

S80

Table S55. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 25.

	x	y	z	U(eq)
H(2)	-4927	1867	1582	54
H(3)	-4981	3083	1351	50
H(7)	-1221	4045	2022	48
H(8)	826	3684	1930	49
H(12)	2694	1996	310	51
H(13)	1727	1114	-448	52
H(17)	-1118	-7	-285	53
H(18)	-2160	-25	827	51
H(21A)	-2761	4088	-94	55
H(21B)	-2824	3320	-176	55
H(22A)	-4815	3363	-24	84
H(22B)	-4510	3762	-700	84
H(22C)	-4732	4137	8	84
H(23A)	-4257	4101	1196	56
H(23B)	-3180	4112	1768	56
H(24A)	-2317	4916	1112	91
H(24B)	-3532	5155	1327	91
H(24C)	-3406	4908	545	91
H(25A)	2997	3117	707	54
H(25B)	2422	3622	1200	54
H(26A)	1825	2694	1873	74
H(26B)	3173	2825	1941	74
H(26C)	2643	2261	1438	74
H(27A)	1991	4372	380	77
H(27B)	647	4371	461	77
H(27C)	1107	4566	-273	77
H(28A)	1894	3773	-986	79
H(28B)	2004	3036	-729	79
H(28C)	2800	3582	-343	79
H(29A)	240	499	-1002	59
H(29B)	-956	503	-1471	59
H(30A)	-249	1252	-2236	106
H(30B)	565	630	-2169	106
H(30C)	940	1281	-1756	106
H(31A)	-1857	2089	-964	57
H(31B)	-1085	2016	-1604	57
H(32A)	-2243	1224	-2117	92
H(32B)	-3092	1773	-1884	92
H(32C)	-2891	1130	-1423	92
H(33)	-2602	436	1858	59
H(34A)	-3720	1412	2548	83
H(34B)	-3160	771	2902	83
H(34C)	-4335	726	2412	83
H(34D)	-2721	-128	1874	86
H(34E)	-2519	187	2640	86
H(34F)	-1575	269	2093	86
H(35A)	-4486	2150	-877	92
H(35B)	-4223	2124	-41	92
H(35C)	-5513	2084	-386	92

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Table S55. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for **25** (cont.).

	x	y	z	U(eq)
H(36A)	-5072	1150	-1500	90
H(36B)	-6134	1119	-1028	90
H(37A)	-5585	106	-594	103
H(37B)	-5547	62	-1431	103
H(38A)	-4311	-782	-652	117
H(38B)	-2995	-628	-732	117
H(38C)	-3878	-695	-1416	117
H(39A)	-2941	2628	2658	82
H(39B)	-2374	3325	2807	82
H(39C)	-2372	2803	3427	82
H(40A)	-1746	1700	2785	66
H(40B)	-959	1936	3468	66
H(41A)	647	1936	2855	72
H(41B)	39	1243	2735	72
H(42A)	1212	1382	1637	76
H(42B)	227	1449	1005	76
H(42C)	108	926	1612	76
H(43A)	-1986	3710	-2173	80
H(43B)	-1720	2989	-1900	80
H(43C)	-733	3413	-2198	80
H(44A)	-210	4459	-1385	84
H(44B)	-1018	4489	-755	84
H(45A)	-1677	5155	-1710	97
H(45B)	-1851	4523	-2194	97
H(46A)	-3615	5462	-1699	80
H(46B)	-4556	4915	-1613	80
H(46C)	-3892	4937	-2307	80

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Table S56. Crystal data and structure refinement for 26.

Identification code	26	
Empirical formula	C <sub>48</sub> H <sub>77</sub> Li <sub>3</sub> N <sub>4</sub> O <sub>8</sub>	
Formula weight	858.96	
Temperature	143(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.0569(15) Å	α = 110.249(19)°
	b = 21.211(4) Å	β = 98.009(13)°
	c = 21.667(4) Å	γ = 96.358(14)°
Volume	5071.9(16) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.125 Mg/m <sup>3</sup>	
Absorption coefficient	0.075 mm <sup>-1</sup>	
F(000)	1864	
Crystal size	0.12 x 0.09 x 0.06 mm <sup>3</sup>	
Theta range for data collection	3.03 to 22.46°	
Index ranges	-12 ≤ h ≤ 12, -22 ≤ k ≤ 22, -22 ≤ l ≤ 22	
Reflections collected	22950	
Independent reflections	11243 [R(int) = 0.0767]	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	11243 / 0 / 1136	
Goodness-of-fit on F <sup>2</sup>	1.645	
Final R indices [I > 2σ(I)]	R1 = 0.1342, wR2 = 0.3874	
R indices (all data)	R1 = 0.1769, wR2 = 0.4351	
Extinction coefficient	0.0024(19)	
Largest diff. peak and hole	0.515 and -0.406 e.Å <sup>-3</sup>	

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Table S57. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **26**.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{\text{ij}}$  tensor.

	x	y	z	U(eq)
Li(1)	3617(10)	2109(6)	3341(6)	50(3)
N(1)	3179(5)	1008(3)	2714(3)	47(2)
C(1)	2806(6)	815(4)	2013(4)	49(2)
C(2)	3403(7)	341(4)	1657(4)	53(2)
C(3)	4181(7)	217(4)	2142(4)	54(2)
C(4)	4033(6)	625(4)	2769(4)	44(2)
C(5)	4707(6)	730(3)	3443(4)	46(2)
N(2)	5118(5)	2001(3)	3805(3)	44(1)
C(6)	5537(6)	1415(4)	3694(4)	47(2)
C(7)	6764(6)	1546(4)	3852(4)	56(2)
C(8)	7077(6)	2234(4)	4057(4)	51(2)
C(9)	6077(6)	2534(4)	4039(4)	47(2)
C(10)	5984(6)	3225(4)	4222(3)	46(2)
N(3)	3880(5)	3107(3)	3919(3)	45(2)
C(11)	4991(6)	3502(4)	4175(4)	48(2)
C(12)	4882(7)	4207(4)	4353(4)	50(2)
C(13)	3739(7)	4229(4)	4206(4)	52(2)
C(14)	3134(6)	3536(4)	3949(4)	45(2)
C(15)	1867(6)	3278(4)	3686(4)	47(2)
N(4)	1904(5)	2116(3)	2796(3)	46(2)
C(16)	1746(6)	2792(3)	2964(4)	44(2)
C(17)	1589(6)	2954(4)	2389(4)	54(2)
C(18)	1612(6)	2348(4)	1836(4)	51(2)
C(19)	1787(6)	1844(4)	2102(4)	43(2)
C(20)	1907(6)	1130(4)	1732(4)	48(2)
C(21)	5446(7)	154(4)	3390(5)	62(2)
C(22)	4771(8)	-552(4)	3259(5)	69(2)
C(23)	3966(6)	756(4)	3978(4)	55(2)
C(24)	4579(7)	868(4)	4681(4)	65(2)
C(25)	7112(6)	3732(4)	4478(4)	49(2)
C(26)	7583(7)	3888(4)	3917(4)	65(2)
C(27)	1205(7)	3867(4)	3720(4)	54(2)
C(28)	1075(7)	4345(4)	4419(4)	61(2)
C(29)	1431(6)	2881(4)	4119(4)	48(2)
C(30)	173(6)	2582(4)	3915(4)	57(2)
C(31)	1266(7)	759(4)	1114(4)	54(2)
C(32)	318(8)	957(5)	731(4)	71(2)
Li(2)	1691(10)	1289(6)	3076(6)	50(3)
C(65)	1816(8)	1511(5)	4667(4)	67(2)
O(1)	1318(4)	1203(3)	3968(3)	56(1)
C(66)	490(9)	614(5)	3816(5)	84(3)
C(67)	-318(11)	502(6)	3247(6)	108(4)
O(2)	142(4)	664(3)	2725(3)	61(2)
C(68)	-740(8)	748(6)	2275(6)	91(3)
Li(4)	-545(10)	-2777(6)	2396(6)	48(3)
N(5)	-553(5)	-1716(3)	2938(3)	50(2)
C(33)	-1540(6)	-1425(3)	2893(4)	46(2)
C(34)	-1653(7)	-1002(4)	3505(4)	51(2)
C(35)	-748(6)	-1031(4)	3989(4)	50(2)
C(36)	-81(6)	-1469(3)	3626(3)	45(2)
C(37)	960(7)	-1716(4)	3888(4)	51(2)

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Table S57. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **26** (cont.).

	x	y	z	U(eq)
N(6)	288(5)	-2941(3)	3182(3)	48(2)
C(38)	670(6)	-2465(4)	3802(4)	52(2)
C(39)	835(7)	-2780(4)	4279(4)	58(2)
C(40)	557(7)	-3466(4)	3946(4)	57(2)
C(41)	224(6)	-3579(4)	3253(4)	51(2)
C(42)	-44(6)	-4202(4)	2697(4)	51(2)
N(7)	-482(5)	-3753(3)	1794(3)	44(2)
C(43)	-352(6)	-4287(4)	2028(4)	50(2)
C(44)	-547(7)	-4912(4)	1449(4)	55(2)
C(45)	-786(7)	-4750(4)	886(5)	62(2)
C(46)	-724(6)	-4032(3)	1118(4)	47(2)
C(47)	-910(6)	-3581(4)	705(4)	49(2)
N(8)	-1386(5)	-2528(3)	1550(3)	46(2)
C(48)	-1744(6)	-3111(3)	981(3)	43(2)
C(49)	-2898(6)	-3213(4)	750(4)	51(2)
C(50)	-3308(7)	-2649(4)	1182(4)	54(2)
C(51)	-2364(6)	-2243(4)	1668(4)	45(2)
C(52)	-2301(6)	-1576(4)	2229(4)	45(2)
C(53)	1400(7)	-1276(4)	4657(4)	59(2)
C(54)	1898(8)	-525(4)	4816(4)	67(2)
C(55)	1900(6)	-1655(4)	3481(4)	56(2)
C(56)	3007(7)	-1871(4)	3716(4)	63(2)
C(57)	-31(7)	-4858(4)	2859(5)	61(2)
C(58)	-1119(8)	-5098(5)	3022(5)	78(3)
C(59)	269(6)	-3127(4)	802(4)	51(2)
C(60)	1194(7)	-3527(4)	495(4)	59(2)
C(61)	-1340(7)	-4015(4)	-46(4)	58(2)
C(62)	-1434(8)	-3633(4)	-513(4)	65(2)
C(63)	-2925(6)	-1096(4)	2170(4)	53(2)
C(64)	-3775(7)	-1132(4)	1570(4)	64(2)
Li(5)	-108(11)	-1738(6)	2051(6)	50(3)
C(81)	-1044(9)	-1265(7)	910(6)	101(4)
O(9)	-243(5)	-1137(3)	1510(3)	72(2)
C(82)	816(8)	-750(5)	1542(5)	75(3)
C(83)	1543(11)	-727(6)	2149(6)	117(5)
O(10)	1584(6)	-1413(4)	2112(5)	103(3)
C(84)	2376(13)	-1761(7)	1819(6)	152(7)
Li(3)	-6151(11)	-2201(7)	-1111(7)	60(3)
C(69)	-6676(13)	-631(6)	-750(7)	128(5)
O(3)	-6146(5)	-1175(3)	-1150(3)	80(2)
C(70)	-6432(8)	-1300(5)	-1842(5)	79(3)
C(71)	-5670(8)	-1767(5)	-2203(5)	71(3)
O(4)	-5782(5)	-2365(3)	-2025(3)	70(2)
C(72)	-5066(9)	-2820(5)	-2350(5)	78(3)
C(73)	-3672(8)	-1407(5)	-527(5)	74(3)
O(5)	-4497(5)	-1946(3)	-534(3)	68(2)
C(74)	-3994(7)	-2547(5)	-578(5)	70(3)
C(75)	-4881(7)	-3085(5)	-560(5)	80(3)
O(6)	-5806(5)	-3198(3)	-1092(3)	76(2)
C(76)	-6658(10)	-3754(6)	-1168(8)	121(5)
C(77)	-6361(10)	-1611(8)	421(6)	119(5)

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Table S57. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **26** (cont.).

	x	y	z	U(eq)
O(7)	-6931(5)	-2020(4)	-246(3)	93(2)
C(78)	-8135(8)	-2062(6)	-347(5)	80(3)
C(79)	-8623(8)	-2553(6)	-1030(5)	78(3)
O(8)	-7984(5)	-2481(3)	-1493(3)	75(2)
C(80)	-8526(8)	-2844(6)	-2184(5)	93(3)
Li(6)	-4871(12)	-3836(7)	2927(7)	62(4)
C(85)	-7404(8)	-3629(6)	2239(5)	87(3)
O(11)	-6309(4)	-3771(3)	2169(3)	65(2)
C(86)	-6250(8)	-4217(6)	1518(5)	89(3)
C(87)	-5025(8)	-4183(6)	1437(5)	83(3)
O(12)	-4373(5)	-4308(3)	1959(3)	64(2)
C(88)	-3211(8)	-4244(5)	1903(5)	77(3)
C(89)	-4262(8)	-2401(5)	2872(5)	74(3)
O(13)	-3981(4)	-2870(3)	3187(3)	59(1)
C(90)	-2776(7)	-2817(4)	3410(5)	67(2)
C(91)	-2619(8)	-3193(4)	3870(5)	73(3)
O(14)	-3299(5)	-3869(3)	3539(3)	67(2)
C(92)	-3314(8)	-4232(5)	3984(5)	79(3)
C(93)	-5431(9)	-2926(5)	4312(4)	75(3)
O(15)	-5805(5)	-3523(3)	3708(3)	68(2)
C(94)	-6402(8)	-4089(6)	3812(6)	84(3)
C(95)	-6684(9)	-4677(6)	3177(5)	82(3)
O(16)	-5667(6)	-4788(3)	2914(3)	79(2)
C(96)	-5717(14)	-5465(6)	2442(7)	123(5)

Table S58. Bond lengths [Å] and angles [°] for 26.

Li(1)-N(3)	2.014(13)	O(1)-C(66)	1.418(10)	C(61)-C(62)	1.500(11)
Li(1)-N(2)	2.021(13)	C(66)-C(67)	1.393(15)	C(63)-C(64)	1.514(11)
Li(1)-N(1)	2.216(13)	C(67)-O(2)	1.452(12)	Li(5)-O(9)	2.014(14)
Li(1)-N(4)	2.237(13)	O(2)-C(68)	1.409(11)	Li(5)-O(10)	2.051(14)
Li(1)-Li(2)	2.605(17)	Li(4)-N(6)	2.010(13)	Li(5)-C(83)	2.688(16)
N(1)-C(4)	1.397(9)	Li(4)-N(7)	2.046(13)	C(81)-O(9)	1.431(11)
N(1)-C(1)	1.418(9)	Li(4)-N(5)	2.151(13)	O(9)-C(82)	1.419(11)
N(1)-Li(2)	2.121(14)	Li(4)-N(8)	2.222(13)	C(82)-C(83)	1.459(13)
C(1)-C(2)	1.380(11)	Li(4)-Li(5)	2.585(17)	C(83)-O(10)	1.435(14)
C(1)-C(20)	1.501(10)	N(5)-C(36)	1.407(9)	O(10)-C(84)	1.364(14)
C(1)-Li(2)	2.771(15)	N(5)-C(33)	1.406(9)	Li(3)-O(4)	2.012(16)
C(2)-C(3)	1.422(11)	N(5)-Li(5)	2.051(14)	Li(3)-O(5)	2.104(14)
C(3)-C(4)	1.383(10)	C(33)-C(34)	1.356(10)	Li(3)-O(7)	2.147(16)
C(4)-C(5)	1.500(10)	C(33)-C(52)	1.503(10)	Li(3)-O(8)	2.186(14)
C(5)-C(6)	1.546(10)	C(33)-Li(5)	2.653(14)	Li(3)-O(3)	2.207(14)
C(5)-C(23)	1.548(11)	C(34)-C(35)	1.427(10)	Li(3)-O(6)	2.212(14)
C(5)-C(21)	1.572(10)	C(35)-C(36)	1.402(10)	C(69)-O(3)	1.454(12)
N(2)-C(6)	1.350(9)	C(36)-C(37)	1.524(10)	O(3)-C(70)	1.413(11)
N(2)-C(9)	1.422(9)	C(37)-C(38)	1.529(10)	C(70)-C(71)	1.517(13)
C(6)-C(7)	1.444(11)	C(37)-C(55)	1.550(11)	C(71)-O(4)	1.446(10)
C(7)-C(8)	1.359(10)	C(37)-C(53)	1.579(10)	O(4)-C(72)	1.434(10)
C(8)-C(9)	1.427(10)	N(6)-C(38)	1.348(9)	C(73)-O(5)	1.425(10)
C(9)-C(10)	1.403(10)	N(6)-C(41)	1.409(9)	O(5)-C(74)	1.451(10)
C(10)-C(11)	1.396(10)	C(38)-C(39)	1.415(11)	C(74)-C(75)	1.489(13)
C(10)-C(25)	1.539(10)	C(39)-C(40)	1.359(11)	C(75)-O(6)	1.422(10)
N(3)-C(14)	1.341(9)	C(40)-C(41)	1.428(11)	O(6)-C(76)	1.423(12)
N(3)-C(11)	1.423(9)	C(41)-C(42)	1.412(11)	C(77)-O(7)	1.427(12)
C(11)-C(12)	1.435(10)	C(42)-C(43)	1.388(11)	O(7)-C(78)	1.425(11)
C(12)-C(13)	1.381(11)	C(42)-C(57)	1.550(11)	C(78)-C(79)	1.475(13)
C(13)-C(14)	1.445(10)	N(7)-C(46)	1.351(9)	C(79)-O(8)	1.386(11)
C(14)-C(15)	1.522(10)	N(7)-C(43)	1.407(10)	O(8)-C(80)	1.442(11)
C(15)-C(16)	1.522(10)	C(43)-C(44)	1.444(11)	Li(6)-O(13)	2.052(14)
C(15)-C(27)	1.542(10)	C(44)-C(45)	1.380(12)	Li(6)-O(15)	2.118(16)
C(15)-C(29)	1.566(10)	C(45)-C(46)	1.420(10)	Li(6)-O(16)	2.128(15)
N(4)-C(19)	1.391(9)	C(46)-C(47)	1.533(11)	Li(6)-O(14)	2.179(15)
N(4)-C(16)	1.393(9)	C(47)-C(48)	1.529(10)	Li(6)-O(12)	2.189(16)
N(4)-Li(2)	2.047(14)	C(47)-C(61)	1.545(10)	Li(6)-O(11)	2.267(15)
C(16)-C(17)	1.398(10)	C(47)-C(59)	1.570(11)	C(85)-O(11)	1.404(11)
C(17)-C(18)	1.428(11)	N(8)-C(48)	1.383(9)	O(11)-C(86)	1.417(11)
C(18)-C(19)	1.399(10)	N(8)-C(51)	1.399(9)	C(86)-C(87)	1.509(14)
C(19)-C(20)	1.483(10)	N(8)-Li(5)	2.016(13)	C(87)-O(12)	1.406(11)
C(19)-Li(2)	2.758(15)	C(48)-C(49)	1.378(10)	O(12)-C(88)	1.418(10)
C(20)-C(31)	1.363(10)	C(49)-C(50)	1.427(10)	C(89)-O(13)	1.432(9)
C(21)-C(22)	1.536(11)	C(50)-C(51)	1.402(11)	O(13)-C(90)	1.445(10)
C(23)-C(24)	1.524(11)	C(51)-C(52)	1.498(10)	C(90)-C(91)	1.481(13)
C(25)-C(26)	1.529(11)	C(51)-Li(5)	2.710(14)	C(91)-O(14)	1.452(10)
C(27)-C(28)	1.544(11)	C(52)-C(63)	1.361(10)	O(14)-C(92)	1.428(10)
C(29)-C(30)	1.517(11)	C(52)-Li(5)	2.765(14)	C(93)-O(15)	1.443(10)
C(31)-C(32)	1.502(11)	C(53)-C(54)	1.539(12)	O(15)-C(94)	1.431(11)
Li(2)-O(2)	2.045(12)	C(55)-C(56)	1.535(11)	C(94)-C(95)	1.467(14)
Li(2)-O(1)	2.109(14)	C(57)-C(58)	1.485(12)	C(95)-O(16)	1.431(12)
C(65)-O(1)	1.433(10)	C(59)-C(60)	1.559(11)	O(16)-C(96)	1.434(12)

Table S58. Bond lengths [Å] and angles [°] for **26** (cont.).

N(3)-Li(1)-N(2)	90.9(5)	C(66)-O(1)-Li(2)	109.9(6)	N(5)-Li(5)-C(33)	31.6(3)
N(3)-Li(1)-N(1)	175.3(7)	C(65)-O(1)-Li(2)	136.0(6)	O(10)-Li(5)-C(33)	134.3(6)
N(2)-Li(1)-N(1)	92.7(5)	C(67)-C(66)-O(1)	112.0(8)	Li(4)-Li(5)-C(33)	73.4(4)
N(3)-Li(1)-N(4)	94.4(5)	C(66)-C(67)-O(2)	113.9(9)	O(9)-Li(5)-C(83)	56.0(4)
N(2)-Li(1)-N(4)	174.3(7)	C(68)-O(2)-C(67)	109.9(8)	N(8)-Li(5)-C(83)	154.2(7)
N(1)-Li(1)-N(4)	81.9(4)	C(68)-O(2)-Li(2)	123.8(6)	N(5)-Li(5)-C(83)	115.6(6)
N(3)-Li(1)-Li(2)	123.9(7)	C(67)-O(2)-Li(2)	112.7(6)	O(10)-Li(5)-C(83)	31.8(4)
N(2)-Li(1)-Li(2)	125.6(6)	N(6)-Li(4)-N(7)	89.5(5)	Li(4)-Li(5)-C(83)	143.5(6)
N(1)-Li(1)-Li(2)	51.4(4)	N(6)-Li(4)-N(5)	95.2(5)	C(33)-Li(5)-C(83)	116.8(5)
N(4)-Li(1)-Li(2)	49.3(4)	N(7)-Li(4)-N(5)	173.4(7)	O(9)-Li(5)-C(51)	91.2(5)
C(4)-N(1)-C(1)	104.4(6)	N(6)-Li(4)-N(8)	176.1(7)	N(8)-Li(5)-C(51)	30.1(3)
C(4)-N(1)-Li(2)	142.7(6)	N(7)-Li(4)-N(8)	93.2(5)	N(5)-Li(5)-C(51)	78.0(4)
C(1)-N(1)-Li(2)	101.2(5)	N(5)-Li(4)-N(8)	81.9(4)	O(10)-Li(5)-C(51)	166.9(7)
C(4)-N(1)-Li(1)	115.4(5)	N(6)-Li(4)-Li(5)	127.2(6)	Li(4)-Li(5)-C(51)	70.7(4)
C(1)-N(1)-Li(1)	118.5(5)	N(7)-Li(4)-Li(5)	123.1(6)	C(33)-Li(5)-C(51)	57.9(3)
Li(2)-N(1)-Li(1)	73.8(5)	N(5)-Li(4)-Li(5)	50.3(4)	C(83)-Li(5)-C(51)	145.4(6)
C(2)-C(1)-N(1)	111.1(6)	N(8)-Li(4)-Li(5)	48.9(4)	O(9)-Li(5)-C(52)	86.5(5)
C(2)-C(1)-C(20)	127.0(7)	C(36)-N(5)-C(33)	105.1(6)	N(8)-Li(5)-C(52)	61.3(4)
N(1)-C(1)-C(20)	121.8(7)	C(36)-N(5)-Li(5)	139.7(6)	N(5)-Li(5)-C(52)	61.5(4)
C(2)-C(1)-Li(2)	149.4(6)	C(33)-N(5)-Li(5)	98.5(6)	O(10)-Li(5)-C(52)	155.2(6)
N(1)-C(1)-Li(2)	48.7(4)	C(36)-N(5)-Li(4)	115.8(5)	Li(4)-Li(5)-C(52)	83.5(5)
C(20)-C(1)-Li(2)	78.1(5)	C(33)-N(5)-Li(4)	122.0(6)	C(33)-Li(5)-C(52)	32.1(3)
C(1)-C(2)-C(3)	106.1(7)	Li(5)-N(5)-Li(4)	75.9(5)	C(83)-Li(5)-C(52)	124.7(6)
C(4)-C(3)-C(2)	107.6(7)	C(34)-C(33)-N(5)	110.9(7)	C(51)-Li(5)-C(52)	31.7(3)
C(3)-C(4)-N(1)	110.7(6)	C(34)-C(33)-C(52)	127.8(7)	C(82)-O(9)-C(81)	113.2(7)
C(3)-C(4)-C(5)	128.9(6)	N(5)-C(33)-C(52)	121.3(6)	C(82)-O(9)-Li(5)	112.8(6)
N(1)-C(4)-C(5)	120.2(6)	C(34)-C(33)-Li(5)	144.1(6)	C(81)-O(9)-Li(5)	127.2(7)
C(4)-C(5)-C(6)	108.4(6)	N(5)-C(33)-Li(5)	49.9(5)	O(9)-C(82)-C(83)	105.2(8)
C(4)-C(5)-C(23)	113.6(6)	C(52)-C(33)-Li(5)	78.0(5)	O(10)-C(83)-C(82)	108.7(8)
C(6)-C(5)-C(23)	107.9(6)	C(33)-C(34)-C(35)	108.0(7)	O(10)-C(83)-Li(5)	48.8(5)
C(4)-C(5)-C(21)	110.5(6)	C(36)-C(35)-C(34)	106.0(6)	C(82)-C(83)-Li(5)	82.2(6)
C(6)-C(5)-C(21)	107.2(6)	C(35)-C(36)-N(5)	109.9(6)	C(84)-O(10)-C(83)	121.0(10)
C(23)-C(5)-C(21)	109.0(6)	C(35)-C(36)-C(37)	128.8(6)	C(84)-O(10)-Li(5)	130.0(8)
C(6)-N(2)-C(9)	106.0(6)	N(5)-C(36)-C(37)	121.2(6)	C(83)-O(10)-Li(5)	99.4(8)
C(6)-N(2)-Li(1)	126.5(6)	C(36)-C(37)-C(38)	110.7(6)	O(4)-Li(3)-O(5)	99.9(6)
C(9)-N(2)-Li(1)	121.5(6)	C(36)-C(37)-C(55)	109.3(6)	O(4)-Li(3)-O(7)	166.7(7)
N(2)-C(6)-C(7)	111.2(6)	C(38)-C(37)-C(55)	107.7(6)	O(5)-Li(3)-O(7)	92.9(6)
N(2)-C(6)-C(5)	119.4(6)	C(36)-C(37)-C(53)	109.7(6)	O(4)-Li(3)-O(8)	93.3(6)
C(7)-C(6)-C(5)	129.4(6)	C(38)-C(37)-C(53)	108.8(6)	O(5)-Li(3)-O(8)	166.4(8)
C(8)-C(7)-C(6)	106.0(6)	C(55)-C(37)-C(53)	110.5(6)	O(7)-Li(3)-O(8)	74.0(5)
C(7)-C(8)-C(9)	108.7(7)	C(38)-N(6)-C(41)	106.4(6)	O(4)-Li(3)-O(3)	79.7(5)
C(10)-C(9)-N(2)	123.0(6)	C(38)-N(6)-Li(4)	125.5(6)	O(5)-Li(3)-O(3)	93.7(6)
C(10)-C(9)-C(8)	128.8(7)	C(41)-N(6)-Li(4)	124.7(6)	O(7)-Li(3)-O(3)	96.3(6)
N(2)-C(9)-C(8)	108.1(6)	N(6)-C(38)-C(39)	110.3(7)	O(8)-Li(3)-O(3)	91.4(5)
C(11)-C(10)-C(9)	127.4(7)	N(6)-C(38)-C(37)	119.4(7)	O(4)-Li(3)-O(6)	94.7(6)
C(11)-C(10)-C(25)	116.7(6)	C(39)-C(38)-C(37)	129.9(7)	O(5)-Li(3)-O(6)	77.6(5)
C(9)-C(10)-C(25)	115.9(6)	C(40)-C(39)-C(38)	107.9(7)	O(7)-Li(3)-O(6)	91.3(6)
C(14)-N(3)-C(11)	108.2(6)	C(39)-C(40)-C(41)	106.9(7)	O(8)-Li(3)-O(6)	98.6(6)
C(14)-N(3)-Li(1)	126.7(6)	N(6)-C(41)-C(42)	122.6(7)	O(3)-Li(3)-O(6)	168.8(8)
C(11)-N(3)-Li(1)	122.1(6)	N(6)-C(41)-C(40)	108.4(7)	C(70)-O(3)-C(69)	112.2(8)
C(10)-C(11)-N(3)	124.2(6)	C(42)-C(41)-C(40)	128.8(7)	C(70)-O(3)-Li(3)	103.9(6)
C(10)-C(11)-C(12)	128.1(7)	C(43)-C(42)-C(41)	126.9(7)	C(69)-O(3)-Li(3)	127.5(8)
N(3)-C(11)-C(12)	107.7(6)	C(43)-C(42)-C(57)	116.9(7)	O(3)-C(70)-C(71)	108.4(7)
C(13)-C(12)-C(11)	107.2(7)	C(41)-C(42)-C(57)	116.1(8)	O(4)-C(71)-C(70)	107.8(7)
C(12)-C(13)-C(14)	107.5(6)	C(46)-N(7)-C(43)	107.3(6)	C(72)-O(4)-C(71)	109.8(7)
N(3)-C(14)-C(13)	109.5(6)	C(46)-N(7)-Li(4)	127.8(6)	C(72)-O(4)-Li(3)	126.9(6)
N(3)-C(14)-C(15)	121.7(6)	C(43)-N(7)-Li(4)	124.2(6)	C(71)-O(4)-Li(3)	114.5(7)
C(13)-C(14)-C(15)	128.6(6)	C(42)-C(43)-N(7)	124.7(7)	C(73)-O(5)-C(74)	110.8(7)



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Table S58. Bond lengths [Å] and angles [°] for 26 (cont.)

C(14)-C(15)-C(16)	106.3(6)	C(42)-C(43)-C(44)	127.9(7)	C(73)-O(5)-Li(3)	123.0(6)
C(14)-C(15)-C(27)	111.7(6)	N(7)-C(43)-C(44)	107.4(7)	C(74)-O(5)-Li(3)	111.9(6)
C(16)-C(15)-C(27)	110.6(6)	C(45)-C(44)-C(43)	107.8(7)	O(5)-C(74)-C(75)	108.6(7)
C(14)-C(15)-C(29)	107.7(6)	C(44)-C(45)-C(46)	106.3(7)	O(6)-C(75)-C(74)	107.4(7)
C(16)-C(15)-C(29)	110.0(6)	N(7)-C(46)-C(45)	111.2(7)	C(76)-O(6)-C(75)	112.4(7)
C(27)-C(15)-C(29)	110.4(6)	N(7)-C(46)-C(47)	120.4(6)	C(76)-O(6)-Li(3)	124.6(7)
C(19)-N(4)-C(16)	106.6(6)	C(45)-C(46)-C(47)	128.4(7)	C(75)-O(6)-Li(3)	108.9(6)
C(19)-N(4)-Li(2)	105.1(5)	C(48)-C(47)-C(46)	109.4(6)	C(78)-O(7)-C(77)	113.8(8)
C(16)-N(4)-Li(2)	143.4(6)	C(48)-C(47)-C(61)	111.1(6)	C(78)-O(7)-Li(3)	117.5(6)
C(19)-N(4)-Li(1)	113.5(5)	C(46)-C(47)-C(61)	111.3(6)	C(77)-O(7)-Li(3)	123.9(7)
C(16)-N(4)-Li(1)	108.2(5)	C(48)-C(47)-C(59)	108.3(6)	O(7)-C(78)-C(79)	108.2(8)
Li(2)-N(4)-Li(1)	74.8(5)	C(46)-C(47)-C(59)	106.9(6)	O(8)-C(79)-C(78)	111.9(8)
N(4)-C(16)-C(17)	109.9(6)	C(61)-C(47)-C(59)	109.7(6)	C(79)-O(8)-C(80)	114.8(7)
N(4)-C(16)-C(15)	122.7(6)	C(48)-N(8)-C(51)	105.2(6)	C(79)-O(8)-Li(3)	114.5(6)
C(17)-C(16)-C(15)	127.1(6)	C(48)-N(8)-Li(5)	144.7(6)	C(80)-O(8)-Li(3)	125.9(7)
C(16)-C(17)-C(18)	106.9(7)	C(51)-N(8)-Li(5)	103.6(5)	O(13)-Li(6)-O(15)	92.9(6)
C(19)-C(18)-C(17)	106.6(7)	C(48)-N(8)-Li(4)	110.7(5)	O(13)-Li(6)-O(16)	165.8(8)
N(4)-C(19)-C(18)	110.1(6)	C(51)-N(8)-Li(4)	113.8(6)	O(15)-Li(6)-O(16)	78.2(5)
N(4)-C(19)-C(20)	122.6(6)	Li(5)-N(8)-Li(4)	75.0(5)	O(13)-Li(6)-O(14)	77.8(5)
C(18)-C(19)-C(20)	127.3(7)	C(49)-C(48)-N(8)	111.8(6)	O(15)-Li(6)-O(14)	97.3(6)
N(4)-C(19)-Li(2)	45.8(4)	C(49)-C(48)-C(47)	127.3(6)	O(16)-Li(6)-O(14)	92.3(6)
C(18)-C(19)-Li(2)	152.5(6)	N(8)-C(48)-C(47)	120.7(6)	O(13)-Li(6)-O(12)	98.4(6)
C(20)-C(19)-Li(2)	78.7(5)	C(48)-C(49)-C(50)	106.5(6)	O(15)-Li(6)-O(12)	164.0(8)
C(31)-C(20)-C(19)	121.6(6)	C(51)-C(50)-C(49)	106.2(7)	O(16)-Li(6)-O(12)	92.7(6)
C(31)-C(20)-C(1)	118.2(7)	N(8)-C(51)-C(50)	110.3(6)	O(14)-Li(6)-O(12)	96.1(6)
C(19)-C(20)-C(1)	120.1(6)	N(8)-C(51)-C(52)	120.8(6)	O(13)-Li(6)-O(11)	97.5(6)
C(22)-C(21)-C(5)	115.0(7)	C(50)-C(51)-C(52)	128.8(7)	O(15)-Li(6)-O(11)	91.7(6)
C(24)-C(23)-C(5)	117.3(7)	N(8)-C(51)-Li(5)	46.3(4)	O(16)-Li(6)-O(11)	93.7(6)
C(26)-C(25)-C(10)	112.8(6)	C(50)-C(51)-Li(5)	151.2(6)	O(14)-Li(6)-O(11)	170.0(8)
C(15)-C(27)-C(28)	117.6(6)	C(52)-C(51)-Li(5)	76.2(5)	O(12)-Li(6)-O(11)	75.7(5)
C(30)-C(29)-C(15)	114.3(6)	C(63)-C(52)-C(51)	122.6(7)	C(85)-O(11)-C(86)	113.7(7)
C(20)-C(31)-C(32)	128.2(7)	C(63)-C(52)-C(33)	117.6(6)	C(85)-O(11)-Li(6)	130.2(7)
N(4)-Li(2)-O(2)	116.9(6)	C(51)-C(52)-C(33)	119.7(6)	C(86)-O(11)-Li(6)	109.8(6)
N(4)-Li(2)-O(1)	131.1(6)	C(63)-C(52)-Li(5)	131.4(6)	O(11)-C(86)-C(87)	109.3(8)
O(2)-Li(2)-O(1)	79.3(5)	C(51)-C(52)-Li(5)	72.1(4)	O(12)-C(87)-C(86)	109.9(9)
N(4)-Li(2)-N(1)	88.9(6)	C(33)-C(52)-Li(5)	69.8(5)	C(87)-O(12)-C(88)	110.1(7)
O(2)-Li(2)-N(1)	122.9(6)	C(54)-C(53)-C(37)	115.0(7)	C(87)-O(12)-Li(6)	112.9(6)
O(1)-Li(2)-N(1)	122.3(6)	C(56)-C(55)-C(37)	114.0(7)	C(88)-O(12)-Li(6)	120.6(6)
N(4)-Li(2)-Li(1)	55.9(4)	C(58)-C(57)-C(42)	113.1(7)	C(89)-O(13)-C(90)	114.1(6)
O(2)-Li(2)-Li(1)	171.0(7)	C(60)-C(59)-C(47)	114.8(6)	C(89)-O(13)-Li(6)	124.6(6)
O(1)-Li(2)-Li(1)	109.5(5)	C(62)-C(61)-C(47)	116.4(7)	C(90)-O(13)-Li(6)	113.2(6)
N(1)-Li(2)-Li(1)	54.8(4)	C(52)-C(63)-C(64)	128.1(7)	O(13)-C(90)-C(91)	108.3(7)
N(4)-Li(2)-C(19)	29.1(3)	O(9)-Li(5)-N(8)	102.8(6)	O(14)-C(91)-C(90)	107.9(7)
O(2)-Li(2)-C(19)	101.3(5)	O(9)-Li(5)-N(5)	134.6(6)	C(92)-O(14)-C(91)	111.3(7)
O(1)-Li(2)-C(19)	157.5(6)	N(8)-Li(5)-N(5)	89.6(5)	C(92)-O(14)-Li(6)	120.7(6)
N(1)-Li(2)-C(19)	76.6(5)	O(9)-Li(5)-O(10)	80.5(5)	C(91)-O(14)-Li(6)	110.9(6)
Li(1)-Li(2)-C(19)	69.8(4)	N(8)-Li(5)-O(10)	142.3(7)	C(94)-O(15)-C(93)	113.6(7)
N(4)-Li(2)-C(1)	78.6(5)	N(5)-Li(5)-O(10)	115.0(7)	C(94)-O(15)-Li(6)	112.4(7)
O(2)-Li(2)-C(1)	102.4(5)	O(9)-Li(5)-Li(4)	159.0(7)	C(93)-O(15)-Li(6)	124.4(7)
O(1)-Li(2)-C(1)	146.5(6)	N(8)-Li(5)-Li(4)	56.1(4)	O(15)-C(94)-C(95)	109.0(8)
N(1)-Li(2)-C(1)	30.1(3)	N(5)-Li(5)-Li(4)	53.8(4)	O(16)-C(95)-C(94)	108.7(8)
Li(1)-Li(2)-C(1)	71.6(4)	O(10)-Li(5)-Li(4)	115.0(6)	C(95)-O(16)-C(96)	114.3(9)
C(19)-Li(2)-C(1)	55.8(3)	O(9)-Li(5)-C(33)	106.6(5)	C(95)-O(16)-Li(6)	107.3(7)
C(66)-O(1)-C(65)	113.0(7)	N(8)-Li(5)-C(33)	81.4(5)	C(96)-O(16)-Li(6)	129.8(8)

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Table S59. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **26**. 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 <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
Li(1)	52(7)	63(8)	27(7)	12(5)	-2(6)	1(6)
N(1)	43(3)	55(4)	39(4)	16(3)	5(3)	5(3)
C(1)	46(4)	48(4)	45(5)	14(4)	0(4)	-2(3)
C(2)	58(5)	60(5)	42(5)	18(4)	13(4)	13(4)
C(3)	58(5)	60(5)	52(5)	24(4)	21(4)	18(4)
C(4)	34(4)	53(4)	50(5)	24(4)	12(3)	10(3)
C(5)	42(4)	46(4)	50(5)	16(3)	14(4)	11(3)
N(2)	43(3)	55(4)	33(3)	16(3)	5(3)	7(3)
C(6)	45(4)	52(4)	46(5)	23(4)	5(4)	12(3)
C(7)	46(5)	64(5)	59(5)	24(4)	7(4)	16(4)
C(8)	36(4)	67(5)	48(5)	21(4)	6(4)	9(4)
C(9)	49(5)	55(5)	40(5)	22(3)	3(4)	10(4)
C(10)	43(4)	62(5)	25(4)	10(3)	6(3)	3(3)
N(3)	34(3)	55(4)	47(4)	19(3)	11(3)	7(3)
C(11)	52(5)	54(4)	31(4)	12(3)	-3(3)	3(4)
C(12)	58(5)	43(4)	46(5)	15(3)	8(4)	4(3)
C(13)	56(5)	43(4)	57(5)	16(4)	17(4)	7(3)
C(14)	40(4)	54(4)	42(5)	18(3)	10(3)	6(3)
C(15)	51(5)	49(4)	43(5)	15(3)	19(4)	14(3)
N(4)	46(4)	47(4)	40(4)	12(3)	1(3)	2(3)
C(16)	36(4)	52(4)	48(5)	25(4)	7(3)	9(3)
C(17)	54(5)	60(5)	49(5)	22(4)	4(4)	12(4)
C(18)	49(5)	60(5)	42(5)	18(4)	6(4)	10(4)
C(19)	31(4)	61(5)	37(5)	20(4)	4(3)	1(3)
C(20)	48(4)	53(5)	47(5)	26(4)	6(4)	7(3)
C(21)	57(5)	54(5)	68(6)	18(4)	-3(4)	17(4)
C(22)	68(6)	51(5)	94(7)	31(5)	21(5)	14(4)
C(23)	46(4)	63(5)	51(5)	20(4)	1(4)	0(4)
C(24)	69(5)	74(6)	55(5)	30(4)	3(4)	12(4)
C(25)	37(4)	56(4)	56(5)	24(4)	7(4)	8(3)
C(26)	60(5)	73(6)	58(6)	22(4)	13(4)	-1(4)
C(27)	49(4)	62(5)	53(5)	25(4)	8(4)	9(4)
C(28)	61(5)	61(5)	61(6)	16(4)	15(4)	25(4)
C(29)	54(5)	51(4)	39(5)	10(3)	20(4)	19(3)
C(30)	52(5)	66(5)	55(5)	23(4)	12(4)	13(4)
C(31)	54(5)	60(5)	41(5)	16(4)	-2(4)	5(4)
C(32)	78(6)	78(6)	50(6)	20(4)	4(5)	6(5)
Li(2)	45(7)	55(7)	36(7)	6(5)	-3(6)	-2(5)
C(65)	70(6)	79(6)	56(6)	28(5)	13(5)	17(4)
O(1)	55(3)	70(3)	49(4)	29(3)	11(3)	6(3)
C(66)	103(8)	73(6)	73(7)	26(5)	35(6)	-16(5)
C(67)	106(9)	117(9)	96(9)	59(7)	-10(7)	-40(7)
O(2)	56(3)	65(3)	57(4)	26(3)	1(3)	-3(3)
C(68)	67(6)	115(8)	83(8)	42(6)	-8(6)	-10(6)
Li(4)	45(7)	58(7)	46(8)	23(6)	16(6)	13(5)
N(5)	57(4)	51(4)	44(4)	15(3)	11(3)	15(3)
C(33)	41(4)	45(4)	48(5)	14(4)	9(3)	7(3)
C(34)	58(5)	43(4)	45(5)	9(4)	9(4)	9(3)
C(35)	47(4)	66(5)	36(5)	16(4)	14(4)	4(4)
C(36)	57(5)	46(4)	21(4)	4(3)	3(3)	-2(3)
C(37)	58(5)	46(4)	42(5)	10(3)	9(4)	8(3)

S90

Table S59. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **26** (cont.).

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
N(6)	54(4)	48(4)	42(4)	16(3)	7(3)	10(3)
C(38)	54(5)	50(4)	46(5)	14(4)	6(4)	9(3)
C(39)	56(5)	69(6)	48(5)	28(4)	-2(4)	5(4)
C(40)	63(5)	70(6)	46(5)	33(4)	8(4)	8(4)
C(41)	44(4)	60(5)	52(5)	23(4)	11(4)	11(3)
C(42)	40(4)	56(5)	57(6)	20(4)	9(4)	9(3)
N(7)	40(3)	50(3)	38(4)	12(3)	10(3)	9(3)
C(43)	38(4)	52(4)	59(6)	20(4)	14(4)	6(3)
C(44)	58(5)	45(4)	60(6)	14(4)	16(4)	10(3)
C(45)	71(6)	47(5)	61(6)	9(4)	18(5)	15(4)
C(46)	34(4)	46(4)	57(6)	15(4)	11(4)	1(3)
C(47)	54(5)	56(4)	28(4)	6(3)	5(3)	5(4)
N(8)	43(4)	48(3)	43(4)	12(3)	10(3)	7(3)
C(48)	44(4)	44(4)	32(4)	7(3)	2(3)	3(3)
C(49)	50(5)	47(4)	47(5)	9(4)	3(4)	6(3)
C(50)	42(4)	69(5)	50(5)	22(4)	5(4)	11(4)
C(51)	49(4)	54(4)	38(4)	21(3)	15(4)	14(3)
C(52)	45(4)	52(4)	36(4)	14(3)	7(3)	5(3)
C(53)	64(5)	68(5)	34(5)	5(4)	2(4)	15(4)
C(54)	75(6)	56(5)	50(5)	1(4)	-4(4)	13(4)
C(55)	48(5)	64(5)	57(5)	23(4)	11(4)	10(4)
C(56)	61(5)	74(6)	59(6)	29(4)	9(4)	16(4)
C(57)	69(5)	55(5)	65(6)	30(4)	10(4)	12(4)
C(58)	80(6)	72(6)	99(8)	48(6)	32(6)	10(5)
C(59)	51(5)	57(5)	41(5)	14(4)	10(4)	4(3)
C(60)	52(5)	64(5)	55(5)	13(4)	15(4)	13(4)
C(61)	69(5)	54(5)	37(5)	-1(4)	7(4)	11(4)
C(62)	80(6)	78(6)	42(5)	23(4)	19(4)	19(5)
C(63)	53(5)	64(5)	48(5)	23(4)	16(4)	23(4)
C(64)	72(6)	67(5)	54(6)	19(4)	14(5)	24(4)
Li(5)	60(8)	40(6)	43(8)	4(5)	20(6)	5(5)
C(81)	87(7)	163(11)	85(8)	86(8)	12(6)	29(7)
O(9)	72(4)	85(4)	72(4)	44(3)	23(3)	9(3)
C(82)	93(7)	61(5)	72(7)	29(5)	18(6)	3(5)
C(83)	126(10)	120(10)	79(8)	50(7)	-33(7)	-58(8)
O(10)	74(4)	132(6)	130(7)	93(6)	6(5)	3(4)
C(84)	158(13)	142(11)	76(9)	-56(8)	77(9)	-57(10)
Li(3)	59(8)	70(8)	58(9)	35(7)	3(7)	12(6)
C(69)	153(12)	103(9)	149(13)	47(9)	60(10)	72(9)
O(3)	74(4)	87(4)	82(5)	31(4)	16(4)	20(3)
C(70)	71(6)	106(7)	88(8)	70(6)	11(6)	16(5)
C(71)	67(6)	90(7)	65(6)	42(5)	15(5)	-3(5)
O(4)	64(4)	95(4)	55(4)	31(3)	18(3)	10(3)
C(72)	88(7)	96(7)	53(6)	20(5)	21(5)	35(6)
C(73)	65(6)	75(6)	77(7)	32(5)	3(5)	-6(5)
O(5)	57(3)	78(4)	70(4)	33(3)	6(3)	7(3)
C(74)	59(5)	81(6)	70(6)	28(5)	1(5)	21(5)
C(75)	56(5)	92(7)	99(8)	54(6)	-9(5)	12(5)
O(6)	73(4)	81(4)	72(4)	35(3)	-5(3)	4(3)
C(76)	98(8)	84(7)	168(13)	66(8)	-37(8)	-16(6)
C(77)	83(8)	186(13)	65(8)	26(8)	10(6)	1(8)
O(7)	60(4)	146(6)	50(4)	14(4)	2(3)	16(4)

S91

Table S59. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 26 (cont.).

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
C(78)	60(6)	123(8)	65(7)	42(6)	15(5)	16(5)
C(79)	54(6)	114(8)	67(7)	33(6)	13(5)	13(5)
O(8)	46(3)	119(5)	50(4)	22(3)	12(3)	-4(3)
C(80)	49(5)	131(9)	60(7)	2(6)	1(5)	-18(5)
Li(6)	69(9)	70(9)	52(9)	29(7)	10(7)	5(7)
C(85)	63(6)	122(9)	72(7)	28(6)	12(5)	31(6)
O(11)	48(3)	88(4)	58(4)	23(3)	17(3)	12(3)
C(86)	65(7)	137(9)	63(7)	34(6)	10(5)	20(6)
C(87)	62(6)	116(8)	75(7)	33(6)	20(5)	29(5)
O(12)	56(4)	84(4)	56(4)	30(3)	12(3)	15(3)
C(88)	62(6)	105(7)	76(7)	35(6)	33(5)	26(5)
C(89)	75(6)	77(6)	87(7)	49(5)	23(5)	14(5)
O(13)	50(3)	68(3)	64(4)	30(3)	11(3)	7(2)
C(90)	58(5)	62(5)	80(7)	31(5)	12(5)	-3(4)
C(91)	62(5)	67(6)	76(7)	15(5)	6(5)	2(4)
O(14)	69(4)	63(4)	69(4)	27(3)	10(3)	8(3)
C(92)	73(6)	85(6)	83(7)	42(6)	3(5)	11(5)
C(93)	99(7)	90(7)	46(6)	24(5)	23(5)	41(5)
O(15)	87(4)	83(4)	49(4)	35(3)	26(3)	22(3)
C(94)	65(6)	121(9)	88(8)	59(7)	32(6)	22(6)
C(95)	76(7)	102(8)	65(7)	38(6)	1(6)	-9(5)
O(16)	91(5)	71(4)	69(4)	20(3)	18(4)	1(3)
C(96)	172(13)	76(8)	115(10)	27(7)	50(10)	5(8)

S92

Table S60. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 26.

	x	y	z	U(eq)
H(2)	3313	138	1184	64
H(3)	4706	-90	2051	65
H(7)	7253	1219	3818	67
H(8)	7836	2475	4191	61
H(12)	5484	4587	4537	60
H(13)	3410	4627	4263	62
H(17)	1487	3385	2369	65
H(18)	1526	2297	1378	61
H(21A)	5872	116	3023	75
H(21B)	6009	294	3812	75
H(22A)	4501	-550	3666	103
H(22B)	5264	-896	3136	103
H(22C)	4120	-661	2893	103
H(23A)	3518	1126	4012	66
H(23B)	3420	322	3813	66
H(24A)	4902	462	4675	98
H(24B)	4038	949	4987	98
H(24C)	5190	1263	4834	98
H(25A)	6993	4163	4813	59
H(25B)	7680	3541	4705	59
H(26A)	7809	3478	3620	97
H(26B)	8245	4254	4111	97
H(26C)	6995	4033	3660	97
H(27A)	434	3667	3447	65
H(27B)	1586	4149	3504	65
H(28A)	520	4108	4589	92
H(28B)	812	4754	4384	92
H(28C)	1811	4476	4726	92
H(29A)	1868	2506	4088	57
H(29B)	1587	3194	4594	57
H(30A)	-271	2952	3974	85
H(30B)	-27	2327	4196	85
H(30C)	5	2275	3444	85
H(31)	1442	319	898	65
H(32A)	64	1352	1036	106
H(32B)	-318	574	536	106
H(32C)	589	1075	373	106
H(65A)	1257	1729	4917	101
H(65B)	2480	1855	4732	101
H(65C)	2053	1160	4830	101
H(66A)	872	212	3744	100
H(66B)	106	668	4202	100
H(67A)	-913	781	3378	130
H(67B)	-686	17	3063	130
H(68A)	-1211	304	2005	137
H(68B)	-413	947	1980	137
H(68C)	-1210	1053	2528	137
H(34)	-2233	-733	3596	61
H(35)	-622	-801	4461	60
H(39)	1095	-2553	4748	69
H(40)	579	-3806	4139	68

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Table S60. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **26** (cont.).

	x	y	z	U(eq)
H(44)	-516	-5356	1455	66
H(45)	-957	-5059	433	74
H(49)	-3336	-3586	378	61
H(50)	-4067	-2565	1147	65
H(53A)	761	-1291	4896	71
H(53B)	1991	-1490	4836	71
H(54A)	2646	-497	4689	100
H(54B)	1977	-267	5297	100
H(54C)	1388	-333	4563	100
H(55A)	1606	-1941	3004	67
H(55B)	2071	-1176	3514	67
H(56A)	3350	-1559	4172	95
H(56B)	3537	-1856	3414	95
H(56C)	2841	-2336	3710	95
H(57A)	130	-5224	2469	73
H(57B)	591	-4769	3244	73
H(58A)	-1332	-4721	3372	117
H(58B)	-1026	-5472	3181	117
H(58C)	-1716	-5259	2619	117
H(59A)	151	-2783	596	61
H(59B)	558	-2878	1287	61
H(60A)	1281	-3890	670	88
H(60B)	1919	-3214	615	88
H(60C)	962	-3727	6	88
H(61A)	-821	-4345	-190	70
H(61B)	-2098	-4281	-97	70
H(62A)	-1888	-3274	-355	98
H(62B)	-1804	-3948	-964	98
H(62C)	-673	-3427	-526	98
H(63)	-2813	-688	2554	63
H(64A)	-3579	-1437	1159	96
H(64B)	-3757	-675	1554	96
H(64C)	-4539	-1307	1608	96
H(81A)	-1107	-835	845	151
H(81B)	-1788	-1473	945	151
H(81C)	-785	-1576	526	151
H(82A)	725	-284	1567	90
H(82B)	1143	-972	1142	90
H(83A)	2318	-487	2192	140
H(83B)	1234	-477	2547	140
H(84A)	2049	-2040	1350	229
H(84B)	2609	-2057	2057	229
H(84C)	3039	-1437	1841	229
H(69A)	-6476	-219	-847	192
H(69B)	-6406	-535	-273	192
H(69C)	-7504	-773	-860	192
H(70A)	-6324	-866	-1918	95
H(70B)	-7240	-1519	-2015	95
H(71A)	-5901	-1899	-2693	86
H(71B)	-4870	-1530	-2066	86
H(72A)	-5331	-2989	-2837	118

Table S60. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **26** (cont.).

	x	y	z	U(eq)
H(72B)	-5095	-3206	-2199	118
H(72C)	-4282	-2577	-2238	118
H(73A)	-3074	-1273	-128	111
H(73B)	-4037	-1014	-519	111
H(73C)	-3337	-1561	-929	111
H(74A)	-3352	-2434	-198	84
H(74B)	-3700	-2713	-1000	84
H(75A)	-4572	-3511	-618	96
H(75B)	-5136	-2934	-125	96
H(76A)	-6316	-4165	-1234	181
H(76B)	-7251	-3832	-1557	181
H(76C)	-6993	-3648	-765	181
H(77A)	-6827	-1277	631	179
H(77B)	-5626	-1372	409	179
H(77C)	-6240	-1903	680	179
H(78A)	-8335	-1609	-294	96
H(78B)	-8441	-2216	-13	96
H(79A)	-8664	-3023	-1033	94
H(79B)	-9407	-2485	-1162	94
H(80A)	-8566	-3336	-2292	139
H(80B)	-8085	-2702	-2475	139
H(80C)	-9296	-2742	-2255	139
H(85A)	-7529	-3246	2099	130
H(85B)	-7477	-3509	2709	130
H(85C)	-7970	-4031	1959	130
H(86A)	-6694	-4084	1177	107
H(86B)	-6580	-4690	1452	107
H(87A)	-4971	-4526	1000	100
H(87B)	-4727	-3726	1443	100
H(88A)	-3130	-4570	1470	116
H(88B)	-2767	-4340	2265	116
H(88C)	-2935	-3780	1936	116
H(89A)	-4022	-1933	3197	111
H(89B)	-5086	-2485	2712	111
H(89C)	-3872	-2464	2493	111
H(90A)	-2420	-2332	3645	80
H(90B)	-2410	-3014	3021	80
H(91A)	-1807	-3227	3975	87
H(91B)	-2865	-2950	4294	87
H(92A)	-2535	-4278	4142	118
H(92B)	-3776	-4686	3748	118
H(92C)	-3639	-3981	4368	118
H(93A)	-6086	-2793	4516	113
H(93B)	-5070	-2552	4202	113
H(93C)	-4883	-3029	4627	113
H(94A)	-7107	-3969	3974	100
H(94B)	-5922	-4203	4155	100
H(95A)	-7013	-5087	3252	99
H(95B)	-7251	-4588	2854	99
H(96A)	-5783	-5791	2669	184
H(96B)	-5023	-5488	2253	184
H(96C)	-6379	-5577	2081	184

Figure S8. Ball-and-stick representation of complex 13 [hydrogens and solvent omitted for clarity].

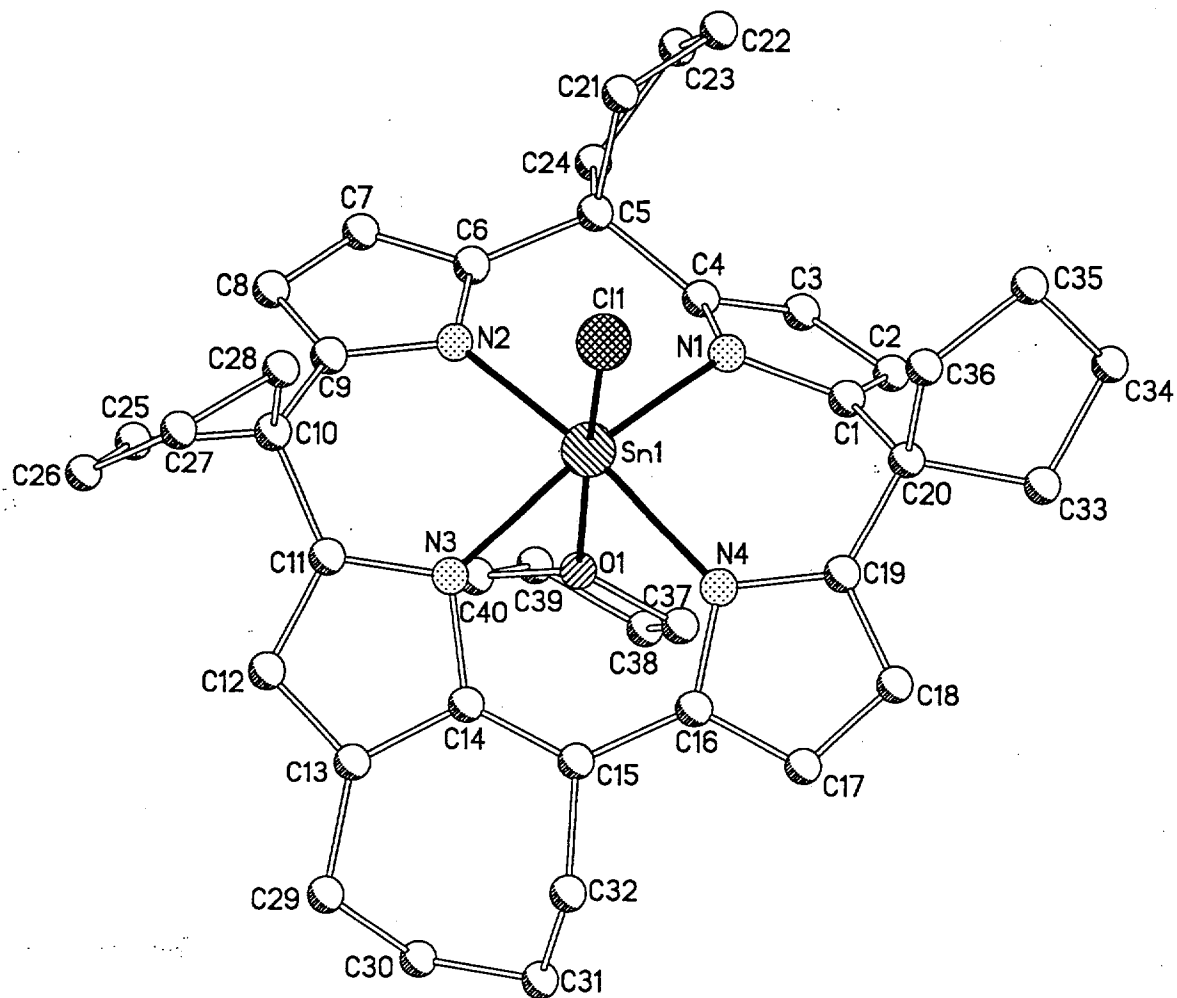
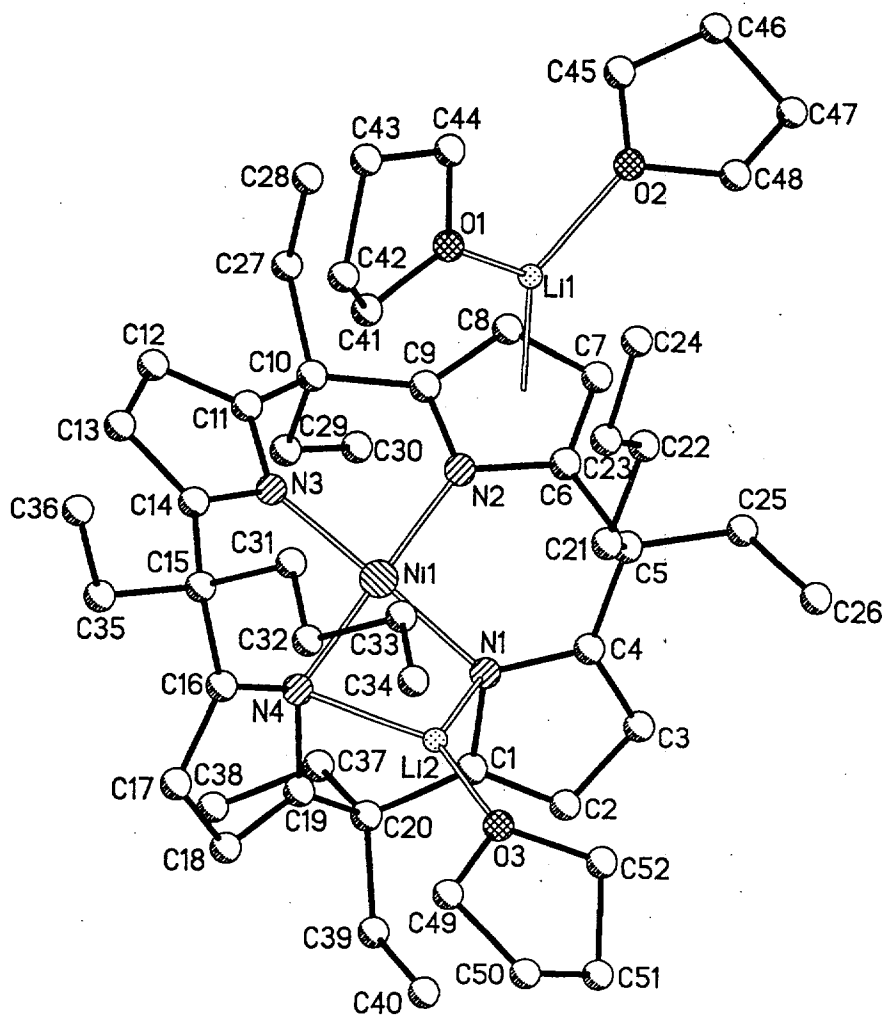




Figure S9. Ball-and-stick representation of complex 19 [hydrogens omitted for clarity].



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Figure S10. Ball-and-stick representation of complex 24 [hydrogens and solvents omitted for clarity].

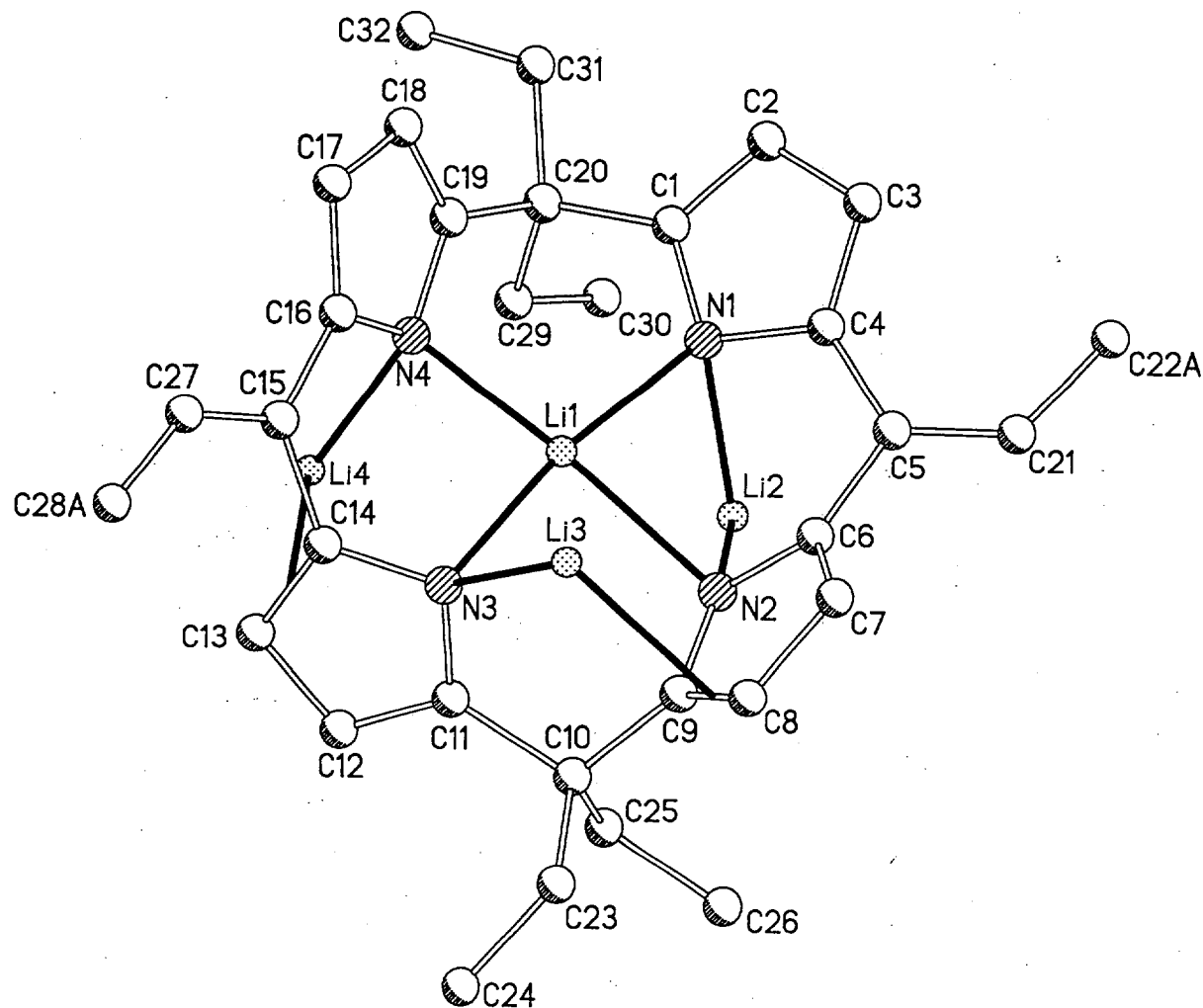
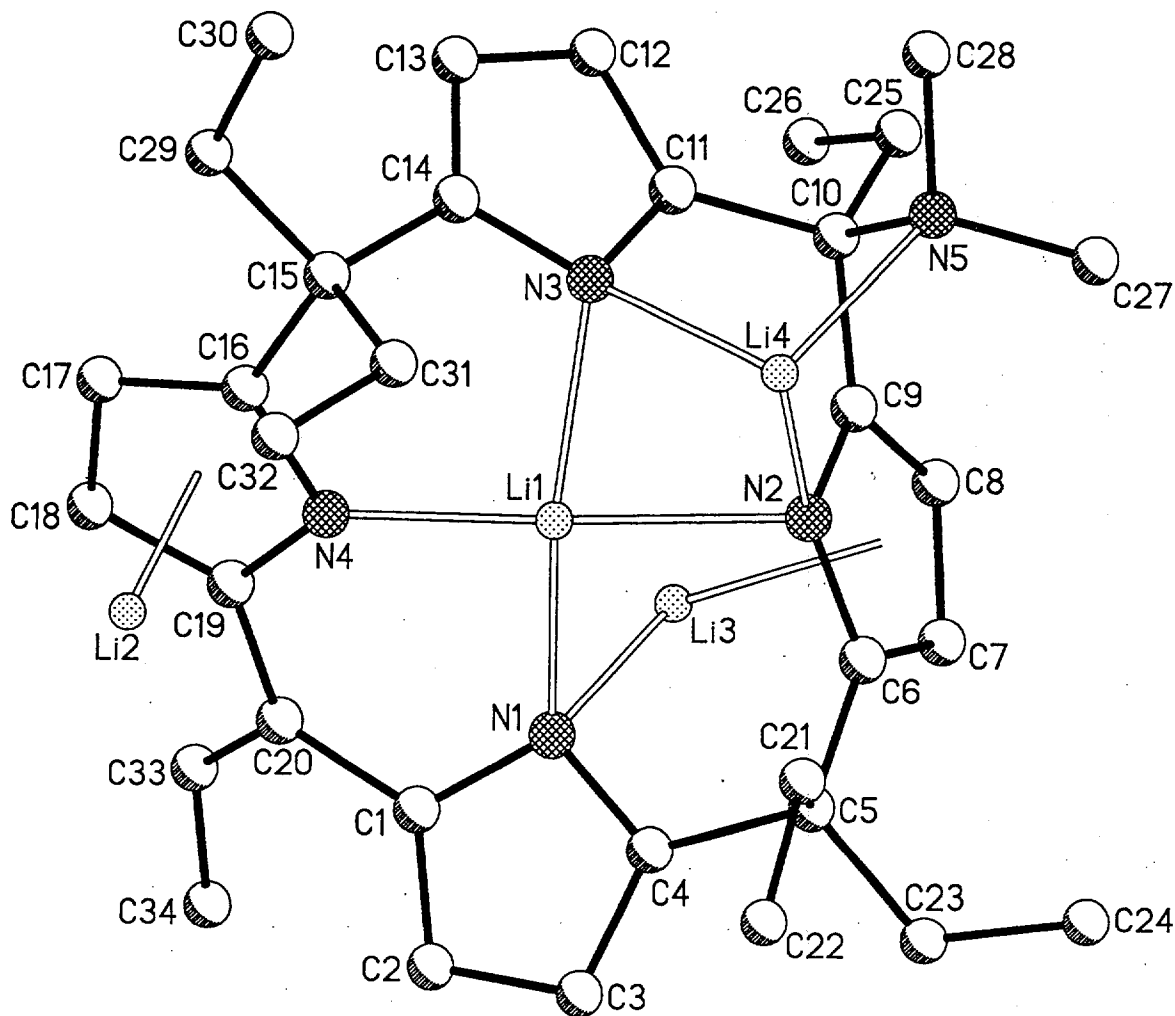


Figure S11. Ball-and-stick representation of complex **25** [hydrogens and solvents omitted for clarity].



S100

Figure S13. ORTEP representation of complex 26 (molecule 2) (50% probability ellipsoids) [hydrogens omitted for clarity].

