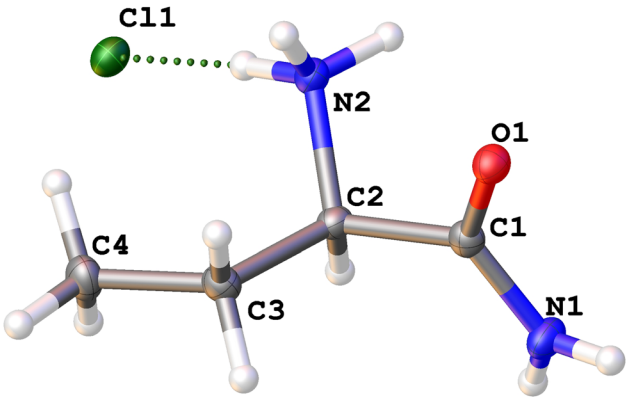
Fengfeng Wang, Lin Luan, Youyou Wang, Xiaowen Hu, Caiyu Zhang and Yang Liu*

The crystal structure of (*R*)-2-aminobutanamide hydrochloride, $C_4H_{11}ClN_2O$



https://doi.org/10.1515/ncrs-2025-0044
Received January 22, 2025; accepted February 17, 2025;
published online March 7, 2025

Abstract

$C_4H_{11}ClN_2O$, orthorhombic, $P2_12_12_1$ (no. 19), a = 4.9699(1) Å, b = 7.5867(2) Å, c = 17.3719(4) Å, V = 655.01(3) Å^3, Z = 4, R_{gt}(F) = 0.0286, wR_{ref}(F^2) = 0.0796, T = 200 K.

CCDC no.: 2411364

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

1 Source of materials

The compound was obtained commercially (Sigma–Aldrich). Crystals suitable for the diffraction test were taken directly from the provided product.

***Corresponding author: Yang Liu**, Institute for Chemical Drug Control, National Institutes for Food and Drug Control, Beijing, 100050 P.R. China, E-mail: yangliu@nifdc.org.cn. https://orcid.org/0000-0001-7714-9194
Fengfeng Wang, Lin Luan, Xiaowen Hu and Caiyu Zhang, Institute for Chemical Drug Control, National Institutes for Food and Drug Control, Beijing, 100050, P.R. China. https://orcid.org/0009-0002-3830-9831 (F. Wang). https://orcid.org/0000-0003-0835-2476 (X. Hu). https://orcid.org/0000-0002-9416-8650 (C. Zhang)
Youyou Wang, Institute for Biological Product Control, National Institutes for Food and Drug Control, Beijing, 100050, P.R. China

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.20 × 0.15 × 0.12 mm
Wavelength:	Cu*K*α radiation (1.54178 Å)
μ:	4.43 mm^{-1}
Diffractometer, scan mode:	Rigaku Synergy, ω scans
θ_{max}, completeness:	75.4°, 100 %
N $(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	2,585, 1,307, 0.022
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1,289
$N(param)_{refined}$:	89
Programs:	CrysAlis^{PRO}[1] Olex2,[2] SHELX[3,4]

2 Experimental details

The positions of hydrogen atoms on carbon atoms were calculated geometrically and refined using the riding model. All the hydrogen atoms on nitrogen atoms were located from difference Fourier map and refined with U_{iso}(H) = 1.5U_{eq}(N). The distance between the hydrogen atoms and the nitrogen atoms were refined freely. A DFIX restrain was used to get a better model for the hydrogen atoms. The absolute structure was established by refinement of the Flack parameter (0.016(12) from 489 selected quotients) using Parsons' method.[5]

3 Comment

The title compound can be used for the synthesis of levetiracetam,[6] and brivaracetam.[7] Despite an extensive search through the Cambridge Structural Database, no reports on the single crystal structure of title compound were identified. The structural analogue, 2-aminobutanoic acid was reported as nitrate,[8] and dihydrogen phosphate.[9–11]

The title compound crystallized in $P2_12_12_1$ space group with one 2-aminobutanamide cation and one chloride anion in its asymmetric unit, forming a 1:1 organic salt. All bond lengths fall in the normal range. The carbon chain exhibits a typical zig-zag-like conformation. The twist angle between C1–C2–C3–C4 is 178.04 (18)°, suggesting that above atoms are nearly coplanar. Protonated amino groups establish hydrogen bonds with two chloride ions and an amide group nearby. H1A atom on the terminal amide group also engages

in hydrogen bonding with a chloride ion, characterized by a DA distance of 3.250 (2) Å.

Conflict of interest: The authors declare no conflicts of interest regarding this article.
Research funding: Institue Building Project Of NIFDC (No.2024HYZX39).
Author contribution: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

References

1. *Rigaku Oxford Diffraction. CrysAlis^{PRO} Software System, Version 1.171.42.92a.;* Rigaku Corporation: Oxford, UK, 2023.
2. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. OLEX2: a Complete Structure Solution, Refinement and Analysis Program. *J. Appl. Crystallogr.* **2009**, *42*, 339–341.
3. Sheldrick, G. M. Crystal Structure Refinement with SHELXL. *Acta Crystallogr.* **2015**, *C71*, 3–8.
4. Sheldrick, G. M. SHELXT – Integrated Space-Group and Crystal-Structure Determination. *Acta Crystallogr.* **2015**, *A71*, 3–8.
5. Parsons, S.; Flack, H. D.; Wagner, T. Use of Intensity Quotients and Differences in Absolute Structure Refinement. *Acta Crystallogr.* **2013**, *B69*, 249–259.
6. Domingo Sanchez, J.; Gómez-Carpintero, J.; González, J. F.; Menéndez, J. C. Twenty-first Century Antiepileptic Drugs. An Overview of Their Targets and Synthetic Approaches. *Eur. J. Med. Chem.* **2024**, *272*, 116476.
7. Manoj, G.; Hanuman, N.; Gyanchander, E.; Bhosale, R. S.; Yadav, J. S. Synthetic Approaches toward the Synthesis of Brivaracetam: An Antiepileptic Drug. *ACS Omega* **2022**, *7*, 2486–2503.
8. Messai, A.; Benali-Cherif, R.; Jeanneau, E.; Benali-Cherif, N. Hydrogen Bonding in 1-carboxypropanaminium Nitrate. *Acta Crystallogr. Sect. E* **2012**, *68*, o1307–o1308.
9. Benali-Cherif, N.; Bendheif, L.; Merazig, H.; Bouchouit, K.; Cherouana, A. Chemical Preparation, Spectroscopic Study and Crystal Structure of DL 2–Ammoniumbutyric Dihydrogenmonophosphate. *Phosphorus, Sulfur Silicon Relat. Elem.* **2002**, *177*, 411–421.
10. Kolev, T.; Spiteller, M.; Sheldrick, W. S.; Mayer–Figge, H. *Acta Crystallogr., Sect. C: Crys. Struct. Commun.* **2006**, *62*, o299.
11. In, Y.; Fujii, M.; Sasada, Y.; Ishida, T. *Acta Crystallogr.* **2001**, *57*, 72.