Crystal structure of imidazolium decanedioate, $C_{18}H_{31}N_2O_6$

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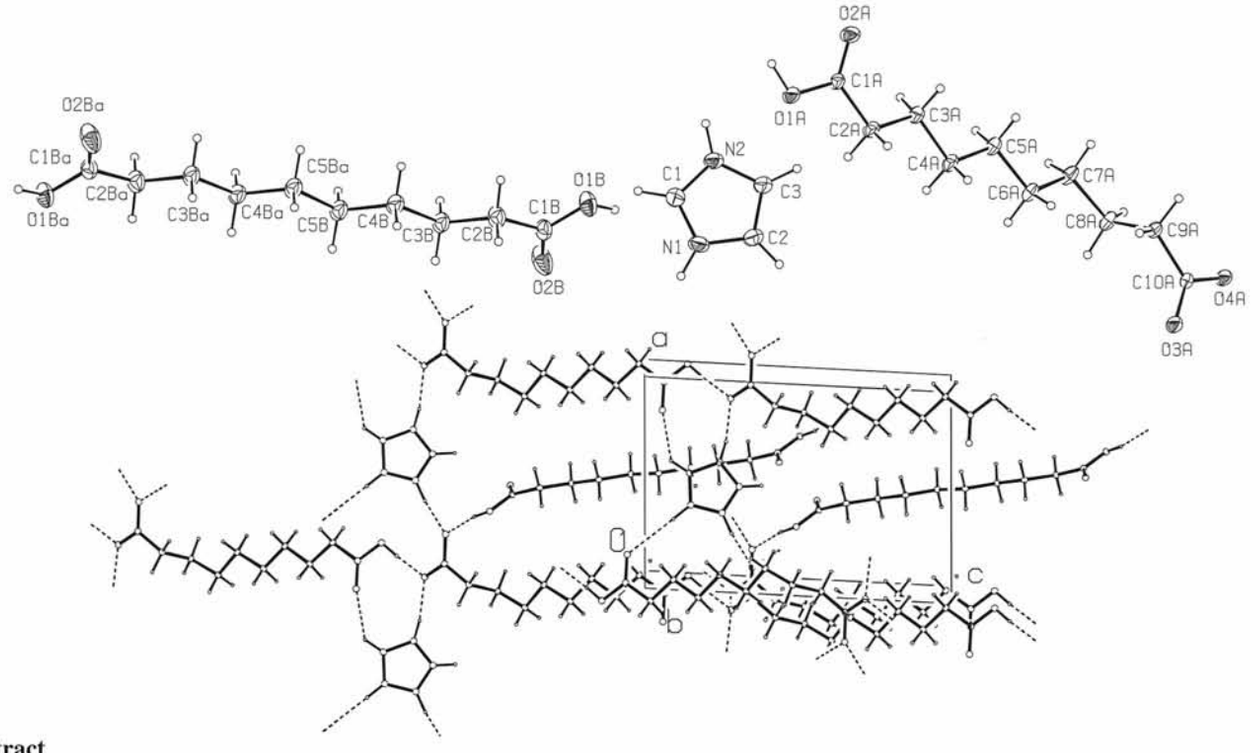

Abstract

$C_{18}H_{31}N_2O_6$, triclinic, $P\bar{1}$ (No. 2), $a = 8.8249(8)$ Å, $b = 8.992(2)$ Å, $c = 12.897(2)$ Å, $\alpha = 95.22(1)°$, $\beta = 92.91(1)°$, $\gamma = 94.62(1)°$, $V = 1014.1$ Å^3, $Z = 2$, $R_{gt}(F) = 0.042$, $wR_{ref}(F^2) = 0.124$, $T = 293$ K.

Source of material

Imidazolium salt was synthesised by mixing of stoichiometric amounts of the decanedioic (sebacic) acid with imidazole (1:2 molar ratio) in ethyl acetate solution. Reaction product was separated by filtration and washed with anhydrous ethyl acetate. The crystals were obtained from ethyl acetate-methanol (3:1) mixture by slow evaporation in room temperature. Colourless, transparent needles were obtained.

Experimental details

The positions H1A, H1B, H4 and H5 were found by difference Fourier synthesis and were refined.

Discussion

The present work is a part of our research on the structure of quaternary imidazolium salts to explain mechanism of conducting properties of such systems [1]. One of the hypotheses assume that the conductivity of organic salts is connected with mobility of protons within the system at given temperature [2]. The present structure is one of the series of imidazolium salts of α/ω dicarboxylic acids.

The unit cell of the title crystal structure contains three acid molecules and two imidazolium rings. This indicates that the substrates didn't react in stoichiomeric proportions. One molecule of the acid (2×) have different conformation comparing to the other one (figure, top). The torsion angle C6A-C7A-C8A-C9A in the aliphatic chain of one molecules is –77.26° (C6A–C7A and C8A–C9A are in *syn* conformation). This is in contrast with the other molecule where all those angles are close to 180°. The first acid molecules with *syn* conformation are arranged in the layers connected by hydrogen bonds between carboxylate anions (figure, bottom). Each layer is created by acid's chains nearly parallel to the *c* axis. The second kind of acid's molecules form hydrogen bonds with the first ones connecting across above layers. The acids of layers are additionally connected along [100] direction by imidazolium cations through net of hydrogen bonds. Each imidazolium ring is engaged in two linkages with surrounded carboxylate anions. Lengths of these N–H···O connections are ranged between 2.67 Å – 2.71 Å with angle ∠N–H···O = 163.9°. Moreover, among the mentioned layers it is possible to distinguish hydrophobic parts composed by aliphatic chains and polar parts assembled by carboxylate anions and imidazolium cations. These polar parts create "channels" along [100] direction. Such channels with positively and negatively charged groups may potentially serve for protons as 'pathways' in the conducting mechanism.

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Table 1. Data collection and handling.

Crystal:	colourless needle, size 0.14 × 0.18 × 0.53 mm
Wavelength:	Cu K_α radiation (1.54178 Å)
μ:	7.51 cm^{-1}
Diffractometer, scan mode:	Kuma KM-4, $\omega/2\theta$
$2\theta_{max}$:	140.24°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	3816, 3651
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 3007
$N(param)_{refined}$:	251
Programs:	SHELXS-97 [3], SHELXL-97 [4]

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

Atom	Site	x	y	z	U_{iso}
H(2A1)	2*i*	0.1037	0.6856	0.0163	0.051
H(2A2)	2*i*	0.1035	0.8148	–0.0575	0.051
H(3A1)	2*i*	–0.1375	0.7220	–0.1284	0.054
H(3A2)	2*i*	–0.1420	0.5953	–0.0527	0.054
H(4A1)	2*i*	0.0589	0.6142	–0.2157	0.053
H(4A2)	2*i*	0.0596	0.4893	–0.1384	0.053
H(5A1)	2*i*	–0.1852	0.3951	–0.2016	0.056
H(5A2)	2*i*	–0.1921	0.5232	–0.2758	0.056
H(6A1)	2*i*	–0.0088	0.4215	–0.3764	0.055
H(6A2)	2*i*	0.0136	0.2997	–0.2987	0.055
H(7A1)	2*i*	–0.2588	0.3128	–0.4208	0.059
H(7A2)	2*i*	–0.2316	0.1886	–0.3458	0.059
H(8A1)	2*i*	–0.0264	0.1195	–0.4557	0.055
H(8A2)	2*i*	–0.1926	0.0730	–0.5027	0.055
H(9A1)	2*i*	–0.1818	0.2681	–0.6072	0.050
H(9A2)	2*i*	–0.0263	0.3368	–0.5516	0.050
H(2B1)	2*i*	0.3243	0.5051	0.6631	0.072
H(2B2)	2*i*	0.4956	0.4912	0.6411	0.072
H(3B1)	2*i*	0.5128	0.3120	0.7571	0.066
H(3B2)	2*i*	0.3381	0.3109	0.7742	0.066
H(4B1)	2*i*	0.5490	0.5607	0.8351	0.069
H(4B2)	2*i*	0.3747	0.5574	0.8535	0.069
H(5B1)	2*i*	0.5797	0.3842	0.9528	0.070
H(5B2)	2*i*	0.4042	0.3689	0.9674	0.070
H(1)	2*i*	0.5188	1.0799	0.3804	0.071
H(2)	2*i*	0.6101	1.0259	0.0861	0.087
H(3)	2*i*	0.3399	1.0634	0.0934	0.084
H(1A)	2*i*	0.008(3)	0.956(3)	0.190(2)	0.091(8)
H(4)	2*i*	0.287(3)	1.097(3)	0.283(2)	0.079(7)
H(5)	2*i*	0.715(3)	1.038(3)	0.265(2)	0.080(7)
H(1B)	2*i*	0.240(3)	0.296(3)	0.444(2)	0.11(1)

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(1A)	2*i*	0.0620(1)	0.9036(1)	0.14117(9)	0.0426(7)	0.0718(8)	0.0429(6)	0.0091(6)	–0.0020(5)	–0.0245(6)
O(2A)	2*i*	–0.1648(1)	0.8730(2)	0.0582(1)	0.0431(7)	0.0844(9)	0.0601(8)	0.0163(6)	–0.0049(6)	–0.0343(7)
O(3A)	2*i*	0.1400(1)	0.1731(1)	–0.65041(8)	0.0373(6)	0.0670(7)	0.0399(6)	0.0039(5)	0.0012(4)	–0.0129(5)
O(4A)	2*i*	–0.0771(1)	0.0593(1)	–0.71835(8)	0.0382(6)	0.0677(7)	0.0411(6)	0.0071(5)	–0.0013(5)	–0.0241(5)
C(1A)	2*i*	–0.0333(2)	0.8471(2)	0.0633(1)	0.0391(9)	0.0387(7)	0.0333(7)	0.0019(6)	0.0028(6)	–0.0060(6)
C(2A)	2*i*	0.0392(2)	0.7510(2)	–0.0181(1)	0.0432(9)	0.0441(8)	0.0379(7)	0.0064(6)	0.0054(6)	–0.0091(6)
C(3A)	2*i*	–0.0754(2)	0.6562(2)	–0.0927(1)	0.0491(9)	0.0478(8)	0.0367(8)	0.0077(7)	0.0023(6)	–0.0126(6)
C(4A)	2*i*	–0.0048(2)	0.5539(2)	–0.1736(1)	0.054(1)	0.0432(8)	0.0337(7)	0.0070(7)	0.0064(6)	–0.0073(6)
C(5A)	2*i*	–0.1247(2)	0.4580(2)	–0.2440(1)	0.056(1)	0.0469(8)	0.0345(7)	0.0079(7)	0.0057(7)	–0.0112(6)
C(6A)	2*i*	–0.0609(2)	0.3587(2)	–0.3297(1)	0.057(1)	0.0440(8)	0.0342(7)	0.0044(7)	0.0106(7)	–0.0086(6)
C(7A)	2*i*	–0.1822(2)	0.2539(2)	–0.3922(1)	0.058(1)	0.0475(9)	0.0390(8)	–0.0022(7)	0.0158(7)	–0.0118(6)
C(8A)	2*i*	–0.1196(2)	0.1580(2)	–0.4810(1)	0.062(1)	0.0373(8)	0.0370(8)	0.0017(7)	0.0122(7)	–0.0096(6)
C(9A)	2*i*	–0.0866(2)	0.2436(2)	–0.5747(1)	0.0486(9)	0.0413(8)	0.0342(7)	0.0115(6)	0.0050(6)	–0.0066(6)
C(10A)	2*i*	–0.0020(2)	0.1534(2)	–0.6537(1)	0.0390(8)	0.0458(8)	0.0260(6)	0.0077(6)	0.0009(5)	–0.0038(5)
O(1B)	2*i*	0.2754(2)	0.3734(2)	0.4936(1)	0.084(1)	0.0634(8)	0.0537(7)	0.0000(7)	–0.0234(7)	–0.0048(6)
O(2B)	2*i*	0.3880(2)	0.1933(2)	0.5612(1)	0.146(2)	0.070(1)	0.082(1)	0.034(1)	–0.052(1)	–0.0225(8)
C(1B)	2*i*	0.3557(2)	0.3198(2)	0.5674(1)	0.057(1)	0.057(1)	0.0435(9)	0.0018(8)	–0.0070(7)	–0.0047(7)
C(2B)	2*i*	0.4024(2)	0.4353(2)	0.6570(1)	0.070(1)	0.057(1)	0.049(1)	0.0028(9)	–0.0114(8)	–0.0085(8)
C(3B)	2*i*	0.4278(2)	0.3740(2)	0.7605(1)	0.055(1)	0.065(1)	0.0421(9)	–0.0030(8)	–0.0025(7)	–0.0093(8)
C(4B)	2*i*	0.4605(2)	0.4966(2)	0.8499(1)	0.052(1)	0.070(1)	0.0450(9)	0.0011(8)	–0.0010(8)	–0.0130(8)
C(5B)	2*i*	0.4893(2)	0.4389(2)	0.9548(1)	0.054(1)	0.073(1)	0.0435(9)	–0.0036(9)	0.0009(7)	–0.0119(8)
N(1)	2*i*	0.6169(2)	1.0481(2)	0.2449(1)	0.0356(8)	0.0663(9)	0.066(1)	0.0099(7)	0.0000(7)	–0.0039(7)
N(2)	2*i*	0.3802(2)	1.0785(2)	0.2521(1)	0.0364(8)	0.0659(9)	0.0572(8)	0.0070(6)	0.0074(6)	–0.0019(7)
C(1)	2*i*	0.5079(2)	1.0707(2)	0.3080(2)	0.048(1)	0.077(1)	0.054(1)	0.0072(9)	0.0024(8)	0.0054(9)
C(2)	2*i*	0.5574(2)	1.0416(3)	0.1462(2)	0.044(1)	0.112(2)	0.057(1)	0.016(1)	0.0066(9)	–0.018(1)
C(3)	2*i*	0.4093(2)	1.0615(3)	0.1499(2)	0.044(1)	0.112(2)	0.052(1)	0.017(1)	–0.0007(8)	–0.015(1)

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