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Table S25. Crystal data and structure refinement [Co(I) (L(0))₂]⁺.

Identification code	ST3339
Empirical formula	C ₄₆ H ₄₆ Co F ₆ N ₆ O ₄ P
Formula weight	950.79
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$\bar{P}1$
Unit cell dimensions	a = 13.142(3) Å alpha = 111.50(3) deg. b = 14.080(3) Å beta = 102.85(3) deg. c = 14.752(3) Å gamma = 110.04(3) deg.
Volume	2188.7(8) Å ³
Z	2
Density (calculated)	1.443 Mg/m ³
Absorption coefficient	0.506 mm ⁻¹
F(000)	984
Crystal size	0.3 x 0.3 x 0.3 mm
Theta range for data collection	2.36 to 24.00 deg.
Index ranges	-18 ≤ h ≤ 13, -20 ≤ k ≤ 14, -19 ≤ l ≤ 21
Reflections collected	8827
Independent reflections	6076 [R(int) = 0.0647]
Absorption correction	Not measured
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	5990 / 0 / 585
Goodness-of-fit on F ²	1.053
Final R indices [I > 2σ(I)]	R1 = 0.0650, wR2 = 0.1533
R indices (all data)	R1 = 0.1170, wR2 = 0.1873
Largest diff. peak and hole	0.472 and -0.362 e.Å ⁻³

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Table S26. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Co}(\text{I})(\text{L}(0))_2]^+$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Co (1)	8440 (1)	5986 (1)	-2311 (1)	30 (1)
O (1)	3973 (3)	6239 (3)	-933 (3)	39 (1)
O (2)	14228 (3)	10483 (3)	976 (3)	39 (1)
O (3)	8692 (4)	7340 (4)	-6339 (3)	47 (1)
O (4)	8269 (4)	871 (4)	-2985 (3)	53 (1)
N (1)	6562 (4)	4939 (4)	-3201 (4)	34 (1)
N (2)	8251 (4)	4705 (4)	-3612 (4)	31 (1)
N (3)	10230 (4)	6386 (4)	-2152 (3)	30 (1)
N (4)	8631 (4)	7447 (4)	-2528 (3)	30 (1)
N (5)	8401 (4)	7080 (4)	-1013 (3)	31 (1)
N (6)	8279 (4)	5138 (4)	-1373 (4)	32 (1)
C (1)	4293 (5)	7435 (5)	-389 (5)	42 (2)
C (2)	4553 (5)	5921 (5)	-1562 (4)	31 (1)
C (3)	5184 (5)	6625 (5)	-1909 (4)	35 (2)
C (4)	5778 (5)	6250 (6)	-2514 (4)	37 (2)
C (5)	5766 (5)	5202 (5)	-2761 (4)	27 (1)
C (6)	5098 (5)	4497 (5)	-2430 (4)	34 (2)
C (7)	4501 (5)	4857 (5)	-1840 (4)	35 (2)
C (8)	6208 (5)	3989 (5)	-4058 (5)	32 (1)
C (9)	4956 (5)	3075 (5)	-4776 (5)	40 (2)
C (10)	7175 (5)	3805 (5)	-4308 (4)	32 (1)
C (11)	7038 (5)	2825 (5)	-5131 (4)	38 (2)
C (12)	8017 (5)	2744 (5)	-5258 (5)	41 (2)
C (13)	9132 (5)	3674 (5)	-4558 (5)	40 (2)
C (14)	9226 (5)	4631 (5)	-3729 (4)	32 (1)
C (15)	10330 (5)	5628 (5)	-2908 (4)	32 (1)
C (16)	11481 (5)	5665 (6)	-2941 (5)	48 (2)
C (17)	11241 (5)	7434 (5)	-1340 (4)	29 (1)
C (18)	11942 (5)	8224 (5)	-1588 (4)	30 (1)
C (19)	12919 (5)	9224 (5)	-801 (4)	32 (1)
C (20)	13223 (5)	9478 (5)	258 (4)	31 (1)
C (21)	12493 (5)	8711 (5)	507 (4)	31 (1)
C (22)	11504 (5)	7722 (5)	-294 (4)	30 (1)
C (23)	14689 (6)	10679 (6)	2023 (5)	48 (2)
C (31)	9479 (6)	8344 (6)	-6325 (5)	55 (2)
C (32)	8751 (5)	7428 (5)	-5366 (5)	34 (2)
C (33)	7835 (5)	6549 (5)	-5385 (5)	33 (1)
C (34)	7838 (5)	6572 (5)	-4439 (4)	32 (1)
C (35)	8705 (5)	7471 (5)	-3472 (4)	31 (1)
C (36)	9637 (5)	8334 (5)	-3466 (5)	35 (2)
C (37)	9656 (5)	8306 (5)	-4409 (5)	37 (2)
C (38)	8640 (5)	8305 (5)	-1768 (4)	32 (1)
C (39)	8653 (6)	9369 (6)	-1798 (5)	44 (2)
C (40)	8485 (5)	8102 (5)	-898 (4)	33 (2)
C (41)	8293 (5)	8810 (6)	-74 (5)	40 (2)
C (42)	7985 (5)	8448 (6)	620 (5)	39 (2)
C (43)	7880 (5)	7393 (6)	493 (4)	40 (2)
C (44)	8095 (5)	6725 (5)	-324 (4)	31 (1)
C (45)	8009 (5)	5582 (5)	-570 (4)	36 (2)
C (46)	7588 (6)	4986 (6)	24 (5)	48 (2)
C (47)	8226 (5)	4016 (5)	-1737 (4)	35 (2)
C (48)	9273 (6)	3946 (6)	-1519 (5)	43 (2)
C (49)	9251 (6)	2881 (6)	-1945 (5)	49 (2)

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C (50)	8175 (6)	1878 (6)	-2602 (5)	43 (2)
C (51)	7138 (6)	1950 (6)	-2788 (5)	44 (2)
C (52)	7168 (5)	3010 (5)	-2351 (5)	41 (2)
C (53)	7267 (7)	-106 (6)	-3846 (5)	58 (2)
P (1)	6517 (2)	9106 (2)	3054 (1)	39 (1)
F (1)	5965 (4)	8329 (3)	3548 (3)	60 (1)
F (2)	6133 (3)	10032 (3)	3691 (3)	57 (1)
F (3)	7051 (4)	9899 (4)	2566 (3)	70 (1)
F (4)	6884 (4)	8204 (4)	2426 (3)	73 (1)
F (5)	7733 (3)	9791 (4)	4057 (3)	64 (1)
F (6)	5279 (4)	8463 (4)	2091 (3)	71 (1)

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Table S27. Bond lengths [Å] and angles [deg] for [Co(I) (L(0))₂]⁺.

Co(1)-N(2)	1.986(5)
Co(1)-N(5)	1.993(5)
Co(1)-N(6)	2.134(5)
Co(1)-N(4)	2.136(5)
Co(1)-N(1)	2.153(5)
Co(1)-N(3)	2.158(4)
O(1)-C(2)	1.373(6)
O(1)-C(1)	1.426(7)
O(2)-C(20)	1.366(7)
O(2)-C(23)	1.409(7)
O(3)-C(32)	1.377(7)
O(3)-C(31)	1.426(7)
O(4)-C(50)	1.381(8)
O(4)-C(53)	1.405(8)
N(1)-C(8)	1.294(7)
N(1)-C(5)	1.431(7)
N(2)-C(10)	1.353(7)
N(2)-C(14)	1.363(7)
N(3)-C(15)	1.300(7)
N(3)-C(17)	1.425(7)
N(4)-C(38)	1.307(7)
N(4)-C(35)	1.428(7)
N(5)-C(40)	1.348(8)
N(5)-C(44)	1.364(7)
N(6)-C(45)	1.310(7)
N(6)-C(47)	1.440(8)
C(2)-C(7)	1.373(8)
C(2)-C(3)	1.388(8)
C(3)-C(4)	1.391(8)
C(4)-C(5)	1.377(8)
C(5)-C(6)	1.393(8)
C(6)-C(7)	1.372(8)
C(8)-C(10)	1.477(7)
C(8)-C(9)	1.504(8)
C(10)-C(11)	1.384(8)
C(11)-C(12)	1.377(8)
C(12)-C(13)	1.396(8)
C(13)-C(14)	1.391(8)
C(14)-C(15)	1.456(8)
C(15)-C(16)	1.508(8)
C(17)-C(22)	1.369(7)
C(17)-C(18)	1.402(8)
C(18)-C(19)	1.371(8)
C(19)-C(20)	1.394(7)
C(20)-C(21)	1.399(8)
C(21)-C(22)	1.376(8)
C(32)-C(37)	1.379(8)
C(32)-C(33)	1.386(8)
C(33)-C(34)	1.383(7)
C(34)-C(35)	1.379(8)
C(35)-C(36)	1.394(8)
C(36)-C(37)	1.383(8)
C(38)-C(40)	1.455(8)
C(38)-C(39)	1.509(9)
C(40)-C(41)	1.399(8)
C(41)-C(42)	1.377(8)
C(42)-C(43)	1.379(9)
C(43)-C(44)	1.385(8)
C(44)-C(45)	1.470(9)

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C(45)-C(46)	1.489(8)
C(47)-C(52)	1.382(8)
C(47)-C(48)	1.388(8)
C(48)-C(49)	1.384(9)
C(49)-C(50)	1.397(9)
C(50)-C(51)	1.376(9)
C(51)-C(52)	1.374(9)
P(1)-F(4)	1.569(4)
P(1)-F(6)	1.582(4)
P(1)-F(5)	1.587(4)
P(1)-F(1)	1.590(4)
P(1)-F(3)	1.593(4)
P(1)-F(2)	1.613(4)

N(2)-Co(1)-N(5)	170.7(2)
N(2)-Co(1)-N(6)	98.4(2)
N(5)-Co(1)-N(6)	75.4(2)
N(2)-Co(1)-N(4)	110.7(2)
N(5)-Co(1)-N(4)	75.4(2)
N(6)-Co(1)-N(4)	150.8(2)
N(2)-Co(1)-N(1)	74.9(2)
N(5)-Co(1)-N(1)	97.7(2)
N(6)-Co(1)-N(1)	87.3(2)
N(4)-Co(1)-N(1)	98.2(2)
N(2)-Co(1)-N(3)	76.2(2)
N(5)-Co(1)-N(3)	111.3(2)
N(6)-Co(1)-N(3)	99.2(2)
N(4)-Co(1)-N(3)	89.8(2)
N(1)-Co(1)-N(3)	151.0(2)
C(2)-O(1)-C(1)	117.3(4)
C(20)-O(2)-C(23)	117.9(5)
C(32)-O(3)-C(31)	116.3(5)
C(50)-O(4)-C(53)	116.0(6)
C(8)-N(1)-C(5)	122.2(5)
C(8)-N(1)-Co(1)	116.8(4)
C(5)-N(1)-Co(1)	120.1(4)
C(10)-N(2)-C(14)	118.4(5)
C(10)-N(2)-Co(1)	121.2(3)
C(14)-N(2)-Co(1)	119.5(4)
C(15)-N(3)-C(17)	120.9(4)
C(15)-N(3)-Co(1)	114.9(4)
C(17)-N(3)-Co(1)	124.0(3)
C(38)-N(4)-C(35)	121.6(5)
C(38)-N(4)-Co(1)	116.6(4)
C(35)-N(4)-Co(1)	121.8(4)
C(40)-N(5)-C(44)	118.9(5)
C(40)-N(5)-Co(1)	120.2(4)
C(44)-N(5)-Co(1)	120.0(4)
C(45)-N(6)-C(47)	121.7(5)
C(45)-N(6)-Co(1)	116.2(4)
C(47)-N(6)-Co(1)	120.9(3)
C(7)-C(2)-O(1)	117.1(5)
C(7)-C(2)-C(3)	119.8(5)
O(1)-C(2)-C(3)	123.1(6)
C(2)-C(3)-C(4)	119.3(6)
C(5)-C(4)-C(3)	121.1(6)
C(4)-C(5)-C(6)	118.5(5)
C(4)-C(5)-N(1)	119.6(5)
C(6)-C(5)-N(1)	121.2(5)
C(7)-C(6)-C(5)	120.7(6)
C(6)-C(7)-C(2)	120.5(5)
N(1)-C(8)-C(10)	114.1(5)
N(1)-C(8)-C(9)	127.3(5)

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C(10)-C(8)-C(9)	118.6(5)
N(2)-C(10)-C(11)	122.1(5)
N(2)-C(10)-C(8)	112.3(5)
C(11)-C(10)-C(8)	125.5(5)
C(12)-C(11)-C(10)	119.9(6)
C(11)-C(12)-C(13)	118.6(5)
C(14)-C(13)-C(12)	119.4(5)
N(2)-C(14)-C(13)	121.5(5)
N(2)-C(14)-C(15)	113.3(5)
C(13)-C(14)-C(15)	125.2(5)
N(3)-C(15)-C(14)	115.6(5)
N(3)-C(15)-C(16)	125.1(5)
C(14)-C(15)-C(16)	119.1(5)
C(22)-C(17)-C(18)	118.6(5)
C(22)-C(17)-N(3)	120.4(5)
C(18)-C(17)-N(3)	120.9(5)
C(19)-C(18)-C(17)	120.4(5)
C(18)-C(19)-C(20)	120.6(5)
O(2)-C(20)-C(19)	115.8(5)
O(2)-C(20)-C(21)	125.4(5)
C(19)-C(20)-C(21)	118.8(5)
C(22)-C(21)-C(20)	119.7(5)
C(17)-C(22)-C(21)	121.7(5)
O(3)-C(32)-C(37)	124.3(5)
O(3)-C(32)-C(33)	116.0(5)
C(37)-C(32)-C(33)	119.7(5)
C(34)-C(33)-C(32)	119.4(5)
C(35)-C(34)-C(33)	121.7(5)
C(34)-C(35)-C(36)	118.3(5)
C(34)-C(35)-N(4)	118.5(5)
C(36)-C(35)-N(4)	123.2(5)
C(37)-C(36)-C(35)	120.4(6)
C(32)-C(37)-C(36)	120.5(5)
N(4)-C(38)-C(40)	114.0(5)
N(4)-C(38)-C(39)	125.6(5)
C(40)-C(38)-C(39)	120.1(5)
N(5)-C(40)-C(41)	121.2(5)
N(5)-C(40)-C(38)	113.7(5)
C(41)-C(40)-C(38)	124.7(6)
C(42)-C(41)-C(40)	119.7(6)
C(41)-C(42)-C(43)	119.2(5)
C(42)-C(43)-C(44)	119.4(6)
N(5)-C(44)-C(43)	121.6(6)
N(5)-C(44)-C(45)	112.4(5)
C(43)-C(44)-C(45)	125.9(6)
N(6)-C(45)-C(44)	114.0(5)
N(6)-C(45)-C(46)	124.4(6)
C(44)-C(45)-C(46)	121.4(5)
C(52)-C(47)-C(48)	119.1(6)
C(52)-C(47)-N(6)	121.9(5)
C(48)-C(47)-N(6)	118.9(5)
C(49)-C(48)-C(47)	120.0(6)
C(48)-C(49)-C(50)	120.0(6)
C(51)-C(50)-O(4)	125.7(6)
C(51)-C(50)-C(49)	119.7(6)
O(4)-C(50)-C(49)	114.6(6)
C(52)-C(51)-C(50)	119.8(6)
C(51)-C(52)-C(47)	121.3(6)
F(4)-P(1)-F(6)	90.7(2)
F(4)-P(1)-F(5)	92.4(3)
F(6)-P(1)-F(5)	176.9(2)
F(4)-P(1)-F(1)	90.7(2)
F(6)-P(1)-F(1)	89.8(2)

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F(5)-P(1)-F(1)	89.6(2)
F(4)-P(1)-F(3)	90.5(2)
F(6)-P(1)-F(3)	89.7(2)
F(5)-P(1)-F(3)	90.8(2)
F(1)-P(1)-F(3)	178.7(3)
F(4)-P(1)-F(2)	179.5(2)
F(6)-P(1)-F(2)	88.9(2)
F(5)-P(1)-F(2)	88.0(2)
F(1)-P(1)-F(2)	89.6(2)
F(3)-P(1)-F(2)	89.2(2)

Symmetry transformations used to generate equivalent atoms:

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Table S28. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for [Co(I)(L(0))₂]⁺. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Co (1)	33 (1)	28 (1)	31 (1)	11 (1)	16 (1)	16 (1)
O (1)	46 (2)	33 (3)	48 (3)	19 (2)	33 (2)	21 (2)
O (2)	45 (3)	29 (2)	31 (2)	9 (2)	13 (2)	14 (2)
O (3)	61 (3)	50 (3)	45 (3)	28 (2)	33 (2)	30 (3)
O (4)	71 (3)	31 (3)	51 (3)	15 (2)	27 (3)	20 (3)
N (1)	33 (3)	30 (3)	33 (3)	10 (2)	16 (2)	12 (2)
N (2)	29 (3)	28 (3)	35 (3)	14 (2)	15 (2)	12 (2)
N (3)	33 (3)	32 (3)	34 (3)	16 (2)	18 (2)	22 (2)
N (4)	26 (3)	36 (3)	29 (3)	14 (2)	15 (2)	16 (2)
N (5)	28 (3)	36 (3)	32 (3)	17 (2)	17 (2)	15 (2)
N (6)	33 (3)	31 (3)	38 (3)	15 (2)	23 (2)	18 (2)
C (1)	43 (4)	38 (4)	42 (4)	10 (3)	23 (3)	20 (3)
C (2)	27 (3)	30 (4)	31 (3)	9 (3)	14 (3)	12 (3)
C (3)	37 (3)	32 (4)	43 (4)	16 (3)	23 (3)	19 (3)
C (4)	34 (3)	44 (4)	34 (3)	20 (3)	15 (3)	17 (3)
C (5)	30 (3)	26 (3)	36 (3)	15 (3)	19 (3)	20 (3)
C (6)	37 (3)	27 (3)	37 (3)	12 (3)	16 (3)	15 (3)
C (7)	35 (3)	28 (4)	42 (4)	17 (3)	21 (3)	12 (3)
C (8)	31 (3)	34 (4)	41 (4)	21 (3)	20 (3)	19 (3)
C (9)	36 (4)	41 (4)	36 (4)	12 (3)	16 (3)	17 (3)
C (10)	35 (3)	31 (4)	29 (3)	13 (3)	18 (3)	15 (3)
C (11)	44 (4)	32 (4)	33 (3)	12 (3)	17 (3)	17 (3)
C (12)	47 (4)	29 (4)	38 (4)	5 (3)	23 (3)	17 (3)
C (13)	41 (4)	39 (4)	40 (4)	12 (3)	23 (3)	23 (3)
C (14)	41 (4)	30 (4)	36 (3)	16 (3)	21 (3)	24 (3)
C (15)	36 (3)	31 (4)	33 (3)	10 (3)	17 (3)	22 (3)
C (16)	41 (4)	40 (4)	48 (4)	8 (3)	19 (3)	18 (3)
C (17)	27 (3)	28 (3)	33 (3)	11 (3)	17 (3)	15 (3)
C (18)	37 (3)	33 (4)	28 (3)	16 (3)	19 (3)	21 (3)
C (19)	37 (3)	31 (4)	32 (3)	15 (3)	18 (3)	17 (3)
C (20)	31 (3)	33 (4)	33 (3)	12 (3)	14 (3)	22 (3)
C (21)	41 (4)	30 (4)	33 (3)	18 (3)	21 (3)	24 (3)
C (22)	36 (3)	29 (3)	34 (3)	15 (3)	20 (3)	19 (3)
C (23)	54 (4)	47 (4)	34 (4)	13 (3)	15 (3)	23 (4)
C (31)	63 (5)	57 (5)	50 (4)	32 (4)	32 (4)	23 (4)
C (32)	38 (4)	35 (4)	40 (4)	17 (3)	24 (3)	25 (3)
C (33)	36 (3)	32 (4)	34 (3)	13 (3)	16 (3)	19 (3)
C (34)	28 (3)	32 (4)	37 (4)	15 (3)	14 (3)	15 (3)
C (35)	30 (3)	31 (4)	36 (3)	15 (3)	18 (3)	19 (3)
C (36)	41 (4)	32 (4)	34 (3)	14 (3)	14 (3)	20 (3)
C (37)	41 (4)	36 (4)	52 (4)	27 (3)	27 (3)	25 (3)
C (38)	30 (3)	33 (4)	30 (3)	10 (3)	12 (3)	16 (3)
C (39)	52 (4)	39 (4)	44 (4)	17 (3)	24 (3)	27 (3)
C (40)	31 (3)	33 (4)	34 (3)	12 (3)	15 (3)	17 (3)
C (41)	48 (4)	34 (4)	43 (4)	13 (3)	24 (3)	25 (3)
C (42)	43 (4)	42 (4)	31 (3)	9 (3)	20 (3)	24 (3)
C (43)	41 (4)	48 (4)	30 (3)	14 (3)	21 (3)	20 (3)
C (44)	28 (3)	32 (4)	31 (3)	12 (3)	9 (3)	16 (3)
C (45)	26 (3)	40 (4)	33 (3)	15 (3)	12 (3)	8 (3)
C (46)	52 (4)	46 (4)	43 (4)	20 (3)	24 (4)	20 (4)
C (47)	44 (4)	32 (4)	32 (3)	17 (3)	17 (3)	19 (3)
C (48)	40 (4)	34 (4)	48 (4)	14 (3)	16 (3)	17 (3)
C (49)	48 (4)	38 (4)	59 (4)	20 (4)	24 (4)	22 (4)

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C (50)	63 (5)	29 (4)	45 (4)	22 (3)	28 (4)	20 (4)
C (51)	49 (4)	27 (4)	39 (4)	13 (3)	6 (3)	11 (3)
C (52)	35 (4)	35 (4)	44 (4)	18 (3)	9 (3)	11 (3)
C (53)	74 (5)	49 (5)	39 (4)	17 (4)	23 (4)	19 (4)
P (1)	45 (1)	34 (1)	36 (1)	16 (1)	20 (1)	15 (1)
F (1)	82 (3)	36 (2)	57 (2)	22 (2)	38 (2)	16 (2)
F (2)	77 (3)	49 (2)	54 (2)	21 (2)	35 (2)	37 (2)
F (3)	105 (3)	66 (3)	70 (3)	48 (2)	59 (3)	42 (3)
F (4)	113 (4)	78 (3)	78 (3)	45 (3)	69 (3)	66 (3)
F (5)	47 (2)	71 (3)	58 (3)	28 (2)	18 (2)	16 (2)
F (6)	66 (3)	69 (3)	48 (2)	14 (2)	12 (2)	25 (2)

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Table S29. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Co}(\text{I})(\text{L}(0))_2]^+$.

	x	y	z	U(eq)
H(1A)	3918(27)	7567(7)	117(22)	64
H(1B)	4028(29)	7674(9)	-904(6)	64
H(1C)	5153(6)	7887(6)	-7(24)	64
H(3)	5209(5)	7355(5)	-1734(4)	42
H(4)	6200(5)	6724(6)	-2762(4)	44
H(6)	5057(5)	3759(5)	-2615(4)	41
H(7)	4048(5)	4365(5)	-1622(4)	41
H(9A)	4804(11)	2386(13)	-4693(23)	60
H(9B)	4834(11)	2875(25)	-5515(5)	60
H(9C)	4413(5)	3368(13)	-4588(21)	60
H(11)	6270(5)	2209(5)	-5608(4)	45
H(12)	7936(5)	2070(5)	-5811(5)	49
H(13)	9820(5)	3654(5)	-4646(5)	48
H(16A)	11591(18)	5787(36)	-3532(21)	71
H(16B)	11467(15)	4933(15)	-3039(33)	71
H(16C)	12134(6)	6300(23)	-2272(14)	71
H(18)	11739(5)	8065(5)	-2306(4)	36
H(19)	13393(5)	9749(5)	-979(4)	39
H(21)	12679(5)	8872(5)	1224(4)	37
H(22)	10991(5)	7225(5)	-115(4)	36
H(23A)	15471(17)	11357(22)	2418(11)	72
H(23B)	14757(35)	10002(16)	2007(5)	72
H(23C)	14160(20)	10814(37)	2370(12)	72
H(31A)	9283(25)	8228(16)	-7051(7)	82
H(31B)	10293(7)	8481(22)	-6026(32)	82
H(31C)	9403(28)	9013(10)	-5887(29)	82
H(33)	7212(5)	5937(5)	-6041(5)	40
H(34)	7226(5)	5952(5)	-4456(4)	38
H(36)	10263(5)	8944(5)	-2811(5)	42
H(37)	10296(5)	8896(5)	-4397(5)	45
H(39A)	9380(16)	10054(6)	-1236(20)	66
H(39B)	7968(19)	9441(18)	-1689(30)	66
H(39C)	8618(34)	9304(15)	-2490(12)	66
H(41)	8374(5)	9536(6)	7(5)	49
H(42)	7847(5)	8918(6)	1180(5)	47
H(43)	7663(5)	7127(6)	961(4)	48
H(46A)	6730(7)	4677(31)	-212(23)	72
H(46B)	7969(27)	5536(10)	786(5)	72
H(46C)	7788(32)	4351(23)	-112(26)	72
H(48)	10005(6)	4630(6)	-1078(5)	52
H(49)	9967(6)	2833(6)	-1789(5)	58
H(51)	6403(6)	1268(6)	-3217(5)	53
H(52)	6448(5)	3052(5)	-2474(5)	50
H(53A)	6662(17)	-398(25)	-3593(8)	87
H(53B)	7484(11)	-707(15)	-4177(23)	87
H(53C)	6955(24)	104(10)	-4369(18)	87

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Table S31. Crystal data and structure refinement for [Ni(II)(L(0))₂]₂+

Identification code	ST3381
Empirical formula	C ₄₆ H ₄₆ F ₁₂ N ₆ Ni O ₄ P ₂
Formula weight	1095.54
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2 ₁ /c
Unit cell dimensions	a = 18.047(2) Å alpha = 90 deg. b = 16.655(2) Å beta = 112.70(2) deg. c = 17.132(2) Å gamma = 90 deg.
Volume	4750.5(10) Å ³
Z	4
Density (calculated)	1.532 Mg/m ³
Absorption coefficient	0.574 mm ⁻¹
F(000)	2248
Crystal size	0.51 x 0.35 x 0.18 mm
Theta range for data collection	1.73 to 23.27 deg.
Index ranges	-20 ≤ h ≤ 13, -18 ≤ k ≤ 18, -14 ≤ l ≤ 19
Reflections collected	32080
Independent reflections	6841 [R(int) = 0.0352]
Absorption correction	SADABS, G.M. Sheldrick, 1994
Max. and min. transmission	0.928 and 0.794
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6825 / 0 / 648
Goodness-of-fit on F ²	1.037
Final R indices [I > 2sigma(I)]	R1 = 0.0281, wR2 = 0.0660
R indices (all data)	R1 = 0.0364, wR2 = 0.0698
Largest diff. peak and hole	0.725 and -0.320 e.Å ⁻³

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Table S32. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ni}(\text{II})(\text{L}(0))_2]2+$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ni(1)	2211(1)	4587(1)	4097(1)	16(1)
O(1)	-1577(1)	3801(1)	1230(1)	30(1)
O(2)	5166(1)	1954(1)	4043(1)	29(1)
O(3)	3655(1)	8079(1)	2944(1)	28(1)
O(4)	2763(1)	4454(1)	8215(1)	26(1)
N(1)	1078(1)	5130(1)	3812(1)	18(1)
N(2)	2480(1)	5518(1)	4869(1)	17(1)
N(3)	3475(1)	4451(1)	4767(1)	17(1)
N(4)	2229(1)	5113(1)	2972(1)	17(1)
N(5)	1923(1)	3677(1)	3306(1)	17(1)
N(6)	2097(1)	3620(1)	4860(1)	16(1)
C(1)	-1937(2)	4190(2)	426(2)	36(1)
C(2)	-937(1)	4178(1)	1833(1)	23(1)
C(3)	-590(1)	3774(1)	2600(1)	25(1)
C(4)	61(1)	4092(1)	3249(1)	22(1)
C(5)	364(1)	4835(1)	3148(1)	18(1)
C(6)	24(1)	5241(1)	2386(1)	23(1)
C(7)	-628(1)	4913(1)	1725(1)	25(1)
C(8)	1096(1)	5803(1)	4187(1)	21(1)
C(9)	396(1)	6343(2)	4057(2)	34(1)
C(10)	1901(1)	6045(1)	4814(1)	19(1)
C(11)	2078(1)	6738(1)	5299(1)	25(1)
C(12)	2866(1)	6860(1)	5853(1)	27(1)
C(13)	3458(1)	6304(1)	5915(1)	24(1)
C(14)	3245(1)	5630(1)	5399(1)	19(1)
C(15)	3799(1)	4981(1)	5353(1)	18(1)
C(16)	4654(1)	5021(1)	5952(2)	28(1)
C(17)	3914(1)	3788(1)	4636(1)	18(1)
C(18)	4402(1)	3287(1)	5280(1)	21(1)
C(19)	4824(1)	2658(1)	5108(1)	21(1)
C(20)	4763(1)	2536(1)	4284(1)	22(1)
C(21)	4259(1)	3020(1)	3633(1)	21(1)
C(22)	3833(1)	3631(1)	3808(1)	19(1)
C(23)	5731(2)	1475(2)	4700(2)	33(1)
C(31)	3256(1)	8817(1)	2965(2)	29(1)
C(32)	3256(1)	7379(1)	2943(1)	22(1)
C(33)	2540(1)	7330(1)	3064(1)	21(1)
C(34)	2196(1)	6582(1)	3054(1)	21(1)
C(35)	2557(1)	5892(1)	2929(1)	17(1)
C(36)	3276(1)	5945(1)	2808(1)	22(1)
C(37)	3622(1)	6685(1)	2813(1)	24(1)
C(38)	1960(1)	4654(1)	2317(1)	18(1)
C(39)	1858(1)	4872(1)	1437(1)	21(1)
C(40)	1760(1)	3822(1)	2485(1)	17(1)
C(41)	1486(1)	3211(1)	1893(1)	20(1)
C(42)	1417(1)	2448(1)	2176(1)	23(1)
C(43)	1610(1)	2301(1)	3028(1)	21(1)
C(44)	1851(1)	2943(1)	3589(1)	17(1)
C(45)	2047(1)	2920(1)	4519(1)	18(1)
C(46)	2179(1)	2126(1)	4955(1)	22(1)
C(47)	2277(1)	3754(1)	5740(1)	19(1)
C(48)	1778(1)	4282(1)	5944(1)	20(1)
C(49)	1951(1)	4499(1)	6773(1)	21(1)

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C(50)	2641 (1)	4204 (1)	7414 (1)	20 (1)
C(51)	3149 (1)	3689 (1)	7216 (1)	23 (1)
C(52)	2960 (1)	3460 (1)	6381 (1)	21 (1)
C(53)	3499 (2)	4208 (2)	8883 (1)	35 (1)
P(1)	115 (1)	6936 (1)	580 (1)	21 (1)
F(11)	758 (1)	6309 (1)	1155 (1)	37 (1)
F(12)	-536 (1)	7572 (1)	2 (1)	28 (1)
F(13)	-221 (1)	7056 (1)	1313 (1)	30 (1)
F(14)	-519 (1)	6224 (1)	186 (1)	30 (1)
F(15)	442 (1)	6825 (1)	-160 (1)	33 (1)
F(16)	738 (1)	7656 (1)	964 (1)	30 (1)
P(2)	4228 (1)	4286 (1)	1515 (1)	24 (1)
F(21)	4990 (1)	3959 (1)	2288 (1)	34 (1)
F(22)	3455 (1)	4620 (1)	748 (1)	40 (1)
F(23)	3681 (1)	4154 (1)	2054 (1)	33 (1)
F(24)	4024 (1)	3396 (1)	1155 (1)	43 (1)
F(25)	4764 (1)	4421 (1)	970 (1)	41 (1)
F(26)	4429 (1)	5177 (1)	1884 (1)	40 (1)

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Table S33. Bond lengths [Å] and angles [deg] for [Ni(II)(L(0))₂]²⁺.

Ni(1)-N(5)	1.965(2)
Ni(1)-N(2)	1.973(2)
Ni(1)-N(1)	2.113(2)
Ni(1)-N(4)	2.129(2)
Ni(1)-N(6)	2.134(2)
Ni(1)-N(3)	2.134(2)
O(1)-C(2)	1.370(3)
O(1)-C(1)	1.431(3)
O(2)-C(20)	1.368(3)
O(2)-C(23)	1.434(3)
O(3)-C(32)	1.370(3)
O(3)-C(31)	1.432(3)
O(4)-C(50)	1.369(3)
O(4)-C(53)	1.438(3)
N(1)-C(8)	1.286(3)
N(1)-C(5)	1.437(3)
N(2)-C(10)	1.339(3)
N(2)-C(14)	1.341(3)
N(3)-C(15)	1.295(3)
N(3)-C(17)	1.426(3)
N(4)-C(38)	1.288(3)
N(4)-C(35)	1.440(3)
N(5)-C(44)	1.341(3)
N(5)-C(40)	1.343(3)
N(6)-C(45)	1.291(3)
N(6)-C(47)	1.432(3)
C(2)-C(7)	1.387(3)
C(2)-C(3)	1.391(3)
C(3)-C(4)	1.374(3)
C(4)-C(5)	1.391(3)
C(5)-C(6)	1.385(3)
C(6)-C(7)	1.392(3)
C(8)-C(10)	1.492(3)
C(8)-C(9)	1.494(3)
C(10)-C(11)	1.385(3)
C(11)-C(12)	1.387(3)
C(12)-C(13)	1.387(3)
C(13)-C(14)	1.389(3)
C(14)-C(15)	1.495(3)
C(15)-C(16)	1.488(3)
C(17)-C(18)	1.392(3)
C(17)-C(22)	1.393(3)
C(18)-C(19)	1.391(3)
C(19)-C(20)	1.388(3)
C(20)-C(21)	1.392(3)
C(21)-C(22)	1.377(3)
C(32)-C(33)	1.388(3)
C(32)-C(37)	1.391(3)
C(33)-C(34)	1.389(3)
C(34)-C(35)	1.379(3)
C(35)-C(36)	1.393(3)
C(36)-C(37)	1.379(3)
C(38)-C(40)	1.488(3)
C(38)-C(39)	1.492(3)
C(40)-C(41)	1.385(3)
C(41)-C(42)	1.383(3)
C(42)-C(43)	1.386(3)
C(43)-C(44)	1.390(3)
C(44)-C(45)	1.493(3)

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C (45) -C (46)	1.494 (3)
C (47) -C (52)	1.386 (3)
C (47) -C (48)	1.396 (3)
C (48) -C (49)	1.378 (3)
C (49) -C (50)	1.394 (3)
C (50) -C (51)	1.389 (3)
C (51) -C (52)	1.390 (3)
P (1) -F (11)	1.5891 (14)
P (1) -F (16)	1.6008 (14)
P (1) -F (15)	1.6013 (14)
P (1) -F (14)	1.6050 (14)
P (1) -F (13)	1.6054 (14)
P (1) -F (12)	1.6088 (13)
P (2) -F (21)	1.5926 (14)
P (2) -F (24)	1.593 (2)
P (2) -F (25)	1.597 (2)
P (2) -F (26)	1.599 (2)
P (2) -F (22)	1.602 (2)
P (2) -F (23)	1.6071 (14)

N (5) -Ni (1) -N (2)	178.55 (7)
N (5) -Ni (1) -N (1)	101.32 (7)
N (2) -Ni (1) -N (1)	77.57 (7)
N (5) -Ni (1) -N (4)	77.54 (7)
N (2) -Ni (1) -N (4)	101.44 (7)
N (1) -Ni (1) -N (4)	88.07 (7)
N (5) -Ni (1) -N (6)	77.18 (7)
N (2) -Ni (1) -N (6)	103.86 (7)
N (1) -Ni (1) -N (6)	98.73 (7)
N (4) -Ni (1) -N (6)	154.65 (7)
N (5) -Ni (1) -N (3)	103.40 (7)
N (2) -Ni (1) -N (3)	77.73 (7)
N (1) -Ni (1) -N (3)	155.26 (7)
N (4) -Ni (1) -N (3)	98.26 (7)
N (6) -Ni (1) -N (3)	85.75 (6)
C (2) -O (1) -C (1)	117.1 (2)
C (20) -O (2) -C (23)	117.2 (2)
C (32) -O (3) -C (31)	117.5 (2)
C (50) -O (4) -C (53)	117.0 (2)
C (8) -N (1) -C (5)	122.4 (2)
C (8) -N (1) -Ni (1)	114.98 (14)
C (5) -N (1) -Ni (1)	121.89 (13)
C (10) -N (2) -C (14)	121.9 (2)
C (10) -N (2) -Ni (1)	118.95 (14)
C (14) -N (2) -Ni (1)	119.05 (14)
C (15) -N (3) -C (17)	122.5 (2)
C (15) -N (3) -Ni (1)	114.44 (14)
C (17) -N (3) -Ni (1)	122.76 (13)
C (38) -N (4) -C (35)	121.0 (2)
C (38) -N (4) -Ni (1)	114.37 (14)
C (35) -N (4) -Ni (1)	124.52 (13)
C (44) -N (5) -C (40)	122.0 (2)
C (44) -N (5) -Ni (1)	119.37 (14)
C (40) -N (5) -Ni (1)	118.52 (14)
C (45) -N (6) -C (47)	124.5 (2)
C (45) -N (6) -Ni (1)	114.23 (14)
C (47) -N (6) -Ni (1)	119.35 (13)
O (1) -C (2) -C (7)	124.7 (2)
O (1) -C (2) -C (3)	115.6 (2)
C (7) -C (2) -C (3)	119.7 (2)
C (4) -C (3) -C (2)	120.7 (2)
C (3) -C (4) -C (5)	119.8 (2)
C (6) -C (5) -C (4)	119.9 (2)

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C(6)-C(5)-N(1)	121.0(2)
C(4)-C(5)-N(1)	118.8(2)
C(5)-C(6)-C(7)	120.3(2)
C(2)-C(7)-C(6)	119.6(2)
N(1)-C(8)-C(10)	115.1(2)
N(1)-C(8)-C(9)	126.4(2)
C(10)-C(8)-C(9)	118.5(2)
N(2)-C(10)-C(11)	120.7(2)
N(2)-C(10)-C(8)	113.0(2)
C(11)-C(10)-C(8)	126.3(2)
C(10)-C(11)-C(12)	118.1(2)
C(13)-C(12)-C(11)	120.7(2)
C(12)-C(13)-C(14)	118.4(2)
N(2)-C(14)-C(13)	120.2(2)
N(2)-C(14)-C(15)	113.6(2)
C(13)-C(14)-C(15)	126.2(2)
N(3)-C(15)-C(16)	127.1(2)
N(3)-C(15)-C(14)	115.0(2)
C(16)-C(15)-C(14)	117.9(2)
C(18)-C(17)-C(22)	118.7(2)
C(18)-C(17)-N(3)	124.0(2)
C(22)-C(17)-N(3)	117.3(2)
C(19)-C(18)-C(17)	120.9(2)
C(20)-C(19)-C(18)	119.4(2)
O(2)-C(20)-C(19)	124.7(2)
O(2)-C(20)-C(21)	115.3(2)
C(19)-C(20)-C(21)	120.1(2)
C(22)-C(21)-C(20)	120.0(2)
C(21)-C(22)-C(17)	120.8(2)
O(3)-C(32)-C(33)	124.7(2)
O(3)-C(32)-C(37)	115.2(2)
C(33)-C(32)-C(37)	120.2(2)
C(32)-C(33)-C(34)	119.2(2)
C(35)-C(34)-C(33)	121.0(2)
C(34)-C(35)-C(36)	119.5(2)
C(34)-C(35)-N(4)	121.0(2)
C(36)-C(35)-N(4)	119.3(2)
C(37)-C(36)-C(35)	120.1(2)
C(36)-C(37)-C(32)	120.1(2)
N(4)-C(38)-C(40)	115.0(2)
N(4)-C(38)-C(39)	126.5(2)
C(40)-C(38)-C(39)	118.5(2)
N(5)-C(40)-C(41)	120.4(2)
N(5)-C(40)-C(38)	113.4(2)
C(41)-C(40)-C(38)	126.0(2)
C(42)-C(41)-C(40)	118.3(2)
C(41)-C(42)-C(43)	120.7(2)
C(42)-C(43)-C(44)	118.5(2)
N(5)-C(44)-C(43)	120.0(2)
N(5)-C(44)-C(45)	113.2(2)
C(43)-C(44)-C(45)	126.8(2)
N(6)-C(45)-C(44)	114.0(2)
N(6)-C(45)-C(46)	127.1(2)
C(44)-C(45)-C(46)	118.9(2)
C(52)-C(47)-C(48)	119.1(2)
C(52)-C(47)-N(6)	123.3(2)
C(48)-C(47)-N(6)	117.2(2)
C(49)-C(48)-C(47)	120.8(2)
C(48)-C(49)-C(50)	119.8(2)
O(4)-C(50)-C(51)	124.5(2)
O(4)-C(50)-C(49)	115.6(2)
C(51)-C(50)-C(49)	119.9(2)
C(50)-C(51)-C(52)	119.9(2)

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C(47)-C(52)-C(51)	120.5(2)
F(11)-P(1)-F(16)	90.52(8)
F(11)-P(1)-F(15)	90.67(8)
F(16)-P(1)-F(15)	89.80(7)
F(11)-P(1)-F(14)	90.35(8)
F(16)-P(1)-F(14)	179.13(8)
F(15)-P(1)-F(14)	90.18(7)
F(11)-P(1)-F(13)	90.17(8)
F(16)-P(1)-F(13)	90.20(7)
F(15)-P(1)-F(13)	179.16(8)
F(14)-P(1)-F(13)	89.81(7)
F(11)-P(1)-F(12)	179.73(8)
F(16)-P(1)-F(12)	89.45(7)
F(15)-P(1)-F(12)	89.60(7)
F(14)-P(1)-F(12)	89.69(7)
F(13)-P(1)-F(12)	89.56(7)
F(21)-P(2)-F(24)	90.04(8)
F(21)-P(2)-F(25)	90.66(8)
F(24)-P(2)-F(25)	90.38(8)
F(21)-P(2)-F(26)	89.83(8)
F(24)-P(2)-F(26)	179.39(9)
F(25)-P(2)-F(26)	90.22(8)
F(21)-P(2)-F(22)	179.02(8)
F(24)-P(2)-F(22)	90.41(8)
F(25)-P(2)-F(22)	90.21(8)
F(26)-P(2)-F(22)	89.71(8)
F(21)-P(2)-F(23)	89.99(7)
F(24)-P(2)-F(23)	89.66(8)
F(25)-P(2)-F(23)	179.35(8)
F(26)-P(2)-F(23)	89.74(8)
F(22)-P(2)-F(23)	89.14(7)

Symmetry transformations used to generate equivalent atoms:

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Table S34. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ni}(\text{II})(\text{L}(0))_2]2+$. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Ni (1)	17 (1)	14 (1)	14 (1)	-1 (1)	5 (1)	-1 (1)
O (1)	24 (1)	37 (1)	20 (1)	4 (1)	-1 (1)	-11 (1)
O (2)	35 (1)	23 (1)	28 (1)	1 (1)	12 (1)	11 (1)
O (3)	25 (1)	14 (1)	43 (1)	2 (1)	12 (1)	-1 (1)
O (4)	33 (1)	28 (1)	17 (1)	-2 (1)	7 (1)	2 (1)
N (1)	20 (1)	16 (1)	17 (1)	1 (1)	7 (1)	-1 (1)
N (2)	19 (1)	17 (1)	15 (1)	-1 (1)	7 (1)	-2 (1)
N (3)	20 (1)	17 (1)	14 (1)	0 (1)	7 (1)	-2 (1)
N (4)	18 (1)	15 (1)	17 (1)	0 (1)	5 (1)	0 (1)
N (5)	14 (1)	17 (1)	18 (1)	-1 (1)	6 (1)	1 (1)
N (6)	15 (1)	20 (1)	15 (1)	0 (1)	5 (1)	-1 (1)
C (1)	29 (1)	48 (2)	21 (1)	4 (1)	-3 (1)	-5 (1)
C (2)	17 (1)	30 (1)	20 (1)	0 (1)	5 (1)	-2 (1)
C (3)	25 (1)	23 (1)	25 (1)	3 (1)	7 (1)	-7 (1)
C (4)	22 (1)	22 (1)	20 (1)	5 (1)	6 (1)	0 (1)
C (5)	15 (1)	20 (1)	19 (1)	-1 (1)	6 (1)	2 (1)
C (6)	23 (1)	20 (1)	26 (1)	4 (1)	8 (1)	-2 (1)
C (7)	23 (1)	28 (1)	20 (1)	9 (1)	4 (1)	1 (1)
C (8)	23 (1)	19 (1)	23 (1)	1 (1)	10 (1)	1 (1)
C (9)	24 (1)	30 (1)	43 (2)	-10 (1)	7 (1)	4 (1)
C (10)	23 (1)	17 (1)	20 (1)	1 (1)	10 (1)	0 (1)
C (11)	29 (1)	21 (1)	27 (1)	-4 (1)	12 (1)	2 (1)
C (12)	35 (1)	20 (1)	25 (1)	-9 (1)	11 (1)	-4 (1)
C (13)	25 (1)	23 (1)	21 (1)	-6 (1)	6 (1)	-5 (1)
C (14)	21 (1)	21 (1)	15 (1)	0 (1)	7 (1)	-3 (1)
C (15)	19 (1)	20 (1)	16 (1)	1 (1)	8 (1)	-3 (1)
C (16)	22 (1)	29 (1)	29 (1)	-10 (1)	7 (1)	-3 (1)
C (17)	15 (1)	16 (1)	21 (1)	-1 (1)	6 (1)	-3 (1)
C (18)	20 (1)	26 (1)	17 (1)	1 (1)	7 (1)	-2 (1)
C (19)	21 (1)	19 (1)	23 (1)	5 (1)	7 (1)	2 (1)
C (20)	22 (1)	16 (1)	29 (1)	-1 (1)	10 (1)	-1 (1)
C (21)	26 (1)	18 (1)	19 (1)	-3 (1)	9 (1)	-3 (1)
C (22)	19 (1)	17 (1)	17 (1)	0 (1)	3 (1)	-3 (1)
C (23)	34 (1)	28 (1)	36 (2)	0 (1)	11 (1)	12 (1)
C (31)	33 (1)	16 (1)	39 (2)	2 (1)	14 (1)	0 (1)
C (32)	22 (1)	17 (1)	22 (1)	3 (1)	4 (1)	-1 (1)
C (33)	23 (1)	16 (1)	24 (1)	-1 (1)	8 (1)	3 (1)
C (34)	21 (1)	21 (1)	22 (1)	2 (1)	9 (1)	1 (1)
C (35)	20 (1)	16 (1)	13 (1)	2 (1)	3 (1)	-1 (1)
C (36)	22 (1)	18 (1)	24 (1)	0 (1)	7 (1)	3 (1)
C (37)	20 (1)	21 (1)	29 (1)	1 (1)	8 (1)	1 (1)
C (38)	15 (1)	20 (1)	18 (1)	0 (1)	5 (1)	4 (1)
C (39)	23 (1)	22 (1)	17 (1)	-1 (1)	6 (1)	-1 (1)
C (40)	14 (1)	20 (1)	16 (1)	-2 (1)	5 (1)	1 (1)
C (41)	19 (1)	22 (1)	18 (1)	-2 (1)	6 (1)	1 (1)
C (42)	23 (1)	20 (1)	24 (1)	-9 (1)	8 (1)	-3 (1)
C (43)	22 (1)	16 (1)	27 (1)	-1 (1)	10 (1)	1 (1)
C (44)	13 (1)	16 (1)	20 (1)	0 (1)	6 (1)	1 (1)
C (45)	13 (1)	17 (1)	22 (1)	1 (1)	7 (1)	0 (1)
C (46)	24 (1)	19 (1)	22 (1)	2 (1)	7 (1)	0 (1)
C (47)	22 (1)	16 (1)	18 (1)	1 (1)	8 (1)	-5 (1)
C (48)	20 (1)	17 (1)	21 (1)	3 (1)	6 (1)	0 (1)
C (49)	27 (1)	17 (1)	23 (1)	1 (1)	13 (1)	1 (1)

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C(50)	27(1)	17(1)	17(1)	0(1)	8(1)	-6(1)
C(51)	23(1)	24(1)	19(1)	3(1)	5(1)	0(1)
C(52)	23(1)	21(1)	21(1)	2(1)	11(1)	1(1)
C(53)	43(2)	41(2)	16(1)	-1(1)	5(1)	5(1)
P(1)	24(1)	19(1)	19(1)	0(1)	8(1)	0(1)
F(11)	33(1)	37(1)	39(1)	12(1)	11(1)	13(1)
F(12)	28(1)	23(1)	32(1)	7(1)	9(1)	3(1)
F(13)	35(1)	34(1)	26(1)	-3(1)	17(1)	-4(1)
F(14)	37(1)	21(1)	30(1)	-2(1)	11(1)	-6(1)
F(15)	44(1)	32(1)	32(1)	-5(1)	24(1)	-1(1)
F(16)	29(1)	33(1)	30(1)	-8(1)	13(1)	-10(1)
P(2)	23(1)	31(1)	17(1)	-1(1)	8(1)	4(1)
F(21)	26(1)	45(1)	25(1)	1(1)	4(1)	10(1)
F(22)	29(1)	68(1)	22(1)	12(1)	9(1)	14(1)
F(23)	36(1)	41(1)	30(1)	12(1)	20(1)	14(1)
F(24)	37(1)	41(1)	49(1)	-21(1)	13(1)	-3(1)
F(25)	33(1)	66(1)	31(1)	1(1)	20(1)	3(1)
F(26)	54(1)	28(1)	40(1)	-3(1)	20(1)	1(1)

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Table S35. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ni}(\text{II})(\text{L}(\text{O}))_2]^{2+}$.

	x	y	z	U(eq)
H(1A)	-2376(7)	3858(5)	46(4)	54
H(1B)	-1532(3)	4266(9)	181(5)	54
H(1C)	-2149(9)	4714(5)	500(2)	54
H(3)	-806(1)	3273(1)	2675(1)	30
H(4)	303(1)	3805(1)	3765(1)	26
H(6)	236(1)	5745(1)	2315(1)	28
H(7)	-860(1)	5191(1)	1202(1)	30
H(9A)	473(5)	6852(4)	3811(10)	52
H(9B)	355(6)	6446(8)	4602(2)	52
H(9C)	-98(2)	6085(4)	3673(8)	52
H(11)	1671(1)	7118(1)	5253(1)	30
H(12)	3002(1)	7330(1)	6193(1)	32
H(13)	3997(1)	6383(1)	6301(1)	29
H(16A)	4697(2)	4845(8)	6514(3)	42
H(16B)	4848(3)	5574(2)	5985(7)	42
H(16C)	4979(2)	4669(7)	5752(5)	42
H(18)	4448(1)	3376(1)	5845(1)	25
H(19)	5150(1)	2316(1)	5550(1)	26
H(21)	4209(1)	2929(1)	3068(1)	25
H(22)	3480(1)	3950(1)	3359(1)	23
H(23A)	5988(7)	1091(7)	4450(2)	50
H(23B)	5450(2)	1183(8)	5000(7)	50
H(23C)	6141(6)	1824(2)	5098(6)	50
H(31A)	3584(5)	9270(1)	2921(10)	44
H(31B)	3177(8)	8854(4)	3499(4)	44
H(31C)	2733(4)	8832(4)	2490(6)	44
H(33)	2288(1)	7803(1)	3152(1)	25
H(34)	1705(1)	6546(1)	3134(1)	25
H(36)	3528(1)	5472(1)	2721(1)	27
H(37)	4111(1)	6721(1)	2729(1)	28
H(39A)	1306(3)	4756(8)	1049(2)	32
H(39B)	2232(6)	4556(6)	1271(3)	32
H(39C)	1969(8)	5445(2)	1412(2)	32
H(41)	1348(1)	3313(1)	1309(1)	24
H(42)	1236(1)	2019(1)	1782(1)	27
H(43)	1578(1)	1774(1)	3225(1)	25
H(46A)	2696(4)	1904(4)	4997(8)	33
H(46B)	1746(5)	1757(3)	4631(5)	33
H(46C)	2181(8)	2194(2)	5524(3)	33
H(48)	1314(1)	4494(1)	5508(1)	24
H(49)	1602(1)	4849(1)	6906(1)	26
H(51)	3624(1)	3494(1)	7650(1)	27
H(52)	3302(1)	3099(1)	6248(1)	25
H(53A)	3538(5)	4457(8)	9416(2)	53
H(53B)	3956(2)	4378(9)	8749(5)	53
H(53C)	3505(5)	3623(2)	8940(7)	53

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Table S37. Crystal data and structure refinement for [Cu(II)(L(0))₂]²⁺.

Identification code	ST3376
Empirical formula	C ₄₆ H ₄₆ Cu F ₁₂ N ₆ O ₄ P ₂
Formula weight	1100.37
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2 ₁ /c
Unit cell dimensions	a = 17.7990(8) Å alpha = 90 deg. b = 16.7966(8) Å beta = 111.890(10) deg. c = 17.1107(8) Å gamma = 90 deg.
Volume	4746.6(4) Å ³
Z	4
Density (calculated)	1.540 Mg/m ³
Absorption coefficient	0.626 mm ⁻¹
F(000)	2252
Crystal size	0.28 x 0.28 x 0.12 mm
Theta range for data collection	1.86 to 33.00 deg.
Index ranges	-27 ≤ h ≤ 27, -25 ≤ k ≤ 25, -26 ≤ l ≤ 26
Reflections collected	97330
Independent reflections	17913 [R(int) = 0.0644]
Absorption correction	Not measured
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	17900 / 0 / 640
Goodness-of-fit on F ²	1.047
Final R indices [I > 2sigma(I)]	R1 = 0.0381, wR2 = 0.0924
R indices (all data)	R1 = 0.0690, wR2 = 0.0989
Largest diff. peak and hole	0.473 and -0.502 e.Å ⁻³

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Table S38. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Cu}(\text{II})(\text{L}(\text{O}))_2]2+$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cu(1)	2776(1)	400(1)	901(1)	14(1)
O(1)	6582(1)	1188(1)	3762(1)	26(1)
O(2)	-217(1)	3036(1)	956(1)	25(1)
O(3)	2217(1)	570(1)	-3215(1)	23(1)
O(4)	1350(1)	-3108(1)	2090(1)	25(1)
N(1)	3945(1)	-150(1)	1190(1)	16(1)
N(2)	2518(1)	-503(1)	137(1)	15(1)
N(3)	1494(1)	567(1)	205(1)	15(1)
N(4)	2933(1)	1416(1)	134(1)	16(1)
N(5)	3064(1)	1291(1)	1693(1)	14(1)
N(6)	2756(1)	-146(1)	2071(1)	16(1)
C(1)	6930(1)	807(1)	4563(1)	31(1)
C(2)	5947(1)	808(1)	3157(1)	20(1)
C(3)	5645(1)	71(1)	3269(1)	22(1)
C(4)	4995(1)	-262(1)	2609(1)	21(1)
C(5)	4655(1)	139(1)	1846(1)	17(1)
C(6)	4955(1)	884(1)	1747(1)	20(1)
C(7)	5604(1)	1210(1)	2393(1)	21(1)
C(8)	3910(1)	-827(1)	829(1)	18(1)
C(9)	4597(1)	-1394(1)	974(1)	31(1)
C(10)	3095(1)	-1037(1)	201(1)	17(1)
C(11)	2918(1)	-1727(1)	-287(1)	22(1)
C(12)	2129(1)	-1833(1)	-858(1)	24(1)
C(13)	1538(1)	-1263(1)	-932(1)	21(1)
C(14)	1753(1)	-597(1)	-412(1)	16(1)
C(15)	1185(1)	52(1)	-389(1)	16(1)
C(16)	336(1)	31(1)	-1017(1)	24(1)
C(17)	1049(1)	1224(1)	337(1)	16(1)
C(18)	1124(1)	1370(1)	1168(1)	17(1)
C(19)	692(1)	1973(1)	1352(1)	19(1)
C(20)	192(1)	2462(1)	710(1)	19(1)
C(21)	143(1)	2353(1)	-113(1)	20(1)
C(22)	571(1)	1733(1)	-296(1)	19(1)
C(23)	-770(1)	3524(1)	314(1)	29(1)
C(31)	1467(1)	800(1)	-3863(1)	30(1)
C(32)	2353(1)	830(1)	-2416(1)	18(1)
C(33)	1853(1)	1357(1)	-2208(1)	20(1)
C(34)	2056(1)	1592(1)	-1373(1)	19(1)
C(35)	2745(1)	1293(1)	-740(1)	16(1)
C(36)	3237(1)	755(1)	-958(1)	17(1)
C(37)	3052(1)	533(1)	-1787(1)	18(1)
C(38)	2945(1)	2089(1)	492(1)	15(1)
C(39)	2781(1)	2894(1)	88(1)	19(1)
C(40)	3138(1)	2026(1)	1422(1)	15(1)
C(41)	3373(1)	2660(1)	1987(1)	18(1)
C(42)	3567(1)	2509(1)	2836(1)	19(1)
C(43)	3498(1)	1747(1)	3110(1)	17(1)
C(44)	3225(1)	1145(1)	2514(1)	14(1)
C(45)	3033(1)	319(1)	2711(1)	15(1)
C(46)	3157(1)	122(1)	3600(1)	19(1)
C(47)	2466(1)	-2344(1)	1962(1)	19(1)
C(48)	2808(1)	-1601(1)	1976(1)	18(1)
C(49)	2439(1)	-919(1)	2126(1)	16(1)

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C(50)	1718(1)	-989(1)	2269(1)	20(1)
C(51)	1374(1)	-1725(1)	2257(1)	22(1)
C(52)	1747(1)	-2412(1)	2097(1)	19(1)
C(53)	1755(1)	-3831(1)	2043(1)	26(1)
P(1)	5102(1)	1935(1)	5577(1)	17(1)
F(1)	5753(1)	1325(1)	6165(1)	35(1)
F(2)	4471(1)	1217(1)	5203(1)	28(1)
F(3)	5447(1)	1812(1)	4845(1)	30(1)
F(4)	5721(1)	2658(1)	5944(1)	28(1)
F(5)	4750(1)	2065(1)	6306(1)	27(1)
F(6)	4441(1)	2552(1)	4986(1)	26(1)
P(2)	-770(1)	-4264(1)	1508(1)	19(1)
F(10)	-574(1)	-5165(1)	1827(1)	34(1)
F(11)	-967(1)	-3362(1)	1200(1)	36(1)
F(12)	-224(1)	-4361(1)	954(1)	34(1)
F(13)	-1549(1)	-4565(1)	729(1)	34(1)
F(14)	-2(1)	-3971(1)	2293(1)	29(1)
F(15)	-1326(1)	-4171(1)	2061(1)	28(1)

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Table S39. Bond lengths [Å] and angles [deg] for [Cu(II)(L(0))₂]²⁺.

Cu(1)-N(2)	1.9419(11)
Cu(1)-N(5)	1.9561(11)
Cu(1)-N(1)	2.1588(11)
Cu(1)-N(3)	2.1626(11)
Cu(1)-N(6)	2.2133(11)
Cu(1)-N(4)	2.2331(11)
O(1)-C(2)	1.373(2)
O(1)-C(1)	1.427(2)
O(2)-C(20)	1.365(2)
O(2)-C(23)	1.429(2)
O(3)-C(32)	1.369(2)
O(3)-C(31)	1.435(2)
O(4)-C(52)	1.363(2)
O(4)-C(53)	1.430(2)
N(1)-C(8)	1.284(2)
N(1)-C(5)	1.427(2)
N(2)-C(10)	1.338(2)
N(2)-C(14)	1.344(2)
N(3)-C(15)	1.292(2)
N(3)-C(17)	1.424(2)
N(4)-C(38)	1.283(2)
N(4)-C(35)	1.421(2)
N(5)-C(40)	1.342(2)
N(5)-C(44)	1.347(2)
N(6)-C(45)	1.284(2)
N(6)-C(49)	1.432(2)
C(2)-C(3)	1.391(2)
C(2)-C(7)	1.394(2)
C(3)-C(4)	1.397(2)
C(4)-C(5)	1.391(2)
C(5)-C(6)	1.395(2)
C(6)-C(7)	1.381(2)
C(8)-C(10)	1.490(2)
C(8)-C(9)	1.496(2)
C(10)-C(11)	1.393(2)
C(11)-C(12)	1.391(2)
C(12)-C(13)	1.392(2)
C(13)-C(14)	1.392(2)
C(14)-C(15)	1.496(2)
C(15)-C(16)	1.493(2)
C(17)-C(22)	1.394(2)
C(17)-C(18)	1.399(2)
C(18)-C(19)	1.377(2)
C(19)-C(20)	1.395(2)
C(20)-C(21)	1.391(2)
C(21)-C(22)	1.393(2)
C(32)-C(33)	1.391(2)
C(32)-C(37)	1.399(2)
C(33)-C(34)	1.394(2)
C(34)-C(35)	1.392(2)
C(35)-C(36)	1.401(2)
C(36)-C(37)	1.383(2)
C(38)-C(39)	1.497(2)
C(38)-C(40)	1.501(2)
C(40)-C(41)	1.394(2)
C(41)-C(42)	1.386(2)
C(42)-C(43)	1.383(2)
C(43)-C(44)	1.389(2)
C(44)-C(45)	1.497(2)

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C(45)-C(46)	1.491(2)
C(47)-C(48)	1.385(2)
C(47)-C(52)	1.388(2)
C(48)-C(49)	1.391(2)
C(49)-C(50)	1.398(2)
C(50)-C(51)	1.377(2)
C(51)-C(52)	1.407(2)
P(1)-F(1)	1.5913(9)
P(1)-F(3)	1.6009(9)
P(1)-F(4)	1.6032(9)
P(1)-F(5)	1.6057(9)
P(1)-F(2)	1.6081(9)
P(1)-F(6)	1.6113(9)
P(2)-F(14)	1.5950(9)
P(2)-F(11)	1.5985(10)
P(2)-F(12)	1.5991(9)
P(2)-F(10)	1.6026(10)
P(2)-F(13)	1.6060(10)
P(2)-F(15)	1.6106(9)

N(2)-Cu(1)-N(5)	178.28(5)
N(2)-Cu(1)-N(1)	77.65(4)
N(5)-Cu(1)-N(1)	100.78(4)
N(2)-Cu(1)-N(3)	78.16(4)
N(5)-Cu(1)-N(3)	103.45(4)
N(1)-Cu(1)-N(3)	155.62(4)
N(2)-Cu(1)-N(6)	101.93(4)
N(5)-Cu(1)-N(6)	77.22(4)
N(1)-Cu(1)-N(6)	87.43(4)
N(3)-Cu(1)-N(6)	100.53(4)
N(2)-Cu(1)-N(4)	104.50(4)
N(5)-Cu(1)-N(4)	76.36(4)
N(1)-Cu(1)-N(4)	98.01(4)
N(3)-Cu(1)-N(4)	85.11(4)
N(6)-Cu(1)-N(4)	153.58(4)
C(2)-O(1)-C(1)	117.13(11)
C(20)-O(2)-C(23)	117.45(11)
C(32)-O(3)-C(31)	116.88(11)
C(52)-O(4)-C(53)	117.31(11)
C(8)-N(1)-C(5)	123.29(12)
C(8)-N(1)-Cu(1)	113.49(9)
C(5)-N(1)-Cu(1)	122.05(9)
C(10)-N(2)-C(14)	121.70(11)
C(10)-N(2)-Cu(1)	119.12(9)
C(14)-N(2)-Cu(1)	119.07(9)
C(15)-N(3)-C(17)	123.08(11)
C(15)-N(3)-Cu(1)	113.42(9)
C(17)-N(3)-Cu(1)	123.25(8)
C(38)-N(4)-C(35)	125.92(11)
C(38)-N(4)-Cu(1)	112.11(9)
C(35)-N(4)-Cu(1)	118.41(8)
C(40)-N(5)-C(44)	121.25(11)
C(40)-N(5)-Cu(1)	119.90(9)
C(44)-N(5)-Cu(1)	118.77(9)
C(45)-N(6)-C(49)	121.99(11)
C(45)-N(6)-Cu(1)	112.90(9)
C(49)-N(6)-Cu(1)	125.06(8)
O(1)-C(2)-C(3)	124.18(12)
O(1)-C(2)-C(7)	115.54(12)
C(3)-C(2)-C(7)	120.28(13)
C(2)-C(3)-C(4)	119.37(13)
C(5)-C(4)-C(3)	120.32(13)
C(4)-C(5)-C(6)	119.71(12)

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C(4)-C(5)-N(1)	121.48(12)
C(6)-C(5)-N(1)	118.42(12)
C(7)-C(6)-C(5)	120.19(12)
C(6)-C(7)-C(2)	120.10(13)
N(1)-C(8)-C(10)	114.61(12)
N(1)-C(8)-C(9)	126.44(13)
C(10)-C(8)-C(9)	118.95(12)
N(2)-C(10)-C(11)	120.85(12)
N(2)-C(10)-C(8)	114.28(11)
C(11)-C(10)-C(8)	124.86(12)
C(12)-C(11)-C(10)	118.13(13)
C(11)-C(12)-C(13)	120.42(13)
C(14)-C(13)-C(12)	118.44(13)
N(2)-C(14)-C(13)	120.43(13)
N(2)-C(14)-C(15)	114.47(11)
C(13)-C(14)-C(15)	125.09(12)
N(3)-C(15)-C(16)	126.96(12)
N(3)-C(15)-C(14)	114.56(12)
C(16)-C(15)-C(14)	118.46(11)
C(22)-C(17)-C(18)	118.75(12)
C(22)-C(17)-N(3)	124.55(12)
C(18)-C(17)-N(3)	116.68(11)
C(19)-C(18)-C(17)	120.78(13)
C(18)-C(19)-C(20)	120.02(13)
O(2)-C(20)-C(21)	124.53(13)
O(2)-C(20)-C(19)	115.46(12)
C(21)-C(20)-C(19)	120.01(13)
C(20)-C(21)-C(22)	119.55(13)
C(21)-C(22)-C(17)	120.75(13)
O(3)-C(32)-C(33)	124.53(13)
O(3)-C(32)-C(37)	115.41(12)
C(33)-C(32)-C(37)	120.06(12)
C(32)-C(33)-C(34)	119.67(13)
C(35)-C(34)-C(33)	120.81(13)
C(34)-C(35)-C(36)	118.81(12)
C(34)-C(35)-N(4)	124.05(12)
C(36)-C(35)-N(4)	116.64(12)
C(37)-C(36)-C(35)	120.87(12)
C(36)-C(37)-C(32)	119.74(13)
N(4)-C(38)-C(39)	127.58(12)
N(4)-C(38)-C(40)	113.64(11)
C(39)-C(38)-C(40)	118.77(11)
N(5)-C(40)-C(41)	120.35(12)
N(5)-C(40)-C(38)	114.74(11)
C(41)-C(40)-C(38)	124.91(12)
C(42)-C(41)-C(40)	118.65(12)
C(43)-C(42)-C(41)	120.41(12)
C(42)-C(43)-C(44)	118.42(12)
N(5)-C(44)-C(43)	120.81(12)
N(5)-C(44)-C(45)	115.23(11)
C(43)-C(44)-C(45)	123.82(12)
N(6)-C(45)-C(46)	126.83(12)
N(6)-C(45)-C(44)	114.76(11)
C(46)-C(45)-C(44)	118.39(11)
C(48)-C(47)-C(52)	119.84(12)
C(47)-C(48)-C(49)	120.76(13)
C(48)-C(49)-C(50)	119.33(12)
C(48)-C(49)-N(6)	120.65(12)
C(50)-C(49)-N(6)	119.84(12)
C(51)-C(50)-C(49)	120.35(13)
C(50)-C(51)-C(52)	119.99(13)
O(4)-C(52)-C(47)	125.14(12)
O(4)-C(52)-C(51)	115.13(12)

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C (47) -C (52) -C (51)	119.73 (12)
F (1) -P (1) -F (3)	90.57 (5)
F (1) -P (1) -F (4)	90.46 (5)
F (3) -P (1) -F (4)	89.75 (5)
F (1) -P (1) -F (5)	90.03 (5)
F (3) -P (1) -F (5)	179.39 (5)
F (4) -P (1) -F (5)	90.17 (5)
F (1) -P (1) -F (2)	90.32 (5)
F (3) -P (1) -F (2)	90.34 (5)
F (4) -P (1) -F (2)	179.21 (5)
F (5) -P (1) -F (2)	89.73 (5)
F (1) -P (1) -F (6)	179.69 (5)
F (3) -P (1) -F (6)	89.73 (5)
F (4) -P (1) -F (6)	89.57 (5)
F (5) -P (1) -F (6)	89.66 (5)
F (2) -P (1) -F (6)	89.65 (5)
F (14) -P (2) -F (11)	89.98 (5)
F (14) -P (2) -F (12)	90.68 (5)
F (11) -P (2) -F (12)	90.47 (5)
F (14) -P (2) -F (10)	89.78 (5)
F (11) -P (2) -F (10)	179.36 (6)
F (12) -P (2) -F (10)	90.13 (5)
F (14) -P (2) -F (13)	179.03 (5)
F (11) -P (2) -F (13)	90.49 (6)
F (12) -P (2) -F (13)	90.17 (5)
F (10) -P (2) -F (13)	89.74 (6)
F (14) -P (2) -F (15)	89.81 (5)
F (11) -P (2) -F (15)	89.66 (5)
F (12) -P (2) -F (15)	179.49 (5)
F (10) -P (2) -F (15)	89.75 (5)
F (13) -P (2) -F (15)	89.34 (5)

Symmetry transformations used to generate equivalent atoms:

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Table S40. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Cu}(\text{II})(\text{L}(\text{O}))_2]_2$. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Cu(1)	16(1)	13(1)	12(1)	-1(1)	4(1)	0(1)
O(1)	23(1)	33(1)	16(1)	3(1)	0(1)	-10(1)
O(2)	31(1)	21(1)	24(1)	0(1)	11(1)	9(1)
O(3)	28(1)	24(1)	13(1)	-2(1)	6(1)	2(1)
O(4)	23(1)	14(1)	40(1)	0(1)	12(1)	-1(1)
N(1)	18(1)	16(1)	14(1)	1(1)	5(1)	0(1)
N(2)	17(1)	16(1)	13(1)	-1(1)	5(1)	-2(1)
N(3)	17(1)	15(1)	13(1)	0(1)	6(1)	-1(1)
N(4)	18(1)	16(1)	13(1)	0(1)	5(1)	0(1)
N(5)	13(1)	14(1)	13(1)	0(1)	4(1)	0(1)
N(6)	18(1)	14(1)	14(1)	0(1)	5(1)	1(1)
C(1)	26(1)	41(1)	18(1)	5(1)	-2(1)	-5(1)
C(2)	17(1)	25(1)	16(1)	1(1)	3(1)	-3(1)
C(3)	22(1)	24(1)	16(1)	6(1)	3(1)	-1(1)
C(4)	23(1)	17(1)	21(1)	5(1)	5(1)	-1(1)
C(5)	18(1)	16(1)	15(1)	0(1)	4(1)	1(1)
C(6)	21(1)	19(1)	16(1)	4(1)	4(1)	-1(1)
C(7)	24(1)	19(1)	19(1)	3(1)	6(1)	-5(1)
C(8)	19(1)	18(1)	18(1)	0(1)	8(1)	0(1)
C(9)	21(1)	26(1)	39(1)	-11(1)	5(1)	5(1)
C(10)	19(1)	16(1)	16(1)	-1(1)	8(1)	0(1)
C(11)	24(1)	20(1)	23(1)	-4(1)	9(1)	2(1)
C(12)	30(1)	21(1)	21(1)	-9(1)	9(1)	-3(1)
C(13)	22(1)	22(1)	17(1)	-6(1)	4(1)	-4(1)
C(14)	19(1)	16(1)	13(1)	-1(1)	6(1)	-2(1)
C(15)	16(1)	16(1)	14(1)	0(1)	6(1)	-2(1)
C(16)	17(1)	26(1)	26(1)	-9(1)	3(1)	-1(1)
C(17)	16(1)	15(1)	16(1)	-1(1)	6(1)	-3(1)
C(18)	17(1)	17(1)	15(1)	1(1)	4(1)	-1(1)
C(19)	24(1)	18(1)	15(1)	-2(1)	8(1)	-2(1)
C(20)	21(1)	15(1)	21(1)	-2(1)	9(1)	-1(1)
C(21)	22(1)	19(1)	19(1)	4(1)	6(1)	2(1)
C(22)	21(1)	21(1)	14(1)	-1(1)	6(1)	-1(1)
C(23)	30(1)	25(1)	30(1)	-1(1)	9(1)	10(1)
C(31)	36(1)	35(1)	13(1)	0(1)	4(1)	4(1)
C(32)	24(1)	17(1)	13(1)	0(1)	6(1)	-3(1)
C(33)	20(1)	22(1)	16(1)	2(1)	5(1)	1(1)
C(34)	21(1)	19(1)	17(1)	1(1)	7(1)	3(1)
C(35)	21(1)	15(1)	12(1)	0(1)	6(1)	-2(1)
C(36)	19(1)	15(1)	16(1)	2(1)	5(1)	1(1)
C(37)	23(1)	15(1)	18(1)	-1(1)	9(1)	1(1)
C(38)	14(1)	16(1)	16(1)	1(1)	5(1)	0(1)
C(39)	24(1)	14(1)	17(1)	2(1)	6(1)	2(1)
C(40)	14(1)	14(1)	15(1)	0(1)	4(1)	0(1)
C(41)	20(1)	15(1)	20(1)	-2(1)	8(1)	-1(1)
C(42)	22(1)	17(1)	19(1)	-7(1)	7(1)	-3(1)
C(43)	18(1)	18(1)	13(1)	-2(1)	4(1)	-1(1)
C(44)	14(1)	15(1)	13(1)	-1(1)	4(1)	1(1)
C(45)	14(1)	16(1)	13(1)	0(1)	4(1)	2(1)
C(46)	23(1)	19(1)	12(1)	1(1)	5(1)	-1(1)
C(47)	23(1)	14(1)	21(1)	-1(1)	7(1)	3(1)
C(48)	19(1)	17(1)	20(1)	0(1)	9(1)	1(1)
C(49)	19(1)	14(1)	12(1)	0(1)	2(1)	-1(1)

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C(50)	20(1)	15(1)	25(1)	-2(1)	7(1)	3(1)
C(51)	17(1)	20(1)	30(1)	0(1)	9(1)	2(1)
C(52)	19(1)	14(1)	20(1)	1(1)	4(1)	-1(1)
C(53)	29(1)	13(1)	36(1)	-1(1)	11(1)	0(1)
P(1)	20(1)	17(1)	16(1)	0(1)	7(1)	1(1)
F(1)	31(1)	36(1)	35(1)	14(1)	9(1)	14(1)
F(2)	36(1)	20(1)	26(1)	-3(1)	9(1)	-8(1)
F(3)	40(1)	30(1)	28(1)	-4(1)	23(1)	1(1)
F(4)	27(1)	31(1)	26(1)	-9(1)	12(1)	-10(1)
F(5)	33(1)	32(1)	21(1)	-4(1)	16(1)	-4(1)
F(6)	25(1)	22(1)	28(1)	8(1)	8(1)	4(1)
P(2)	19(1)	25(1)	14(1)	1(1)	6(1)	-3(1)
F(10)	49(1)	23(1)	32(1)	2(1)	17(1)	-1(1)
F(11)	34(1)	32(1)	42(1)	17(1)	13(1)	4(1)
F(12)	28(1)	56(1)	25(1)	1(1)	16(1)	-2(1)
F(13)	25(1)	59(1)	16(1)	-9(1)	6(1)	-11(1)
F(14)	23(1)	37(1)	20(1)	-1(1)	2(1)	-7(1)
F(15)	30(1)	36(1)	22(1)	-9(1)	15(1)	-10(1)

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Table S41. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Cu}(\text{II})(\text{L}(\text{O}))_2]2+$.

	x	y	z	U(eq)
H(1A)	7375 (1)	1134 (1)	4938 (1)	47
H(1B)	7138 (1)	283 (1)	4493 (1)	47
H(1C)	6516 (1)	744 (1)	4808 (1)	47
H(3)	5879 (1)	-204 (1)	3789 (1)	26
H(4)	4784 (1)	-764 (1)	2682 (1)	25
H(6)	4711 (1)	1167 (1)	1234 (1)	23
H(7)	5817 (1)	1710 (1)	2317 (1)	25
H(9A)	5090 (1)	-1175 (1)	1402 (1)	46
H(9B)	4684 (1)	-1473 (1)	447 (1)	46
H(9C)	4468 (1)	-1906 (1)	1170 (1)	46
H(11)	3324 (1)	-2114 (1)	-230 (1)	27
H(12)	1993 (1)	-2296 (1)	-1201 (1)	29
H(13)	1000 (1)	-1329 (1)	-1327 (1)	25
H(16A)	37 (1)	489 (1)	-928 (1)	37
H(16B)	74 (1)	-463 (1)	-948 (1)	37
H(16C)	341 (1)	52 (1)	-1588 (1)	37
H(18)	1476 (1)	1049 (1)	1610 (1)	20
H(19)	735 (1)	2056 (1)	1916 (1)	23
H(21)	-179 (1)	2700 (1)	-548 (1)	25
H(22)	535 (1)	1656 (1)	-859 (1)	23
H(23A)	-1022 (1)	3909 (1)	571 (1)	44
H(23B)	-1189 (1)	3189 (1)	-85 (1)	44
H(23C)	-477 (1)	3809 (1)	16 (1)	44
H(31A)	1438 (1)	580 (1)	-4404 (1)	44
H(31B)	1435 (1)	1382 (1)	-3900 (1)	44
H(31C)	1014 (1)	595 (1)	-3727 (1)	44
H(33)	1375 (1)	1555 (1)	-2634 (1)	24
H(34)	1721 (1)	1960 (1)	-1234 (1)	22
H(36)	3704 (1)	540 (1)	-530 (1)	21
H(37)	3399 (1)	180 (1)	-1929 (1)	22
H(39A)	2666 (1)	2841 (1)	-516 (1)	29
H(39B)	3256 (1)	3235 (1)	346 (1)	29
H(39C)	2313 (1)	3132 (1)	170 (1)	29
H(41)	3400 (1)	3186 (1)	1794 (1)	22
H(42)	3748 (1)	2930 (1)	3232 (1)	23
H(43)	3634 (1)	1638 (1)	3691 (1)	20
H(46A)	3008 (1)	-435 (1)	3635 (1)	28
H(46B)	2817 (1)	469 (1)	3791 (1)	28
H(46C)	3727 (1)	202 (1)	3959 (1)	28
H(47)	2724 (1)	-2806 (1)	1861 (1)	23
H(48)	3300 (1)	-1556 (1)	1883 (1)	22
H(50)	1465 (1)	-526 (1)	2376 (1)	24
H(51)	885 (1)	-1769 (1)	2356 (1)	27
H(53A)	1410 (1)	-4285 (1)	2042 (1)	40
H(53B)	2266 (1)	-3868 (1)	2530 (1)	40
H(53C)	1867 (1)	-3834 (1)	1523 (1)	40

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Table S43. Crystal data and structure refinement for [Zn(II) (L(0))₂]²⁺.

Identification code	ST3300
Empirical formula	C ₄₆ H ₄₆ F ₁₂ N ₆ O ₄ P ₂ Zn
Formula weight	1102.20
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2 ₁ /c
Unit cell dimensions	a = 17.807(2) Å alpha = 90 deg. b = 16.825(2) Å beta = 111.38(2) deg. c = 17.037(2) Å gamma = 90 deg.
Volume	4753.1(10) Å ³
Z	4
Density (calculated)	1.540 Mg/m ³
Absorption coefficient	0.682 mm ⁻¹
F(000)	2256
Crystal size	0.20 x 0.20 x 0.19 mm
Theta range for data collection	2.74 to 32.50 deg.
Index ranges	-27<=h<=27, -25<=k<=25, -26<=l<=26
Reflections collected	33840
Independent reflections	17173 [R(int) = 0.0344]
Absorption correction	Not measured
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	17161 / 0 / 648
Goodness-of-fit on F ²	1.035
Final R indices [I>2sigma(I)]	R1 = 0.0349, wR2 = 0.0808
R indices (all data)	R1 = 0.0631, wR2 = 0.0859
Largest diff. peak and hole	0.556 and -0.374 e.Å ⁻³

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Table S44. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Zn(II)(L(0))}_2]^{2+}$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Zn(1)	2224(1)	9587(1)	4090(1)	15(1)
O(1)	3641(1)	13077(1)	2933(1)	25(1)
O(2)	2813(1)	9417(1)	8180(1)	24(1)
O(3)	-1571(1)	8848(1)	1292(1)	28(1)
O(4)	5214(1)	6992(1)	4032(1)	25(1)
N(1)	2231(1)	10112(1)	2910(1)	16(1)
N(2)	1932(1)	8667(1)	3256(1)	15(1)
N(3)	2082(1)	8556(1)	4824(1)	16(1)
N(4)	1062(1)	10168(1)	3856(1)	17(1)
N(5)	2495(1)	10529(1)	4905(1)	16(1)
N(6)	3525(1)	9468(1)	4811(1)	15(1)
C(1)	3234(1)	13799(1)	2977(1)	27(1)
C(2)	3242(1)	12377(1)	2914(1)	19(1)
C(3)	3616(1)	11698(1)	2755(1)	21(1)
C(4)	3275(1)	10962(1)	2732(1)	20(1)
C(5)	2550(1)	10889(1)	2865(1)	16(1)
C(6)	2177(1)	11563(1)	3017(1)	19(1)
C(7)	2518(1)	12310(1)	3041(1)	20(1)
C(8)	1965(1)	9658(1)	2264(1)	15(1)
C(9)	1856(1)	9869(1)	1377(1)	19(1)
C(10)	1768(1)	8824(1)	2439(1)	15(1)
C(11)	1487(1)	8235(1)	1836(1)	18(1)
C(12)	1411(1)	7473(1)	2107(1)	21(1)
C(13)	1604(1)	7310(1)	2955(1)	19(1)
C(14)	1852(1)	7937(1)	3525(1)	15(1)
C(15)	2051(1)	7882(1)	4461(1)	16(1)
C(16)	2204(1)	7082(1)	4867(1)	21(1)
C(17)	2271(1)	8680(1)	5703(1)	16(1)
C(18)	2953(1)	8373(1)	6331(1)	19(1)
C(19)	3160(1)	8614(1)	7164(1)	20(1)
C(20)	2670(1)	9152(1)	7379(1)	19(1)
C(21)	1979(1)	9452(1)	6756(1)	19(1)
C(22)	1790(1)	9226(1)	5925(1)	18(1)
C(23)	3559(1)	9186(1)	8825(1)	31(1)
C(31)	-1918(1)	9234(1)	496(1)	34(1)
C(32)	-940(1)	9226(1)	1896(1)	21(1)
C(33)	-593(1)	8816(1)	2651(1)	23(1)
C(34)	56(1)	9136(1)	3298(1)	21(1)
C(35)	348(1)	9885(1)	3206(1)	18(1)
C(36)	-2(1)	10295(1)	2452(1)	21(1)
C(37)	-644(1)	9967(1)	1791(1)	23(1)
C(38)	1101(1)	10841(1)	4225(1)	19(1)
C(39)	416(1)	11398(1)	4103(1)	34(1)
C(40)	1918(1)	11060(1)	4844(1)	18(1)
C(41)	2095(1)	11754(1)	5323(1)	24(1)
C(42)	2882(1)	11867(1)	5878(1)	26(1)
C(43)	3472(1)	11299(1)	5950(1)	22(1)
C(44)	3254(1)	10629(1)	5436(1)	17(1)
C(45)	3821(1)	9978(1)	5410(1)	17(1)
C(46)	4658(1)	9993(1)	6047(1)	27(1)
C(47)	3971(1)	8810(1)	4677(1)	16(1)
C(48)	4455(1)	8308(1)	5306(1)	19(1)
C(49)	4875(1)	7686(1)	5118(1)	21(1)

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C(50)	4812(1)	7567(1)	4290(1)	20(1)
C(51)	4305(1)	8050(1)	3649(1)	20(1)
C(52)	3881(1)	8658(1)	3841(1)	18(1)
C(53)	5771(1)	6510(1)	4673(1)	30(1)
P(1)	-106(1)	8099(1)	-609(1)	19(1)
F(11)	-739(1)	7393(1)	-982(1)	28(1)
F(12)	538(1)	8800(1)	-228(1)	29(1)
F(13)	237(1)	7969(1)	-1350(1)	28(1)
F(14)	540(1)	7466(1)	-38(1)	26(1)
F(15)	-441(1)	8220(1)	137(1)	31(1)
F(16)	-741(1)	8726(1)	-1177(1)	35(1)
P(2)	5770(1)	14257(1)	3524(1)	20(1)
F(21)	5012(1)	13943(1)	2748(1)	30(1)
F(22)	6539(1)	14579(1)	4292(1)	34(1)
F(23)	6329(1)	14154(1)	2971(1)	29(1)
F(24)	5565(1)	15147(1)	3179(1)	35(1)
F(25)	5221(1)	14365(1)	4077(1)	36(1)
F(26)	5977(1)	13368(1)	3858(1)	38(1)

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Table S45. Bond lengths [Å] and angles [deg] for [Zn(II)(L(0))₂]²⁺.

Zn(1)-N(2)	2.0369(10)
Zn(1)-N(5)	2.0464(10)
Zn(1)-N(4)	2.1893(11)
Zn(1)-N(1)	2.1997(11)
Zn(1)-N(6)	2.2003(12)
Zn(1)-N(3)	2.2051(10)
O(1)-C(2)	1.368(2)
O(1)-C(1)	1.431(2)
O(2)-C(20)	1.368(2)
O(2)-C(23)	1.435(2)
O(3)-C(32)	1.372(2)
O(3)-C(31)	1.426(2)
O(4)-C(50)	1.368(2)
O(4)-C(53)	1.429(2)
N(1)-C(8)	1.282(2)
N(1)-C(5)	1.438(2)
N(2)-C(14)	1.336(2)
N(2)-C(10)	1.339(2)
N(3)-C(15)	1.283(2)
N(3)-C(17)	1.426(2)
N(4)-C(38)	1.284(2)
N(4)-C(35)	1.430(2)
N(5)-C(44)	1.334(2)
N(5)-C(40)	1.336(2)
N(6)-C(45)	1.290(2)
N(6)-C(47)	1.428(2)
C(2)-C(7)	1.387(2)
C(2)-C(3)	1.398(2)
C(3)-C(4)	1.373(2)
C(4)-C(5)	1.395(2)
C(5)-C(6)	1.386(2)
C(6)-C(7)	1.389(2)
C(8)-C(9)	1.494(2)
C(8)-C(10)	1.502(2)
C(10)-C(11)	1.384(2)
C(11)-C(12)	1.387(2)
C(12)-C(13)	1.385(2)
C(13)-C(14)	1.393(2)
C(14)-C(15)	1.505(2)
C(15)-C(16)	1.492(2)
C(17)-C(18)	1.393(2)
C(17)-C(22)	1.398(2)
C(18)-C(19)	1.391(2)
C(19)-C(20)	1.395(2)
C(20)-C(21)	1.394(2)
C(21)-C(22)	1.383(2)
C(32)-C(33)	1.389(2)
C(32)-C(37)	1.391(2)
C(33)-C(34)	1.383(2)
C(34)-C(35)	1.394(2)
C(35)-C(36)	1.389(2)
C(36)-C(37)	1.393(2)
C(38)-C(39)	1.492(2)
C(38)-C(40)	1.499(2)
C(40)-C(41)	1.393(2)
C(41)-C(42)	1.388(2)
C(42)-C(43)	1.392(2)
C(43)-C(44)	1.394(2)
C(44)-C(45)	1.500(2)

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C (45) -C (46)	1.491 (2)
C (47) -C (48)	1.389 (2)
C (47) -C (52)	1.398 (2)
C (48) -C (49)	1.389 (2)
C (49) -C (50)	1.389 (2)
C (50) -C (51)	1.396 (2)
C (51) -C (52)	1.380 (2)
P (1) -F (16)	1.5908 (9)
P (1) -F (15)	1.6015 (9)
P (1) -F (11)	1.6015 (9)
P (1) -F (13)	1.6056 (9)
P (1) -F (12)	1.6075 (9)
P (1) -F (14)	1.6100 (9)
P (2) -F (26)	1.5952 (9)
P (2) -F (21)	1.5958 (9)
P (2) -F (25)	1.5972 (9)
P (2) -F (24)	1.6016 (9)
P (2) -F (22)	1.6056 (10)
P (2) -F (23)	1.6108 (9)

N (2) -Zn (1) -N (5)	178.50 (4)
N (2) -Zn (1) -N (4)	103.25 (4)
N (5) -Zn (1) -N (4)	75.56 (4)
N (2) -Zn (1) -N (1)	75.69 (4)
N (5) -Zn (1) -N (1)	103.30 (4)
N (4) -Zn (1) -N (1)	88.49 (4)
N (2) -Zn (1) -N (6)	105.62 (4)
N (5) -Zn (1) -N (6)	75.61 (4)
N (4) -Zn (1) -N (6)	151.02 (4)
N (1) -Zn (1) -N (6)	101.01 (4)
N (2) -Zn (1) -N (3)	75.24 (4)
N (5) -Zn (1) -N (3)	105.78 (4)
N (4) -Zn (1) -N (3)	99.13 (4)
N (1) -Zn (1) -N (3)	150.92 (4)
N (6) -Zn (1) -N (3)	85.82 (4)
C (2) -O (1) -C (1)	117.64 (10)
C (20) -O (2) -C (23)	117.39 (11)
C (32) -O (3) -C (31)	117.08 (11)
C (50) -O (4) -C (53)	117.06 (10)
C (8) -N (1) -C (5)	121.67 (10)
C (8) -N (1) -Zn (1)	114.99 (8)
C (5) -N (1) -Zn (1)	123.25 (8)
C (14) -N (2) -C (10)	121.92 (10)
C (14) -N (2) -Zn (1)	119.34 (8)
C (10) -N (2) -Zn (1)	118.55 (8)
C (15) -N (3) -C (17)	125.98 (11)
C (15) -N (3) -Zn (1)	114.58 (8)
C (17) -N (3) -Zn (1)	116.63 (8)
C (38) -N (4) -C (35)	123.08 (11)
C (38) -N (4) -Zn (1)	115.24 (9)
C (35) -N (4) -Zn (1)	120.47 (8)
C (44) -N (5) -C (40)	121.90 (11)
C (44) -N (5) -Zn (1)	119.17 (9)
C (40) -N (5) -Zn (1)	118.73 (9)
C (45) -N (6) -C (47)	123.50 (11)
C (45) -N (6) -Zn (1)	115.10 (9)
C (47) -N (6) -Zn (1)	120.98 (8)
O (1) -C (2) -C (7)	124.74 (11)
O (1) -C (2) -C (3)	115.37 (11)
C (7) -C (2) -C (3)	119.89 (12)
C (4) -C (3) -C (2)	120.35 (12)
C (3) -C (4) -C (5)	120.13 (12)
C (6) -C (5) -C (4)	119.45 (12)

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C(6)-C(5)-N(1)	120.58(11)
C(4)-C(5)-N(1)	119.78(11)
C(5)-C(6)-C(7)	120.80(12)
C(2)-C(7)-C(6)	119.37(12)
N(1)-C(8)-C(9)	126.73(11)
N(1)-C(8)-C(10)	115.16(11)
C(9)-C(8)-C(10)	118.09(10)
N(2)-C(10)-C(11)	120.85(11)
N(2)-C(10)-C(8)	114.44(10)
C(11)-C(10)-C(8)	124.59(11)
C(10)-C(11)-C(12)	117.88(12)
C(13)-C(12)-C(11)	120.88(12)
C(12)-C(13)-C(14)	118.19(12)
N(2)-C(14)-C(13)	120.20(11)
N(2)-C(14)-C(15)	114.06(10)
C(13)-C(14)-C(15)	125.74(11)
N(3)-C(15)-C(16)	127.30(12)
N(3)-C(15)-C(14)	114.04(11)
C(16)-C(15)-C(14)	118.64(11)
C(18)-C(17)-C(22)	118.94(11)
C(18)-C(17)-N(3)	123.93(11)
C(22)-C(17)-N(3)	116.60(11)
C(19)-C(18)-C(17)	120.58(12)
C(18)-C(19)-C(20)	119.86(12)
O(2)-C(20)-C(21)	115.70(12)
O(2)-C(20)-C(19)	124.42(12)
C(21)-C(20)-C(19)	119.88(12)
C(22)-C(21)-C(20)	119.85(12)
C(21)-C(22)-C(17)	120.86(12)
O(3)-C(32)-C(33)	115.51(12)
O(3)-C(32)-C(37)	124.37(12)
C(33)-C(32)-C(37)	120.12(12)
C(34)-C(33)-C(32)	120.38(13)
C(33)-C(34)-C(35)	119.95(12)
C(36)-C(35)-C(34)	119.56(12)
C(36)-C(35)-N(4)	121.56(12)
C(34)-C(35)-N(4)	118.45(11)
C(35)-C(36)-C(37)	120.62(12)
C(32)-C(37)-C(36)	119.33(12)
N(4)-C(38)-C(39)	126.21(12)
N(4)-C(38)-C(40)	115.21(11)
C(39)-C(38)-C(40)	118.57(11)
N(5)-C(40)-C(41)	120.75(12)
N(5)-C(40)-C(38)	114.32(11)
C(41)-C(40)-C(38)	124.92(12)
C(42)-C(41)-C(40)	118.08(13)
C(41)-C(42)-C(43)	120.50(12)
C(42)-C(43)-C(44)	118.15(13)
N(5)-C(44)-C(43)	120.59(12)
N(5)-C(44)-C(45)	114.47(11)
C(43)-C(44)-C(45)	124.93(12)
N(6)-C(45)-C(46)	126.75(12)
N(6)-C(45)-C(44)	115.10(11)
C(46)-C(45)-C(44)	118.14(11)
C(48)-C(47)-C(52)	118.82(11)
C(48)-C(47)-N(6)	125.01(11)
C(52)-C(47)-N(6)	116.13(11)
C(47)-C(48)-C(49)	121.06(12)
C(48)-C(49)-C(50)	119.44(12)
O(4)-C(50)-C(49)	124.75(12)
O(4)-C(50)-C(51)	115.24(11)
C(49)-C(50)-C(51)	120.01(12)
C(52)-C(51)-C(50)	119.97(12)

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C(51)-C(52)-C(47)	120.57(12)
F(16)-P(1)-F(15)	90.65(5)
F(16)-P(1)-F(11)	90.49(5)
F(15)-P(1)-F(11)	89.85(5)
F(16)-P(1)-F(13)	90.07(5)
F(15)-P(1)-F(13)	179.27(5)
F(11)-P(1)-F(13)	90.04(5)
F(16)-P(1)-F(12)	90.20(5)
F(15)-P(1)-F(12)	90.25(5)
F(11)-P(1)-F(12)	179.30(5)
F(13)-P(1)-F(12)	89.85(5)
F(16)-P(1)-F(14)	179.58(5)
F(15)-P(1)-F(14)	89.75(5)
F(11)-P(1)-F(14)	89.63(5)
F(13)-P(1)-F(14)	89.53(5)
F(12)-P(1)-F(14)	89.68(5)
F(26)-P(2)-F(21)	90.04(5)
F(26)-P(2)-F(25)	90.43(5)
F(21)-P(2)-F(25)	90.64(5)
F(26)-P(2)-F(24)	179.33(5)
F(21)-P(2)-F(24)	89.71(5)
F(25)-P(2)-F(24)	90.19(5)
F(26)-P(2)-F(22)	90.45(5)
F(21)-P(2)-F(22)	178.99(5)
F(25)-P(2)-F(22)	90.23(5)
F(24)-P(2)-F(22)	89.79(5)
F(26)-P(2)-F(23)	89.82(5)
F(21)-P(2)-F(23)	89.85(5)
F(25)-P(2)-F(23)	179.44(5)
F(24)-P(2)-F(23)	89.56(5)
F(22)-P(2)-F(23)	89.27(5)

Symmetry transformations used to generate equivalent atoms:

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Table S46. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Zn}(\text{II})(\text{L}(0))_2]2+$. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Zn(1)	18(1)	13(1)	12(1)	-1(1)	4(1)	0(1)
O(1)	23(1)	14(1)	38(1)	1(1)	12(1)	-2(1)
O(2)	30(1)	27(1)	13(1)	-3(1)	6(1)	2(1)
O(3)	24(1)	36(1)	17(1)	4(1)	-1(1)	-11(1)
O(4)	30(1)	22(1)	24(1)	0(1)	11(1)	10(1)
N(1)	19(1)	14(1)	15(1)	0(1)	6(1)	0(1)
N(2)	16(1)	14(1)	15(1)	-1(1)	5(1)	0(1)
N(3)	18(1)	18(1)	14(1)	-1(1)	6(1)	0(1)
N(4)	17(1)	17(1)	15(1)	1(1)	5(1)	-1(1)
N(5)	19(1)	16(1)	14(1)	-1(1)	7(1)	-2(1)
N(6)	17(1)	17(1)	14(1)	0(1)	7(1)	-1(1)
C(1)	30(1)	14(1)	38(1)	0(1)	13(1)	0(1)
C(2)	20(1)	16(1)	19(1)	1(1)	4(1)	-1(1)
C(3)	17(1)	21(1)	27(1)	1(1)	9(1)	1(1)
C(4)	22(1)	16(1)	21(1)	-1(1)	8(1)	2(1)
C(5)	19(1)	16(1)	12(1)	1(1)	3(1)	-1(1)
C(6)	19(1)	19(1)	20(1)	0(1)	10(1)	0(1)
C(7)	22(1)	14(1)	23(1)	0(1)	9(1)	2(1)
C(8)	15(1)	18(1)	13(1)	1(1)	5(1)	2(1)
C(9)	22(1)	20(1)	14(1)	2(1)	5(1)	0(1)
C(10)	15(1)	17(1)	13(1)	0(1)	4(1)	1(1)
C(11)	19(1)	21(1)	15(1)	-3(1)	6(1)	-1(1)
C(12)	23(1)	19(1)	20(1)	-7(1)	7(1)	-4(1)
C(13)	21(1)	15(1)	22(1)	-3(1)	9(1)	-1(1)
C(14)	15(1)	16(1)	15(1)	-1(1)	6(1)	0(1)
C(15)	15(1)	17(1)	17(1)	2(1)	6(1)	0(1)
C(16)	26(1)	16(1)	20(1)	2(1)	8(1)	2(1)
C(17)	20(1)	17(1)	13(1)	1(1)	7(1)	-2(1)
C(18)	21(1)	21(1)	18(1)	2(1)	9(1)	1(1)
C(19)	22(1)	21(1)	17(1)	3(1)	6(1)	1(1)
C(20)	25(1)	19(1)	14(1)	-1(1)	7(1)	-3(1)
C(21)	23(1)	17(1)	18(1)	-1(1)	10(1)	1(1)
C(22)	19(1)	17(1)	16(1)	2(1)	6(1)	1(1)
C(23)	36(1)	39(1)	13(1)	0(1)	2(1)	6(1)
C(31)	29(1)	46(1)	19(1)	5(1)	-3(1)	-7(1)
C(32)	17(1)	27(1)	17(1)	2(1)	4(1)	-2(1)
C(33)	24(1)	22(1)	21(1)	4(1)	5(1)	-6(1)
C(34)	21(1)	21(1)	18(1)	5(1)	4(1)	-1(1)
C(35)	17(1)	19(1)	16(1)	0(1)	5(1)	1(1)
C(36)	22(1)	19(1)	21(1)	4(1)	6(1)	-1(1)
C(37)	21(1)	25(1)	17(1)	7(1)	2(1)	-1(1)
C(38)	20(1)	19(1)	20(1)	0(1)	8(1)	1(1)
C(39)	23(1)	30(1)	43(1)	-12(1)	5(1)	5(1)
C(40)	21(1)	17(1)	18(1)	-1(1)	8(1)	0(1)
C(41)	26(1)	21(1)	26(1)	-6(1)	10(1)	2(1)
C(42)	32(1)	21(1)	24(1)	-10(1)	11(1)	-4(1)
C(43)	23(1)	24(1)	19(1)	-6(1)	5(1)	-4(1)
C(44)	19(1)	18(1)	13(1)	-1(1)	6(1)	-2(1)
C(45)	18(1)	18(1)	15(1)	-1(1)	6(1)	-3(1)
C(46)	19(1)	28(1)	28(1)	-10(1)	2(1)	-1(1)
C(47)	16(1)	17(1)	17(1)	-2(1)	6(1)	-2(1)
C(48)	19(1)	23(1)	16(1)	1(1)	7(1)	0(1)
C(49)	21(1)	20(1)	21(1)	4(1)	7(1)	2(1)

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C(50)	21(1)	16(1)	23(1)	-1(1)	9(1)	1(1)
C(51)	24(1)	18(1)	17(1)	-3(1)	9(1)	-1(1)
C(52)	19(1)	17(1)	16(1)	1(1)	5(1)	0(1)
C(53)	31(1)	26(1)	33(1)	0(1)	10(1)	11(1)
P(1)	22(1)	19(1)	16(1)	0(1)	8(1)	0(1)
F(11)	27(1)	33(1)	26(1)	-7(1)	10(1)	-10(1)
F(12)	36(1)	21(1)	27(1)	-2(1)	8(1)	-7(1)
F(13)	33(1)	32(1)	23(1)	-2(1)	16(1)	-3(1)
F(14)	26(1)	23(1)	27(1)	7(1)	8(1)	3(1)
F(15)	42(1)	32(1)	27(1)	-4(1)	22(1)	1(1)
F(16)	31(1)	36(1)	35(1)	12(1)	8(1)	12(1)
P(2)	20(1)	26(1)	15(1)	2(1)	7(1)	-3(1)
F(21)	24(1)	40(1)	24(1)	-2(1)	3(1)	-8(1)
F(22)	26(1)	58(1)	18(1)	-9(1)	6(1)	-11(1)
F(23)	30(1)	38(1)	24(1)	-10(1)	16(1)	-11(1)
F(24)	49(1)	25(1)	34(1)	3(1)	16(1)	0(1)
F(25)	30(1)	57(1)	27(1)	1(1)	17(1)	-1(1)
F(26)	35(1)	34(1)	45(1)	18(1)	13(1)	4(1)

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Table S47. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Zn}(\text{II})(\text{L}(\text{O}))_2]2+$.

	x	y	z	U(eq)
H(1A)	3573(3)	14254(1)	2963(6)	40
H(1B)	3128(5)	13810(3)	3502(3)	40
H(1C)	2723(3)	13829(3)	2495(3)	40
H(3)	4108(1)	11745(1)	2662(1)	26
H(4)	3533(1)	10503(1)	2626(1)	24
H(6)	1683(1)	11515(1)	3106(1)	23
H(7)	2258(1)	12770(1)	3144(1)	23
H(9A)	1304(2)	9742(5)	1004(1)	28
H(9B)	2238(4)	9566(4)	1202(2)	28
H(9C)	1954(5)	10439(1)	1343(1)	28
H(11)	1350(1)	8349(1)	1254(1)	22
H(12)	1224(1)	7056(1)	1706(1)	25
H(13)	1568(1)	6784(1)	3143(1)	23
H(16A)	2727(3)	6883(2)	4886(5)	31
H(16B)	1778(3)	6714(2)	4540(3)	31
H(16C)	2207(6)	7123(1)	5442(2)	31
H(18)	3280(1)	7996(1)	6189(1)	23
H(19)	3633(1)	8412(1)	7587(1)	24
H(21)	1639(1)	9811(1)	6901(1)	23
H(22)	1328(1)	9444(1)	5500(1)	21
H(23A)	3618(3)	9462(5)	9351(2)	47
H(23B)	4009(1)	9329(6)	8651(3)	47
H(23C)	3560(3)	8611(1)	8913(5)	47
H(31A)	-2348(4)	8900(3)	114(2)	51
H(31B)	-1502(2)	9319(6)	255(3)	51
H(31C)	-2143(6)	9747(3)	571(1)	51
H(33)	-802(1)	8313(1)	2722(1)	28
H(34)	302(1)	8846(1)	3806(1)	25
H(36)	199(1)	10804(1)	2386(1)	26
H(37)	-876(1)	10246(1)	1274(1)	27
H(39A)	492(3)	11879(3)	3816(6)	51
H(39B)	397(4)	11541(5)	4653(1)	51
H(39C)	-91(1)	11140(2)	3761(6)	51
H(41)	1689(1)	12139(1)	5270(1)	29
H(42)	3018(1)	12336(1)	6211(1)	31
H(43)	4008(1)	11367(1)	6338(1)	27
H(46A)	4660(1)	9769(5)	6579(2)	40
H(46B)	4853(2)	10542(1)	6139(5)	40
H(46C)	5011(1)	9676(5)	5843(3)	40
H(48)	4500(1)	8392(1)	5873(1)	23
H(49)	5202(1)	7345(1)	5553(1)	25
H(51)	4252(1)	7960(1)	3080(1)	24
H(52)	3525(1)	8976(1)	3402(1)	21
H(53A)	6027(5)	6130(4)	4414(1)	45
H(53B)	5484(1)	6222(5)	4977(4)	45
H(53C)	6185(4)	6850(1)	5068(4)	45