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2-Amino-4,6-dimethoxypyrimidin-1-ium 1-methyl-5-sulfamoyl-1*H*-pyrazole-4-carboxylate

Y.-F Liu,* H.-T Xia and S.-A Li

Department of Chemical Engineering, Huaihai Institute of Technology, Lianyungang Jiangsu 222005, People's Republic of China

Correspondence e-mail: xht161006@hhit.edu.cn

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In the title compound, $C_6H_{10}N_3O_2^+\cdot C_5H_6N_3O_4S^-$, the pyrimidinium cation acts as a strong hydrogen-bond donor *via* the NH_2 and NH groups, with the carboxylate groups of the pyrazole group acting as the acceptors. These hydrogen bonds lead to fused $R_2^2(8)$ rings, which form sheets parallel to the $[10\bar{1}]$ plane

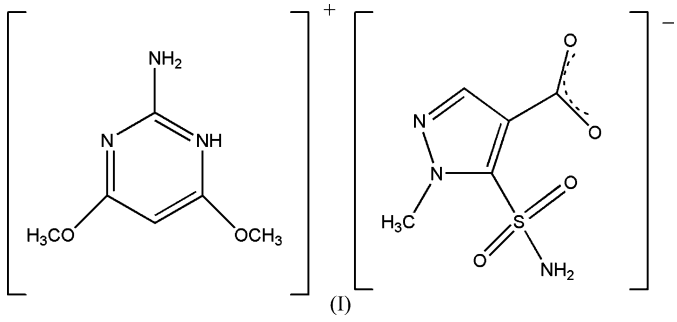
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.054
wR factor = 0.152
Data-to-parameter ratio = 13.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

During the course of studies on the coordination chemistry of pyrazosulfuronethyl by hydrothermal methods, we obtained crystals of the title compound, (I); we now report the structure and supramolecular arrangement of (I) (Fig. 1).



(I)

In the crystal structure of (I), ions are linked into chains involving two $R_2^2(8)$ rings (Bernstein *et al.*, 1995) through C—H···O, C—H···N and N—H···O hydrogen bonds (Fig. 2 and Table 2). Neighboring chains are linked into sheets by two N—H···O hydrogen bonds (Fig. 3). Neighboring sheets are connected by C—H···O and N—H···O hydrogen bonds, resulting in a three-dimensional network structure (Fig. 4).

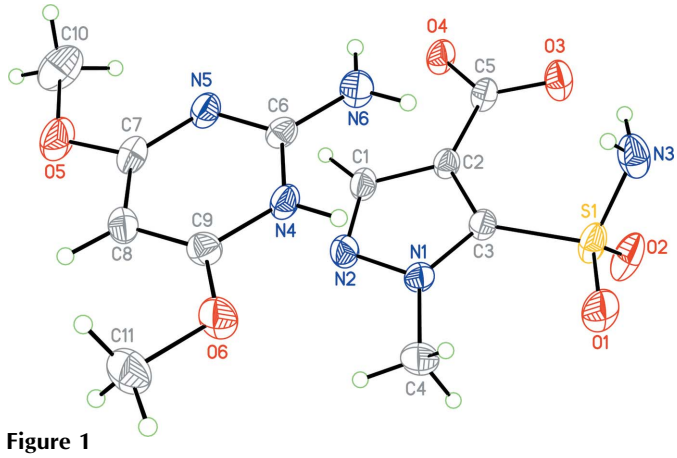


Figure 1
The asymmetric unit of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level.

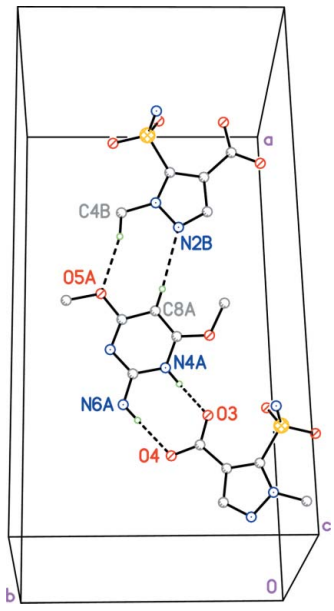


Figure 2
Part of the crystal structure of (I), showing the formation of a hydrogen-bonded chain built from two $R_2^2(8)$ rings. For clarity, H atoms not involved in the hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds [symmetry codes: (A) $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}-z$; (B) $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z$].

Experimental

Solutions of pyrazosulfuronethyl (1 mmol) in water (20 ml) and cupric nitrate (1 mmol) in water (10 ml) were mixed; the mixture was maintained at 393 K for 5 h by the hydrothermal method and left overnight at room temperature; the solution was allowed to stand, slowly producing crystals of (I) slowly.

Crystal data

$C_6H_{10}N_3O_2^+\cdot C_5H_6N_3O_4S^-$
M_r = 360.36
Monoclinic, $C2/c$
a = 22.843 (10) Å
b = 10.484 (5) Å
c = 13.921 (6) Å
β = 104.411 (7)°
V = 3229 (3) Å^3
Z = 8
D_x = 1.483 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 298 (2) K
Block, dark pink
0.42 × 0.40 × 0.21 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.905, T_{max} = 0.951
8217 measured reflections
2845 independent reflections
1467 reflections with $I > 2\sigma(I)$
R_{int} = 0.065
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.152
S = 1.00
2845 reflections
218 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0793P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

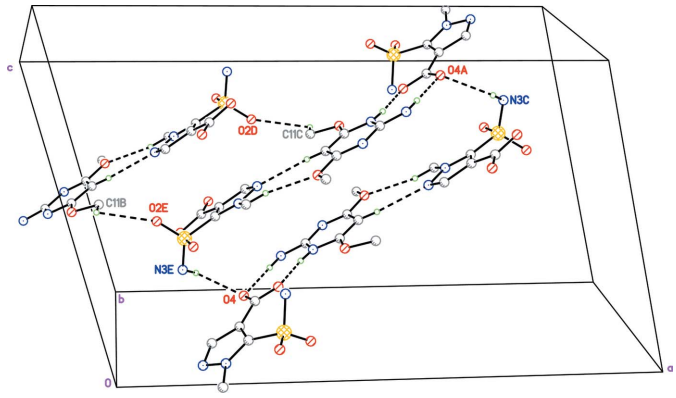


Figure 4
different view of the crystal structure of (I); the formation of a three-dimensional network structure built from C—H···O and N—H···O interactions. For clarity, H atoms not involved in the hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds [symmetry codes: (A) $1-x,1-y,1-z$; (B) $-x,1+y,\frac{1}{2}-z$; (C) $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z$; (D) $x,1-y,\frac{1}{2}+z$; (E) $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}-z$].

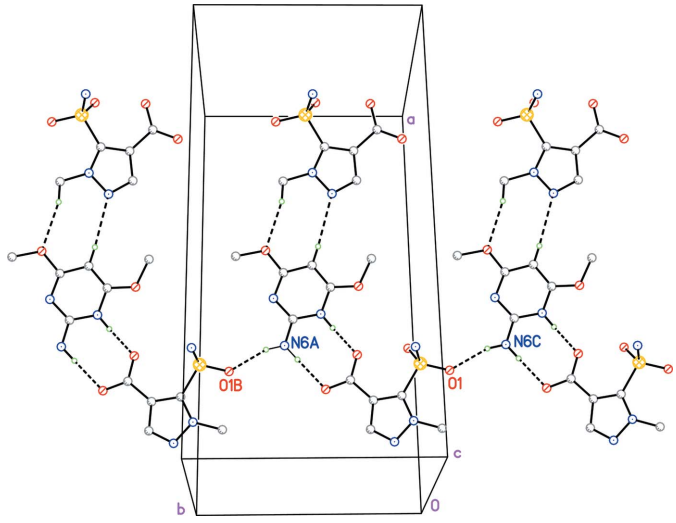


Figure 3
A larger portion of the crystal structure of (I); the formation of a hydrogen-bonded sheet built from N—H···O interactions. For clarity, H atoms not involved in the hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds [symmetry codes: (A) $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}-z$; (B) $x,1+y,z$; (C) $\frac{1}{2}-x,-\frac{1}{2}+y,\frac{1}{2}-z$].

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···N2^{i}	0.93	2.57	3.503 (5)	176
C11—H11A···O2^{ii}	0.96	2.71	3.080 (5)	104
N4—H4···O3^{iii}	0.86	1.73	2.583 (4)	175
C4—H4B···O5^{i}	0.96	2.45	3.383 (5)	164
N6—H6A···O1^{iv}	0.86	2.12	2.948 (4)	161
N6—H6B···O4^{iii}	0.86	1.98	2.842 (4)	179
N3—H3A···O4^{iii}	0.89	2.03	2.902 (5)	166

Symmetry codes: (i) $-x,-y,-z$; (ii) $x-\frac{1}{2},y-\frac{1}{2},z$; (iii) $-x+\frac{1}{2},y-\frac{1}{2},-z+\frac{1}{2}$; (iv) $-x+\frac{1}{2},y+\frac{1}{2},-z+\frac{1}{2}$.

All H atoms were located in difference Fourier maps and then treated as riding atoms, with C—H distances of 0.93 (aryl) and 0.96 Å (methyl), N—H distances of 0.86 and 0.89 Å, and U_{iso}(H) = 1.2(C aryl, N) or 1.5U_{eq}(C methyl).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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