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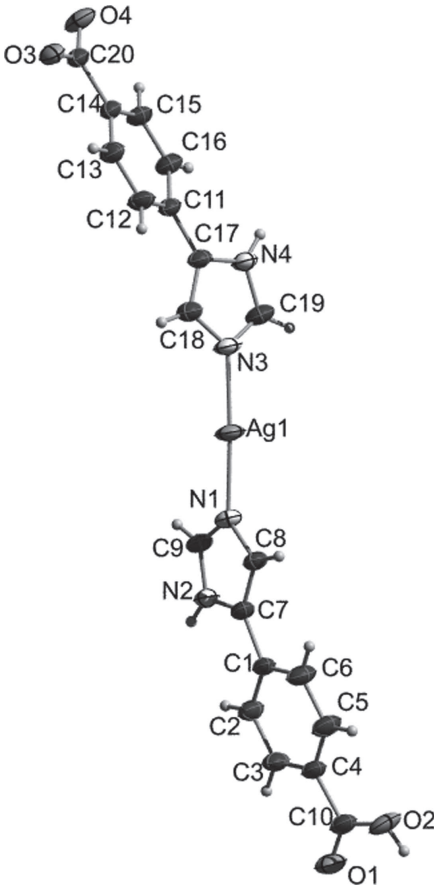
Liang-Quan Sheng*

Crystal structure of (4-(1*H*-imidazol-5-yl)benzoic acid-κ*N*) (4-(1*H*-imidazol-5-yl)benzoato-κ*N*) silver(I), $C_{20}H_{15}N_4O_4Ag$



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Abstract

$C_{20}H_{15}N_4O_4Ag$, monoclinic, $P2_1/n$ (no. 14), $a = 12.6344(8)$ Å, $b = 9.7274(6)$ Å, $c = 15.7567(10)$ Å, $\beta = 109.06(1)°$, $V = 1830.3(2)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0244$, $wR_{ref}(F^2) = 0.0674$, $T = 296(2)$ K.

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***Corresponding author: Liang-Quan Sheng,** Department of Chemistry, Fuyang Normal College, Fuyang, Anhui 236041, China, e-mail: sscfync@163.com

Table 1: Data collection and handling.

Crystal:	Colorless, block, size 0.12×0.15×0.18 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	11.38 cm^{-1}
Diffractometer, scan mode:	Bruker Smart Apex CCD, φ and ω scans
$2\theta_{max}$:	55.1°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	11772, 4196
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 3467
$N(param)_{refined}$:	263
Programs:	SHELX [12], Bruker Software [13]

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(2)	4*e*	0.6661	0.2494	−0.1025	0.0480
H(3)	4*e*	0.7557	0.2702	−0.2081	0.0490
H(5)	4*e*	0.5408	0.5659	−0.3323	0.0520
H(6)	4*e*	0.4540	0.5486	−0.2246	0.0500
H(8)	4*e*	0.3447	0.4982	−0.1315	0.0390
H(9)	4*e*	0.4276	0.2232	0.0600	0.0430
H(12)	4*e*	−0.0343	0.6230	0.2292	0.0450
H(13)	4*e*	−0.1109	0.6798	0.3392	0.0440
H(15)	4*e*	−0.2473	0.3047	0.3203	0.0390
H(16)	4*e*	−0.1714	0.2478	0.2098	0.0390
H(18)	4*e*	0.1016	0.5015	0.1621	0.0440
H(19)	4*e*	−0.0291	0.2232	−0.0221	0.0470
H(2A)	4*e*	0.5699	0.2287	−0.0081	0.0400
H(4)	4*e*	−0.1481	0.2491	0.0664	0.0420
H(2B)	4*e*	0.6800	0.4811	−0.4646	0.0750

The crystal structure is shown in the figure. Tables 1–3 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

All reagents and solvents were used as obtained commercially without further purification. A mixture containing $AgNO_3$ (16 g, 0.1 mmol), 4-(1H-imidazol-5-yl)benzoic acid (HL)

Table 3: Fractional atomic coordinate and displacement parameters (Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ag(1)	4*e*	0.20690(1)	0.37603(2)	0.01126(1)	0.0356(1)	0.0597(1)	0.0473(1)	0.00280(7)	0.03130(8)	0.00458(7)
C(1)	4*e*	0.5485(2)	0.3946(2)	−0.1535(1)	0.0275(9)	0.043(1)	0.0280(8)	−0.0073(8)	0.0166(7)	−0.0040(7)
C(2)	4*e*	0.6404(2)	0.3131(3)	−0.1487(1)	0.036(1)	0.056(1)	0.0335(9)	0.009(1)	0.0201(8)	0.0111(9)
C(3)	4*e*	0.6942(2)	0.3255(3)	−0.2123(1)	0.033(1)	0.057(1)	0.040(1)	0.007(1)	0.0230(9)	0.006(1)
C(4)	4*e*	0.6575(2)	0.4191(2)	−0.2816(1)	0.032(1)	0.044(1)	0.0313(9)	−0.0053(9)	0.0208(8)	−0.0027(8)
C(5)	4*e*	0.5664(2)	0.5023(2)	−0.2860(1)	0.049(1)	0.053(1)	0.039(1)	0.007(1)	0.0294(9)	0.0112(9)
C(6)	4*e*	0.5137(2)	0.4908(2)	−0.2218(1)	0.042(1)	0.050(1)	0.044(1)	0.012(1)	0.0295(9)	0.0100(9)
C(7)	4*e*	0.4832(2)	0.3748(2)	−0.0924(1)	0.0290(9)	0.039(1)	0.0264(8)	−0.0039(8)	0.0155(7)	0.0004(7)
C(8)	4*e*	0.3840(2)	0.4300(2)	−0.0926(1)	0.0298(9)	0.043(1)	0.0317(9)	−0.0001(9)	0.0188(7)	0.0025(8)
C(9)	4*e*	0.4288(2)	0.2797(2)	0.0127(1)	0.035(1)	0.048(1)	0.0332(9)	−0.0043(9)	0.0212(8)	0.0031(8)
C(10)	4*e*	0.7112(2)	0.4214(2)	−0.3533(1)	0.040(1)	0.049(1)	0.036(1)	−0.006(1)	0.0248(9)	−0.0027(9)
C(11)	4*e*	−0.0939(2)	0.4297(2)	0.2083(1)	0.0277(9)	0.040(1)	0.0264(8)	0.0061(8)	0.0153(7)	0.0025(7)
C(12)	4*e*	−0.0769(2)	0.5586(2)	0.2474(1)	0.037(1)	0.046(1)	0.040(1)	−0.0061(9)	0.0256(9)	−0.0005(9)
C(13)	4*e*	−0.1228(2)	0.5926(2)	0.3136(1)	0.038(1)	0.042(1)	0.0353(9)	−0.0043(9)	0.0204(8)	−0.0072(8)
C(14)	4*e*	−0.1864(2)	0.4973(2)	0.3419(1)	0.0280(9)	0.043(1)	0.0230(8)	0.0051(8)	0.0132(7)	0.0011(7)
C(15)	4*e*	−0.2043(2)	0.3688(2)	0.3024(1)	0.037(1)	0.037(1)	0.0308(8)	0.0014(8)	0.0207(8)	0.0041(8)
C(16)	4*e*	−0.1587(2)	0.3346(2)	0.2359(1)	0.038(1)	0.034(1)	0.0330(9)	0.0030(9)	0.0219(8)	0.0011(7)
C(17)	4*e*	−0.0432(2)	0.3923(2)	0.1396(1)	0.0296(9)	0.038(1)	0.0308(8)	0.0056(8)	0.0181(7)	0.0033(7)
C(18)	4*e*	0.0533(2)	0.4354(2)	0.1276(1)	0.033(1)	0.047(1)	0.0367(9)	0.0016(9)	0.0206(8)	0.0009(9)
C(19)	4*e*	−0.0177(2)	0.2826(2)	0.0263(1)	0.042(1)	0.048(1)	0.037(1)	0.002(1)	0.0268(9)	−0.0015(9)
C(20)	4*e*	−0.2348(2)	0.5320(2)	0.4151(1)	0.0288(9)	0.047(1)	0.0243(8)	0.0050(9)	0.0139(7)	0.0007(8)
N(1)	4*e*	0.3507(1)	0.3695(2)	−0.0263(1)	0.0311(8)	0.045(1)	0.0335(8)	−0.0012(7)	0.0208(7)	0.0005(7)
N(2)	4*e*	0.5109(1)	0.2793(2)	−0.0242(1)	0.0288(8)	0.043(1)	0.0340(8)	0.0019(7)	0.0187(6)	0.0050(7)
N(3)	4*e*	0.0686(2)	0.3658(2)	0.0562(1)	0.0346(9)	0.051(1)	0.0408(9)	0.0033(8)	0.0272(7)	0.0032(7)
N(4)	4*e*	−0.0872(1)	0.2945(2)	0.0746(1)	0.0337(8)	0.043(1)	0.0359(8)	−0.0018(8)	0.0226(7)	−0.0010(7)
O(1)	4*e*	0.7947(1)	0.3548(2)	−0.3479(1)	0.0466(9)	0.089(1)	0.0499(9)	0.0132(9)	0.0336(8)	0.0076(8)
O(2)	4*e*	0.6571(1)	0.4977(2)	−0.4227(1)	0.064(1)	0.062(1)	0.0408(8)	0.0099(8)	0.0397(7)	0.0087(7)
O(3)	4*e*	−0.2148(1)	0.6503(2)	0.45001(9)	0.0357(7)	0.053(1)	0.0363(7)	−0.0022(7)	0.0207(6)	−0.0121(6)
O(4)	4*e*	−0.2942(1)	0.4440(2)	0.43549(9)	0.062(1)	0.0507(9)	0.0412(7)	−0.0059(8)	0.0379(7)	−0.0033(7)

(42.2 mg, 0.2 mmol), DMF (*N*:*N*′-dimethylformamide, 1 mL), 10 mL H_2O was sealed in a 16 mL Teflon-lined stainless steel container and heated at 453 K for 72 h. After cooling to room temperature within 12 h, colorless crystals were obtained in 42% yield. Analysis calculated (%): C, 49.71; H, 3.13; N, 11.59%; Found: C, 49.48; H, 3.29; N, 11.38%.

Experimental details

H atoms bonded to C atoms were placed geometrically and treated as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$ for the CH or NH while $U_{iso}(H) = 1.5U_{eq}(O)$ for the OH group.

Discussion

The design and synthesis of metal-organic frameworks (MOFs) have attracted considerable attention because of their potential applications as functional materials as well as their structural diversity and intriguing variety of topologies [1–4]. The organic linkers with N and O donors often have been employed as effective building blocks in the construction of MOFs [5–7]. For example, the N-containing heterocyclic ring ligands including substituted tetrazole, imidazole, benzimidazole, 1,2,4-triazole have been extensively used to construct interesting MOFs [8–10]. On the other hand, carboxylate ligands play an important role in coordination chemistry, which may adopt diverse binding modes such as monodentate, chelating, and bridging configurations. Especially, the designable ligands incorporating multi-N and carboxylate groups may be a useful strategy for construction of novel MOFs [11]. In this paper, we report a silver(I) complex based on the anionic (4-(1*H*-imidazol-5-yl)benzoato-*κ*N) ligand (L-) and the neutral (4-(1*H*-imidazol-5-yl)benzoic acid ligand (HL). The asymmetric unit consists of one Ag(I) atom, and the ligands HL and L-. Both ligands coordinate the AgI as terminal ligands. The monovalent Ag^I ion adopts a linear coordination geometry with two N atoms from two different ligands as shown in the Figure.

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