Z. Kristallogr. NCS **230** (2015) 243-244 / **DOI** 10.1515/ncrs-2015-0023

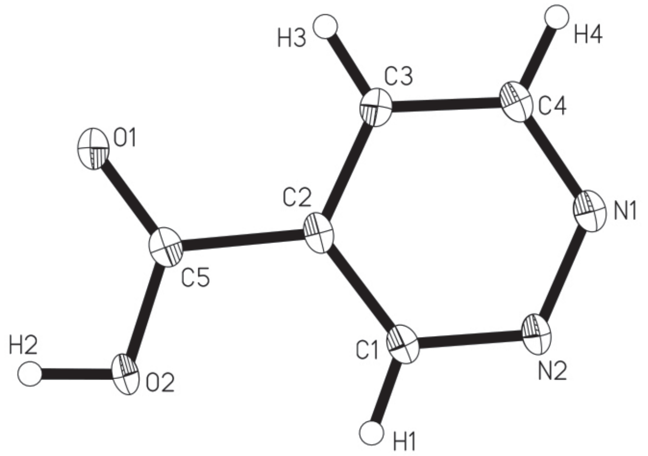
© 2015 Walter de Gruyter GmbH, Berlin/Munich/Boston

Crystal structure of 4-pyridazinecarboxylic acid, $C_5H_4N_2O_2$

Shengjun Deng*, Jie Chen, Yijian Liu and Ning Zhang*

Institute of Applied Chemistry, College of Chemistry, Nanchang University, Nanchang 330031, Jiangxi Province, P. R. China

Received February 09, 2015, accepted July 06, 2015, available online July 27, 2015, CCDC no. 1267/4357



Abstract

$C_5H_4N_2O_2$, orthorhombic, *Pnma* (no. 62), $a = 11.165(2)$ Å, $b = 6.215(1)$ Å, $c = 7.413(2)$ Å, $V = 514.4$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0567$, $wR_{ref}(F^2) = 0.1515$, $T = 153$ K.

Table 1. Data collection and handling.

Crystal:	light yellow blocks, size 0.25×0.28×0.32 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	1.28 cm^{-1}
Diffractometer, scan mode:	SuperNova, Dual, Cu at zero, Eos, ω
$2\theta_{max}$:	51.96°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1793, 553
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 470
$N(param)_{refined}$:	55
Programs:	SHELX [5]

Source of material

4-pyridazinecarboxylic acid (0.0124 g, 0.1 mmol), $Pr(NO_3)_3 \cdot 6H_2O$ (0.0435 g, 0.1 mmol), triethylamine (0.01 mL), and H_2O (8 mL) were added respectively to a 15-mL Teflon-lined steel autoclave, which was sealed and heated to 443 K for 3 days and then cooled to room temperature. The obtained clear solution was evaporated at room temperature. Clear light yellow block-shaped crystals formed over a 1-month period.

Experimental details

All H atoms were located from the difference Fourier map and refined using riding model, with $U_{iso}(H) = 1.2\ U_{eq}(C, N)$.

Discussion

The construction of metal-organic coordination polymers is of current interest in the fields of supramolecular chemistry and crystal engineering [1]. Up to date, metal-organic coordination polymers based on pyridazine derivatives are very rare [2, 3]. The synthesis of title compound is out of the expectation of our original purpose. The asymmetric unit is composed of one half 4-pyridazinecarboxylic acid molecule, located on a mirror plane in the orthorhombic, centrosymmetric space group *Pnma*. All bond lengths are within normal ranges [4]. In the crystal, intermolecular O2–H2···N1 hydrogen bonds link the molecules into infinite chains. The chains are further connected by the weak supramolecular interactions into a 3D supramolecular network.

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{iso}
H(3)	4*c*	−0.0085	¼	0.5082	0.026
H(4)	4*c*	0.0285	¼	0.2006	0.026
H(1)	4*c*	0.3523	¼	0.5689	0.026
H(2)	4*c*	0.2322	¼	0.9939	0.026

* Correspondence author
(e-mail: dshj1028@126.com, nzhang.ncu@163.com)

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	4*c*	0.2818(2)	¼	0.5013(4)	0.028(2)	0.020(2)	0.017(2)	0	−0.002(1)	0
C(2)	4*c*	0.1684(2)	¼	0.5785(4)	0.029(2)	0.015(1)	0.015(2)	0	−0.001(1)	0
C(3)	4*c*	0.0713(2)	¼	0.4658(4)	0.024(2)	0.023(2)	0.019(2)	0	0.003(1)	0
C(4)	4*c*	0.0941(2)	¼	0.2796(4)	0.030(2)	0.024(2)	0.017(2)	0	−0.003(1)	0
C(5)	4*c*	0.1504(2)	¼	0.7812(4)	0.028(2)	0.018(2)	0.019(2)	0	−0.001(1)	0
N(1)	4*c*	0.2039(2)	¼	0.2149(3)	0.031(1)	0.020(1)	0.018(1)	0	−0.0007(9)	0
N(2)	4*c*	0.3004(2)	¼	0.3227(3)	0.030(1)	0.023(1)	0.014(1)	0	0.0005(9)	0
O(1)	4*c*	0.0517(2)	¼	0.8455(3)	0.028(1)	0.044(2)	0.017(1)	0	0.0025(8)	0
O(2)	4*c*	0.2516(2)	¼	0.8715(3)	0.029(1)	0.027(1)	0.012(1)	0	−0.0008(7)	0

Acknowledgments. This work was supported by the National Natural Science Foundations of China (No. 21263014), the Natural Science Foundations of Jiangxi Province (No. 2011ZBAB203013 and 20122BAB203010), and the Foundation of Educational Department of Jiangxi Province (No. GJJ12103).

References

1. Li, M.; Li, D.; O'Keeffe, M.; Yaghi, O. M.: Topological Analysis of Metal-Organic Frameworks with Polytopic Linkers and/or Multiple Building Units and the Minimal Transitivity Principle. Chem. Rev. **114** (2014) 1343–1370.
2. Henry, N.; Costenoble, S.; Lagrenee, M.; Loiseau, T.; Abraham, F.: Lanthanide-based 0D and 2D molecular assemblies with the pyridazine-3,6-dicarboxylate linker. CrystEngComm. **13** (2011) 251–258.
3. Cepeda, J.; Beobide, G.; Castillo, O.; Luque, A.; Pérez-Yáñez, S.; Román, P.: Structure-Directing Effect of Organic Cations in the Assembly of Anionic In(III)/Diazinedicarboxylate Architectures. Cryst. Growth Des. **12** (2012) 1501–1512.
4. Allen, F. H.; Kennard, O.; Watson, D. G.; Brammer, L.; Orpen, A. G.; Taylor, R.: Tables of Bond Lengths determined by X-Ray and Neutron Diffraction. Part I. Bond Lengths in Organic Compounds. J. Chem. Soc. Perkin Trans. (1987) S1-S19.
5. Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. **A64** (2008) 112–122.