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Di-4-pyridyl sulfide–isophthalic acid (1/1)

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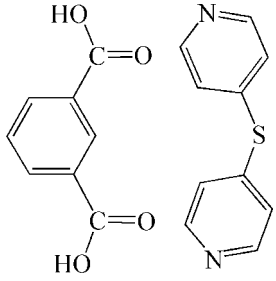
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.007 Å; R factor = 0.080; wR factor = 0.269; data-to-parameter ratio = 13.5.

In the heteromolecular title structure, $C_{10}H_8N_2S\cdot C_8H_6O_4$, the two components are linked by O—H···N hydrogen bonds to form a one-dimensional chain. These chains are further interconnected by weak intermolecular C—H···O hydrogen bonds and weak C—H···π interactions to generate a three-dimensional supramolecular structure.

Related literature

For C—H···O hydrogen bonds, see: Bhogala *et al.* (2005); Wang *et al.* (2008). For C—H···π interactions, see: Fun & Kia (2008).



Experimental

Crystal data

$C_{10}H_8N_2S\cdot C_8H_6O_4$
M_r = 354.37
Triclinic, $P\overline{1}$
a = 6.618 (6) Å
b = 8.200 (7) Å
c = 16.013 (13) Å
α = 88.808 (11)°
β = 79.340 (11)°
γ = 79.275 (11)°
V = 839.0 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 291 (2) K
0.47 × 0.30 × 0.11 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.905, T_{max} = 0.977
6280 measured reflections
3084 independent reflections
1885 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.080
$wR(F^2)$ = 0.269
S = 1.08
3084 reflections
228 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.05 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C17—H17···O2^{i}	0.93	2.45	3.334 (6)	159
C16—H16···O2^{ii}	0.93	2.58	3.180 (6)	123
C13—H13···O4^{iii}	0.93	2.31	3.141 (6)	148
C12—H12···$Cg1^{iv}$	0.93	2.98	3.570 (6)	123
O3—H3D···N1^{v}	0.82	1.83	2.634 (5)	164
O1—H1D···N2^{vi}	0.82	1.84	2.662 (5)	179

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, y, z+1$; (iii) $x-1, y+1, z$; (iv) $-x+1, -y+2, -z+1$; (v) $x, y-1, z$; (vi) $x, y, z-1$. $Cg1$ is the centroid of the C2–C7 isophthalic acid ring.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2125).

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