Zheng-Jun Liu*, Xiao-Miao Chen, Jing-Song Cheng, Tao-Li Deng and Lan Qin

Crystal structure of poly-[(μ_2 -(carboxylatomethyl)((3-nitrophenyl)sulfonyl)amido- $\kappa^3 N:O:O'$)(μ_2 -4,4'-bipyridine- $\kappa^2 N:N'$) nickel(II)], $C_{18}H_{14}NiN_4O_6S$

Table 1: Data collection and handling.

Crystal:	Green block
Size:	0.26 × 0.25 × 0.21 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.19 mm ⁻¹
Diffractometer, scan mode:	CCD, φ and ω
$\theta_{\max}$, completeness:	28.4°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	17895, 4697, 0.046
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3385
$N(\text{param})_{\text{refined}}$:	271
Programs:	Bruker [1], SHELX [2, 3], Olex2 [4]

<https://doi.org/10.1515/ncrs-2018-0551>

Received December 2, 2018; accepted January 31, 2019; available online February 21, 2019

Abstract

$C_{18}H_{14}NiN_4O_6S$, trigonal, $R\bar{3}$ (no. 148), $a = 31.014(11)$ Å, $b = 31.014(11)$ Å, $c = 10.125(7)$ Å, $V = 8434(8)$ Å³, $Z = 18$, $R_{\text{gt}}(F) = 0.0380$, $wR_{\text{ref}}(F^2) = 0.0941$, $T = 296(2)$ K.

CCDC no.: 1503985

The title crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

To a 20 mL Teflon-lined reaction vessel was added nickel(II) acetate tetrahydrate (124.4 mg, 0.5 mmol), 3-nitrobenzenesulfonylglycine (H_2nbs) (130.1 mg, 0.5 mmol), 4,4'-bipyridine (4,4'-bipy) (78.1 mg, 0.5 mmol) and 15 mL

water. Then the pH of the resulting mixture was adjusted to 7 with 1 mol/L NaOH aqueous solution. After heating at 120 °C for 24 h, the mixture was cooled to room temperature at a rate of 10 °C per hour to give green block crystals.

Experimental details

The structure was solved with the ShelXT [2] structure solution program using intrinsic phasing and refined with the ShelXL [3] refinement package.

Comment

The sulfonylated amino acid has a plurality of coordination sites because it contains both an amino group and a carboxyl group. It can be used to assemble MOFs and CPs [5–8] which have potential applications in gas adsorption and separations [9–11], sensors [12, 13], catalysis [14, 15], and fluorescent materials [16].

In this paper, we report the synthesis and the crystal structure of a new nickel(II) complex with 4,4'-bipyridine (4,4'-bipy) and 3-nitrobenzenesulfonylglycine (H_2nbs). The asymmetric unit is composed of one Ni(II) ion, one nbs ligand and one 4,4'-bipy ligand. The Ni^{2+} ion is five-coordinated by two N atoms (N3, N4) from 4,4'-bipy group, two O atoms (O5, O6) and one N atom (N2) from nbs group (Ni–O, 1.9500(18) ~ 2.0255(17) Å, Ni–N, 2.013(2) ~ 2.168(2) Å). A three-dimensional coordination polymer was formed by Ni–O and Ni–N bonds.

*Corresponding author: Zheng-Jun Liu, Special and Key Laboratory of Functional Materials and Resource chemistry of Guizhou Provincial Education Department, Anshun University, Anshun 561000, P.R. China, e-mail: liuzhengjun_chem@163.com

Xiao-Miao Chen, Jing-Song Cheng, Tao-Li Deng and Lan Qin: Special and Key Laboratory of Functional Materials and Resource Chemistry of Guizhou Provincial Education Department, Anshun University, Anshun 561000, P.R. China

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
Ni1	0.08130(2)	0.38507(2)	0.30183(3)	0.02756(10)
S1	0.18734(2)	0.45589(2)	0.15518(6)	0.03231(15)
O1	0.30621(9)	0.49945(10)	0.5643(3)	0.0795(8)
O2	0.34202(8)	0.57868(9)	0.5889(2)	0.0738(7)
O3	0.20460(6)	0.48022(7)	0.02977(17)	0.0475(5)
O4	0.20257(7)	0.42085(6)	0.1921(2)	0.0483(5)
O5	0.02357(6)	0.40384(6)	−0.02796(16)	0.0347(4)
O6	0.03396(6)	0.37658(6)	0.16340(18)	0.0426(5)
N1	0.31029(9)	0.53977(11)	0.5402(2)	0.0523(6)
N2	0.12992(7)	0.43266(7)	0.16831(19)	0.0337(5)
N3	0.29729(7)	0.39022(8)	0.9094(2)	0.0355(5)
N4	0.12869(7)	0.39010(7)	0.44477(19)	0.0321(4)
C1	0.27523(9)	0.54153(10)	0.4478(2)	0.0382(6)
C2	0.26979(11)	0.58229(11)	0.4457(3)	0.0540(8)
H2	0.287904	0.608859	0.502744	0.065*
C3	0.23679(13)	0.58319(12)	0.3571(4)	0.0694(10)
H3	0.232237	0.610637	0.355221	0.083*
C4	0.21033(11)	0.54449(10)	0.2712(3)	0.0500(7)
H4	0.188198	0.545817	0.211622	0.060*
C5	0.21684(8)	0.50364(9)	0.2741(2)	0.0316(5)
C6	0.24906(8)	0.50160(9)	0.3649(2)	0.0349(6)
H6	0.252952	0.473796	0.369855	0.042*
C7	0.10423(9)	0.44162(11)	0.0608(3)	0.0458(7)
H7A	0.118012	0.439278	−0.023119	0.055*
H7B	0.108962	0.474891	0.068488	0.055*
C8	0.05012(8)	0.40429(8)	0.0654(2)	0.0278(5)
C9	0.29295(10)	0.37192(10)	0.7890(3)	0.0455(7)
H9	0.312951	0.358632	0.765952	0.055*
C10	0.26046(10)	0.37155(10)	0.6965(3)	0.0455(7)
H10	0.258981	0.358804	0.612450	0.055*
C11	0.22997(9)	0.39044(9)	0.7304(2)	0.0335(5)
C12	0.23376(10)	0.40843(11)	0.8551(3)	0.0448(7)
H12	0.213720	0.421264	0.881758	0.054*
C13	0.26746(10)	0.40744(11)	0.9411(3)	0.0446(7)
H13	0.269361	0.419559	1.026188	0.054*
C14	0.19494(9)	0.39122(9)	0.6324(2)	0.0319(5)
C15	0.18187(9)	0.42784(10)	0.6293(3)	0.0397(6)
H15	0.194955	0.453482	0.691006	0.048*
C16	0.14956(9)	0.42597(9)	0.5346(3)	0.0375(6)
H16	0.141732	0.451267	0.533027	0.045*
C17	0.14134(9)	0.35504(9)	0.4487(2)	0.0374(6)
H17	0.127091	0.329374	0.387226	0.045*
C18	0.17387(9)	0.35459(9)	0.5374(3)	0.0380(6)
H18	0.181986	0.329515	0.534166	0.046*

Acknowledgements: The project was supported by Key Project of Guizhou Provincial Education Department (KY[2015]385), Youth Science and Technology Talents Growth Project of Guizhou Provincial Education Department (KY[2018]329) and Platform Project of Anshun University (2015PT03).

References

1. BRUKER. SAINT, APEX2 and SADABS. Bruker AXS Inc., Madison, WI, USA (2009).

2. Sheldrick, G. M.: SHELXT-integrated space-group and crystal-structure determination. *Acta Crystallogr.* **A71** (2015) 3–8.
3. Sheldrick, G. M.: Crystal structure refinement with SHELXL. *Acta Crystallogr.* **C71** (2015) 3–8.
4. 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.* **42** (2009) 339–341.
5. Chen, X.; Liu, Z.; Deng, T.: Crystal structure of poly-{diaqua-bis[(μ₂-3-nitrobenzenesulfonyl)glycine-κ³N:O:O']}(4,4'-bipyridine)manganese(II)]-dimethylformamide (1/1), C₃₉H₃₅Mn₂N₉O₁₅S₂. *Z. Kristallogr. NCS* **233** (2018) 893–895.
6. Liu, Z. J.; Chen, X. M.; Hao, S. Y.; Cheng, M. Q.: Syntheses, crystal structures, and thermal properties of two transition metal complexes with 4-chlorobenzenesulfonyl-glycine acid ligand. *Synth. React. Inorg. Met.-Org. Nano-Met. Chem.* **46** (2016) 529–533.
7. Cheng, M. Q.; Chen, X. M.; Liu, Z. J.; Li, Y. J.: Crystal structure of ((4-acetamidophenyl)sulfonyl)(carboxylatomethyl) amide-κ²N,O)bis(1,10-phenantroline-κ²N,N') nickel(II) heptahydrate, [Ni(abgly)(phen)₂]-7 H₂O, C₃₄H₄₀N₆NiO₁₂S. *Z. Kristallogr. NCS* **228** (2013) 491–493.
8. Cheng, M. Q.; Chen, X. M.; Liu, Z. J.; Feng, C. Q.: Syntheses, structures, and thermal properties of two new Mn(II) and Ni(II) complexes of 3-nitrobenzenesulfonyl-glycine acid and 4-chlorobenzenesulfonyl-glycine acid ligands. *Synth. React. Inorg. Met.-Org. Nano-Met. Chem.* **44** (2013) 27–32.
9. Alhamami, M.; Doan, H.; Cheng, C.: A review on breathing behaviors of metal-organic-frameworks (MOFs) for gas adsorption. *Materials* **7** (2014) 3198–3250.
10. Wang, Z.; Sezen, H.; Liu, J.; Yang, C.; Roggenbuck, S. E.; Peikert, K.; Fröba, M.; Mavrandonakis, A.; Supronowicz, B.; Heine, T.; Gliemann, H.; Wöll, C.: Tunable coordinative defects in UHM-3 surface-mounted MOFs for gas adsorption and separation: a combined experimental and theoretical study. *Mesoporous Mater.* **207** (2015) 53–60.
11. Adil, K.; Belmabkhout, Y.; Pillai, R. S.: Gas/vapour separation using ultra-microporous metal–organic frameworks: insights into the structure/separation relationship. *Chem. Soc. Rev.* **46** (2017) 3402–3430.
12. Schönfeld, F.; Meyer, L. V.; Mühlbach, F.; Zottnick, S. H.; Müller-Buschbaum, K.: Optical isotherms as a fundamental characterization method for gas sensing with luminescent MOFs by comparison of open and dense frameworks. *J. Mater. Chem. C* **6** (2018) 2588–2595.
13. Wu, Y.; Xu, G.; Dong, W.; Zhao, J.; Li, D.-S.; Zhang, J.; Bu, X.: Anionic lanthanide MOFs as a platform for iron-selective sensing, systematic color tuning, and efficient nanoparticle catalysis. *Inorg. Chem.* **56** (2017) 1402–1411.
14. Deria, P.; Gómez-Gualdrón, D. A.; Hod, I.: Framework-topology-dependent catalytic activity of zirconium-based (porphinato)zinc(II) MOFs. *J. Am. Chem. Soc.* **138** (2016) 14449–14457.
15. Chen, L.; Xu, Q.: Converting MOFs into amination catalysts. *Science* **358** (2017) 304–305.
16. Chen, C.; Qiu, Q.; Pan, M.; Cao, C.-C.; Zhu, N.-X.; Wang, H.-P.; Jiang, J.-J.; Wei, Z.-W.; Su, C.-Y.: Tunability of fluorescent metal-organic frameworks through dynamic spacer installation with multivariate fluorophores. *Chem. Commun.* **54** (2018) 13666–13669.