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

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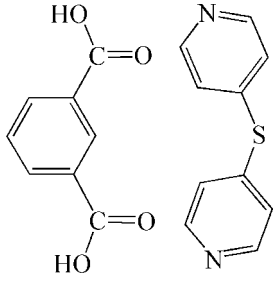
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.007 Å; R factor = 0.080; wR factor = 0.269; data-to-parameter ratio = 13.5.

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*.

The authors thank Luo Yang Normal University for supporting this work.

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

References

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supporting information

Acta Cryst. (2008). E**64**, o2279 [doi:10.1107/S1600536808035496]

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

Jian-Hua Qin, Xiao-Dong Li and Jian-Ge Wang

S1. Comment

The asymmetric unit consists of one 4,4′-dipyridyl sulfide molecule and one isophthalic acid molecule (Fig. 1). The hetero-molecularar components of (I) are linked by O—H···N hydrogen bonds to form a one-dimensional chain (Table 1 & Fig. 2). These chains interact with each other *via* weak intermolecular C—H···O hydrogen bonds and C—H···π interactions. Within the asymmetric unit, the atoms C13, C16 and C17 act as hydrogen-bond donors (Table 1). The bond lengths and angles of these three hydrogen bonds are comparable with literature data (Bhogala *et al.*, 2005; Wang *et al.*, 2008). These hydrogen bonds, albeit rather weak, link the chains into two-dimensional double layers structure, which are further connected by weak intermolecular C—H···π interactions (Table 1) to generate a three-dimensional supramolecular structure (Fig. 3).

S2. Experimental

4,4′-dipyridyl sulfide (18.84 mg, 0.1 mmol), isophthalic acid (16.51 mg, 0.1 mmol), and NaOH (8.13 mg, 0.2 mmol) were added to a H_2O solution (15 ml) in a Teflonlined stainless steel reactor. The mixture was heated at 473 K for 3 d, and then slowly cooled down to room temperature. Colorless crystals of the title compound were obtained.

S3. Refinement

All hydrogen atoms were positioned geometrically and treated as riding, with C—H bonding lengths constrained to 0.93 (aromatic CH) and O—H bonding lengths constrained to 0.82 (OH), and with U_{iso}(H) = 1.2U_{eq}(C) and U_{iso}(H) = 1.5U_{eq}(O).

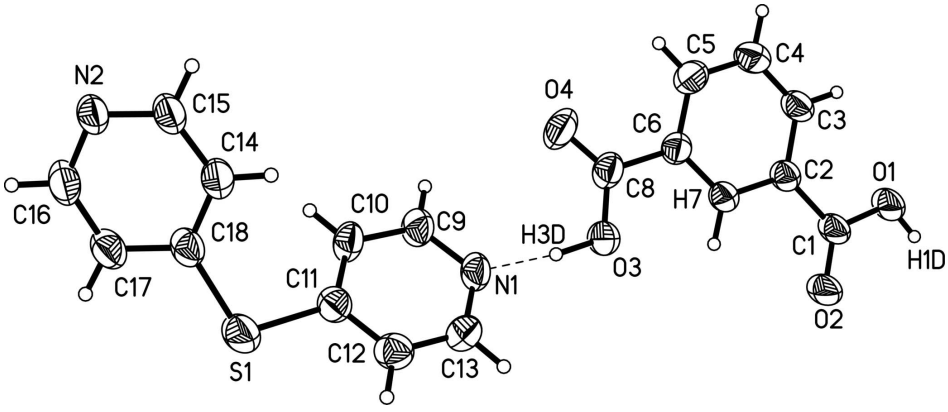

Figure 1

A view of the hetero-molecular components of the title compound with the atom labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

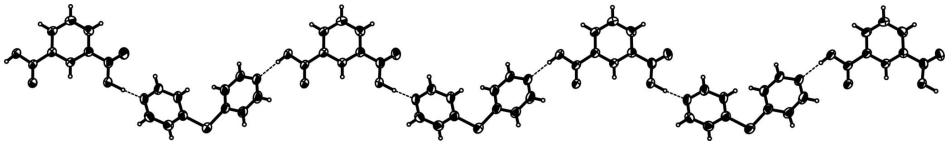

Figure 2

A view of the one-dimensional hydrogen-bond chain motif.

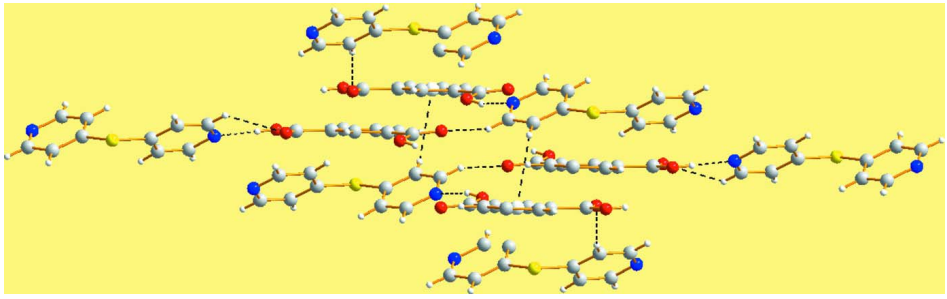

Figure 3

A view of the C—H···O hydrogen bond and the C—H···π interactions in the crystal structure of the title compound.

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

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
F(000) = 368
D_x = 1.403 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1298 reflections
θ = 2.9–21.2°
μ = 0.22 mm^{-1}
T = 291 K
Block, colorless
0.47 × 0.30 × 0.11 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
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
θ_{max} = 25.5°, θ_{min} = 2.5°
h = −8→7
k = −9→9
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.080
$wR(F^2)$ = 0.269
S = 1.08
3084 reflections
228 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1354P)^2 + 0.4871P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 1.05$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.2928 (2)	0.9132 (2)	0.77591 (8)	0.1000 (6)
O1	0.9948 (5)	0.7101 (5)	0.0723 (2)	0.0868 (10)
H1D	0.9203	0.7396	0.0371	0.130*
O2	0.7255 (6)	0.5957 (5)	0.1306 (2)	0.0993 (12)
O3	0.7222 (6)	0.3409 (5)	0.4098 (2)	0.0958 (12)
H3D	0.6703	0.3073	0.4560	0.144*
O4	1.0069 (6)	0.2941 (6)	0.4653 (2)	0.1133 (14)
N1	0.5677 (7)	1.1790 (5)	0.5430 (2)	0.0733 (10)
N2	0.7476 (6)	0.8077 (5)	0.9602 (2)	0.0777 (11)
C1	0.8967 (7)	0.6270 (6)	0.1321 (3)	0.0716 (12)
C2	1.0110 (6)	0.5765 (5)	0.2024 (3)	0.0636 (10)
C3	1.2038 (7)	0.6166 (6)	0.2056 (3)	0.0724 (12)
H3	1.2694	0.6727	0.1605	0.087*
C4	1.2987 (7)	0.5754 (6)	0.2735 (3)	0.0833 (14)
H4	1.4264	0.6058	0.2751	0.100*
C5	1.2062 (7)	0.4887 (6)	0.3400 (3)	0.0772 (12)
H5	1.2721	0.4597	0.3861	0.093*
C6	1.0141 (6)	0.4447 (5)	0.3378 (3)	0.0639 (10)
C7	0.9189 (6)	0.4878 (5)	0.2695 (2)	0.0637 (10)
H7	0.7912	0.4574	0.2677	0.076*
C8	0.9164 (7)	0.3505 (6)	0.4099 (3)	0.0734 (12)
C9	0.6939 (8)	1.0749 (6)	0.5857 (3)	0.0761 (13)
H9	0.8376	1.0583	0.5661	0.091*
C10	0.6199 (8)	0.9931 (6)	0.6562 (3)	0.0750 (12)
H10	0.7120	0.9208	0.6834	0.090*
C11	0.4099 (7)	1.0177 (6)	0.6868 (3)	0.0691 (11)
C12	0.2817 (8)	1.1212 (6)	0.6439 (3)	0.0782 (13)
H12	0.1377	1.1399	0.6631	0.094*
C13	0.3637 (8)	1.1986 (6)	0.5722 (3)	0.0795 (13)
H13	0.2728	1.2673	0.5429	0.095*
C14	0.6067 (8)	0.9811 (6)	0.8561 (3)	0.0833 (14)
H14	0.6056	1.0787	0.8254	0.100*
C15	0.7391 (8)	0.9425 (6)	0.9127 (3)	0.0842 (15)
H15	0.8286	1.0150	0.9182	0.101*
C16	0.6162 (10)	0.7091 (7)	0.9505 (3)	0.0917 (16)
H16	0.6169	0.6143	0.9834	0.110*
C17	0.4795 (8)	0.7377 (6)	0.8952 (3)	0.0855 (15)
H17	0.3896	0.6644	0.8916	0.103*
C18	0.4760 (7)	0.8763 (6)	0.8449 (3)	0.0716 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0992 (10)	0.1442 (14)	0.0722 (9)	−0.0626 (10)	−0.0181 (7)	0.0271 (8)
O1	0.091 (2)	0.117 (3)	0.0667 (19)	−0.058 (2)	−0.0187 (16)	0.0361 (18)
O2	0.097 (2)	0.150 (3)	0.076 (2)	−0.074 (2)	−0.0345 (18)	0.054 (2)
O3	0.093 (2)	0.138 (3)	0.074 (2)	−0.057 (2)	−0.0301 (18)	0.053 (2)
O4	0.085 (2)	0.152 (4)	0.103 (3)	−0.016 (2)	−0.032 (2)	0.068 (3)
N1	0.095 (3)	0.077 (2)	0.0527 (19)	−0.028 (2)	−0.0184 (19)	0.0174 (17)
N2	0.099 (3)	0.088 (3)	0.056 (2)	−0.045 (2)	−0.0143 (19)	0.0178 (19)
C1	0.074 (3)	0.094 (3)	0.056 (2)	−0.043 (2)	−0.010 (2)	0.018 (2)
C2	0.062 (2)	0.071 (3)	0.059 (2)	−0.021 (2)	−0.0061 (19)	0.0076 (19)
C3	0.069 (3)	0.084 (3)	0.070 (3)	−0.035 (2)	−0.007 (2)	0.011 (2)
C4	0.063 (3)	0.100 (4)	0.092 (3)	−0.031 (3)	−0.013 (2)	0.011 (3)
C5	0.069 (3)	0.089 (3)	0.074 (3)	−0.010 (2)	−0.020 (2)	0.010 (2)
C6	0.061 (2)	0.067 (3)	0.063 (2)	−0.0106 (19)	−0.0114 (19)	0.010 (2)
C7	0.061 (2)	0.073 (3)	0.060 (2)	−0.023 (2)	−0.0099 (19)	0.012 (2)
C8	0.072 (3)	0.082 (3)	0.063 (3)	−0.008 (2)	−0.012 (2)	0.017 (2)
C9	0.076 (3)	0.091 (3)	0.058 (2)	−0.016 (2)	−0.005 (2)	0.016 (2)
C10	0.082 (3)	0.080 (3)	0.057 (2)	−0.007 (2)	−0.008 (2)	0.019 (2)
C11	0.079 (3)	0.076 (3)	0.058 (2)	−0.025 (2)	−0.014 (2)	0.003 (2)
C12	0.071 (3)	0.092 (3)	0.072 (3)	−0.019 (2)	−0.010 (2)	−0.001 (2)
C13	0.084 (3)	0.084 (3)	0.077 (3)	−0.017 (3)	−0.033 (3)	0.012 (3)
C14	0.107 (4)	0.085 (3)	0.072 (3)	−0.043 (3)	−0.027 (3)	0.024 (2)
C15	0.108 (4)	0.096 (3)	0.063 (3)	−0.056 (3)	−0.017 (3)	0.021 (2)
C16	0.136 (5)	0.087 (3)	0.068 (3)	−0.058 (3)	−0.024 (3)	0.022 (2)
C17	0.111 (4)	0.093 (3)	0.068 (3)	−0.059 (3)	−0.019 (3)	0.008 (3)
C18	0.083 (3)	0.086 (3)	0.049 (2)	−0.033 (2)	−0.002 (2)	0.005 (2)

Geometric parameters (Å, º)

S1—C18	1.767 (5)	C5—H5	0.9300
S1—C11	1.776 (5)	C6—C7	1.369 (6)
O1—C1	1.308 (5)	C6—C8	1.490 (6)
O1—H1D	0.8200	C7—H7	0.9300
O2—C1	1.212 (5)	C9—C10	1.361 (6)
O3—C8	1.302 (6)	C9—H9	0.9300
O3—H3D	0.8200	C10—C11	1.364 (6)
O4—C8	1.198 (5)	C10—H10	0.9300
N1—C13	1.325 (6)	C11—C12	1.356 (6)
N1—C9	1.347 (6)	C12—C13	1.373 (7)
N2—C16	1.323 (6)	C12—H12	0.9300
N2—C15	1.327 (6)	C13—H13	0.9300
C1—C2	1.480 (6)	C14—C18	1.364 (6)
C2—C3	1.385 (6)	C14—C15	1.367 (7)
C2—C7	1.394 (5)	C14—H14	0.9300
C3—C4	1.360 (6)	C15—H15	0.9300
C3—H3	0.9300	C16—C17	1.366 (7)

C4—C5	1.380 (6)	C16—H16	0.9300
C4—H4	0.9300	C17—C18	1.379 (6)
C5—C6	1.391 (6)	C17—H17	0.9300

C18—S1—C11	106.3 (2)	N1—C9—H9	118.6
C1—O1—H1D	109.5	C10—C9—H9	118.6
C8—O3—H3D	109.5	C9—C10—C11	119.6 (4)
C13—N1—C9	117.0 (4)	C9—C10—H10	120.2
C16—N2—C15	115.8 (4)	C11—C10—H10	120.2
O2—C1—O1	122.8 (4)	C12—C11—C10	118.0 (4)
O2—C1—C2	122.8 (4)	C12—C11—S1	117.9 (4)
O1—C1—C2	114.3 (4)	C10—C11—S1	124.0 (4)
C3—C2—C7	118.4 (4)	C11—C12—C13	120.2 (4)
C3—C2—C1	122.9 (4)	C11—C12—H12	119.9
C7—C2—C1	118.7 (4)	C13—C12—H12	119.9
C4—C3—C2	121.1 (4)	N1—C13—C12	122.4 (4)
C4—C3—H3	119.5	N1—C13—H13	118.8
C2—C3—H3	119.5	C12—C13—H13	118.8
C3—C4—C5	120.3 (4)	C18—C14—C15	119.8 (4)
C3—C4—H4	119.9	C18—C14—H14	120.1
C5—C4—H4	119.9	C15—C14—H14	120.1
C4—C5—C6	119.8 (4)	N2—C15—C14	123.9 (4)
C4—C5—H5	120.1	N2—C15—H15	118.1
C6—C5—H5	120.1	C14—C15—H15	118.1
C7—C6—C5	119.6 (4)	N2—C16—C17	124.2 (4)
C7—C6—C8	121.2 (4)	N2—C16—H16	117.9
C5—C6—C8	119.2 (4)	C17—C16—H16	117.9
C6—C7—C2	120.9 (4)	C16—C17—C18	119.3 (4)
C6—C7—H7	119.6	C16—C17—H17	120.3
C2—C7—H7	119.6	C18—C17—H17	120.3
O4—C8—O3	122.8 (4)	C14—C18—C17	116.9 (4)
O4—C8—C6	122.5 (4)	C14—C18—S1	124.6 (4)
O3—C8—C6	114.7 (4)	C17—C18—S1	118.4 (4)
N1—C9—C10	122.8 (4)		

O2—C1—C2—C3	−178.0 (5)	N1—C9—C10—C11	−1.0 (8)
O1—C1—C2—C3	1.2 (7)	C9—C10—C11—C12	1.5 (7)
O2—C1—C2—C7	0.6 (7)	C9—C10—C11—S1	177.7 (4)
O1—C1—C2—C7	179.8 (4)	C18—S1—C11—C12	−152.0 (4)
C7—C2—C3—C4	−2.1 (7)	C18—S1—C11—C10	31.8 (5)
C1—C2—C3—C4	176.5 (4)	C10—C11—C12—C13	−0.4 (7)
C2—C3—C4—C5	1.6 (8)	S1—C11—C12—C13	−176.8 (4)
C3—C4—C5—C6	−0.6 (8)	C9—N1—C13—C12	1.9 (7)
C4—C5—C6—C7	0.1 (7)	C11—C12—C13—N1	−1.4 (8)
C4—C5—C6—C8	179.8 (4)	C16—N2—C15—C14	−0.5 (8)
C5—C6—C7—C2	−0.6 (7)	C18—C14—C15—N2	−1.3 (8)
C8—C6—C7—C2	179.7 (4)	C15—N2—C16—C17	0.9 (8)
C3—C2—C7—C6	1.6 (6)	N2—C16—C17—C18	0.7 (9)

C1—C2—C7—C6	−177.0 (4)	C15—C14—C18—C17	2.7 (8)
C7—C6—C8—O4	170.8 (5)	C15—C14—C18—S1	178.4 (4)
C5—C6—C8—O4	−8.8 (7)	C16—C17—C18—C14	−2.4 (8)
C7—C6—C8—O3	−12.1 (6)	C16—C17—C18—S1	−178.4 (4)
C5—C6—C8—O3	168.3 (4)	C11—S1—C18—C14	34.9 (5)
C13—N1—C9—C10	−0.7 (7)	C11—S1—C18—C17	−149.5 (4)

Hydrogen-bond geometry (Å, º)

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···*Cg*1^{iv}	0.93	2.98	3.570 (6)	123
O3—H3*D*···N1^{v}	0.82	1.83	2.634 (5)	164
O1—H1*D*···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.