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Linear chains in the 1:1 complex of thiophene-2,5-dicarboxylic acid and 4,4′-bipyridine

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.055
wR factor = 0.145
Data-to-parameter ratio = 15.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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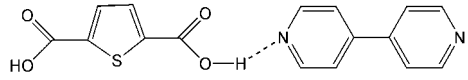
In the crystal structure of the title complex, $C_{10}H_8N_2{\cdot}C_6H_4O_4S$ or bpy·tdc (bpy is 4,4′-bipyridine and tdc is thiophene-2,5-dicarboxylic acid), bpy and tdc form one-dimensional zigzag chains as a result of O—H···N hydrogen bonds. These chains are further assembled into layers by van der Waals attractions, which are extended into a three-dimensional network by van der Waals and aromatic π–π stacking interactions.

Comment

Crystals of many organic compounds grow from solution and commonly contain only one kind of molecule. Hydrogen-bonding interactions, van der Waals attractions and aromatic π–π stacking interactions are the primary interactions involved in the creation of a variety of molecular architectures for organic crystals. We report here the crystal structure of the title 1:1 complex, bpy·tdc (bpy is 4,4′-bipyridine and tdc is thiophene-2,5-dicarboxylic acid), (I), which crystallizes in the space group $P2_1/c$. In (I), bpy and tdc form one-dimensional zigzag chains as a result of O—H···N hydrogen bonds (Fig. 2 and Table 1). These chains are assembled into layers by van der Waals attractions (Fig. 3), which are further extended into a three-dimensional network by van der Waals and aromatic π–π stacking interactions (Fig. 4); the thiophene plane (S1/C12–C15) makes a dihedral angle of 9.3° with the adjacent pyridine plane (N1/C1–C5) and the distance between the two planes is 3.5 Å. The unique strength and direction of the hydrogen-bonding interactions play a very important role in the creation of the observed molecular architecture for this crystal structure.



(I)

Experimental

4,4′-Bipyridine (0.2 mmol) and thiophene-2,5-dicarboxylic acid (0.2 mmol) were dissolved in a water–alcohol (4:1 v/v, 20 ml) mixture. The solution was stirred for 1 h at 333 K and then filtered. The resulting solution was allowed to stand in air at room temperature for one week and yielded colorless crystals.

Crystal data

$C_{10}H_8N_2{\cdot}C_6H_4O_4S$
M_r = 328.34
Monoclinic, $P2_1/c$
a = 6.8598 (6) Å
b = 10.3438 (9) Å
c = 21.1315 (18) Å
β = 95.718 (2)°
V = 1492.0 (2) Å^3
Z = 4
D_x = 1.462 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 2–27°
μ = 0.24 mm^{-1}
T = 293 (2) K
Block, colorless
0.52 × 0.46 × 0.18 mm

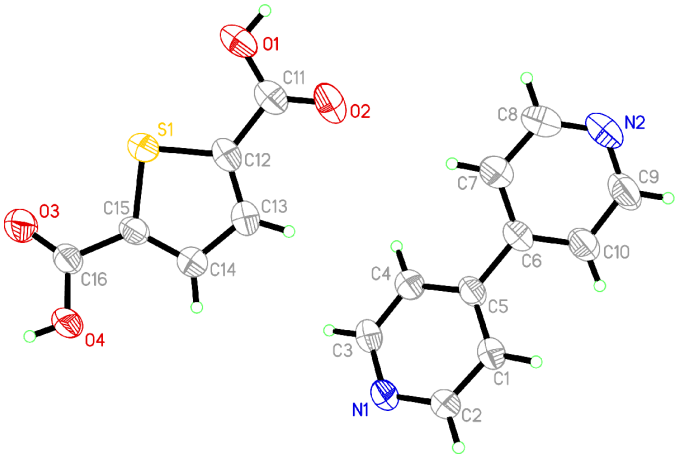


Figure 1
The component molecules of (I), shown with 50% probability displacement ellipsoids.

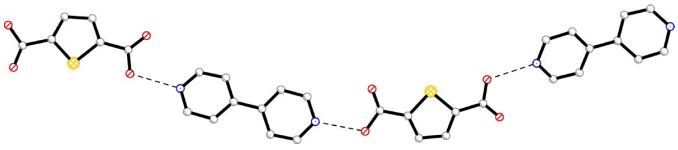


Figure 2
Perspective view of the one-dimensional chain in (I). Hydrogen bonds are shown as dashed lines and H atoms have been omitted.

Data collection

Siemens *R*3*m* diffractometer
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.886, T_{max} = 0.958
8861 measured reflections
3243 independent reflections
2620 reflections with $I > 2\sigma(I)$

R_{int} = 0.021
θ_{max} = 27.0°
$h = -8 \rightarrow 7$
$k = -10 \rightarrow 13$
$l = -26 \rightarrow 26$
2 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.145
S = 1.07
3243 reflections
208 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0724P)^2 + 0.482P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N2^{i}	0.82	1.84	2.662 (2)	175
O4—H4B···N1^{ii}	0.82	1.80	2.616 (2)	175

Symmetry codes: (i) $-1-x, 1-y, 1-z$; (ii) $1-x, y-\frac{1}{2}, \frac{1}{2}-z$.

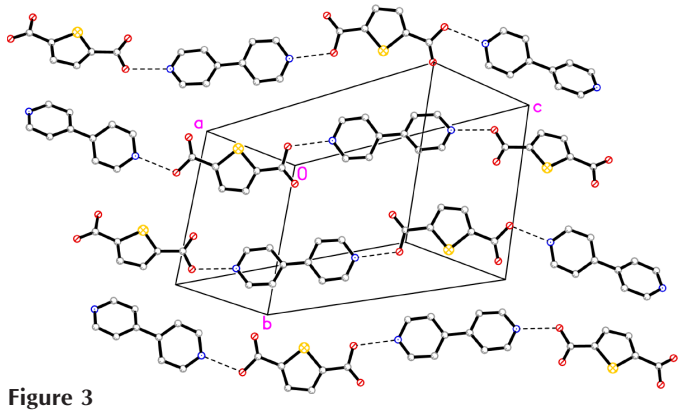


Figure 3
Perspective view of the layers consisting of chains. H atoms have been omitted. Dashed lines indicate hydrogen bonds.

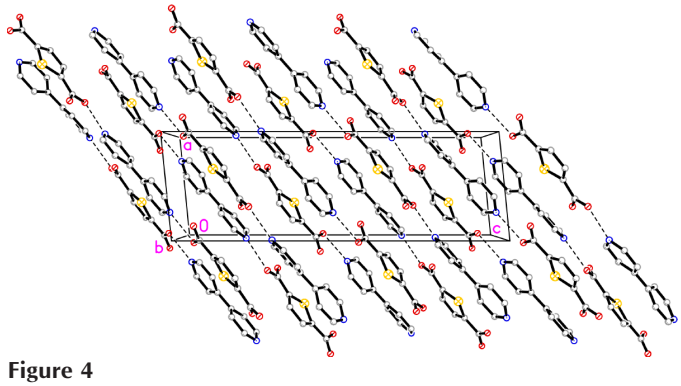


Figure 4
The molecular packing, viewed along the *b* axis. H atoms have been omitted. Dashed lines indicate hydrogen bonds.

H atoms bonded to C atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C). H atoms linking with O atoms were located in difference maps, adjusted to give O—H = 0.85 Å, and refined as riding on their parent atoms, with U_{iso}(H) = 1.5U_{eq}(O).

Data collection: *R*3*m Software* (Siemens, 1990); cell refinement: *R*3*m Software*; data reduction: *R*3*m Software*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1998); software used to prepare material for publication: *SHELXL*97.

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