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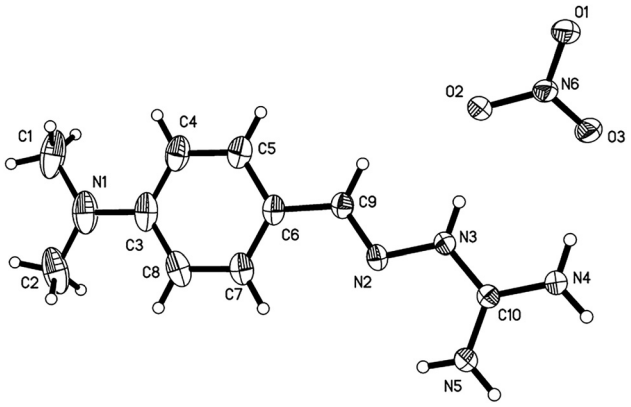
# Crystal structure of (*E*)-amino(2-(4-(dimethylamino)benzylidene)hydrazineyl) methaniminium nitrate, $C_{10}H_{16}N_6O_3$




https://doi.org/10.1515/ncrs-2021-0092
Received March 15, 2021; accepted April 8, 2021;
published online April 26, 2021

**Abstract**

$C_{10}H_{16}N_6O_3$, monoclinic, $P2_1/c$ (no. 14), $a$ = 7.2312(1) Å, $b$ = 17.7721(3) Å, $c$ = 11.0146(2) Å, $\beta$ = 104.557°, $V$ = 1370.08(4) Å$^3$, $Z$ = 4, $R_{gt}(F)$ = 0.0532, $wR_{ref}(F^2)$ = 0.1537, $T$ = 170.0 K.

**CCDC no.:** 2076114

The asymmetric unit of the title crystal structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Colourless block |
| Size: | 0.32 × 0.21 × 0.18 mm |
| Wavelength: | Cu *K*α radiation (1.54184 Å) |
| $\mu$: | 0.84 mm$^{-1}$ |
| Diffractometer, scan mode: | XtaLAB Synergy R, $\omega$ |
| $\theta_{max}$, completeness: | 75.1°, >99% |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 9426, 2698, 0.022 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs}$ > 2 σ($I_{obs}$), 2450 |
| $N(param)_{refined}$: | 174 |
| Programs: | CrysAlis$^{PRO}$ [1], SHELX [2, 3], Olex2 [4] |

## Source of material

4-(Dimethylamino)benzaldehyde (1.49 g, 0.01 mol) was dissolved in 15 ml ethanol at room temperature, aminoguanidine nitrate (1.37 g, 0.01 mol) was put into the aqueous ethanol (10 ml water and 8 ml ethanol), heated at 60° centigrade, and stirred for 8 h, then cooled down to room temperature, finally we obtained the colorless transparent crystal.

## Experimental details

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

## Comment

Guanidine compounds, as an organic base and nitrogen-containing heterocyclic ligands, have been the research focus of chemistry [5], medicine [6] and materials science [7]. Because of their insensitivity and low flame temperature, high energy materials containing guanidine compounds can make significant contributions in the field of emerging propulsion technology [8]. More than 20 years ago, Tadao Taguchi et al. have synthesized aminoguanidine Schiff base from guanidine and pyrrolaldehyde, which has important biological toxicological significance [9]. In order to explore

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

| Atom | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | −0.05663 (16) | 0.82525 (8) | 0.17718 (11) | 0.0485 (3) |
| O2 | 0.1338 (2) | 0.75088 (12) | 0.30474 (14) | 0.0740 (6) |
| O3 | 0.19151 (18) | 0.77955 (8) | 0.12752 (12) | 0.0511 (4) |
| N6 | 0.08941 (19) | 0.78554 (9) | 0.20231 (13) | 0.0433 (4) |
| N1 | 0.4130 (4) | 0.41106 (12) | 0.9114 (2) | 0.0874 (7) |
| N2 | 0.5414 (2) | 0.63944 (7) | 0.48320 (12) | 0.0365 (3) |
| N3 | 0.50076 (18) | 0.68666 (7) | 0.37950 (12) | 0.0356 (3) |
| H3 | 0.38460 (18) | 0.69524 (7) | 0.33897 (12) | 0.0428 (4)* |
| N4 | 0.6058 (2) | 0.76428 (8) | 0.24555 (13) | 0.0409 (4) |
| H4a | 0.4889 (2) | 0.77271 (8) | 0.20653 (13) | 0.0490 (4)* |
| H4b | 0.6968 (2) | 0.78549 (8) | 0.22081 (13) | 0.0490 (4)* |
| N5 | 0.82308 (19) | 0.70476 (8) | 0.40629 (13) | 0.0400 (3) |
| H5a | 0.84588 (19) | 0.67518 (8) | 0.47013 (13) | 0.0480 (4)* |
| H5b | 0.91620 (19) | 0.72539 (8) | 0.38310 (13) | 0.0480 (4)* |
| C1 | 0.2356 (6) | 0.38566 (16) | 0.9365 (3) | 0.1026 (12) |
| H1a | 0.1575 (19) | 0.42840 (18) | 0.943 (3) | 0.1538 (18)* |
| H1b | 0.169 (2) | 0.3538 (13) | 0.8692 (14) | 0.1538 (18)* |
| H1c | 0.2630 (6) | 0.3579 (14) | 1.0138 (14) | 0.1538 (18)* |
| C2 | 0.5905 (6) | 0.38315 (15) | 0.9887 (3) | 0.0955 (11) |
| H2a | 0.6540 (19) | 0.3535 (13) | 0.9385 (6) | 0.1433 (16)* |
| H2b | 0.6705 (17) | 0.42474 (15) | 1.024 (2) | 0.1433 (16)* |
| H2c | 0.5656 (6) | 0.3526 (13) | 1.0546 (15) | 0.1433 (16)* |
| C3 | 0.4114 (4) | 0.45815 (10) | 0.8108 (2) | 0.0634 (6) |
| C4 | 0.2373 (4) | 0.48138 (11) | 0.7309 (2) | 0.0611 (6) |
| H4 | 0.1224 (4) | 0.46415 (11) | 0.7440 (2) | 0.0733 (7)* |
| C5 | 0.2372 (3) | 0.52957 (11) | 0.63359 (19) | 0.0525 (5) |
| H5 | 0.1209 (3) | 0.54447 (11) | 0.58139 (19) | 0.0630 (6)* |
| C6 | 0.4061 (3) | 0.55698 (9) | 0.61038 (16) | 0.0436 (4) |
| C7 | 0.5785 (3) | 0.53392 (10) | 0.68853 (17) | 0.0504 (5) |
| H7 | 0.6929 (3) | 0.55124 (10) | 0.67480 (17) | 0.0604 (6)* |
| C8 | 0.5807 (4) | 0.48495 (11) | 0.78743 (19) | 0.0601 (6) |
| H8 | 0.6972 (4) | 0.46975 (11) | 0.83901 (19) | 0.0721 (7)* |
| C9 | 0.3938 (2) | 0.60792 (9) | 0.50545 (15) | 0.0388 (4) |
| H9 | 0.2744 (2) | 0.61804 (9) | 0.45245 (15) | 0.0465 (5)* |
| C10 | 0.6459 (2) | 0.71842 (8) | 0.34418 (14) | 0.0328 (3) |

the properties of guanidine Schiff base ligands or even its complexes, we have synthesized a new ligand whose crystal structure has not been reported.

Bond lengths and angles in the title guanidinium salt are within normal ranges [10, 11]. The bond length between C9 and N2 is 1.282(2) Å, indicating that the reaction of Schiff base has taken place, and the C=N was also formed.

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

**Research funding:** 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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