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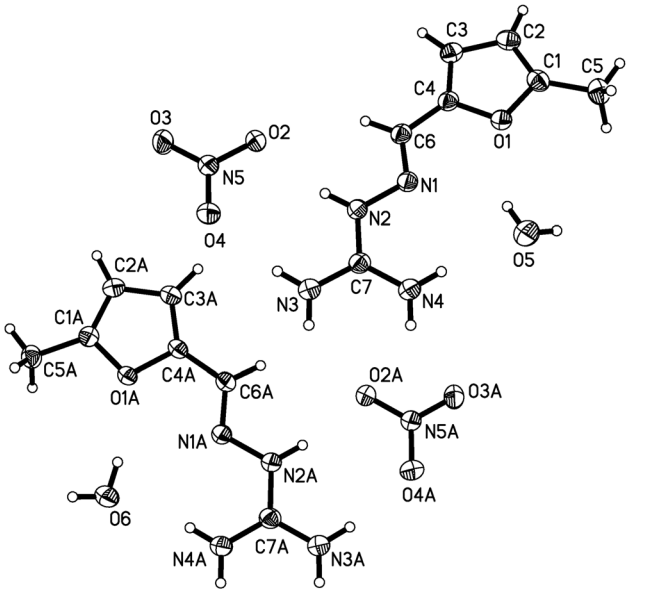
Crystal structure of (*E*)-amino(2-((5-methylfuran-2-yl)methylene)hydrazinyl) methaniminium nitrate monohydrate, $C_{14}H_{26}N_{10}O_{10}$



https://doi.org/10.1515/ncrs-2021-0419
Received October 25, 2021; accepted December 2, 2021; published online December 16, 2021

Abstract

$C_{14}H_{26}N_{10}O_{10}$, monoclinic, $P2_1$ (no. 4), a = 12.3337(3) Å, b = 3.87010(10) Å, c = 24.2368(6) Å, β = 97.644(2)°, V = 1146.61(5) Å^3, Z = 2, $R_{gt}(F)$ = 0.0400, $wR_{ref}(F^2)$ = 0.1092, T = 170 K.

CCDC no.: 2125809

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Table 1: Data collection and handling.

Crystal:	Yellow plate
Size:	0.42 × 0.11 × 0.01 mm
Wavelength:	Cu *K*α radiation (1.54184 Å)
μ:	1.06 mm^{-1}
Diffractometer, scan mode:	XtaLAB Synergy R, ω
θ_{max}, completeness:	75.1°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	10,934, 4198, 0.041
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 3982
$N(param)_{refined}$:	312
Programs:	CrysAlis^{PRO} [1], SHELX [2], Olex2 [3]

Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

5-Methylfurfural (1.10 g, 0.01 mol) was placed in 15 ml ethanol at room temperature, added into aminoguanidine nitrate (1.37 g, 0.01 mol) solution containing 10 ml water and 8 ml ethanol, heated and stirred for 8 h cooled to room temperature, then the precipitate was removed, and the filtrate was left standing to precipitate light yellow crystal.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

Guanidine groups easy form hydrogen bonds, have good stability and strong physiological activity, and are used as intermediates in the synthesis of drugs [4, 5]. Schiff base compounds and their metal complexes are used in medicine [6], catalysis [7], analytical chemistry [8], and an important application in the field of photochromism [9].

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
O1	0.26216 (12)	0.6229 (5)	0.55776 (6)	0.0427 (4)
N1	0.38488 (16)	0.9592 (6)	0.64397 (8)	0.0411 (4)
N2	0.43925 (15)	1.1364 (6)	0.68867 (8)	0.0419 (4)
H2	0.407808	1.179062	0.717537	0.050*
N3	0.59227 (16)	1.4148 (7)	0.72964 (9)	0.0495 (5)
H3A	0.658960	1.480600	0.730010	0.059*
H3B	0.557878	1.461439	0.757354	0.059*
N4	0.59248 (17)	1.1657 (7)	0.64332 (9)	0.0502 (5)
H4A	0.659176	1.229094	0.642849	0.060*
H4B	0.558661	1.052957	0.615647	0.060*
C1	0.1824 (2)	0.4463 (7)	0.52321 (10)	0.0462 (6)
C2	0.0960 (2)	0.3859 (8)	0.55111 (11)	0.0487 (6)
H2A	0.031852	0.271008	0.537299	0.058*
C3	0.1210 (2)	0.5293 (7)	0.60506 (11)	0.0464 (6)
H3	0.076973	0.526809	0.633356	0.056*
C4	0.22208 (18)	0.6711 (7)	0.60727 (9)	0.0406 (5)
C5	0.2069 (3)	0.3684 (9)	0.46697 (12)	0.0582 (7)
H5A	0.214299	0.580204	0.447200	0.087*
H5B	0.148404	0.234001	0.447550	0.087*
H5C	0.273905	0.239891	0.469318	0.087*
C6	0.28879 (18)	0.8536 (7)	0.65051 (10)	0.0414 (5)
H6	0.262060	0.896467	0.683965	0.050*
C7	0.54233 (18)	1.2409 (7)	0.68622 (10)	0.0413 (5)
O1A	0.76376 (11)	1.3943 (5)	0.94291 (6)	0.0396 (4)
N1A	0.87729 (15)	1.2428 (6)	0.85690 (8)	0.0423 (5)
N2A	0.93133 (15)	1.1463 (7)	0.81334 (8)	0.0465 (5)
H2AA	0.898660	1.028638	0.785936	0.056*
N3A	1.08727 (17)	1.1520 (8)	0.77224 (9)	0.0554 (6)
H3AA	1.154823	1.206798	0.772184	0.066*
H3AB	1.052959	1.039691	0.744658	0.066*
N4A	1.08741 (16)	1.4126 (7)	0.85745 (9)	0.0503 (5)
H4AA	1.154966	1.469234	0.857971	0.060*
H4AB	1.053087	1.468296	0.884792	0.060*
C1A	0.68667 (18)	1.4417 (7)	0.97817 (9)	0.0410 (5)
C2A	0.58899 (19)	1.3233 (7)	0.95376 (11)	0.0448 (5)
H2AB	0.523651	1.327295	0.968980	0.054*
C3A	0.60408 (18)	1.1913 (7)	0.90055 (10)	0.0436 (5)
H3AC	0.551014	1.091883	0.874508	0.052*
C4A	0.71098 (18)	1.2390 (6)	0.89532 (10)	0.0395 (5)
C5A	0.7272 (2)	1.5969 (8)	1.03287 (10)	0.0499 (6)
H5AA	0.791151	1.474605	1.049336	0.075*
H5AB	0.671395	1.581509	1.056854	0.075*
H5AC	0.745324	1.835055	1.027883	0.075*
C6A	0.77561 (18)	1.1574 (7)	0.85241 (9)	0.0418 (5)
H6A	0.743827	1.040961	0.820770	0.050*
C7A	1.03632 (19)	1.2400 (7)	0.81460 (10)	0.0441 (6)
O2	0.30805 (13)	1.3944 (7)	0.76875 (7)	0.0540 (5)
O3	0.31049 (15)	1.6358 (8)	0.84949 (8)	0.0645 (6)
O4	0.45007 (14)	1.6807 (7)	0.80558 (8)	0.0565 (5)
N5	0.35664 (15)	1.5716 (6)	0.80870 (8)	0.0447 (5)
O2A	0.80373 (14)	0.7363 (6)	0.73062 (8)	0.0582 (6)
O3A	0.80719 (17)	0.4827 (7)	0.65154 (8)	0.0649 (6)
O4A	0.94760 (16)	0.7633 (9)	0.68933 (10)	0.0806 (9)
N5A	0.85311 (16)	0.6597 (8)	0.69018 (8)	0.0492 (5)
O5	0.48651 (18)	0.8605 (12)	0.53592 (10)	0.0981 (11)
H5D	0.480166	0.689310	0.513761	0.147*
H5E	0.434336	0.807510	0.553971	0.147*
O6	0.99548 (15)	1.6258 (8)	0.95986 (8)	0.0637 (6)
H6B	0.992218	1.796659	0.981628	0.096*
H6C	0.929169	1.582980	0.947335	0.096*

According to previous studies [10, 11] we synthesized the title compound by the method of amine carbonyl condensation.

The structure of the title compound contains pairs of crystallographically independent cations, anions and water molecules (see the figure). The N–N and C=N bond distances in the two molecules are almost the same, N(1)–N(2) is 1.378(3) Å, N(1A)–N(2A) is 1.373(3) Å, N1=C6 is 1.283(3) Å, N(1A) = C(6A) is 1.288(3) Å, and all other bond lengths and bond angles are within the normal range [11].

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Research funding: This study was financially supported by Henan University of Science and Technology Distinguished Professor Open Fund (Grant No. 135100001).

Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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