

Supplementary Materials for

Further Insights in the Crystal Engineering of High Explosives of 1:2 Salts of the s-Tetrazine Ligand-Picrate Anion Series

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Table S1. Crystal data and refinement parameters for (H₂L4)(picrate)₂ new polymorph and (H₂L5)(picrate)₂

	(H ₂ L4)(picrate) ₂ new polymorph	(H ₂ L5)(picrate) ₂
Empirical formula	C ₃₀ H ₃₈ N ₁₂ O ₁₆	C ₂₄ H ₁₄ N ₁₂ O ₁₄
Formula weight	822.72	694.47
Temperature (K)	100(2)	100(2)
Crystal system	monoclinic	triclinic
space group	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> -1
<i>a</i> (Å)	15.0432(9)	12.848(5)
<i>b</i> (Å)	12.9768(10)	16.337(7)
<i>c</i> (Å)	19.2547(12)	16.353(6)
α (°)	90	117.71(2)
β (°)	106.479(4)	90.12(1)
γ (°)	90	111.57(1)
Volume (Å ³)	3604.4(4)	2763(2)
<i>Z</i> / <i>Z'</i>	4/1	4/2
Independent reflections / <i>R</i> (int)	3758/0.1083	7536/0.1054
μ (mm ⁻¹)	1.072	1.230
<i>R</i> indices [<i>I</i> >2 σ (<i>I</i>)] ^a	<i>R</i> 1 = 0.1079	<i>R</i> 1 = 0.1049
	<i>wR</i> 2 = 0.2772	<i>wR</i> 2 = 0.2855
<i>R</i> indices (all data) ^a	<i>R</i> 1 = 0.1339	<i>R</i> 1 = 0.1484
	<i>wR</i> 2 = 0.3003	<i>wR</i> 2 = 0.3302

$$^a R1 = \sum ||F_o| - |F_c|| / \sum |F_o| ; wR2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}$$

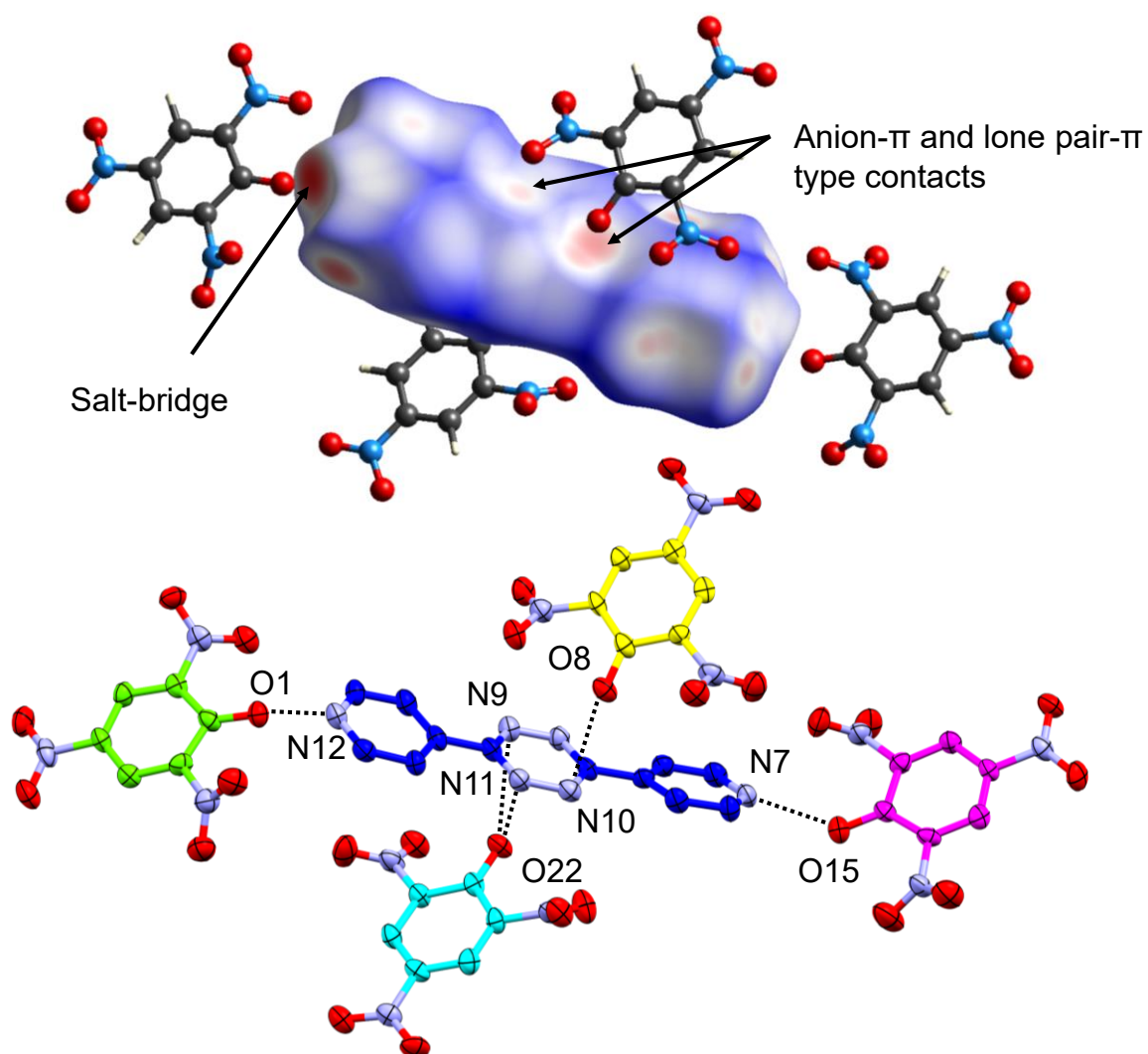


Figure S1. Top: Hirshfeld surface of the blue ligand in the $(H_2L5)_2(Picr)_4$ crystals showing pyridinium-phenolate salt-bridges, anion- π and lone pair- π interactions as the most noticeable forces governing the crystal packing. Bottom: Details of short intramolecular contacts and labels of the interacting atoms. Hydrogen atoms omitted for clarity.

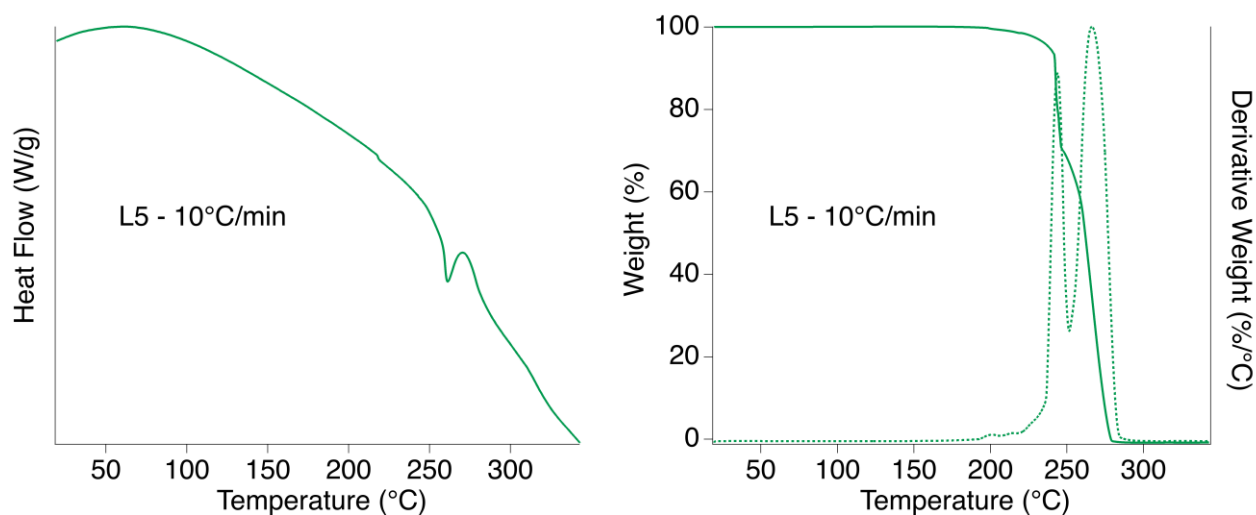


Figure S2. Heat flow and TG/DTG profiles of the ligand L5.

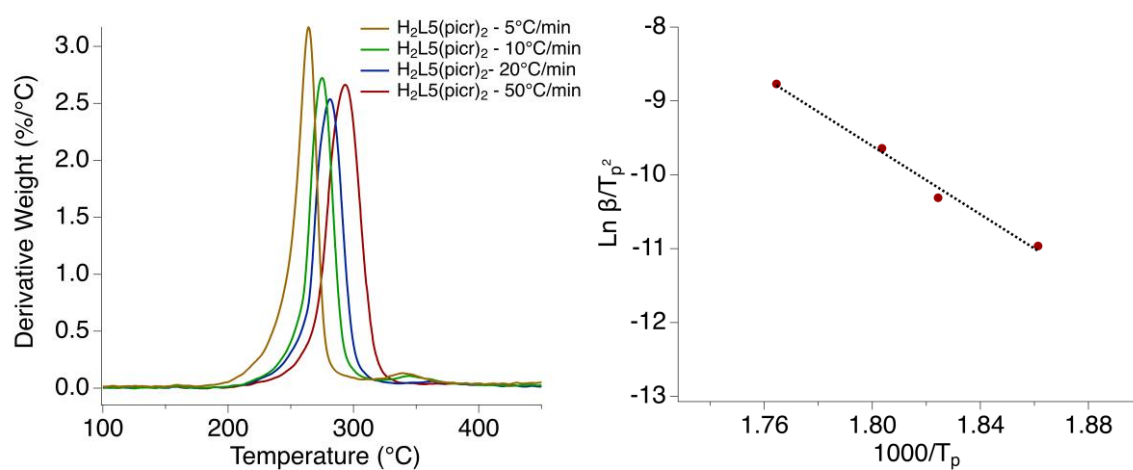


Figure S3. Left: DTG profile of the picrate complex of L5 at different heating rates. Right: Kissinger model extrapolation of thermokinetic parameters.