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Table S28. Bond lengths [Å] and angles [°] for 23.

N(1)-C(1)	1.376(5)	C(10)-C(27)	1.552(6)	C(35)-C(36)	1.539(6)
N(1)-C(4)	1.394(5)	C(10)-C(25)	1.555(5)	Li(1)-O(1)	2.358(9)
N(1)-Li(2)	2.025(6)	C(11)-C(12)	1.379(6)	Li(1)-Li(2)	2.726(9)
N(1)-Li(1)	2.145(7)	C(11)-Li(4)	2.329(9)	Li(1)-Li(3)	2.804(10)
N(2)-C(9)	1.379(5)	C(12)-C(13)	1.417(5)	Li(1)-Li(4)	2.977(12)
N(2)-C(6)	1.402(5)	C(12)-Li(4)	2.315(10)	O(1)-C(37)	1.403(7)
N(2)-Li(2)	2.077(7)	C(13)-C(14)	1.378(6)	O(1)-C(40)	1.428(6)
N(2)-Li(1)	2.213(7)	C(13)-Li(4)	2.289(10)	O(1)-Li(4)	2.012(10)
N(3)-C(11)	1.387(5)	C(14)-C(15)	1.524(5)	C(37)-C(38)	1.419(9)
N(3)-C(14)	1.393(5)	C(14)-Li(4)	2.305(10)	C(38)-C(39)	1.515(9)
N(3)-Li(3)	2.136(8)	C(14)-Li(3)	2.671(8)	C(39)-C(40)	1.563(8)
N(3)-Li(1)	2.261(7)	C(15)-C(16)	1.522(5)	C(40)-Li(4)	2.776(11)
N(3)-Li(4)	2.354(9)	C(15)-N(6)	1.542(5)	Li(2)-O(2)	1.936(7)
N(4)-C(19)	1.383(5)	C(15)-C(31)	1.556(5)	O(2)-C(41)	1.445(5)
N(4)-C(16)	1.388(5)	C(15)-Li(3)	2.600(7)	O(2)-C(44)	1.467(4)
N(4)-Li(3)	2.061(7)	C(16)-C(17)	1.385(5)	C(41)-C(42)	1.523(6)
N(4)-Li(1)	2.195(7)	C(16)-Li(3)	2.637(7)	C(42)-C(43)	1.528(6)
C(1)-C(2)	1.398(5)	C(17)-C(18)	1.400(6)	C(43)-C(44)	1.508(6)
C(1)-C(20)	1.527(5)	C(18)-C(19)	1.390(5)	Li(3)-O(3)	1.993(7)
C(2)-C(3)	1.413(5)	C(19)-C(20)	1.531(5)	O(3)-C(48)	1.434(5)
C(3)-C(4)	1.389(5)	C(20)-C(33)	1.542(5)	O(3)-C(45)	1.449(6)
C(4)-C(5)	1.525(5)	C(20)-C(35)	1.543(5)	C(45)-C(46)	1.519(9)
C(4)-Li(2)	2.601(7)	N(5)-C(21)	1.466(5)	C(46)-C(47)	1.354(10)
C(5)-C(6)	1.518(6)	N(5)-C(22)	1.470(6)	C(47)-C(48)	1.475(8)
C(5)-N(5)	1.546(5)	N(5)-Li(2)	2.103(7)	Li(4)-O(4)	2.003(10)
C(5)-C(23)	1.553(5)	C(23)-C(24)	1.530(7)	O(4)-C(52)	1.341(7)
C(5)-Li(2)	2.538(7)	C(25)-C(26)	1.534(5)	O(4)-C(49)	1.391(7)
C(6)-C(7)	1.372(6)	C(27)-C(28)	1.533(5)	C(49)-C(50)	1.511(10)
C(6)-Li(2)	2.609(8)	N(6)-C(30)	1.469(5)	C(50)-C(51)	1.530(11)
C(7)-C(8)	1.408(6)	N(6)-C(29)	1.480(5)	C(51)-C(52)	1.459(11)
C(8)-C(9)	1.382(6)	N(6)-Li(3)	2.172(7)	C(53)-C(54)	1.502(8)
C(9)-C(10)	1.534(5)	C(31)-C(32)	1.506(6)	C(53)-C(53) ^a	1.525(11)
C(10)-C(11)	1.535(5)	C(33)-C(34)	1.524(5)	C(54)-C(55)	1.559(9)
C(1)-N(1)-C(4)	106.4(3)	N(6)-C(15)-Li(3)	56.5(2)	C(5)-Li(2)-C(6)	34.27(15)
C(1)-N(1)-Li(2)	144.5(3)	C(31)-C(15)-Li(3)	168.4(3)	C(4)-Li(2)-C(6)	58.62(18)
C(4)-N(1)-Li(2)	97.3(3)	C(17)-C(16)-N(4)	110.2(3)	O(2)-Li(2)-Li(1)	127.7(3)
C(1)-N(1)-Li(1)	111.7(3)	C(17)-C(16)-C(15)	128.1(3)	N(1)-Li(2)-Li(1)	51.1(2)
C(4)-N(1)-Li(1)	112.6(3)	N(4)-C(16)-C(15)	120.1(3)	N(2)-Li(2)-Li(1)	52.8(2)
Li(2)-N(1)-Li(1)	81.6(3)	C(17)-C(16)-Li(3)	145.6(3)	N(5)-Li(2)-Li(1)	121.8(3)
C(9)-N(2)-C(6)	105.7(3)	N(4)-C(16)-Li(3)	50.7(2)	C(5)-Li(2)-Li(1)	84.3(3)
C(9)-N(2)-Li(2)	145.8(3)	C(15)-C(16)-Li(3)	71.8(2)	C(4)-Li(2)-Li(1)	67.8(2)
C(6)-N(2)-Li(2)	95.2(3)	C(16)-C(17)-C(18)	106.9(3)	C(6)-Li(2)-Li(1)	69.8(2)
C(9)-N(2)-Li(1)	115.3(3)	C(19)-C(18)-C(17)	107.0(3)	C(41)-O(2)-C(44)	109.3(3)
C(6)-N(2)-Li(1)	113.4(3)	N(4)-C(19)-C(18)	110.1(3)	C(41)-O(2)-Li(2)	119.4(3)
Li(2)-N(2)-Li(1)	78.8(3)	N(4)-C(19)-C(20)	120.6(3)	C(44)-O(2)-Li(2)	115.1(3)
C(11)-N(3)-C(14)	105.8(3)	C(18)-C(19)-C(20)	129.2(3)	O(2)-C(41)-C(42)	106.4(3)
C(11)-N(3)-Li(3)	141.4(3)	C(1)-C(20)-C(19)	108.8(3)	C(41)-C(42)-C(43)	102.7(4)
C(14)-N(3)-Li(3)	96.1(3)	C(1)-C(20)-C(33)	109.2(3)	C(44)-C(43)-C(42)	102.3(3)
C(11)-N(3)-Li(1)	116.0(3)	C(19)-C(20)-C(33)	110.0(3)	O(2)-C(44)-C(43)	105.3(3)
C(14)-N(3)-Li(1)	117.4(3)	C(1)-C(20)-C(35)	109.6(3)	O(3)-Li(3)-N(4)	136.9(4)
Li(3)-N(3)-Li(1)	79.2(3)	C(19)-C(20)-C(35)	108.5(3)	O(3)-Li(3)-N(3)	130.9(3)

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Table S28. Bond lengths [Å] and angles [°] for **23** (cont.)

C(11)-N(3)-Li(4)	71.8(3)	C(33)-C(20)-C(35)	110.7(3)	N(4)-Li(3)-N(3)	86.5(3)
C(14)-N(3)-Li(4)	70.7(3)	C(21)-N(5)-C(22)	109.2(3)	O(3)-Li(3)-N(6)	108.5(3)
Li(3)-N(3)-Li(4)	146.6(3)	C(21)-N(5)-C(5)	114.5(3)	N(4)-Li(3)-N(6)	89.8(3)
Li(1)-N(3)-Li(4)	80.3(3)	C(22)-N(5)-C(5)	113.9(3)	N(3)-Li(3)-N(6)	89.2(3)
C(19)-N(4)-C(16)	105.8(3)	C(21)-N(5)-Li(2)	117.8(3)	O(3)-Li(3)-C(15)	144.7(3)
C(19)-N(4)-Li(3)	140.0(3)	C(22)-N(5)-Li(2)	113.3(3)	N(4)-Li(3)-C(15)	64.3(2)
C(16)-N(4)-Li(3)	97.8(3)	C(5)-N(5)-Li(2)	86.8(3)	N(3)-Li(3)-C(15)	63.7(2)
C(19)-N(4)-Li(1)	113.6(3)	C(24)-C(23)-C(5)	118.3(4)	N(6)-Li(3)-C(15)	36.32(16)
C(16)-N(4)-Li(1)	116.6(3)	C(26)-C(25)-C(10)	115.3(3)	O(3)-Li(3)-C(16)	150.0(4)
Li(3)-N(4)-Li(1)	82.4(3)	C(28)-C(27)-C(10)	113.5(3)	N(4)-Li(3)-C(16)	31.43(14)
N(1)-C(1)-C(2)	110.0(3)	C(30)-N(6)-C(29)	109.1(3)	N(3)-Li(3)-C(16)	78.4(2)
N(1)-C(1)-C(20)	121.1(3)	C(30)-N(6)-C(15)	113.6(3)	N(6)-Li(3)-C(16)	59.64(19)
C(2)-C(1)-C(20)	128.8(3)	C(29)-N(6)-C(15)	113.8(3)	C(15)-Li(3)-C(16)	33.77(14)
C(1)-C(2)-C(3)	106.8(3)	C(30)-N(6)-Li(3)	113.7(3)	O(3)-Li(3)-C(14)	143.5(3)
C(4)-C(3)-C(2)	106.8(3)	C(29)-N(6)-Li(3)	118.2(3)	N(4)-Li(3)-C(14)	79.4(2)
C(3)-C(4)-N(1)	109.9(3)	C(15)-N(6)-Li(3)	87.1(3)	N(3)-Li(3)-C(14)	31.24(14)
C(3)-C(4)-C(5)	129.6(3)	C(32)-C(31)-C(15)	115.4(3)	N(6)-Li(3)-C(14)	59.1(2)
N(1)-C(4)-C(5)	119.5(3)	C(34)-C(33)-C(20)	114.4(3)	C(15)-Li(3)-C(14)	33.57(14)
C(3)-C(4)-Li(2)	149.9(3)	C(36)-C(35)-C(20)	114.8(3)	C(16)-Li(3)-C(14)	57.83(18)
N(1)-C(4)-Li(2)	50.6(2)	N(1)-Li(1)-N(4)	97.0(3)	O(3)-Li(3)-Li(1)	130.5(3)
C(5)-C(4)-Li(2)	70.5(2)	N(1)-Li(1)-N(2)	83.2(3)	N(4)-Li(3)-Li(1)	50.9(2)
C(6)-C(5)-C(4)	113.9(3)	N(4)-Li(1)-N(2)	159.3(4)	N(3)-Li(3)-Li(1)	52.4(2)
C(6)-C(5)-N(5)	104.5(3)	N(1)-Li(1)-N(3)	161.0(4)	N(6)-Li(3)-Li(1)	120.9(3)
C(4)-C(5)-N(5)	105.1(3)	N(4)-Li(1)-N(3)	80.4(2)	C(15)-Li(3)-Li(1)	84.5(3)
C(6)-C(5)-C(23)	111.5(3)	N(2)-Li(1)-N(3)	92.7(3)	C(16)-Li(3)-Li(1)	68.8(2)
C(4)-C(5)-C(23)	111.4(3)	N(1)-Li(1)-O(1)	107.5(3)	C(14)-Li(3)-Li(1)	70.3(2)
N(5)-C(5)-C(23)	109.9(3)	N(4)-Li(1)-O(1)	100.3(3)	C(48)-O(3)-C(45)	107.9(3)
C(6)-C(5)-Li(2)	75.4(3)	N(2)-Li(1)-O(1)	99.3(3)	C(48)-O(3)-Li(3)	133.3(3)
C(4)-C(5)-Li(2)	75.0(2)	N(3)-Li(1)-O(1)	91.5(3)	C(45)-O(3)-Li(3)	118.7(3)
N(5)-C(5)-Li(2)	55.8(2)	N(1)-Li(1)-Li(2)	47.3(2)	O(3)-C(45)-C(46)	105.7(5)
C(23)-C(5)-Li(2)	165.7(3)	N(4)-Li(1)-Li(2)	118.2(3)	C(47)-C(46)-C(45)	105.8(6)
C(7)-C(6)-N(2)	110.0(3)	N(2)-Li(1)-Li(2)	48.4(2)	C(46)-C(47)-C(48)	110.1(6)
C(7)-C(6)-C(5)	129.0(4)	N(3)-Li(1)-Li(2)	117.5(3)	O(3)-C(48)-C(47)	106.2(4)
N(2)-C(6)-C(5)	120.3(3)	O(1)-Li(1)-Li(2)	134.1(3)	O(4)-Li(4)-O(1)	105.6(4)
C(7)-C(6)-Li(2)	149.8(3)	N(1)-Li(1)-Li(3)	117.0(4)	O(4)-Li(4)-C(13)	104.3(4)
N(2)-C(6)-Li(2)	52.4(2)	N(4)-Li(1)-Li(3)	46.8(2)	O(1)-Li(4)-C(13)	138.4(5)
C(5)-C(6)-Li(2)	70.3(3)	N(2)-Li(1)-Li(3)	114.9(3)	O(4)-Li(4)-C(14)	137.0(5)
C(6)-C(7)-C(8)	107.0(4)	N(3)-Li(1)-Li(3)	48.4(2)	O(1)-Li(4)-C(14)	106.1(5)
C(9)-C(8)-C(7)	107.1(4)	O(1)-Li(1)-Li(3)	125.6(3)	C(13)-Li(4)-C(14)	34.9(2)
N(2)-C(9)-C(8)	110.2(3)	Li(2)-Li(1)-Li(3)	99.6(3)	O(4)-Li(4)-C(12)	97.5(4)
N(2)-C(9)-C(10)	121.0(3)	N(1)-Li(1)-Li(4)	146.5(4)	O(1)-Li(4)-C(12)	155.9(5)
C(8)-C(9)-C(10)	128.8(4)	N(4)-Li(1)-Li(4)	102.4(3)	C(13)-Li(4)-C(12)	35.85(19)
C(9)-C(10)-C(11)	109.1(3)	N(2)-Li(1)-Li(4)	87.8(3)	C(14)-Li(4)-C(12)	58.2(3)
C(9)-C(10)-C(27)	110.7(3)	N(3)-Li(1)-Li(4)	51.2(2)	O(4)-Li(4)-C(11)	123.1(5)
C(11)-C(10)-C(27)	108.7(3)	O(1)-Li(1)-Li(4)	42.4(2)	O(1)-Li(4)-C(11)	122.6(4)
C(9)-C(10)-C(25)	109.4(3)	Li(2)-Li(1)-Li(4)	136.0(3)	C(13)-Li(4)-C(11)	58.1(2)
C(11)-C(10)-C(25)	108.2(3)	Li(3)-Li(1)-Li(4)	96.1(3)	C(14)-Li(4)-C(11)	57.2(2)
C(27)-C(10)-C(25)	110.7(3)	C(37)-O(1)-C(40)	106.2(4)	C(12)-Li(4)-C(11)	34.56(19)
C(12)-C(11)-N(3)	110.5(3)	C(37)-O(1)-Li(4)	136.9(4)	O(4)-Li(4)-N(3)	155.6(5)
C(12)-C(11)-C(10)	129.6(3)	C(40)-O(1)-Li(4)	106.3(5)	O(1)-Li(4)-N(3)	98.2(4)
N(3)-C(11)-C(10)	119.9(3)	C(37)-O(1)-Li(1)	105.5(4)	C(13)-Li(4)-N(3)	58.5(2)
C(12)-C(11)-Li(4)	72.2(3)	C(40)-O(1)-Li(1)	114.6(3)	C(14)-Li(4)-N(3)	34.78(17)
N(3)-C(11)-Li(4)	73.8(3)	Li(4)-O(1)-Li(1)	85.5(3)	C(12)-Li(4)-N(3)	58.2(2)
C(10)-C(11)-Li(4)	121.6(3)	O(1)-C(37)-C(38)	108.1(5)	C(11)-Li(4)-N(3)	34.45(17)

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Table S28. Bond lengths [Å] and angles [°] for **23** (cont.)

C(11)-C(12)-C(13)	106.6(3)	C(37)-C(38)-C(39)	107.7(5)	O(4)-Li(4)-C(40)	83.9(3)
C(11)-C(12)-Li(4)	73.3(3)	C(38)-C(39)-C(40)	98.4(5)	O(1)-Li(4)-C(40)	29.6(2)
C(13)-C(12)-Li(4)	71.1(3)	O(1)-C(40)-C(39)	101.6(4)	C(13)-Li(4)-C(40)	168.0(5)
C(14)-C(13)-C(12)	107.1(3)	O(1)-C(40)-Li(4)	44.1(3)	C(14)-Li(4)-C(40)	134.4(4)
C(14)-C(13)-Li(4)	73.2(3)	C(39)-C(40)-Li(4)	112.2(4)	C(12)-Li(4)-C(40)	153.2(4)
C(12)-C(13)-Li(4)	73.1(3)	O(2)-Li(2)-N(1)	133.5(3)	C(11)-Li(4)-C(40)	124.8(4)
C(13)-C(14)-N(3)	110.1(3)	O(2)-Li(2)-N(2)	128.2(3)	N(3)-Li(4)-C(40)	116.2(4)
C(13)-C(14)-C(15)	128.9(3)	N(1)-Li(2)-N(2)	89.7(3)	O(4)-Li(4)-Li(1)	150.8(5)
N(3)-C(14)-C(15)	120.2(3)	O(2)-Li(2)-N(5)	110.5(3)	O(1)-Li(4)-Li(1)	52.2(3)
C(13)-C(14)-Li(4)	71.9(3)	N(1)-Li(2)-N(5)	91.5(3)	C(13)-Li(4)-Li(1)	104.7(4)
N(3)-C(14)-Li(4)	74.5(3)	N(2)-Li(2)-N(5)	91.6(3)	C(14)-Li(4)-Li(1)	72.1(3)
C(15)-C(14)-Li(4)	128.7(3)	O(2)-Li(2)-C(5)	147.8(3)	C(12)-Li(4)-Li(1)	103.9(3)
C(13)-C(14)-Li(3)	147.2(3)	N(1)-Li(2)-C(5)	66.0(2)	C(11)-Li(4)-Li(1)	71.1(3)
N(3)-C(14)-Li(3)	52.7(2)	N(2)-Li(2)-C(5)	65.7(2)	N(3)-Li(4)-Li(1)	48.5(2)
C(15)-C(14)-Li(3)	70.7(3)	N(5)-Li(2)-C(5)	37.44(16)	C(40)-Li(4)-Li(1)	68.1(3)
Li(4)-C(14)-Li(3)	119.5(3)	O(2)-Li(2)-C(4)	151.2(3)	C(52)-O(4)-C(49)	106.1(5)
C(16)-C(15)-C(14)	114.9(3)	N(1)-Li(2)-C(4)	32.10(14)	C(52)-O(4)-Li(4)	118.8(5)
C(16)-C(15)-N(6)	104.7(3)	N(2)-Li(2)-C(4)	80.6(2)	C(49)-O(4)-Li(4)	126.3(5)
C(14)-C(15)-N(6)	104.6(3)	N(5)-Li(2)-C(4)	61.33(19)	O(4)-C(49)-C(50)	109.5(6)
C(16)-C(15)-C(31)	111.1(3)	C(5)-Li(2)-C(4)	34.49(14)	C(49)-C(50)-C(51)	103.7(7)
C(14)-C(15)-C(31)	109.5(3)	O(2)-Li(2)-C(6)	145.0(3)	C(52)-C(51)-C(50)	101.7(7)
N(6)-C(15)-C(31)	111.9(3)	N(1)-Li(2)-C(6)	81.6(2)	O(4)-C(52)-C(51)	114.6(7)
C(16)-C(15)-Li(3)	74.4(2)	N(2)-Li(2)-C(6)	32.35(15)	C(54)-C(53)-C(53) ^a	115.8(6)
C(14)-C(15)-Li(3)	75.8(3)	N(5)-Li(2)-C(6)	60.8(2)	C(53)-C(54)-C(55)	115.3(5)

Symmetry transformations used to generate equivalent atoms:

^a -x,-y-1,-z+1

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Table S39. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **23**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
N(1)	36(2)	34(2)	32(2)	-2(1)	-3(1)	-6(1)
N(2)	39(2)	35(2)	35(2)	2(1)	-4(1)	-9(1)
N(3)	35(2)	38(2)	32(2)	-3(1)	-1(1)	-5(1)
N(4)	35(2)	37(2)	34(2)	-4(1)	-1(1)	-8(1)
C(1)	33(2)	37(2)	32(2)	-1(2)	-2(1)	-8(2)
C(2)	37(2)	46(2)	33(2)	-1(2)	5(2)	-9(2)
C(3)	38(2)	42(2)	38(2)	-6(2)	0(2)	-3(2)
C(4)	43(2)	31(2)	34(2)	-2(2)	-1(2)	-1(2)
C(5)	45(2)	34(2)	37(2)	2(2)	-3(2)	-4(2)
C(6)	47(2)	35(2)	44(3)	-3(2)	3(2)	-7(2)
C(7)	80(3)	37(2)	50(3)	5(2)	13(2)	2(2)
C(8)	65(3)	42(3)	43(3)	13(2)	6(2)	-4(2)
C(9)	40(2)	41(2)	34(2)	5(2)	-5(2)	-9(2)
C(10)	40(2)	44(2)	32(2)	1(2)	0(2)	-9(2)
C(11)	41(2)	38(2)	32(2)	-1(2)	-1(2)	-7(2)
C(12)	47(2)	47(2)	30(2)	0(2)	-1(2)	-13(2)
C(13)	42(2)	46(2)	35(2)	-5(2)	-4(2)	-5(2)
C(14)	35(2)	35(2)	34(2)	-4(2)	-3(1)	-3(2)
C(15)	38(2)	38(2)	35(2)	-3(2)	-3(2)	-6(2)
C(16)	37(2)	35(2)	34(2)	1(2)	-4(2)	-5(2)
C(17)	38(2)	55(3)	40(2)	-5(2)	-5(2)	-16(2)
C(18)	36(2)	46(2)	40(2)	-3(2)	1(2)	-11(2)
C(19)	35(2)	37(2)	36(2)	-5(2)	4(2)	-7(2)
C(20)	37(2)	36(2)	29(2)	1(2)	0(1)	-6(2)
N(5)	47(2)	42(2)	42(2)	1(2)	-3(1)	-12(2)
C(21)	55(2)	51(3)	76(3)	-10(2)	-8(2)	-18(2)
C(22)	60(3)	65(3)	41(3)	-5(2)	-10(2)	-5(2)
C(23)	65(3)	37(2)	46(3)	-3(2)	4(2)	-9(2)
C(24)	71(3)	52(3)	55(3)	-1(2)	8(2)	8(2)
C(25)	49(2)	47(2)	32(2)	3(2)	-1(2)	-12(2)
C(26)	48(2)	63(3)	47(3)	7(2)	3(2)	-22(2)
C(27)	38(2)	46(2)	37(2)	-1(2)	-5(2)	-6(2)
C(28)	42(2)	55(3)	40(2)	-3(2)	1(2)	-7(2)
N(6)	49(2)	40(2)	37(2)	-7(2)	3(1)	-2(1)
C(29)	74(3)	60(3)	37(3)	-11(2)	1(2)	10(2)
C(30)	70(3)	44(3)	64(3)	2(2)	-10(2)	-15(2)
C(31)	49(2)	52(3)	40(2)	-1(2)	-8(2)	-16(2)
C(32)	41(2)	71(3)	47(3)	5(2)	-11(2)	-9(2)
C(33)	40(2)	38(2)	35(2)	0(2)	-1(2)	-9(2)
C(34)	47(2)	40(2)	51(3)	2(2)	0(2)	-5(2)
C(35)	42(2)	38(2)	36(2)	-1(2)	1(2)	-12(2)
C(36)	55(2)	47(2)	37(2)	3(2)	-4(2)	-14(2)
Li(1)	55(4)	56(4)	36(4)	0(3)	2(3)	-24(3)
O(1)	58(2)	74(2)	96(3)	-43(2)	-1(2)	-11(2)
C(37)	89(4)	89(4)	76(4)	-1(3)	5(3)	-7(3)
C(38)	53(3)	121(5)	87(4)	-9(4)	5(3)	-22(3)
C(39)	88(4)	53(3)	118(5)	-12(3)	-27(4)	9(3)
C(40)	65(3)	78(4)	100(5)	-23(3)	-3(3)	-10(3)
Li(2)	40(3)	35(3)	36(4)	2(3)	-3(2)	-5(3)
O(2)	34(1)	52(2)	39(2)	2(1)	-4(1)	-5(1)

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Table S29. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **23** (cont.).

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(41)	45(2)	64(3)	42(3)	9(2)	-3(2)	-2(2)
C(42)	42(2)	69(3)	40(3)	6(2)	-6(2)	0(2)
C(43)	41(2)	56(3)	40(2)	1(2)	-7(2)	-6(2)
C(44)	39(2)	58(3)	38(2)	-3(2)	1(2)	-10(2)
Li(3)	39(3)	55(4)	38(4)	-2(3)	-1(3)	-3(3)
O(3)	47(2)	48(2)	51(2)	-2(1)	-3(1)	0(1)
C(45)	81(4)	74(4)	155(7)	-46(4)	-43(4)	16(3)
C(46)	95(5)	78(5)	233(10)	-52(6)	-76(6)	28(4)
C(47)	133(6)	126(7)	200(10)	-84(7)	-101(7)	74(5)
C(48)	51(2)	63(3)	54(3)	-10(2)	-11(2)	6(2)
Li(4)	69(5)	74(6)	64(6)	-1(5)	-16(4)	13(4)
O(4)	99(3)	73(3)	95(3)	-9(2)	-33(2)	-1(2)
C(49)	121(5)	95(5)	79(5)	11(4)	-51(4)	-10(4)
C(50)	120(6)	125(7)	114(6)	-29(5)	-31(5)	-34(5)
C(51)	154(8)	134(8)	153(9)	-17(7)	32(7)	-48(7)
C(52)	102(5)	113(6)	89(5)	46(4)	-41(4)	-36(4)
C(53)	76(3)	61(3)	80(4)	3(3)	3(3)	-10(3)
C(54)	104(5)	78(4)	85(5)	2(3)	-29(3)	-9(3)
C(55)	123(5)	67(4)	119(6)	7(4)	-42(5)	-8(4)

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Table S30. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 23.

	x	y	z	U(eq)
H(2)	619	405	4398	46
H(3)	1201	2446	4219	48
H(7)	3846	4405	2469	69
H(8)	4795	3675	1446	62
H(12)	4022	1241	226	49
H(13)	2281	-8	248	49
H(17)	-236	-1983	2102	52
H(18)	-87	-2083	3267	49
H(21A)	5487	3586	3862	89
H(21B)	5796	3055	3199	89
H(21C)	6470	2448	3795	89
H(22A)	5299	1531	4611	83
H(22B)	3885	1398	4528	83
H(22C)	4268	2641	4641	83
H(23A)	2820	3724	4125	59
H(23B)	3617	4324	3586	59
H(24A)	1918	4532	2944	92
H(24B)	1567	5178	3572	92
H(24C)	1119	3949	3492	92
H(25A)	6140	1244	505	51
H(25B)	5376	2448	690	51
H(26A)	7008	2667	1364	78
H(26B)	7429	2712	642	78
H(26C)	7789	1556	1070	78
H(27A)	6897	493	1852	48
H(27B)	5767	-205	2064	48
H(28A)	6028	-1178	1135	69
H(28B)	7307	-1361	1470	69
H(28C)	7110	-440	890	69
H(29A)	4271	-3422	799	88
H(29B)	3948	-2073	601	88
H(29C)	3007	-2959	479	88
H(30A)	1866	-3812	1359	88
H(30B)	2134	-3529	2047	88
H(30C)	3171	-4284	1638	88
H(31A)	1340	-1648	521	55
H(31B)	575	-2256	1072	55
H(32A)	-463	-467	1335	79
H(32B)	-604	-616	615	79
H(32C)	355	185	822	79
H(33A)	4017	-1596	3354	45
H(33B)	3889	-1781	4092	45
H(34A)	3314	-3629	4015	70
H(34B)	4595	-3551	3628	70
H(34C)	3340	-3442	3276	70
H(35A)	561	-1484	4236	46
H(35B)	1319	-2728	4123	46
H(36A)	2655	-2535	4891	69
H(36B)	1289	-2191	5185	69
H(36C)	2115	-1199	4951	69

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Table S30. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **23** (cont.).

	x	y	z	U(eq)
H(37A)	462	861	2821	103
H(37B)	-48	640	2165	103
H(38A)	-911	2289	2918	103
H(38B)	-1420	2068	2262	103
H(39A)	-424	3946	2425	104
H(39B)	-378	3425	1748	104
H(40A)	1758	3231	1935	96
H(40B)	1508	2879	2662	96
H(41A)	6205	-1747	4054	62
H(41B)	5902	-507	4351	62
H(42A)	8275	-1714	4036	61
H(42B)	7895	-897	4608	61
H(43A)	7918	789	3974	55
H(43B)	9051	-35	3654	55
H(44A)	7252	825	2994	54
H(44B)	7880	-483	2894	54
H(45A)	6050	-3631	1443	123
H(45B)	5131	-4298	1902	123
H(46A)	6664	-5157	2476	161
H(46B)	7544	-4862	1879	161
H(47A)	8140	-3497	2277	185
H(47B)	7689	-4127	2915	185
H(48A)	6167	-2764	3067	68
H(48B)	6846	-2011	2534	68
H(49A)	-82	3204	335	117
H(49B)	720	2017	140	117
H(50A)	689	4048	-517	139
H(50B)	1675	2919	-639	139
H(51A)	3149	3749	-230	175
H(51B)	2176	4900	-135	175
H(52A)	2996	3482	765	121
H(52B)	1778	4399	821	121
H(53A)	1078	-4568	4725	87
H(53B)	378	-4133	5352	87
H(54A)	1563	-6430	5233	106
H(54B)	947	-5920	5862	106
H(55A)	2950	-4842	5291	154
H(55B)	3273	-6065	5667	154
H(55C)	2569	-4980	6015	154

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Table S31. Crystal data and structure refinement for 30.

Identification code	30	
Empirical formula	C ₃₉ H ₄₂ N ₄ Ni O	
Formula weight	641.48	
Temperature	143(2) K	
Wavelength	0.71070 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 16.370(3) Å	$\alpha = 90^\circ$.
	b = 12.068(2) Å	$\beta = 116.82(3)^\circ$.
	c = 17.840(4) Å	$\gamma = 90^\circ$.
Volume	3145.3(11) Å ³	
Z	4	
Density (calculated)	1.355 Mg/m ³	
Absorption coefficient	0.656 mm ⁻¹	
F(000)	1360	
Crystal size	0.18 x 0.15 x 0.10 mm ³	
Theta range for data collection	1.40 to 24.44°	
Index ranges	-18 < = h < = 18, -13 < = k < = 13, -20 < = l < = 20	
Reflections collected	12695	
Independent reflections	4187 [R(int) = 0.0841]	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4187 / 0 / 407	
Goodness-of-fit on F ²	0.943	
Final R indices [I > 2sigma(I)]	R1 = 0.0685, wR2 = 0.1725	
R indices (all data)	R1 = 0.1124, wR2 = 0.2004	
Extinction coefficient	0.0141(16)	
Largest diff. peak and hole	0.509 and -1.057 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 30. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni(1)	1223(1)	681(1)	-1382(1)	42(1)
O(1)	4106(3)	-37(4)	-2803(3)	61(1)
N(1)	1415(4)	2020(4)	-777(4)	42(1)
N(2)	-36(4)	806(4)	-1727(3)	43(1)
N(3)	1015(3)	-621(4)	-2020(3)	41(1)
N(4)	2465(4)	602(4)	-1100(3)	43(1)
C(1)	2184(5)	2335(5)	-108(5)	45(2)
C(2)	2089(5)	3413(5)	161(5)	53(2)
C(3)	1226(5)	3754(5)	-392(5)	52(2)
C(4)	789(5)	2886(5)	-966(4)	43(2)
C(5)	-138(5)	2799(5)	-1524(4)	45(2)
C(6)	-538(5)	1794(5)	-1880(4)	43(2)
C(7)	-1479(5)	1541(6)	-2267(4)	52(2)
C(8)	-1564(5)	403(6)	-2337(4)	55(2)
C(9)	-661(5)	-29(5)	-2000(4)	44(2)
C(10)	-348(4)	-1216(5)	-1871(4)	44(2)
C(11)	312(4)	-1319(5)	-2247(4)	44(2)
C(12)	289(5)	-2089(5)	-2860(4)	50(2)
C(13)	1037(5)	-1857(5)	-2993(4)	49(2)
C(14)	1516(5)	-959(5)	-2454(4)	46(2)
C(15)	2381(5)	-567(5)	-2267(4)	42(2)
C(16)	2863(5)	146(5)	-1584(4)	47(2)
C(17)	3820(5)	373(5)	-1183(4)	50(2)
C(18)	4007(5)	927(5)	-451(4)	49(2)
C(19)	3163(5)	1068(5)	-420(4)	43(2)
C(20)	3004(4)	1577(5)	276(4)	46(2)
C(21)	-743(5)	3791(5)	-1650(5)	53(2)
C(22)	-1089(5)	3871(6)	-981(5)	67(2)
C(23)	194(5)	-1436(5)	-906(5)	50(2)
C(24)	-383(5)	-1306(6)	-433(5)	62(2)
C(25)	-1160(5)	-2016(5)	-2263(5)	55(2)
C(26)	-928(5)	-3236(5)	-1972(5)	67(2)
C(27)	2882(5)	-1052(5)	-2732(4)	49(2)
C(28)	3549(5)	-1957(5)	-2254(5)	64(2)
C(29)	3270(5)	-134(5)	-3066(4)	50(2)
C(30)	2631(5)	666(5)	-3713(4)	53(2)
C(31)	2983(6)	1616(7)	-3878(5)	73(2)
C(32)	2417(7)	2349(7)	-4477(6)	89(3)
C(33)	1491(6)	2129(7)	-4921(5)	77(2)
C(34)	1147(6)	1179(7)	-4761(5)	73(2)
C(35)	1705(6)	461(6)	-4146(5)	60(2)
C(36)	2753(5)	617(5)	734(4)	51(2)
C(37)	3475(5)	-281(6)	1104(5)	64(2)
C(38)	3856(5)	2185(5)	937(5)	59(2)
C(39)	4201(5)	3164(6)	633(5)	73(2)

Table S33. Bond lengths [Å] and angles [°] for 30.

Ni(1)-N(4)	1.864(5)	C(5)-C(6)	1.388(9)	C(19)-C(20)	1.509(8)
Ni(1)-N(2)	1.872(5)	C(5)-C(21)	1.505(8)	C(20)-C(38)	1.546(9)
Ni(1)-N(3)	1.879(5)	C(6)-C(7)	1.408(9)	C(20)-C(36)	1.575(8)
Ni(1)-N(1)	1.889(5)	C(7)-C(8)	1.380(9)	C(21)-C(22)	1.537(8)
O(1)-C(29)	1.236(7)	C(8)-C(9)	1.420(9)	C(23)-C(24)	1.532(7)
N(1)-C(1)	1.341(8)	C(9)-C(10)	1.504(9)	C(25)-C(26)	1.550(9)
N(1)-C(4)	1.395(7)	C(10)-C(11)	1.514(7)	C(27)-C(28)	1.508(9)
N(2)-C(9)	1.360(8)	C(10)-C(25)	1.532(8)	C(27)-C(29)	1.526(8)
N(2)-C(6)	1.403(7)	C(10)-C(23)	1.563(9)	C(29)-C(30)	1.506(9)
N(3)-C(11)	1.334(7)	C(11)-C(12)	1.422(8)	C(30)-C(31)	1.374(9)
N(3)-C(14)	1.417(6)	C(12)-C(13)	1.377(8)	C(30)-C(35)	1.377(10)
N(4)-C(19)	1.358(8)	C(13)-C(14)	1.426(8)	C(31)-C(32)	1.374(11)
N(4)-C(16)	1.407(7)	C(14)-C(15)	1.384(8)	C(32)-C(33)	1.383(11)
C(1)-C(2)	1.420(8)	C(15)-C(16)	1.407(9)	C(33)-C(34)	1.363(10)
C(1)-C(20)	1.509(9)	C(15)-C(27)	1.522(7)	C(34)-C(35)	1.373(10)
C(2)-C(3)	1.371(9)	C(16)-C(17)	1.425(9)	C(36)-C(37)	1.517(9)
C(3)-C(4)	1.413(9)	C(17)-C(18)	1.374(9)	C(38)-C(39)	1.512(9)
C(4)-C(5)	1.393(9)	C(18)-C(19)	1.418(8)		
N(4)-Ni(1)-N(2)	176.4(2)	C(5)-C(6)-N(2)	122.7(6)	C(17)-C(18)-C(19)	107.0(6)
N(4)-Ni(1)-N(3)	89.9(2)	C(5)-C(6)-C(7)	126.8(6)	N(4)-C(19)-C(18)	110.9(5)
N(2)-Ni(1)-N(3)	89.8(2)	N(2)-C(6)-C(7)	109.0(5)	N(4)-C(19)-C(20)	121.1(5)
N(4)-Ni(1)-N(1)	90.6(2)	C(8)-C(7)-C(6)	107.7(6)	C(18)-C(19)-C(20)	127.9(6)
N(2)-Ni(1)-N(1)	89.6(2)	C(7)-C(8)-C(9)	106.4(6)	C(1)-C(20)-C(19)	108.7(6)
N(3)-Ni(1)-N(1)	177.9(2)	N(2)-C(9)-C(8)	110.6(6)	C(1)-C(20)-C(38)	111.7(5)
C(1)-N(1)-C(4)	107.2(5)	N(2)-C(9)-C(10)	120.1(6)	C(19)-C(20)-C(38)	112.9(5)
C(1)-N(1)-Ni(1)	126.7(4)	C(8)-C(9)-C(10)	129.2(6)	C(1)-C(20)-C(36)	107.2(5)
C(4)-N(1)-Ni(1)	126.0(5)	C(9)-C(10)-C(11)	105.8(4)	C(19)-C(20)-C(36)	108.0(5)
C(9)-N(2)-C(6)	106.2(5)	C(9)-C(10)-C(25)	111.4(5)	C(38)-C(20)-C(36)	108.0(6)
C(9)-N(2)-Ni(1)	126.7(4)	C(11)-C(10)-C(25)	113.1(5)	C(5)-C(21)-C(22)	112.5(5)
C(6)-N(2)-Ni(1)	126.4(4)	C(9)-C(10)-C(23)	108.4(5)	C(24)-C(23)-C(10)	113.8(6)
C(11)-N(3)-C(14)	106.5(5)	C(11)-C(10)-C(23)	108.1(5)	C(10)-C(25)-C(26)	114.5(6)
C(11)-N(3)-Ni(1)	127.4(4)	C(25)-C(10)-C(23)	109.9(5)	C(28)-C(27)-C(15)	113.6(5)
C(14)-N(3)-Ni(1)	125.5(4)	N(3)-C(11)-C(12)	111.5(5)	C(28)-C(27)-C(29)	115.1(5)
C(19)-N(4)-C(16)	105.9(5)	N(3)-C(11)-C(10)	120.3(5)	C(15)-C(27)-C(29)	110.9(5)
C(19)-N(4)-Ni(1)	126.5(4)	C(12)-C(11)-C(10)	128.2(6)	O(1)-C(29)-C(30)	119.9(6)
C(16)-N(4)-Ni(1)	127.3(5)	C(13)-C(12)-C(11)	106.4(5)	O(1)-C(29)-C(27)	120.4(7)
N(1)-C(1)-C(2)	111.0(6)	C(12)-C(13)-C(14)	107.4(5)	C(30)-C(29)-C(27)	119.7(6)
N(1)-C(1)-C(20)	121.2(6)	C(15)-C(14)-N(3)	123.4(6)	C(31)-C(30)-C(35)	119.5(7)
C(2)-C(1)-C(20)	127.8(7)	C(15)-C(14)-C(13)	127.9(5)	C(31)-C(30)-C(29)	119.0(7)
C(3)-C(2)-C(1)	105.5(7)	N(3)-C(14)-C(13)	108.1(5)	C(35)-C(30)-C(29)	121.5(6)
C(2)-C(3)-C(4)	108.7(6)	C(14)-C(15)-C(16)	122.1(5)	C(30)-C(31)-C(32)	120.2(8)
C(5)-C(4)-N(1)	124.1(6)	C(14)-C(15)-C(27)	118.8(6)	C(31)-C(32)-C(33)	120.1(8)
C(5)-C(4)-C(3)	127.3(6)	C(16)-C(15)-C(27)	118.5(6)	C(34)-C(33)-C(32)	119.4(8)
N(1)-C(4)-C(3)	107.6(6)	N(4)-C(16)-C(15)	122.4(6)	C(33)-C(34)-C(35)	120.6(8)
C(6)-C(5)-C(4)	122.0(6)	N(4)-C(16)-C(17)	109.0(6)	C(34)-C(35)-C(30)	120.1(7)
C(6)-C(5)-C(21)	119.0(6)	C(15)-C(16)-C(17)	127.8(5)	C(37)-C(36)-C(20)	114.7(5)
C(4)-C(5)-C(21)	118.5(6)	C(18)-C(17)-C(16)	107.0(5)	C(39)-C(38)-C(20)	116.8(6)

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Table S34. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **30**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Ni(1)	53(1)	41(1)	55(1)	-2(1)	46(1)	0(1)
O(1)	64(4)	74(3)	73(4)	-10(3)	55(3)	-7(3)
N(1)	58(4)	40(3)	56(4)	2(3)	49(4)	-1(3)
N(2)	58(4)	39(3)	59(4)	-3(3)	50(3)	-3(3)
N(3)	50(3)	42(3)	55(4)	-2(3)	44(3)	-3(3)
N(4)	58(4)	44(3)	53(4)	-6(3)	48(3)	-1(3)
C(1)	60(5)	44(4)	56(5)	2(3)	47(4)	3(4)
C(2)	61(5)	52(4)	70(6)	-4(4)	52(5)	-1(4)
C(3)	74(6)	40(4)	75(6)	-8(4)	61(5)	-2(4)
C(4)	65(5)	31(4)	61(5)	-2(3)	52(4)	4(3)
C(5)	66(5)	42(4)	54(5)	9(3)	53(4)	14(4)
C(6)	58(5)	38(4)	57(5)	4(3)	47(4)	4(3)
C(7)	59(5)	45(5)	70(5)	10(3)	43(4)	10(3)
C(8)	55(5)	60(5)	70(5)	3(4)	46(4)	0(4)
C(9)	44(4)	57(4)	52(5)	8(3)	41(4)	7(3)
C(10)	54(5)	40(4)	66(5)	0(3)	52(4)	2(3)
C(11)	57(5)	40(4)	62(5)	-5(3)	52(4)	-5(3)
C(12)	57(5)	51(4)	59(5)	-10(3)	43(4)	-13(3)
C(13)	67(5)	49(4)	56(5)	-12(3)	49(4)	-13(4)
C(14)	63(5)	48(4)	57(5)	-3(3)	53(4)	-3(3)
C(15)	57(5)	39(4)	54(5)	-2(3)	47(4)	5(3)
C(16)	68(5)	42(4)	60(5)	7(4)	54(4)	9(4)
C(17)	60(5)	52(4)	64(5)	0(3)	52(4)	-1(3)
C(18)	47(4)	54(4)	67(5)	-4(4)	45(4)	-5(3)
C(19)	51(5)	46(4)	50(5)	0(3)	40(4)	2(3)
C(20)	51(5)	50(4)	55(5)	-13(3)	39(4)	-6(3)
C(21)	63(5)	49(4)	65(5)	-3(4)	44(4)	7(4)
C(22)	78(6)	75(5)	75(6)	-5(4)	58(5)	18(4)
C(23)	63(5)	42(4)	74(6)	-3(3)	56(5)	-4(3)
C(24)	80(6)	63(5)	84(6)	6(4)	74(5)	1(4)
C(25)	53(5)	43(4)	92(6)	-11(4)	55(5)	-11(3)
C(26)	81(6)	58(5)	92(7)	-5(4)	64(5)	-7(4)
C(27)	61(5)	50(4)	67(5)	-9(4)	56(4)	-4(3)
C(28)	88(6)	57(5)	87(6)	-5(4)	74(5)	12(4)
C(29)	62(5)	59(4)	57(5)	-12(4)	50(5)	-7(4)
C(30)	66(6)	61(5)	53(5)	4(4)	46(4)	6(4)
C(31)	76(6)	84(6)	72(7)	11(5)	43(5)	-11(5)
C(32)	97(8)	80(6)	87(7)	14(5)	41(6)	-29(6)
C(33)	80(7)	70(6)	85(7)	21(5)	40(6)	-7(5)
C(34)	74(6)	75(6)	81(7)	6(5)	46(5)	-2(5)
C(35)	68(6)	59(5)	75(6)	-3(4)	53(5)	-7(4)
C(36)	67(5)	55(4)	55(5)	2(3)	49(4)	1(4)
C(37)	82(6)	56(4)	75(6)	6(4)	55(5)	6(4)
C(38)	63(5)	61(5)	71(5)	-12(4)	45(5)	-4(4)
C(39)	78(6)	65(5)	95(7)	-10(4)	56(6)	-8(4)

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Table S35. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 30.

	x	y	z	U(eq)
H(2)	2530	3814	626	63
H(3)	966	4457	-389	63
H(7)	-1967	2060	-2447	63
H(8)	-2118	-10	-2566	66
H(12)	-154	-2652	-3126	60
H(13)	1204	-2227	-3374	59
H(17)	4248	179	-1385	60
H(18)	4592	1169	-42	59
H(21A)	-1275	3747	-2212	64
H(21B)	-397	4471	-1631	64
H(22A)	-1467	3223	-1021	101
H(22B)	-1455	4546	-1073	101
H(22C)	-565	3896	-421	101
H(23A)	445	-2197	-817	60
H(23B)	717	-916	-664	60
H(24A)	-677	-576	-554	93
H(24B)	12	-1375	172	93
H(24C)	-854	-1884	-615	93
H(25A)	-1404	-1990	-2881	65
H(25B)	-1649	-1757	-2124	65
H(26A)	-399	-3478	-2049	101
H(26B)	-1455	-3708	-2305	101
H(26C)	-783	-3294	-1377	101
H(27)	2398	-1420	-3241	59
H(28A)	3991	-1675	-1704	96
H(28B)	3874	-2200	-2571	96
H(28C)	3215	-2585	-2176	96
H(31)	3620	1767	-3577	88
H(32)	2662	3008	-4586	106
H(33)	1098	2635	-5334	93
H(34)	515	1012	-5077	87
H(35)	1453	-179	-4018	72
H(36A)	2645	943	1190	61
H(36B)	2173	271	328	61
H(37A)	3666	-522	683	95
H(37B)	3220	-913	1274	95
H(37C)	4005	12	1596	95
H(38A)	3713	2445	1391	71
H(38B)	4360	1640	1188	71
H(39A)	4436	2905	246	109
H(39B)	4692	3534	1114	109
H(39C)	3698	3686	341	109

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Table S36. Crystal data and structure refinement for 13.

Identification code	13	
Empirical formula	C43 H54 Cl N4 O Sn	
Formula weight	797.04	
Temperature	143(2) K	
Wavelength	0.71070 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 28.497(6) Å	$\alpha = 90^\circ$.
	b = 14.481(3) Å	$\beta = 98.57(3)^\circ$.
	c = 17.548(4) Å	$\gamma = 90^\circ$.
Volume	7161(2) Å ³	
Z	8	
Density (calculated)	1.479 Mg/m ³	
Absorption coefficient	0.830 mm ⁻¹	
F(000)	3320	
Crystal size	0.27 x 0.20 x 0.13 mm ³	
Theta range for data collection	1.45 to 24.49°	
Index ranges	-32 ≤ h ≤ 33, -16 ≤ k ≤ 16, -18 ≤ l ≤ 20	
Reflections collected	16050	
Independent reflections	5287 [R(int) = 0.0721]	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5287 / 35 / 462	
Goodness-of-fit on F ²	0.977	
Final R indices [I > 2sigma(I)]	R1 = 0.0561, wR2 = 0.1402	
R indices (all data)	R1 = 0.0831, wR2 = 0.1597	
Extinction coefficient	0.00279(19)	
Largest diff. peak and hole	1.359 and -0.816 e.Å ⁻³	

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Table S37. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 13. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Sn(1)	-1420(1)	-218(1)	1772(1)	32(1)
Cl(1)	-1081(1)	-557(1)	630(1)	38(1)
O(1)	-1671(2)	108(3)	2934(2)	38(1)
N(1)	-1830(2)	-1411(4)	1747(3)	37(1)
N(2)	-1995(2)	561(4)	1252(3)	36(1)
N(3)	-1045(2)	1045(4)	2054(3)	35(1)
N(4)	-871(2)	-899(4)	2535(3)	37(1)
C(1)	-1671(2)	-2198(4)	2189(4)	39(2)
C(2)	-2045(2)	-2569(5)	2474(4)	45(2)
C(3)	-2449(2)	-2022(4)	2228(4)	42(2)
C(4)	-2315(2)	-1322(4)	1776(4)	40(2)
C(5)	-2625(2)	-716(4)	1220(3)	33(2)
C(6)	-2473(2)	291(4)	1195(4)	34(2)
C(7)	-2749(2)	1042(4)	987(4)	39(2)
C(8)	-2451(2)	1806(5)	926(4)	41(2)
C(9)	-1997(2)	1507(4)	1085(3)	34(2)
C(10)	-1548(2)	2058(4)	1082(3)	33(2)
C(11)	-1206(2)	1908(4)	1808(4)	36(2)
C(12)	-993(2)	2575(4)	2330(4)	40(2)
C(13)	-685(2)	2132(4)	2902(4)	37(2)
C(14)	-712(2)	1181(4)	2729(3)	34(2)
C(15)	-435(2)	483(5)	3121(4)	36(2)
C(16)	-485(2)	-482(5)	3018(3)	36(2)
C(17)	-211(2)	-1164(5)	3411(4)	43(2)
C(18)	-411(2)	-2000(5)	3181(4)	47(2)
C(19)	-821(2)	-1829(4)	2645(4)	36(2)
C(20)	-1165(2)	-2527(4)	2262(4)	42(2)
C(21)	-2664(2)	-1144(5)	412(4)	41(2)
C(22)	-2976(3)	-1980(5)	454(4)	54(2)
C(23)	-3367(3)	-1636(5)	899(4)	57(2)
C(24)	-3151(2)	-791(5)	1376(4)	46(2)
C(25)	-1656(2)	3104(4)	967(4)	41(2)
C(26)	-1230(2)	3526(4)	664(4)	45(2)
C(27)	-997(3)	2729(5)	300(4)	55(2)
C(28)	-1299(2)	1867(5)	368(4)	41(2)
C(29)	-427(3)	2592(5)	3605(4)	47(2)
C(30)	-466(2)	2053(5)	4342(4)	50(2)
C(31)	-154(2)	1191(5)	4446(3)	41(2)
C(32)	-18(2)	804(4)	3698(3)	38(2)
C(33)	-1113(3)	-3460(5)	2693(4)	52(2)
C(34)	-1315(3)	-4196(5)	2118(4)	60(2)
C(35)	-1306(3)	-3772(5)	1337(4)	64(2)
C(36)	-1041(2)	-2846(5)	1465(4)	47(2)
C(37)	-1667(2)	-523(5)	3568(4)	43(2)
C(38)	-2087(3)	-249(5)	3948(4)	53(2)
C(39A)	-2335(6)	434(11)	3485(10)	54(5)
C(39B)	-2087(9)	802(15)	3813(12)	30(7)
C(40)	-1964(3)	883(5)	3056(4)	47(2)
C(41)	-182(7)	4925(11)	205(11)	236(10)
C(42)	121(9)	5314(15)	896(11)	297(13)
C(43)	-9(8)	5042(14)	1713(11)	289(13)

Table S38. Bond lengths [Å] and angles [°] for 13.

Sn(1)-N(1)	2.082(5)	C(5)-C(21)	1.537(8)	C(21)-C(22)	1.510(9)
Sn(1)-N(2)	2.082(5)	C(5)-C(24)	1.567(8)	C(22)-C(23)	1.538(9)
Sn(1)-N(3)	2.138(5)	C(6)-C(7)	1.360(9)	C(23)-C(24)	1.556(10)
Sn(1)-N(4)	2.143(5)	C(7)-C(8)	1.408(9)	C(25)-C(26)	1.524(8)
Sn(1)-O(1)	2.307(4)	C(8)-C(9)	1.353(8)	C(26)-C(27)	1.520(9)
Sn(1)-Cl(1)	2.4028(16)	C(9)-C(10)	1.510(8)	C(27)-C(28)	1.531(9)
O(1)-C(40)	1.434(7)	C(10)-C(11)	1.499(9)	C(29)-C(30)	1.528(9)
O(1)-C(37)	1.438(7)	C(10)-C(25)	1.553(8)	C(30)-C(31)	1.528(9)
N(1)-C(4)	1.397(8)	C(10)-C(28)	1.555(8)	C(31)-C(32)	1.528(8)
N(1)-C(1)	1.415(8)	C(11)-C(12)	1.406(9)	C(33)-C(34)	1.522(10)
N(2)-C(9)	1.400(8)	C(12)-C(13)	1.388(9)	C(34)-C(35)	1.505(10)
N(2)-C(6)	1.407(8)	C(13)-C(14)	1.409(8)	C(35)-C(36)	1.539(10)
N(3)-C(11)	1.378(8)	C(13)-C(29)	1.494(9)	C(37)-C(38)	1.508(9)
N(3)-C(14)	1.418(8)	C(14)-C(15)	1.399(9)	C(38)-C(39A)	1.402(14)
N(4)-C(19)	1.365(8)	C(15)-C(16)	1.415(9)	C(38)-C(39B)	1.54(2)
N(4)-C(16)	1.418(8)	C(15)-C(32)	1.514(9)	C(39A)-C(40)	1.533(15)
C(1)-C(2)	1.354(8)	C(16)-C(17)	1.380(9)	C(39B)-C(40)	1.430(17)
C(1)-C(20)	1.507(9)	C(17)-C(18)	1.373(9)	C(41)-C(41) ^a	1.37(3)
C(2)-C(3)	1.410(9)	C(18)-C(19)	1.409(9)	C(41)-C(42)	1.490(17)
C(3)-C(4)	1.375(9)	C(19)-C(20)	1.496(9)	C(41)-C(42) ^a	2.00(3)
C(4)-C(5)	1.498(9)	C(20)-C(33)	1.545(9)	C(42)-C(43)	1.585(16)
C(5)-C(6)	1.523(9)	C(20)-C(36)	1.562(9)	C(42)-C(41) ^a	2.00(3)
N(1)-Sn(1)-N(2)	92.2(2)	C(4)-C(5)-C(21)	108.6(5)	C(18)-C(19)-C(20)	127.2(6)
N(1)-Sn(1)-N(3)	166.90(19)	C(6)-C(5)-C(21)	110.0(5)	C(19)-C(20)-C(1)	112.3(5)
N(2)-Sn(1)-N(3)	88.36(19)	C(4)-C(5)-C(24)	109.3(5)	C(19)-C(20)-C(33)	111.2(6)
N(1)-Sn(1)-N(4)	89.3(2)	C(6)-C(5)-C(24)	110.8(5)	C(1)-C(20)-C(33)	109.8(6)
N(2)-Sn(1)-N(4)	167.52(18)	C(21)-C(5)-C(24)	101.1(5)	C(19)-C(20)-C(36)	112.4(5)
N(3)-Sn(1)-N(4)	87.45(19)	C(7)-C(6)-N(2)	108.3(6)	C(1)-C(20)-C(36)	111.0(6)
N(1)-Sn(1)-O(1)	86.69(17)	C(7)-C(6)-C(5)	128.1(6)	C(33)-C(20)-C(36)	99.3(5)
N(2)-Sn(1)-O(1)	87.13(17)	N(2)-C(6)-C(5)	122.6(5)	C(22)-C(21)-C(5)	103.9(5)
N(3)-Sn(1)-O(1)	80.27(17)	C(6)-C(7)-C(8)	108.4(6)	C(21)-C(22)-C(23)	104.0(6)
N(4)-Sn(1)-O(1)	80.58(17)	C(9)-C(8)-C(7)	107.6(6)	C(22)-C(23)-C(24)	105.6(5)
N(1)-Sn(1)-Cl(1)	96.13(14)	C(8)-C(9)-N(2)	109.4(6)	C(23)-C(24)-C(5)	105.9(5)
N(2)-Sn(1)-Cl(1)	97.67(13)	C(8)-C(9)-C(10)	127.9(6)	C(26)-C(25)-C(10)	106.5(5)
N(3)-Sn(1)-Cl(1)	96.77(13)	N(2)-C(9)-C(10)	122.7(5)	C(27)-C(26)-C(25)	105.3(5)
N(4)-Sn(1)-Cl(1)	94.50(14)	C(11)-C(10)-C(9)	111.3(5)	C(26)-C(27)-C(28)	107.5(5)
O(1)-Sn(1)-Cl(1)	174.32(12)	C(11)-C(10)-C(25)	110.1(5)	C(27)-C(28)-C(10)	104.3(5)
C(40)-O(1)-C(37)	108.7(5)	C(9)-C(10)-C(25)	111.4(5)	C(13)-C(29)-C(30)	112.5(6)
C(40)-O(1)-Sn(1)	123.7(4)	C(11)-C(10)-C(28)	110.0(5)	C(31)-C(30)-C(29)	113.8(5)
C(37)-O(1)-Sn(1)	125.8(4)	C(9)-C(10)-C(28)	113.5(5)	C(30)-C(31)-C(32)	114.4(5)
C(4)-N(1)-C(1)	106.9(5)	C(25)-C(10)-C(28)	100.0(5)	C(15)-C(32)-C(31)	114.4(5)
C(4)-N(1)-Sn(1)	118.6(4)	N(3)-C(11)-C(12)	109.1(6)	C(34)-C(33)-C(20)	106.8(6)
C(1)-N(1)-Sn(1)	121.6(4)	N(3)-C(11)-C(10)	122.8(6)	C(35)-C(34)-C(33)	105.2(6)
C(9)-N(2)-C(6)	106.3(5)	C(12)-C(11)-C(10)	128.1(6)	C(34)-C(35)-C(36)	107.3(6)
C(9)-N(2)-Sn(1)	126.9(4)	C(13)-C(12)-C(11)	108.7(6)	C(35)-C(36)-C(20)	102.5(5)
C(6)-N(2)-Sn(1)	124.8(4)	C(12)-C(13)-C(14)	106.6(6)	O(1)-C(37)-C(38)	105.0(5)
C(11)-N(3)-C(14)	106.6(5)	C(12)-C(13)-C(29)	124.9(6)	C(39A)-C(38)-C(37)	107.1(7)
C(11)-N(3)-Sn(1)	124.8(4)	C(14)-C(13)-C(29)	128.1(6)	C(39A)-C(38)-C(39B)	39.3(8)
C(14)-N(3)-Sn(1)	124.2(4)	C(15)-C(14)-C(13)	126.2(6)	C(37)-C(38)-C(39B)	100.0(8)
C(19)-N(4)-C(16)	106.2(5)	C(15)-C(14)-N(3)	124.7(6)	C(38)-C(39A)-C(40)	105.0(10)
C(19)-N(4)-Sn(1)	126.4(4)	C(13)-C(14)-N(3)	109.0(5)	C(40)-C(39B)-C(38)	103.3(13)
C(16)-N(4)-Sn(1)	127.3(4)	C(14)-C(15)-C(16)	127.8(6)	C(39B)-C(40)-O(1)	107.6(9)

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Table S38. Bond lengths [Å] and angles [°] for 13.

C(2)-C(1)-N(1)	108.5(6)	C(14)-C(15)-C(32)	115.8(6)	C(39B)-C(40)-C(39A)	39.1(8)
C(2)-C(1)-C(20)	129.8(6)	C(16)-C(15)-C(32)	116.3(6)	O(1)-C(40)-C(39A)	101.6(7)
N(1)-C(1)-C(20)	121.7(6)	C(17)-C(16)-C(15)	127.2(6)	C(41) ^a -C(41)-C(42)	88.5(18)
C(1)-C(2)-C(3)	108.4(6)	C(17)-C(16)-N(4)	109.0(6)	C(41) ^a -C(41)-C(42) ^a	48.3(11)
C(4)-C(3)-C(2)	107.9(6)	C(15)-C(16)-N(4)	123.5(6)	C(42)-C(41)-C(42) ^a	136.8(12)
C(3)-C(4)-N(1)	108.3(6)	C(18)-C(17)-C(16)	107.7(6)	C(41)-C(42)-C(43)	117.1(19)
C(3)-C(4)-C(5)	128.4(6)	C(17)-C(18)-C(19)	107.9(6)	C(41)-C(42)-C(41) ^a	43.2(12)
N(1)-C(4)-C(5)	121.3(5)	N(4)-C(19)-C(18)	109.1(6)	C(43)-C(42)-C(41) ^a	154.1(17)
C(4)-C(5)-C(6)	116.0(5)	N(4)-C(19)-C(20)	123.7(6)		

Symmetry transformations used to generate equivalent atoms:

^a -x,-y+1,-z

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Table S39. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 13. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Sn(1)	29(1)	34(1)	34(1)	-2(1)	4(1)	-1(1)
Cl(1)	37(1)	42(1)	37(1)	-4(1)	9(1)	0(1)
O(1)	40(3)	33(2)	41(3)	2(2)	9(2)	9(2)
N(1)	31(3)	41(3)	40(3)	1(3)	7(2)	1(3)
N(2)	35(3)	38(3)	36(3)	-5(2)	11(2)	-7(3)
N(3)	29(3)	41(3)	32(3)	-4(2)	1(2)	3(3)
N(4)	35(3)	41(3)	36(3)	-1(3)	6(3)	-3(3)
C(1)	38(4)	37(4)	40(4)	-2(3)	2(3)	0(3)
C(2)	53(5)	37(4)	45(4)	1(3)	7(4)	-10(4)
C(3)	40(4)	40(4)	45(4)	-2(3)	5(3)	-1(3)
C(4)	39(4)	38(4)	43(4)	-1(3)	8(3)	-4(3)
C(5)	24(3)	36(4)	38(4)	-5(3)	2(3)	-5(3)
C(6)	27(4)	39(4)	35(4)	-3(3)	2(3)	-1(3)
C(7)	26(3)	45(4)	44(4)	1(3)	3(3)	3(3)
C(8)	38(4)	36(4)	49(4)	2(3)	4(3)	3(3)
C(9)	35(4)	39(4)	27(3)	3(3)	7(3)	2(3)
C(10)	34(4)	31(3)	33(3)	3(3)	2(3)	-2(3)
C(11)	33(4)	38(4)	39(4)	0(3)	8(3)	-3(3)
C(12)	42(4)	29(4)	47(4)	-2(3)	4(3)	-3(3)
C(13)	33(4)	39(4)	38(4)	-6(3)	3(3)	-4(3)
C(14)	26(3)	42(4)	33(3)	-2(3)	5(3)	-2(3)
C(15)	29(4)	44(4)	36(4)	-3(3)	9(3)	-2(3)
C(16)	31(4)	42(4)	35(4)	-6(3)	6(3)	-1(3)
C(17)	39(4)	42(4)	44(4)	0(3)	-7(3)	6(4)
C(18)	43(4)	41(4)	53(4)	7(4)	0(4)	10(4)
C(19)	27(3)	37(4)	43(4)	-6(3)	3(3)	-1(3)
C(20)	49(4)	29(4)	48(4)	0(3)	2(3)	8(3)
C(21)	34(4)	43(4)	45(4)	-9(3)	0(3)	-3(3)
C(22)	55(5)	54(5)	52(4)	-7(4)	-3(4)	-15(4)
C(23)	46(4)	54(5)	68(5)	4(4)	-3(4)	-12(4)
C(24)	34(4)	38(4)	67(5)	0(4)	16(4)	-1(3)
C(25)	39(4)	38(4)	44(4)	0(3)	3(3)	-1(3)
C(26)	49(4)	33(4)	49(4)	1(3)	-1(3)	-3(3)
C(27)	52(5)	49(5)	66(5)	8(4)	14(4)	-9(4)
C(28)	37(4)	47(4)	37(4)	2(3)	5(3)	-7(3)
C(29)	52(4)	39(4)	47(4)	-3(3)	-3(4)	-2(4)
C(30)	46(4)	59(5)	44(4)	-8(4)	2(3)	3(4)
C(31)	38(4)	48(4)	34(4)	-7(3)	1(3)	1(3)
C(32)	31(4)	41(4)	40(4)	-1(3)	4(3)	4(3)
C(33)	52(5)	41(4)	60(5)	9(4)	-1(4)	0(4)
C(34)	75(6)	37(4)	66(5)	-1(4)	3(4)	2(4)
C(35)	84(6)	40(4)	62(5)	-3(4)	-6(5)	-1(4)
C(36)	45(4)	43(4)	52(4)	-6(3)	3(3)	7(4)
C(37)	51(4)	46(4)	36(4)	6(3)	16(3)	7(4)
C(38)	59(5)	49(5)	53(5)	0(4)	14(4)	6(4)
C(39A)	53(10)	59(10)	56(10)	5(8)	27(8)	5(8)
C(39B)	28(12)	40(13)	23(10)	-4(9)	6(9)	-9(10)
C(40)	56(5)	40(4)	45(4)	-5(3)	7(4)	18(4)
C(41)	300(20)	129(12)	330(20)	-65(14)	200(20)	-116(13)
C(42)	350(30)	149(17)	410(30)	-99(19)	130(20)	-69(18)
C(43)	220(20)	290(30)	350(30)	-100(20)	20(30)	-50(20)

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Table S40. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 13.

	x	y	z	U(eq)
H(2)	-2037	-3106	2786	54
H(3)	-2758	-2119	2353	51
H(7)	-3086	1050	898	46
H(8)	-2551	2419	796	50
H(12)	-1050	3221	2296	47
H(17)	67	-1072	3776	52
H(18)	-294	-2590	3353	56
H(21A)	-2812	-705	13	50
H(21B)	-2348	-1325	292	50
H(22A)	-2794	-2492	732	65
H(22B)	-3112	-2194	-68	65
H(23A)	-3457	-2125	1244	68
H(23B)	-3653	-1451	539	68
H(24A)	-3161	-887	1931	55
H(24B)	-3329	-221	1208	55
H(25A)	-1948	3197	593	49
H(25B)	-1701	3395	1462	49
H(26A)	-1333	4010	277	54
H(26B)	-1008	3803	1090	54
H(27A)	-670	2631	572	66
H(27B)	-980	2864	-248	66
H(28A)	-1098	1308	448	49
H(28B)	-1535	1783	-101	49
H(29A)	-559	3219	3649	57
H(29B)	-88	2657	3549	57
H(30A)	-377	2465	4790	60
H(30B)	-800	1867	4337	60
H(31A)	-323	705	4694	49
H(31B)	141	1340	4799	49
H(32A)	155	1287	3454	45
H(32B)	201	277	3825	45
H(33A)	-775	-3588	2886	62
H(33B)	-1290	-3448	3138	62
H(34A)	-1118	-4762	2181	72
H(34B)	-1644	-4357	2188	72
H(35A)	-1633	-3671	1072	76
H(35B)	-1140	-4186	1016	76
H(36A)	-1157	-2397	1054	56
H(36B)	-695	-2929	1484	56
H(37A)	-1368	-466	3933	52
H(37B)	-1700	-1169	3381	52
H(38A)	-2294	-789	3991	64
H(38B)	-1979	-5	4472	64
H(39A)	-2473	895	3806	65
H(39B)	-2594	157	3118	65
H(39C)	-2404	1070	3838	36
H(39D)	-1850	1112	4198	36
H(40A)	-2112	1158	2561	56
H(40B)	-1781	1364	3373	56
H(41A)	-262	4265	256	80
H(41B)	-470	5295	26	80
H(42A)	111	5996	853	80
H(42B)	452	5121	879	80
H(43A)	-320	5303	1771	80
H(43B)	232	5286	2119	80
H(43C)	-22	4368	1756	80

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Table S41. Crystal data and structure refinement for 19.

Identification code	19	
Empirical formula	C ₅₂ H ₈₀ Li ₂ N ₄ Ni O ₃	
Formula weight	881.79	
Temperature	143(2) K	
Wavelength	0.71070 Å	
Crystal system	Monoclinic	
Space group	Cc	
Unit cell dimensions	a = 18.394(4) Å	$\alpha = 90^\circ$.
	b = 14.212(3) Å	$\beta = 98.13(3)^\circ$.
	c = 18.563(4) Å	$\gamma = 90^\circ$.
Volume	4803.9(17) Å ³	
Z	4	
Density (calculated)	1.219 Mg/m ³	
Absorption coefficient	0.449 mm ⁻¹	
F(000)	1912	
Crystal size	0.30 x 0.25 x 0.17 mm ³	
Theta range for data collection	1.82 to 24.52°	
Index ranges	-21 ≤ h ≤ 21, -16 ≤ k ≤ 15, -20 ≤ l ≤ 21	
Reflections collected	11914	
Independent reflections	6268 [R(int) = 0.0346]	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	6268 / 2 / 560	
Goodness-of-fit on F ²	0.987	
Final R indices [I > 2sigma(I)]	R1 = 0.0469, wR2 = 0.1178	
R indices (all data)	R1 = 0.0561, wR2 = 0.1252	
Absolute structure parameter	-0.004(14)	
Extinction coefficient	0.0110(6)	
Largest diff. peak and hole	0.429 and -0.284 e.Å ⁻³	

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Table S42. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 19. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni(1)	-2346(1)	2377(1)	-1804(1)	37(1)
N(1)	-2558(2)	1340(2)	-1237(2)	38(1)
N(2)	-1805(2)	1614(2)	-2351(2)	39(1)
N(3)	-2168(2)	3408(2)	-2363(2)	39(1)
N(4)	-2901(2)	3133(2)	-1258(2)	40(1)
C(1)	-3247(2)	1153(3)	-1044(2)	43(1)
C(2)	-3283(2)	216(3)	-832(3)	48(1)
C(3)	-2587(2)	-189(3)	-910(3)	44(1)
C(4)	-2156(2)	507(3)	-1142(2)	39(1)
C(5)	-1387(2)	485(3)	-1334(2)	38(1)
C(6)	-1441(2)	793(3)	-2122(2)	39(1)
C(7)	-1193(2)	364(3)	-2716(2)	41(1)
C(8)	-1425(3)	931(3)	-3335(3)	44(1)
C(9)	-1788(2)	1699(3)	-3092(2)	40(1)
C(10)	-2210(3)	2477(3)	-3529(3)	39(1)
C(11)	-2138(2)	3386(3)	-3102(2)	42(1)
C(12)	-2092(3)	4312(3)	-3354(3)	46(1)
C(13)	-2088(3)	4910(3)	-2740(3)	49(1)
C(14)	-2137(2)	4339(3)	-2138(2)	40(1)
C(15)	-2142(2)	4584(3)	-1340(2)	42(1)
C(16)	-2785(2)	4075(3)	-1097(3)	44(1)
C(17)	-3333(3)	4393(3)	-707(3)	49(1)
C(18)	-3795(3)	3617(3)	-634(3)	49(1)
C(19)	-3536(2)	2854(3)	-972(3)	42(1)
C(20)	-3850(2)	1883(3)	-1135(2)	41(1)
C(21)	-897(2)	1192(3)	-830(2)	43(1)
C(22)	-87(2)	1240(3)	-934(3)	48(1)
C(23)	316(3)	2048(4)	-528(3)	58(1)
C(24)	1116(3)	2146(4)	-657(4)	68(2)
C(25)	-1057(3)	-514(3)	-1253(2)	46(1)
C(26)	-868(3)	-878(4)	-478(3)	57(1)
C(27)	-1943(3)	2606(3)	-4269(3)	47(1)
C(28)	-1127(3)	2875(3)	-4254(3)	52(1)
C(29)	-3037(2)	2211(3)	-3665(3)	48(1)
C(30)	-3224(3)	1220(4)	-3961(3)	62(1)
C(31)	-1411(2)	4245(3)	-880(3)	47(1)
C(32)	-1325(3)	4445(3)	-70(3)	54(1)
C(33)	-634(4)	4025(5)	343(3)	76(2)
C(34)	-461(4)	4313(6)	1125(3)	92(2)
C(35)	-2218(3)	5655(3)	-1233(3)	47(1)
C(36)	-1547(3)	6252(3)	-1322(3)	58(1)
C(37)	-4219(2)	1846(3)	-1950(3)	48(1)
C(38)	-4869(3)	2502(3)	-2147(3)	61(1)
C(39)	-4437(2)	1656(4)	-641(3)	49(1)
C(40)	-4179(3)	1595(4)	164(3)	60(1)
Li(1)	-370(5)	1554(6)	-2739(5)	59(2)
O(1)	20(2)	2749(2)	-2540(2)	57(1)
O(2)	458(2)	879(2)	-3019(2)	57(1)
C(41)	-359(3)	3507(4)	-2253(3)	65(2)
C(42)	179(4)	4189(5)	-1976(4)	89(2)
C(43)	769(3)	4095(4)	-2480(4)	77(2)
C(44)	718(3)	3084(4)	-2705(4)	73(2)
C(45)	584(5)	767(6)	-3740(4)	113(3)
C(46)	955(4)	-81(5)	-3858(4)	87(2)
C(47)	967(4)	-597(4)	-3129(4)	85(2)
C(48)	846(3)	144(5)	-2615(3)	79(2)
Li(2)	-2397(5)	2317(6)	-385(5)	53(2)
O(3)	-2161(2)	2180(2)	618(2)	58(1)
C(49)	-2321(4)	2844(4)	1157(4)	81(2)
C(50)	-2302(4)	2313(4)	1866(3)	77(2)
C(51)	-2493(3)	1321(4)	1608(3)	68(2)
C(52)	-2102(3)	1240(4)	930(3)	67(2)

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Table S43. Bond lengths [Å] and angles [°] for 19.

Ni(1)-N(3)	1.851(4)	C(7)-Li(1)	2.275(10)	C(27)-C(28)	1.546(7)
Ni(1)-N(2)	1.866(4)	C(8)-C(9)	1.387(6)	C(29)-C(30)	1.534(7)
Ni(1)-N(4)	1.875(4)	C(8)-Li(1)	2.273(11)	C(31)-C(32)	1.517(7)
Ni(1)-N(1)	1.885(4)	C(9)-C(10)	1.519(6)	C(32)-C(33)	1.511(7)
Ni(1)-Li(2)	2.651(8)	C(9)-Li(1)	2.605(10)	C(33)-C(34)	1.499(8)
N(1)-C(1)	1.390(5)	C(10)-C(11)	1.513(6)	C(35)-C(36)	1.527(6)
N(1)-C(4)	1.394(5)	C(10)-C(27)	1.534(6)	C(37)-C(38)	1.519(7)
N(1)-Li(2)	2.093(9)	C(10)-C(29)	1.551(7)	C(39)-C(40)	1.504(7)
N(2)-C(6)	1.382(5)	C(11)-C(12)	1.404(6)	Li(1)-O(1)	1.860(9)
N(2)-C(9)	1.384(6)	C(12)-C(13)	1.421(6)	Li(1)-O(2)	1.933(10)
N(3)-C(11)	1.379(6)	C(13)-C(14)	1.394(6)	O(1)-C(41)	1.427(6)
N(3)-C(14)	1.387(5)	C(14)-C(15)	1.524(6)	O(1)-C(44)	1.443(6)
N(4)-C(16)	1.382(6)	C(15)-C(16)	1.508(6)	O(2)-C(45)	1.400(7)
N(4)-C(19)	1.408(5)	C(15)-C(35)	1.544(6)	O(2)-C(48)	1.418(6)
N(4)-Li(2)	2.100(10)	C(15)-C(31)	1.564(6)	C(41)-C(42)	1.428(8)
C(1)-C(2)	1.392(7)	C(16)-C(17)	1.396(6)	C(42)-C(43)	1.537(8)
C(1)-C(20)	1.511(6)	C(17)-C(18)	1.410(7)	C(43)-C(44)	1.496(8)
C(1)-Li(2)	2.477(10)	C(18)-C(19)	1.372(6)	C(45)-C(46)	1.416(9)
C(2)-C(3)	1.430(6)	C(19)-C(20)	1.510(6)	C(46)-C(47)	1.538(9)
C(3)-C(4)	1.374(6)	C(19)-Li(2)	2.349(10)	C(47)-C(48)	1.459(8)
C(4)-C(5)	1.507(6)	C(20)-C(39)	1.546(6)	Li(2)-O(3)	1.861(9)
C(5)-C(6)	1.517(6)	C(20)-C(37)	1.569(7)	O(3)-C(49)	1.435(7)
C(5)-C(25)	1.543(6)	C(21)-C(22)	1.530(6)	O(3)-C(52)	1.455(6)
C(5)-C(21)	1.568(6)	C(22)-C(23)	1.509(7)	C(49)-C(50)	1.513(9)
C(6)-C(7)	1.391(6)	C(23)-C(24)	1.531(7)	C(50)-C(51)	1.514(8)
C(6)-Li(1)	2.645(10)	C(25)-C(26)	1.522(6)	C(51)-C(52)	1.539(8)
C(7)-C(8)	1.420(6)				
N(3)-Ni(1)-N(2)	90.28(15)	C(9)-C(8)-Li(1)	87.2(3)	C(36)-C(35)-C(15)	116.4(4)
N(3)-Ni(1)-N(4)	90.15(15)	C(7)-C(8)-Li(1)	71.9(3)	C(38)-C(37)-C(20)	115.4(4)
N(2)-Ni(1)-N(4)	179.13(17)	N(2)-C(9)-C(8)	109.5(4)	C(40)-C(39)-C(20)	116.9(4)
N(3)-Ni(1)-N(1)	178.13(17)	N(2)-C(9)-C(10)	120.8(4)	O(1)-Li(1)-O(2)	102.1(5)
N(2)-Ni(1)-N(1)	91.05(15)	C(8)-C(9)-C(10)	129.2(4)	O(1)-Li(1)-C(8)	137.0(5)
N(4)-Ni(1)-N(1)	88.51(15)	N(2)-C(9)-Li(1)	84.6(3)	O(2)-Li(1)-C(8)	109.1(4)
N(3)-Ni(1)-Li(2)	128.1(2)	C(8)-C(9)-Li(1)	60.6(3)	O(1)-Li(1)-C(7)	156.1(5)
N(2)-Ni(1)-Li(2)	128.2(2)	C(10)-C(9)-Li(1)	127.6(3)	O(2)-Li(1)-C(7)	100.8(4)
N(4)-Ni(1)-Li(2)	51.9(2)	C(11)-C(10)-C(9)	109.9(4)	C(8)-Li(1)-C(7)	36.4(2)
N(1)-Ni(1)-Li(2)	51.7(2)	C(11)-C(10)-C(27)	110.6(4)	O(1)-Li(1)-C(9)	108.8(4)
C(1)-N(1)-C(4)	107.0(3)	C(9)-C(10)-C(27)	111.2(4)	O(2)-Li(1)-C(9)	140.4(5)
C(1)-N(1)-Ni(1)	124.2(3)	C(11)-C(10)-C(29)	107.7(4)	C(8)-Li(1)-C(9)	32.13(19)
C(4)-N(1)-Ni(1)	125.9(3)	C(9)-C(10)-C(29)	109.0(4)	C(7)-Li(1)-C(9)	54.4(2)
C(1)-N(1)-Li(2)	88.2(4)	C(27)-C(10)-C(29)	108.3(4)	O(1)-Li(1)-C(6)	125.3(5)
C(4)-N(1)-Li(2)	116.9(4)	N(3)-C(11)-C(12)	108.9(4)	O(2)-Li(1)-C(6)	125.2(4)
Ni(1)-N(1)-Li(2)	83.4(3)	N(3)-C(11)-C(10)	121.8(4)	C(8)-Li(1)-C(6)	54.2(2)
C(6)-N(2)-C(9)	107.5(3)	C(12)-C(11)-C(10)	129.1(4)	C(7)-Li(1)-C(6)	31.73(18)
C(6)-N(2)-Ni(1)	126.6(3)	C(11)-C(12)-C(13)	106.6(4)	C(9)-Li(1)-C(6)	50.3(2)
C(9)-N(2)-Ni(1)	125.4(3)	C(14)-C(13)-C(12)	107.5(4)	C(41)-O(1)-C(44)	109.1(4)
C(11)-N(3)-C(14)	108.3(4)	N(3)-C(14)-C(13)	108.6(4)	C(41)-O(1)-Li(1)	124.6(4)
C(11)-N(3)-Ni(1)	125.1(3)	N(3)-C(14)-C(15)	120.4(4)	C(44)-O(1)-Li(1)	126.1(4)
C(14)-N(3)-Ni(1)	126.1(3)	C(13)-C(14)-C(15)	131.0(4)	C(45)-O(2)-C(48)	106.4(4)
C(16)-N(4)-C(19)	107.6(3)	C(16)-C(15)-C(14)	107.1(4)	C(45)-O(2)-Li(1)	123.9(5)
C(16)-N(4)-Ni(1)	126.3(3)	C(16)-C(15)-C(35)	110.2(4)	C(48)-O(2)-Li(1)	125.5(4)
C(19)-N(4)-Ni(1)	126.0(3)	C(14)-C(15)-C(35)	111.3(4)	O(1)-C(41)-C(42)	107.2(4)
C(16)-N(4)-Li(2)	109.3(4)	C(16)-C(15)-C(31)	109.8(4)	C(41)-C(42)-C(43)	103.6(5)

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Table S43. Bond lengths [Å] and angles [°] for **19** (cont.).

C(19)-N(4)-Li(2)	81.5(4)	C(14)-C(15)-C(31)	109.7(4)	C(44)-C(43)-C(42)	103.4(5)
Ni(1)-N(4)-Li(2)	83.4(3)	C(35)-C(15)-C(31)	108.7(4)	O(1)-C(44)-C(43)	106.3(4)
N(1)-C(1)-C(2)	109.7(4)	N(4)-C(16)-C(17)	108.9(4)	O(2)-C(45)-C(46)	113.2(6)
N(1)-C(1)-C(20)	121.4(4)	N(4)-C(16)-C(15)	120.2(4)	C(45)-C(46)-C(47)	102.5(5)
C(2)-C(1)-C(20)	128.7(4)	C(17)-C(16)-C(15)	130.8(4)	C(48)-C(47)-C(46)	104.3(5)
N(1)-C(1)-Li(2)	57.6(3)	C(16)-C(17)-C(18)	106.7(4)	O(2)-C(48)-C(47)	107.3(5)
C(2)-C(1)-Li(2)	123.4(4)	C(19)-C(18)-C(17)	108.7(4)	O(3)-Li(2)-N(1)	132.4(5)
C(20)-C(1)-Li(2)	89.9(3)	C(18)-C(19)-N(4)	108.0(4)	O(3)-Li(2)-N(4)	147.7(5)
C(1)-C(2)-C(3)	106.1(4)	C(18)-C(19)-C(20)	131.9(4)	N(1)-Li(2)-N(4)	77.5(3)
C(4)-C(3)-C(2)	107.8(4)	N(4)-C(19)-C(20)	119.7(4)	O(3)-Li(2)-C(19)	124.4(5)
C(3)-C(4)-N(1)	109.3(4)	C(18)-C(19)-Li(2)	112.9(4)	N(1)-Li(2)-C(19)	81.0(3)
C(3)-C(4)-C(5)	131.4(4)	N(4)-C(19)-Li(2)	62.2(3)	N(4)-Li(2)-C(19)	36.3(2)
N(1)-C(4)-C(5)	119.2(3)	C(20)-C(19)-Li(2)	95.0(3)	O(3)-Li(2)-C(1)	117.8(4)
C(4)-C(5)-C(6)	106.6(3)	C(19)-C(20)-C(1)	110.6(4)	N(1)-Li(2)-C(1)	34.12(19)
C(4)-C(5)-C(25)	111.4(3)	C(19)-C(20)-C(39)	110.5(4)	N(4)-Li(2)-C(1)	79.0(3)
C(6)-C(5)-C(25)	109.3(3)	C(1)-C(20)-C(39)	110.7(4)	C(19)-Li(2)-C(1)	61.9(3)
C(4)-C(5)-C(21)	109.0(3)	C(19)-C(20)-C(37)	109.0(3)	O(3)-Li(2)-Ni(1)	164.1(5)
C(6)-C(5)-C(21)	110.1(3)	C(1)-C(20)-C(37)	107.2(4)	N(1)-Li(2)-Ni(1)	44.94(19)
C(25)-C(5)-C(21)	110.3(3)	C(39)-C(20)-C(37)	108.8(4)	N(4)-Li(2)-Ni(1)	44.65(19)
N(2)-C(6)-C(7)	109.0(4)	C(22)-C(21)-C(5)	116.2(3)	C(19)-Li(2)-Ni(1)	71.5(3)
N(2)-C(6)-C(5)	120.2(4)	C(23)-C(22)-C(21)	112.9(4)	C(1)-Li(2)-Ni(1)	68.9(2)
C(7)-C(6)-C(5)	130.8(4)	C(22)-C(23)-C(24)	114.0(4)	C(49)-O(3)-C(52)	109.7(4)
N(2)-C(6)-Li(1)	83.1(3)	C(26)-C(25)-C(5)	116.0(4)	C(49)-O(3)-Li(2)	125.9(5)
C(7)-C(6)-Li(1)	59.3(3)	C(10)-C(27)-C(28)	116.5(4)	C(52)-O(3)-Li(2)	119.2(4)
C(5)-C(6)-Li(1)	125.7(3)	C(30)-C(29)-C(10)	116.5(4)	O(3)-C(49)-C(50)	107.3(5)
C(6)-C(7)-C(8)	107.3(4)	C(32)-C(31)-C(15)	116.4(4)	C(49)-C(50)-C(51)	102.3(5)
C(6)-C(7)-Li(1)	88.9(3)	C(33)-C(32)-C(31)	113.0(4)	C(50)-C(51)-C(52)	102.4(5)
C(8)-C(7)-Li(1)	71.7(4)	C(34)-C(33)-C(32)	115.5(5)	O(3)-C(52)-C(51)	103.8(4)
C(9)-C(8)-C(7)	106.7(4)				

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Table S44. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 19. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni(1)	43(1)	34(1)	35(1)	1(1)	11(1)	3(1)
N(1)	40(2)	39(2)	38(2)	0(2)	13(2)	5(2)
N(2)	41(2)	37(2)	38(2)	8(2)	8(2)	3(2)
N(3)	46(2)	33(2)	39(2)	-5(2)	11(2)	3(2)
N(4)	43(2)	33(2)	45(2)	1(2)	8(2)	-3(2)
C(1)	41(2)	46(3)	43(3)	-2(2)	9(2)	3(2)
C(2)	46(3)	40(3)	60(3)	6(2)	14(2)	-5(2)
C(3)	47(3)	34(2)	53(3)	5(2)	14(2)	3(2)
C(4)	44(2)	34(2)	40(2)	-1(2)	9(2)	7(2)
C(5)	42(2)	31(2)	43(2)	1(2)	12(2)	7(2)
C(6)	43(2)	35(2)	39(2)	1(2)	7(2)	-3(2)
C(7)	50(3)	36(2)	38(3)	-1(2)	13(2)	5(2)
C(8)	53(3)	43(2)	38(2)	-5(2)	14(2)	3(2)
C(9)	48(3)	30(2)	40(2)	1(2)	6(2)	2(2)
C(10)	54(3)	37(2)	28(3)	4(2)	11(2)	3(2)
C(11)	45(2)	44(3)	40(3)	0(2)	12(2)	3(2)
C(12)	62(3)	37(2)	41(3)	3(2)	16(2)	2(2)
C(13)	67(3)	37(2)	45(3)	6(2)	15(2)	1(2)
C(14)	52(3)	27(2)	43(3)	-2(2)	15(2)	1(2)
C(15)	50(3)	37(2)	42(3)	2(2)	13(2)	4(2)
C(16)	47(3)	39(3)	46(3)	1(2)	11(2)	2(2)
C(17)	48(3)	43(3)	58(3)	-12(2)	19(2)	2(2)
C(18)	47(3)	49(3)	54(3)	-8(2)	22(2)	3(2)
C(19)	40(2)	39(2)	49(3)	1(2)	10(2)	0(2)
C(20)	40(2)	39(2)	46(3)	7(2)	17(2)	2(2)
C(21)	43(2)	46(3)	42(3)	0(2)	7(2)	8(2)
C(22)	44(2)	54(3)	46(3)	-3(2)	8(2)	-1(2)
C(23)	58(3)	59(3)	57(3)	-8(3)	4(2)	2(2)
C(24)	55(3)	72(4)	75(4)	-10(3)	2(3)	-5(3)
C(25)	51(3)	40(2)	48(3)	7(2)	13(2)	7(2)
C(26)	68(3)	52(3)	52(3)	13(2)	15(2)	15(2)
C(27)	61(3)	47(3)	35(3)	4(2)	13(2)	5(2)
C(28)	69(3)	50(3)	42(3)	9(2)	23(2)	8(2)
C(29)	49(3)	53(3)	41(3)	-2(2)	4(2)	4(2)
C(30)	59(3)	60(3)	68(4)	-15(3)	10(3)	-3(2)
C(31)	51(3)	45(3)	44(3)	-7(2)	10(2)	-6(2)
C(32)	71(3)	47(3)	44(3)	-7(2)	8(2)	1(2)
C(33)	86(4)	83(4)	53(3)	-15(3)	-6(3)	16(3)
C(34)	82(4)	128(6)	63(4)	-18(4)	-1(3)	14(4)
C(35)	58(3)	35(2)	51(3)	-8(2)	13(2)	-2(2)
C(36)	66(3)	46(3)	65(3)	-8(2)	16(2)	-7(2)
C(37)	52(3)	40(3)	51(3)	1(2)	6(2)	-3(2)
C(38)	56(3)	61(3)	64(4)	11(3)	4(3)	7(2)
C(39)	46(3)	52(3)	52(3)	1(2)	18(2)	-1(2)
C(40)	56(3)	73(4)	57(3)	6(3)	25(2)	-3(2)
Li(1)	77(6)	43(5)	59(6)	3(4)	17(4)	-1(4)
O(1)	58(2)	50(2)	68(2)	-6(2)	23(2)	-5(2)
O(2)	64(2)	56(2)	53(2)	0(2)	15(2)	7(2)
C(41)	59(3)	59(3)	81(4)	-13(3)	25(3)	-1(2)
C(42)	79(4)	77(4)	119(6)	-30(4)	43(4)	-24(3)
C(43)	65(4)	74(4)	98(5)	-24(3)	37(3)	-22(3)
C(44)	70(4)	73(4)	83(4)	-17(3)	37(3)	-16(3)
C(45)	183(8)	108(6)	62(4)	25(4)	64(5)	65(6)
C(46)	105(5)	84(4)	75(4)	1(4)	28(4)	29(4)
C(47)	110(5)	58(4)	95(5)	9(3)	47(4)	23(3)
C(48)	66(4)	115(5)	55(3)	6(3)	0(3)	36(3)
Li(2)	70(6)	57(5)	31(5)	-5(3)	9(4)	-1(4)
O(3)	84(2)	48(2)	41(2)	0(2)	8(2)	3(2)
C(49)	128(6)	60(3)	60(4)	-12(3)	28(4)	-10(3)
C(50)	102(5)	79(4)	53(4)	-9(3)	25(3)	-21(3)
C(51)	75(4)	66(4)	63(4)	8(3)	13(3)	5(3)
C(52)	86(4)	59(3)	58(3)	6(3)	14(3)	13(3)

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Table S45. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **19**.

	x	y	z	U(eq)
H(2)	-3688	-92	-668	57
H(3)	-2447	-826	-819	53
H(7)	-920	-204	-2708	49
H(8)	-1348	809	-3821	53
H(12)	-2069	4502	-3841	55
H(13)	-2057	5577	-2740	59
H(17)	-3384	5011	-526	58
H(18)	-4216	3623	-391	58
H(21A)	-1111	1829	-912	52
H(21B)	-924	1021	-318	52
H(22A)	156	642	-764	58
H(22B)	-53	1305	-1459	58
H(23A)	304	1961	0	70
H(23B)	53	2640	-677	70
H(24A)	1384	1567	-505	102
H(24B)	1344	2677	-373	102
H(24C)	1133	2257	-1175	102
H(25A)	-1411	-956	-1526	55
H(25B)	-605	-525	-1486	55
H(26A)	-432	-549	-237	85
H(26B)	-768	-1555	-488	85
H(26C)	-1282	-765	-210	85
H(27A)	-2247	3099	-4542	56
H(27B)	-2033	2012	-4546	56
H(28A)	-1011	3420	-3935	78
H(28B)	-1035	3033	-4747	78
H(28C)	-815	2343	-4070	78
H(29A)	-3237	2280	-3200	57
H(29B)	-3294	2672	-4011	57
H(30A)	-2999	1121	-4403	93
H(30B)	-3758	1154	-4076	93
H(30C)	-3034	752	-3594	93
H(31A)	-1368	3558	-948	56
H(31B)	-996	4545	-1079	56
H(32A)	-1318	5134	7	65
H(32B)	-1756	4189	130	65
H(33A)	-678	3331	322	91
H(33B)	-214	4203	91	91
H(34A)	-324	4979	1154	138
H(34B)	-52	3932	1365	138
H(34C)	-894	4214	1369	138
H(35A)	-2636	5882	-1585	57
H(35B)	-2345	5765	-739	57
H(36A)	-1144	6094	-937	87
H(36B)	-1670	6920	-1289	87
H(36C)	-1394	6125	-1798	87
H(37A)	-3842	2000	-2263	57
H(37B)	-4384	1193	-2064	57
H(38A)	-5279	2293	-1902	91
H(38B)	-5019	2493	-2675	91
H(38C)	-4728	3143	-1991	91

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Table S45. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **19** (cont.).

	x	y	z	U(eq)
H(39A)	-4823	2145	-722	59
H(39B)	-4668	1049	-801	59
H(40A)	-3845	1058	263	91
H(40B)	-4603	1511	423	91
H(40C)	-3920	2176	329	91
H(41A)	-625	3278	-1859	78
H(41B)	-719	3788	-2640	78
H(42A)	384	4048	-1465	107
H(42B)	-34	4830	-2001	107
H(43A)	664	4516	-2907	92
H(43B)	1263	4244	-2218	92
H(44A)	744	3023	-3232	88
H(44B)	1126	2717	-2433	88
H(45A)	879	1305	-3875	136
H(45B)	108	778	-4063	136
H(46A)	1459	45	-3963	104
H(46B)	684	-446	-4264	104
H(47A)	572	-1076	-3161	102
H(47B)	1446	-910	-2983	102
H(48A)	556	-101	-2245	95
H(48B)	1321	379	-2363	95
H(49A)	-2812	3126	1012	97
H(49B)	-1951	3355	1211	97
H(50A)	-2669	2564	2158	92
H(50B)	-1809	2340	2158	92
H(51A)	-3031	1240	1481	81
H(51B)	-2304	852	1981	81
H(52A)	-1581	1057	1066	81
H(52B)	-2348	771	584	81

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Table S46. Crystal data and structure refinement for **24**.

Identification code	24	
Empirical formula	C ₅₆ H ₇₈ Li ₄ N ₄ O ₉	
Formula weight	978.98	
Temperature	293(2) K	
Wavelength	0.71070 Å	
Crystal system	Monoclinic	
Space group	I2/a	
Unit cell dimensions	a = 24.353(5) Å	$\alpha = 90^\circ$.
	b = 20.315(4) Å	$\beta = 115.97(3)^\circ$.
	c = 25.646(5) Å	$\gamma = 90^\circ$.
Volume	11406(4) Å ³	
Z	8	
Density (calculated)	1.140 Mg/m ³	
Absorption coefficient	0.075 mm ⁻¹	
F(000)	4208	
Crystal size	0.15 x 0.10 x 0.08 mm ³	
Theta range for data collection	1.34 to 23.48°	
Index ranges	-22 ≤ h ≤ 25, -22 ≤ k ≤ 19, -24 ≤ l ≤ 27	
Reflections collected	17344	
Independent reflections	5940 [R(int) = 0.0948]	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5940 / 0 / 614	
Goodness-of-fit on F ²	1.190	
Final R indices [I > 2sigma(I)]	R1 = 0.1379, wR2 = 0.3383	
R indices (all data)	R1 = 0.2178, wR2 = 0.3868	
Extinction coefficient	0.0080(10)	
Largest diff. peak and hole	1.320 and -0.449 e.Å ⁻³	

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Table S47. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **24**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	590(3)	-145(3)	-1239(3)	60(2)
N(2)	1420(3)	307(3)	-1692(4)	64(2)
N(3)	1609(3)	-1086(4)	-2023(3)	63(2)
N(4)	602(3)	-1578(3)	-1715(3)	61(2)
C(1)	181(4)	-470(5)	-1097(5)	67(3)
C(2)	204(5)	-221(5)	-599(5)	86(3)
C(3)	642(5)	278(5)	-407(5)	84(3)
C(4)	876(4)	336(4)	-807(4)	61(2)
C(5)	1354(4)	780(5)	-808(4)	67(3)
C(6)	1712(4)	567(4)	-1136(5)	67(3)
C(7)	2316(5)	647(5)	-980(5)	84(3)
C(8)	2418(5)	439(5)	-1458(5)	76(3)
C(9)	1874(5)	248(4)	-1882(5)	67(3)
C(10)	1713(4)	-22(4)	-2479(4)	65(3)
C(11)	1492(4)	-743(5)	-2520(5)	62(2)
C(12)	1224(4)	-1139(6)	-2990(5)	84(3)
C(13)	1181(4)	-1768(6)	-2783(6)	80(3)
C(14)	1419(4)	-1722(5)	-2188(5)	65(3)
C(15)	1411(4)	-2232(5)	-1783(5)	74(3)
C(16)	1012(4)	-2103(4)	-1510(4)	66(3)
C(17)	944(5)	-2425(4)	-1064(5)	79(3)
C(18)	478(5)	-2086(5)	-1002(4)	76(3)
C(19)	273(4)	-1589(4)	-1393(4)	66(3)
C(20)	-170(4)	-1049(4)	-1440(5)	71(3)
C(21)	1485(4)	1352(5)	-532(4)	69(3)
C(22A)	1199(5)	1648(5)	-176(5)	76(4)
C(22B)	1890(30)	2010(30)	-610(20)	110(20)
C(23)	2289(4)	7(5)	-2583(5)	77(3)
C(24)	2210(4)	-186(5)	-3188(5)	87(3)
C(25)	1188(4)	398(5)	-2933(4)	77(3)
C(26)	1349(5)	1119(5)	-2943(5)	95(3)
C(27)	1705(6)	-2788(7)	-1745(6)	101(4)
C(28A)	2131(7)	-3039(7)	-1962(8)	82(7)
C(28B)	1810(16)	-3260(20)	-1340(20)	240(40)
C(29)	-542(4)	-852(5)	-2085(5)	75(3)
C(30)	-1013(4)	-306(5)	-2203(5)	93(3)
C(31)	-623(5)	-1292(5)	-1195(5)	93(3)
C(32)	-1072(5)	-1836(5)	-1537(5)	101(4)
Li(1)	1069(6)	-695(7)	-1622(6)	65(4)
Li(2)	552(6)	431(7)	-1890(7)	68(4)
Li(3)	2332(6)	-743(8)	-1293(7)	80(5)
Li(4)	-277(6)	3342(7)	-2399(7)	73(4)
O(1)	-39(3)	1064(3)	-2277(3)	79(2)
O(2)	58(3)	2444(3)	-2192(3)	84(2)
O(3)	3108(3)	-1075(3)	-1227(3)	91(2)
O(4)	4130(4)	-1864(5)	-1029(5)	143(4)
O(5)	350(3)	3807(4)	-1729(3)	101(2)
O(6)	1185(5)	4189(9)	-677(6)	251(7)
O(7)	2311(3)	-1023(4)	-583(3)	117(3)

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Table S47. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **24** (cont.).

	x	y	z	U(eq)
C(33)	-105(5)	1474(5)	-2756(4)	77(3)
C(34)	246(5)	2085(5)	-2563(5)	87(3)
C(35)	127(5)	2041(5)	-1693(5)	84(3)
C(36)	-233(5)	1428(5)	-1900(5)	86(3)
C(37)	3080(6)	-1647(9)	-1545(8)	192(9)
C(38)	3534(8)	-2092(7)	-1256(9)	216(10)
C(39)	4198(5)	-1300(6)	-693(5)	97(4)
C(40)	3716(5)	-814(5)	-1025(5)	93(3)
C(41)	974(7)	3564(8)	-1416(7)	151(5)
C(42)	1040(14)	3507(13)	-905(12)	310(15)
C(43)	551(11)	4399(15)	-975(11)	315(14)
C(44)	312(7)	4453(7)	-1568(6)	135(5)
C(45)	1857(4)	-1050(5)	-367(5)	76(3)
C(46A)	2818(8)	-1516(9)	-111(8)	67(8)
C(46B)	2844(8)	-534(10)	-159(9)	83(9)
C(47)	2205(10)	1800(13)	-4250(11)	226(8)
C(48)	2389(9)	1433(10)	-3757(11)	194(7)
C(49)	2740(8)	1656(10)	-3186(8)	165(6)
C(50)	2868(8)	2302(11)	-3077(9)	180(6)
C(51)	2757(10)	2756(11)	-3510(12)	211(8)
C(52)	2409(10)	2539(13)	-4117(12)	232(9)
O(8)	72(15)	3038(13)	-107(13)	377(12)
O(9A)	209(16)	4490(20)	295(16)	270(20)
O(9B)	90(20)	3910(20)	546(19)	270(30)
C(53)	-520(12)	3427(15)	-292(11)	237(9)
C(54)	-550(20)	3990(20)	-50(20)	390(20)
C(55)	653(16)	3920(20)	493(14)	292(13)
C(56)	518(15)	3294(18)	339(14)	261(11)

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Table S48. Bond lengths [Å] and angles [°] for 24.

N(1)-C(1)	1.372(10)	C(13)-Li(4)#1	2.454(16)	O(2)-C(35)	1.467(11)
N(1)-C(4)	1.412(10)	C(14)-C(15)	1.473(13)	O(3)-C(37)	1.405(13)
N(1)-Li(2)	2.007(16)	C(14)-Li(4)#1	2.508(16)	O(3)-C(40)	1.436(10)
N(1)-Li(1)	2.140(15)	C(15)-C(27)	1.317(14)	O(4)-C(38)	1.385(16)
N(2)-C(6)	1.390(11)	C(15)-C(16)	1.447(12)	O(4)-C(39)	1.398(13)
N(2)-C(9)	1.396(10)	C(16)-C(17)	1.390(12)	O(5)-C(44)	1.391(14)
N(2)-Li(2)	1.963(16)	C(16)-Li(4)#1	2.732(19)	O(5)-C(41)	1.459(15)
N(2)-Li(1)	2.246(15)	C(17)-C(18)	1.394(12)	O(6)-C(43)	1.46(2)
N(3)-C(11)	1.369(10)	C(18)-C(19)	1.354(12)	O(6)-C(42)	1.48(3)
N(3)-C(14)	1.377(11)	C(19)-C(20)	1.506(12)	O(7)-C(45)	1.438(10)
N(3)-Li(3)	2.050(17)	C(20)-C(29)	1.553(13)	O(7)-C(46B)	1.618(17)
N(3)-Li(1)	2.144(15)	C(20)-C(31)	1.569(12)	O(7)-C(46A)	1.638(18)
N(4)-C(19)	1.381(10)	C(21)-C(22A)	1.494(13)	C(33)-C(34)	1.464(13)
N(4)-C(16)	1.398(10)	C(21)-C(22B)	1.72(5)	C(35)-C(36)	1.481(13)
N(4)-Li(4)#1	2.060(17)	C(23)-C(24)	1.531(12)	C(37)-C(38)	1.37(2)
N(4)-Li(1)	2.081(15)	C(25)-C(26)	1.520(12)	C(39)-C(40)	1.485(13)
C(1)-C(2)	1.352(12)	C(27)-C(28B)	1.35(5)	C(41)-C(42)	1.26(2)
C(1)-C(20)	1.493(12)	C(27)-C(28A)	1.47(2)	C(43)-C(44)	1.38(2)
C(2)-C(3)	1.394(12)	C(29)-C(30)	1.528(11)	C(45)-C(46A)#3	1.475(19)
C(3)-C(4)	1.379(12)	C(31)-C(32)	1.532(13)	C(45)-C(46B)#3	1.61(2)
C(4)-C(5)	1.474(12)	Li(1)-Li(2)	2.56(2)	C(46A)-C(45)#3	1.475(19)
C(4)-Li(2)	2.542(19)	Li(1)-Li(3)	2.811(19)	C(46A)-C(46A)#3	1.87(3)
C(5)-C(21)	1.325(11)	Li(1)-Li(4)#1	3.10(2)	C(46B)-C(45)#3	1.61(2)
C(5)-C(6)	1.515(12)	Li(2)-O(1)	1.858(15)	C(47)-C(48)	1.36(3)
C(5)-Li(2)	2.698(18)	Li(2)-C(36)	2.777(17)	C(47)-C(52)	1.57(3)
C(6)-C(7)	1.353(12)	Li(3)-O(7)	1.93(2)	C(48)-C(49)	1.41(2)
C(6)-Li(2)	2.649(18)	Li(3)-O(3)	1.944(15)	C(49)-C(50)	1.35(2)
C(7)-C(8)	1.420(12)	Li(3)-C(46B)	2.65(3)	C(50)-C(51)	1.38(2)
C(8)-C(9)	1.352(12)	Li(4)-O(5)	1.969(17)	C(51)-C(52)	1.48(3)
C(8)-Li(3)	2.462(19)	Li(4)-O(2)	1.973(16)	O(8)-C(56)	1.29(3)
C(9)-C(10)	1.507(13)	Li(4)-N(4)#2	2.060(17)	O(8)-C(53)	1.53(3)
C(9)-Li(3)	2.470(19)	Li(4)-C(13)#2	2.454(16)	O(9A)-C(55)	1.52(4)
C(10)-C(23)	1.539(11)	Li(4)-C(14)#2	2.508(16)	O(9B)-C(55)	1.42(4)
C(10)-C(11)	1.547(12)	Li(4)-C(16)#2	2.732(19)	O(9B)-C(54)	1.65(5)
C(10)-C(25)	1.553(12)	Li(4)-Li(1)#2	3.10(2)	O(9B)-C(56)	1.84(5)
C(11)-C(12)	1.357(12)	O(1)-C(33)	1.434(10)	C(53)-C(54)	1.33(4)
C(12)-C(13)	1.405(13)	O(1)-C(36)	1.452(10)	C(55)-C(56)	1.32(4)
C(13)-C(14)	1.378(12)	O(2)-C(34)	1.423(11)		
C(1)-N(1)-C(4)	106.8(7)	C(19)-C(18)-C(17)	109.9(9)	N(3)-Li(3)-Li(1)	49.3(5)
C(1)-N(1)-Li(2)	136.7(7)	C(18)-C(19)-N(4)	109.4(8)	C(8)-Li(3)-Li(1)	94.6(6)
C(4)-N(1)-Li(2)	94.5(7)	C(18)-C(19)-C(20)	128.4(10)	C(9)-Li(3)-Li(1)	69.3(5)
C(1)-N(1)-Li(1)	118.4(7)	N(4)-C(19)-C(20)	121.6(8)	C(46B)-Li(3)-Li(1)	104.6(7)
C(4)-N(1)-Li(1)	122.8(7)	C(1)-C(20)-C(19)	108.8(7)	O(5)-Li(4)-O(2)	97.9(7)
Li(2)-N(1)-Li(1)	76.1(6)	C(1)-C(20)-C(29)	109.9(8)	O(5)-Li(4)-N(4)#2	134.6(8)
C(6)-N(2)-C(9)	105.4(7)	C(19)-C(20)-C(29)	109.7(8)	O(2)-Li(4)-N(4)#2	106.5(8)
C(6)-N(2)-Li(2)	103.1(8)	C(1)-C(20)-C(31)	109.4(8)	O(5)-Li(4)-C(13)#2	107.2(8)
C(9)-N(2)-Li(2)	148.1(8)	C(19)-C(20)-C(31)	110.1(8)	O(2)-Li(4)-C(13)#2	99.5(7)
C(6)-N(2)-Li(1)	107.7(7)	C(29)-C(20)-C(31)	108.9(8)	N(4)#2-Li(4)-C(13)#2	105.8(7)
C(9)-N(2)-Li(1)	109.7(6)	C(5)-C(21)-C(22A)	127.6(9)	O(5)-Li(4)-C(14)#2	133.3(8)
Li(2)-N(2)-Li(1)	74.5(6)	C(5)-C(21)-C(22B)	129(2)	O(2)-Li(4)-C(14)#2	108.5(7)
C(11)-N(3)-C(14)	106.7(8)	C(22A)-C(21)-C(22B)	102(2)	N(4)#2-Li(4)-C(14)#2	73.6(6)
C(11)-N(3)-Li(3)	115.0(8)	C(10)-C(23)-C(24)	116.6(8)	C(13)#2-Li(4)-C(14)#2	32.2(3)

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Table S48. Bond lengths [Å] and angles [°] for **24** (cont.).

C(14)-N(3)-Li(3)	129.8(8)	C(26)-C(25)-C(10)	114.1(8)	O(5)-Li(4)-C(16)#2	164.3(8)
C(11)-N(3)-Li(1)	109.6(7)	C(15)-C(27)-C(28B)	125(2)	O(2)-Li(4)-C(16)#2	88.7(6)
C(14)-N(3)-Li(1)	107.5(6)	C(15)-C(27)-C(28A)	136.2(13)	N(4)#2-Li(4)-C(16)#2	29.9(3)
Li(3)-N(3)-Li(1)	84.2(6)	C(28B)-C(27)-C(28A)	97(2)	C(13)#2-Li(4)-C(16)#2	85.6(6)
C(19)-N(4)-C(16)	105.6(7)	C(30)-C(29)-C(20)	115.8(8)	C(14)#2-Li(4)-C(16)#2	56.1(4)
C(19)-N(4)-Li(4)#1	127.9(7)	C(32)-C(31)-C(20)	116.6(8)	O(5)-Li(4)-Li(1)#2	111.9(7)
C(16)-N(4)-Li(4)#1	102.7(7)	N(4)-Li(1)-N(3)	92.6(6)	O(2)-Li(4)-Li(1)#2	146.9(8)
C(19)-N(4)-Li(1)	112.2(6)	N(4)-Li(1)-N(1)	97.0(6)	N(4)#2-Li(4)-Li(1)#2	41.8(4)
C(16)-N(4)-Li(1)	110.5(6)	N(3)-Li(1)-N(1)	170.1(8)	C(13)#2-Li(4)-Li(1)#2	85.3(6)
Li(4)#1-N(4)-Li(1)	97.0(6)	N(4)-Li(1)-N(2)	168.7(8)	C(14)#2-Li(4)-Li(1)#2	60.6(5)
C(2)-C(1)-N(1)	109.7(8)	N(3)-Li(1)-N(2)	87.9(6)	C(16)#2-Li(4)-Li(1)#2	58.9(5)
C(2)-C(1)-C(20)	128.9(9)	N(1)-Li(1)-N(2)	82.3(5)	C(33)-O(1)-C(36)	109.0(7)
N(1)-C(1)-C(20)	121.2(9)	N(4)-Li(1)-Li(2)	124.1(7)	C(33)-O(1)-Li(2)	129.1(7)
C(1)-C(2)-C(3)	108.3(9)	N(3)-Li(1)-Li(2)	122.4(7)	C(36)-O(1)-Li(2)	113.5(8)
C(4)-C(3)-C(2)	107.6(9)	N(1)-Li(1)-Li(2)	49.6(5)	C(34)-O(2)-C(35)	110.4(7)
C(3)-C(4)-N(1)	107.6(8)	N(2)-Li(1)-Li(2)	47.7(5)	C(34)-O(2)-Li(4)	120.7(7)
C(3)-C(4)-C(5)	129.7(9)	N(4)-Li(1)-Li(3)	118.4(7)	C(35)-O(2)-Li(4)	128.8(7)
N(1)-C(4)-C(5)	122.7(9)	N(3)-Li(1)-Li(3)	46.5(5)	C(37)-O(3)-C(40)	107.2(7)
C(3)-C(4)-Li(2)	141.9(7)	N(1)-Li(1)-Li(3)	128.7(7)	C(37)-O(3)-Li(3)	116.0(8)
N(1)-C(4)-Li(2)	51.9(5)	N(2)-Li(1)-Li(3)	69.6(5)	C(40)-O(3)-Li(3)	135.4(8)
C(5)-C(4)-Li(2)	79.6(6)	Li(2)-Li(1)-Li(3)	117.2(7)	C(38)-O(4)-C(39)	110.8(8)
C(21)-C(5)-C(4)	122.8(9)	N(4)-Li(1)-Li(4)#1	41.3(4)	C(44)-O(5)-C(41)	110.2(10)
C(21)-C(5)-C(6)	119.0(8)	N(3)-Li(1)-Li(4)#1	70.9(5)	C(44)-O(5)-Li(4)	125.8(9)
C(4)-C(5)-C(6)	118.2(8)	N(1)-Li(1)-Li(4)#1	115.5(6)	C(41)-O(5)-Li(4)	122.6(9)
C(21)-C(5)-Li(2)	132.6(7)	N(2)-Li(1)-Li(4)#1	129.1(7)	C(43)-O(6)-C(42)	93.0(18)
C(4)-C(5)-Li(2)	67.9(6)	Li(2)-Li(1)-Li(4)#1	106.7(6)	C(45)-O(7)-C(46B)	106.8(9)
C(6)-C(5)-Li(2)	71.8(6)	Li(3)-Li(1)-Li(4)#1	115.6(6)	C(45)-O(7)-C(46A)	98.6(9)
C(7)-C(6)-N(2)	110.5(9)	O(1)-Li(2)-N(2)	136.2(8)	C(46B)-O(7)-C(46A)	75.8(10)
C(7)-C(6)-C(5)	128.0(10)	O(1)-Li(2)-N(1)	126.2(8)	C(45)-O(7)-Li(3)	135.8(7)
N(2)-C(6)-C(5)	121.2(8)	N(2)-Li(2)-N(1)	93.3(7)	C(46B)-O(7)-Li(3)	96.2(9)
C(7)-C(6)-Li(2)	154.3(9)	O(1)-Li(2)-C(4)	115.7(8)	C(46A)-O(7)-Li(3)	123.8(9)
N(2)-C(6)-Li(2)	46.2(5)	N(2)-Li(2)-C(4)	85.6(6)	O(1)-C(33)-C(34)	112.0(9)
C(5)-C(6)-Li(2)	75.3(6)	N(1)-Li(2)-C(4)	33.6(4)	O(2)-C(34)-C(33)	110.4(8)
C(6)-C(7)-C(8)	106.8(9)	O(1)-Li(2)-Li(1)	159.6(8)	O(2)-C(35)-C(36)	109.5(9)
C(9)-C(8)-C(7)	107.4(9)	N(2)-Li(2)-Li(1)	57.8(5)	O(1)-C(36)-C(35)	110.6(8)
C(9)-C(8)-Li(3)	74.4(6)	N(1)-Li(2)-Li(1)	54.3(5)	O(1)-C(36)-Li(2)	37.8(5)
C(7)-C(8)-Li(3)	94.7(7)	C(4)-Li(2)-Li(1)	75.9(5)	C(35)-C(36)-Li(2)	108.2(7)
C(8)-C(9)-N(2)	109.9(9)	O(1)-Li(2)-C(6)	130.3(7)	C(38)-C(37)-O(3)	114.3(13)
C(8)-C(9)-C(10)	130.5(9)	N(2)-Li(2)-C(6)	30.7(4)	C(37)-C(38)-O(4)	117.0(13)
N(2)-C(9)-C(10)	119.5(8)	N(1)-Li(2)-C(6)	78.8(6)	O(4)-C(39)-C(40)	109.9(10)
C(8)-C(9)-Li(3)	73.8(7)	C(4)-Li(2)-C(6)	59.2(4)	O(3)-C(40)-C(39)	113.2(8)
N(2)-C(9)-Li(3)	94.1(6)	Li(1)-Li(2)-C(6)	69.8(5)	C(42)-C(41)-O(5)	103.4(18)
C(10)-C(9)-Li(3)	100.0(7)	O(1)-Li(2)-C(5)	114.2(7)	C(41)-C(42)-O(6)	103(2)
C(9)-C(10)-C(23)	108.0(8)	N(2)-Li(2)-C(5)	63.5(5)	C(44)-C(43)-O(6)	116(2)
C(9)-C(10)-C(11)	109.9(8)	N(1)-Li(2)-C(5)	63.1(5)	C(43)-C(44)-O(5)	101.7(17)
C(23)-C(10)-C(11)	109.9(7)	C(4)-Li(2)-C(5)	32.5(3)	O(7)-C(45)-C(46A)#3	97.0(9)
C(9)-C(10)-C(25)	109.0(7)	Li(1)-Li(2)-C(5)	84.8(6)	O(7)-C(45)-C(46B)#3	99.1(9)
C(23)-C(10)-C(25)	111.3(8)	C(6)-Li(2)-C(5)	32.9(3)	C(46A)#3-C(45)-C(46B) ^c	80.8(11)
C(11)-C(10)-C(25)	108.8(7)	O(1)-Li(2)-C(36)	28.6(4)	C(45)#3-C(46A)-O(7)	100.3(10)
C(12)-C(11)-N(3)	110.4(9)	N(2)-Li(2)-C(36)	139.1(7)	C(45)#3-C(46A)-C(46A) ^c	87.8(12)
C(12)-C(11)-C(10)	129.7(10)	N(1)-Li(2)-C(36)	102.3(7)	O(7)-C(46A)-C(46A)#3	76.6(10)
N(3)-C(11)-C(10)	119.6(9)	C(4)-Li(2)-C(36)	87.0(5)	C(45)#3-C(46B)-O(7)	95.7(10)
C(11)-C(12)-C(13)	106.8(10)	Li(1)-Li(2)-C(36)	155.7(7)	C(45)#3-C(46B)-Li(3)	129.8(11)

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Table S48. Bond lengths [Å] and angles [°] for **24** (cont.).

C(14)-C(13)-C(12)	107.1(10)	C(6)-Li(2)-C(36)	116.1(6)	O(7)-C(46B)-Li(3)	46.4(7)
C(14)-C(13)-Li(4)#1	76.1(7)	C(5)-Li(2)-C(36)	90.2(5)	C(48)-C(47)-C(52)	112(2)
C(12)-C(13)-Li(4)#1	102.1(7)	O(7)-Li(3)-O(3)	104.0(8)	C(47)-C(48)-C(49)	126(2)
N(3)-C(14)-C(13)	109.0(9)	O(7)-Li(3)-N(3)	113.2(8)	C(50)-C(49)-C(48)	120.7(19)
N(3)-C(14)-C(15)	123.4(10)	O(3)-Li(3)-N(3)	112.0(8)	C(49)-C(50)-C(51)	123(2)
C(13)-C(14)-C(15)	127.2(10)	O(7)-Li(3)-C(8)	119.4(8)	C(50)-C(51)-C(52)	118(2)
N(3)-C(14)-Li(4)#1	104.1(6)	O(3)-Li(3)-C(8)	101.5(7)	C(51)-C(52)-C(47)	120(2)
C(13)-C(14)-Li(4)#1	71.7(6)	N(3)-Li(3)-C(8)	106.2(8)	C(56)-O(8)-C(53)	112(3)
C(15)-C(14)-Li(4)#1	88.9(6)	O(7)-Li(3)-C(9)	128.8(8)	C(55)-O(9B)-C(54)	118(4)
C(27)-C(15)-C(16)	125.3(10)	O(3)-Li(3)-C(9)	119.8(8)	C(55)-O(9B)-C(56)	45.7(19)
C(27)-C(15)-C(14)	118.7(10)	N(3)-Li(3)-C(9)	75.0(6)	C(54)-O(9B)-C(56)	104(3)
C(16)-C(15)-C(14)	115.5(8)	C(8)-Li(3)-C(9)	31.8(4)	C(54)-C(53)-O(8)	123(3)
C(17)-C(16)-N(4)	110.2(8)	O(7)-Li(3)-C(46B)	37.4(5)	C(53)-C(54)-O(9B)	97(4)
C(17)-C(16)-C(15)	131.3(10)	O(3)-Li(3)-C(46B)	89.3(7)	C(56)-C(55)-O(9B)	84(3)
N(4)-C(16)-C(15)	118.5(9)	N(3)-Li(3)-C(46B)	149.3(9)	C(56)-C(55)-O(9A)	126(3)
C(17)-C(16)-Li(4)#1	137.5(7)	C(8)-Li(3)-C(46B)	89.9(7)	O(9B)-C(55)-O(9A)	58(2)
N(4)-C(16)-Li(4)#1	47.3(5)	C(9)-Li(3)-C(46B)	114.3(8)	O(8)-C(56)-C(55)	131(4)
C(15)-C(16)-Li(4)#1	81.0(7)	O(7)-Li(3)-Li(1)	79.4(6)	O(8)-C(56)-O(9B)	100(3)
C(18)-C(17)-C(16)	104.9(9)	O(3)-Li(3)-Li(1)	158.8(8)	C(55)-C(56)-O(9B)	50(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+0,y-1/2,-z-1/2 #2 -x+0,y+1/2,-z-1/2 #3 -x+1/2,y,-z

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Table S49. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **24**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
N(1)	66(5)	53(5)	55(5)	3(4)	22(4)	10(4)
N(2)	62(5)	61(5)	67(6)	-1(4)	27(5)	1(4)
N(3)	57(4)	63(5)	64(6)	-4(5)	22(4)	4(4)
N(4)	61(4)	58(5)	68(6)	0(4)	33(4)	4(4)
C(1)	68(6)	72(7)	68(8)	-6(6)	38(6)	-9(5)
C(2)	99(8)	94(8)	78(9)	-18(7)	52(7)	-29(7)
C(3)	107(8)	82(8)	69(8)	-10(6)	43(7)	4(7)
C(4)	63(6)	52(6)	55(7)	-1(5)	15(6)	3(5)
C(5)	59(6)	59(7)	68(7)	8(6)	13(5)	17(5)
C(6)	63(7)	57(6)	67(8)	-5(5)	15(6)	1(5)
C(7)	65(7)	87(7)	94(9)	-17(6)	27(7)	2(5)
C(8)	66(7)	77(7)	85(8)	-11(6)	35(7)	-5(5)
C(9)	63(6)	56(6)	77(8)	-5(5)	26(7)	-5(5)
C(10)	59(6)	71(7)	64(7)	-1(6)	26(5)	-2(5)
C(11)	62(6)	69(7)	55(7)	2(6)	26(5)	4(5)
C(12)	93(7)	90(8)	57(8)	-4(7)	21(6)	-9(6)
C(13)	70(6)	86(9)	81(10)	-6(7)	30(6)	-8(5)
C(14)	62(6)	67(8)	67(9)	-9(6)	30(6)	10(5)
C(15)	74(6)	49(7)	98(9)	13(6)	38(6)	20(5)
C(16)	67(6)	50(6)	74(8)	0(5)	23(6)	-5(5)
C(17)	86(7)	44(6)	87(9)	13(6)	20(6)	-6(5)
C(18)	88(7)	72(7)	72(8)	-5(6)	40(6)	-15(6)
C(19)	76(6)	45(6)	67(7)	2(5)	22(6)	-4(5)
C(20)	81(6)	68(6)	82(9)	-13(6)	51(7)	-15(6)
C(21)	63(6)	55(6)	81(8)	-18(6)	23(5)	-3(5)
C(22A)	81(8)	57(8)	78(10)	-3(7)	25(7)	2(6)
C(22B)	120(50)	150(60)	60(40)	20(40)	30(30)	-30(40)
C(23)	67(6)	87(7)	80(8)	-3(6)	35(6)	-10(5)
C(24)	80(7)	77(7)	101(10)	-2(6)	36(6)	6(5)
C(25)	80(6)	79(7)	70(8)	7(6)	30(6)	10(6)
C(26)	111(8)	78(8)	103(10)	20(6)	54(7)	16(6)
C(27)	91(9)	82(10)	115(12)	11(8)	31(9)	-8(8)
C(28A)	68(11)	44(10)	138(19)	-13(10)	50(12)	17(8)
C(28B)	90(20)	240(60)	260(70)	-70(50)	-60(30)	50(30)
C(29)	59(6)	79(7)	93(9)	-8(6)	39(6)	-4(5)
C(30)	71(6)	89(8)	117(10)	-10(7)	40(6)	15(6)
C(31)	111(8)	80(7)	115(10)	-8(7)	73(8)	-4(6)
C(32)	100(7)	91(8)	141(11)	-23(7)	81(8)	-30(6)
Li(1)	76(9)	53(9)	66(11)	-8(8)	32(8)	-7(7)
Li(2)	69(9)	57(9)	70(11)	7(8)	21(8)	-1(7)
Li(3)	58(9)	84(11)	83(13)	-19(9)	19(9)	3(8)
Li(4)	68(9)	76(11)	75(12)	5(9)	30(9)	-3(8)
O(1)	86(4)	70(4)	92(5)	12(4)	48(4)	18(3)
O(2)	93(5)	74(4)	92(6)	17(4)	46(4)	19(4)
O(3)	70(5)	91(5)	115(6)	-24(4)	44(4)	-1(4)
O(4)	104(6)	110(7)	258(12)	-15(7)	119(7)	15(5)
O(5)	80(5)	106(6)	94(6)	0(4)	18(4)	-8(4)
O(6)	128(9)	350(20)	188(13)	-87(12)	-10(8)	-12(10)
O(7)	84(5)	208(9)	50(5)	-12(5)	20(4)	17(5)
C(33)	99(7)	74(7)	78(8)	24(6)	56(6)	31(6)
C(34)	88(7)	78(8)	106(10)	29(7)	52(7)	31(6)
C(35)	86(7)	86(8)	79(8)	25(7)	34(6)	32(6)
C(36)	89(7)	82(8)	95(9)	20(7)	49(7)	20(6)
C(37)	89(9)	236(18)	280(20)	-182(18)	113(13)	-48(11)
C(38)	152(14)	110(12)	460(30)	-92(16)	201(19)	-5(11)
C(39)	77(7)	118(10)	103(10)	19(8)	46(7)	18(7)
C(40)	89(8)	85(8)	108(9)	23(7)	47(7)	3(7)
C(45)	60(6)	96(8)	76(8)	7(7)	35(6)	1(5)
C(46A)	75(13)	64(13)	53(15)	0(11)	19(11)	28(10)
C(46B)	82(14)	92(16)	70(17)	-9(12)	29(13)	-59(12)

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Table S50. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for 24.

	x	y	z	U(eq)
H(2)	-31	-358	-415	80
H(3)	756	526	-71	80
H(7)	2607	808	-627	80
H(8)	2792	434	-1476	80
H(12)	1093	-1018	-3376	80
H(13)	1023	-2144	-3005	80
H(17)	1162	-2787	-852	80
H(18)	330	-2186	-734	80
H(21)	1791	1599	-563	80
H(22A)	1383	2068	-30	80
H(22B)	1262	1361	143	80
H(22C)	769	1704	-413	80
H(22D)	1908	2352	-347	80
H(22E)	1681	2174	-1003	80
H(22F)	2291	1872	-537	80
H(23A)	2594	-280	-2302	80
H(23B)	2448	452	-2503	80
H(24A)	2596	-150	-3204	80
H(24B)	1919	102	-3471	80
H(24C)	2067	-632	-3269	80
H(25A)	1073	211	-3315	80
H(25B)	835	369	-2852	80
H(26A)	1006	1346	-3233	80
H(26B)	1692	1154	-3033	80
H(26C)	1452	1312	-2570	80
H(27)	1622	-3100	-1525	80
H(28A)	2234	-3487	-1840	80
H(28B)	2495	-2775	-1811	80
H(28C)	1942	-3018	-2378	80
H(28D)	2022	-3619	-1411	80
H(28E)	1429	-3408	-1360	80
H(28F)	2056	-3077	-963	80
H(29A)	-258	-712	-2236	80
H(29B)	-752	-1239	-2301	80
H(30A)	-1217	-219	-2612	80
H(30B)	-811	87	-2002	80
H(30C)	-1307	-442	-2068	80
H(31A)	-384	-1448	-802	80
H(31B)	-857	-916	-1173	80
H(32A)	-1323	-1947	-1347	80
H(32B)	-848	-2218	-1554	80
H(32C)	-1325	-1684	-1923	80
H(33A)	-534	1581	-2981	80
H(33B)	31	1235	-3005	80
H(34A)	677	1982	-2358	80
H(34B)	185	2352	-2898	80
H(35A)	-14	2285	-1450	80
H(35B)	555	1933	-1463	80
H(36A)	-181	1157	-1570	80
H(36B)	-663	1537	-2110	80
H(37A)	2689	-1859	-1651	80
H(37B)	3101	-1522	-1901	80
H(38A)	3495	-2451	-1520	80
H(38B)	3465	-2275	-941	80
H(39A)	4597	-1108	-587	80
H(39B)	4169	-1418	-339	80
H(40A)	3757	-436	-780	80
H(40B)	3776	-665	-1355	80
H(41A)	1023	3143	-1569	80
H(41B)	1265	3875	-1439	80
H(42A)	1371	3208	-684	80
H(42B)	668	3351	-896	80
H(43A)	303	4090	-883	80
H(43B)	514	4824	-820	80
H(44A)	553	4748	-1683	80
H(44B)	-108	4606	-1734	80

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Table S51. Crystal data and structure refinement for **25**.

Identification code	25	
Empirical formula	C ₄₆ H ₇₃ Li ₄ N ₅ O ₆	
Formula weight	819.85	
Temperature	143(2) K	
Wavelength	0.71070 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 11.755(2) Å	$\alpha = 90^\circ$.
	b = 20.644(4) Å	$\beta = 95.22(3)^\circ$.
	c = 19.117(4) Å	$\gamma = 90^\circ$.
Volume	4619.9(16) Å ³	
Z	4	
Density (calculated)	1.179 Mg/m ³	
Absorption coefficient	0.076 mm ⁻¹	
F(000)	1776	
Crystal size	0.17 x 0.15 x 0.13 mm ³	
Theta range for data collection	1.45 to 24.40°.	
Index ranges	-13 ≤ h ≤ 13, -23 ≤ k ≤ 23, -22 ≤ l ≤ 22	
Reflections collected	24492	
Independent reflections	7078 [R(int) = 0.0531]	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	7078 / 0 / 561	
Goodness-of-fit on F ²	1.040	
Final R indices [I > 2sigma(I)]	R1 = 0.0789, wR2 = 0.2282	
R indices (all data)	R1 = 0.1051, wR2 = 0.2481	
Extinction coefficient	0.046(4)	
Largest diff. peak and hole	1.003 and -0.582 e.Å ⁻³	

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Table S52. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **25**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Li(1)	-1442(4)	2319(3)	362(3)	43(1)
N(1)	-2596(2)	2423(1)	1097(1)	36(1)
C(1)	-3251(3)	1909(2)	1302(2)	39(1)
C(2)	-4324(3)	2125(2)	1433(2)	45(1)
C(3)	-4356(3)	2799(2)	1306(2)	42(1)
C(4)	-3289(3)	2960(2)	1100(2)	37(1)
C(5)	-2855(3)	3618(2)	861(2)	38(1)
N(2)	-867(2)	3320(1)	593(1)	38(1)
C(6)	-1571(3)	3628(1)	1027(2)	36(1)
C(7)	-940(3)	3821(2)	1640(2)	40(1)
C(8)	197(3)	3623(2)	1588(2)	41(1)
C(9)	223(2)	3320(2)	938(2)	37(1)
C(10)	1224(2)	3123(2)	536(2)	37(1)
N(3)	76(2)	2288(1)	-171(1)	38(1)
C(11)	1093(3)	2460(2)	203(2)	38(1)
C(12)	1919(3)	1989(2)	119(2)	42(1)
C(13)	1385(3)	1503(2)	-303(2)	43(1)
C(14)	264(3)	1695(2)	-471(2)	39(1)
C(15)	-729(3)	1315(2)	-836(2)	41(1)
N(4)	-1861(2)	1394(1)	214(1)	39(1)
C(16)	-1346(2)	1003(2)	-250(2)	39(1)
C(17)	-1405(3)	356(2)	-52(2)	44(1)
C(18)	-1977(3)	347(2)	568(2)	43(1)
C(19)	-2225(3)	991(2)	727(2)	39(1)
C(20)	-2803(3)	1239(2)	1329(2)	39(1)
C(21)	-3147(3)	3695(2)	61(2)	46(1)
C(22)	-4414(3)	3743(2)	-186(2)	56(1)
C(23)	-3419(3)	4161(2)	1261(2)	46(1)
C(24)	-3144(3)	4845(2)	1042(2)	61(1)
C(25)	2360(3)	3178(2)	1006(2)	45(1)
C(26)	2514(3)	2696(2)	1620(2)	50(1)
N(5)	1170(2)	3607(1)	-81(1)	42(1)
C(27)	1234(3)	4285(2)	140(2)	51(1)
C(28)	2040(3)	3490(2)	-577(2)	52(1)
C(29)	-298(3)	776(2)	-1298(2)	49(1)
C(30)	291(4)	1005(2)	-1919(2)	71(1)
C(31)	-1539(3)	1772(2)	-1281(2)	48(1)
C(32)	-2530(3)	1445(2)	-1715(2)	61(1)
C(33)	-2963(3)	847(2)	1874(2)	49(1)
C(34A)	-3596(4)	947(3)	2483(3)	55(2)
C(34B)	-2396(14)	242(7)	2143(8)	57(5)
Li(2)	-3212(5)	781(3)	-290(3)	49(1)
C(35)	-4721(3)	1962(2)	-442(2)	61(1)
O(1)	-4632(2)	1264(1)	-474(1)	59(1)
C(36)	-5326(3)	993(2)	-1050(3)	75(1)
C(37)	-5197(4)	271(3)	-997(3)	86(2)
O(2)	-4013(2)	127(1)	-902(1)	63(1)
C(38)	-3781(4)	-546(2)	-927(3)	78(1)
Li(3)	-1061(5)	2664(3)	1699(3)	48(1)
C(39)	-2317(3)	2863(2)	2922(2)	55(1)

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Table S52. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **25** (cont.).

	x	y	z	U(eq)
O(3)	-1246(2)	2618(1)	2740(1)	49(1)
C(40)	-1070(3)	1963(2)	2950(2)	55(1)
C(41)	-46(3)	1713(2)	2642(2)	60(1)
O(4)	-178(2)	1828(1)	1902(1)	53(1)
C(42)	386(3)	1360(2)	1508(2)	51(1)
Li(4)	-460(5)	3221(3)	-426(3)	45(1)
C(43)	-1407(8)	3426(3)	-1933(3)	178(4)
O(5)	-1108(2)	3658(1)	-1277(1)	59(1)
C(44)	-975(4)	4343(2)	-1246(2)	70(1)
C(45)	-1855(4)	4687(3)	-1708(3)	81(1)
O(6)	-2959(4)	4592(3)	-1470(3)	136(2)
C(46)	-3824(6)	5010(4)	-1798(5)	156(3)

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Table S53. Bond lengths [Å] and angles [°] for **25**.

Li(1)-N(4)	1.984(6)	C(9)-Li(4)	2.664(7)	C(23)-C(24)	1.517(5)
Li(1)-N(1)	2.050(6)	C(10)-C(11)	1.512(4)	C(25)-C(26)	1.537(5)
Li(1)-N(3)	2.136(6)	C(10)-N(5)	1.543(4)	N(5)-C(27)	1.462(4)
Li(1)-N(2)	2.206(6)	C(10)-C(25)	1.544(4)	N(5)-C(28)	1.476(4)
Li(1)-Li(3)	2.653(8)	C(10)-Li(4)	2.584(7)	N(5)-Li(4)	2.123(6)
Li(1)-Li(4)	2.718(7)	N(3)-C(14)	1.379(4)	C(29)-C(30)	1.503(5)
N(1)-C(4)	1.376(4)	N(3)-C(11)	1.382(4)	C(31)-C(32)	1.523(5)
N(1)-C(1)	1.388(4)	N(3)-Li(4)	2.070(6)	C(33)-C(34A)	1.452(6)
N(1)-Li(3)	2.110(7)	C(11)-C(12)	1.395(4)	C(33)-C(34B)	1.484(14)
C(1)-C(2)	1.382(4)	C(11)-Li(4)	2.616(6)	Li(2)-O(1)	1.948(6)
C(1)-C(20)	1.480(4)	C(12)-C(13)	1.399(5)	Li(2)-O(2)	1.970(6)
C(2)-C(3)	1.412(5)	C(13)-C(14)	1.385(4)	C(35)-O(1)	1.446(5)
C(3)-C(4)	1.389(4)	C(14)-C(15)	1.521(4)	O(1)-C(36)	1.425(5)
C(4)-C(5)	1.536(4)	C(15)-C(16)	1.532(4)	C(36)-C(37)	1.501(6)
C(5)-C(6)	1.514(4)	C(15)-C(29)	1.536(4)	C(37)-O(2)	1.419(5)
C(5)-C(23)	1.540(4)	C(15)-C(31)	1.541(5)	O(2)-C(38)	1.418(5)
C(5)-C(21)	1.544(5)	N(4)-C(16)	1.379(4)	Li(3)-O(3)	2.024(6)
N(2)-C(6)	1.380(4)	N(4)-C(19)	1.385(4)	Li(3)-O(4)	2.034(6)
N(2)-C(9)	1.387(4)	N(4)-Li(2)	2.185(6)	C(39)-O(3)	1.430(4)
N(2)-Li(4)	2.057(6)	C(16)-C(17)	1.393(5)	O(3)-C(40)	1.419(4)
N(2)-Li(3)	2.538(6)	C(16)-Li(2)	2.234(6)	C(40)-C(41)	1.480(5)
C(6)-C(7)	1.386(5)	C(17)-C(18)	1.414(5)	C(41)-O(4)	1.428(4)
C(6)-Li(3)	2.415(6)	C(17)-Li(2)	2.306(7)	O(4)-C(42)	1.426(4)
C(7)-C(8)	1.410(4)	C(18)-C(19)	1.400(5)	Li(4)-O(5)	1.954(6)
C(7)-Li(3)	2.395(7)	C(18)-Li(2)	2.273(7)	C(43)-O(5)	1.357(6)
C(8)-C(9)	1.394(4)	C(19)-C(20)	1.479(4)	O(5)-C(44)	1.424(5)
C(8)-Li(3)	2.490(6)	C(19)-Li(2)	2.215(7)	C(44)-C(45)	1.479(6)
C(9)-C(10)	1.517(4)	C(20)-C(33)	1.347(5)	C(45)-O(6)	1.426(6)
C(9)-Li(3)	2.574(6)	C(21)-C(22)	1.524(4)	O(6)-C(46)	1.434(7)
N(4)-Li(1)-N(1)	91.6(2)	N(3)-C(11)-C(12)	109.8(3)	O(2)-C(37)-C(36)	108.0(3)
N(4)-Li(1)-N(3)	96.4(2)	N(3)-C(11)-C(10)	120.0(3)	C(38)-O(2)-C(37)	113.0(3)
N(1)-Li(1)-N(3)	164.5(3)	C(12)-C(11)-C(10)	129.4(3)	C(38)-O(2)-Li(2)	127.6(3)
N(4)-Li(1)-N(2)	175.3(3)	N(3)-C(11)-Li(4)	51.80(19)	C(37)-O(2)-Li(2)	110.1(3)
N(1)-Li(1)-N(2)	88.5(2)	C(12)-C(11)-Li(4)	146.0(3)	O(3)-Li(3)-O(4)	82.6(2)
N(3)-Li(1)-N(2)	82.5(2)	C(10)-C(11)-Li(4)	71.9(2)	O(3)-Li(3)-N(1)	111.2(3)
N(4)-Li(1)-Li(3)	114.5(3)	C(11)-C(12)-C(13)	106.6(3)	O(4)-Li(3)-N(1)	107.5(3)
N(1)-Li(1)-Li(3)	51.40(18)	C(14)-C(13)-C(12)	107.2(3)	O(3)-Li(3)-C(7)	96.1(2)
N(3)-Li(1)-Li(3)	113.1(3)	N(3)-C(14)-C(13)	110.0(3)	O(4)-Li(3)-C(7)	145.5(3)
N(2)-Li(1)-Li(3)	62.17(19)	N(3)-C(14)-C(15)	120.2(3)	N(1)-Li(3)-C(7)	105.1(3)
N(4)-Li(1)-Li(4)	133.8(3)	C(13)-C(14)-C(15)	129.3(3)	O(3)-Li(3)-C(6)	121.3(3)
N(1)-Li(1)-Li(4)	130.4(3)	C(14)-C(15)-C(16)	106.0(3)	O(4)-Li(3)-C(6)	154.0(3)
N(3)-Li(1)-Li(4)	48.69(17)	C(14)-C(15)-C(29)	110.9(3)	N(1)-Li(3)-C(6)	75.2(2)
N(2)-Li(1)-Li(4)	48.01(17)	C(16)-C(15)-C(29)	108.6(3)	C(7)-Li(3)-C(6)	33.50(13)
Li(3)-Li(1)-Li(4)	107.8(3)	C(14)-C(15)-C(31)	110.4(3)	O(3)-Li(3)-C(8)	103.9(3)
C(4)-N(1)-C(1)	105.7(2)	C(16)-C(15)-C(31)	110.6(2)	O(4)-Li(3)-C(8)	113.2(3)
C(4)-N(1)-Li(1)	121.1(2)	C(29)-C(15)-C(31)	110.2(3)	N(1)-Li(3)-C(8)	128.7(3)
C(1)-N(1)-Li(1)	122.1(3)	C(16)-N(4)-C(19)	106.6(3)	C(7)-Li(3)-C(8)	33.49(13)
C(4)-N(1)-Li(3)	106.5(2)	C(16)-N(4)-Li(1)	122.5(2)	C(6)-Li(3)-C(8)	54.60(16)
C(1)-N(1)-Li(3)	119.7(2)	C(19)-N(4)-Li(1)	124.5(3)	O(3)-Li(3)-N(2)	150.5(3)
Li(1)-N(1)-Li(3)	79.2(2)	C(16)-N(4)-Li(2)	73.8(2)	O(4)-Li(3)-N(2)	121.9(3)
C(2)-C(1)-N(1)	110.1(3)	C(19)-N(4)-Li(2)	72.9(2)	N(1)-Li(3)-N(2)	78.9(2)
C(2)-C(1)-C(20)	128.5(3)	Li(1)-N(4)-Li(2)	141.3(3)	C(7)-Li(3)-N(2)	54.48(15)
N(1)-C(1)-C(20)	121.3(3)	N(4)-C(16)-C(17)	110.6(3)	C(6)-Li(3)-N(2)	32.23(11)
C(1)-C(2)-C(3)	107.3(3)	N(4)-C(16)-C(15)	119.2(3)	C(8)-Li(3)-N(2)	53.61(15)
C(4)-C(3)-C(2)	105.9(3)	C(17)-C(16)-C(15)	129.9(3)	O(3)-Li(3)-C(9)	134.6(3)
N(1)-C(4)-C(3)	111.0(3)	N(4)-C(16)-Li(2)	69.9(2)	O(4)-Li(3)-C(9)	103.8(2)
N(1)-C(4)-C(5)	119.9(3)	C(17)-C(16)-Li(2)	74.9(2)	N(1)-Li(3)-C(9)	109.4(3)
C(3)-C(4)-C(5)	129.1(3)	C(15)-C(16)-Li(2)	126.2(3)	C(7)-Li(3)-C(9)	53.77(15)

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Table S53. Bond lengths [Å] and angles [°] for **25** (cont.).

C(6)-C(5)-C(4)	107.5(2)	C(16)-C(17)-C(18)	106.2(3)	C(6)-Li(3)-C(9)	52.85(15)
C(6)-C(5)-C(23)	110.6(3)	C(16)-C(17)-Li(2)	69.4(2)	C(8)-Li(3)-C(9)	31.90(12)
C(4)-C(5)-C(23)	109.0(2)	C(18)-C(17)-Li(2)	70.8(2)	N(2)-Li(3)-C(9)	31.49(11)
C(6)-C(5)-C(21)	109.5(2)	C(19)-C(18)-C(17)	107.2(3)	O(3)-Li(3)-Li(1)	155.6(3)
C(4)-C(5)-C(21)	109.6(3)	C(19)-C(18)-Li(2)	69.6(2)	O(4)-Li(3)-Li(1)	89.6(2)
C(23)-C(5)-C(21)	110.5(3)	C(17)-C(18)-Li(2)	73.3(2)	N(1)-Li(3)-Li(1)	49.40(18)
C(6)-N(2)-C(9)	107.0(3)	N(4)-C(19)-C(18)	109.4(3)	C(7)-Li(3)-Li(1)	103.2(2)
C(6)-N(2)-Li(4)	145.0(3)	N(4)-C(19)-C(20)	122.4(3)	C(6)-Li(3)-Li(1)	72.4(2)
C(9)-N(2)-Li(4)	99.5(2)	C(18)-C(19)-C(20)	128.1(3)	C(8)-Li(3)-Li(1)	100.4(2)
C(6)-N(2)-Li(1)	111.3(2)	N(4)-C(19)-Li(2)	70.5(2)	N(2)-Li(3)-Li(1)	50.25(17)
C(9)-N(2)-Li(1)	110.4(2)	C(18)-C(19)-Li(2)	74.1(2)	C(9)-Li(3)-Li(1)	69.70(19)
Li(4)-N(2)-Li(1)	79.1(2)	C(20)-C(19)-Li(2)	120.6(2)	C(40)-O(3)-C(39)	112.2(3)
C(6)-N(2)-Li(3)	69.0(2)	C(33)-C(20)-C(19)	120.0(3)	C(40)-O(3)-Li(3)	107.3(3)
C(9)-N(2)-Li(3)	75.7(2)	C(33)-C(20)-C(1)	121.0(3)	C(39)-O(3)-Li(3)	113.5(3)
Li(4)-N(2)-Li(3)	141.5(2)	C(19)-C(20)-C(1)	119.0(3)	O(3)-C(40)-C(41)	108.8(3)
Li(1)-N(2)-Li(3)	67.6(2)	C(22)-C(21)-C(5)	115.9(3)	O(4)-C(41)-C(40)	108.5(3)
N(2)-C(6)-C(7)	109.7(3)	C(24)-C(23)-C(5)	115.4(3)	C(42)-O(4)-C(41)	113.4(3)
N(2)-C(6)-C(5)	120.5(3)	C(26)-C(25)-C(10)	115.7(3)	C(42)-O(4)-Li(3)	136.8(3)
C(7)-C(6)-C(5)	128.9(3)	C(27)-N(5)-C(28)	108.8(2)	C(41)-O(4)-Li(3)	109.7(3)
N(2)-C(6)-Li(3)	78.8(2)	C(27)-N(5)-C(10)	113.6(3)	O(5)-Li(4)-N(2)	129.5(3)
C(7)-C(6)-Li(3)	72.5(2)	C(28)-N(5)-C(10)	113.7(3)	O(5)-Li(4)-N(3)	135.4(3)
C(5)-C(6)-Li(3)	107.2(2)	C(27)-N(5)-Li(4)	118.1(2)	N(2)-Li(4)-N(3)	87.8(2)
C(6)-C(7)-C(8)	107.2(3)	C(28)-N(5)-Li(4)	113.5(3)	O(5)-Li(4)-N(5)	110.9(3)
C(6)-C(7)-Li(3)	74.0(2)	C(10)-N(5)-Li(4)	88.2(2)	N(2)-Li(4)-N(5)	87.2(2)
C(8)-C(7)-Li(3)	77.0(2)	C(30)-C(29)-C(15)	115.2(3)	N(3)-Li(4)-N(5)	91.7(2)
C(9)-C(8)-C(7)	106.9(3)	C(32)-C(31)-C(15)	115.8(3)	O(5)-Li(4)-C(10)	147.6(3)
C(9)-C(8)-Li(3)	77.3(2)	C(20)-C(33)-C(34A)	130.8(4)	N(2)-Li(4)-C(10)	64.12(18)
C(7)-C(8)-Li(3)	69.5(2)	C(20)-C(33)-C(34B)	133.1(6)	N(3)-Li(4)-C(10)	64.10(18)
N(2)-C(9)-C(8)	109.3(3)	C(34A)-C(33)-C(34B)	95.1(6)	N(5)-Li(4)-C(10)	36.64(13)
N(2)-C(9)-C(10)	119.0(3)	O(1)-Li(2)-O(2)	83.6(2)	O(5)-Li(4)-C(11)	149.6(3)
C(8)-C(9)-C(10)	130.7(3)	O(1)-Li(2)-N(4)	111.1(3)	N(2)-Li(4)-C(11)	80.6(2)
N(2)-C(9)-Li(3)	72.8(2)	O(2)-Li(2)-N(4)	161.5(3)	N(3)-Li(4)-C(11)	31.66(13)
C(8)-C(9)-Li(3)	70.8(2)	O(1)-Li(2)-C(19)	115.5(3)	N(5)-Li(4)-C(11)	60.72(17)
C(10)-C(9)-Li(3)	131.8(2)	O(2)-Li(2)-C(19)	147.0(3)	C(10)-Li(4)-C(11)	33.80(12)
N(2)-C(9)-Li(4)	49.58(18)	N(4)-Li(2)-C(19)	36.67(14)	O(5)-Li(4)-C(9)	147.1(3)
C(8)-C(9)-Li(4)	151.3(3)	O(1)-Li(2)-C(16)	136.4(3)	N(2)-Li(4)-C(9)	30.90(12)
C(10)-C(9)-Li(4)	70.3(2)	O(2)-Li(2)-C(16)	125.2(3)	N(3)-Li(4)-C(9)	77.5(2)
Li(3)-C(9)-Li(4)	111.9(2)	N(4)-Li(2)-C(16)	36.34(14)	N(5)-Li(4)-C(9)	58.99(17)
C(11)-C(10)-C(9)	113.6(2)	C(19)-Li(2)-C(16)	59.71(18)	C(10)-Li(4)-C(9)	33.56(12)
C(11)-C(10)-N(5)	105.6(2)	O(1)-Li(2)-C(18)	144.3(3)	C(11)-Li(4)-C(9)	57.38(15)
C(9)-C(10)-N(5)	103.5(2)	O(2)-Li(2)-C(18)	113.4(3)	O(5)-Li(4)-Li(1)	128.7(3)
C(11)-C(10)-C(25)	111.1(3)	N(4)-Li(2)-C(18)	61.27(19)	N(2)-Li(4)-Li(1)	52.87(18)
C(9)-C(10)-C(25)	110.9(3)	C(19)-Li(2)-C(18)	36.31(15)	N(3)-Li(4)-Li(1)	50.81(18)
N(5)-C(10)-C(25)	111.8(2)	C(16)-Li(2)-C(18)	59.71(18)	N(5)-Li(4)-Li(1)	120.2(3)
C(11)-C(10)-Li(4)	74.3(2)	O(1)-Li(2)-C(17)	171.7(3)	C(10)-Li(4)-Li(1)	83.6(2)
C(9)-C(10)-Li(4)	76.1(2)	O(2)-Li(2)-C(17)	103.8(3)	C(11)-Li(4)-Li(1)	69.37(19)
N(5)-C(10)-Li(4)	55.20(19)	N(4)-Li(2)-C(17)	60.92(18)	C(9)-Li(4)-Li(1)	67.43(19)
C(25)-C(10)-Li(4)	166.9(2)	C(19)-Li(2)-C(17)	60.07(19)	C(43)-O(5)-C(44)	114.0(4)
C(14)-N(3)-C(11)	106.2(3)	C(16)-Li(2)-C(17)	35.68(14)	C(43)-O(5)-Li(4)	131.0(4)
C(14)-N(3)-Li(4)	141.8(3)	C(18)-Li(2)-C(17)	35.97(15)	C(44)-O(5)-Li(4)	113.0(3)
C(11)-N(3)-Li(4)	96.5(2)	C(36)-O(1)-C(35)	112.6(3)	O(5)-C(44)-C(45)	112.6(4)
C(14)-N(3)-Li(1)	113.4(2)	C(36)-O(1)-Li(2)	111.1(3)	O(6)-C(45)-C(44)	110.5(4)
C(11)-N(3)-Li(1)	117.7(2)	C(35)-O(1)-Li(2)	124.4(3)	C(45)-O(6)-C(46)	114.0(5)
Li(4)-N(3)-Li(1)	80.5(2)	O(1)-C(36)-C(37)	106.9(4)		

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Table S54. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **25**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Li(1)	46(3)	44(3)	39(3)	2(2)	5(2)	1(2)
N(1)	36(1)	36(2)	38(2)	2(1)	5(1)	0(1)
C(1)	40(2)	38(2)	39(2)	0(1)	4(1)	-5(1)
C(2)	37(2)	50(2)	48(2)	0(2)	7(2)	-5(1)
C(3)	35(2)	42(2)	50(2)	-1(2)	7(2)	-1(1)
C(4)	38(2)	37(2)	37(2)	-2(1)	6(1)	-2(1)
C(5)	36(2)	35(2)	42(2)	2(1)	6(1)	2(1)
N(2)	36(1)	38(2)	40(2)	0(1)	5(1)	-1(1)
C(6)	40(2)	33(2)	38(2)	0(1)	9(1)	0(1)
C(7)	43(2)	39(2)	39(2)	-4(1)	9(1)	-2(1)
C(8)	40(2)	43(2)	39(2)	-4(1)	3(1)	-2(1)
C(9)	34(2)	41(2)	38(2)	1(1)	5(1)	-2(1)
C(10)	34(2)	40(2)	39(2)	2(1)	8(1)	-3(1)
N(3)	37(1)	38(2)	41(2)	-2(1)	6(1)	-3(1)
C(11)	36(2)	39(2)	39(2)	-2(1)	8(1)	-3(1)
C(12)	33(2)	46(2)	49(2)	1(2)	9(1)	1(1)
C(13)	44(2)	39(2)	49(2)	-5(2)	11(2)	3(1)
C(14)	42(2)	38(2)	39(2)	-3(1)	10(2)	1(1)
C(15)	43(2)	40(2)	39(2)	-4(1)	6(2)	-3(1)
N(4)	37(1)	40(2)	40(2)	-1(1)	2(1)	-1(1)
C(16)	36(2)	41(2)	40(2)	-5(1)	5(1)	-3(1)
C(17)	42(2)	37(2)	52(2)	-5(2)	2(2)	1(1)
C(18)	44(2)	36(2)	49(2)	3(2)	5(2)	0(1)
C(19)	39(2)	39(2)	39(2)	0(1)	4(1)	-4(1)
C(20)	39(2)	39(2)	38(2)	0(1)	0(1)	-5(1)
C(21)	42(2)	49(2)	46(2)	8(2)	3(2)	1(1)
C(22)	46(2)	64(3)	57(2)	8(2)	-6(2)	4(2)
C(23)	41(2)	38(2)	62(2)	-3(2)	17(2)	0(1)
C(24)	56(2)	37(2)	92(3)	-4(2)	18(2)	2(2)
C(25)	37(2)	51(2)	47(2)	-6(2)	4(2)	-5(1)
C(26)	43(2)	57(2)	48(2)	-3(2)	-1(2)	1(2)
N(5)	49(2)	37(2)	42(2)	2(1)	15(1)	0(1)
C(27)	63(2)	40(2)	52(2)	-2(2)	12(2)	-4(2)
C(28)	56(2)	52(2)	53(2)	4(2)	24(2)	-1(2)
C(29)	52(2)	52(2)	46(2)	-13(2)	9(2)	-6(2)
C(30)	73(3)	80(3)	64(3)	-21(2)	29(2)	-21(2)
C(31)	53(2)	50(2)	40(2)	1(2)	4(2)	-1(2)
C(32)	63(2)	72(3)	48(2)	4(2)	-3(2)	-8(2)
C(33)	50(2)	50(2)	47(2)	6(2)	4(2)	-3(2)
C(34A)	60(3)	60(3)	46(3)	1(2)	5(2)	-7(2)
C(34B)	85(11)	40(9)	47(9)	20(7)	7(7)	-1(7)
Li(2)	44(3)	55(4)	49(3)	-1(3)	3(3)	-4(3)
C(35)	58(2)	58(3)	66(3)	3(2)	2(2)	10(2)
O(1)	49(1)	64(2)	62(2)	-2(1)	-7(1)	-3(1)
C(36)	53(2)	90(4)	79(3)	-11(3)	-16(2)	-6(2)
C(37)	58(3)	90(4)	106(4)	-20(3)	-16(3)	-16(2)
O(2)	59(2)	57(2)	71(2)	-7(1)	-8(1)	-12(1)
C(38)	91(3)	54(3)	89(3)	-19(2)	6(3)	-13(2)
Li(3)	52(3)	44(3)	49(3)	3(3)	10(3)	1(2)
C(39)	49(2)	67(3)	49(2)	-2(2)	12(2)	6(2)
O(3)	49(1)	53(2)	46(1)	3(1)	7(1)	4(1)

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Table S54. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **25** (cont.).

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(40)	63(2)	53(2)	49(2)	10(2)	10(2)	5(2)
C(41)	70(3)	66(3)	44(2)	14(2)	3(2)	14(2)
O(4)	57(2)	56(2)	45(1)	7(1)	8(1)	12(1)
C(42)	47(2)	50(2)	57(2)	0(2)	10(2)	8(2)
Li(4)	50(3)	44(3)	42(3)	-2(2)	8(3)	4(2)
C(43)	325(12)	104(5)	89(5)	46(4)	-74(6)	-78(6)
O(5)	80(2)	50(2)	46(2)	5(1)	3(1)	8(1)
C(44)	81(3)	57(3)	72(3)	5(2)	6(2)	9(2)
C(45)	81(3)	76(3)	84(3)	6(3)	0(3)	11(2)
O(6)	118(3)	146(4)	144(4)	39(3)	15(3)	12(3)
C(46)	139(6)	131(6)	192(8)	29(6)	-13(6)	43(5)