Supporting Information

to the paper entitled

Proficiency of the electron-deficient 1,3,5-triazine ring to generate anion−π and lone-pair−π interactions

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Table S1 Crystal data and structure refinement details for **cspat**

Empirical formula	$C_{29}H_{26}Cl_1N_7S_2$	
Fw (g mol^{-1})	572.14	
Crystal system	Orthorhombic	
Space group	*Pbnm*	
Crystal colour and size	colourless	$0.16 \times 0.16 \times 0.04$ mm^3
Temperature (K)	293(2)	
Unit cell parameters	a = 10.6745(2) Å	α = 90°
	b = 11.5441(2) Å	β = 90°
	c = 22.9797(3) Å	γ = 90°
V (Å^3)	2831.73(8)	
Z	4	
ρ_{calcd} (Mg/m^3)	1.342	
μ (mm^{-1})	0.315	
F(000)	1192	
θ for data collection (deg)	3.27 − 27.09	
Reflections collected	5896	
Independent reflections	3193 (R_{int} = 0.0405)	
Reflections with $F^2>2\sigma$	2027	
Data / restraints / parameters	3193 / 0 / 182	
Final R indices [$F^2>2\sigma$]	R_1 = 0.0504	wR_2 = 0.1215
R indices (all data)	R_1 = 0.0953	wR_2 = 0.1393
goodness of fit on F^2 [a]	1.062	
largest diff. peak and hole (e Å^3)	0.229 and −0.291	

[a] Goodness-of-fit $S = \{\Sigma[w(F_o^2 - F_c^2)^2]/(n - p)\}^{1/2}$, where n is the number of reflections and p the number of parameters.

CCDC reference number 770310

Figure S1. ORTEP view of the single-crystal X-ray structure of the ligand 2-chloro-4,6-bis-*N*-[2-methylsulfanyl-*N*-(pyridin-2-ylmethyl)aniline]-1,3,5-triazine (**cspat**). H atoms are omitted for clarity.

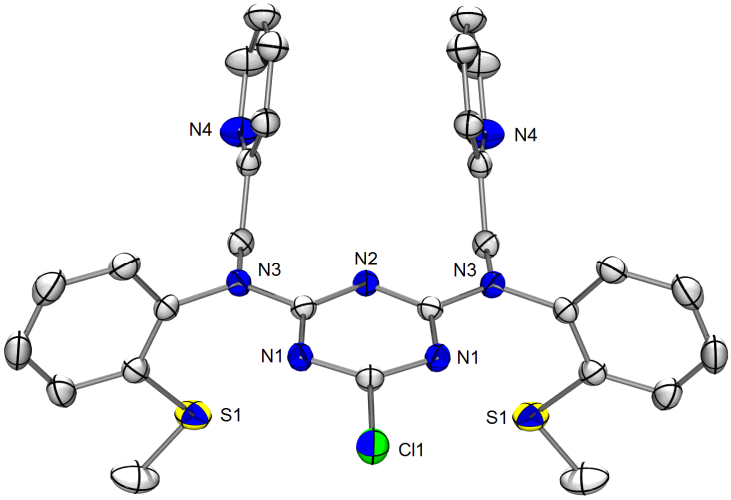

Figure S2. Illustration showing the close contact between the coordinated nitrate anion (oxygen atom O48) and the 1,3,5-triazine ring in **3**, characterized by a O41···triazine centroid distance of 2.940(5) Å. The N26−H26···O53 hydrogen bond distance is 2.630(4) Å and the angle N26−H26−O53 is 167.00º.

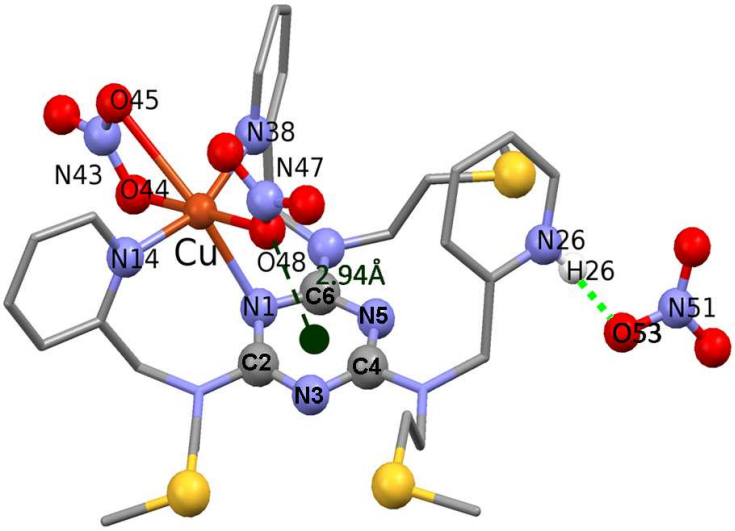

Figure S3. A) Scheme illustrating the supramolecular dimerization through double lone pair−pi contacts; **B** and **C**) Two views (in space-filling mode) of the anion−pi/lone pair−pi/pi−lone pair/pi−anion supramolecular association observed in the crystal structure of **3**.