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Interaction of cobalt(II) and nickel(II) with a γ -linked, bis- β -diketone ligand to yield an unusual coordination motif

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Table 1S. Pertinent Geometry Details (bond lengths in Å, angles in °) for [CoL(H₂O)₂].H₂O and [NiL(H₂O)₂].H₂O (LH₂ = 2)

[CoL(H ₂ O) ₂].H ₂ O		[NiL(H ₂ O) ₂].H ₂ O	
Co(1)-O(1)	2.0330(9)	Ni(1)-O(1)	2.0235(9)
Co(1)-O(3)	2.0723(9)	Ni(1)-O(3)	2.0549(10)
Co(1)-S(1)	2.4810(5)	Ni(1)-S(1)	2.4074(5)
O(1)-Co(1)-O(3)	100.92(4)	O(1)-Ni(1)-O(3)	96.84(4)
O(1)-Co(1)-O(1 ¹)	165.58(5)	O(1)-Ni(1)-O(1 ¹)	173.65(5)
O(1)-Co(1)-O(3 ¹)	89.53(4)	O(1)-Ni(1)-O(3 ¹)	87.76(4)
O(1)-Co(1)-S(1)	79.55(3)	O(1)-Ni(1)-S(1)	82.07(3)
O(1)-Co(1)-S(1 ¹)	90.18(3)	O(1)-Ni(1)-S(1 ¹)	93.46(3)
O(3)-Co(1)-O(3 ¹)	87.62(6)	O(3)-Ni(1)-O(3 ¹)	87.46(6)
O(3)-Co(1)-S(1)	92.48(3)	O(3)-Ni(1)-S(1)	91.73(3)
O(3)-Co(1)-S(1 ¹)	168.90(3)	O(3)-Ni(1)-S(1 ¹)	169.63(3)
S(1)-Co(1)-S(1 ¹)	89.55(2)	S(1)-Ni(1)-S(1 ¹)	90.89(2)
symmetry operator: $-x + 1, y, -z + \frac{1}{2}$			

Table 2S. Hydrogen Bond Parameters (distances in Å, angles in °) for [CoL(H₂O)₂] \cdot H₂O and [NiL(H₂O)₂] \cdot H₂O (LH₂ = 2)

compound 1	atoms	distance	distance	distance	angle
	D-H \cdots A	D-H	H \cdots A	D \cdots A	DHA
	O(3)-H(3O) \cdots O(4)	0.77(2)	1.99(2)	2.735(2)	163(2)
	O(3)-H(3OB) \cdots O(2 ²)	0.85(2)	1.79(2)	2.627(1)	173(2)
	O(4)-H(4O) \cdots O(1 ³)	0.76(2)	2.15(2)	2.878(2)	160(2)
symmetry operators: ² ; $-x + 3/2, -y + 1/2, -z + 1.$ ³ ; $x, -y, z - 1/2$					
compound 2	D-H \cdots A	D-H	H \cdots A	D \cdots A	DHA
	O(3)-H(3OB) \cdots O(4)	0.77(2)	2.00(2)	2.734(2)	160(2)
	O(3)-H(3O) \cdots O(2 ²)	0.81(2)	1.83(2)	2.639(1)	172(2)
	O(4)-H(4O) \cdots O(1 ³)	0.76(2)	2.13(2)	2.854(1)	158(2)
symmetry operators: ² ; $-x + 1/2, -y + 1/2, -z.$ ³ ; $-x + 1, -y, -z.$					

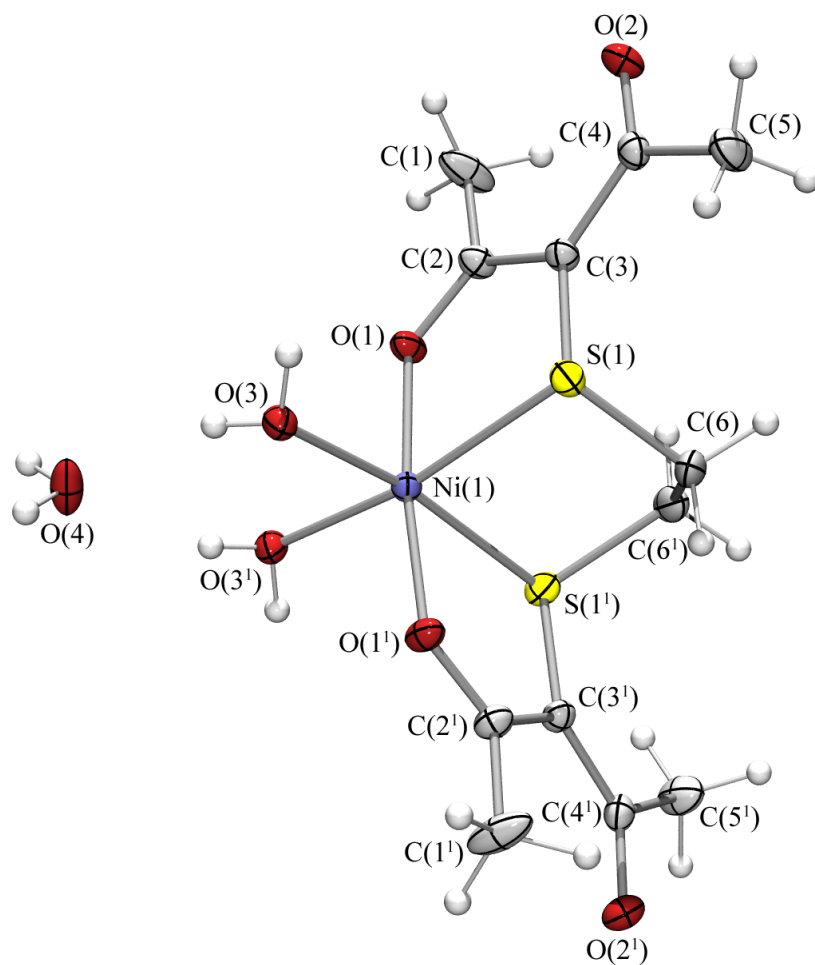


Figure 1S. ORTEP representation of [NiL(H₂O)₂]·H₂O (LH₂ = 2) with ellipsoids drawn at the 50% probability level. Symmetry code ¹; $-x + 1, y, -z + 1/2$.