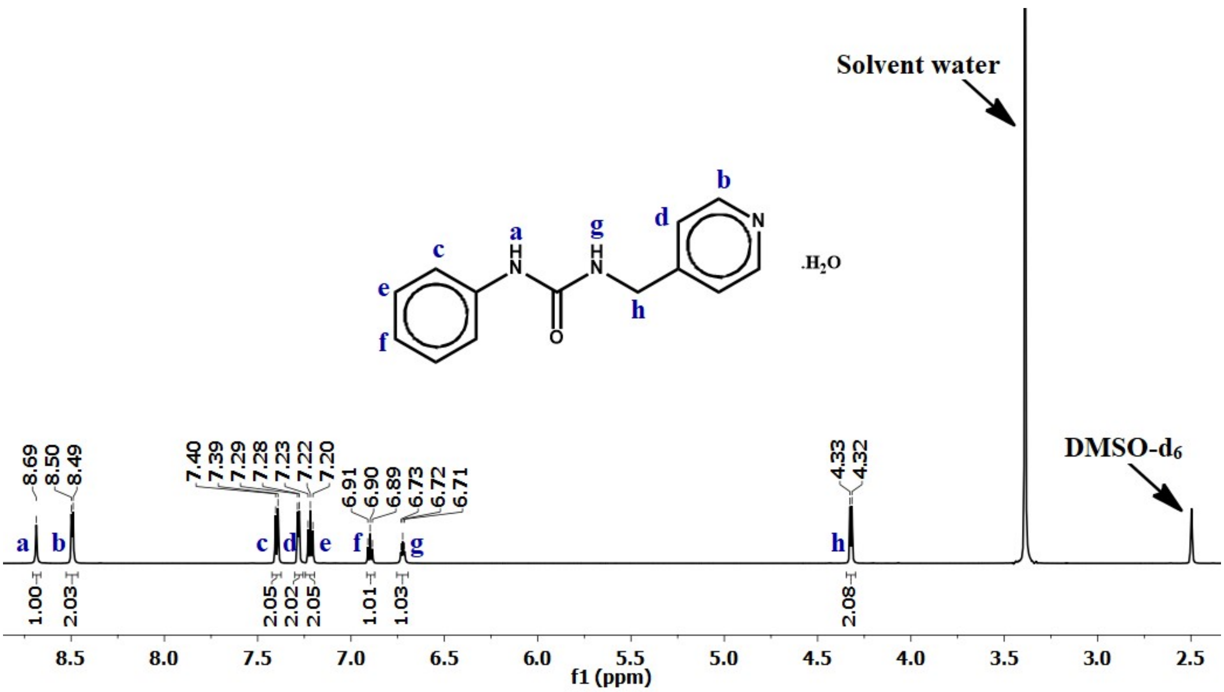


Figure S23. [1]H-NMR (600 MHz, DMSO-d$_6$) spectrum of *phenurea.H$_2$O*.

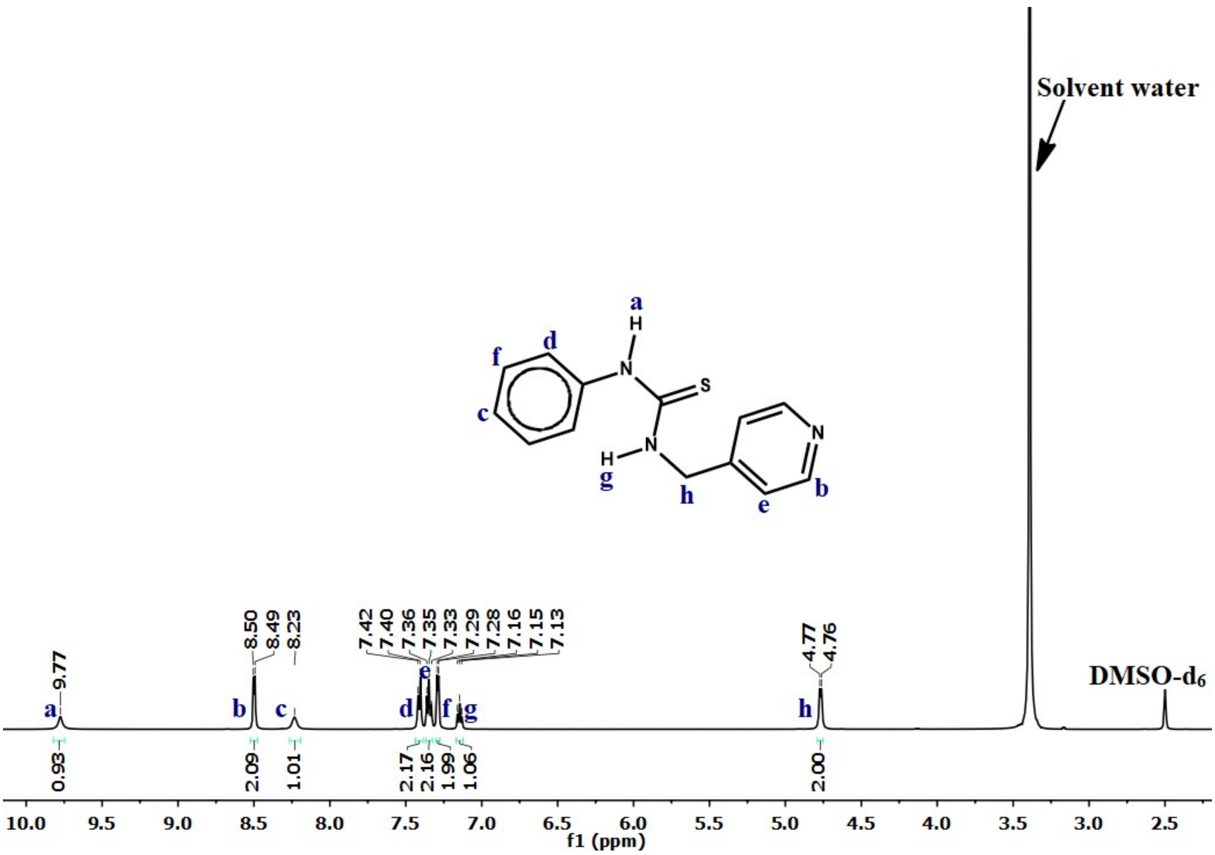


Figure S24. [1]H-NMR (500 MHz, DMSO-d_6) spectrum of *phenthiourea*.

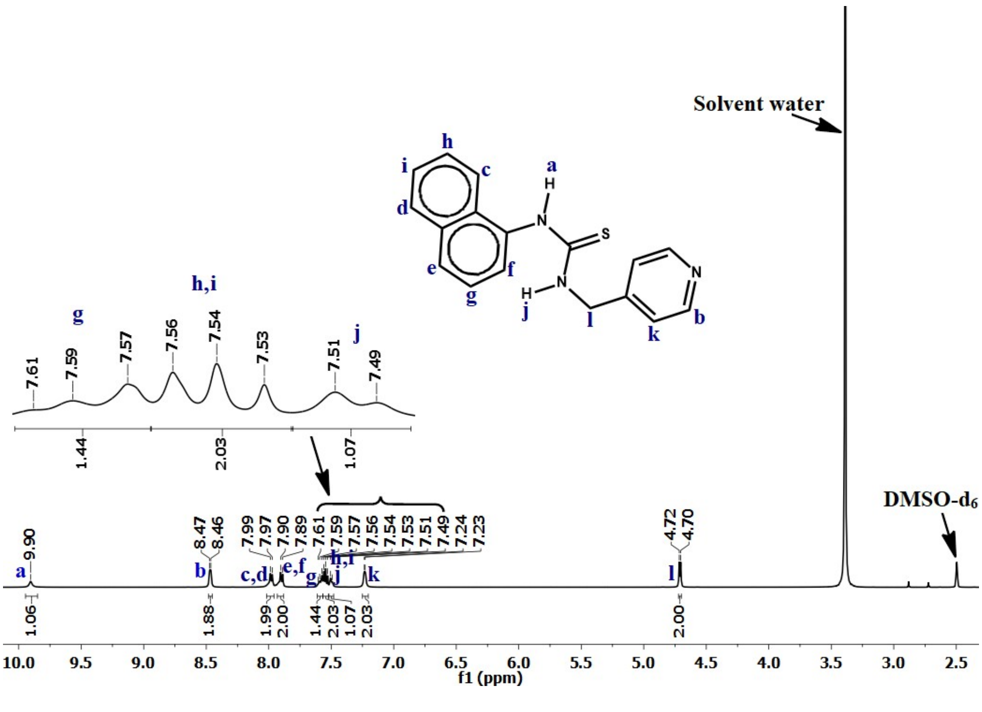


Figure S25. [1]H-NMR (500 MHz, DMSO-d_6) spectrum of *naphurea.H_2O*.

Figure S26. [1]H-NMR (500 MHz, DMSO-d_6) spectrum of *naphthiourea*.

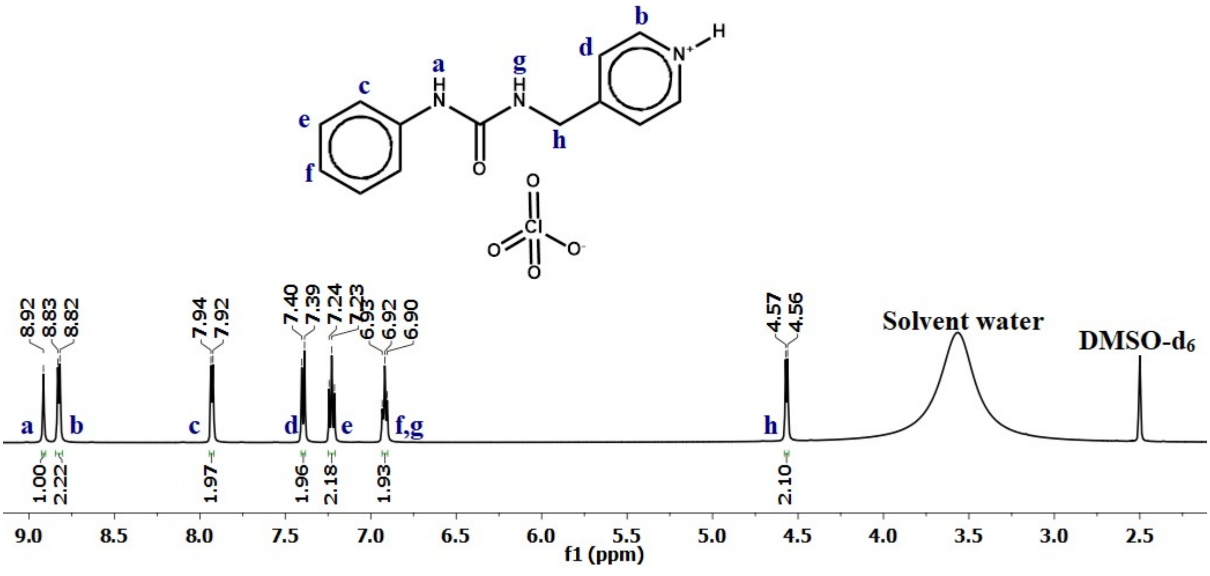


Figure S27. [1]H-NMR (500 MHz, DMSO-d_6) spectrum of *Hphenurea.ClO_4*.

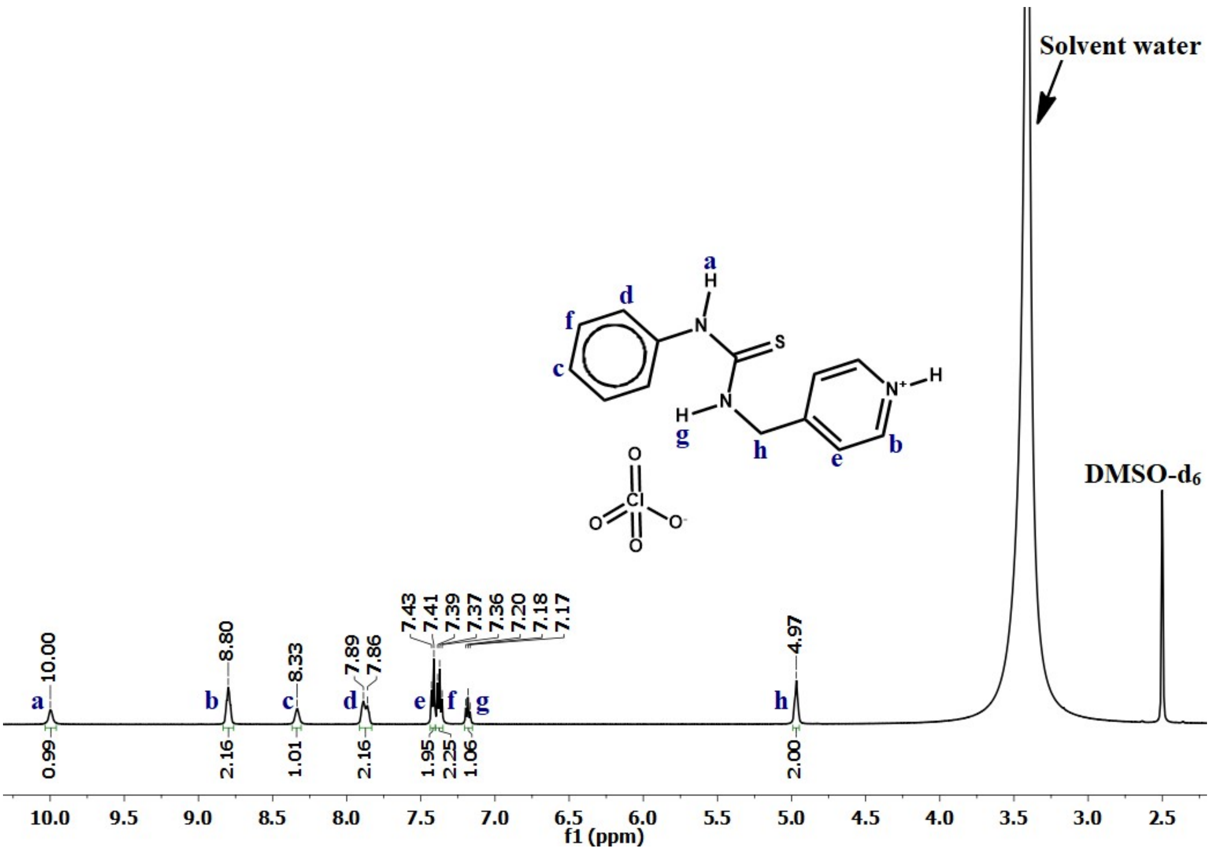


Figure S28. [1]H-NMR (500 MHz, DMSO-d_6) spectrum of *Hphenthiourea.ClO_4*.

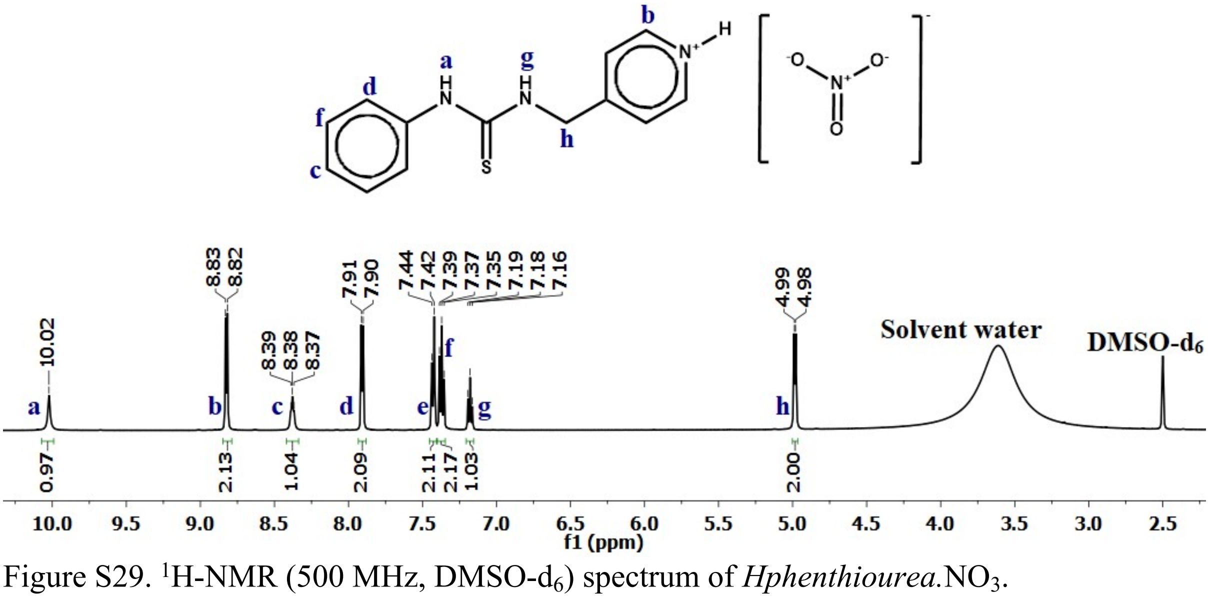


Figure S29. [1]H-NMR (500 MHz, DMSO-d_6) spectrum of *Hphenthiourea.*NO_3.

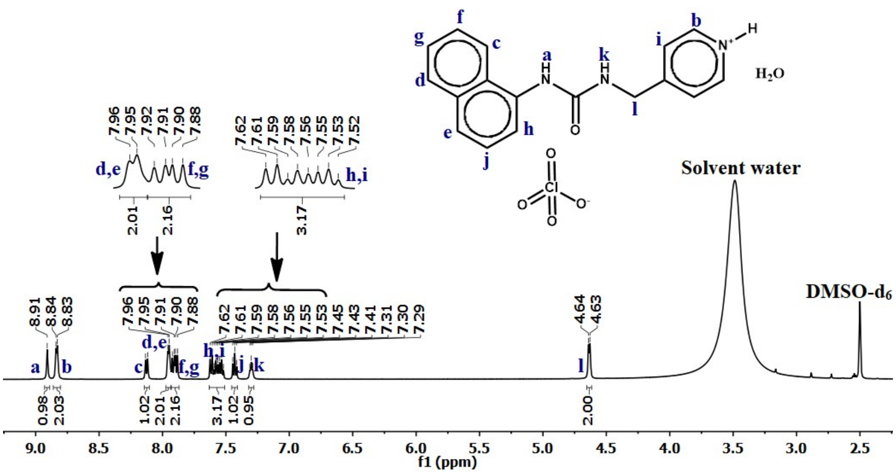


Figure S30. [1]H-NMR (500 MHz, DMSO-d_6) spectrum of *Hnaphurea.ClO_4.H_2O*.

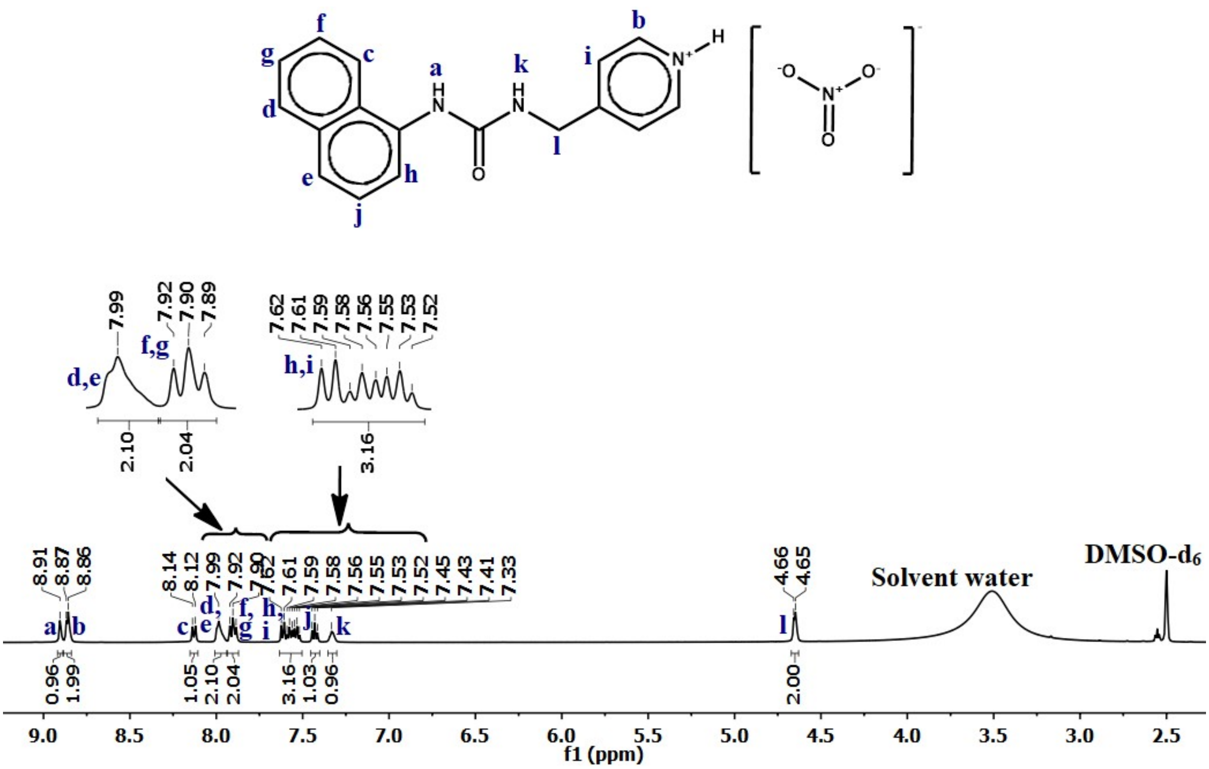


Figure S31. [1]H-NMR (500 MHz, DMSO-d_6) spectrum of *Hnaphurea.NO_3*.

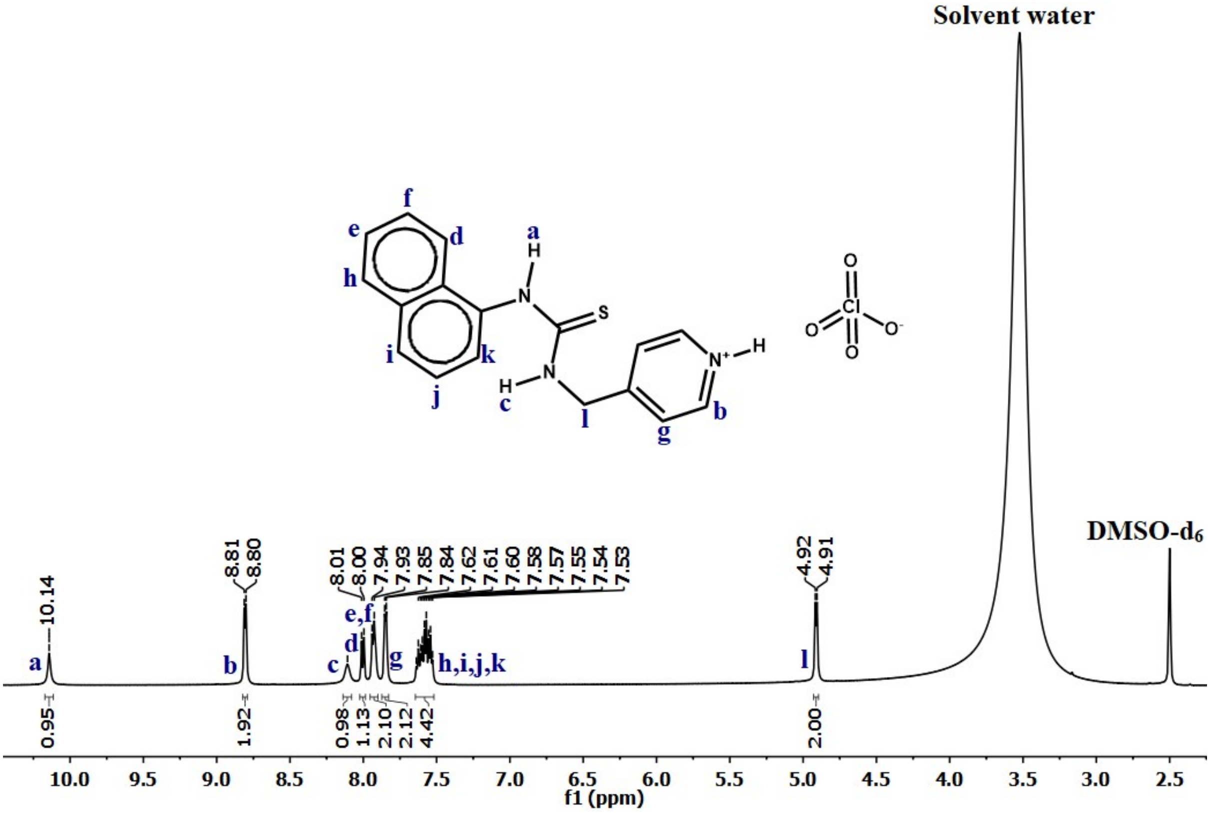


Figure S32. ^{1}H-NMR (500 MHz, DMSO-d_6) spectrum of *Hnaphthiourea.ClO$_4$*.

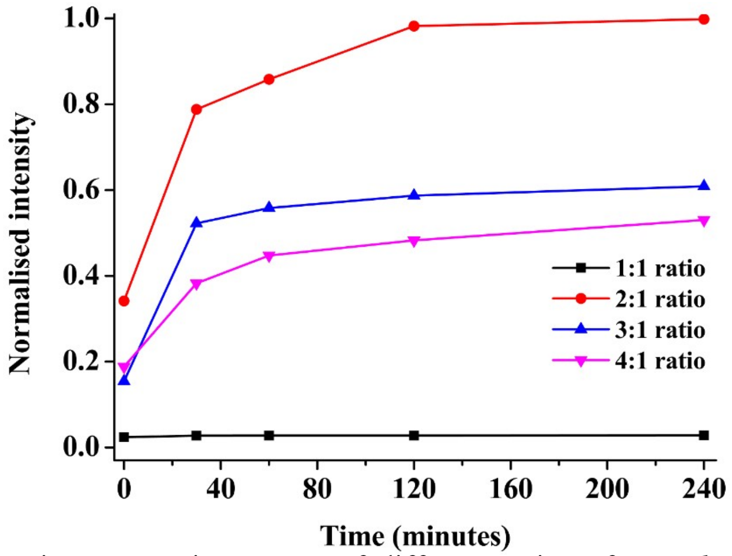


Figure S33. Intensity versus time curve of different ratios of *Hnaphurea*@CaO pellets in water (λ_{ex} = 258 nm, λ_{em} = 385 nm).

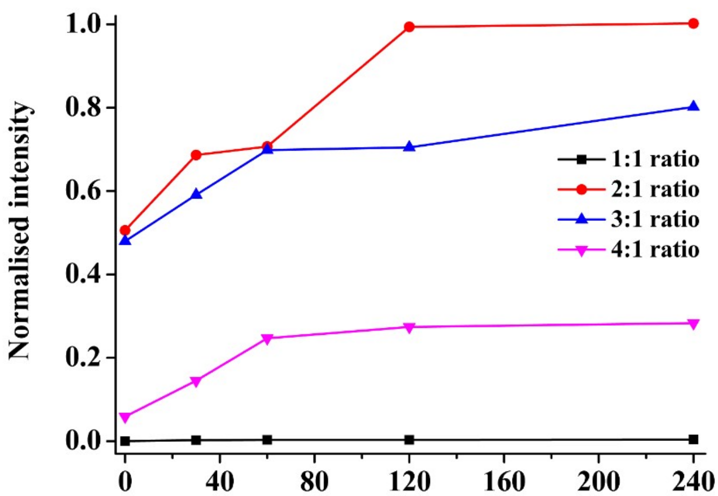


Figure S34. Intensity versus time curve of different ratios of *Hnaphurea.NO_3* @CaO pellets in water (λ_{ex} = 258 nm, λ_{em} = 385 nm).

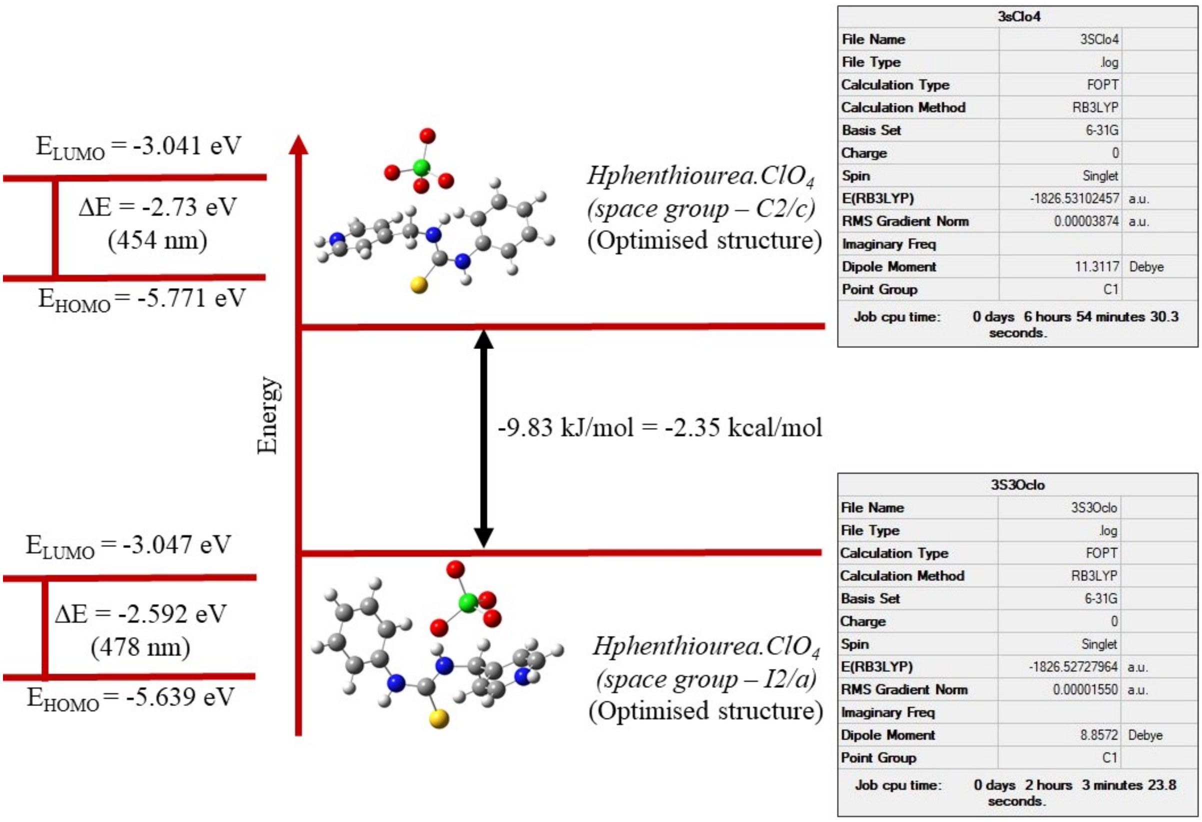


Figure S35. Electronic energy levels calculated by DFT showing the HOMO-LUMO gap in *Hphenthiourea.ClO_4* with space groups C2/c and I2/a and total energy difference between these two forms (calculated by Gaussian software using the B3LYP functional and the 6-31G basis set).

Table S3. X, Y, Z coordinates of *Hphenthiourea.ClO_4* (space group - C2/c).

Center Number	Atomic Number	Coordinates (Å) X	Y	Z
1	17	0.059190	-2.793878	0.201967
2	8	1.704025	-2.629749	0.731428
3	8	-0.945688	-1.868863	1.297897
4	8	-0.443323	-4.427454	0.148811
5	8	-0.065290	-2.047936	-1.378851
6	16	0.864983	3.255294	0.025398
7	7	-1.587179	2.197330	-0.333411
8	7	-0.057201	0.809679	0.781390
9	6	-2.750179	1.357218	-0.300075
10	6	-0.340552	1.984269	0.172929
11	6	2.406182	0.588431	0.500144

12	7	4.649394	0.387566	-1.103620
13	6	-2.710357	0.019479	-0.717476
14	1	-1.790375	-0.433290	-1.069846
15	6	1.221103	0.580421	1.440428
16	1	1.159845	-0.420632	1.886377
17	1	1.382216	1.318498	2.232746
18	6	2.336841	-0.046197	-0.761577
19	1	1.412793	-0.499994	-1.106186
20	6	-3.963672	1.932623	0.112950
21	1	-3.982398	2.968218	0.439162
22	6	-3.882531	-0.744835	-0.685799
23	1	-3.838659	-1.784476	-0.990810
24	6	3.654421	1.089430	0.929223
25	1	3.743255	1.580380	1.889973
26	6	-5.092893	-0.177049	-0.276102
27	1	-5.998175	-0.774839	-0.261040
28	6	-5.131922	1.167657	0.115299
29	1	-6.066979	1.616944	0.434020
30	6	3.464642	-0.130848	-1.547757
31	1	3.473711	-0.613533	-2.515097
32	6	4.763181	0.987413	0.117317
33	1	5.739074	1.365590	0.388285
34	1	-1.706070	3.124584	-0.718881
35	1	-0.721211	0.031850	0.843279
36	1	5.468520	0.313835	-1.693620

Table S4. X, Y, Z coordinates of *Hphenthiourea.ClO₄* (space group - I2/a).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	16	-1.191556	-3.839159	-0.474492
2	7	-2.650634	-1.644204	0.067563
3	1	-3.273922	-2.384167	0.361282
4	7	-0.472983	-1.198569	-0.649700
5	1	-0.573322	-0.202429	-0.417704
6	7	4.033665	-0.662776	1.441715
7	1	4.764571	-0.341422	2.064335
8	6	-4.272934	2.253624	0.401058
9	1	-4.696346	3.247562	0.496801
10	6	-4.518881	1.285029	1.381583
11	1	-5.137886	1.522797	2.240593
12	6	-3.955946	0.012165	1.269019
13	1	-4.126709	-0.734177	2.039247
14	6	-3.153243	-0.308125	0.161348
15	6	-2.926571	0.653831	-0.835878
16	1	-2.340562	0.407761	-1.713069
17	6	-3.475038	1.932715	-0.701748

18	1	-3.278743	2.675907	-1.466786
19	6	-1.438570	-2.107989	-0.363216
20	6	0.819093	-1.558281	-1.211132
21	1	0.988501	-0.984719	-2.127300
22	1	0.778268	-2.630464	-1.457884
23	6	1.960887	-1.292671	-0.264748
24	6	1.784139	-1.338484	1.132175
25	1	0.816723	-1.584096	1.546549
26	6	2.828542	-1.009366	1.970886
27	1	2.742920	-0.989860	3.048002
28	6	4.249158	-0.610658	0.100290
29	1	5.221669	-0.273158	-0.227585
30	6	3.228351	-0.940607	-0.767298
31	1	3.388084	-0.846358	-1.832356
32	17	1.445587	2.216612	-0.302678
33	8	0.098523	1.374201	0.431453
34	8	2.833999	1.967445	0.705428
35	8	1.728859	1.472792	-1.848780
36	8	1.097672	3.882149	-0.471577