

SUPPLEMENTARY INFORMATION FOR

**Adaptive binding and selection of compressed 1, ω -
diammonium-alkanes *via* molecular encapsulation in
water**

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Table S1. Crystallographic information on data collection and structure refinement

	PTS{1}₂	PTSG{1}	PTSG{2a}	PTSG{2b}	PTSG{3}
Formula	C ₁₆ H ₆ O ₁₂ S ₄ , 2(C ₁₀ H ₂₆ N ₂), 4(H ₂ O)	C ₁₆ H ₆ O ₁₂ S ₄ , C ₁₀ H ₂₆ N ₂ , 2(CH ₆ N ₃),2(H ₂ O))	C ₁₆ H ₆ O ₁₂ S ₄ , C ₁₁ H ₂₈ N ₂ , 2(CH ₆ N ₃),2(H ₂ O)	C ₁₆ H ₆ O ₁₂ S ₄ , C ₁₁ H ₂₈ N ₂ , 2(CH ₆ N ₃),2(H ₂ O)	C ₁₆ H ₆ O ₁₂ S ₄ , C ₁₂ H ₃₀ N ₂ , 2(CH ₆ N ₃),2(H ₂ O)
Crystal Class	Triclinic	Triclinic	Triclinic	Triclinic	Triclinic
Space Group	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1
<i>a</i> (Å)	7.8956(4)	9.7336(8)	9.8126(4)	9.8826(4)	9.7985(3)
<i>b</i> (Å)	9.6557(3)	9.7556(8)	10.2605(4)	10.2939(4)	9.8928(3)
<i>c</i> (Å)	14.9160(6)	10.1940(7)	19.4731(7)	9.8156(4)	10.2589(4)
<i>α</i> (°)	77.311(3)	95.207(6)	96.737(3)	96.289(3)	94.489(3)
<i>β</i> (°)	81.835(4)	95.926(6)	95.763(3)	95.622(3)	97.927(3)
<i>γ</i> (°)	86.214(3)	95.224(7)	94.085(3)	94.839(3)	95.090(3)
Volume (Å ³)	1097.43(8)	953.91(13)	1930.36(13)	983.19(7)	976.92(6)
<i>Z</i>	1	1	2	1	1
Radiation type	Mo- <i>Kα</i>	Mo- <i>Kα</i>	Mo- <i>Kα</i>	Mo- <i>Kα</i>	Mo- <i>Kα</i>
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
<i>ρ</i> (gcm ⁻³)	1.421	1.478	1.485	1.458	1.490
Temperature (K)	175	175	125	293	175
Diffractometer type	Gemini	Gemini	Gemini	Gemini	Gemini
Scan type	ω	ω	ω	ω	ω
Reflections measured	15468	36619	15112	31497	35243
Independent reflex.	4495	5743	6676	5199	5973
<i>R</i> _{int}	0.032	0.038	0.022	0.038	0.038
Average size (mm)	0.25x0.35x0.50	0.30x0.40x0.60	0.30x0.50x0.70	0.40x0.45x0.50	0.30x0.50x0.70
Refinement on	<i>F</i>	<i>F</i>	<i>F</i>	<i>F</i>	<i>F</i>
<i>R</i> -factor	0.0437	0.0353	0.0418	0.0479	0.0404
<i>wR</i>	0.0483	0.0299	0.0489	0.0539	0.0494
< <i>σ</i> (<i>I</i>)/ <i>I</i> >	0.0422	0.0408	0.0368	0.0473	0.0433
Number of parameters	289	244	496	298	299
Goodness of fit	1.0944	0.9998	0.9891	1.02233	1.0533

	PTS{1}(H ₂ O) ₄	PTS{1}(H ₂ O) ₄ *	PTSG{1} _{0.5} {3} _{0.5}
Formula	C ₁₀ H ₂₆ N ₂ , 0.5(C ₁₆ H ₆ O ₁₂ S ₄),2(H ₂ O)	C ₁₆ H ₆ O ₁₂ S ₄ , 2(C ₁₀ H ₂₆ N ₂), 4(H ₂ O)	C ₁₆ H ₆ O ₁₂ S ₄ , 2(H ₂ O), 2(CH ₆ N ₃), 0.6224(C ₁₀ H ₂₆ N ₂), 0.1888(C ₁₂ H ₃₀ N ₂), 0.1888(C ₁₂ H ₃₀ N ₂)
Crystal Class	Triclinic	Monoclinic	Triclinic
Space Group	<i>P</i> -1	<i>I</i> 2/c	<i>P</i> -1
<i>a</i> (Å)	7.8956(4)	19.4827(5)	9.7673(3)
<i>b</i> (Å)	9.6557(3)	7.7013(2)	9.8143(3)
<i>c</i> (Å)	14.9160(6)	30.1416(7)	10.2046(4)
<i>α</i> (°)	77.311(3)	90	94.880(3)
<i>β</i> (°)	81.835(4)	101.758(2)	96.822(3)
<i>γ</i> (°)	86.214(3)	90	95.184(3)
Volume (Å ³)	1097.43(4)	4427.63(11)	962.75(6)
Z	2	4	1
Radiation type	Mo- <i>Kα</i>	Mo- <i>Kα</i>	Mo- <i>Kα</i>
Wavelength (Å)	0.71073	0.71073	0.71073
ρ (gcm ⁻³)	1.421	1.409	1.483
Temperature (K)	175	175	125
Diffractometer type	Gemini	Gemini	Gemini
Scan type	ω	ω	ω
Reflections measured	15468	12680	14777
Independent reflex.	4468	4256	5557
<i>R</i> _{int}	0.032	0.029	0.027
Average size (mm)	0.12x0.18x0.36	0.30x0.40x0.50	0.20x0.50x0.55
Refinement on	<i>F</i>	<i>F</i>	<i>F</i>
<i>R</i> -factor	0.0433	0.0746	0.0586
<i>wR</i>	0.0461	0.0767	0.0649
< <i>σ</i> (<i>I</i>)/ <i>I</i> >	0.0422	0.0438	0.0400
Number of parameters	311	301	241
Goodness of fit	1.0815	1.0486	0.9213

Table S2. Dimensions of the pyrene box in all the three cases. Length was defined as the distance between the 1 and ω- nitrogen atoms, width as the distance between the opposing guanidinium planes and height as the distance between the opposing pyrene rings. The theoretical elongated length was calculated using the Gaussian09 computation packadge at the B3-LYP level of theory.

Pyrene box	1,10-diammonium decane (1)	1,11-diammonium undecane (2)	1,12-diammonium dodecane (3)
Length (Å)	13.807	14.239	14.465
Theoretical N-N elongated length	13.810	15.036	16.534
Compression rate (%)	0	5	13
Width (Å)	7.386	7.952	7.949
Height (Å)	8.137	8.161	8.508

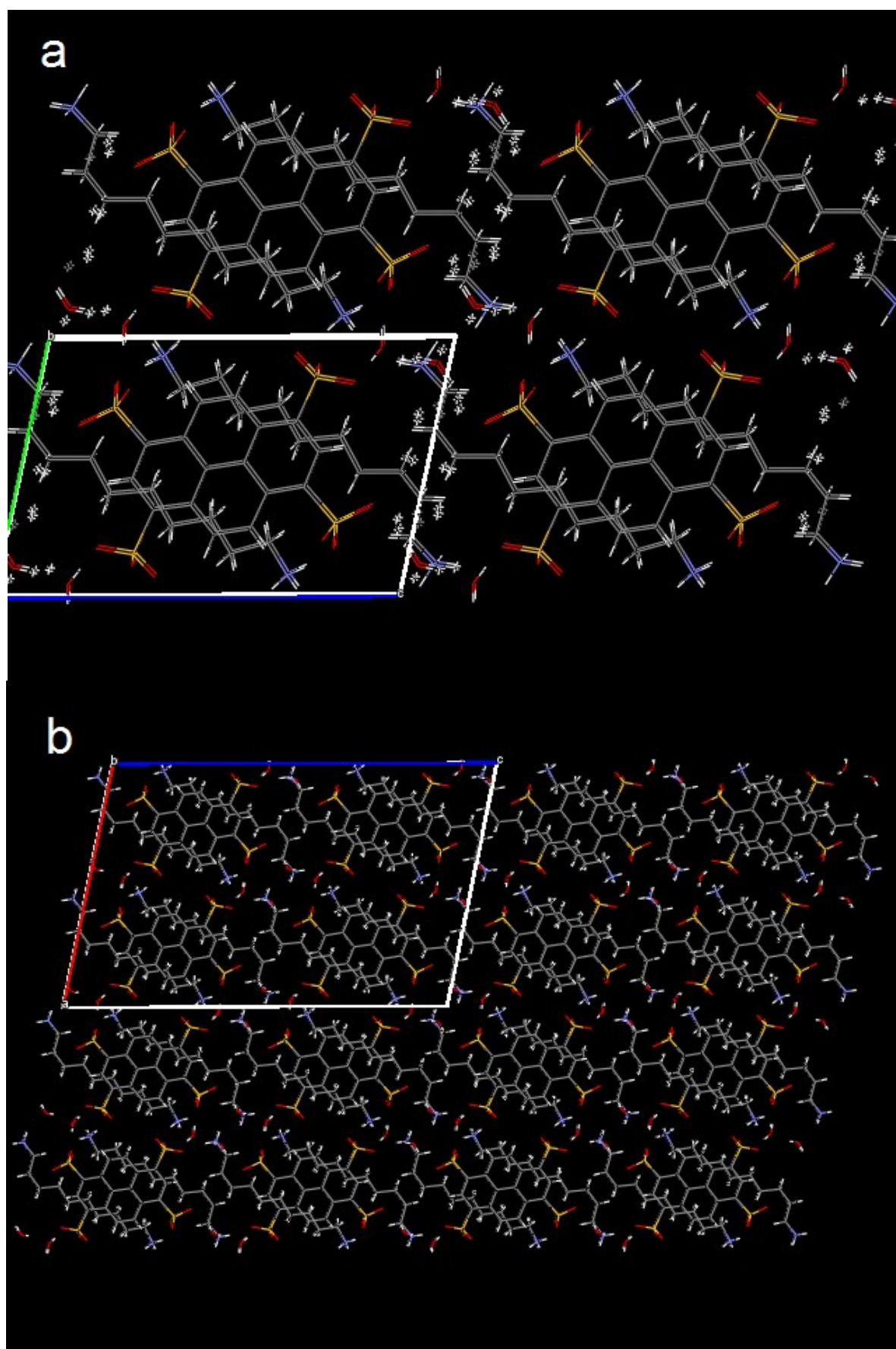
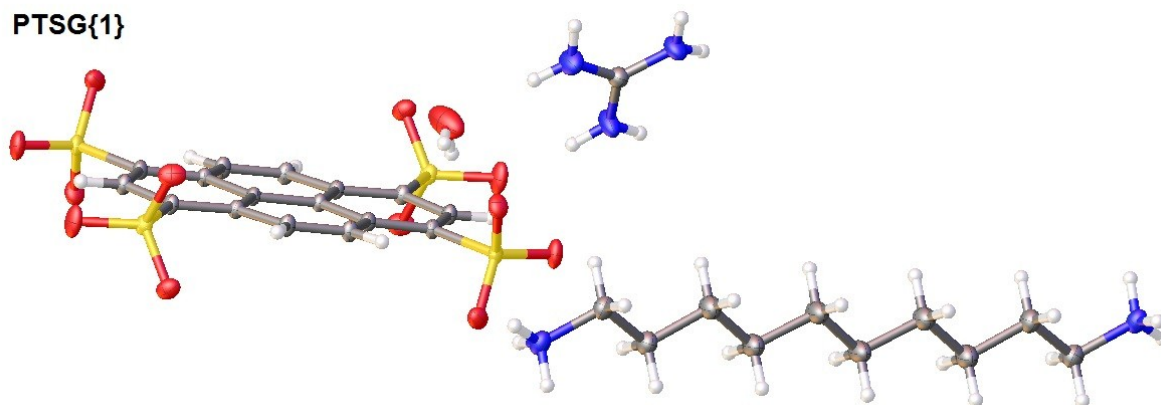
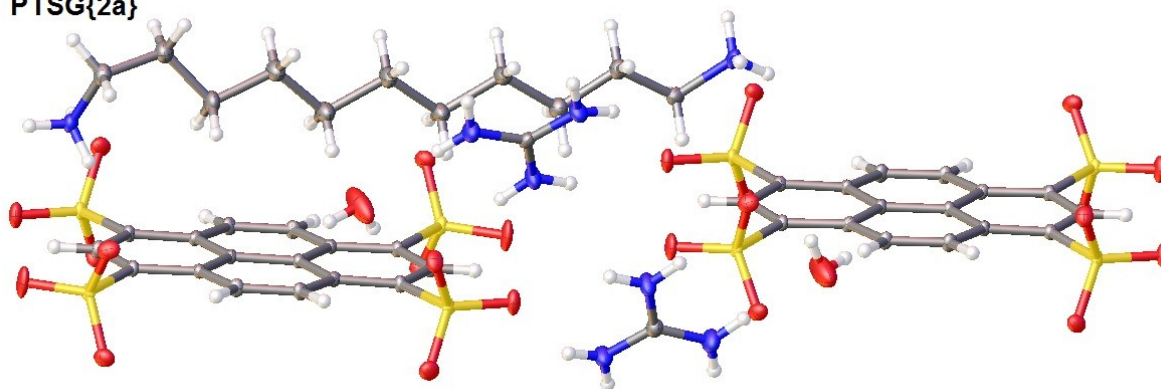


Figure S1: Comparison between the packing behaviors of polymorphs a) **PTS{1}(H₂O)₄** and b) **PTS{1}(H₂O)₄***

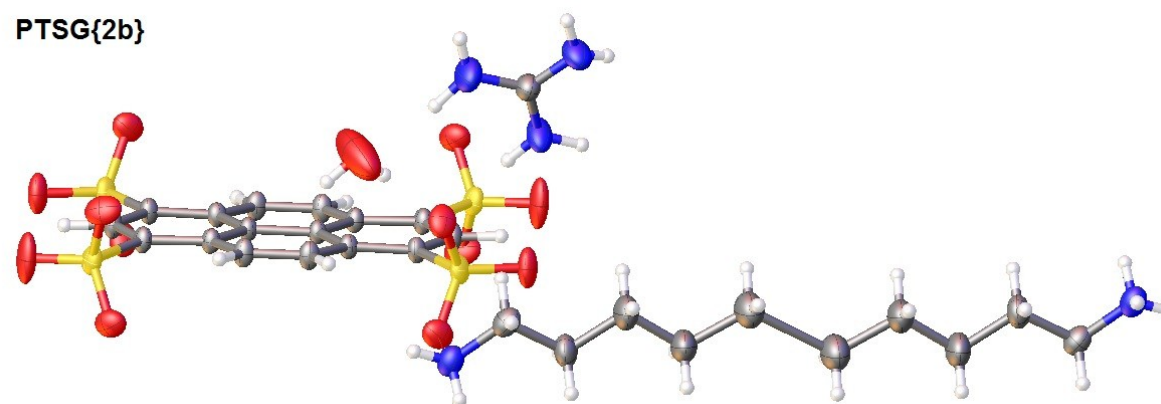
PTSG{1}



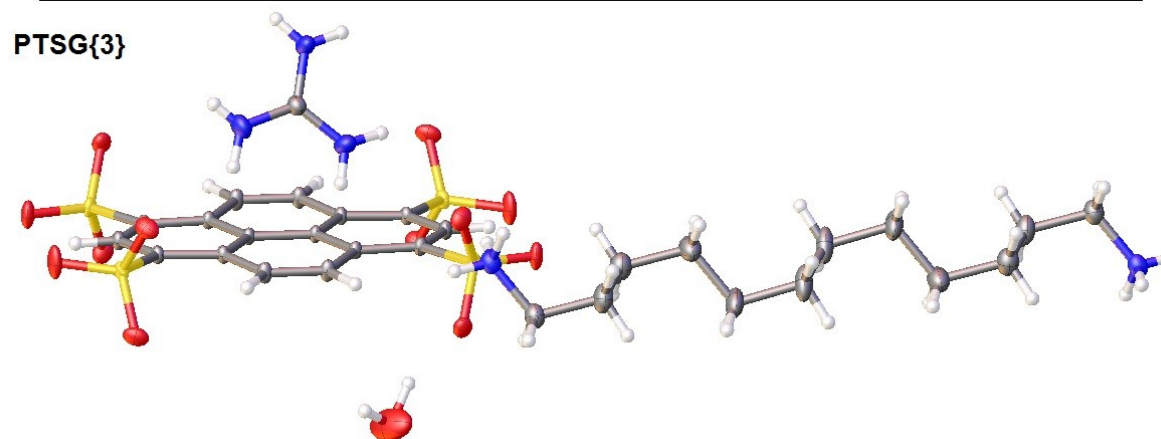
PTSG{2a}

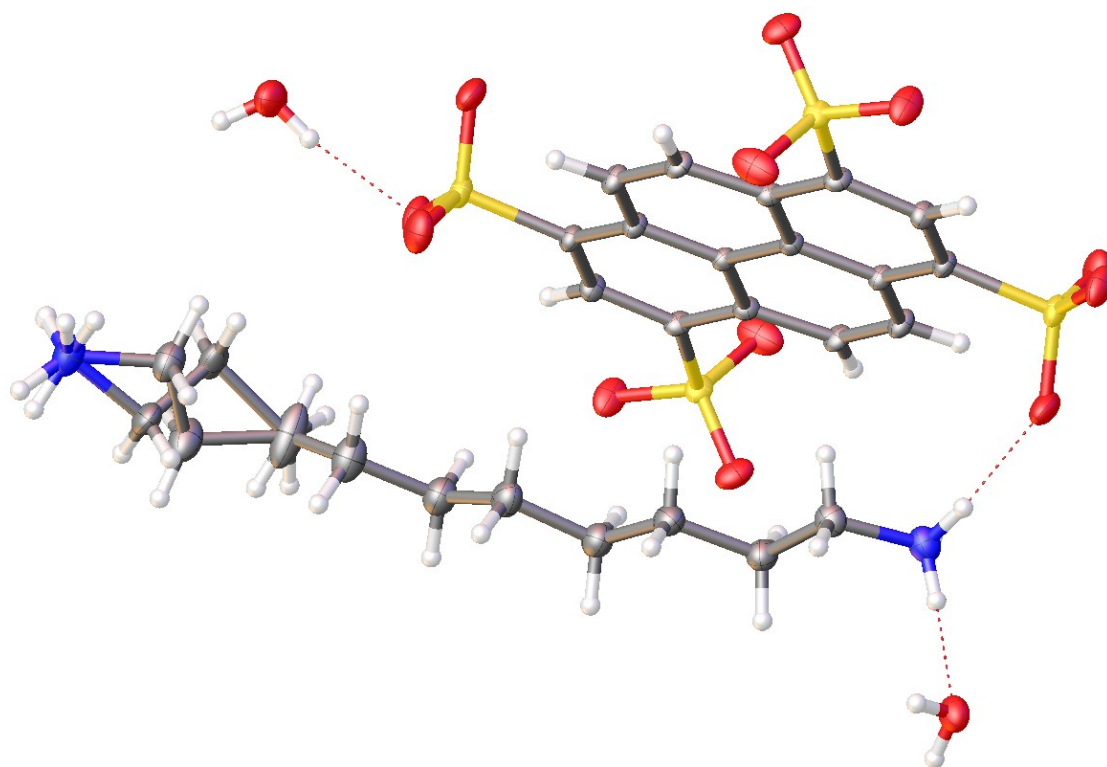


PTSG{2b}

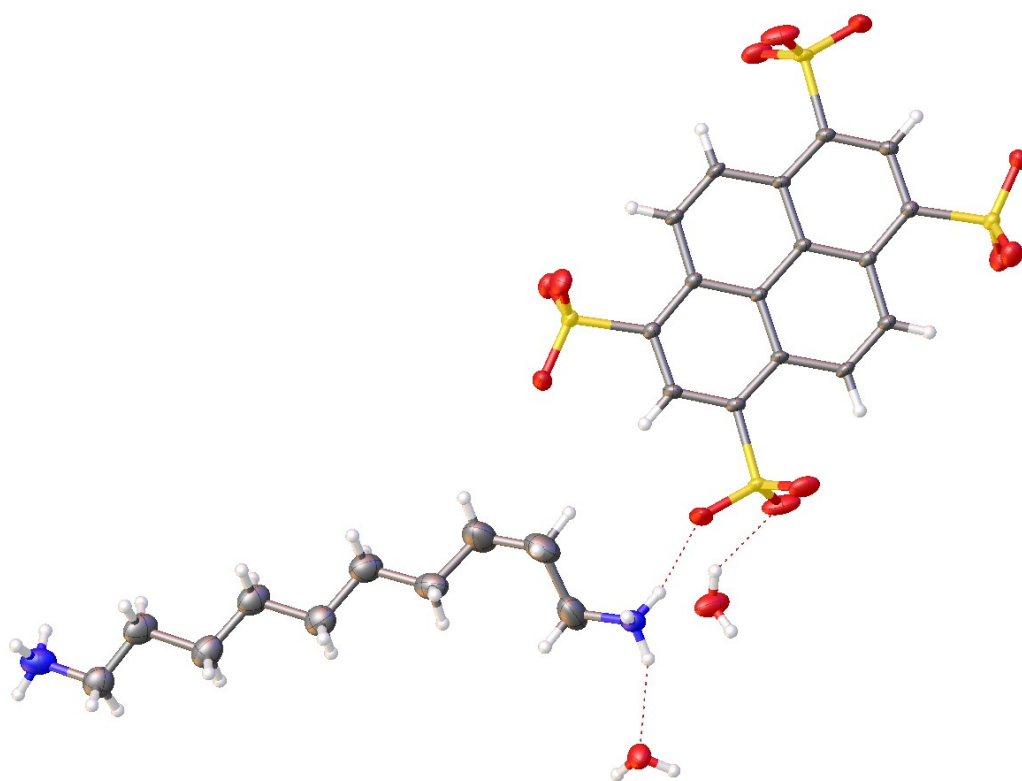


PTSG{3}





$\text{PTS}\{1\}(\text{H}_2\text{O})_4$



$\text{PTS}\{1\}(\text{H}_2\text{O})_4^*$

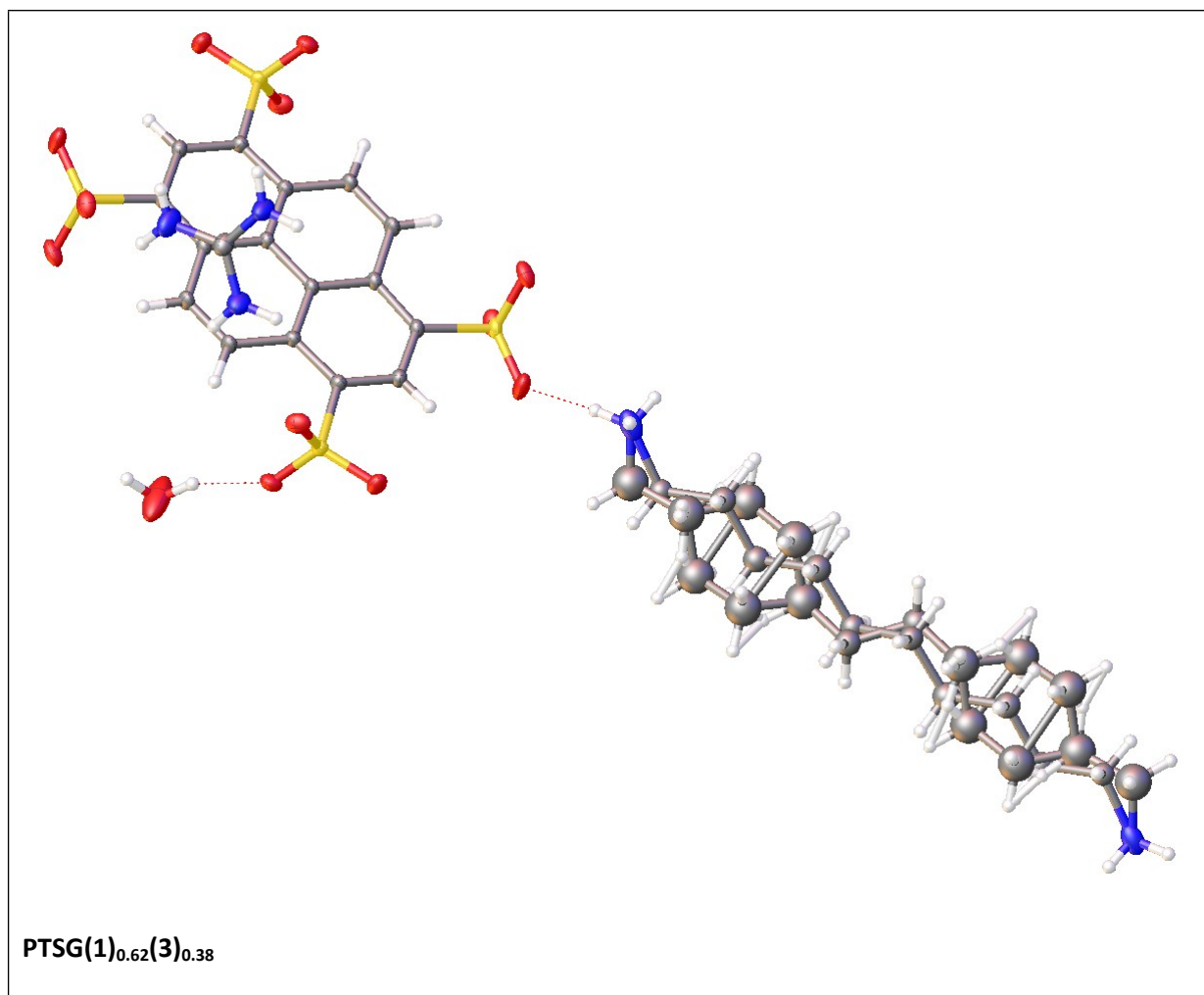


Figure S2. ORTEP diagrams of structures. Thermal ellipsoids are drawn at 50% probability.