Electronic Supplementary Information

Elucidating the Elusive Crystal Structure of 2,4,6-tris(2-pyrimidyl)-1,3,5-triazine (TPymT) Through Powder X-ray Diffraction

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Experimental XRPD patterns, measured from two different samples of ***α*-TPymT**, clearly testify to a preferred orientation along the (100) direction. Description of one ***α*-TPymT** molecule in the asymmetric unit required 9 independent parameters (3 for position, 3 for orientation and 3 for torsion angles between the triazine and pyrimidine rings). One additional parameter was required for the March-Dollase coefficient. Thus, description of the ***α*-TPymT** structure in the $P6_1$ or $P3_112$ space groups, with one molecule in the asymmetric unit, requires 9 + 1 = 10 independent parameters, while the $P3_1$ space group, with two molecules in the asymmetric unit, requires 9 × 2 + 1 = 19 parameters. Refinement in the $P6_1$ and $P3_112$ space groups affords reasonable crystal structures, but fits were unsatisfactory (Fig. S1 in ESI†). For instance, in $P6_1$ the first low-angle peak was fitted poorly, with a significant difference between the calculated and observed intensities. Similar discrepancies were found for the refinement in the $P3_112$ space group. Refinement in $P3_1$ resulted in a much better fit (Fig. S1 in ESI†), but required a larger number of parameters and we were cautious about "overrefinement". To verify our choice of a space group, we compared models obtained in refinements with different space groups and checked the difference between them. As an example, we give here comparison of models in the $P3_1$ and $P6_1$ space groups. In both models the crystal structure consists of similar flat layers, formed by molecules of ***α*-TPymT**. However, these models differ significantly in the way in which the layers pack. An overlay of the models in the $P3_1$ and $P6_1$ space groups are shown in Fig. S2 in ESI†. It is clearly seen that the model in the trigonal $P3_1$ space group is not a distorted model of the one in the hexagonal $P6_1$ space group. All corresponding layers from 2 to 6 differ significantly. This also testifies that the model in the $P3_1$ space group is not merely a deformation of the one in the $P6_1$ super group.

Since the experimental XRPD pattern was cut up to $2\theta = 60°$ (~1.55 $Å^{-1}$ resolution), we cannot expect an atomic resolution for the structure; however, this resolution is definitely sufficient to select one of the two models. An additional check of the symmetry in the PLATON program also revealed no missing symmetry elements in the $P3_1$ model. All these arguments allowed us to refine the crystal structure of ***α*-TPymT** in the $P3_1$ space group based on the XRPD data.

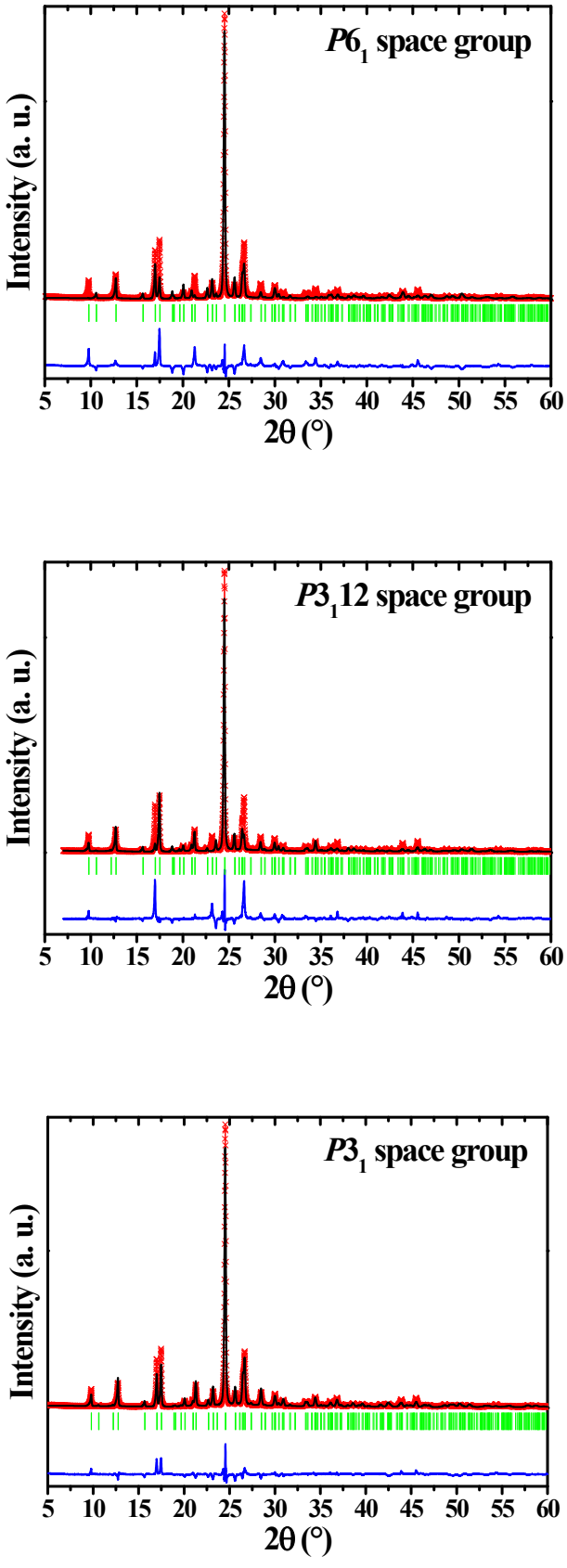

Fig. S1 Rietveld refinement plots (Cu-Kα) of ***α*-TPymT** modeled in the $P6_1$, $P3_112$ and $P3_1$ space groups. Experimental and calculated data are shown in red symbols and black line, respectively. Blue line shows the difference curve, while green marks show Bragg positions.

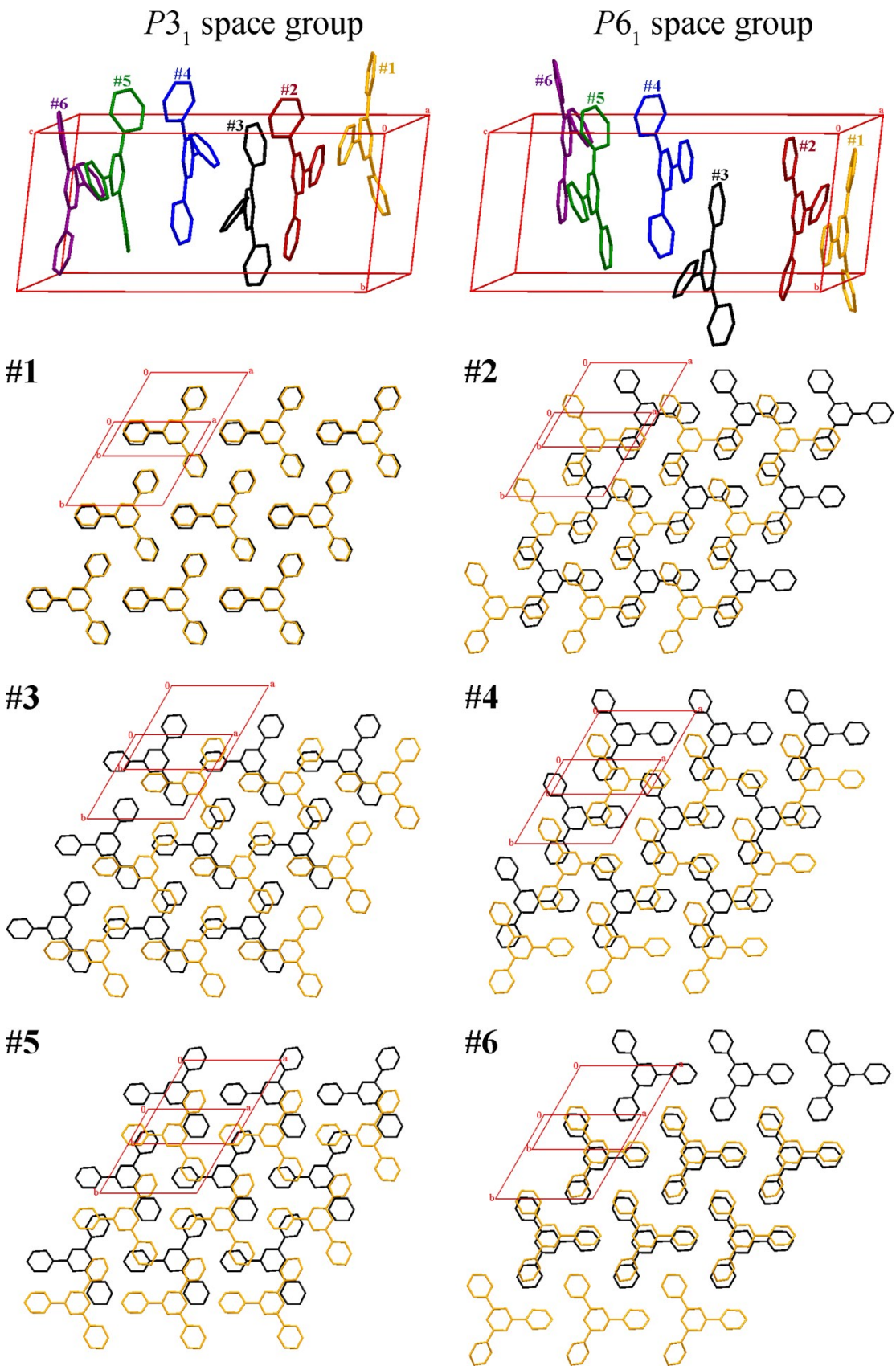

Fig. S2 Unit cell packing of ***α*-TPymT** in different space groups (top) and an overlay of the corresponding layers of ***α*-TPymT**, formed by the corresponding molecules along the c axis, with the first layers being best overlaid (bottom). Numbers on the top figure corresponds to the layers order on the bottom one. Layers on the bottom figure, formed by the corresponding molecules in the $P3_1$ and $P6_1$ space groups, are shown in gold and black, respectively. H-atoms were omitted for clarity.

Table S1. Selected bond lengths (Å) and bond angles (°) for 2-cyanopyrimidine

Bond lengths							
N(1)–C(1)	1.350(2)	N(2)–C(3)	1.350(2)	N(3)–C(5)	1.136(2)	C(2)–C(3)	1.370(3)
N(1)–C(4)	1.326(3)	N(2)–C(4)	1.327(3)	C(1)–C(2)	1.370(3)	C(4)–C(5)	1.469(2)
Bond angles							
C(1)–N(1)–C(4)	116.08(18)	N(1)–C(1)–C(2)	121.28(17)	N(2)–C(3)–C(2)	121.30(18)	N(3)–C(5)–C(4)	179.94(18)
C(3)–N(2)–C(4)	116.08(17)	N(1)–C(4)–C(5)	116.55(17)	N(2)–C(4)–C(5)	116.52(16)	C(1)–C(2)–C(3)	118.31(16)
N(1)–C(4)–N(2)	126.93(16)						
Dihedral angles							
C(4)–N(1)–C(1)–C(2)	0.0(3)	C(1)–N(1)–C(4)–C(5)	–178.97(16)	C(3)–N(2)–C(4)–N(1)	–0.8(3)	N(1)–C(1)–C(2)–C(3)	–0.7(3)
C(1)–N(1)–C(4)–N(2)	0.8(3)	C(4)–N(2)–C(3)–C(2)	0.0(3)	C(3)–N(2)–C(4)–C(5)	178.97(16)	C(1)–C(2)–C(3)–N(2)	0.7(3)

Table S2. Selected bond lengths (Å) and bond angles (°) for pyrimidine-2-carboximidamide

Bond lengths							
N(1)–C(1)	1.339(5)	N(3)–C(3)	1.352(3)	N(4)–C(5)	1.357(3)	C(3)–C(4)	1.358(4)
N(2)–C(1)	1.295(4)	N(4)–C(2)	1.282(4)	C(1)–C(2)	1.504(3)	C(4)–C(5)	1.371(4)
N(3)–C(2)	1.316(4)						
Bond angles							
C(2)–N(3)–C(3)	114.4(3)	N(3)–C(2)–N(4)	128.9(2)	N(3)–C(2)–C(1)	116.1(2)	N(4)–C(5)–C(4)	120.9(3)
C(2)–N(4)–C(5)	116.1(3)	N(1)–C(1)–C(2)	115.5(2)	N(3)–C(3)–C(4)	122.4(3)	C(3)–C(4)–C(5)	117.3(2)
N(1)–C(1)–N(2)	122.1(2)	N(2)–C(1)–C(2)	121.8(3)	N(4)–C(2)–C(1)	114.9(3)		
Dihedral angles							
C(3)–N(3)–C(2)–N(4)	0.5(4)	C(5)–N(4)–C(2)–N(3)	–1.2(4)	N(1)–C(1)–C(2)–N(3)	–171.3(2)	N(2)–C(1)–C(2)–N(4)	–177.6(3)
C(3)–N(3)–C(2)–C(1)	–176.2(2)	C(5)–N(4)–C(2)–C(1)	175.6(2)	N(1)–C(1)–C(2)–N(4)	11.5(3)	N(3)–C(3)–C(4)–C(5)	0.5(4)
C(2)–N(3)–C(3)–C(4)	–0.1(4)	C(2)–N(4)–C(5)–C(4)	1.4(4)	N(2)–C(1)–C(2)–N(3)	–0.4(4)	C(3)–C(4)–C(5)–N(4)	–1.1(4)

Table S3. Hydrogen bond lengths (Å) and angles (°) for pyrimidine-2-carboximidamide[a]

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠(DHA)
N(1)–H(11)···N(2)$^{\#1}$	0.859(3)	2.452(3)	3.125(3)	135.8(3)
N(1)–H(12)···N(4)	0.858(4)	2.316(4)	2.631(3)	101.9(3)
N(1)–H(12)···N(4)$^{\#2}$	0.858(4)	2.611(4)	3.376(4)	149.0(3)
N(2)–H(21)···N(3)	0.860(4)	2.317(3)	2.766(3)	112.7(3)

[a] Symmetry transformations used to generate equivalent atoms: #1 $-x$, $1-y$, $2-z$; #2 $1-x$, $1-y$, $1-z$.

Table S4. π···π bond lengths (Å) and angles (°) for pyrimidine-2-carboximidamide[a]

Cg(*I*)	Cg(*J*)[b]	*d*[Cg(*I*)–Cg(*J*)]	*α*	*β*
Cg(1)	Cg(1)$^{\#1}$	4.1779(13)	0.03	35.76
Cg(1)	Cg(1)$^{\#2}$	3.7449(13)	0.03	21.64

[a] Cg(*I*)–Cg(*J*): distance between ring centroids; *α*: dihedral angle between planes Cg(*I*) and Cg(*J*); *β*: angle Cg(*I*) → Cg(*J*) vector and normal to plane *I*. Cg(1): N(3)–C(2)–N(4)–C(5)–C(4)–C(3).

[b] Symmetry transformations used to generate equivalent atoms: #1 $-x$, $1-y$, $1-z$; #2 $-x$, $2-y$, $1-z$.

Table S5. Selected bond lengths (Å) and bond angles (°) for ***α*-TPymT**

Molecule **A**				Molecule **B**			
Bond lengths							
N(1)–C(2)	1.340(3)	N(20)–C(19)	1.394(4)	N(25)–C(26)	1.340(3)	N(44)–C(43)	1.390(3)
N(1)–C(6)	1.339(3)	N(20)–C(21)	1.399(3)	N(25)–C(30)	1.340(3)	N(44)–C(45)	1.393(3)
N(3)C(2)	1.343(3)	N(24)–C(19)	1.391(4)	N(27)–C(26)	1.343(3)	N(48)–C(43)	1.394(3)
N(3)–C(4)	1.345(3)	N(24)–C(23)	1.393(3)	N(27)–C(28)	1.344(3)	N(48)–C(47)	1.399(3)
N(5)–C(4)	1.345(3)	C(2)–C(7)	1.495(3)	N(29)–C(28)	1.346(3)	C(26)–C(31)	1.494(3)
N(5)–C(6)	1.343(3)	C(4)–C(13)	1.489(3)	N(29)–C(30)	1.344(3)	C(28)–C(37)	1.488(3)
N(8)–C(7)	1.394(4)	C(6)–C(19)	1.494(3)	N(32)–C(31)	1.391(3)	C(30)–C(43)	1.494(3)
N(8)–C(9)	1.399(3)	C(9)–C(10)	1.339(3)	N(32)–C(33)	1.393(3)	C(33)–C(34)	1.335(4)
N(12)–C(7)	1.391(3)	C(10)–C(11)	1.335(4)	N(36)–C(31)	1.394(4)	C(34)–C(35)	1.338(3)
N(12)–C(11)	1.393(3)	C(15)–C(16)	1.334(3)	N(36)–C(35)	1.399(3)	C(39)–C(40)	1.333(3)
N(14)–C(13)	1.387(3)	C(16)–C(17)	1.334(3)	N(38)–C(37)	1.387(4)	C(40)–C(41)	1.334(4)
N(14)–C(15)	1.391(3)	C(21)–C(22)	1.339(4)	N(38)–C(39)	1.391(3)	C(45)–C(46)	1.336(3)
N(18)–C(13)	1.387(3)	C(22)–C(23)	1.336(4)	N(42)–C(37)	1.388(3)	C(46)–C(47)	1.338(3)
N(18)–C(17)	1.392(3)			N(42)–C(41)	1.391(3)		
Bond angles							
C(2)–N(1)–C(6)	115.1(2)	N(8)–C(7)–N(12)	118.05(18)	C(26)–N(25)–C(30)	115.10(18)	N(32)–C(31)–N(36)	118.04(18)
C(2)–N(3)–C(4)	114.68(18)	N(8)–C(7)–C(2)	121.04(19)	C(26)–N(27)–C(28)	114.8(2)	N(32)–C(31)–C(26)	120.9(2)
C(4)–N(5)–C(6)	114.73(18)	N(12)–C(7)–C(2)	120.9(2)	C(28)–N(29)–C(30)	114.63(18)	N(36)–C(31)–C(26)	121.0(2)
C(7)–N(8)–C(9)	118.4(2)	N(8)–C(9)–C(10)	124.1(2)	C(31)–N(32)–C(33)	118.8(2)	N(32)–C(33)–C(34)	124.2(2)
C(7)–N(12)–C(11)	118.8(2)	C(9)–C(10)–C(11)	116.41(19)	C(31)–N(36)–C(35)	118.4(2)	C(33)–C(34)–C(35)	116.43(19)
C(13)–N(14)–C(15)	118.81(19)	N(12)–C(11)–C(10)	124.2(2)	C(37)–N(38)–C(39)	118.8(2)	N(36)–C(35)–C(34)	124.1(2)
C(13)–N(18)–C(17)	118.78(19)	N(14)–C(13)–N(18)	117.8(2)	C(37)–N(42)–C(41)	118.8(2)	N(38)–C(37)–N(42)	117.71(19)
C(19)–N(20)–C(21)	118.5(2)	N(14)–C(13)–C(4)	121.14(19)	C(43)–N(44)–C(45)	118.81(19)	N(38)–C(37)–C(28)	121.2(2)
C(19)–N(24)–C(23)	118.8(2)	N(18)–C(13)–C(4)	121.11(18)	C(43)–N(48)–C(47)	118.44(19)	N(42)–C(37)–C(28)	121.2(2)
N(1)–C(2)–N(3)	125.15(19)	N(14)–C(15)–C(16)	124.34(19)	N(25)–C(26)–N(27)	125.10(19)	N(38)–C(39)–C(40)	124.3(2)
N(1)–C(2)–C(7)	117.8(2)	C(15)–C(16)–C(17)	116.0(2)	N(25)–C(26)–C(31)	117.83(17)	C(39)–C(40)–C(41)	115.98(19)
N(3)–C(2)–C(7)	117.05(17)	N(18)–C(17)–C(16)	124.3(2)	N(27)–C(26)–C(31)	117.1(2)	N(42)–C(41)–C(40)	124.4(2)
N(3)–C(4)–N(5)	125.2(2)	N(20)–C(19)–N(24)	118.02(18)	N(27)–C(28)–N(29)	125.21(19)	N(44)–C(43)–N(48)	118.0(2)
N(3)–C(4)–C(13)	117.40(18)	N(20)–C(19)–C(6)	121.1(2)	N(27)–C(28)–C(37)	117.4(2)	N(44)–C(43)–C(30)	120.96(18)
N(5)–C(4)–C(13)	117.42(18)	N(24)–C(19)–C(6)	120.9(2)	N(29)–C(28)–C(37)	117.38(17)	N(48)–C(43)–C(30)	121.00(18)
N(1)–C(6)–N(5)	125.09(18)	N(20)–C(21)–C(22)	124.1(2)	N(25)–C(30)–N(29)	125.2(2)	N(44)–C(45)–C(46)	124.20(19)
N(1)–C(6)–C(19)	117.9(2)	C(21)–C(22)–C(23)	116.39(19)	N(25)–C(30)–C(43)	117.84(18)	C(45)–C(46)–C(47)	116.4(2)
N(5)–C(6)–C(19)	117.01(17)	N(24)–C(23)–C(22)	124.2(3)	N(29)–C(30)–C(43)	116.97(18)	N(48)–C(47)–C(46)	124.14(19)
Dihedral angles							
C(6)–N(1)–C(2)–N(3)	–0.8(6)	C(21)–N(20)–C(19)–N(24)	0.7(5)	C(30)–N(25)–C(26)–N(27)	–0.8(5)	C(45)–N(44)–C(43)–N(48)	–0.1(5)
C(6)–N(1)–C(2)–C(7)	179.3(3)	C(21)–N(20)–C(19)–C(6)	179.9(3)	C(30)–N(25)–C(26)–C(31)	179.3(3)	C(45)–N(44)–C(43)–C(30)	–179.3(3)
C(2)–N(1)–C(6)–N(5)	–0.8(6)	C(19)–N(20)–C(21)–C(22)	–0.7(5)	C(26)–N(25)–C(30)–N(29)	–0.8(5)	C(43)–N(44)–C(45)–C(46)	–0.7(5)
C(2)–N(1)–C(6)–C(19)	179.3(3)	C(23)–N(24)–C(19)–N(20)	–0.1(5)	C(26)–N(25)–C(30)–C(43)	179.3(3)	C(47)–N(48)–C(43)–N(44)	0.8(5)
C(4)–N(3)–C(2)–N(1)	1.5(6)	C(23)–N(24)–C(19)–C(6)	–179.3(3)	C(28)–N(27)–C(26)–N(25)	1.5(5)	C(47)–N(48)–C(43)–C(30)	179.9(3)
C(4)–N(3)–C(2)–C(7)	–178.6(3)	C(19)–N(24)–C(23)–C(22)	–0.8(5)	C(28)–N(27)–C(26)–C(31)	–178.6(3)	C(43)–N(48)–C(47)–C(46)	–0.7(5)
C(2)–N(3)–C(4)–N(5)	–0.7(6)	N(1)–C(2)–C(7)–N(8)	27.1(5)	C(26)–N(27)–C(28)–N(29)	–0.7(5)	N(25)–C(26)–C(31)–N(32)	–32.8(5)
C(2)–N(3)–C(4)–C(13)	179.3(3)	N(1)–C(2)–C(7)–N(12)	–153.8(4)	C(26)–N(27)–C(28)–C(37)	179.3(3)	N(25)–C(26)–C(31)–N(36)	148.1(3)
C(6)–N(5)–C(4)–N(3)	–0.7(6)	N(3)–C(2)–C(7)–N(8)	–152.8(3)	C(30)–N(29)–C(28)–N(27)	–0.7(5)	N(27)–C(26)–C(31)–N(32)	147.3(3)
C(6)–N(5)–C(4)–C(13)	179.3(3)	N(3)–C(2)–C(7)–N(12)	26.3(5)	C(30)–N(29)–C(28)–C(37)	179.3(3)	N(27)–C(26)–C(31)–N(36)	–31.8(5)
C(4)–N(5)–C(6)–N(1)	1.5(6)	N(3)–C(4)–C(13)–N(14)	–20.1(5)	C(28)–N(29)–C(30)–N(25)	1.5(5)	N(27)–C(28)–C(37)–N(38)	–39.3(5)
C(4)–N(5)–C(6)–C(19)	–178.6(3)	N(3)–C(4)–C(13)–N(18)	159.9(4)	C(28)–N(29)–C(30)–C(43)	–178.6(3)	N(27)–C(28)–C(37)–N(42)	140.7(3)
C(9)–N(8)–C(7)–N(12)	0.8(5)	N(5)–C(4)–C(13)–N(14)	159.9(4)	C(33)–N(32)–C(31)–N(36)	–0.1(5)	N(29)–C(28)–C(37)–N(38)	140.7(3)
C(9)–N(8)–C(7)–C(2)	179.9(3)	N(5)–C(4)–C(13)–N(18)	–20.1(5)	C(33)–N(32)–C(31)–C(26)	–179.2(3)	N(29)–C(28)–C(37)–N(42)	–39.3(5)
C(7)–N(8)–C(9)–C(10)	–0.7(5)	N(1)–C(6)–C(19)–N(20)	144.7(3)	C(31)–N(32)–C(33)–C(34)	–0.7(5)	N(25)–C(30)–C(43)–N(44)	–164.7(3)
C(11)–N(12)–C(7)–N(8)	–0.1(5)	N(1)–C(6)–C(19)–N(24)	–36.1(5)	C(35)–N(36)–C(31)–N(32)	0.8(5)	N(25)–C(30)–C(43)–N(48)	16.2(5)
C(11)–N(12)–C(7)–C(2)	–179.2(3)	N(5)–C(6)–C(19)–N(20)	–35.2(5)	C(35)–N(36)–C(31)–C(26)	179.9(3)	N(29)–C(30)–C(43)–N(44)	15.4(5)
C(7)–N(12)–C(11)–C(10)	–0.7(6)	N(5)–C(6)–C(19)–N(24)	144.0(3)	C(31)–N(36)–C(35)–C(34)	–0.7(5)	N(29)–C(30)–C(43)–N(48)	–163.7(3)
C(15)–N(14)–C(13)–N(18)	–0.5(5)	N(8)–C(9)–C(10)–C(11)	–0.1(5)	C(39)–N(38)–C(37)–N(42)	–0.5(4)	N(32)–C(33)–C(34)–C(35)	0.8(5)
C(15)–N(14)–C(13)–C(4)	179.5(3)	C(9)–C(10)–C(11)–N(12)	0.8(5)	C(39)–N(38)–C(37)–C(28)	179.5(3)	C(33)–C(34)–C(35)–N(36)	–0.1(5)
C(13)–N(14)–C(15)–C(16)	1.2(6)	N(14)–C(15)–C(16)–C(17)	–0.6(6)	C(37)–N(38)–C(39)–C(40)	1.2(5)	N(38)–C(39)–C(40)–C(41)	–0.6(5)

C(17)–N(18)–C(13)–N(14)	–0.7(5)	C(15)–C(16)–C(17)–N(18)	–0.7(6)	C(41)–N(42)–C(37)–N(38)	–0.6(4)	C(39)–C(40)–C(41)–N(42)	–0.7(5)
C(17)–N(18)–C(13)–C(4)	179.4(3)	N(20)–C(21)–C(22)–C(23)	–0.1(5)	C(41)–N(42)–C(37)–C(28)	179.4(3)	N(44)–C(45)–C(46)–C(47)	0.8(5)
C(13)–N(18)–C(17)–C(16)	1.3(6)	C(21)–C(22)–C(23)–N(24)	0.8(5)	C(37)–N(42)–C(41)–C(40)	1.3(5)	C(45)–C(46)–C(47)–N(48)	–0.1(5)

Table S6. π···π bond lengths (Å) and angles (°) for ***α*-TPymT**[a]

Cg(*I*)	Cg(*J*)[b]	*d*[Cg(*I*)–Cg(*J*)]	*α*	*β*	Cg(*I*)	Cg(*J*)[b]	*d*[Cg(*I*)–Cg(*J*)]	*α*	*β*
Cg(1)	Cg(5)$^{\#1}$	4.7512(18)	2.11	39.93	Cg(5)	Cg(2)$^{\#6}$	4.9402(16)	24.38	47.71
Cg(1)	Cg(5)$^{\#2}$	4.8142(17)	1.79	43.39	Cg(5)	Cg(2)$^{\#7}$	4.9915(18)	25.84	42.01
Cg(1)	Cg(8)$^{\#1}$	4.3692(18)	17.16	32.3	Cg(5)	Cg(3)$^{\#1}$	4.3677(18)	17.84	35.56
Cg(1)	Cg(8)$^{\#2}$	4.8769(19)	16.59	38.99	Cg(5)	Cg(4)$^{\#5}$	4.6431(18)	41.18	40.09
Cg(2)	Cg(5)$^{\#3}$	4.9401(16)	24.38	44.02	Cg(6)	Cg(1)$^{\#6}$	4.9790(16)	34.65	44
Cg(2)	Cg(5)$^{\#4}$	4.9915(18)	26.03	40.05	Cg(6)	Cg(2)$^{\#6}$	3.699(2)	8.32	18.14
Cg(2)	Cg(6)$^{\#3}$	3.699(2)	8.32	12.94	Cg(6)	Cg(4)$^{\#5}$	3.807(2)	0	27.44
Cg(2)	Cg(7)$^{\#4}$	3.892(2)	0	21.7	Cg(7)	Cg(1)$^{\#7}$	4.8181(18)	38.42	48.59
Cg(3)	Cg(5)$^{\#1}$	4.3677(18)	17.84	49.03	Cg(7)	Cg(2)$^{\#7}$	3.892(2)	32.22	30.77
Cg(3)	Cg(7)$^{\#1}$	3.9933(19)	31.4	11.26	Cg(7)	Cg(3)$^{\#1}$	3.9933(19)	31.4	38.4
Cg(3)	Cg(8)$^{\#2}$	3.983(2)	15.47	30.05	Cg(8)	Cg(1)$^{\#1}$	4.3693(18)	17.16	46.24
Cg(4)	Cg(6)$^{\#2}$	3.807(2)	45.86	14.94	Cg(8)	Cg(1)$^{\#5}$	4.8768(18)	10.74	51.55
Cg(4)	Cg(8)$^{\#1}$	4.1827(19)	45.39	51.95	Cg(8)	Cg(3)$^{\#5}$	3.983(2)	34.06	4.68
Cg(5)	Cg(1)$^{\#1}$	4.7512(18)	2.11	39.79	Cg(8)	Cg(4)$^{\#1}$	4.1828(19)	45.39	13.06
Cg(5)	Cg(1)$^{\#5}$	4.8143(18)	5.29	39.08					

[a] Cg(*I*)–Cg(*J*): distance between ring centroids; *α*: dihedral angle between planes Cg(*I*) and Cg(*J*); *β*: angle Cg(*I*) → Cg(*J*) vector and normal to plane *I*. Cg(1): N(1)–C(2)–N(3)–C(4)–N(5)–C(6), Cg(2): N(8)–C(7)–N(12)–C(11)–C(10)–C(9), Cg(3): N(14)–C(13)–N(18)–C(17)–C(16)–C(15), Cg(4): N(20)–C(19)–N(24)–C(23)–C(22)–C(21), Cg(5): N(25)–C(26)–N(27)–C(28)–N(29)–C(30), Cg(6): N(32)–C(31)–N(36)–C(35)–C(34)–C(33), Cg(7): N(38)–C(37)–N(42)–C(41)–C(40)–C(39), Cg(8): N(44)–C(43)–N(48)–C(47)–C(46)–C(45).

[b] Symmetry transformations used to generate equivalent atoms: #1 *x*, *y*, *z*; #2 1 – *x* + *y*, 1 – *x*, –1/3 + *z*; #3 *x*, –1 + *y*, *z*; #4 1 – *x* + *y*, –*x*, –1/3 + *z*; #5 1 – *y*, *x* – *y*, 1/3 + *z*; #6 *x*, 1 + *y*, *z*; #7 –*y*, –1 + *x* – *y*, 1/3 + *z*.