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Sodium 1-(4-chlorophenyl)-5-methyl-1*H*-1,2,3-triazole-4-carboxylate

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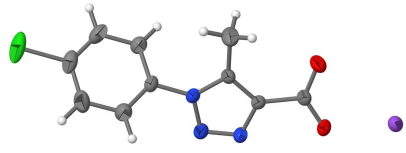
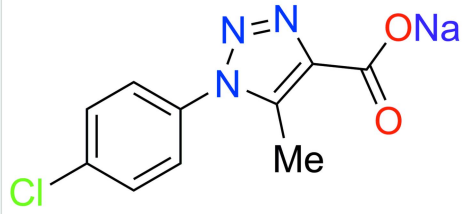
Structural data: full structural data are available from iucrdata.iucr.org

In the title molecular salt, $Na^{+}\cdot C_{10}H_7ClN_3O_2^{-}$, the dihedral angles between the planes of adjacent chlorophenyl, methyltriazole and carboxylate groups of the anion are 50.2 (1) and 9.0 (3)°, respectively. The shortest distance between sodium cations is 4.0595 (9) Å. The sodium cation is coordinated by two N atoms and three O atoms, generating layers of ions lying parallel to the *bc* plane.

3D view



Chemical scheme



Structure description

1,2,3-Triazole-4-carboxylic acids are important precursors for various biologically active compounds that act as xanthine oxidase inhibitors (Zhang *et al.*, 2017; Ojha *et al.*, 2017) and antibacterial (Maji & Haldar, 2017) and antitubercular (Kamal *et al.*, 2013) agents. As part of our studies in this area, we now describe the synthesis and structure of the title salt.

The asymmetric unit comprises a Na^{+} cation and a $C_{10}H_7ClN_3O_2^{-}$ anion (Fig. 1). The anion consists of chlorophenyl, methyltriazolyl and carboxylate groups, and the twist angles between the planes through adjacent groups are 50.2 (1) and 9.0 (3)°, respectively. The shortest distance between sodium cations is 4.0595 (9) Å and each cation is coordinated by two N atoms, with an average Na—N distance of 2.5654 (6) Å, and by three O atoms, with an average Na···O distance of 2.37 (4) Å. The resulting coordination polyhedron is a very distorted trigonal bipyramid with one N atom and one O atom in the axial sites. The extended structure generates layers of ions parallel to the *bc* plane (Fig. 2). A short C—H···N contact is also observed (Table 1).

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4A···N2^{i}	0.96	2.52	3.432 (3)	159

Symmetry code: (i) $x, y-1, z$.

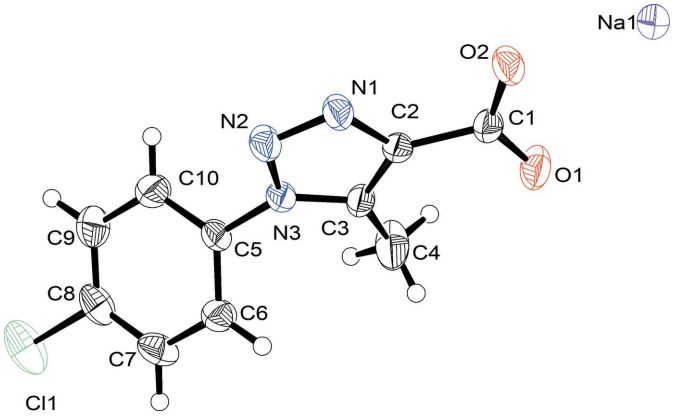


Figure 1
The asymmetric unit of the title salt, showing 50% probability displacement ellisoids.

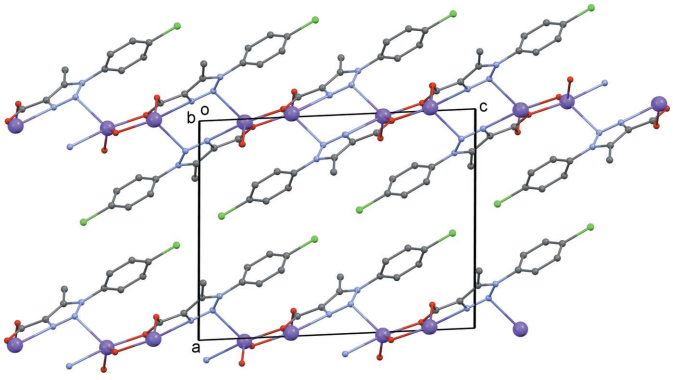


Figure 2
The crystal packing of the title salt, viewed down the b axis.

Synthesis and crystallization

The title compound was synthesized from the reaction of 1-(4-chlorophenyl)-5-methyl-1*H*-1,2,3-triazole-4-carboxylic acid and sodium hydroxide (10%) in ethanol under reflux for 4 h. The crude product obtained after work-up was recrystallized from dimethylformamide solution to give colourless blocks.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Table 2
Experimental details.

Crystal data	
Chemical formula	$Na^{+}\cdot C_{10}H_7ClN_3O_2^{-}$
M_r	259.63
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	11.6462 (8), 6.3754 (4), 14.7003 (9)
β (°)	92.711 (7)
V (Å^3)	1090.26 (12)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.38
Crystal size (mm)	0.42 × 0.16 × 0.07
Data collection	
Diffractometer	Rigaku OD SuperNova Dual source diffractometer with an Atlas detector
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.467, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8333, 2665, 1875
R_{int}	0.030
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.696
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.115, 1.05
No. of reflections	2665
No. of parameters	155
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.40

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXS97* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *CHEMDRAW* Ultra (Cambridge Soft, 2001).

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full crystallographic data

IUCrData (2018). **3**, x181127 [https://doi.org/10.1107/S2414314618011276]

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Crystal data

$Na^+ \cdot C_{10}H_7ClN_3O_2^-$
M_r = 259.63
Monoclinic, $P2_1/c$
a = 11.6462 (8) Å
b = 6.3754 (4) Å
c = 14.7003 (9) Å
β = 92.711 (7)°
V = 1090.26 (12) Å^3
Z = 4
$F(000)$ = 528
D_x = 1.582 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2649 reflections
θ = 3.5–29.2°
μ = 0.38 mm^{-1}
T = 293 K
Block, colourless
0.42 × 0.16 × 0.07 mm

Data collection

Rigaku OD SuperNova Dual source diffractometer with an Atlas detector
ω scans
Absorption correction: gaussian (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.467, T_{max} = 1.000
8333 measured reflections
2665 independent reflections
1875 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 29.7°, θ_{min} = 3.2°
h = −14→15
k = −8→8
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.115
S = 1.05
2665 reflections
155 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0446P)^2 + 0.2829P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.08988 (16)	0.5137 (3)	0.64261 (13)	0.0306 (4)
C2	0.12619 (15)	0.6087 (3)	0.55520 (12)	0.0277 (4)
C3	0.19398 (17)	0.5260 (3)	0.48997 (13)	0.0304 (4)
C4	0.2601 (2)	0.3285 (3)	0.48670 (17)	0.0597 (8)
H4A	0.209664	0.215967	0.467891	0.090*
H4B	0.294116	0.298547	0.546045	0.090*
H4C	0.319562	0.342836	0.444051	0.090*
C5	0.25655 (16)	0.6837 (3)	0.34347 (13)	0.0302 (4)
C6	0.24624 (18)	0.5191 (3)	0.28293 (14)	0.0378 (5)
H6	0.201366	0.403343	0.296042	0.045*
C7	0.30294 (19)	0.5273 (4)	0.20265 (14)	0.0448 (6)
H7	0.297119	0.416527	0.161513	0.054*
C8	0.36800 (18)	0.7002 (4)	0.18405 (14)	0.0421 (5)
C9	0.3785 (2)	0.8660 (4)	0.24377 (15)	0.0481 (6)
H9	0.422407	0.982653	0.230039	0.058*
C10	0.32262 (19)	0.8562 (3)	0.32453 (15)	0.0429 (5)
H10	0.329600	0.965933	0.366091	0.052*
N1	0.09199 (14)	0.8041 (2)	0.52889 (11)	0.0337 (4)
N2	0.13405 (15)	0.8474 (2)	0.45008 (11)	0.0355 (4)
N3	0.19683 (13)	0.6783 (2)	0.42611 (10)	0.0292 (4)
O1	0.11449 (14)	0.3261 (2)	0.65583 (10)	0.0469 (4)
O2	0.03699 (12)	0.6316 (2)	0.69418 (9)	0.0406 (4)
Cl1	0.43802 (6)	0.70889 (13)	0.08201 (4)	0.0687 (3)
Na1	−0.01461 (7)	0.49886 (11)	0.83416 (5)	0.0360 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0339 (11)	0.0277 (10)	0.0310 (10)	−0.0038 (8)	0.0085 (9)	0.0010 (8)
C2	0.0327 (10)	0.0239 (9)	0.0269 (9)	−0.0009 (7)	0.0067 (8)	−0.0022 (7)
C3	0.0376 (11)	0.0241 (9)	0.0303 (10)	−0.0014 (7)	0.0100 (9)	0.0016 (8)
C4	0.0875 (19)	0.0378 (12)	0.0569 (15)	0.0222 (12)	0.0378 (14)	0.0114 (11)
C5	0.0345 (10)	0.0332 (9)	0.0234 (9)	0.0004 (8)	0.0067 (8)	−0.0006 (8)
C6	0.0419 (12)	0.0384 (11)	0.0336 (11)	−0.0062 (9)	0.0081 (9)	−0.0057 (9)
C7	0.0498 (14)	0.0542 (13)	0.0310 (11)	0.0016 (10)	0.0075 (10)	−0.0134 (10)
C8	0.0330 (11)	0.0646 (14)	0.0293 (11)	0.0056 (10)	0.0081 (9)	0.0040 (10)
C9	0.0502 (14)	0.0527 (13)	0.0425 (13)	−0.0119 (11)	0.0142 (11)	0.0075 (11)
C10	0.0533 (14)	0.0382 (11)	0.0381 (12)	−0.0091 (10)	0.0119 (10)	−0.0050 (9)
N1	0.0462 (10)	0.0287 (8)	0.0271 (8)	0.0056 (7)	0.0107 (7)	0.0023 (7)
N2	0.0487 (10)	0.0299 (8)	0.0287 (9)	0.0090 (7)	0.0103 (8)	0.0025 (7)
N3	0.0363 (9)	0.0265 (8)	0.0253 (8)	0.0013 (6)	0.0079 (7)	−0.0016 (6)
O1	0.0652 (10)	0.0282 (7)	0.0494 (9)	0.0057 (7)	0.0242 (8)	0.0101 (7)
O2	0.0584 (9)	0.0334 (7)	0.0318 (7)	0.0055 (7)	0.0205 (7)	0.0019 (6)
Cl1	0.0569 (4)	0.1123 (6)	0.0390 (3)	0.0133 (4)	0.0240 (3)	0.0101 (3)
Na1	0.0500 (5)	0.0288 (4)	0.0300 (4)	−0.0048 (3)	0.0083 (4)	0.0008 (3)

Geometric parameters (Å, º)

Na1—N1^{i}	2.5649 (16)	C4—H4C	0.9600
Na1—N2^{ii}	2.5658 (19)	C5—C6	1.377 (3)
Na1—O1^{iii}	2.3964 (16)	C5—C10	1.378 (3)
Na1—O2	2.3299 (14)	C5—N3	1.429 (2)
Na1—O2^{i}	2.3902 (15)	C6—C7	1.380 (3)
Na1—Na1^{i}	4.0595 (9)	C6—H6	0.9300
Na1—Na1^{iii}	4.0595 (9)	C7—C8	1.373 (3)
C1—O1	1.243 (2)	C7—H7	0.9300
C1—O2	1.250 (2)	C8—C9	1.376 (3)
C1—C2	1.499 (2)	C8—Cl1	1.742 (2)
C2—N1	1.359 (2)	C9—C10	1.382 (3)
C2—C3	1.375 (2)	C9—H9	0.9300
C3—N3	1.352 (2)	C10—H10	0.9300
C3—C4	1.478 (3)	N1—N2	1.308 (2)
C4—H4A	0.9600	N2—N3	1.358 (2)
C4—H4B	0.9600		
O1—C1—O2	126.89 (17)	N1—N2—N3	106.93 (14)
O1—C1—C2	116.76 (16)	N1—N2—Na1^{iv}	113.55 (12)
O2—C1—C2	116.34 (16)	N3—N2—Na1^{iv}	119.04 (12)
O1—C1—Na1	85.80 (11)	C3—N3—N2	111.00 (14)
O2—C1—Na1	41.15 (9)	C3—N3—C5	129.55 (15)
C2—C1—Na1	157.39 (12)	N2—N3—C5	119.42 (14)
N1—C2—C3	108.84 (15)	C1—O1—Na1^{i}	137.58 (14)
N1—C2—C1	121.58 (15)	C1—O2—Na1	118.17 (12)
C3—C2—C1	129.59 (17)	C1—O2—Na1^{iii}	122.42 (11)
N3—C3—C2	104.06 (15)	Na1—O2—Na1^{iii}	118.64 (6)
N3—C3—C4	124.00 (16)	O2—Na1—O2^{i}	103.44 (4)
C2—C3—C4	131.76 (18)	O2—Na1—O1^{iii}	83.35 (5)
C3—C4—H4A	109.5	O2^{i}—Na1—O1^{iii}	144.50 (7)
C3—C4—H4B	109.5	O2—Na1—N1^{i}	169.72 (6)
H4A—C4—H4B	109.5	O2^{i}—Na1—N1^{i}	67.86 (5)
C3—C4—H4C	109.5	O1^{iii}—Na1—N1^{i}	100.58 (5)
H4A—C4—H4C	109.5	O2—Na1—N2^{ii}	104.69 (6)
H4B—C4—H4C	109.5	O2^{i}—Na1—N2^{ii}	123.69 (6)
C6—C5—C10	120.64 (17)	O1^{iii}—Na1—N2^{ii}	86.61 (6)
C6—C5—N3	120.01 (16)	N1^{i}—Na1—N2^{ii}	85.11 (5)
C10—C5—N3	119.33 (16)	O2—Na1—C1	20.68 (5)
C5—C6—C7	119.56 (18)	O2^{i}—Na1—C1	85.20 (5)
C5—C6—H6	120.2	O1^{iii}—Na1—C1	103.90 (5)
C7—C6—H6	120.2	N1^{i}—Na1—C1	152.77 (5)
C8—C7—C6	119.43 (19)	N2^{ii}—Na1—C1	107.94 (5)
C8—C7—H7	120.3	O2—Na1—Na1^{i}	73.40 (4)
C6—C7—H7	120.3	O2^{i}—Na1—Na1^{i}	30.25 (3)
C7—C8—C9	121.55 (18)	O1^{iii}—Na1—Na1^{i}	140.89 (6)
C7—C8—Cl1	118.84 (17)	N1^{i}—Na1—Na1^{i}	98.11 (4)

C9—C8—Cl1	119.61 (17)	N2^{ii}—Na1—Na1^{i}	129.16 (5)
C8—C9—C10	118.82 (19)	C1—Na1—Na1^{i}	55.00 (4)
C8—C9—H9	120.6	O2—Na1—Na1^{iii}	31.12 (4)
C10—C9—H9	120.6	O2^{i}—Na1—Na1^{iii}	132.42 (5)
C5—C10—C9	119.99 (19)	O1^{iii}—Na1—Na1^{iii}	53.76 (3)
C5—C10—H10	120.0	N1^{i}—Na1—Na1^{iii}	154.32 (4)
C9—C10—H10	120.0	N2^{ii}—Na1—Na1^{iii}	91.80 (4)
N2—N1—C2	109.17 (14)	C1—Na1—Na1^{iii}	51.60 (4)
N2—N1—Na1^{iii}	138.87 (11)	Na1^{i}—Na1—Na1^{iii}	103.49 (3)
C2—N1—Na1^{iii}	109.24 (11)		

Symmetry codes: (i) $-x$, $y-1/2$, $-z+3/2$; (ii) x, $-y+3/2$, $z+1/2$; (iii) $-x$, $y+1/2$, $-z+3/2$; (iv) x, $-y+3/2$, $z-1/2$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4*A*···N2^{v}	0.96	2.52	3.432 (3)	159

Symmetry code: (v) x, $y-1$, z.