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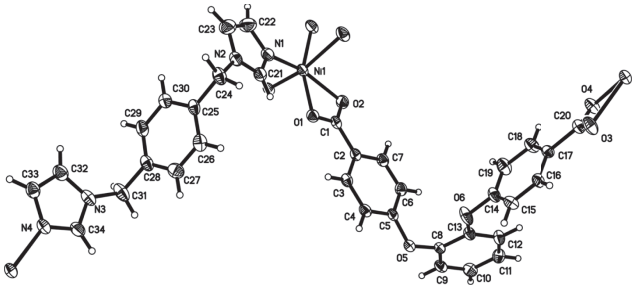
# Crystal structure of poly[($\mu_2$-1,4-bis((1*H*-imidiazol-1-yl)methyl)benzene-$\kappa^2N$:$N'$)-($\mu_2$-4,4′-(1,2-phenylenebis(oxy)dibenzoato-$\kappa^4O$,$O'$:$O''$,$O'''$) nickel(II)], $C_{34}H_{26}O_6N_4Ni$

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## Abstract

$C_{34}H_{26}O_6N_4Ni$, monoclinic, $P2_1/c$, $a = 11.4709(19)$ Å, $b = 13.328(2)$ Å, $c = 20.062(3)$ Å, $\beta = 94.305(3)°$, $V = 3058.5(9)$ Å$^3$, $Z = 4$, $R_{gt}(F) = 0.0393$, $wR_{ref}(F^2) = 0.0868$, $T = 293$ K.

**CCDC no.:** 1434883

## Source of material

The synthesis was performed under hydrothermal conditions. A mixture of $NiCl_2{\cdot}6(H_2O)$, (0.2 mmol, 0.050 g), 4,4′-(1,2-phenylenebis(oxy))dibenzoic acid (0.2 mmol, 0.086 g), NaOH (0.4 mmol, 0.016 g) and $H_2O$ (15 mL) in a 25 mL stainless steel reactor with a Teflon liner was heated from 293 to 433 K in 2 h and a constant temperature was maintained at 433 K for 72 h. After cooling to room temperature, green block crystals were collected in 68% yield based on the added amounts of $NiCl_2{\cdot}6(H_2O)$.

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**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Green, Block, size 0.20×0.21×0.26 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71073 Å) |
| $\mu$: | 6.87 cm$^{-1}$ |
| Diffractometer, scan mode: | Bruker APEXII CCD, $\varphi$ and $\omega$ scans |
| $2\theta_{max}$: | 56.48° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 18815, 7373 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\,\sigma(I_{obs})$, 5012 |
| $N(param)_{refined}$: | 406 |
| Programs: | SHELXTL [8] |

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

| Atom | Site | *x* | *y* | *z* | $U_{iso}$ |
|---|---|---|---|---|---|
| H(3) | 4*e* | 1.0184 | −0.1074 | 0.8783 | 0.047 |
| H(4) | 4*e* | 0.9854 | −0.1781 | 0.9799 | 0.049 |
| H(6) | 4*e* | 0.7253 | 0.0189 | 1.0014 | 0.051 |
| H(7) | 4*e* | 0.7614 | 0.0913 | 0.901 | 0.05 |
| H(9) | 4*e* | 0.8173 | −0.0275 | 1.1668 | 0.053 |
| H(10) | 4*e* | 0.652 | 0.0009 | 1.2239 | 0.061 |
| H(11) | 4*e* | 0.4752 | −0.0655 | 1.1841 | 0.06 |
| H(12) | 4*e* | 0.461 | −0.1616 | 1.0879 | 0.057 |
| H(15) | 4*e* | 0.5585 | −0.3887 | 0.9954 | 0.058 |
| H(16) | 4*e* | 0.3907 | −0.4439 | 0.9357 | 0.053 |
| H(18) | 4*e* | 0.2953 | −0.16 | 0.8971 | 0.059 |
| H(19) | 4*e* | 0.4679 | −0.1042 | 0.9525 | 0.068 |
| H(21) | 4*e* | 1.1056 | −0.0704 | 0.6978 | 0.056 |
| H(22) | 4*e* | 1.0607 | 0.1178 | 0.5497 | 0.082 |
| H(23) | 4*e* | 1.1841 | −0.0182 | 0.5137 | 0.084 |
| H(24A) | 4*e* | 1.2592 | −0.1885 | 0.5674 | 0.064 |
| H(24B) | 4*e* | 1.1934 | −0.2235 | 0.6291 | 0.064 |
| H(26) | 4*e* | 1.3188 | −0.2653 | 0.722 | 0.061 |
| H(27) | 4*e* | 1.4926 | −0.2491 | 0.7881 | 0.065 |
| H(29) | 4*e* | 1.5856 | −0.0212 | 0.6745 | 0.065 |
| H(30) | 4*e* | 1.4147 | −0.04 | 0.607 | 0.063 |
| H(31A) | 4*e* | 1.6929 | −0.0503 | 0.7809 | 0.076 |
| H(31B) | 4*e* | 1.6587 | −0.1398 | 0.8262 | 0.076 |
| H(32) | 4*e* | 1.7953 | −0.126 | 0.6636 | 0.066 |
| H(33) | 4*e* | 1.958 | −0.2443 | 0.6658 | 0.06 |
| H(34) | 4*e* | 1.8125 | −0.2729 | 0.8345 | 0.061 |

**Table 3:** Atomic displacement parameters (Å$^2$).

| Atom | Site | *x* | *y* | *z* | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| C(1) | 4*e* | 0.9152(2) | 0.0475(2) | 0.8137(1) | 0.026(1) | 0.037(1) | 0.049(1) | −0.0035(8) | −0.0033(9) | −0.0020(9) |
| C(2) | 4*e* | 0.8939(2) | 0.0008(1) | 0.8791(1) | 0.028(1) | 0.034(1) | 0.043(1) | −0.0027(8) | −0.0016(8) | −0.0018(9) |
| C(3) | 4*e* | 0.9603(2) | −0.0816(2) | 0.9032(1) | 0.031(1) | 0.041(1) | 0.047(1) | 0.0053(9) | 0.0037(9) | −0.004(1) |
| C(4) | 4*e* | 0.9399(2) | −0.1244(2) | 0.9637(1) | 0.033(1) | 0.037(1) | 0.052(1) | 0.0045(9) | −0.0028(9) | 0.003(1) |
| C(5) | 4*e* | 0.8514(2) | −0.0873(2) | 1.0006(1) | 0.0263(9) | 0.041(1) | 0.041(1) | −0.0047(8) | −0.0039(8) | −0.0018(9) |
| C(6) | 4*e* | 0.7844(2) | −0.0061(2) | 0.9768(1) | 0.036(1) | 0.043(1) | 0.050(1) | 0.0062(9) | 0.0070(9) | −0.001(1) |
| C(7) | 4*e* | 0.8063(2) | 0.0369(2) | 0.9168(1) | 0.035(1) | 0.038(1) | 0.054(1) | 0.0060(9) | 0.0017(9) | 0.002(1) |
| C(8) | 4*e* | 0.7378(2) | −0.1110(2) | 1.0933(1) | 0.029(1) | 0.042(1) | 0.040(1) | −0.0005(9) | −0.0032(8) | 0.0051(9) |
| C(9) | 4*e* | 0.7457(2) | −0.0544(2) | 1.1508(1) | 0.040(1) | 0.045(1) | 0.047(1) | −0.004(1) | −0.010(1) | −0.003(1) |
| C(10) | 4*e* | 0.6469(2) | −0.0374(2) | 1.1850(1) | 0.054(1) | 0.051(1) | 0.048(1) | 0.002(1) | −0.002(1) | −0.010(1) |
| C(11) | 4*e* | 0.5415(2) | −0.0773(2) | 1.1613(1) | 0.046(1) | 0.054(1) | 0.052(1) | 0.001(1) | 0.013(1) | −0.003(1) |
| C(12) | 4*e* | 0.5327(2) | −0.1348(2) | 1.1036(1) | 0.035(1) | 0.054(1) | 0.055(1) | −0.009(1) | 0.004(1) | −0.008(1) |
| C(13) | 4*e* | 0.6307(2) | −0.1521(2) | 1.0698(1) | 0.034(1) | 0.045(1) | 0.042(1) | −0.0034(9) | −0.0012(9) | −0.0071(9) |
| C(14) | 4*e* | 0.5284(2) | −0.2410(2) | 0.9801(1) | 0.032(1) | 0.061(1) | 0.045(1) | −0.004(1) | −0.0014(9) | −0.018(1) |
| C(15) | 4*e* | 0.5061(2) | −0.3428(2) | 0.9752(1) | 0.042(1) | 0.050(1) | 0.050(1) | 0.006(1) | −0.010(1) | −0.001(1) |
| C(16) | 4*e* | 0.4051(2) | −0.3755(2) | 0.9399(1) | 0.044(1) | 0.036(1) | 0.051(1) | −0.000(1) | −0.006(1) | −0.004(1) |
| C(17) | 4*e* | 0.3250(2) | −0.3077(1) | 0.91064(9) | 0.034(1) | 0.037(1) | 0.035(1) | −0.0006(8) | −0.0006(8) | −0.0052(8) |
| C(18) | 4*e* | 0.3487(2) | −0.2062(2) | 0.9162(1) | 0.045(1) | 0.039(1) | 0.061(2) | 0.002(1) | −0.011(1) | −0.005(1) |
| C(19) | 4*e* | 0.4513(2) | −0.1725(2) | 0.9501(1) | 0.052(1) | 0.039(1) | 0.077(2) | −0.008(1) | −0.007(1) | −0.014(1) |
| C(20) | 4*e* | 0.2165(2) | −0.3438(2) | 0.8711(1) | 0.033(1) | 0.041(1) | 0.044(1) | −0.0007(9) | 0.0000(9) | −0.0071(9) |
| C(21) | 4*e* | 1.1092(2) | −0.0400(2) | 0.6563(1) | 0.037(1) | 0.054(1) | 0.048(1) | 0.004(1) | 0.002(1) | −0.002(1) |
| C(22) | 4*e* | 1.0850(2) | 0.0626(2) | 0.5755(1) | 0.075(2) | 0.075(2) | 0.053(2) | 0.019(2) | 0.003(1) | 0.012(1) |
| C(23) | 4*e* | 1.1532(2) | −0.0125(2) | 0.5551(1) | 0.070(2) | 0.093(2) | 0.048(2) | 0.018(2) | 0.008(1) | −0.002(2) |
| C(24) | 4*e* | 1.2390(2) | −0.1694(2) | 0.6118(1) | 0.038(1) | 0.054(1) | 0.068(2) | 0.004(1) | 0.002(1) | −0.019(1) |
| C(25) | 4*e* | 1.3503(2) | −0.1561(2) | 0.6567(1) | 0.031(1) | 0.042(1) | 0.053(1) | 0.0028(9) | 0.0061(9) | −0.012(1) |
| C(26) | 4*e* | 1.3731(2) | −0.2171(2) | 0.7116(1) | 0.046(1) | 0.040(1) | 0.067(2) | −0.002(1) | 0.010(1) | −0.005(1) |
| C(27) | 4*e* | 1.4773(2) | −0.2068(2) | 0.7516(1) | 0.055(1) | 0.047(1) | 0.060(2) | 0.012(1) | −0.002(1) | −0.001(1) |
| C(28) | 4*e* | 1.5580(2) | −0.1342(2) | 0.7375(1) | 0.034(1) | 0.050(1) | 0.058(2) | 0.008(1) | 0.000(1) | −0.013(1) |
| C(29) | 4*e* | 1.5330(2) | −0.0715(2) | 0.6838(1) | 0.034(1) | 0.058(1) | 0.070(2) | −0.009(1) | 0.004(1) | 0.002(1) |
| C(30) | 4*e* | 1.4300(2) | −0.0826(2) | 0.6434(1) | 0.039(1) | 0.064(2) | 0.055(1) | −0.004(1) | 0.002(1) | 0.009(1) |
| C(31) | 4*e* | 1.6713(2) | −0.1206(2) | 0.7807(1) | 0.042(1) | 0.068(2) | 0.077(2) | 0.016(1) | −0.010(1) | −0.025(1) |
| C(32) | 4*e* | 1.8184(2) | −0.1698(2) | 0.6982(1) | 0.048(1) | 0.049(1) | 0.068(2) | 0.005(1) | −0.000(1) | 0.009(1) |
| C(33) | 4*e* | 1.9082(2) | −0.2353(2) | 0.6999(1) | 0.041(1) | 0.043(1) | 0.067(2) | −0.002(1) | 0.005(1) | 0.005(1) |
| C(34) | 4*e* | 1.8291(2) | −0.2514(2) | 0.7922(1) | 0.040(1) | 0.061(2) | 0.049(1) | 0.008(1) | −0.006(1) | −0.005(1) |
| N(1) | 4*e* | 1.0571(2) | 0.0454(1) | 0.63946(9) | 0.038(1) | 0.051(1) | 0.046(1) | 0.0032(8) | −0.0022(8) | −0.0002(9) |
| N(2) | 4*e* | 1.1677(2) | −0.0779(1) | 0.60693(9) | 0.0333(9) | 0.054(1) | 0.048(1) | 0.0020(8) | −0.0014(8) | −0.0082(9) |
| N(3) | 4*e* | 1.7682(2) | −0.1804(1) | 0.7574(1) | 0.037(1) | 0.048(1) | 0.062(1) | 0.0086(8) | −0.0094(9) | −0.0108(9) |
| N(4) | 4*e* | 1.9152(1) | −0.2869(1) | 0.75928(9) | 0.0322(9) | 0.044(1) | 0.052(1) | 0.0008(8) | −0.0050(8) | −0.0033(9) |
| O(1) | 4*e* | 0.9873(1) | 0.0073(1) | 0.77702(7) | 0.0371(8) | 0.0441(8) | 0.0436(8) | 0.0039(6) | 0.0021(6) | −0.0007(7) |
| O(2) | 4*e* | 0.8621(1) | 0.1270(1) | 0.79455(8) | 0.0392(8) | 0.0477(9) | 0.059(1) | 0.0108(7) | 0.0058(7) | 0.0119(7) |
| O(3) | 4*e* | 0.2095(1) | −0.4330(1) | 0.85160(8) | 0.0397(8) | 0.0415(9) | 0.077(1) | −0.0014(7) | −0.0099(8) | −0.0170(8) |
| O(4) | 4*e* | 0.1347(1) | −0.2823(1) | 0.85696(8) | 0.0376(8) | 0.0459(8) | 0.063(1) | 0.0064(7) | −0.0111(7) | −0.0121(7) |
| O(5) | 4*e* | 0.8381(1) | −0.1335(1) | 1.06134(7) | 0.0298(7) | 0.0554(9) | 0.0435(8) | 0.0033(6) | −0.0003(6) | 0.0076(7) |
| O(6) | 4*e* | 0.6339(1) | −0.2113(1) | 1.01313(8) | 0.0319(8) | 0.087(1) | 0.066(1) | −0.0054(8) | −0.0025(7) | −0.037(1) |
| Ni(1) | 4*e* | 0.95763(2) | 0.11701(2) | 0.70466(1) | 0.0282(1) | 0.0387(2) | 0.0474(2) | 0.0008(1) | −0.0033(1) | 0.0033(1) |

## Experimental details

All H atoms were refined using a riding model, with C—H distances of 0.93 Å and $U_{iso}$(H) values of 1.2$U_{eq}$(C) for aromatic hydrogen atoms and those at the imidazole rings and 0.97° A and $U_{iso}$(H) values of 1.2$U_{eq}$(C) for the hydrogen atoms of methylene groups.

## Discussion

Metal-organic-frameworks (MOFs), composed of metal ions (or cluster) as nodes and multitopic organic ligands as linkers have received tremendous attention not only owing to their fascinating structures but also for their potential applications in gas storage, chemical separation, optical sensing/detection, catalysis and drug delivery [1–6]. The structures and properties of such systems depend on the coordination and geometric preferences of both the central metal ions and the bridging building blocks, as well as on the influence of weaker non-covalent interactions, such as hydrogen bonds and π-π stacking interactions [7]. Multidentate ligands containing rich coordination sites (N and/or O donors) are

often employed to produce polymeric networks with a structural diversity owing to their various coordination modes. Recently, we obtained the title compound by the reaction of nickel chloride with 6-(1*H*-Benzoimidazol-2-yl)-pyridine-2-carboxylic acid and 1-(4-((1*H*-imidazol-1-yl)methyl)benzyl)-1*H*-imidazole using hydrothermal method and its crystal structure is reported here.

In the title compound, $Ni(C_{20}H_{12}O_6)(C_{14}H_{14}N_4)$, the Ni(II) atom has an octahedral environment with four O atoms from two 4,4′-(1,2-phenylenebis(oxy))dibenzoate ligands and two N atoms from two neutral 1,4-bis-((1*H*-imidazol-1-yl)methyl)benzene ligands. The Ni—O bond lengths are 2.0709(14) Å, 2.1837(16) Å, 2.2516(15) Å, and 2.0633(14) Å, respectively. And the Ni—N bond lengths are 2.0368(18) Å and 2.0328(17) Å, respectively. The Ni(II) coordination angles are in the normal range from 60.83(5)° to 158.38(6)°. The complex moieties of the title compound are connected into a two-dimensional structure.

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