

**Appendix A. Supplementary material**

CCDC 1056388-1056391 (**1-4**) and 1402098 (**5**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* [www.ccdc.cam.ac.uk/data\\_request/cif](http://www.ccdc.cam.ac.uk/data_request/cif). Supplementary data associated with this article can be found, in the online version.

**Table S1.** Selected Bond Lengths (Å) and Angles (deg) for **1-4**.**Compound 1**

Cr(1)—O(1)	2.006(2)	O(3)—Cr(1)—O(1)	157.03(8)
Cr(1)—O(3)	1.9841(19)	O(3)—Cr(1)—O(6)	90.04(8)
Cr(1)—O(6)	2.001(2)	O(6)—Cr(1)—O(1)	93.88(8)
Cr(1)—O(8)	2.013(2)	N(2)—Cr(1)—O(8)	78.04(9)
Cr(1)—N(1)	1.967(2)	N(2)—Cr(1)—N(1)	177.53(10)
Cr(1)—N(2)	1.969(2)	C(1)—O(1)—Cr(1)	117.77(18)
O(1)—C(1)	1.286(3)	C(7)—O(3)—Cr(1)	117.90(17)
O(2)—C(1)	1.236(3)	N(1)—Cr(1)—O(1)	78.12(9)
O(3)—C(7)	1.300(3)	N(1)—Cr(1)—O(3)	78.91(9)
O(4)—C(7)	1.222(3)	C(2)—N(1)—C(6)	121.9(2)
O(5)—C(4)	1.324(3)	C(6)—N(1)—Cr(1)	118.52(18)

**Compound 2**

Cr(1)—O(1)	1.997(3)	O(3)—Cr(1)—O(1)	157.57(12)
Cr(1)—O(3)	1.988(3)	O(6)—Cr(1)—O(1)	91.72(12)
Cr(1)—O(6)	1.97(3)	O(6)—Cr(1)—O(3)	91.67(10)
Cr(1)—O(8)	1.986(3)	O(6)—Cr(1)—O(8)	158.32(12)
Cr(1)—N(1)	1.964(3)	N(1)—Cr(1)—O(1)	78.52(12)
Cr(1)—N(2)	1.955(3)	N(1)—Cr(1)—O(3)	79.07(12)
O(1)—C(1)	1.289(5)	N(1)—Cr(1)—O(6)	100.74(12)
O(2)—C(1)	1.225(5)	N(1)—Cr(1)—O(8)	100.92(12)
O(3)—C(7)	1.298(4)	C(1)—O(1)—Cr(1)	118.3(2)
O(4)—C(7)	1.226(5)	C(7)—O(3)—Cr(1)	117.5(2)
O(5)—C(4)	1.332(5)	C(8)—O(6)—Cr(1)	117.3(2)

**Compound 3**

Co(1)—O(7)	2.0163 (14)	O(7)—Co(1)—N(1)	173.50 (6)
Co(1)—N(1)	2.0268 (16)	O(7)—Co(1)—O(8)	85.68 (6)
Co(1)—O(8)	2.1244 (17)	N(1)—Co(1)—O(8)	93.22 (6)
Co(1)—O(6)	2.1312 (15)	O(7)—Co(1)—O(6)	86.06 (6)
Co(1)—O(1)A	2.160 (4)	N(1)—Co(1)—O(6)	95.49 (6)
Co(1)—O(1)	2.1596 (19)	O(8)—Co(1)—O(6)	170.56 (6)
Co(1)—O(3)	2.1988 (15)		
O(1)—C(1)	1.273 (9)	O(7)—Co(1)—O(1)A	98.5 (7)
O(2)—C(1)	1.248 (3)	N(1)—Co(1)—O(1)A	75.1 (8)
O(3)—C(7)	1.278 (2)	O(8)—Co(1)—O(1)A	91 (4)
O(4)—C(7)	1.237 (3)	O(6)—Co(1)—O(1)A	95(4)

**Compound 4**

Ni(1)—N(1)	1.964 (2)	N(1)—Ni(1)—O(7)	176.40 (9)
Ni(1)—O(7)	2.010 (2)	N(1)—Ni(1)—O(6)	95.17 (9)
Ni(1)—O(6)	2.079 (2)	O(7)—Ni(1)—O(6)	85.76 (9)
Ni(1)—O(8)	2.081 (2)	N(1)—Ni(1)—O(8)	95.05 (9)
Ni(1)—O(1)A	2.121 (2)	O(7)—Ni(1)—O(8)	86.210 (9)
Ni(1)—O(1)	2.121 (2)	O(6)—Ni(1)—O(8)	171.20 (9)
Ni(1)—O(3)	2.190 (2)	N(1)—Ni(1)—O(1)	79.0 (3)
O(3)—C(7)	1.281 (3)	O(7)—Ni(1)—O(1)	97.6 (3)

O(2)—C(1)	1.248 (4)	O(6)—Ni(1)—O(1)	90.7(2)
O(3)—C(7)	1.281 (3)	O(8)—Ni(1)—O(1)	94.07 (2)
O(4)—C(7)	1.240 (3)	N(1)—Ni(1)—O(3)	76.64 (8)

**Table S2.** Selected Hydrogen-bond geometry (Å, °) **1-4**

**Compound 1**

DHA<D—H...A	d(D—H)	d(H...A)	d(D...A)	d(D—H...A)
O(5)—H(5A)···O(28) <sup>a</sup>	0.84	1.74	2.574(3)	172
O(10)—H(10A)···O(14) <sup>b</sup>	0.84	1.77	2.599(3)	168
O(15)—H(15A)···O(26) <sup>c</sup>	0.84	1.73	2.557(3)	168
O(20)—H(20A)···O(22) <sup>d</sup>	0.84	1.67	2.509(3)	176
N(5)—H(5N)···O(25) <sup>b</sup>	0.91	1.86	2.768(5)	177
N(7)—H(7N)···O(23) <sup>e</sup>	0.91	1.80	2.666(6)	159
O(21)—H(21A)···O(19) <sup>g</sup>	0.84	1.93	2.766(3)	174
O(21)—H(21B)O(9)	0.84	1.87	2.696(3)	170
O(22)—H(22A)···O(4)	0.84	1.89	2.708(3)	164
O(22)—H(22B)···O(21) <sup>b</sup>	0.84	1.84	2.672(3)	170
O(23)—H(23A)···O(21) <sup>f</sup>	0.84	1.92	2.761(5)	175
O(23)—H(23B)···O(17) <sup>h</sup>	0.84	2.19	2.903(6)	143
O(24)—H(24A)···O(9) <sup>f</sup>	0.84	2.11	2.897(6)	156
O(24)—H(24B)···O(13) <sup>h</sup>	0.84	2.03	2.861(6)	172
O(25)—H(25A)···O(16) <sup>h</sup>	0.84	2.11	2.944(4)	172

**Compound 2**

O(5)—H(5O)···O(12)	0.84	1.80	2.625(4)	166
O(10)—H(10O)···O(11) <sup>a</sup>	0.84	1.83	2.613(4)	154
N(5)—H(5A)···O(1) <sup>b</sup>	0.91	2.04	2.881(4)	153
N(5)—H(5B)···N(7) <sup>c</sup>	0.91	2.14	3.046(5)	170
N(6)—H(6N)···O(13)	0.91	2.11	2.698(5)	166
N(8)—H(8A)···O(8) <sup>d</sup>	0.91	2.11	2.893(4)	144
N(8)—H(8B)···N(4) <sup>e</sup>	0.91	2.03	2.933(5)	172
O(11)—H(11A)···O(4) <sup>f</sup>	0.84	2.14	2.904(4)	157

**Compound 3**

O(5)—H(5A)···O(3) <sup>a</sup>	0.84	1.80	2.632 (2)	170
O(6)—H(6B)···O(4) <sup>b</sup>	0.84	2.02	2.823 (2)	160
O(6)—H(6B)···O(9) <sup>c</sup>	0.84	2.03	2.846 (2)	165
O(7)—H(7B)···O(1) <sup>d</sup>	0.84	1.91	2.710 (14)	160
O(8)—H(8A)···O(9) <sup>d</sup>	0.84	1.95	2.782 (14)	169
O(8)—H(8B)···O(4) <sup>e</sup>	0.84	1.90	2.708 (2)	162
C(3)—H(3)···O(7) <sup>a</sup>	0.95	2.62	3.519 (2)	1586
O(9)—H(9A)···O(2) <sup>c</sup>	0.84	2.28	2.882 (2)	129

**Compound 4**

O(9)—H(9B)···O(2) <sup>a</sup>	0.84	2.08	2.898 (4)	163
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O(9)—H(9)A···O(2)	0.84	1.90	2.717 (4)	166
O(8)—H(8B)···O(4) <sup>b</sup>	0.84	2.04	2.836 (3)	157
O(8)—H(8A)···O(9) <sup>a</sup>	0.84	2.02	2.830 (3)	161
O(7)—H(7A)···O(1) <sup>c</sup>	0.84	1.94	2.756 (10)	164
O(6)—H(6B)···O(9) <sup>c</sup>	0.84	1.96	2.797 (3)	170
O(6)—H(6A)···O(4) <sup>d</sup>	0.84	1.88	2.699 (3)	165
O(5)—H(5A)···O(3) <sup>e</sup>	0.84	1.80	2.619 (3)	166

Footnotes indicating symmetry operations for Table S2.

**Compound 1:** <sup>a</sup>x,y,-1+z; <sup>b</sup>x,1+y,z; <sup>c</sup>x,-1+y,z; <sup>d</sup>x,-1+y,1+z; <sup>e</sup>x,1+y,1+z; <sup>f</sup>1+x,y,z; <sup>g</sup>-x,-1-y,1-z; <sup>h</sup>1-x,-y,1-z.

**Compound 2:** <sup>a</sup>1+x,y,1+z; <sup>b</sup>-0.5+x,1.5-y,-1+z; <sup>c</sup>x,1+y,-1+z; <sup>d</sup>x,-1+y,z; <sup>e</sup>x,-1+y,1+z; <sup>f</sup>-0.5+x,0.5-y,-1+z.

**Compound 3:** <sup>a</sup>0.5+x,0.5+y,z; <sup>b</sup>1-x,1-y,1-z; <sup>c</sup>1.5-x,-0.5+y,0.5-z; <sup>d</sup>1-x,y,0.5-z; <sup>e</sup>1-x,2-y,1-z.

**Compound 4:** <sup>a</sup>0.5-x,0.5-y,1.5-z; <sup>b</sup>1-x,1-y,1-z; <sup>c</sup>1-x,y,1.5-z; <sup>d</sup>1-x,-y,1-z; <sup>e</sup>-0.5+x,-0.5+y,z.