Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

A cocrystal of pyridine-2,4-dicarboxylic acid and serine

Peng Liang

College of Chemical Engineering & Materials Science, Liaodong University, Dandong 118003, People's Republic of China
Correspondence e-mail: liangpenglong@163.com

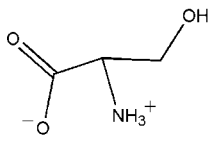
Received 8 November 2007; accepted 22 November 2007

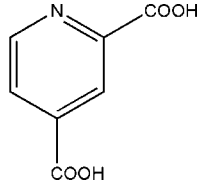
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.036; wR factor = 0.090; data-to-parameter ratio = 7.0.

The title compound, pyridine-2,4-dicarboxylic acid–*S*-serine (1/1), $C_7H_5NO_4{\cdot}C_3H_7NO_3$, has serine in its zwitterionic form. The crystal structure is stabilized by an extensive series of intermolecular O—H···O, N—H···N and N—H···O hydrogen bonds, forming a three-dimensional network.

Related literature

For related structures of organic acids and amino acids, see: Coupar *et al.* (1997); Pandiarajan *et al.* (2001); Sobczyk *et al.* (2000); Srinivasan *et al.* (2002).





Experimental

Crystal data

$C_7H_5NO_4{\cdot}C_3H_7NO_3$
M_r = 272.22
Triclinic, $P1$
a = 4.4941 (13) Å
b = 6.4512 (18) Å
c = 10.123 (3) Å
α = 81.273 (3)°
β = 87.060 (3)°
γ = 86.247 (3)°
V = 289.22 (14) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 298 (2) K
0.37 × 0.33 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.952, T_{max} = 0.961
2493 measured reflections
1287 independent reflections
1202 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.090
S = 1.05
1287 reflections
184 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O5^{i}	0.82	1.77	2.590 (3)	173
O4—H4···O6^{ii}	0.82	1.81	2.598 (3)	162
O7—H7···O6^{iii}	0.82	1.94	2.754 (3)	171
N2—H2A···N1^{iv}	0.89 (3)	2.05 (2)	2.872 (3)	152 (4)
N2—H2A···O1^{iv}	0.89 (3)	2.55 (4)	3.023 (3)	113 (3)
N2—H2B···O7^{v}	0.90 (3)	2.01 (2)	2.848 (3)	155 (4)
N2—H2C···O2^{vi}	0.90 (4)	2.07 (4)	2.925 (3)	158 (4)
N2—H2C···O5^{v}	0.90 (4)	2.48 (4)	2.998 (3)	117 (3)

Symmetry codes: (i) $x+1, y-1, z-1$; (ii) $x-1, y-1, z$; (iii) $x, y-1, z$; (iv) $x, y, z+1$; (v) $x+1, y, z$; (vi) $x, y+1, z+1$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

The author acknowledges Liaodong University for funding this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2422).

References

Bruker (1998). *SMART* (Version 5.628) and *SAINT* (Version 6.02) and *SHELXTL* (Version 5.1). Bruker AXS Inc., Madison, Wisconsin, USA.
Coupar, P. I., Glidewell, C. & Ferguson, G. (1997). *Acta Cryst.* B**53**, 521–533.
Pandiarajan, S., Sridhar, B. & Rajaram, R. K. (2001). *Acta Cryst.* E**57**, o466–o468.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sobczyk, L., Lis, T., Olejnik, Z. & Majerz, I. (2000). *J. Mol. Struct.* **552**, 233–241.
Srinivasan, N., Sridhar, B. & Rajaram, R. K. (2002). *Acta Cryst.* E**58**, o95–o97.

 © 2008 International Union of Crystallography

supporting information

Acta Cryst. (2008). E**64**, o43 [https://doi.org/10.1107/S160053680706240X]

A cocrystal of pyridine-2,4-dicarboxylic acid and serine

Peng Liang

S1. Comment

The interactions of organic acids with amino acids in the solid state have been widely investigated due to their interesting hydrogen-bonding interactions (Coupar *et al.*, 1997; Sobczyk *et al.*, 2000; Pandiarajan *et al.*, 2001; Srinivasan *et al.*, 2002). We report here the structure of the title co-crystal (I), Fig.1, formed from pyridine-2,4-dicarboxylic acid and serine in its zwitterionic form.

The crystal is stabilized by an extensive array of intermolecular O–H···O, N–H···N, and N–H···O hydrogen bonds (Table 1), forming a three-dimensional network (Fig. 2).

S2. Experimental

The compound was crystallized by slow evaporation of an equimolar solution of pyridine-2,4-dicarboxylic acid and serine in a solution of ethanol/water (1:1, *v*/*v*).

S3. Refinement

In the absence of significant anomalous dispersion effects, Friedel pairs were averaged. The H2A, H2B, and H2C atoms of the serine NH_3 group were located from a difference Fourier map and refined isotropically, with N–H distances restrained to 0.90 (1) Å, H···H distances restrained to 1.43 (2) Å, and with U_{iso}(H) values fixed at 0.08 Å^2. The other H atoms were placed in idealized positions and constrained to ride on their parent atoms with C–H distances in the range 0.93–0.98 Å, O–H distances of 0.82 Å, and with U_{iso}(H) set at 1.2U_{eq}(C) and 1.5U_{eq}(O).

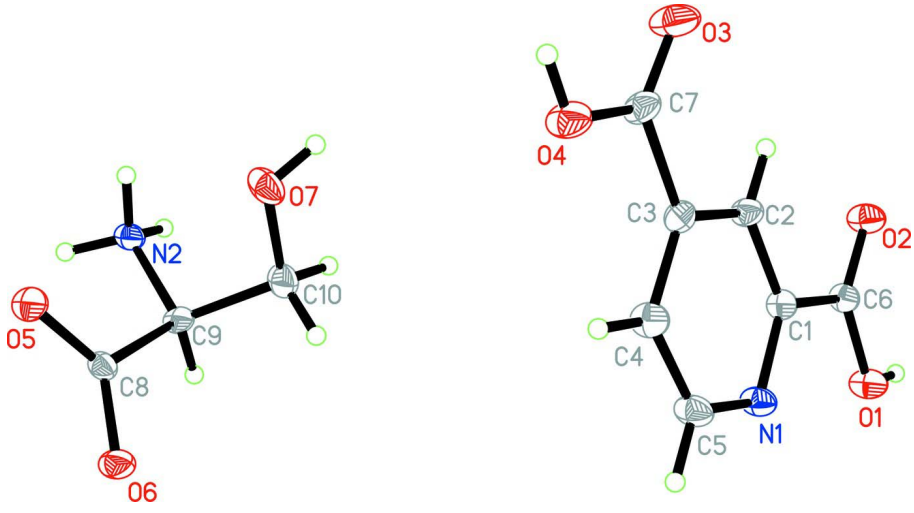


Figure 1

The asymmetric unit of the compound, showing 30% probability displacement and the atom-numbering scheme.

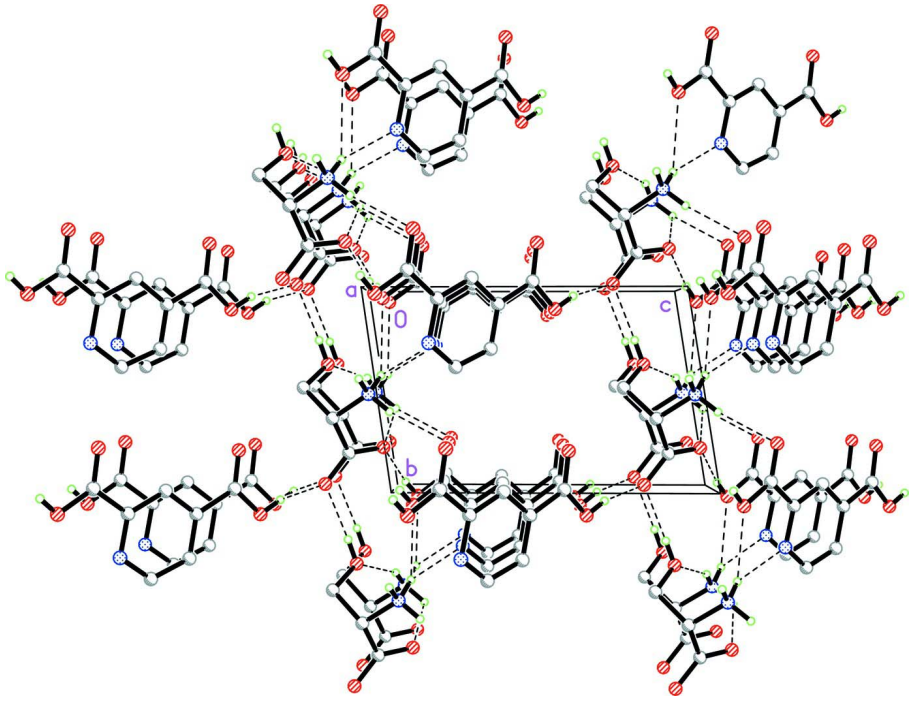


Figure 2

The molecular packing of the compound. Intermolecular hydrogen bonds are shown as dashed lines.

pyridine-2,4-dicarboxylic acid–serine (1/1)

Crystal data

$C_7H_5NO_4{\cdot}C_3H_7NO_3$
M_r = 272.22
Triclinic, $P1$
Hall symbol: P 1
a = 4.4941 (13) Å
b = 6.4512 (18) Å
c = 10.123 (3) Å
α = 81.273 (3)°
β = 87.060 (3)°
γ = 86.247 (3)°
V = 289.22 (14) Å^3
Z = 1
F(000) = 142
D_x = 1.563 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1233 reflections
θ = 2.7–27.8°
μ = 0.14 mm^{-1}
T = 298 K
Block, colorless
0.37 × 0.33 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.952, T_{max} = 0.961
2493 measured reflections
1287 independent reflections
1202 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 27.5°, θ_{min} = 2.0°
$h = -5 \rightarrow 5$
$k = -8 \rightarrow 8$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.090$
$S = 1.05$
1287 reflections
184 parameters
9 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0577P)^2 + 0.006P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	1.0517 (4)	0.0560 (3)	0.0626 (2)	0.0334 (5)
H1	1.1822	−0.0201	0.0317	0.050*
O2	0.9510 (4)	−0.2405 (3)	0.1977 (2)	0.0356 (5)
O3	0.1493 (6)	−0.2074 (3)	0.5583 (2)	0.0516 (7)
O4	−0.0519 (5)	0.1089 (3)	0.5859 (2)	0.0434 (6)
H4	−0.1431	0.0430	0.6491	0.065*
O5	0.4623 (4)	0.7963 (3)	0.9831 (2)	0.0337 (5)
O6	0.5883 (5)	0.9761 (3)	0.7854 (2)	0.0359 (5)
O7	0.4881 (4)	0.3780 (3)	0.8451 (2)	0.0377 (5)
H7	0.4986	0.2569	0.8290	0.057*
N1	0.6382 (5)	0.2780 (3)	0.1903 (2)	0.0293 (5)
N2	0.9518 (5)	0.5231 (3)	0.9729 (2)	0.0269 (5)
C1	0.6767 (6)	0.0717 (4)	0.2350 (3)	0.0249 (5)
C2	0.5179 (6)	−0.0277 (4)	0.3443 (3)	0.0271 (5)
H2	0.5490	−0.1714	0.3717	0.033*
C3	0.3112 (6)	0.0908 (4)	0.4122 (3)	0.0270 (5)
C4	0.2762 (6)	0.3039 (4)	0.3694 (3)	0.0327 (6)
H4A	0.1446	0.3884	0.4148	0.039*
C5	0.4416 (6)	0.3894 (4)	0.2573 (3)	0.0333 (6)
H5	0.4132	0.5326	0.2274	0.040*
C6	0.9072 (6)	−0.0535 (4)	0.1629 (3)	0.0261 (5)
C7	0.1307 (6)	−0.0215 (4)	0.5278 (3)	0.0320 (6)
C8	0.6098 (5)	0.8204 (4)	0.8753 (3)	0.0236 (5)
C9	0.8388 (5)	0.6435 (4)	0.8475 (3)	0.0253 (5)

H9	1.0081	0.7073	0.7955	0.030*
C10	0.7075 (6)	0.4937 (4)	0.7658 (3)	0.0329 (6)
H10A	0.6184	0.5730	0.6870	0.039*
H10B	0.8645	0.3982	0.7367	0.039*
H2A	0.826 (7)	0.433 (5)	1.017 (4)	0.080*
H2B	1.120 (5)	0.448 (5)	0.955 (4)	0.080*
H2C	0.998 (9)	0.607 (6)	1.031 (4)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0327 (10)	0.0268 (10)	0.0373 (11)	0.0043 (8)	0.0169 (8)	−0.0029 (8)
O2	0.0397 (11)	0.0250 (10)	0.0390 (11)	0.0046 (8)	0.0125 (8)	−0.0022 (8)
O3	0.0690 (16)	0.0327 (12)	0.0461 (14)	0.0018 (10)	0.0271 (12)	0.0043 (10)
O4	0.0507 (13)	0.0357 (12)	0.0398 (12)	0.0011 (9)	0.0226 (10)	−0.0022 (10)
O5	0.0320 (10)	0.0297 (10)	0.0364 (11)	0.0046 (7)	0.0156 (8)	−0.0036 (8)
O6	0.0460 (11)	0.0237 (10)	0.0335 (10)	0.0063 (8)	0.0135 (8)	0.0015 (8)
O7	0.0352 (11)	0.0269 (10)	0.0526 (13)	−0.0027 (8)	0.0124 (9)	−0.0153 (9)
N1	0.0300 (12)	0.0222 (11)	0.0337 (12)	0.0017 (9)	0.0082 (9)	−0.0023 (9)
N2	0.0275 (11)	0.0197 (11)	0.0317 (11)	0.0013 (8)	0.0099 (9)	−0.0024 (8)
C1	0.0227 (11)	0.0253 (12)	0.0262 (12)	0.0008 (9)	0.0023 (10)	−0.0043 (10)
C2	0.0315 (13)	0.0224 (12)	0.0259 (12)	0.0014 (9)	0.0043 (10)	−0.0015 (10)
C3	0.0272 (13)	0.0301 (13)	0.0234 (12)	−0.0022 (10)	0.0034 (10)	−0.0041 (10)
C4	0.0319 (14)	0.0282 (14)	0.0359 (14)	0.0054 (11)	0.0112 (12)	−0.0056 (12)
C5	0.0363 (15)	0.0224 (13)	0.0390 (15)	0.0027 (11)	0.0090 (12)	−0.0031 (11)
C6	0.0255 (12)	0.0243 (13)	0.0282 (14)	0.0005 (10)	0.0053 (10)	−0.0058 (10)
C7	0.0346 (15)	0.0335 (16)	0.0254 (14)	0.0007 (12)	0.0087 (11)	−0.0014 (11)
C8	0.0239 (11)	0.0189 (11)	0.0280 (12)	−0.0015 (8)	0.0049 (10)	−0.0050 (9)
C9	0.0243 (12)	0.0229 (12)	0.0261 (12)	0.0019 (9)	0.0122 (10)	−0.0009 (9)
C10	0.0372 (14)	0.0279 (14)	0.0341 (14)	0.0000 (11)	0.0089 (11)	−0.0104 (11)

Geometric parameters (Å, º)

O1—C6	1.315 (3)	N2—H2C	0.90 (4)
O1—H1	0.8200	C1—C2	1.381 (3)
O2—C6	1.211 (3)	C1—C6	1.500 (3)
O3—C7	1.191 (4)	C2—C3	1.386 (3)
O4—C7	1.318 (4)	C2—H2	0.9300
O4—H4	0.8200	C3—C4	1.378 (4)
O5—C8	1.242 (3)	C3—C7	1.508 (4)
O6—C8	1.251 (3)	C4—C5	1.386 (4)
O7—C10	1.417 (3)	C4—H4A	0.9300
O7—H7	0.8200	C5—H5	0.9300
N1—C5	1.327 (4)	C8—C9	1.535 (3)
N1—C1	1.342 (3)	C9—C10	1.528 (4)
N2—C9	1.479 (3)	C9—H9	0.9800
N2—H2A	0.89 (3)	C10—H10A	0.9700
N2—H2B	0.90 (3)	C10—H10B	0.9700

C6—O1—H1	109.5	N1—C5—H5	118.2
C7—O4—H4	109.5	C4—C5—H5	118.2
C10—O7—H7	109.5	O2—C6—O1	124.4 (2)
C5—N1—C1	117.4 (2)	O2—C6—C1	120.9 (2)
C9—N2—H2A	115 (3)	O1—C6—C1	114.7 (2)
C9—N2—H2B	110 (3)	O3—C7—O4	125.2 (3)
H2A—N2—H2B	107 (2)	O3—C7—C3	122.6 (3)
C9—N2—H2C	112 (3)	O4—C7—C3	112.2 (2)
H2A—N2—H2C	106 (2)	O5—C8—O6	126.1 (2)
H2B—N2—H2C	107 (2)	O5—C8—C9	117.8 (2)
N1—C1—C2	123.1 (2)	O6—C8—C9	116.2 (2)
N1—C1—C6	117.7 (2)	N2—C9—C10	109.4 (2)
C2—C1—C6	119.3 (2)	N2—C9—C8	111.60 (19)
C1—C2—C3	118.7 (2)	C10—C9—C8	111.4 (2)
C1—C2—H2	120.6	N2—C9—H9	108.1
C3—C2—H2	120.6	C10—C9—H9	108.1
C4—C3—C2	118.7 (2)	C8—C9—H9	108.1
C4—C3—C7	123.3 (2)	O7—C10—C9	109.5 (2)
C2—C3—C7	118.1 (2)	O7—C10—H10A	109.8
C3—C4—C5	118.6 (2)	C9—C10—H10A	109.8
C3—C4—H4A	120.7	O7—C10—H10B	109.8
C5—C4—H4A	120.7	C9—C10—H10B	109.8
N1—C5—C4	123.6 (2)	H10A—C10—H10B	108.2

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O5^{i}	0.82	1.77	2.590 (3)	173
O4—H4···O6^{ii}	0.82	1.81	2.598 (3)	162
O7—H7···O6^{iii}	0.82	1.94	2.754 (3)	171
N2—H2*A*···N1^{iv}	0.89 (3)	2.05 (2)	2.872 (3)	152 (4)
N2—H2*A*···O1^{iv}	0.89 (3)	2.55 (4)	3.023 (3)	113 (3)
N2—H2*B*···O7^{v}	0.90 (3)	2.01 (2)	2.848 (3)	155 (4)
N2—H2*C*···O2^{vi}	0.90 (4)	2.07 (4)	2.925 (3)	158 (4)
N2—H2*C*···O5^{v}	0.90 (4)	2.48 (4)	2.998 (3)	117 (3)

Symmetry codes: (i) $x+1, y-1, z-1$; (ii) $x-1, y-1, z$; (iii) $x, y-1, z$; (iv) $x, y, z+1$; (v) $x+1, y, z$; (vi) $x, y+1, z+1$.