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2-Aminopyrimidine-3,3,3-triphenyl- propanoic acid (1/1)

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organic compounds

2-Aminopyrimidine–3,3,3-triphenylpropanoic acid (1/1)

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The title bimolecular compound, $C_4H_5N_3·C_{21}H_{18}O_2$, constructed from 2-aminopyrimidine and 3,3,3-triphenylpropanoic acid, forms a tetramolecular hydrogen-bonded motif *via* O—H···N, N—H···O and N—H···N contacts. This aggregate organizes to give crystal-packing motifs with hydrophilic and hydrophobic regions.

Comment

Over the past decade, the field of supramolecular chemistry has emerged as a significant contributor to the broad area of materials science owing in part to advances in decoding the structural features responsible for molecular cohesion. While much of this progress has been documented in the literature, many areas still require attention before prediction of complex high-order motifs can be successfully achieved with regularity. To this end, two areas that continue to prove useful for understanding the fundamental principles of supramolecular chemistry include new synthon identification and thorough assessment of the recognition profiles of known molecular contacts.

The packing tendencies of Ph_3X groups (X = C or P; Scudder & Dance, 1998, 2000; Steiner, 2000) and their use in practical applications (Garcia-Garibay, 2005; Jarowski *et al.*, 2007) have been reported in the literature. Crystallographic studies of molecules containing Ph_3X groups show several salient packing motifs, such as the sixfold (6PE) and fourfold (4PE) phenyl embraces (Scudder & Dance, 2000). Although these phenyl embrace motifs have been exploited as a tool for constructing supramolecular assemblies, extending their use to include additional molecular contacts (*e.g.* hydrogen bonds) has seen less attention. It has been reported by Steiner (1999) that 3,3,3-triphenylpropanoic acid crystallizes with molecules organized into linear motifs *via* a combination of carboxyl–carboxyl and 6PE interactions. We wondered if the observed linear assemblage could be transferred and extended by cocrystallizing the triphenylpropanoic acid with a complementary hydrogen-bond spacer such as 2-aminopyrimidine.

(I)
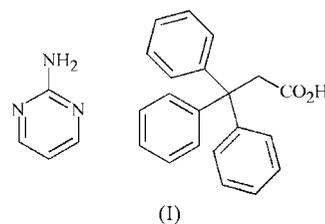
Cocrystallization of 3,3,3-triphenylpropanoic acid and 2-aminopyrimidine produced the expected bimolecular compound, (I); the C—O distances in the acid component (Table 1) are consistent with the location of the hydroxy H atom as deduced from the refinement. The asymmetric unit of (I) shows the formation of a hydrogen-bonded $R_2^2(8)$ motif involving both 2-aminopyrimidine and 3,3,3-triphenylpropanoic acid components (Fig. 1). As anticipated, this molecular assemblage is further linked to give a tetrameric motif by use of two additional inversion-related N—H···N hydrogen bonds (Table 2; Lynch *et al.*, 1998). Unlike the structure of 3,3,3-triphenylpropanoic acid, the terminal triphenylmethyl (TPM) groups of our tetrameric unit lack participation in 6PE interactions. Rather, the TPM groups of (I) assemble by use of van der Waals contacts to give hydrophobic and hydrophilic regions (Fig. 2)

The most effective packing of 6PE motifs involves a concerted cycle of six local edge-to-face Ph···Ph interactions.
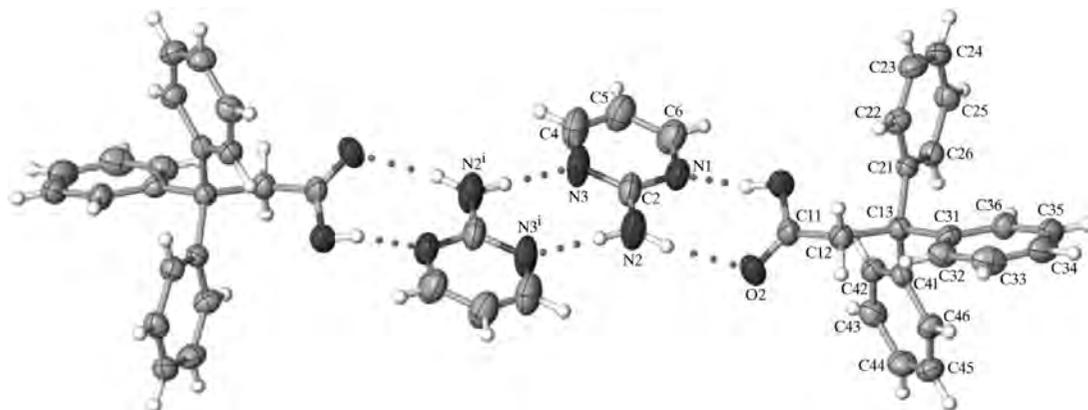
Figure 1
A molecular diagram of (I), showing the labeling scheme, asymmetric unit (50% probability displacement ellipsoids) and hydrogen-bonded tetramer. [Symmetry code: (i) $-x + 1, -y + 2, -z + 1$.]
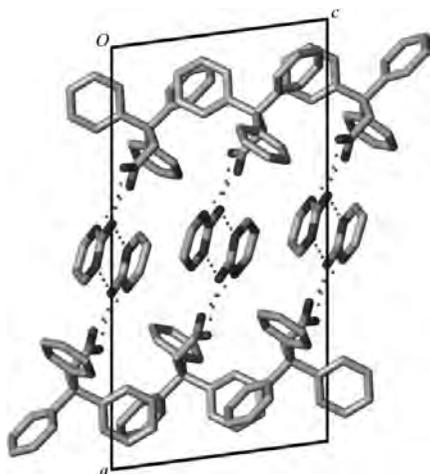
Figure 2
A projection of the unit-cell contents of (I), showing hydrophobic and hydrophilic crystal regions. H atoms have been omitted for the sake of clarity.

Compounds that align in this manner possess TPM conformations that approach a rotor with pseudo-threefold symmetry. This structural feature is easily quantified by assessing the twist of the three phenyl groups around their C—C_{ipso} bond. Cases that exhibit rotor conformations show similar twist angles of the phenyl groups. For (I), these torsion angles (Table 1) differ markedly and they are consistent with the previously described 'flipper' conformation (Scudder & Dance, 2000). Although this arrangement of phenyl groups is capable of forming several phenyl embrace motifs (*e.g.* 6PE and 4PE), (I) crystallizes with phenyl groups aligned in a skewed 4PE arrangement. In conclusion, this study highlights the successful use of building blocks (*i.e.* 3,3,3-triphenyl-propanoic acid and 2-aminopyrimidine) that form the expected hydrogen-bonded tetramolecular unit with additional, less well defined, phenyl embrace contacts for organizing the supramolecular assembly.

Experimental

Single crystals of (I) were prepared by slow evaporation at room temperature of an acetone solution containing equimolar quantities of 2-aminopyrimidine and 3,3,3-triphenylpropionic acid (m.p. 383–384 K).

Crystal data

$C_4H_5N_3 \cdot C_{21}H_{18}O_2$	$V = 2065.6$ (5) Å^3
$M_r = 397.46$	$Z = 4$
Monoclinic, $P2_1/c$	Cu $K\alpha$ radiation
$a = 20.590$ (2) Å	$\mu = 0.66$ mm^{-1}
$b = 9.5109$ (8) Å	$T = 298$ (2) K
$c = 10.640$ (2) Å	$0.45 \times 0.42 \times 0.20$ mm
$\beta = 97.518$ (15)°	

Data collection

Bruker *P*4 diffractometer	2048 reflections with $I > 2\sigma(I)$
Absorption correction: analytical (*XPREP*; Bruker, 2001)	$R_{int} = 0.043$
$T_{min} = 0.757$, $T_{max} = 0.880$	$\theta_{max} = 61.8°$
4193 measured reflections	3 standard reflections
3144 independent reflections	every 97 reflections
	intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.057$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.149$	
$S = 1.04$	
3144 reflections	$\Delta\rho_{max} = 0.17$ e Å^{-3}
278 parameters	$\Delta\rho_{min} = -0.23$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C11	1.318 (3)	N3—C2	1.348 (4)
O2—C11	1.213 (4)	N3—C4	1.331 (5)
N1—C2	1.338 (4)	C4—C5	1.355 (6)
N1—C6	1.329 (4)	C5—C6	1.373 (5)
N2—C2	1.336 (5)		
C12—C13—C21—C22	50.3 (3)	C12—C13—C41—C42	78.5 (3)
C12—C13—C31—C32	6.1 (4)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1—H1C$\cdots$N1	0.96 (5)	1.85 (5)	2.790 (3)	166 (4)
N2—H2A$\cdots$O2	0.89 (4)	2.11 (4)	2.990 (4)	167 (4)
N2—H2B$\cdots$N3^i	0.94 (5)	2.13 (5)	3.068 (5)	173 (4)

Symmetry code: (i) $-x + 1, -y + 2, -z + 1$.

H atoms bonded to N or O atoms were refined without constraint. All other H atoms were included as riding atoms in geometrically idealized positions [C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C)].

Data collection and cell refinement: *XSCANS* (Bruker, 1999); data reduction: *XPREP* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics and preparation of material for publication: *X-SEED* (Barbour, 2001).

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