

Srinivas Basavoju, C. Malla  
Reddy and Gautam R. Desiraju\*School of Chemistry, University of Hyderabad,  
Hyderabad 500 046, IndiaCorrespondence e-mail:  
gautam\_desiraju@yahoo.com

## Key indicators

Single-crystal X-ray study  
 $T = 298$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
 $R$  factor = 0.071  
 $wR$  factor = 0.177  
Data-to-parameter ratio = 13.9For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

## 2-(Methylsulfanyl)nicotinic acid

The title compound,  $\text{C}_7\text{H}_7\text{NO}_2\text{S}$ , forms centrosymmetric acid dimers which are connected through weak  $\text{C}-\text{H}\cdots\text{O}$  interactions to form a tape. Adjacent tapes are arranged in a zigzag fashion with weak methyl–methyl interactions.

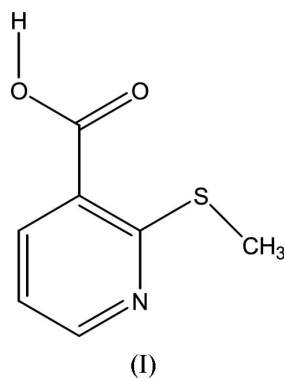
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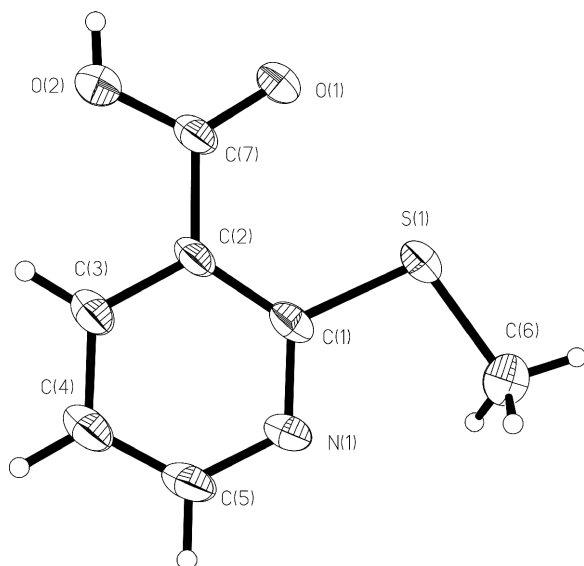
Online 4 March 2005

## Comment

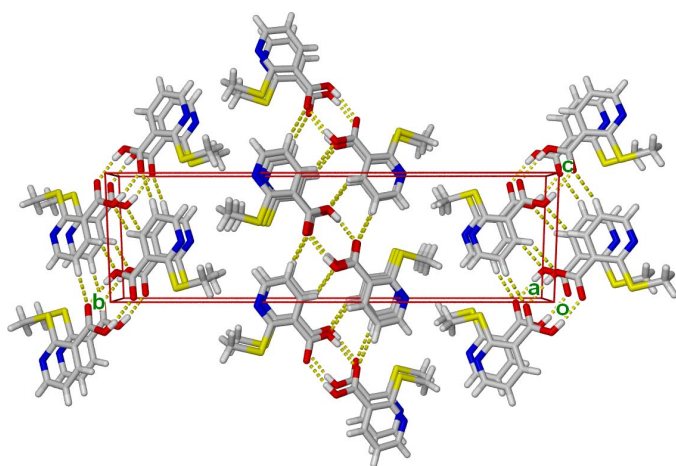
In the course of our research on intermolecular interactions, the crystal structure of 2-(methylsulfanyl)nicotinic acid, (I) (Fig. 1), was undertaken. Coordination polymers of (I) with  $\text{Sn}^{\text{II}}$  and  $\text{Cu}^{\text{II}}$  have been reported (Gielen *et al.*, 1992; Miklos *et al.*, 2001; Segl'a *et al.*, 2004). The acid group of (I) binds to the central Sn atom in diethylbis(2-methylthionicotinato- $\kappa^2O,O'$ )tin(II) as a bidentate ligand (Gielen *et al.*, 1992). Compound (I) acts as a counter-ion in diaqua(diethylenetriamine)copper(II) bis(2-methylthionicotinate), (Miklos *et al.*, 2001), while in diaquabis(2-methylthionicotinato- $\kappa^2O,O'$ )-dipyridylcopper(II), it acts as a monodentate ligand (Segl'a *et al.*, 2004).



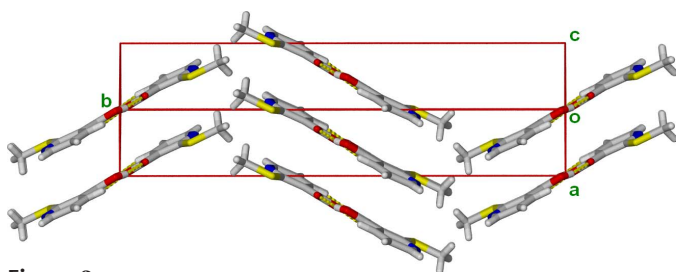
The molecule is nearly planar and forms centrosymmetric acid dimers *via*  $\text{O}2-\text{H}1\cdots\text{O}1^{\text{i}}$  hydrogen bonds [1.85 (5) Å and  $169$  (5) $^\circ$ ; symmetry code: (i)  $-x, 1-y, 1-z$ ]. These dimers are connected *via* weak  $\text{C}3-\text{H}3\cdots\text{O}2^{\text{ii}}$  [2.63 Å and  $141$  $^\circ$ ; symmetry code: (ii)  $-1-x, 1-y, -z$ ] and  $\text{C}4-\text{H}4\cdots\text{O}1^{\text{iii}}$  [2.70 Å and  $157$  $^\circ$ ; symmetry code: (iii)  $-1+x, y, -1+z$ ] interactions parallel to the  $(\bar{2}72)$  or  $(27\bar{2})$  planes to form tapes (Fig. 2). Translation-related tapes are stacked along [100] (Fig. 3). Adjacent tapes are arranged in a zigzag fashion with weak methyl–methyl interactions (Fig. 3). Surprisingly, the pyridine group is not intermolecularly bonded to the carboxylic acid group *via*  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bonds, because of steric hindrance created by the presence of the SMe group. There are no short contacts to the S and N atoms.



**Figure 1**  
The structure and numbering scheme of (I). Displacement ellipsoids are drawn at the 50% probability level.



**Figure 2**  
The zigzag arrangement of molecules in (I), showing O—H...O and C—H...O hydrogen bonds (dashed lines) parallel to the  $(\bar{2}72)$  or  $(272)$  plane forming tapes.



**Figure 3**  
The stacking of dimers in (I).

## Experimental

The material was purchased from the Lancaster Chemical Company and crystallized from  $\text{CH}_2\text{Cl}_2$  by slow evaporation at ambient temperature to obtain diffraction-quality single crystals.

## Crystal data

$\text{C}_7\text{H}_7\text{NO}_2\text{S}$   
 $M_r = 169.20$   
Monoclinic,  $P2_1/c$   
 $a = 3.9834$  (10) Å  
 $b = 25.373$  (7) Å  
 $c = 7.465$  (2) Å  
 $\beta = 101.380$  (4)°  
 $V = 739.7$  (3) Å<sup>3</sup>  
 $Z = 4$

$D_x = 1.519$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
Cell parameters from 1108 reflections  
 $\theta = 3.2$ – $26.5^\circ$   
 $\mu = 0.38$  mm<sup>-1</sup>  
 $T = 298$  (2) K  
Block, colourless  
 $0.20 \times 0.13 \times 0.10$  mm

## Data collection

Bruker SMART APEX CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)  
 $T_{\min} = 0.943$ ,  $T_{\max} = 0.960$   
4393 measured reflections

1462 independent reflections  
1181 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.040$   
 $\theta_{\text{max}} = 26.1^\circ$   
 $h = -4 \rightarrow 4$   
 $k = -31 \rightarrow 28$   
 $l = -9 \rightarrow 8$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.071$   
 $wR(F^2) = 0.177$   
 $S = 1.10$   
1462 reflections  
105 parameters  
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0967P)^2 + 0.4717P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.95$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.38$  e Å<sup>-3</sup>

The carboxylic acid H atom was located in a difference map and refined freely. Other H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and allowed to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.2$  (aromatic) or 1.5 (methyl) times  $U_{\text{eq}}(\text{H})$ .

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2000); software used to prepare material for publication: SHELXTL.

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