Crystal structure of dimethylamonium hydrogen 2-propyl-4,5-imidazoledicarboxylate, $[C_2H_8N][C_8H_9N_2O_4]$

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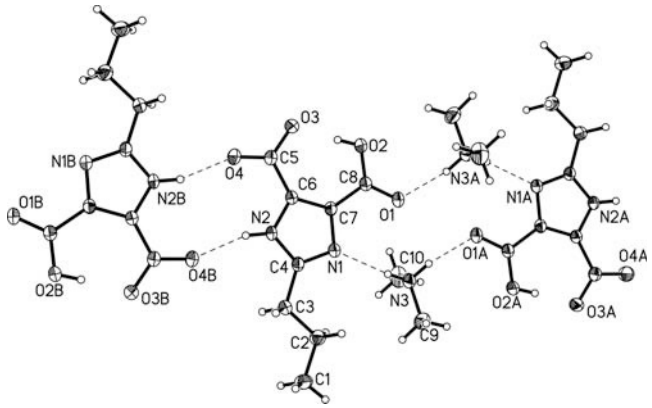

Abstract

$C_{10}H_{17}N_3O_4$, monoclinic, $P2_1/n$ (no. 14), a = 9.179(1) Å, b = 15.203(2) Å, c = 9.289(1) Å, β = 112.015(2)°, V = 1201.8 Å^3, Z = 4, $R_{gt}(F)$ = 0.047, $wR_{ref}(F^2)$ = 0.119, T = 296 K.

Source of material

Dimethylamine (0.2 mmol) and 2-propyl-4,5-imidazoledicarboxylic acid (0.2 mmol) were dissolved in methanol (5 ml) and water (10 ml) at room temperature. The single crystals of the title compound were obtained from the solution after five days.

Discussion

Designing the solid state with molecules that encode well defined non-covalent motifs has recently become a rapidly growing area of research due to their fascinating molecular and/or supramolecular structural diversity and potential applications for catalysis [3,4] and material sciences [5,6]. Among the noncovalent motifs, hydrogen bonding, metal-ligand coordination, and π-π stacking have been employed as synthetic paradigms to rational design of superstructures. Except for other interactions, one of the best strategies to design high-dimensional supramolecular systems is to utilize the hydrogen bonding of the bridging ligand in addition to their coordination capability. The 2-propyl-4,5-imidazoledicarboxylic acid, possesses several interesting characteristics: (a) it has two carboxyl groups which may be completely or partially deprotonated, inducing various coordination modes and allowing interesting structures with higher dimensions; (b) the two carboxyl groups can act not only as hydrogen-bond acceptor but also as hydrogen-bond donor, depending upon the numbers of deprotonated carboxyl groups; (c) the two N atoms also can participate in hydrogen bonds. To propagate non-covalent interactions only along one direction, each unit must have two-point interactions with two adjacent neighbors.

The crystal structure of the title compound comprises a dimethylamonium cation and a mono-deprotonated 2-propyl-4,5-imidazoledicarboxylate anion per asymmetric unit. The two components are linked by N–H···N and N–H···O hydrogen bonds to form an 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.

Table 1. Data collection and handling.

Crystal:	colorless block, size 0.19 × 0.23 × 0.27 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	1.05 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, φ/ω
$2\theta_{max}$:	55°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	10454, 2749
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1665
$N(param)_{refined}$:	158
Programs:	SHELXS-97, SHELXL-97, SHELXTL [7]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(2)	4*e*	0.0812	1.1009	0.0464	0.071
H(2D)	4*e*	0.1316	0.9595	0.4854	0.045
H(3A)	4*e*	0.5210	0.9017	0.2302	0.056
H(3B)	4*e*	0.5901	0.9245	0.1177	0.056
H(1A)	4*e*	0.6501	0.7886	0.7841	0.080
H(1B)	4*e*	0.7025	0.7266	0.6774	0.080
H(1C)	4*e*	0.5418	0.7105	0.6960	0.080
H(2A)	4*e*	0.6076	0.8579	0.5460	0.054
H(2B)	4*e*	0.4991	0.7799	0.4581	0.054
H(3C)	4*e*	0.3188	0.8171	0.5687	0.054
H(3D)	4*e*	0.4277	0.8940	0.6599	0.054
H(9A)	4*e*	0.7086	0.7943	0.3307	0.107
H(9B)	4*e*	0.7787	0.8896	0.3533	0.107
H(9C)	4*e*	0.7880	0.8299	0.2194	0.107
H(10A)	4*e*	0.5253	0.7929	–0.0007	0.110
H(10B)	4*e*	0.3748	0.8397	0.0036	0.110
H(10C)	4*e*	0.4565	0.7654	0.1237	0.110

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Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	4*e*	0.3662(2)	1.02223(9)	0.0498(2)	0.0523(8)	0.0644(9)	0.0571(9)	0.0135(7)	0.0388(7)	0.0190(7)
O(2)	4*e*	0.1450(2)	1.09441(9)	0.0047(2)	0.0481(8)	0.0589(9)	0.0459(8)	0.0130(7)	0.0296(7)	0.0171(7)
O(3)	4*e*	–0.0452(2)	1.11903(9)	0.1276(2)	0.0532(9)	0.0589(9)	0.0527(8)	0.0194(7)	0.0309(7)	0.0216(7)
O(4)	4*e*	–0.0818(2)	1.0740(1)	0.3385(2)	0.073(1)	0.093(1)	0.070(1)	0.0402(9)	0.0550(9)	0.0350(9)
N(1)	4*e*	0.3540(2)	0.94255(9)	0.3157(2)	0.0373(8)	0.0406(9)	0.0353(8)	0.0022(7)	0.0196(7)	0.0036(7)
N(2)	4*e*	0.1787(2)	0.96398(9)	0.4213(2)	0.0399(8)	0.0468(9)	0.0352(8)	0.0056(7)	0.0243(7)	0.0070(7)
N(3)	4*e*	0.5731(2)	0.8799(1)	0.1731(2)	0.054(1)	0.048(1)	0.050(1)	0.0104(8)	0.0331(8)	0.0084(8)
C(1)	4*e*	0.6143(2)	0.7545(1)	0.6902(2)	0.050(1)	0.054(1)	0.052(1)	0.011(1)	0.014(1)	0.006(1)
C(2)	4*e*	0.5329(2)	0.8145(1)	0.5527(2)	0.047(1)	0.048(1)	0.043(1)	0.0052(9)	0.0175(9)	–0.0007(9)
C(3)	4*e*	0.3935(2)	0.8609(1)	0.5636(2)	0.045(1)	0.054(1)	0.043(1)	0.0090(9)	0.0238(9)	0.0127(9)
C(4)	4*e*	0.3118(2)	0.9219(1)	0.4332(2)	0.036(1)	0.038(1)	0.038(1)	0.0002(8)	0.0199(8)	0.0012(8)
C(5)	4*e*	–0.0090(2)	1.0726(1)	0.2509(2)	0.044(1)	0.049(1)	0.046(1)	0.0080(9)	0.0261(9)	0.008(1)
C(6)	4*e*	0.1309(2)	1.0150(1)	0.2907(2)	0.0366(9)	0.037(1)	0.0335(9)	0.0022(8)	0.0177(8)	0.0035(8)
C(7)	4*e*	0.2411(2)	1.0012(1)	0.2256(2)	0.0348(9)	0.035(1)	0.0350(9)	–0.0015(8)	0.0178(8)	0.0004(8)
C(8)	4*e*	0.2534(2)	1.0403(1)	0.0854(2)	0.039(1)	0.039(1)	0.038(1)	0.0001(9)	0.0198(8)	0.0027(9)
C(9)	4*e*	0.7253(3)	0.8454(2)	0.2782(3)	0.060(2)	0.100(2)	0.066(2)	0.031(1)	0.038(1)	0.024(2)
C(10)	4*e*	0.4738(3)	0.8138(2)	0.0656(3)	0.083(2)	0.065(2)	0.084(2)	–0.013(1)	0.046(2)	–0.013(1)

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