Supporting Information

Structural, Electrochemical, DNA Binding and Cleavage Properties of Nickel(II) Complex $[Ni(H_2biim)_2(H_2O)_2]^{2+}$ of 2,2'-Biimidazole

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Abstract

Computing details

Data collection: APEX2 (Bruker, 2004); cell refinement: APEX2/SAINT (Bruker, 2004); data reduction: SAINT/XPREP (Bruker, 2004); program(s) used to solve structure: SIR92 (Altornare *et al.*, 1993); program(s) used to refine structure: SHELXL-97 (Sheldrick, 1997); molecular graphics: ORTEP3 (Farrugia, 1997) and Mercury (Bruno *et al.*, 2002); software used to prepare material for publication: SHELXL-97 (Sheldrick, 1997).

References

NOT FOUND

(shelxl)

Crystal data

$C_{12}H_{12}N_8NiO_2{\cdot}2(ClO_4){\cdot}H_2O$	$Z = 2$
$M_r = 575.92$	$F(000) = 584$
Triclinic, $P\bar{1}$	$D_x = 1.686$ Mg m^{-3}
$a = 7.8784$ (4) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 11.1228$ (4) Å	Cell parameters from 5815 reflections
$c = 13.2269$ (6) Å	$\theta = 4.6$–$52.7°$
$\alpha = 84.916$ (2)°	$\mu = 1.16$ mm^{-1}
$\beta = 88.864$ (2)°	$T = 296$ K
$\gamma = 79.305$ (1)°	Block, colorless
$V = 1134.45$ (9) Å^3	0.30 × 0.20 × 0.20 mm

Data collection

Bruker axs kappa apex2 CCD Diffractometer	5471 independent reflections
Radiation source: fine-focus sealed tube	4001 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.023$
ω and ϕ scan	$\theta_{max} = 28.2°$, $\theta_{min} = 1.6°$
Absorption correction: multi-scan SADABS (Bruker, 1999)	$h = -10 \rightarrow 10$
$T_{min} = 0.722$, $T_{max} = 0.801$	$k = -14 \rightarrow 14$
13943 measured reflections	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.065$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.227$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.02$	$w = 1/[\sigma^2(F_o^2) + (0.150P)^2 + 0.933P]$ where $P = (F_o^2 + 2F_c^2)/3$
5471 reflections	$(\Delta/\sigma)_{max} = 0.044$
326 parameters	$\Delta\rangle_{max} = 1.16$ e Å^{-3}
3 restraints	$\Delta\rangle_{min} = -0.72$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni2	1.0000	1.0000	0.5000	0.0449 (2)
Ni1	1.0000	0.5000	0.0000	0.0399 (2)
Cl1	0.77447 (19)	0.90315 (10)	0.16068 (9)	0.0656 (4)
Cl2	0.35791 (15)	0.60809 (10)	0.68055 (9)	0.0592 (3)
O1S	-0.1327 (6)	0.4959 (4)	-0.3038 (3)	0.0781 (11)
N5	0.8085 (5)	1.1091 (3)	0.5813 (3)	0.0519 (8)
N6	0.7349 (6)	1.2796 (4)	0.6547 (3)	0.0626 (10)
H6N6	0.7394	1.3501	0.6754	0.075*
N8	1.0861 (6)	1.3385 (3)	0.5648 (3)	0.0566 (9)
O2	1.1093 (5)	0.9208 (3)	0.6393 (3)	0.0689 (9)
N2	0.8993 (6)	0.8525 (4)	-0.1342 (4)	0.0678 (11)
H2N2	0.9404	0.9189	-0.1452	0.081*
N3	1.1815 (4)	0.6096 (3)	0.0202 (3)	0.0469 (8)
O1	0.8847 (4)	0.5517 (3)	0.1392 (2)	0.0558 (7)
O3	0.9139 (10)	0.9433 (7)	0.1297 (8)	0.185 (4)
N7	1.1125 (5)	1.1563 (3)	0.5076 (3)	0.0521 (8)
C4	1.1367 (6)	0.7218 (4)	-0.0266 (3)	0.0492 (9)
C6	1.3358 (6)	0.6079 (5)	0.0662 (4)	0.0605 (11)
H6	1.3981	0.5413	0.1055	0.073*
N4	1.2543 (6)	0.7897 (4)	-0.0125 (4)	0.0665 (11)
O10	0.3735 (10)	0.5637 (12)	0.7785 (6)	0.237 (6)
C10	0.8530 (6)	1.2134 (4)	0.5995 (3)	0.0496 (9)
C11	0.6049 (7)	1.2148 (5)	0.6726 (5)	0.0710 (14)
H11	0.5035	1.2392	0.7085	0.085*
C12	0.6512 (6)	1.1082 (5)	0.6282 (4)	0.0620 (12)
H12	0.5878	1.0455	0.6292	0.074*
C9	1.0154 (6)	1.2390 (4)	0.5587 (3)	0.0495 (9)
C8	1.2411 (7)	1.3173 (5)	0.5139 (4)	0.0653 (13)
H8	1.3204	1.3697	0.5052	0.078*
C7	1.2556 (7)	1.2056 (4)	0.4791 (4)	0.0605 (11)
H7	1.3482	1.1677	0.4415	0.073*
N1	0.8769 (4)	0.6647 (3)	-0.0795 (3)	0.0463 (7)
C3	0.9750 (6)	0.7502 (4)	-0.0812 (3)	0.0488 (9)
C2	0.7456 (8)	0.8336 (5)	-0.1680 (5)	0.0755 (15)

H2	0.6650	0.8899	-0.2066	0.091*
C1	0.7322 (6)	0.7172 (4)	-0.1347 (4)	0.0593 (11)
H1	0.6401	0.6790	-0.1471	0.071*
C5	1.3841 (7)	0.7185 (6)	0.0457 (5)	0.0759 (15)
H5	1.4846	0.7415	0.0667	0.091*
O4	0.6887 (8)	0.9618 (7)	0.2400 (6)	0.152 (3)
O5	0.7414 (11)	0.7935 (6)	0.1497 (10)	0.210 (5)
O9	0.4491 (12)	0.7032 (8)	0.6665 (7)	0.191 (4)
O8	0.437 (2)	0.5264 (11)	0.6204 (13)	0.308 (8)
O7	0.1892 (9)	0.6430 (10)	0.6601 (9)	0.228 (6)
O6	0.6673 (19)	0.9476 (16)	0.0794 (9)	0.290 (8)
H4N4	1.225 (10)	0.862 (7)	-0.054 (6)	0.11 (3)*
H8N8	1.045 (6)	1.399 (5)	0.604 (4)	0.048 (12)*
H2S	-0.063 (6)	0.476 (5)	-0.255 (3)	0.078 (19)*
H1S	-0.179 (9)	0.571 (3)	-0.303 (6)	0.12 (3)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni2	0.0498 (4)	0.0375 (4)	0.0475 (4)	-0.0083 (3)	-0.0041 (3)	-0.0035 (3)
Ni1	0.0417 (4)	0.0353 (3)	0.0441 (4)	-0.0128 (3)	-0.0013 (3)	0.0014 (3)
Cl1	0.0965 (9)	0.0467 (6)	0.0621 (7)	-0.0335 (6)	-0.0030 (6)	-0.0078 (5)
Cl2	0.0568 (6)	0.0531 (6)	0.0653 (7)	-0.0098 (5)	0.0043 (5)	0.0054 (5)
O1S	0.105 (3)	0.064 (2)	0.067 (2)	-0.011 (2)	-0.017 (2)	-0.0170 (19)
N5	0.055 (2)	0.0447 (18)	0.056 (2)	-0.0093 (15)	-0.0002 (16)	-0.0063 (15)
N6	0.071 (3)	0.051 (2)	0.067 (3)	-0.0064 (18)	0.009 (2)	-0.0185 (18)
N8	0.077 (3)	0.0418 (18)	0.054 (2)	-0.0170 (17)	-0.0067 (19)	-0.0030 (16)
O2	0.086 (2)	0.0586 (19)	0.060 (2)	-0.0091 (17)	-0.0217 (17)	0.0014 (15)
N2	0.075 (3)	0.0439 (19)	0.081 (3)	-0.0136 (18)	-0.001 (2)	0.0161 (19)
N3	0.0444 (17)	0.0430 (17)	0.056 (2)	-0.0165 (14)	-0.0025 (15)	0.0001 (14)
O1	0.0672 (19)	0.0513 (16)	0.0507 (17)	-0.0164 (14)	0.0092 (14)	-0.0046 (13)
O3	0.150 (6)	0.159 (6)	0.288 (10)	-0.107 (5)	0.114 (7)	-0.115 (7)
N7	0.058 (2)	0.0464 (19)	0.054 (2)	-0.0151 (16)	0.0014 (16)	-0.0069 (16)
C4	0.052 (2)	0.043 (2)	0.055 (2)	-0.0191 (17)	0.0037 (18)	-0.0030 (17)
C6	0.052 (2)	0.063 (3)	0.068 (3)	-0.017 (2)	-0.012 (2)	0.002 (2)
N4	0.074 (3)	0.053 (2)	0.080 (3)	-0.033 (2)	0.000 (2)	0.001 (2)
O10	0.145 (5)	0.431 (15)	0.149 (6)	-0.174 (8)	-0.067 (5)	0.162 (8)

C10	0.057 (2)	0.043 (2)	0.048 (2)	-0.0065 (17)	-0.0040 (18)	-0.0025 (16)
C11	0.062 (3)	0.072 (3)	0.080 (4)	-0.010 (2)	0.015 (3)	-0.019 (3)
C12	0.055 (3)	0.060 (3)	0.073 (3)	-0.014 (2)	0.007 (2)	-0.008 (2)
C9	0.058 (2)	0.045 (2)	0.046 (2)	-0.0131 (18)	-0.0065 (18)	-0.0001 (16)
C8	0.073 (3)	0.061 (3)	0.068 (3)	-0.031 (2)	-0.001 (2)	0.000 (2)
C7	0.059 (3)	0.057 (3)	0.069 (3)	-0.021 (2)	0.005 (2)	-0.008 (2)
N1	0.0498 (18)	0.0398 (16)	0.0489 (18)	-0.0101 (14)	-0.0042 (14)	0.0031 (14)
C3	0.056 (2)	0.0367 (18)	0.053 (2)	-0.0097 (16)	0.0043 (18)	0.0038 (16)
C2	0.075 (4)	0.062 (3)	0.081 (4)	-0.001 (3)	-0.009 (3)	0.018 (3)
C1	0.057 (3)	0.057 (2)	0.062 (3)	-0.007 (2)	-0.009 (2)	0.002 (2)
C5	0.065 (3)	0.091 (4)	0.085 (4)	-0.046 (3)	-0.002 (3)	-0.011 (3)
O4	0.115 (4)	0.203 (7)	0.172 (6)	-0.080 (5)	0.035 (4)	-0.113 (6)
O5	0.166 (7)	0.072 (3)	0.409 (15)	-0.047 (4)	0.111 (8)	-0.077 (6)
O9	0.210 (8)	0.213 (8)	0.188 (7)	-0.153 (7)	0.050 (6)	0.003 (6)
O8	0.350 (18)	0.194 (10)	0.40 (2)	-0.028 (11)	0.082 (14)	-0.191 (12)
O7	0.097 (4)	0.268 (11)	0.299 (12)	-0.067 (6)	-0.081 (6)	0.173 (10)
O6	0.292 (14)	0.40 (2)	0.188 (10)	-0.104 (14)	-0.119 (10)	0.045 (12)

Geometric parameters (Å, º)

Ni2—N5	2.096 (4)	N8—C8	1.375 (7)
Ni2—N5^{i}	2.096 (4)	N8—H8N8	0.89 (5)
Ni2—O2^{i}	2.099 (3)	N2—C3	1.328 (6)
Ni2—O2	2.099 (3)	N2—C2	1.357 (8)
Ni2—N7^{i}	2.104 (3)	N2—H2N2	0.8600
Ni2—N7	2.104 (3)	N3—C4	1.332 (5)
Ni1—N3^{ii}	2.079 (3)	N3—C6	1.367 (6)
Ni1—N3	2.079 (3)	N7—C9	1.311 (6)
Ni1—N1	2.107 (3)	N7—C7	1.375 (6)
Ni1—N1^{ii}	2.107 (3)	C4—N4	1.325 (6)
Ni1—O1^{ii}	2.115 (3)	C4—C3	1.446 (6)
Ni1—O1	2.115 (3)	C6—C5	1.358 (7)
Cl1—O3	1.306 (6)	C6—H6	0.9300
Cl1—O5	1.314 (6)	N4—C5	1.374 (8)
Cl1—O4	1.383 (6)	N4—H4N4	0.93 (8)
Cl1—O6	1.378 (11)	C10—C9	1.445 (6)
Cl2—O8	1.322 (10)	C11—C12	1.356 (7)

Cl2—O7	1.340 (6)	C11—H11	0.9300
Cl2—O10	1.344 (6)	C12—H12	0.9300
Cl2—O9	1.383 (6)	C8—C7	1.347 (7)
O1S—H2S	0.844 (19)	C8—H8	0.9300
O1S—H1S	0.85 (2)	C7—H7	0.9300
N5—C10	1.315 (5)	N1—C3	1.330 (5)
N5—C12	1.375 (6)	N1—C1	1.373 (6)
N6—C10	1.325 (6)	C2—C1	1.353 (7)
N6—C11	1.363 (7)	C2—H2	0.9300
N6—H6N6	0.8600	C1—H1	0.9300
N8—C9	1.337 (5)	C5—H5	0.9300
N5—Ni2—N5^{i}	180.00 (16)	C3—N2—C2	107.9 (4)
N5—Ni2—O2^{i}	91.70 (15)	C3—N2—H2N2	126.0
N5^{i}—Ni2—O2^{i}	88.30 (15)	C2—N2—H2N2	126.0
N5—Ni2—O2	88.30 (15)	C4—N3—C6	105.9 (3)
N5^{i}—Ni2—O2	91.71 (15)	C4—N3—Ni1	112.2 (3)
O2^{i}—Ni2—O2	180.0 (3)	C6—N3—Ni1	142.0 (3)
N5—Ni2—N7^{i}	100.26 (14)	C9—N7—C7	105.3 (4)
N5^{i}—Ni2—N7^{i}	79.74 (14)	C9—N7—Ni2	111.6 (3)
O2^{i}—Ni2—N7^{i}	91.81 (14)	C7—N7—Ni2	143.0 (3)
O2—Ni2—N7^{i}	88.18 (14)	N4—C4—N3	111.0 (4)
N5—Ni2—N7	79.74 (14)	N4—C4—C3	131.2 (4)
N5^{i}—Ni2—N7	100.26 (14)	N3—C4—C3	117.9 (3)
O2^{i}—Ni2—N7	88.18 (14)	C5—C6—N3	109.4 (5)
O2—Ni2—N7	91.82 (14)	C5—C6—H6	125.3
N7^{i}—Ni2—N7	180.00 (8)	N3—C6—H6	125.3
N3^{ii}—Ni1—N3	180.0	C4—N4—C5	107.8 (4)
N3^{ii}—Ni1—N1	99.56 (13)	C4—N4—H4N4	107 (5)
N3—Ni1—N1	80.44 (13)	C5—N4—H4N4	144 (5)
N3^{ii}—Ni1—N1^{ii}	80.44 (13)	N5—C10—N6	111.6 (4)
N3—Ni1—N1^{ii}	99.56 (13)	N5—C10—C9	118.2 (4)
N1—Ni1—N1^{ii}	180.0	N6—C10—C9	130.2 (4)
N3^{ii}—Ni1—O1^{ii}	88.68 (13)	C12—C11—N6	107.1 (4)
N3—Ni1—O1^{ii}	91.32 (13)	C12—C11—H11	126.4
N1—Ni1—O1^{ii}	87.63 (13)	N6—C11—H11	126.4

N1^{ii}—Ni1—O1^{ii}	92.37 (13)	C11—C12—N5	108.1 (4)
N3^{ii}—Ni1—O1	91.32 (13)	C11—C12—H12	126.0
N3—Ni1—O1	88.68 (13)	N5—C12—H12	126.0
N1—Ni1—O1	92.37 (13)	N7—C9—N8	112.2 (4)
N1^{ii}—Ni1—O1	87.63 (13)	N7—C9—C10	118.5 (4)
O1^{ii}—Ni1—O1	180.000 (1)	N8—C9—C10	129.2 (4)
O3—Cl1—O5	125.8 (4)	C7—C8—N8	106.6 (4)
O3—Cl1—O4	114.8 (4)	C7—C8—H8	126.7
O5—Cl1—O4	115.2 (5)	N8—C8—H8	126.7
O3—Cl1—O6	100.0 (8)	C8—C7—N7	109.5 (5)
O5—Cl1—O6	88.2 (8)	C8—C7—H7	125.3
O4—Cl1—O6	102.7 (8)	N7—C7—H7	125.3
O8—Cl2—O7	112.9 (10)	C3—N1—C1	105.9 (4)
O8—Cl2—O10	111.1 (10)	C3—N1—Ni1	110.9 (3)
O7—Cl2—O10	107.9 (5)	C1—N1—Ni1	143.1 (3)
O8—Cl2—O9	103.7 (8)	N2—C3—N1	110.6 (4)
O7—Cl2—O9	113.4 (6)	N2—C3—C4	130.8 (4)
O10—Cl2—O9	107.8 (6)	N1—C3—C4	118.5 (3)
H2S—O1S—H1S	110 (4)	C1—C2—N2	106.8 (5)
C10—N5—C12	106.1 (4)	C1—C2—H2	126.6
C10—N5—Ni2	111.9 (3)	N2—C2—H2	126.6
C12—N5—Ni2	141.9 (3)	C2—C1—N1	108.7 (5)
C10—N6—C11	107.0 (4)	C2—C1—H1	125.6
C10—N6—H6N6	126.5	N1—C1—H1	125.6
C11—N6—H6N6	126.5	C6—C5—N4	106.0 (4)
C9—N8—C8	106.3 (4)	C6—C5—H5	127.0
C9—N8—H8N8	124 (3)	N4—C5—H5	127.0
C8—N8—H8N8	129 (3)		

Symmetry codes: (i) -*x*+2, -*y*+2, -*z*+1; (ii) -*x*+2, -*y*+1, -*z*.