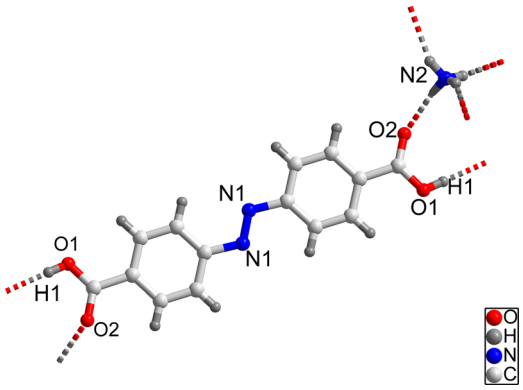
Wang Jian-Ge and Wang Hua-Rui*

The crystal structure of ammonium (E)-4-((4-carboxyphenyl)diazenyl)benzoate, $C_{14}H_{13}N_3O_4$



https://doi.org/10.1515/ncrs-2022-0138
Received March 23, 2022; accepted April 19, 2022;
published online May 5, 2022

Abstract

$C_{14}H_{13}N_3O_4$, monoclinic, *I*2/*a* (no. 15), a = 11.4188(4) Å, b = 3.7968(2) Å, c = 30.2320(18) Å, β = 96.037(6)°, V = 1303.44(11) Å^3, Z = 4, $R_{gt}(F)$ = 0.0656, w$R_{ref}(F^2)$ = 0.2073, T = 293(2) K.

CCDC no.: 2167333

The molecular 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.

Source of material

Azobenzene-4,4′-dicarboxylic acid (0.1 mmol, 27 mg), three drops of concentrated ammonia were added to the mixture of water (3 mL) and methanol (7 mL) in a Teflon-lined stainless steel reactor. The mixture was heated at 373 K for three days, and then slowly cooled down to room temperature. Orange crystals of the title compound were obtained.

Table 1: Data collection and handling.

Crystal:	Orange block
Size:	0.28 × 0.24 × 0.23 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.11 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	28.4°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	21200, 1529, 0.053
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 1324
$N(param)_{refined}$:	96
Programs:	CrysAlis^{PRO} [1], Olex2 [2], SHELX [3, 4]

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
O1	0.44240 (11)	0.0278 (5)	0.46280 (4)	0.0461 (5)
H1[a]	0.4840	−0.0278	0.4855	0.069*
O2	0.61501 (12)	0.1780 (5)	0.44090 (5)	0.0466 (5)
N1	0.30224 (14)	0.2952 (5)	0.25445 (5)	0.0350 (5)
C1	0.44840 (15)	0.1825 (5)	0.38706 (6)	0.0287 (5)
C2	0.33171 (16)	0.0804 (6)	0.37579 (6)	0.0318 (5)
H2	0.2881	−0.0118	0.3974	0.038*
C3	0.28105 (16)	0.1167 (5)	0.33250 (6)	0.0327 (5)
H3	0.2034	0.0477	0.3249	0.039*
C4	0.34623 (16)	0.2567 (5)	0.30019 (6)	0.0297 (5)
C5	0.46176 (16)	0.3651 (5)	0.31145 (6)	0.0335 (5)
H5	0.5049	0.4613	0.2900	0.040*
C6	0.51208 (15)	0.3287 (5)	0.35479 (6)	0.0320 (5)
H6	0.5892	0.4025	0.3625	0.038*
C7	0.50794 (16)	0.1305 (5)	0.43302 (6)	0.0332 (5)
N2	0.7500	0.6115 (8)	0.5000	0.0458 (7)
H2A	0.7183	0.4827	0.4818	0.069*
H2B	0.7132	0.7498	0.5164	0.069*

[a]Occupancy: 0.5.

Experimental details

The crystallographic data of title complex was collected on a SuperNova, EosS2 diffractometer at room temperature.

***Corresponding author: Wang Hua-Rui**, College of Chemistry and Chemical Engineering, and Henan Key Laboratory of Function-Oriented Porous Materials, LuoYang Normal University, Luoyang, Henan 471934, P. R. China, E-mail: wanghrly@126.com. https://orcid.org/0000-0003-4069-3350
Wang Jian-Ge, College of Chemistry and Chemical Engineering, and Henan Key Laboratory of Function-Oriented Porous Materials, LuoYang Normal University, Luoyang, Henan 471934, P. R. China

Using Olex2 [2], the structure was solved with the SHELXT [3] structure solution program using Intrinsic Phasing and refined with the SHELXL [4] refinement package. The H atoms bonded to C atoms were fixed, with C–H distance of 0.93 Å; and/or positioned geometrically in the riding-model approximation, with C–H distance of 0.97 Å; U_{iso}(H) = 1.2U_{eq}(C), U_{iso}(H) = 1.5U_{eq}(N), U_{iso}(H) = 1.5U_{eq}(O). The occupancy of carboxyl hydrogen atom is one-half.

Comment

Hydrogen-bonded organic framework (HOFs) is an interesting porous polymer materials, which can be self-assembled by hydrogen bonding between organic connectors [5, 6]. Compared with other intermolecular forces (such as π–π interaction, electrostatic interaction and van der Waals force), hydrogen bonding has high efficiency, directionality and reversibility [7–9]. HOFs often show high crystallinity, solution processability, easy healing and purification [10–12]. Azobenzene-4,4′- dicarboxylic acid (H_2abd), has two carboxyl groups, which can be completely or partially deprotonated or not deprotonated, as hydrogen bond acceptors or hydrogen bond donors, depending on the number of deprotonated carboxyl groups [13, 14]. Its molecular structure has good planarity and is conducive to the orderly arrangement of azobenzene molecules [15–17]. For these reasons, we decided to use H_2abd to construct novel molecular structure and study the formation conditions of HOFs.

The asymmetric unit of the title compound contains one Habd$^-$ anion and one ammonium ion. In the compound, the Habd$^-$ anions are hydrogen bonded via both O–H/O and N–H/O interactions; the monoanionic carboxylate is involved in strong O–H···O [distance: 2.492 Å, angle: 163.54°] hydrogen bonding involving carboxylate (COO^-) and carboxylic acid (COOH) resulting in a 1D chain, whereas the ammonium ion forms various N–H···O [distance: 2.7746(1)–2.913 Å, angle: 152.60–170.55°] interactions with the carboxylic acid resulting into an overall 2D network. Geometric parameters of the anion are similar to that in H_2abd [18].

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

Research funding: This work was supported by LuoYang Normal University.

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

References

1. Agilent Technologies. CrysAlis^{PRO}. Agilent Technologies; Santa Clara: CA, USA, 2017.
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. *SHELXTL* – integrated space-group and crystal-structure determination. *Acta Crystallogr.* 2015, *A71*, 3–8.
4. Sheldrick G. M. Crystal structure refinement with SHELXL. *Acta Crystallogr.* 2015, *C71*, 3–8.
5. Lin R. B., He Y., Li P., Wang H., Zhou W., Chen B. Multifunctional porous hydrogen-bonded organic framework materials. *Chem. Soc. Rev.* 2019, *48*, 1362–1389.
6. Dang L.-L., Li T.-T., Cui Z., Sui D., Ma L.-F., Jin G.-X. Selective construction and stability studies of molecular trefoil knot and Solomon link. *Dalton Trans.* 2021, *50*, 16984–16989.
7. Song P.-A., Wang H. High-performance polymeric materials through hydrogen-bond cross-linking. *Adv. Mater.* 2020, *32*, 1901244.
8. Qin J.-H., Qin W.-J., Xiao Z., Yang J.-K., Wang H.-R., Yang X.-G., Li D.-S., Ma L.-F. Efficient energy-transfer-induced high photoelectric conversion in a dye-encapsulated ionic pyrene-based metal-organic framework. *Inorg. Chem.* 2021, *60*, 18593–18597.
9. Liu J. Q., Luo Z. D., Ying P., Singh A. K., Trivedi M., Kumar A. Recent developments in luminescent coordination polymers: designing strategies, sensing application and theoretical evidences. *Coord. Chem. Rev.* 2020, *406*, 213145.
10. Yang J., Wang J., Hou B., Huang X., Wang T., Bao Y., Hao H. Porous hydrogen-bonded organic frameworks (HOFs): from design to potential applications. *Chem. Eng. J.* 2020, *399*, 125873.
11. Wang B., Lin R. B., Zhang Z., Xiang S., Chen B. Hydrogen-bonded organic frameworks as a tunable platform for functional materials. *J. Am. Chem. Soc.* 2020, *142*, 14399–14416.
12. Wang H.-R., Yang X.-G., Qin J.-H., Ma L.-F. Long-lived room temperature phosphorescence of organic-inorganic hybrid systems. *Inorg. Chem. Front.* 2021, *8*, 1942–1950.
13. Zhang X.-Y., Ma Q.-Q., Liu X.-F., Niu H.-W., Luo L., Li R.-F., Feng X. A turn-off Eu-MOF@Fe^{2+} sensor for the selective and sensitive fluorescence detection of bromate in wheat flour. *Food Chem.* 2022, *382*, 132379.
14. Lukasik N., Hemine K., Anusiewicz I., Skurski P., Paluszkiewicz E. Photoresponsive amide-based derivatives of azobenzene-4,4'-dicarboxylic acid—experimental and theoretical studies. *Materials* 2021, *14*, 3995.
15. Chen S., Wang C., Yin Y., Chen K. Synthesis of photo-responsive azobenzene molecules with different hydrophobic chain length for controlling foam stability. *RSC Adv.* 2016, *6*, 60138–60144.
16. Xue L., Pan Y., Zhang S., Chen Y., Yu H., Yang Y., Mo L., Sun Z., Li L., Yang H. Fluorescent azobenzene-containing compounds: from structure to mechanism. *Crystals* 2021, *11*, 840.
17. Dutta A., Pan Y., Liu J.-Q., Kumar A. Multicomponent isoreticular metal-organic frameworks: principles, current status and challenges. *Coord. Chem. Rev.* 2021, *445*, 214074.
18. Yu Q.-D., Liu Y.-Y. 4,4'-azinodibenzoic acid. *Acta Crystallogr.* 2009, *E65*, o2326.