

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

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

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

College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang 471022, People's Republic of China
Correspondence e-mail: jh_q128105@126.com

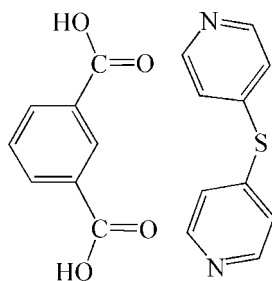
Received 21 October 2008; accepted 30 October 2008

Key indicators: single-crystal X-ray study; $T = 291$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.080; wR factor = 0.269; data-to-parameter ratio = 13.5.

In the heteromolecular title structure, $\text{C}_{10}\text{H}_8\text{N}_2\text{S}\cdot\text{C}_8\text{H}_6\text{O}_4$, the two components are linked by $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds to form a one-dimensional chain. These chains are further interconnected by weak intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds and weak $\text{C}-\text{H}\cdots\pi$ interactions to generate a three-dimensional supramolecular structure.

Related literature

For $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, see: Bhogala *et al.* (2005); Wang *et al.* (2008). For $\text{C}-\text{H}\cdots\pi$ interactions, see: Fun & Kia (2008).


Experimental
Crystal data

$\text{C}_{10}\text{H}_8\text{N}_2\text{S}\cdot\text{C}_8\text{H}_6\text{O}_4$
 $M_r = 354.37$
Triclinic, $P\bar{1}$
 $a = 6.618$ (6) Å

$b = 8.200$ (7) Å
 $c = 16.013$ (13) Å
 $\alpha = 88.808$ (11)°
 $\beta = 79.340$ (11)°

$\gamma = 79.275$ (11)°
 $V = 839.0$ (12) Å³
 $Z = 2$
Mo $K\alpha$ radiation

$\mu = 0.22$ mm⁻¹
 $T = 291$ (2) K
 $0.47 \times 0.30 \times 0.11$ 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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.020$

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, °).

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

- Bhogala, B. R., Basavoju, S. & Nangia, A. (2005). *Cryst. Growth Des.* **5**, 1683–1686.
Bruker (1997). SMART, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
Fun, H.-K. & Kia, R. (2008). *Acta Cryst.* **E64**, m1116–m1117.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Wang, Y.-T., Tang, G.-M., Zhang, Y.-C. & Wan, W.-Z. (2008). *Acta Cryst.* **E64**, o1753.