



Synthesis and crystal structure of 1,3-diisopropyl-4,5-dimethylimidazolium 4-methyl-benzenesulfinate

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ABSTRACT

New different types of 2,3-dihydroimidazole-2-ylidenes (**1**) have been successfully synthesized and characterized by NMR and X-ray, 1,3-diisopropyl-4, 5-dimethylimidazolium 4-methylbenzenethiolate (**2**) was very sensitive toward atmosphere, so it enhance the oxidation probability of the methyl thio phenol ion and formed benzenesulfinateImidazolium salt (**3**). Single crystals of **3** that suitable for X-ray crystal structure analysis were obtained by allowing diethyl ether vapor diffuse into an acetone solution at RT. The compound is crystalline in the monoclinic space group $P2_1/c$.

Key words: Imidazolium, Synthesis, X-ray, benzenesulfinate.

INTRODUCTION

Poor water solubility of drug candidates is a major problem in the pharmaceutical industry, and it has been estimated that 40% of all newly developed drugs are poorly soluble or insoluble in water [1]. Room temperature ionic liquids are organic salts which are liquids at ambient temperature; they are composed of ions comprising a relatively large asymmetric organic cation (e.g. dialkylimidazolium ions) and an inorganic or organic anion (e.g. halide, hexafluorophosphate). Imidazolium salts are also known as precursors for stable carbenes with many applications in organic synthesis [2].

N-Heterocyclic carbenes have been in the center of our interest as strong nucleophiles and organic bases; they react with Brønsted acids and have consequently been used as selective deprotonation reagents [3]. The nature of the hydrogen bonds in the imidazolium salts depends on the properties of the counterions, and appears to be weaker with hard and less basic counterions. The close interaction of the C–H···X (X = S, O, N) hydrogen bonds have attracted considerable interest in various organic compounds to understand their crystal structures [4, 5].

This work will shed more light for 1,3-diisopropyl-4,5-dimethylimidazol-2-ylidene(**1**) reactions to obtain new imidazolium salts (**2** and **3**) on the route of possible drugs (Fig. 1).

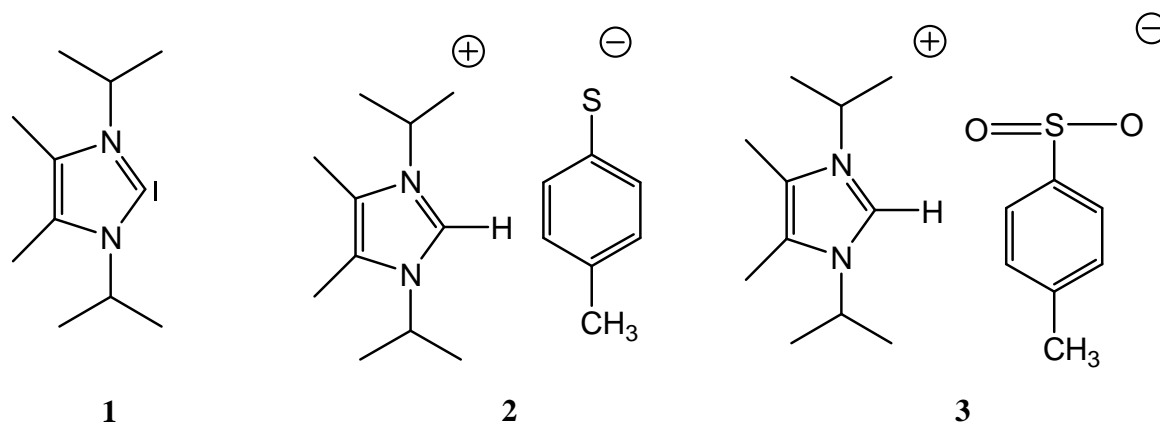


Figure 1: Structures of the title compound with N-heterocyclic carbenes

EXPERIMENTAL SECTION

Mass spectra

Mass spectra were recorded on a Finnigan Triple-Stage-Quadrupol spectrometer (TSQ-70) from Finnigan-Mat. High-resolution mass spectra were measured on a modified AMD Inectra MAT 711 A and reported as mass / charge (m/z). The used mass spectrometric ionization methods were electron-impact (EI) by 70 eV at 200°C or Fast-atom bombardment (FAB) by 70 eV in Nitrobenzylalcohol-Matrix at 60°C.

NMR spectra

The high resolution NMR spectra were acquired by a Bruker DRX 400 NMR spectrometer which operated at 400.13 MHz for ^1H , 100.61 MHz for ^{13}C and 161.98 MHz for ^{19}F nuclei, respectively. The spectra were measured relative to TMS (^1H , ^{13}C) as an internal standards. All experiments were performed at 25 °C. Data are reported as follows: chemical shift (multiplicity: s = singlet, d = doublet, t = triplet, q = quartet, sept = septet, m = multiplet, J = coupling constant (Hz) in italic form).

Crystal structure analyses

The crystals were mounted on a glass fiber with epoxy cement at room temperature. Preliminary examination and data collection were performed with a Stoe IPDS 2 diffractometer with graphite-monochromated Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$).

Data collection: CAD-4 Software (Enraf–Nonius, 1998); cell refinement:CAD-4 Software); data reduction: HELENA/PLATON (Spek, 2009); program(s) used to solve structure: SHELXS97 (Sheldrick,2008); program(s) used to refine structure: SHELXL97 (Sheldrick,2008 [6]); molecular graphics: SHELXTL (Sheldrick, 2008 [6]); software used to prepare material for publication: SHELXTL.

Synthesis of 1,3-diisopropyl-4, 5-dimethylimidazolium 4-methyl- benzenesulfinate (3)

The title compound was prepared by addition of 4-methylbenzenethiol (0.250 g, 2.01 mmol) to a solution containing 0.362g (2.01 mmol) of 1,3-diisopropyl-4,5-dimethylimidazol-2-ylidene [7], in 30 ml of dry diethylether at -50 °C. After stirring over night at room temperature, the precipitate was filtered off, washed with dry diethylether and dried under reduced pressure to form 1,3-diisopropyl-4, 5-dimethylimidazolium 4-methylbenzenethiolate (2) (Yield: 0.50 g, 74%).

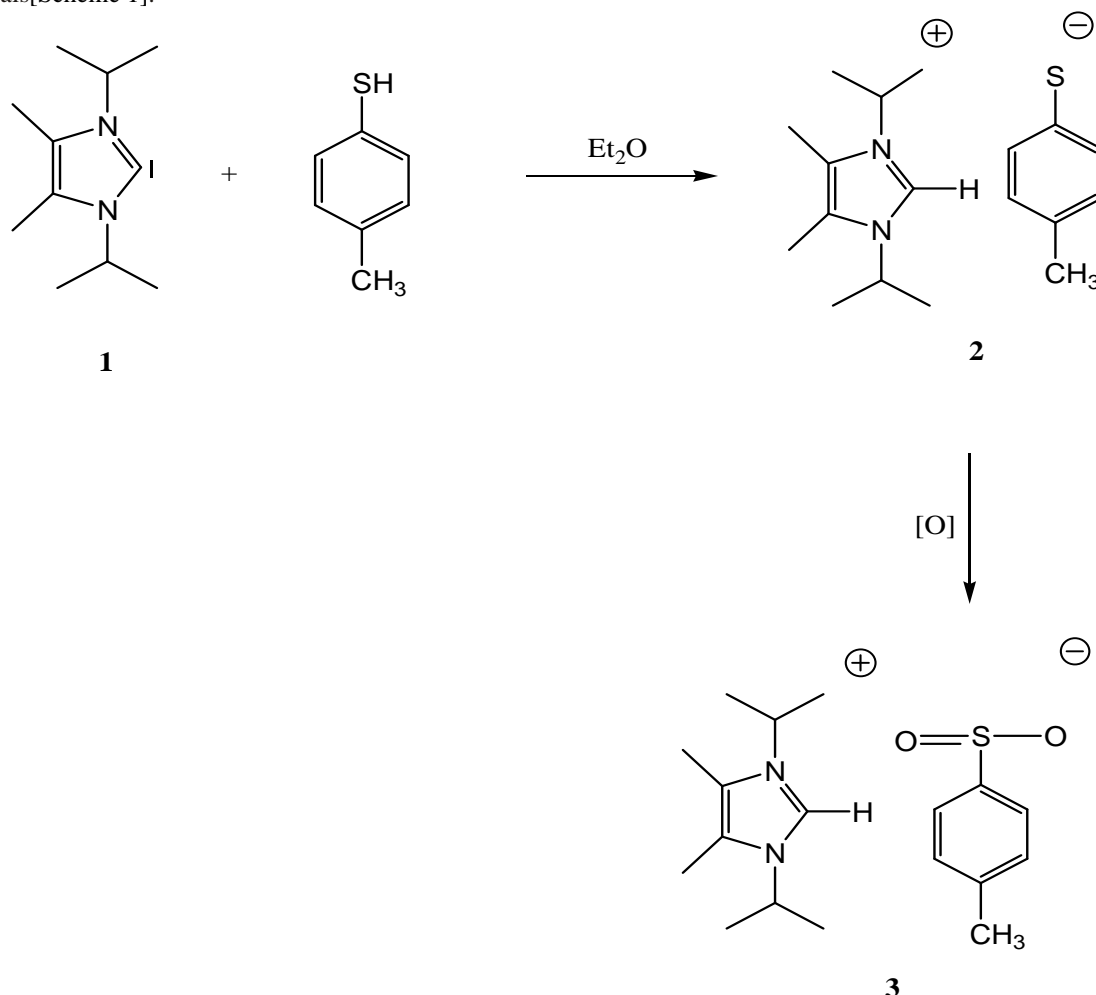
The compound 2 was elucidated on the bases of:

$^1\text{H NMR (CD}_2\text{Cl}_2)$: $\delta = 1.67$ (d, 12H, 1,3- CHMe_2 , $^3J = 6.71$ Hz), 2.25 (s, 6H, 4,5-Me), 4.50 (sept, 2H, 1,3- CHMe_2), 2.32 (PhCH_3), 7.14 (d, 2 H, $\text{C}_{\text{Ph}}^{3,5}$), 7.29 (d, 2 H, $\text{C}_{\text{Ph}}^{2,6}$), 10.67 (s, 1 H, C_{Im}^2).

$^{13}\text{C}\{^1\text{H}\} \text{NMR (CD}_2\text{Cl}_2)$: $\delta = 8.84$ (4,5-Me) , 23.01 (1,3- CHMe_2), 51.30 (1,3- CHMe_2), 21.15 (PhCH_3), 130.07 ($\text{C}_{\text{Ph}}^{2,6}$), 131.60 ($\text{C}_{\text{Ph}}^{3,5}$), 137.81 (C_{Ph}^1), 138.89 (C_{Ph}^4), 130.34 (C_{Im}^2), 134.29 ($\text{C}_{\text{Im}}^{4,5}$). **Anal. Calcd.** for $\text{C}_{18}\text{H}_{28}\text{N}_2\text{S}$

(304.49 g/mol): (C, 71.00; H, 9.27; N, 9.20; S, 10.53) %. **Found** for C₁₈H₂₈N₂S: (C, 71.65; H, 9.89; N, 8.81; S, 10.68) %. **MS (FAB neg.):** m/z (%) = 123.0 [100].

Compound **2** was very sensitive toward atmosphere, so it enhance the oxidation probability of the methyl thio phenol ion and formed the titled compound (**3**) which was recrystallized from acetone /diethylether as colourless crystals [Scheme 1].



Scheme 1: Synthesis of the title compound (3)

RESULTS AND DISCUSSION

The formation of stable C-H...O bonds between the components of 2*H*-imidazolium cation pairs may act as an additional stabilizing factor in their crystal structures [3]. By continuing our investigations on the structural chemistry of imidazolium salts [8, 9], we became interested in the structure produced from the reaction of imidazolcarbene with 4-methylbenzenethiol, surprisingly, 1,3-diisopropyl-4, 5-dimethylimidazolium methyl benzenesulfinate was obtained due to air oxidation of the 4-methylbenzenethiolate. Apparently their properties are influenced by interionic interactions which have been detected mainly in their 2*H*-derivatives as hydrogen bonds. The C-H...X interaction is typically weak and it acts as an additional stabilizing factor in their crystal structures [4, 10].

In the title compound (Fig. 2), the bond distances and angles in the imidazolium cation are in agreement with similar published moieties in literature [3, 8]. In the case of the anion, it is consisted of sulfinate moiety connected to a benzene ring. The distances S1-O1 and S1-O2 are approximately similar, 1.484 (3) Å and 1.452(4) Å, respectively. These distances are in agreement with that of SO₃ in imidazolium benzenesulfonate [11] and show a resonance

structure of single and double bond. The O-S-O angle is 111.5(2) ° that is in agreement of other angles found in literature for Sulfur atom in trigonal pyramidal geometry [12].

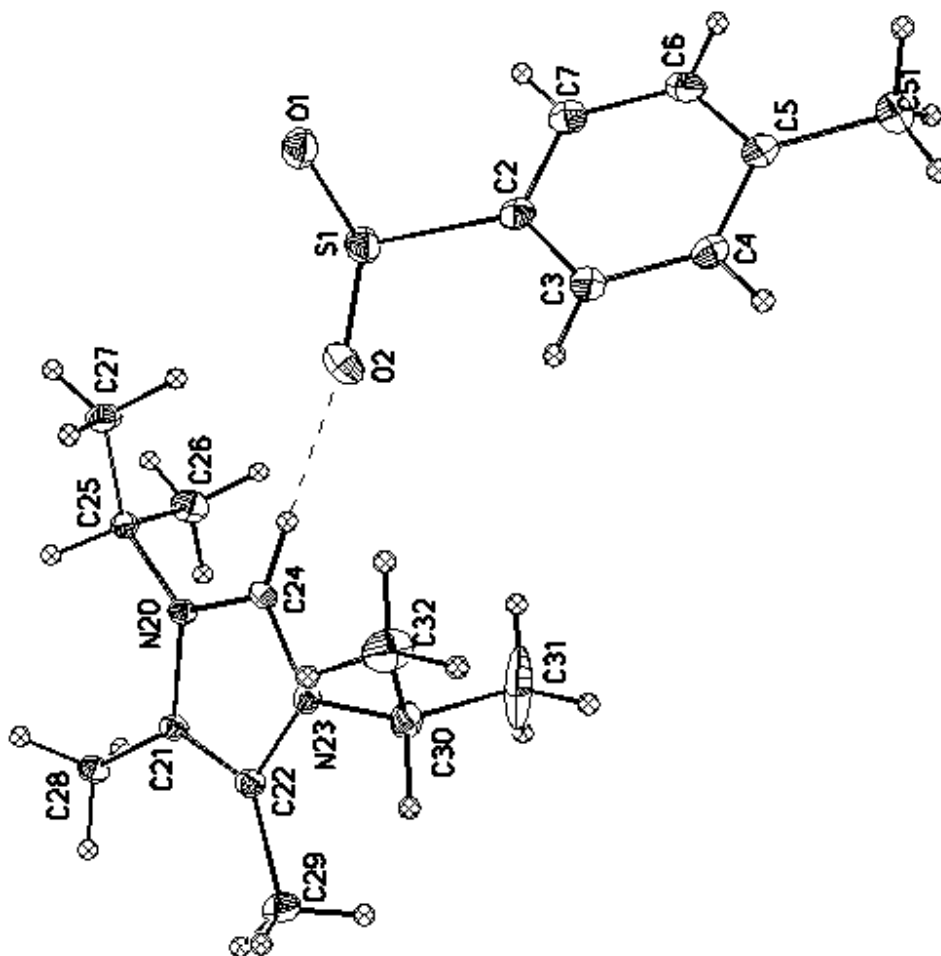


Figure 2: Crystal structure of the title compound (3)

Table 1: Selected bond lengths (Å) and angles (deg) for $C_{18}H_{28}N_2O_2S$ (3)

H(24)-C(24)	0.950(3)
S(1)-O(1)	1.484(3)
S(1)-O(2)	1.452(4)
S(1)-C(2)	1.805(4)
C(2)-C(3)	1.382(6)
N(20)-C(24)	1.330(5)
N(23)-C(24)	1.333(5)
O(2)-S(1)-O(1)	111.5(2)
O(2)-S(1)-C(2)	103.7(2)
O(1)-S(1)-C(2)	101.71(18)
C(24)-N(20)-C(21)	108.9(3)
C(24)-N(20)-C(25)	126.5(3)
C(21)-N(20)-C(25)	124.2(3)

Table 2: Crystal data and structure refinement for (3)

Identification code	kuhmal207	
Empirical formula	C18 H28 N2 O2 S	
Formula weight	336.48	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 14.1151(17) Å b = 8.4634(7) Å c = 16.379(2) Å	$\alpha = 90^\circ$ $\beta = 104.491(10)^\circ$ $\gamma = 90^\circ$
Volume	1894.4(4) Å ³	
Z	4	
Density (calculated)	1.180 Mg/m ³	
Absorption coefficient	0.182 mm ⁻¹	
F(000)	728	
Crystal size	0.25 x 0.15 x 0.15 mm ³	
Theta range for data collection	3.26 to 26.37°	
Index ranges	-17<=h<=17, -10<=k<=10, -20<=l<=20	
Reflections collected	24973	
Independent reflections	3873 [R(int) = 0.1064]	
Completeness to theta = 26.37°	99.8 %	
Absorption correction	None	
Max. and min. transmission	0.9733 and 0.9560	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3873 / 0 / 215	
Goodness-of-fit on F ²	1.114	
Final R indices [I>2sigma(I)]	R1 = 0.0956, wR2 = 0.2207	
R indices (all data)	R1 = 0.1199, wR2 = 0.2350	
Largest diff. peak and hole	1.888 and -0.468 e.Å ⁻³	

Table 3: Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å²x 10³) for (3). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
S(1)	2184(1)	4922(2)	1864(1)	44(1)
N(20)	997(2)	3641(4)	4443(2)	25(1)
N(23)	2136(2)	5282(4)	5032(2)	27(1)
O(1)	1587(2)	5727(4)	1103(2)	45(1)
O(2)	2127(3)	5734(6)	2631(2)	68(1)
C(2)	3412(3)	5332(5)	1782(2)	35(1)
C(3)	3991(3)	6462(6)	2277(3)	43(1)
C(4)	4910(3)	6800(6)	2155(3)	48(1)
C(5)	5269(3)	6007(6)	1553(3)	42(1)
C(6)	4690(3)	4849(6)	1077(3)	41(1)
C(7)	3768(3)	4523(5)	1183(3)	38(1)
C(21)	1024(3)	3673(4)	5303(2)	25(1)
C(22)	1742(3)	4697(4)	5670(2)	28(1)
C(24)	1676(3)	4619(4)	4302(2)	27(1)
C(25)	389(3)	2541(5)	3829(2)	29(1)
C(26)	919(4)	963(5)	3890(3)	43(1)
C(27)	141(3)	3229(6)	2944(2)	41(1)
C(28)	340(3)	2718(5)	5662(2)	32(1)
C(29)	2119(3)	5175(6)	6573(2)	42(1)
C(30)	2951(3)	6439(5)	5144(3)	38(1)
C(31)	3877(4)	5565(8)	5138(7)	116(4)
C(32)	2702(5)	7700(7)	4485(3)	63(2)
C(51)	6265(4)	6396(8)	1413(3)	61(2)

Table 4: Bond lengths [Å] and angles [°] for (3)

S(1)-O(2)	1.452(4)
S(1)-O(1)	1.484(3)
S(1)-C(2)	1.805(4)
N(20)-C(24)	1.330(5)
N(20)-C(21)	1.400(4)
N(20)-C(25)	1.478(5)
N(23)-C(24)	1.333(5)
N(23)-C(22)	1.393(5)
N(23)-C(30)	1.487(5)
C(2)-C(3)	1.382(6)
C(2)-C(7)	1.389(6)
C(3)-C(4)	1.391(6)
C(3)-H(3)	0.9500
C(4)-C(5)	1.388(6)
C(4)-H(4)	0.9500
C(5)-C(6)	1.385(7)
C(5)-C(51)	1.516(7)
C(6)-C(7)	1.382(6)
C(6)-H(6)	0.9500
C(7)-H(7)	0.9500
C(21)-C(22)	1.354(5)
C(21)-C(28)	1.488(5)
C(22)-C(29)	1.496(5)
C(24)-H(24)	0.9500
C(25)-C(27)	1.519(5)
C(25)-C(26)	1.522(6)
C(25)-H(25)	1.0000
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-C(32)	1.496(7)
C(30)-C(31)	1.504(7)
C(30)-H(30)	1.0000
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
O(2)-S(1)-O(1)	11.5(2)
O(2)-S(1)-C(2)	103.7(2)
O(1)-S(1)-C(2)	101.71(18)
C(24)-N(20)-C(21)	108.9(3)
C(24)-N(20)-C(25)	126.5(3)
C(21)-N(20)-C(25)	124.2(3)
C(24)-N(23)-C(22)	109.1(3)
C(24)-N(23)-C(30)	125.2(3)
C(22)-N(23)-C(30)	125.7(3)
C(3)-C(2)-C(7)	119.3(4)
C(3)-C(2)-S(1)	121.8(3)
C(7)-C(2)-S(1)	118.8(3)
C(2)-C(3)-C(4)	119.6(4)
C(2)-C(3)-H(3)	120.2
C(4)-C(3)-H(3)	120.2
C(5)-C(4)-C(3)	121.5(4)
C(5)-C(4)-H(4)	119.3

C(3)-C(4)-H(4)	119.3
C(6)-C(5)-C(4)	118.2(4)
C(6)-C(5)-C(51)	120.5(4)
C(4)-C(5)-C(51)	121.3(4)
C(7)-C(6)-C(5)	120.8(4)
C(7)-C(6)-H(6)	119.6
C(5)-C(6)-H(6)	119.6
C(6)-C(7)-C(2)	120.6(4)
C(6)-C(7)-H(7)	119.7
C(2)-C(7)-H(7)	119.7
C(22)-C(21)-N(20)	106.7(3)
C(22)-C(21)-C(28)	131.3(3)
N(20)-C(21)-C(28)	122.0(3)
C(21)-C(22)-N(23)	106.8(3)
C(21)-C(22)-C(29)	130.8(4)
N(23)-C(22)-C(29)	122.3(3)
N(20)-C(24)-N(23)	108.5(3)
N(20)-C(24)-H(24)	125.8
N(23)-C(24)-H(24)	125.8
N(20)-C(25)-C(27)	111.3(3)
N(20)-C(25)-C(26)	108.4(3)
C(27)-C(25)-C(26)	113.0(3)
N(20)-C(25)-H(25)	108.0
C(27)-C(25)-H(25)	108.0
C(26)-C(25)-H(25)	108.0
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(21)-C(28)-H(28A)	109.5
C(21)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(21)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(22)-C(29)-H(29A)	109.5
C(22)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(22)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
N(23)-C(30)-C(32)	110.2(4)
N(23)-C(30)-C(31)	108.8(4)
C(32)-C(30)-C(31)	113.2(6)
N(23)-C(30)-H(30)	108.2
C(32)-C(30)-H(30)	108.2
C(31)-C(30)-H(30)	108.2
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(5)-C(51)-H(51A)	109.5
C(5)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5

C(5)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5

Symmetry transformations used to generate equivalent atoms:

There is no classical hydrogen bonding. However, a noncovalent bond between the hydrogen of the imidazolium part and one of the SO₂ oxygen can be suggested with a distance C24...O2 of 3.111(5)Å. Bond lengths in 4-Methylbenzenethiol anion are similar to those found in ethyl phenylsulfonyleacetate compound [13].

Table 5: Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (3). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
S(1)	39(1)	52(1)	42(1)	14(1)	14(1)	4(1)
N(20)	28(2)	25(2)	22(1)	2(1)	8(1)	-2(1)
N(23)	25(2)	28(2)	29(2)	-2(1)	6(1)	-2(1)
O(1)	37(2)	51(2)	47(2)	6(2)	10(1)	4(1)
O(2)	52(2)	107(3)	55(2)	1(2)	31(2)	-11(2)
C(2)	37(2)	38(2)	28(2)	13(2)	3(2)	4(2)
C(3)	37(2)	58(3)	34(2)	-6(2)	9(2)	1(2)
C(4)	40(2)	67(3)	35(2)	-15(2)	4(2)	-6(2)
C(5)	36(2)	57(3)	31(2)	4(2)	4(2)	2(2)
C(6)	50(3)	48(3)	28(2)	3(2)	12(2)	9(2)
C(7)	46(2)	33(2)	34(2)	2(2)	7(2)	4(2)
C(21)	30(2)	25(2)	20(2)	4(1)	7(1)	3(2)
C(22)	31(2)	30(2)	24(2)	3(2)	6(2)	5(2)
C(24)	26(2)	32(2)	25(2)	2(2)	11(1)	-2(2)
C(25)	28(2)	35(2)	25(2)	-3(2)	8(1)	-10(2)
C(26)	57(3)	30(2)	44(2)	-9(2)	16(2)	-6(2)
C(27)	44(2)	55(3)	24(2)	1(2)	8(2)	-15(2)
C(28)	35(2)	37(2)	26(2)	5(2)	12(2)	-1(2)
C(29)	48(2)	50(3)	27(2)	-2(2)	4(2)	0(2)
C(30)	32(2)	36(2)	47(2)	-13(2)	11(2)	-12(2)
C(31)	26(3)	66(4)	251(11)	-48(6)	29(4)	-11(3)
C(32)	80(4)	55(3)	53(3)	0(3)	17(3)	-38(3)
C(51)	43(3)	94(4)	48(3)	-1(3)	15(2)	-2(3)

Table 6: Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (3)

	x	y	z	U(eq)
H(3)	3763	7004	2699	52
H(4)	5301	7591	2490	58
H(6)	4929	4272	673	50
H(7)	3375	3740	843	46
H(24)	1811	4812	3771	32
H(25)	-238	2369	3996	35
H(26A)	1511	1084	3687	65
H(26B)	488	177	3544	65
H(26C)	1098	611	4479	65
H(27A)	-97	4313	2959	62
H(27B)	-367	2585	2575	62
H(27C)	728	3232	2727	62
H(28A)	524	1601	5670	48
H(28B)	-329	2851	5313	48
H(28C)	373	3072	6238	48
H(29A)	1805	4531	6928	64
H(29B)	1971	6293	6636	64
H(29C)	2829	5014	6745	64
H(30)	3039	6949	5709	46
H(31A)	4006	4767	5585	173
H(31B)	4425	6312	5234	173
H(31C)	3804	5047	4590	173
H(32A)	2610	7223	3925	94
H(32B)	3235	8473	4575	94
H(32C)	2097	8230	4522	94
H(51A)	6578	7217	1812	92

H(51B)	6187	6779	835	92
H(51C)	6674	5445	1501	92

Table 7: Torsion angles [°] for (3)

O(2)-S(1)-C(2)-C(3)	-12.2(4)
O(1)-S(1)-C(2)-C(3)	103.7(4)
O(2)-S(1)-C(2)-C(7)	170.0(3)
O(1)-S(1)-C(2)-C(7)	-74.1(3)
C(7)-C(2)-C(3)-C(4)	1.6(7)
S(1)-C(2)-C(3)-C(4)	-176.2(4)
C(2)-C(3)-C(4)-C(5)	-1.1(7)
C(3)-C(4)-C(5)-C(6)	-0.6(7)
C(3)-C(4)-C(5)-C(51)	179.1(5)
C(4)-C(5)-C(6)-C(7)	1.7(7)
C(51)-C(5)-C(6)-C(7)	-177.9(4)
C(5)-C(6)-C(7)-C(2)	-1.3(6)
C(3)-C(2)-C(7)-C(6)	-0.5(6)
S(1)-C(2)-C(7)-C(6)	177.4(3)
C(24)-N(20)-C(21)-C(22)	-0.2(4)
C(25)-N(20)-C(21)-C(22)	173.0(3)
C(24)-N(20)-C(21)-C(28)	179.1(3)
C(25)-N(20)-C(21)-C(28)	-7.8(5)
N(20)-C(21)-C(22)-N(23)	0.5(4)
C(28)-C(21)-C(22)-N(23)	-178.7(4)
N(20)-C(21)-C(22)-C(29)	-178.2(4)
C(28)-C(21)-C(22)-C(29)	2.6(7)
C(24)-N(23)-C(22)-C(21)	-0.6(4)
C(30)-N(23)-C(22)-C(21)	-179.6(3)
C(24)-N(23)-C(22)-C(29)	178.2(4)
C(30)-N(23)-C(22)-C(29)	-0.7(6)
C(21)-N(20)-C(24)-N(23)	-0.2(4)
C(25)-N(20)-C(24)-N(23)	-173.1(3)
C(22)-N(23)-C(24)-N(20)	0.5(4)
C(30)-N(23)-C(24)-N(20)	179.5(3)
C(24)-N(20)-C(25)-C(27)	-34.5(5)
C(21)-N(20)-C(25)-C(27)	153.6(3)
C(24)-N(20)-C(25)-C(26)	90.4(4)
C(21)-N(20)-C(25)-C(26)	-81.5(4)
C(24)-N(23)-C(30)-C(32)	47.4(5)
C(22)-N(23)-C(30)-C(32)	-133.8(4)
C(24)-N(23)-C(30)-C(31)	-77.3(6)
C(22)-N(23)-C(30)-C(31)	101.5(6)

Symmetry transformations used to generate equivalent atoms:

CONCLUSION

New different types of 2,3-dihydroimidazole-2-ylidenes have successfully synthesized on the route to possible drugs (scheme 1). The resulting compounds are classified as salt derivatives, these compounds play an important role in the construction of ionic liquids [14], which can be potentially used as pharmaceutical solvents [1]. Apparently their properties are influenced by interionic interactions which have been detected mainly in their 2H-derivatives as hydrogen bonds [3]. The close interaction of the C-H...X (X = S, O, N) hydrogen bonds have attracted considerable interest and suggested in various organic compounds to understand their crystal structures.

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