Inorganic Chemistry
including bioinorganic chemistry
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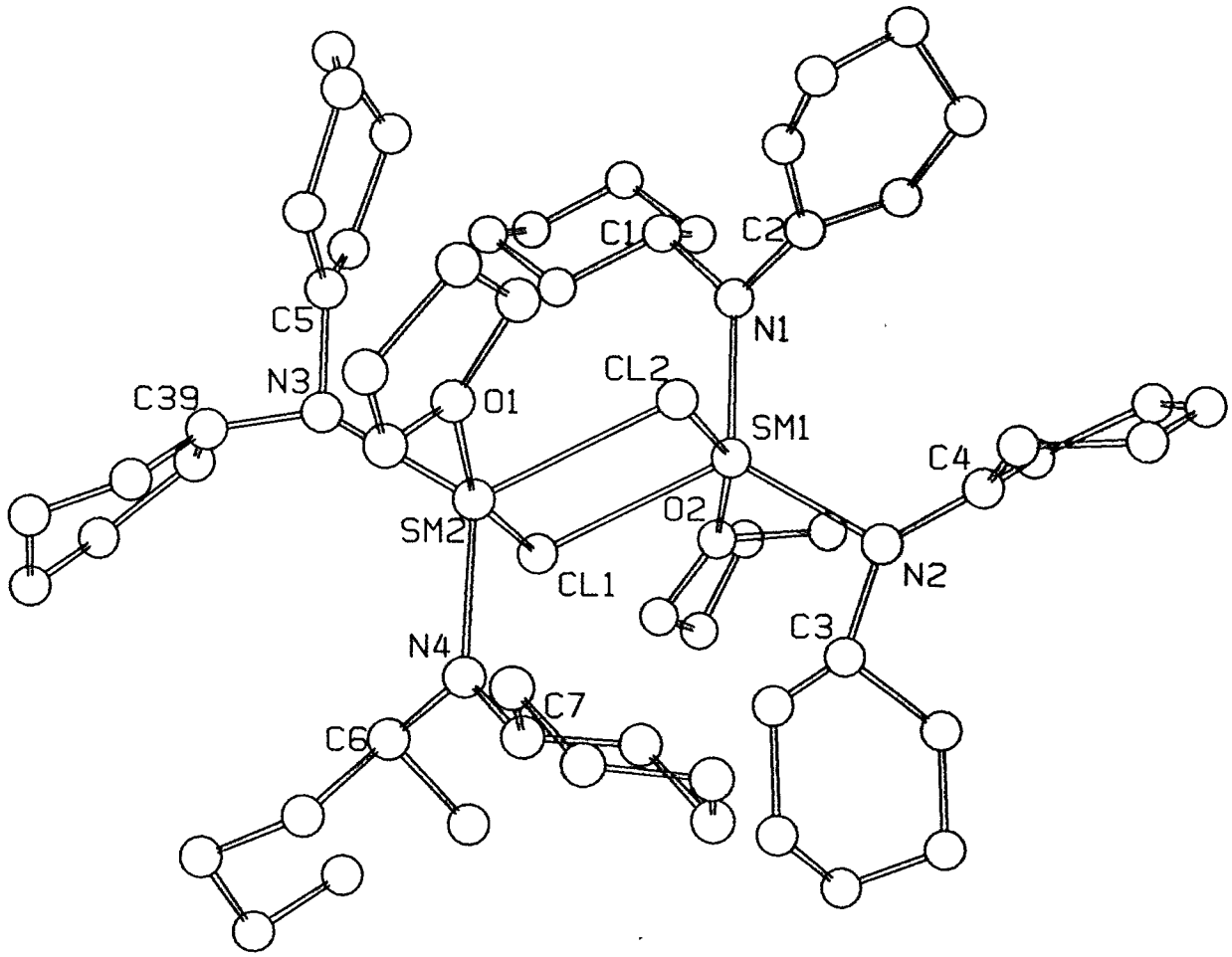
P-1873-MI

65 sg

Complex 1

Figure 1



P-1873-M2

Table S1

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{56}H_{104}O_2Sm_2N_4Cl_2$
Formula Weight	1238.18
Crystal Color, Habit	orange, cube
Crystal Dimensions (mm)	0.400 X 0.400 X 0.400
Crystal System	triclinic
No. Reflections Used for Unit Cell Determination (2θ range)	20 (47.0 - 49.5°)
Omega Scan Peak Width at Half-height	0.42
Lattice Parameters:	
	a = 14.344 (1)Å
	b = 23.897 (2)Å
	c = 10.2031 (9)Å
	α = 88.479 (9)°
	β = 121.83 (1)°
	γ = 93.73 (1)°
	V = 2965 (1)Å^3
Space Group	$P\bar{1}$ (#2)
Z value	2
D_{calc}	1.387 g/cm^3
F_{000}	1286
$\mu_{(MoK\alpha)}$	20.99 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC6S
Radiation	MoKα (λ = 0.71069 Å)
Temperature	-156°C
Take-off Angle	6.0°

P-1873-M3

Detector Aperture	6.0 mm horizontal 6.0 mm vertical
Crystal to Detector Distance	40 cm
Scan Type	ω-2θ
Scan Rate	4.0°/min (in omega) (3 rescans)
Scan Width	(1.42 + 0.30 tanθ)°
$2\theta_{max}$	51.5°
No. of Reflections Measured	Total: 5396 Unique: 5168 (R_{int} = .013)
Corrections	Lorentz-polarization Secondary Extinction (coefficient: 0.29627E-06)

C. Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares
Function Minimized	Σ w (|Fo| - |Fc|)^2
Least-squares Weights	$4Fo^2/\sigma^2(Fo^2)$
p-factor	0.03
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	4801
No. Variables	595
Reflection/Parameter Ratio	8.07
Residuals: R; R_w	0.031; 0.042
Goodness of Fit Indicator	2.15
Max Shift/Error in Final Cycle	0.79
Maximum Peak in Final Diff. Map	0.89 $e^-/Å^3$
Minimum Peak in Final Diff. Map	-1.69 $e^-/Å^3$

P-1873-MY

Table S2

Positional parameters and B(eq)[5] for 65sg

atom	x	y	z	B(eq)
Sm(1)	0.17534(5)	0.31784(3)	0.54046(8)	2.69(2)
Sm(2)	0.32466(5)	0.18216(3)	0.45954(8)	2.69(2)
Cl(1)	0.2531(3)	0.2129(2)	0.6558(4)	3.0(1)
Cl(2)	0.2469(3)	0.2871(2)	0.3442(4)	3.0(1)
O(1)	0.3914(6)	0.1861(3)	0.2909(7)	2.3(2)
O(2)	0.1326(6)	0.3115(3)	0.7558(7)	2.5(2)
N(1)	0.290(1)	0.3899(6)	0.662(1)	3.1(4)
N(2)	0.002(1)	0.3327(6)	0.361(2)	3.2(4)
N(3)	0.497(1)	0.1675(6)	0.640(2)	3.5(4)
N(4)	0.207(1)	0.1085(6)	0.346(1)	3.3(4)
C(1)	0.399(1)	0.4015(6)	0.825(1)	2.7(3)
C(2)	0.283(1)	0.4289(9)	0.546(2)	4.7(6)
C(3)	-0.0514(7)	0.2781(4)	0.360(1)	2.2(3)
C(4)	-0.033(1)	0.3815(5)	0.260(1)	4.6(4)
C(5)	0.581(1)	0.2154(6)	0.693(1)	4.1(4)
C(6)	0.222(1)	0.0694(8)	0.464(2)	4.2(6)
C(7)	0.125(1)	0.0977(6)	0.198(2)	2.9(4)
C(8)	0.227(1)	0.0064(5)	0.419(1)	4.3(4)
C(9)	0.1082(7)	0.0734(5)	0.473(1)	3.1(3)
C(10)	0.6042(5)	0.2510(3)	0.8037(7)	2.0(2)
C(11)	0.3547(8)	0.4392(5)	0.492(1)	3.7(4)
C(12)	-0.0330(9)	0.2331(5)	0.384(1)	6.3(5)
C(13)	-0.0514(7)	0.4304(4)	0.357(1)	2.7(3)
C(14)	0.167(1)	0.0188(6)	0.635(1)	4.7(5)
C(15)	0.190(1)	-0.0382(6)	0.602(2)	6.3(6)
C(16)	0.3715(9)	0.4594(6)	0.386(1)	4.6(4)
C(17)	0.345(1)	0.5186(6)	0.396(1)	5.4(5)
C(18)	0.3803(7)	0.4337(3)	0.9383(9)	3.2(3)
C(19)	-0.1764(7)	0.2925(5)	0.336(1)	4.6(4)
C(20)	0.406(1)	0.2310(5)	0.188(2)	3.6(4)
C(21)	0.459(1)	0.2099(6)	0.121(1)	4.7(5)
C(22)	0.121(1)	0.2656(7)	0.828(1)	4.0(4)
C(23)	0.080(1)	0.2911(7)	0.927(1)	4.7(4)
C(24)	-0.214(1)	0.1966(5)	0.348(2)	7.0(6)
C(25)	-0.0282(7)	0.3933(4)	0.147(1)	2.9(3)
C(26)	0.524(1)	0.3870(5)	1.174(1)	4.1(4)
C(27)	0.543(1)	0.3515(4)	1.072(1)	4.4(4)
C(28)	0.6558(7)	0.3093(3)	0.8101(8)	3.0(3)
C(29)	0.4421(7)	0.3442(3)	0.909(1)	3.4(3)
C(30)	-0.118(1)	0.4297(6)	-0.001(2)	4.6(4)
C(31)	-0.139(1)	0.4775(6)	0.053(1)	5.6(5)
C(32)	-0.100(1)	0.4804(5)	0.208(2)	7.0(6)
C(33)	0.4863(8)	0.4412(4)	1.101(1)	3.9(3)
C(34)	0.0523(6)	0.3623(3)	0.725(1)	2.3(3)
C(35)	0.1141(9)	0.3485(4)	0.939(1)	4.9(4)
C(36)	0.4007(7)	0.1374(5)	0.217(1)	3.8(4)
C(37)	0.275(1)	-0.0363(6)	0.556(2)	6.4(5)
C(38)	0.452(1)	0.1437(5)	0.138(1)	6.4(5)
C(39)	0.5716(7)	0.1249(5)	0.747(1)	3.2(3)

P-1873-MS

Positional parameters and B(eq) for 65sg

atom	x	y	z	B(eq)
C(40)	0.583(1)	0.0737(5)	0.702(1)	3.7(4)
C(41)	0.6353(7)	0.2202(4)	0.592(1)	3.0(3)
C(42)	0.6929(7)	0.2776(3)	0.604(1)	3.1(3)
C(43)	0.243(1)	0.5190(6)	0.408(2)	6.2(5)
C(44)	0.591(1)	0.0628(8)	0.963(2)	4.9(5)
C(45)	0.1602(7)	0.0973(4)	0.082(1)	3.9(3)
C(46)	0.062(1)	0.0845(5)	-0.081(1)	5.6(5)
C(47)	-0.033(1)	0.1248(5)	-0.127(2)	5.0(4)
C(48)	0.0375(7)	0.1385(5)	0.156(1)	5.3(4)
C(49)	-0.0626(8)	0.1253(7)	-0.007(2)	7.6(6)
C(50)	-0.126(1)	0.1827(5)	0.311(2)	9.8(7)
C(51)	-0.263(1)	0.2459(6)	0.277(2)	7.8(6)
C(52)	0.573(1)	0.1236(5)	0.904(1)	5.3(5)
C(53)	0.631(1)	0.0267(5)	0.763(1)	5.2(4)
C(54)	0.595(1)	0.0121(4)	0.878(1)	3.8(4)
C(56)	0.237(1)	0.4837(6)	0.537(2)	5.6(5)
C(57)	0.7435(7)	0.3064(3)	0.7708(9)	3.1(3)
H(1)	0.4548	0.4218	0.8129	3.7
H(2)	0.2277	0.4159	0.4441	4.9
H(3)	-0.0887	0.2736	0.2472	2.4
H(4)	-0.1092	0.3709	0.2029	5.4
H(5)	0.5222	0.2422	0.6310	6.6
H(6)	0.2863	0.0824	0.5464	4.4
H(7)	0.0961	0.0623	0.1934	2.8
H(8)	0.1572	-0.0028	0.3470	5.5
H(9)	0.2743	0.0064	0.3781	5.5
H(10)	0.5380	0.2584	0.8020	2.4
H(11)	0.6550	0.2332	0.8986	2.4
H(12)	0.4126	0.4583	0.5810	4.0
H(13)	0.3772	0.4016	0.4935	4.0
H(14)	0.0085	0.2253	0.3393	7.8
H(15)	0.0089	0.2319	0.4909	7.8
H(16)	-0.1052	0.4202	0.3802	3.1
H(17)	0.0149	0.4399	0.4487	3.1
H(18)	0.2118	-0.0626	0.6856	7.9
H(19)	0.1217	-0.0537	0.5134	7.9
H(20)	0.4442	0.4563	0.4089	5.0
H(21)	0.3220	0.4448	0.2854	5.0
H(22)	0.4028	0.5352	0.4862	6.6
H(23)	0.3313	0.5389	0.3077	6.6
H(24)	0.3498	0.4692	0.8971	4.0
H(25)	0.3280	0.4122	0.9489	4.0
H(26)	-0.1601	0.3004	0.4398	5.5
H(27)	-0.2048	0.3247	0.2762	5.5
H(28)	0.3423	0.2457	0.1134	5.6
H(29)	0.4549	0.2614	0.2577	5.6
H(30)	0.4281	0.2198	0.0202	5.9
H(31)	0.5380	0.2205	0.1784	5.9
H(32)	0.0643	0.2418	0.7515	3.6
H(33)	0.1847	0.2473	0.8885	3.6

P-1873-ML

Positional parameters and B(eq) for 65sg

atom	x	y	z	B(eq)
H(34)	0.0009	0.2868	0.8753	4.6
H(35)	0.1129	0.2725	1.0223	4.6
H(37)	-0.2721	0.1673	0.2739	15.6
H(38)	0.0390	0.4113	0.1838	2.5
H(39)	-0.0276	0.3576	0.1030	2.5
H(40)	0.4697	0.3694	1.1857	4.7
H(41)	0.5902	0.3901	1.2697	4.7
H(42)	0.6006	0.3676	1.0603	5.3
H(43)	0.5664	0.3148	1.1134	5.3
H(44)	0.5980	0.3325	0.7278	3.2
H(45)	0.6821	0.3264	0.9034	3.2
H(46)	0.3879	0.3270	0.9167	4.1
H(47)	0.4631	0.3214	0.8504	4.1
H(48)	-0.0863	0.4401	-0.0598	5.2
H(49)	-0.1816	0.4085	-0.0619	5.2
H(50)	-0.1114	0.5080	0.0310	6.3
H(51)	-0.2162	0.4794	0.0077	6.3
H(52)	-0.1534	0.5001	0.2258	8.5
H(53)	-0.0356	0.5065	0.2575	8.5
H(54)	0.5418	0.4583	1.0907	4.6
H(55)	0.4710	0.4637	1.1638	4.6
H(56)	0.4461	0.1102	0.3022	4.2
H(57)	0.3329	0.1218	0.1541	4.2
H(58)	0.2852	-0.0722	0.5215	7.6
H(59)	0.3455	-0.0253	0.6427	7.6
H(60)	0.4124	0.1272	0.0398	7.3
H(61)	0.5261	0.1273	0.1925	7.3
H(62)	0.6364	0.1905	0.7676	6.8
H(63)	0.0985	0.1096	0.5055	3.8
H(64)	0.0422	0.0630	0.3822	3.8
H(65)	0.2345	0.0318	0.7177	5.4
H(66)	0.1160	0.0143	0.6672	5.4
H(67)	-0.1991	0.1941	0.4356	15.6
H(68)	0.0659	0.3971	0.6934	3.0
H(69)	-0.0261	0.3543	0.6562	3.0
H(70)	0.0806	0.3729	0.9791	5.6
H(71)	0.1897	0.3542	0.9951	5.6
H(72)	0.6429	0.1411	0.7829	3.8
H(73)	0.5083	0.0626	0.6372	4.2
H(74)	0.6128	0.0821	0.6409	4.2
H(75)	0.6881	0.1916	0.6196	3.9
H(76)	0.5783	0.2151	0.4845	3.9
H(77)	0.7479	0.2744	0.5823	3.3
H(78)	0.6388	0.3048	0.5338	3.3
H(79)	0.2211	0.5569	0.4123	7.7
H(80)	0.1789	0.5041	0.3084	7.7
H(81)	0.6636	0.0616	1.0543	6.2
H(82)	0.5385	0.0548	0.9846	6.2
H(83)	0.1920	0.1335	0.0830	4.8
H(84)	0.2157	0.0699	0.1115	4.8

P-1873-M7

Positional parameters and B(eq) for 65sg

atom	x	y	z	B(eq)
H(85)	0.0808	0.0895	-0.1567	6.5
H(86)	0.0358	0.0481	-0.0857	6.5
H(87)	-0.0105	0.1622	-0.1285	6.6
H(88)	-0.0950	0.1150	-0.2181	6.6
H(89)	0.0139	0.1342	0.2303	6.3
H(90)	0.0591	0.1746	0.1578	6.3
H(91)	-0.1182	0.1520	-0.0281	8.5
H(92)	-0.0905	0.0887	-0.0007	8.5
H(93)	-0.1459	0.1702	0.2268	8.4
H(94)	-0.0882	0.1507	0.3972	8.4
H(95)	-0.3189	0.2554	0.2960	8.5
H(96)	-0.2998	0.2466	0.1613	8.5
H(97)	0.6330	0.1471	0.9797	6.1
H(98)	0.5071	0.1376	0.8880	6.1
H(99)	0.6102	-0.0012	0.6921	6.7
H(100)	0.7081	0.0319	0.8233	6.7
H(101)	0.6406	-0.0152	0.9466	5.3
H(102)	0.5204	-0.0023	0.8177	5.3
H(103)	0.1646	0.4814	0.5115	7.9
H(104)	0.2800	0.5052	0.6292	7.9
H(105)	0.7757	0.3433	0.7758	4.8
H(106)	0.8067	0.2841	0.8491	4.8

U values for 65sg

ATOM	U11	U22	U33	U12	U13	U23
Sm(1)	0.0433(3)	0.0260(4)	0.0470(3)	0.0039(3)	0.0332(2)	-0.0012(3)
Sm(2)	0.0433(3)	0.0260(4)	0.0470(3)	0.0039(3)	0.0332(2)	-0.0012(3)
Cl(1)	0.049(1)	0.032(2)	0.044(1)	0.003(1)	0.032(1)	-0.003(1)
Cl(2)	0.049(1)	0.032(2)	0.044(1)	0.003(1)	0.032(1)	-0.003(1)
O(1)	0.048(3)	0.025(3)	0.016(3)	0.006(2)	0.018(2)	0.006(2)
O(2)	0.054(3)	0.031(3)	0.017(3)	0.003(3)	0.025(2)	0.002(2)
N(1)	0.061(5)	0.029(6)	0.044(4)	-0.004(5)	0.040(3)	-0.000(4)
N(2)	0.048(5)	0.028(7)	0.068(6)	0.013(5)	0.044(4)	0.013(5)
N(3)	0.053(5)	0.026(7)	0.069(6)	0.012(5)	0.041(4)	0.013(5)
N(4)	0.048(5)	0.034(7)	0.061(5)	-0.005(5)	0.042(3)	-0.010(5)
C(1)	0.036(5)	0.029(5)	0.030(4)	-0.005(4)	0.013(3)	-0.006(4)
C(2)	0.055(7)	0.07(1)	0.053(7)	-0.012(7)	0.029(5)	-0.002(8)
C(3)	0.039(4)	0.013(4)	0.039(4)	0.015(3)	0.025(3)	0.012(3)
C(4)	0.062(7)	0.040(6)	0.064(6)	0.017(5)	0.025(6)	0.007(5)
C(5)	0.055(6)	0.056(7)	0.052(6)	0.026(5)	0.031(4)	0.020(5)
C(6)	0.080(7)	0.05(1)	0.052(6)	-0.026(7)	0.051(4)	0.001(6)
C(7)	0.038(5)	0.019(5)	0.064(6)	-0.000(4)	0.033(4)	-0.006(4)
C(8)	0.054(6)	0.032(5)	0.065(7)	-0.018(5)	0.025(5)	0.007(5)
C(9)	0.025(4)	0.067(7)	0.030(4)	-0.012(4)	0.019(3)	-0.007(4)
C(10)	0.036(3)	0.019(3)	0.035(3)	0.009(2)	0.026(2)	-0.001(2)
C(11)	0.033(5)	0.055(6)	0.052(5)	-0.012(5)	0.023(4)	-0.011(5)
C(12)	0.061(6)	0.085(8)	0.103(8)	0.021(5)	0.048(5)	0.025(6)
C(13)	0.036(4)	0.028(4)	0.039(5)	0.008(3)	0.020(3)	0.004(4)
C(14)	0.056(6)	0.08(1)	0.043(5)	-0.021(6)	0.028(4)	0.003(6)
C(15)	0.09(1)	0.054(8)	0.082(8)	0.004(7)	0.039(7)	0.036(6)
C(16)	0.045(5)	0.087(9)	0.042(5)	-0.015(5)	0.023(4)	0.004(5)
C(17)	0.071(7)	0.069(9)	0.054(6)	-0.012(6)	0.027(5)	0.033(6)
C(18)	0.061(5)	0.034(4)	0.032(4)	0.011(4)	0.025(3)	-0.000(3)
C(19)	0.035(4)	0.068(7)	0.080(6)	-0.010(4)	0.035(4)	-0.038(5)
C(20)	0.044(5)	0.029(5)	0.071(6)	0.013(4)	0.036(4)	0.013(4)
C(21)	0.086(7)	0.051(6)	0.059(6)	-0.011(6)	0.051(5)	-0.000(5)
C(22)	0.036(4)	0.091(9)	0.040(4)	0.022(5)	0.031(3)	0.034(5)
C(23)	0.053(5)	0.098(9)	0.033(4)	-0.026(5)	0.029(4)	-0.028(5)
C(24)	0.067(6)	0.037(6)	0.18(1)	0.013(5)	0.080(7)	0.019(8)
C(25)	0.044(4)	0.029(4)	0.047(4)	0.000(3)	0.032(3)	-0.005(3)

U values for 65sg

ATOM	U11	U22	U33	U12	U13	U23
C(26)	0.071(6)	0.032(6)	0.042(5)	-0.007(5)	0.023(4)	-0.003(4)
C(27)	0.062(6)	0.036(5)	0.048(6)	0.013(5)	0.014(4)	0.013(4)
C(28)	0.053(4)	0.028(4)	0.034(3)	0.011(3)	0.023(3)	-0.001(3)
C(29)	0.047(4)	0.025(4)	0.050(5)	0.010(3)	0.020(4)	-0.001(3)
C(30)	0.042(6)	0.040(6)	0.064(8)	0.005(5)	0.010(5)	0.033(5)
C(31)	0.078(8)	0.077(8)	0.048(6)	0.030(6)	0.026(5)	0.039(6)
C(32)	0.16(1)	0.048(7)	0.086(8)	0.058(7)	0.080(7)	0.040(6)
C(33)	0.071(6)	0.046(5)	0.027(4)	-0.001(4)	0.023(4)	0.003(4)
C(34)	0.036(4)	0.021(3)	0.039(4)	0.002(3)	0.026(3)	-0.000(3)
C(35)	0.088(5)	0.058(6)	0.079(5)	-0.020(5)	0.073(4)	-0.028(5)
C(36)	0.038(4)	0.052(5)	0.065(6)	-0.007(4)	0.035(4)	-0.024(5)
C(37)	0.114(9)	0.051(7)	0.106(8)	0.017(6)	0.077(6)	0.027(6)
C(38)	0.15(1)	0.057(6)	0.080(6)	0.051(6)	0.090(5)	0.031(5)
C(39)	0.043(4)	0.027(4)	0.076(5)	0.014(4)	0.048(3)	0.024(4)
C(40)	0.074(7)	0.039(5)	0.027(4)	0.018(5)	0.026(4)	0.011(4)
C(41)	0.029(4)	0.044(5)	0.044(4)	0.003(3)	0.020(3)	0.009(4)
C(42)	0.055(4)	0.022(4)	0.054(4)	-0.002(4)	0.039(3)	0.005(3)
C(43)	0.115(8)	0.056(8)	0.094(7)	0.018(6)	0.076(6)	0.044(6)
C(44)	0.051(7)	0.069(9)	0.052(7)	0.001(6)	0.018(5)	0.004(6)
C(45)	0.045(5)	0.059(6)	0.035(4)	0.011(4)	0.015(3)	0.000(4)
C(46)	0.071(7)	0.083(8)	0.040(5)	-0.008(6)	0.017(5)	0.001(5)
C(47)	0.054(6)	0.027(6)	0.058(9)	0.007(5)	-0.006(6)	0.005(6)
C(48)	0.031(4)	0.072(7)	0.077(7)	0.012(4)	0.013(4)	-0.025(6)
C(49)	0.033(5)	0.11(1)	0.09(1)	0.023(6)	-0.009(6)	-0.026(8)
C(50)	0.074(7)	0.048(7)	0.25(2)	-0.018(6)	0.09(1)	-0.05(1)
C(51)	0.062(6)	0.11(1)	0.13(1)	-0.008(6)	0.050(7)	-0.038(8)
C(52)	0.102(8)	0.061(7)	0.061(6)	0.034(6)	0.056(5)	0.029(5)
C(53)	0.117(6)	0.044(6)	0.087(6)	0.041(5)	0.087(4)	0.029(5)
C(54)	0.072(6)	0.035(5)	0.036(5)	0.021(4)	0.026(4)	0.017(4)
C(56)	0.074(8)	0.049(7)	0.062(7)	-0.031(6)	0.021(6)	0.015(5)
C(57)	0.050(4)	0.034(4)	0.039(4)	-0.010(3)	0.027(3)	-0.007(3)
H(1)	0.0474					
H(2)	0.0623					
H(3)	0.0301					
H(4)	0.0688					
H(5)	0.0832					

P-1873-MS

U values for 65sg

ATOM	U11	U22	U33	U12	U13	U23
H(6)	0.0561					
H(7)	0.0350					
H(8)	0.0702					
H(9)	0.0702					
H(10)	0.0306					
H(11)	0.0306					
H(12)	0.0512					
H(13)	0.0512					
H(14)	0.0982					
H(15)	0.0982					
H(16)	0.0398					
H(17)	0.0398					
H(18)	0.1004					
H(19)	0.1004					
H(20)	0.0637					
H(21)	0.0637					
H(22)	0.0839					
H(23)	0.0839					
H(24)	0.0511					
H(25)	0.0511					
H(26)	0.0695					
H(27)	0.0695					
H(28)	0.0714					
H(29)	0.0714					
H(30)	0.0742					
H(31)	0.0742					
H(32)	0.0452					
H(33)	0.0452					
H(34)	0.0588					
H(35)	0.0588					
H(37)	0.1979					
H(38)	0.0313					
H(39)	0.0313					
H(40)	0.0601					
H(41)	0.0601					
H(42)	0.0674					

P-1873-M10

U values for 65sg

ATOM	U11	U22	U33	U12	U13	U23
H(43)	0.0674					
H(44)	0.0400					
H(45)	0.0400					
H(46)	0.0521					
H(47)	0.0521					
H(48)	0.0664					
H(49)	0.0664					
H(50)	0.0803					
H(51)	0.0803					
H(52)	0.1081					
H(53)	0.1081					
H(54)	0.0580					
H(55)	0.0580					
H(56)	0.0528					
H(57)	0.0528					
H(58)	0.0958					
H(59)	0.0958					
H(60)	0.0924					
H(61)	0.0924					
H(62)	0.0859					
H(63)	0.0487					
H(64)	0.0487					
H(65)	0.0688					
H(66)	0.0688					
H(67)	0.1979					
H(68)	0.0381					
H(69)	0.0381					
H(70)	0.0704					
H(71)	0.0704					
H(72)	0.0487					
H(73)	0.0538					
H(74)	0.0538					
H(75)	0.0490					
H(76)	0.0490					
H(77)	0.0421					
H(78)	0.0421					

p-1873-m11

U values for 65sg

ATOM	U11	U22	U33	U12	U13	U23
H(79)	0.0981					
H(80)	0.0981					
H(81)	0.0786					
H(82)	0.0786					
H(83)	0.0606					
H(84)	0.0606					
H(85)	0.0823					
H(86)	0.0823					
H(87)	0.0838					
H(88)	0.0838					
H(89)	0.0792					
H(90)	0.0792					
H(91)	0.1079					
H(92)	0.1079					
H(93)	0.1068					
H(94)	0.1068					
H(95)	0.1076					
H(96)	0.1076					
H(97)	0.0778					
H(98)	0.0778					
H(99)	0.0852					
H(100)	0.0852					
H(101)	0.0665					
H(102)	0.0665					
H(103)	0.1001					
H(104)	0.1001					
H(105)	0.0607					
H(106)	0.0607					

P-1873-M12

Table S4

Intramolecular Distances Involving the Nonhydrogen Atoms

atom	atom	distance	atom	atom	distance
SM1	CL1	2.782(4)	C3	C12	1.11(1)
SM1	CL2	2.819(5)	C3	C19	1.73(1)
SM1	O2	2.573(8)	C4	C13	1.67(2)
SM1	N1	2.19(1)	C4	C25	1.21(2)
SM1	N2	2.23(1)	C5	C10	1.32(1)
SM2	CL1	2.819(5)	C5	C41	1.59(2)
SM2	CL2	2.782(4)	C6	C8	1.60(2)
SM2	O1	2.368(9)	C6	C9	1.69(2)
SM2	N3	2.21(1)	C7	C45	1.52(2)
SM2	N4	2.22(1)	C7	C48	1.50(2)
O1	C20	1.56(2)	C8	C37	1.58(2)
O1	C36	1.46(1)	C9	C14	1.92(2)
O2	C22	1.35(2)	C10	C28	1.52(1)
O2	C34	1.64(1)	C11	C16	1.30(2)
N1	C1	1.59(1)	C12	C50	1.61(2)
N1	C2	1.45(3)	C13	C32	1.77(2)
N2	C3	1.46(2)	C14	C15	1.51(2)
N2	C4	1.47(2)	C15	C37	1.52(2)
N3	C5	1.49(2)	C16	C17	1.51(2)
N3	C39	1.49(2)	C17	C43	1.52(2)
N4	C6	1.44(2)	C18	C33	1.56(1)
N4	C7	1.35(2)	C19	C51	1.49(2)
C1	C18	1.55(2)	C20	C21	1.38(2)
C1	C29	1.57(2)	C21	C38	1.59(2)
C2	C11	1.41(3)	C22	C23	1.57(2)
C2	C56	1.48(3)	C23	C35	1.41(2)

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Distances Involving the Nonhydrogen Atoms (cont)

atom	atom	distance	atom	atom	distance
C24	C50	1.55(2)			
C24	C51	1.39(2)			
C25	C30	1.65(1)			
C26	C27	1.50(2)			
C26	C33	1.46(2)			
C27	C29	1.53(1)			
C28	C57	1.51(1)			
C30	C31	1.40(2)			
C31	C32	1.37(2)			
C34	C35	1.91(1)			
C36	C38	1.35(2)			
C39	C40	1.37(2)			
C39	C52	1.59(2)			
C40	C53	1.31(2)			
C41	C42	1.53(1)			
C42	C57	1.61(1)			
C43	C56	1.58(2)			
C44	C52	1.54(2)			
C44	C54	1.54(2)			
C45	C46	1.53(1)			
C46	C47	1.57(2)			
C47	C49	1.49(2)			
C48	C49	1.54(1)			
C53	C54	1.53(1)			

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

P-1873-M15

Table S5

Intramolecular Bond Angles Involving the Nonhydrogen Atoms

atom	atom	atom	angle	atom	atom	atom	angle
CL1	SM1	CL2	78.9(1)	SM1	O2	C34	106.0(4)
CL1	SM1	O2	80.9(2)	C22	O2	C34	116.8(9)
CL1	SM1	N1	115.8(3)	SM1	N1	C1	136.5(9)
CL1	SM1	N2	124.4(4)	SM1	N1	C2	107.4(9)
CL2	SM1	O2	159.8(2)	C1	N1	C2	112(1)
CL2	SM1	N1	100.6(4)	SM1	N2	C3	100.2(7)
CL2	SM1	N2	98.5(5)	SM1	N2	C4	124.3(9)
O2	SM1	N1	88.8(4)	C3	N2	C4	134.3(9)
O2	SM1	N2	92.2(5)	SM2	N3	C5	118.8(9)
N1	SM1	N2	119.1(5)	SM2	N3	C39	144.2(9)
CL1	SM2	CL2	78.9(1)	C5	N3	C39	97.0(9)
CL1	SM2	O1	162.6(2)	SM2	N4	C6	107.9(8)
CL1	SM2	N3	97.9(5)	SM2	N4	C7	133(1)
CL1	SM2	N4	98.2(4)	C6	N4	C7	119(1)
CL2	SM2	O1	85.6(2)	N1	C1	C18	113(1)
CL2	SM2	N3	124.4(4)	N1	C1	C29	110(1)
CL2	SM2	N4	116.6(3)	C18	C1	C29	103.6(9)
O1	SM2	N3	84.4(5)	N1	C2	C11	130(2)
O1	SM2	N4	95.7(5)	N1	C2	C56	117(2)
N3	SM2	N4	118.7(5)	C11	C2	C56	105(2)
SM1	CL1	SM2	101.1(1)	N2	C3	C12	141(1)
SM1	CL2	SM2	101.1(1)	N2	C3	C19	105.6(9)
SM2	O1	C20	137.1(7)	C12	C3	C19	113(1)
SM2	O1	C36	124.4(6)	N2	C4	C13	105(1)
C20	O1	C36	96.4(8)	N2	C4	C25	132(1)
SM1	O2	C22	129.1(8)	C13	C4	C25	121(1)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

P-1873-M16

Intramolecular Bond Angles Involving the Nonhydrogen Atoms (cont)

atom	atom	atom	angle	atom	atom	atom	angle
N3	C5	C10	125(1)	C4	C25	C30	125(1)
N3	C5	C41	111(1)	C27	C26	C33	109(1)
C10	C5	C41	124(1)	C26	C27	C29	113(1)
N4	C6	C8	112(1)	C10	C28	C57	110.3(6)
N4	C6	C9	104(1)	C1	C29	C27	113.1(7)
C8	C6	C9	109(1)	C25	C30	C31	109(1)
N4	C7	C45	115(1)	C30	C31	C32	117(1)
N4	C7	C48	108(1)	C13	C32	C31	134(1)
C45	C7	C48	112(1)	C18	C33	C26	111.3(8)
C6	C8	C37	115(1)	O2	C34	C35	77.7(5)
C6	C9	C14	88.0(8)	C23	C35	C34	97.7(7)
C5	C10	C28	120.8(8)	O1	C36	C38	119(1)
C2	C11	C16	149(1)	C8	C37	C15	102(1)
C3	C12	C50	123(1)	C21	C38	C36	102(1)
C4	C13	C32	95.4(8)	N3	C39	C40	125(1)
C9	C14	C15	119(1)	N3	C39	C52	111(1)
C14	C15	C37	114(1)	C40	C39	C52	113.7(9)
C11	C16	C17	95(1)	C39	C40	C53	140(1)
C16	C17	C43	111(1)	C5	C41	C42	113.1(8)
C1	C18	C33	112.5(8)	C41	C42	C57	112.5(7)
C3	C19	C51	116.9(9)	C17	C43	C56	120(1)
O1	C20	C21	111(1)	C52	C44	C54	126(1)
C20	C21	C38	106(1)	C7	C45	C46	111.2(9)
O2	C22	C23	102(1)	C45	C46	C47	112(1)
C22	C23	C35	104(1)	C46	C47	C49	111(1)
C50	C24	C51	111(1)	C7	C48	C49	110(1)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

P-1873-MIN

Intramolecular Bond Angles Involving the Nonhydrogen Atoms (cont)

atom	atom	atom	angle	atom	atom	atom	angle
C47	C49	C48	113(1)				
C12	C50	C24	106(1)				
C19	C51	C24	108(1)				
C39	C52	C44	107(1)				
C40	C53	C54	103(1)				
C44	C54	C53	115(1)				
C2	C56	C43	107(2)				
C28	C57	C42	110.5(6)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

P-1873-M18

Table S6

Torsion or Conformation Angles

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
SM1	CL1	SM2	CL2	0.0(1)	SM2	O1	C20	C21	175.3(7)
SM1	CL1	SM2	O1	27.3(6)	SM2	O1	C36	C38	-172.0(8)
SM1	CL1	SM2	N3	123.7(4)	SM2	N3	C5	C10	87(1)
SM1	CL1	SM2	N4	-115.6(3)	SM2	N3	C5	C41	-90(1)
SM1	CL2	SM2	CL1	0.0(1)	SM2	N3	C39	C40	56(3)
SM1	CL2	SM2	O1	-172.1(2)	SM2	N3	C39	C52	-86(2)
SM1	CL2	SM2	N3	-92.0(6)	SM2	N4	C6	C8	-134(1)
SM1	CL2	SM2	N4	93.7(5)	SM2	N4	C6	C9	108.2(9)
SM1	O2	C22	C23	-172.4(5)	SM2	N4	C7	C45	62(2)
SM1	O2	C34	C35	-157.2(4)	SM2	N4	C7	C48	-64(2)
SM1	N1	C1	C18	-104(2)	CL1	SM1	O2	C22	-20.8(7)
SM1	N1	C1	C29	11(2)	CL1	SM1	O2	C34	-167.6(4)
SM1	N1	C2	C11	-103(2)	CL1	SM1	N1	C1	-19(2)
SM1	N1	C2	C56	113(1)	CL1	SM1	N1	C2	137(1)
SM1	N2	C3	C12	-27(2)	CL1	SM1	N2	C3	13(1)
SM1	N2	C3	C19	142.1(7)	CL1	SM1	N2	C4	-156(1)
SM1	N2	C4	C13	-88(1)	CL1	SM2	O1	C20	-16(1)
SM1	N2	C4	C25	76(2)	CL1	SM2	O1	C36	-175.2(5)
SM2	CL1	SM1	CL2	0.0(1)	CL1	SM2	N3	C5	-89(1)
SM2	CL1	SM1	O2	179.3(2)	CL1	SM2	N3	C39	87(2)
SM2	CL1	SM1	N1	-96.5(5)	CL1	SM2	N4	C6	-58(1)
SM2	CL1	SM1	N2	92.8(6)	CL1	SM2	N4	C7	115(2)
SM2	CL2	SM1	CL1	0.0(1)	CL2	SM1	O2	C22	-19(1)
SM2	CL2	SM1	O2	-2.0(5)	CL2	SM1	O2	C34	-165.5(4)
SM2	CL2	SM1	N1	114.5(3)	CL2	SM1	N1	C1	-101(2)
SM2	CL2	SM1	N2	-123.6(4)	CL2	SM1	N1	C2	54(1)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Torsion or Conformation Angles (cont)

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
CL2	SM1	N2	C3	95.2(9)	N1	C2	C11	C16	161(2)
CL2	SM1	N2	C4	-74(1)	N1	C2	C56	C43	177(1)
CL2	SM2	O1	C20	10.8(8)	N2	SM1	O2	C22	103.7(8)
CL2	SM2	O1	C36	-148.3(6)	N2	SM1	O2	C34	-43.0(5)
CL2	SM2	N3	C5	-7(2)	N2	SM1	N1	C1	153(2)
CL2	SM2	N3	C39	169(2)	N2	SM1	N1	C2	-52(1)
CL2	SM2	N4	C6	-140(1)	N2	C3	C12	C50	-157(2)
CL2	SM2	N4	C7	34(2)	N2	C3	C19	C51	159(1)
O1	SM2	N3	C5	74(1)	N2	C4	C13	C32	-176.4(9)
O1	SM2	N3	C39	-110(2)	N2	C4	C25	C30	148(1)
O1	SM2	N4	C6	132(1)	N3	SM2	O1	C20	-114.5(8)
O1	SM2	N4	C7	-54(2)	N3	SM2	O1	C36	86.4(7)
O1	C20	C21	C38	16(1)	N3	SM2	N4	C6	46(1)
O1	C36	C38	C21	-14(1)	N3	SM2	N4	C7	-141(2)
O2	SM1	N1	C1	61(2)	N3	C5	C10	C28	-157(1)
O2	SM1	N1	C2	-144(1)	N3	C5	C41	C42	161.6(9)
O2	SM1	N2	C3	-67.7(9)	N3	C39	C40	C53	-172(2)
O2	SM1	N2	C4	123(1)	N3	C39	C52	C44	148(1)
O2	C22	C23	C35	-21(1)	N4	SM2	O1	C20	127.1(8)
O2	C34	C35	C23	-57.2(8)	N4	SM2	O1	C36	-32.0(7)
N1	SM1	O2	C22	-137.2(8)	N4	SM2	N3	C5	167(1)
N1	SM1	O2	C34	76.0(5)	N4	SM2	N3	C39	-17(2)
N1	SM1	N2	C3	-157.6(8)	N4	C6	C8	C37	164(1)
N1	SM1	N2	C4	33(2)	N4	C6	C9	C14	-179(1)
N1	C1	C18	C33	176.3(9)	N4	C7	C45	C46	180(1)
N1	C1	C29	C27	-176(1)	N4	C7	C48	C49	-176(1)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

P-1873-M20

Torsion or Conformation Angles (cont)

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
C1	N1	C2	C11	59(2)	C7	C45	C46	C47	53(1)
C1	N1	C2	C56	-85(2)	C7	C48	C49	C47	-56(2)
C1	C18	C33	C26	-63(1)	C8	C6	C9	C14	61(1)
C1	C29	C27	C26	57(1)	C8	C37	C15	C14	-54(1)
C2	N1	C1	C18	101(2)	C9	C6	C8	C37	-81(1)
C2	N1	C1	C29	-144(1)	C9	C14	C15	C37	62(1)
C2	C11	C16	C17	59(3)	C10	C5	N3	C39	-90(1)
C2	C56	C43	C17	-42(2)	C10	C5	C41	C42	-15(1)
C3	N2	C4	C13	107(2)	C10	C28	C57	C42	56.6(8)
C3	N2	C4	C25	-89(2)	C11	C2	C56	C43	25(1)
C3	C12	C50	C24	-52(2)	C11	C16	C17	C43	-43(1)
C3	C19	C51	C24	41(2)	C12	C3	C19	C51	-28(2)
C4	N2	C3	C12	140(2)	C12	C50	C24	C51	63(2)
C4	N2	C3	C19	-51(2)	C13	C4	C25	C30	-50(1)
C4	C13	C32	C31	16(2)	C13	C32	C31	C30	-16(3)
C4	C25	C30	C31	47(2)	C16	C11	C2	C56	-52(3)
C5	N3	C39	C40	-128(1)	C16	C17	C43	C56	54(2)
C5	N3	C39	C52	90(1)	C18	C1	C29	C27	-55(1)
C5	C10	C28	C57	-41(1)	C18	C33	C26	C27	57(1)
C5	C41	C42	C57	31(1)	C19	C3	C12	C50	34(2)
C6	N4	C7	C45	-125(2)	C19	C51	C24	C50	-61(2)
C6	N4	C7	C48	109(2)	C20	O1	C36	C38	22(1)
C6	C8	C37	C15	65(1)	C20	C21	C38	C36	-2(1)
C6	C9	C14	C15	-60(1)	C21	C20	O1	C36	-22(1)
C7	N4	C6	C8	51(2)	C22	O2	C34	C35	51.2(8)
C7	N4	C6	C9	-66(2)	C22	C23	C35	C34	51.9(9)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

P-1873-M21

Torsion or Conformation Angles (cont)

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
C23	C22	O2	C34	-28.6(9)					
C25	C4	C13	C32	18(1)					
C25	C30	C31	C32	-11(2)					
C28	C10	C5	C41	20(1)					
C28	C57	C42	C41	-54.3(9)					
C29	C1	C18	C33	58(1)					
C29	C27	C26	C33	-55(1)					
C39	N3	C5	C41	93(1)					
C39	C40	C53	C54	50(2)					
C39	C52	C44	C54	-5(2)					
C40	C39	C52	C44	2(1)					
C40	C53	C54	C44	-38(1)					
C45	C7	C48	C49	56(1)					
C45	C46	C47	C49	-52(1)					
C46	C45	C7	C48	-56(1)					
C46	C47	C49	C48	53(2)					
C52	C39	C40	C53	-31(2)					
C52	C44	C54	C53	25(2)					

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

P-1873-M22

Table S7 **Complex 2**

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{24}H_{60}SmN_6Li_2Cl_3$
Formula Weight	703.42
Crystal Color, Habit	yellow, cube
Crystal Dimensions (mm)	0.400 X 0.400 X 0.400
Crystal System	triclinic
No. Reflections Used for Unit Cell Determination (2θ range)	23 (39.4 - 43.3°)
Omega Scan Peak Width at Half-height	0.32
Lattice Parameters:	a = 11.552 (1)Å b = 15.483 (1)Å c = 11.330 (1)Å α = 101.69 (1)° β = 106.13 (1)° γ = 88.89 (2)° V = 1904.8 (6)Å^3
Space Group	$P\bar{1}$ (#2)
Z value	2
D_{calc}	1.226 g/cm^3
F_{000}	730
$\mu_{(MoK\alpha)}$	17.78 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC6S
Radiation	MoKα (λ = 0.71069 Å)
Temperature	-145°C
Take-off Angle	6.0°

Detector Aperture	6.0 mm horizontal 6.0 mm vertical
Crystal to Detector Distance	40 cm
Scan Type	ω
Scan Rate	4.0°/min (in omega) (3 rescans)
Scan Width	(1.39 + 0.30 tanθ)°
$2\theta_{max}$	45.0°
No. of Reflections Measured	Total: 4470 Unique: 4171 (R_{int} = .016)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.94 - 1.10)

C. Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w (\|Fo\| - \|Fc\|)^2$
Least-squares Weights	$4Fo^2/\sigma^2(Fo^2)$
p-factor	0.03
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>2.50σ(I)) No. Variables Reflection/Parameter Ratio	3849 315 12.22
Residuals: R; R_w	0.035; 0.047
Goodness of Fit Indicator	2.19
Max Shift/Error in Final Cycle	0.36
Maximum Peak in Final Diff. Map Minimum Peak in Final Diff. Map	0.32 $e^-/Å^3$ -0.44 $e^-/Å^3$

P-1873-M24

Table S8

Positional parameters and B(eq) for 106sg

atom	x	y	z	B(eq)
Sm(1)	0.25423(3)	0.24891(2)	0.39791(3)	2.54(2)
Cl(1)	0.1212(2)	0.3953(1)	0.4473(1)	3.83(7)
Cl(2)	0.3944(2)	0.1088(1)	0.4543(1)	3.52(6)
Cl(3)	0.2952(2)	0.2741(1)	0.6661(1)	4.03(7)
N(1)	0.3794(4)	0.3126(3)	0.3213(4)	3.0(2)
N(2)	0.1016(5)	0.1663(3)	0.2649(5)	3.4(2)
N(3)	0.0199(5)	0.3733(4)	0.7319(5)	4.4(2)
N(4)	0.2168(5)	0.5022(3)	0.7897(5)	3.9(2)
N(5)	0.3931(5)	0.0593(4)	0.7575(5)	4.1(2)
N(6)	0.5952(5)	0.1770(4)	0.7844(5)	4.3(2)
C(1)	0.3171(6)	0.3397(4)	0.2043(6)	3.9(3)
C(2)	0.3703(8)	0.3035(5)	0.0962(7)	5.8(4)
C(3)	0.3037(7)	0.4383(5)	0.2197(6)	4.5(3)
C(4)	0.5061(6)	0.3400(4)	0.3756(7)	4.2(3)
C(5)	0.5289(7)	0.3721(6)	0.5171(8)	6.4(4)
C(6)	0.5912(7)	0.2691(5)	0.349(1)	6.3(4)
C(7)	0.035(1)	0.4683(9)	0.818(1)	6.7(3)
C(8)	0.130(1)	0.5073(7)	0.860(1)	5.9(2)
C(9)	0.0265(9)	0.297(1)	0.783(1)	10.6(8)
C(10)	0.337(1)	0.4960(6)	0.8720(9)	8.6(5)
C(11)	0.0539(8)	0.1309(6)	0.1308(7)	6.3(4)
C(12)	0.0331(7)	0.1367(6)	0.3437(8)	5.8(4)
C(13)	0.310(1)	0.0850(5)	0.8326(8)	6.7(4)
C(14)	0.515(1)	0.0429(7)	0.8249(9)	7.9(5)
C(15)	-0.0961(7)	0.3729(5)	0.6437(7)	4.8(3)
C(16)	0.2140(7)	0.5781(5)	0.7326(7)	5.0(3)
C(17)	0.3462(8)	-0.0238(5)	0.672(1)	6.4(4)
C(18)	0.592(1)	0.1207(7)	0.8755(8)	7.4(4)
C(19)	0.6250(8)	0.2677(6)	0.8530(9)	7.2(4)
C(20)	0.6811(7)	0.1473(6)	0.7136(8)	6.2(4)
C(21)	0.0387(9)	0.0389(7)	0.340(1)	8.5(5)
C(22)	-0.092(1)	0.1697(8)	0.326(1)	7.9(6)
C(23)	-0.012(1)	0.202(1)	0.066(1)	8.8(7)
C(24)	0.152(1)	0.0931(9)	0.081(1)	9.2(6)
Li(1)	0.160(1)	0.3876(6)	0.655(1)	3.2(4)
Li(2)	0.420(1)	0.1533(7)	0.664(1)	3.4(4)
H(1)	0.2347	0.3143	0.1787	4.8
H(2)	0.3678	0.2397	0.0790	6.9
H(3)	0.3265	0.3214	0.0206	6.9
H(4)	0.4522	0.3235	0.1169	6.9
H(5)	0.3823	0.4673	0.2469	5.5
H(6)	0.2618	0.4538	0.1407	5.5
H(7)	0.2611	0.4604	0.2790	5.5
H(8)	0.5226	0.3894	0.3401	5.1
H(9)	0.5115	0.3273	0.5556	7.6
H(10)	0.6122	0.3929	0.5577	7.6
H(11)	0.4800	0.4222	0.5358	7.6
H(12)	0.5781	0.2190	0.3829	7.6
H(13)	0.5772	0.2480	0.2594	7.6

P-1873-M25

Positional parameters and B(eq) for 106sg

atom	x	y	z	B(eq)
H(14)	0.6735	0.2884	0.3835	7.6
H(15)	-0.0316	0.4901	0.7954	17.8
H(16)	0.0292	0.4395	0.9001	17.8
H(17)	0.1671	0.5018	0.9418	10.7
H(18)	0.0948	0.5651	0.8609	10.7
H(19)	-0.0367	0.2890	0.8190	13.9
H(20)	0.0146	0.2415	0.7112	13.9
H(21)	0.1015	0.2888	0.8379	13.9
H(22)	0.3434	0.4458	0.9093	9.4
H(23)	0.3963	0.4898	0.8232	9.4
H(24)	0.3614	0.5477	0.9359	9.4
H(25)	-0.0057	0.0832	0.1208	7.7
H(26)	0.0761	0.1624	0.4291	7.3
H(27)	0.3369	0.1396	0.8916	8.2
H(28)	0.2305	0.0937	0.7809	8.2
H(29)	0.3018	0.0413	0.8793	8.2
H(30)	0.5160	0.0150	0.8931	9.5
H(31)	0.5539	0.0051	0.7701	9.5
H(32)	-0.1056	0.4251	0.6080	5.8
H(33)	-0.1085	0.3227	0.5745	5.8
H(34)	-0.1602	0.3707	0.6819	5.8
H(35)	0.2346	0.6319	0.7973	5.9
H(36)	0.2706	0.5742	0.6850	5.9
H(37)	0.1355	0.5846	0.6799	5.9
H(38)	0.2622	-0.0192	0.6219	7.3
H(39)	0.3907	-0.0419	0.6110	7.3
H(40)	0.3448	-0.0717	0.7134	7.3
H(41)	0.6725	0.1058	0.9139	8.7
H(42)	0.5628	0.1564	0.9420	8.7
H(43)	0.7016	0.2723	0.9143	8.5
H(44)	0.6284	0.3054	0.7959	8.5
H(45)	0.5653	0.2890	0.8941	8.5
H(46)	0.6635	0.0868	0.6701	7.3
H(47)	0.6810	0.1824	0.6540	7.3
H(48)	0.7625	0.1499	0.7691	7.3
H(49)	-0.0051	0.0193	0.3907	9.5
H(50)	0.0054	0.0049	0.2546	9.5
H(51)	0.1209	0.0199	0.3672	9.5
H(52)	-0.0890	0.2340	0.3443	11.7
H(53)	-0.1385	0.1516	0.2391	11.7
H(54)	-0.1331	0.1501	0.3770	11.7
H(55)	0.0429	0.2505	0.0767	14.5
H(56)	-0.0462	0.1802	-0.0221	14.5
H(57)	-0.0764	0.2247	0.1007	14.5
H(58)	0.1885	0.0453	0.1217	12.6
H(59)	0.1225	0.0664	-0.0079	12.6
H(60)	0.2127	0.1355	0.0917	12.6

U values for 106sg

ATOM	U11	U22	U33	U12	U13	U23
Sm(1)	0.0303(2)	0.0385(2)	0.0258(2)	0.0052(2)	0.0063(1)	0.0051(1)
Cl(1)	0.055(1)	0.057(1)	0.0373(9)	0.0254(9)	0.0156(8)	0.0163(8)
Cl(2)	0.053(1)	0.045(1)	0.0353(8)	0.0170(8)	0.0146(8)	0.0064(7)
Cl(3)	0.063(1)	0.055(1)	0.0320(8)	0.029(1)	0.0109(8)	0.0082(7)
N(1)	0.033(3)	0.040(3)	0.040(3)	0.001(3)	0.010(3)	0.008(2)
N(2)	0.039(3)	0.053(3)	0.037(3)	0.002(3)	0.007(3)	0.009(3)
N(3)	0.033(4)	0.084(4)	0.056(4)	-0.005(3)	0.013(3)	0.027(3)
N(4)	0.057(4)	0.049(3)	0.042(3)	-0.001(3)	0.017(3)	0.008(3)
N(5)	0.053(4)	0.060(4)	0.050(3)	0.012(3)	0.026(3)	0.018(3)
N(6)	0.049(4)	0.050(4)	0.053(4)	0.004(3)	0.001(3)	0.006(3)
C(1)	0.053(5)	0.049(4)	0.043(4)	-0.002(4)	0.013(4)	0.006(3)
C(2)	0.107(7)	0.069(5)	0.045(4)	-0.002(5)	0.031(5)	-0.002(4)
C(3)	0.070(5)	0.055(4)	0.050(4)	0.011(4)	0.015(4)	0.020(3)
C(4)	0.038(5)	0.048(4)	0.074(5)	-0.001(4)	0.008(4)	0.021(4)
C(5)	0.063(6)	0.080(6)	0.074(6)	-0.013(5)	-0.015(5)	0.004(5)
C(6)	0.054(5)	0.068(5)	0.135(8)	0.014(4)	0.039(5)	0.043(5)
C(7)	0.085(4)					
C(8)	0.075(3)					
C(9)	0.035(6)	0.26(2)	0.18(1)	0.049(8)	0.047(8)	0.20(1)
C(10)	0.14(1)	0.067(6)	0.073(6)	0.008(6)	-0.036(6)	0.003(5)
C(11)	0.093(7)	0.089(6)	0.046(5)	-0.047(5)	0.002(5)	0.004(4)
C(12)	0.067(6)	0.089(6)	0.064(5)	-0.013(5)	0.018(5)	0.011(5)
C(13)	0.135(8)	0.063(5)	0.078(6)	0.013(5)	0.066(6)	0.010(4)
C(14)	0.092(8)	0.14(1)	0.080(7)	0.007(7)	0.001(6)	0.071(7)
C(15)	0.048(5)	0.068(5)	0.066(5)	0.010(4)	0.014(4)	0.017(4)
C(16)	0.066(5)	0.051(4)	0.074(5)	-0.003(4)	0.015(4)	0.021(4)
C(17)	0.099(7)	0.038(4)	0.128(8)	0.005(4)	0.071(6)	0.012(5)
C(18)	0.094(7)	0.099(7)	0.071(6)	0.009(6)	-0.019(5)	0.036(5)
C(19)	0.076(6)	0.076(6)	0.085(6)	0.001(5)	-0.014(5)	-0.020(5)
C(20)	0.044(5)	0.090(6)	0.081(6)	0.008(5)	-0.003(5)	-0.005(5)
C(21)	0.093(8)	0.13(1)	0.105(8)	-0.033(7)	0.013(6)	0.064(7)
C(22)	0.051(7)	0.098(9)	0.15(1)	-0.023(6)	0.060(8)	-0.027(8)
C(23)	0.072(9)	0.17(1)	0.074(8)	-0.07(1)	-0.065(7)	0.09(1)
C(24)	0.12(1)	0.16(1)	0.063(7)	-0.09(1)	0.070(8)	-0.065(7)
Li(1)	0.048(7)	0.033(5)	0.039(6)	0.003(5)	0.012(5)	0.006(4)

U values for 106sg

ATOM	U11	U22	U33	U12	U13	U23
Li(2)	0.043(7)	0.047(6)	0.039(6)	0.009(5)	0.008(5)	0.013(5)
H(1)	0.0614					
H(2)	0.0877					
H(3)	0.0877					
H(4)	0.0877					
H(5)	0.0701					
H(6)	0.0701					
H(7)	0.0701					
H(8)	0.0650					
H(9)	0.0966					
H(10)	0.0966					
H(11)	0.0966					
H(12)	0.0964					
H(13)	0.0964					
H(14)	0.0964					
H(15)	0.2260					
H(16)	0.2260					
H(17)	0.1355					
H(18)	0.1355					
H(19)	0.1761					
H(20)	0.1761					
H(21)	0.1761					
H(22)	0.1186					
H(23)	0.1186					
H(24)	0.1186					
H(25)	0.0972					
H(26)	0.0919					
H(27)	0.1034					
H(28)	0.1034					
H(29)	0.1034					
H(30)	0.1197					
H(31)	0.1197					
H(32)	0.0735					
H(33)	0.0735					
H(34)	0.0735					
H(35)	0.0746					

U values for 106sg

ATOM	U11	U22	U33	U12	U13	U23
H(36)	0.0746					
H(37)	0.0746					
H(38)	0.0922					
H(39)	0.0922					
H(40)	0.0922					
H(41)	0.1099					
H(42)	0.1099					
H(43)	0.1070					
H(44)	0.1070					
H(45)	0.1070					
H(46)	0.0920					
H(47)	0.0920					
H(48)	0.0920					
H(49)	0.1198					
H(50)	0.1198					
H(51)	0.1198					
H(52)	0.1477					
H(53)	0.1477					
H(54)	0.1477					
H(55)	0.1840					
H(56)	0.1840					
H(57)	0.1840					
H(58)	0.1596					
H(59)	0.1596					
H(60)	0.1596					

P-1873-M28

P-1873-M29

Table S10
Intramolecular Distances Involving the Nonhydrogen Atoms

atom	atom	distance	atom	atom	distance
SM1	CL1	2.764(2)	N4	LI1	2.07(1)
SM1	CL2	2.754(2)	N5	C13	1.45(1)
SM1	CL3	2.888(2)	N5	C14	1.45(1)
SM1	N1	2.218(5)	N5	C17	1.454(9)
SM1	N2	2.202(5)	N5	LI2	2.04(1)
CL1	LI1	2.29(1)	N6	C18	1.49(1)
CL2	LI2	2.28(1)	N6	C19	1.457(9)
CL3	LI1	2.33(1)	N6	C20	1.45(1)
CL3	LI2	2.34(1)	N6	LI2	2.10(1)
N1	C1	1.462(8)	C1	C2	1.52(1)
N1	C4	1.455(8)	C1	C3	1.511(9)
N2	C11	1.457(9)	C4	C5	1.53(1)
N2	C12	1.48(1)	C4	C6	1.50(1)
N3	C7	1.58(1)	C7	C8	1.19(2)
N3	C9	1.41(1)	C11	C23	1.52(1)
N3	C15	1.431(9)	C11	C24	1.46(1)
N3	LI1	2.08(1)	C12	C21	1.51(1)
N4	C8	1.44(1)	C12	C22	1.49(1)
N4	C10	1.45(1)	C14	C18	1.43(1)
N4	C16	1.449(9)			

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

P-1873-M30

Table S11
Intramolecular Bond Angles Involving the Nonhydrogen Atoms

atom	atom	atom	angle	atom	atom	atom	angle
CL1	SM1	CL2	155.69(5)	C15	N3	LI1	112.4(5)
CL1	SM1	CL3	78.08(5)	C8	N4	C10	109.7(7)
CL1	SM1	N1	97.0(1)	C8	N4	C16	111.5(6)
CL1	SM1	N2	95.7(1)	C8	N4	LI1	102.3(6)
CL2	SM1	CL3	77.74(4)	C10	N4	C16	109.7(6)
CL2	SM1	N1	97.1(1)	C10	N4	LI1	112.4(5)
CL2	SM1	N2	94.9(1)	C16	N4	LI1	111.2(5)
CL3	SM1	N1	119.9(1)	C13	N5	C14	116.2(7)
CL3	SM1	N2	121.7(1)	C13	N5	C17	107.3(6)
N1	SM1	N2	118.3(2)	C13	N5	LI2	113.1(5)
SM1	CL1	LI1	92.2(2)	C14	N5	C17	105.6(7)
SM1	CL2	LI2	93.1(3)	C14	N5	LI2	102.5(6)
SM1	CL3	LI1	88.5(2)	C17	N5	LI2	111.9(5)
SM1	CL3	LI2	88.5(3)	C18	N6	C19	108.5(7)
LI1	CL3	LI2	175.5(4)	C18	N6	C20	112.1(6)
SM1	N1	C1	112.1(4)	C18	N6	LI2	100.7(6)
SM1	N1	C4	130.6(4)	C19	N6	C20	110.5(7)
C1	N1	C4	116.9(5)	C19	N6	LI2	115.5(5)
SM1	N2	C11	140.0(5)	C20	N6	LI2	109.3(5)
SM1	N2	C12	105.4(4)	N1	C1	C2	113.7(6)
C11	N2	C12	114.5(6)	N1	C1	C3	113.2(5)
C7	N3	C9	121.1(9)	C2	C1	C3	111.1(6)
C7	N3	C15	104.0(7)	N1	C4	C5	108.4(6)
C7	N3	LI1	96.7(6)	N1	C4	C6	113.8(6)
C9	N3	C15	108.6(7)	C5	C4	C6	110.1(7)
C9	N3	LI1	113.3(6)	N3	C7	C8	122(1)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

P-1873-M31

Intramolecular Bond Angles Involving the Nonhydrogen Atoms (cont)

atom	atom	atom	angle	atom	atom	atom	angle
N4	C8	C7	122(1)				
N2	C11	C23	109.7(8)				
N2	C11	C24	109.3(8)				
C23	C11	C24	114(1)				
N2	C12	C21	113.0(7)				
N2	C12	C22	114.8(8)				
C21	C12	C22	113.2(8)				
N5	C14	C18	114.2(8)				
N6	C18	C14	115.1(7)				
CL1	LI1	CL3	100.8(4)				
CL1	LI1	N3	120.7(5)				
CL1	LI1	N4	118.4(5)				
CL3	LI1	N3	114.1(5)				
CL3	LI1	N4	115.2(5)				
N3	LI1	N4	88.6(4)				
CL2	LI2	CL3	100.3(4)				
CL2	LI2	N5	116.6(5)				
CL2	LI2	N6	118.7(5)				
CL3	LI2	N5	117.6(5)				
CL3	LI2	N6	115.7(5)				
N5	LI2	N6	89.1(4)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

P-1873-M32

Table S12
Torsion or Conformation Angles

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
SM1	CL1	LI1	CL3	5.7(3)	CL1	SM1	N2	C12	-76.7(4)
SM1	CL1	LI1	N3	-121.0(5)	CL1	LI1	CL3	LI2	-53(5)
SM1	CL1	LI1	N4	132.2(5)	CL1	LI1	N3	C7	-110.6(7)
SM1	CL2	LI2	CL3	4.6(3)	CL1	LI1	N3	C9	121.3(9)
SM1	CL2	LI2	N5	132.8(5)	CL1	LI1	N3	C15	-2.4(8)
SM1	CL2	LI2	N6	-122.4(5)	CL1	LI1	N4	C8	124.6(6)
SM1	CL3	LI1	CL1	-5.4(3)	CL1	LI1	N4	C10	-117.8(7)
SM1	CL3	LI1	N3	125.5(4)	CL1	LI1	N4	C16	5.6(8)
SM1	CL3	LI1	N4	-134.1(5)	CL2	SM1	CL1	LI1	1.3(3)
SM1	CL3	LI2	CL2	-4.4(3)	CL2	SM1	CL3	LI1	-173.0(3)
SM1	CL3	LI2	N5	-131.9(5)	CL2	SM1	CL3	LI2	3.7(3)
SM1	CL3	LI2	N6	124.7(5)	CL2	SM1	N1	C1	134.7(4)
SM1	N1	C1	C2	-125.7(5)	CL2	SM1	N1	C4	-53.5(5)
SM1	N1	C1	C3	106.3(5)	CL2	SM1	N2	C11	-94.9(8)
SM1	N1	C4	C5	-34.6(8)	CL2	SM1	N2	C12	81.4(4)
SM1	N1	C4	C6	88.3(7)	CL2	LI2	CL3	LI1	43(5)
SM1	N2	C11	C23	-79(1)	CL2	LI2	N5	C13	-128.5(6)
SM1	N2	C11	C24	47(1)	CL2	LI2	N5	C14	105.6(7)
SM1	N2	C12	C21	-112.4(6)	CL2	LI2	N5	C17	-7.1(8)
SM1	N2	C12	C22	115.7(7)	CL2	LI2	N6	C18	-126.9(6)
CL1	SM1	CL2	LI2	-9.7(3)	CL2	LI2	N6	C19	116.4(7)
CL1	SM1	CL3	LI1	4.5(3)	CL2	LI2	N6	C20	-8.8(8)
CL1	SM1	CL3	LI2	-178.8(3)	CL3	SM1	CL1	LI1	-4.6(3)
CL1	SM1	N1	C1	-65.1(4)	CL3	SM1	CL2	LI2	-3.8(3)
CL1	SM1	N1	C4	106.6(5)	CL3	SM1	N1	C1	-145.4(3)
CL1	SM1	N2	C11	107.0(8)	CL3	SM1	N1	C4	26.4(6)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

P-1873 M33

Torsion or Conformation Angles (cont)

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
CL3	SM1	N2	C11	-173.5(7)	N3	C7	C8	N4	36(2)
CL3	SM1	N2	C12	2.8(5)	N3	LI1	CL3	LI2	78(5)
CL3	LI1	N3	C7	129.1(7)	N3	LI1	N4	C8	0.1(6)
CL3	LI1	N3	C9	1(1)	N3	LI1	N4	C10	117.7(7)
CL3	LI1	N3	C15	-122.7(6)	N3	LI1	N4	C16	-119.0(5)
CL3	LI1	N4	C8	-116.0(6)	N4	LI1	CL3	LI2	178(4)
CL3	LI1	N4	C10	1.5(8)	N4	LI1	N3	C7	12.0(6)
CL3	LI1	N4	C16	124.9(6)	N4	LI1	N3	C9	-116.1(9)
CL3	LI2	N5	C13	-9.2(8)	N4	LI1	N3	C15	120.2(6)
CL3	LI2	N5	C14	-135.1(7)	N5	C14	C18	N6	-51(1)
CL3	LI2	N5	C17	112.1(6)	N5	LI2	CL3	LI1	-84(5)
CL3	LI2	N6	C18	113.7(6)	N5	LI2	N6	C18	-6.7(6)
CL3	LI2	N6	C19	-3.0(8)	N5	LI2	N6	C19	-123.4(7)
CL3	LI2	N6	C20	-128.2(6)	N5	LI2	N6	C20	111.4(6)
N1	SM1	CL1	LI1	-123.8(3)	N6	LI2	CL3	LI1	172(4)
N1	SM1	CL2	LI2	115.4(3)	N6	LI2	N5	C13	109.5(6)
N1	SM1	CL3	LI1	95.8(3)	N6	LI2	N5	C14	-16.4(6)
N1	SM1	CL3	LI2	-87.6(3)	N6	LI2	N5	C17	-129.1(5)
N1	SM1	N2	C11	5.9(8)	C1	N1	C4	C5	136.8(6)
N1	SM1	N2	C12	-177.8(4)	C1	N1	C4	C6	-100.3(7)
N2	SM1	CL1	LI1	116.7(3)	C2	C1	N1	C4	61.3(8)
N2	SM1	CL2	LI2	-125.2(3)	C3	C1	N1	C4	-66.7(7)
N2	SM1	CL3	LI1	-84.8(3)	C7	C8	N4	C10	-139(1)
N2	SM1	CL3	LI2	91.8(3)	C7	C8	N4	C16	100(1)
N2	SM1	N1	C1	35.2(4)	C7	C8	N4	LI1	-19(1)
N2	SM1	N1	C4	-153.0(5)	C8	C7	N3	C9	93(1)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

P-1873-M34

Torsion or Conformation Angles (cont)

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
C8	C7	N3	C15	-144(1)					
C8	C7	N3	LI1	-29(1)					
C11	N2	C12	C21	65.0(9)					
C11	N2	C12	C22	-67(1)					
C12	N2	C11	C23	104.4(8)					
C12	N2	C11	C24	-129.6(8)					
C13	N5	C14	C18	-84.7(9)					
C14	C18	N6	C19	152.6(9)					
C14	C18	N6	C20	-85(1)					
C14	C18	N6	LI2	31(1)					
C17	N5	C14	C18	156.5(8)					
C18	C14	N5	LI2	39.1(9)					

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Table S13 **Complex 3** 38

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{80}H_{148}Cl_6Sm_4N_6O_2$
Formula Weight	2040.41
Crystal Color, Habit	orange, plates
Crystal Dimensions (mm)	0.100 X 0.200 X 0.300
Crystal System	triclinic
No. Reflections Used for Unit Cell Determination (2θ range)	4 (28.4 - 31.0°)
Omega Scan Peak Width at Half-height	0.31
Lattice Parameters:	
	a = 16.508 (1)Å
	b = 16.7795 (9)Å
	c = 16.4030 (8)Å
	α = 89.794 (1)°
	β = 88.688 (2)°
	γ = 79.531 (1)°
	V = 4466.8 (7)Å^3
Space Group	$P\bar{1}$ (#2)
Z value	2
D_{calc}	1.517 g/cm^3
F_{000}	2072
$\mu_{(MoK\alpha)}$	28.26 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC6S
Radiation	MoKα (λ = 0.71069 Å)
Temperature	-140°C
Take-off Angle	6.0°

P-1873-M36

Detector Aperture	6.0 mm horizontal 6.0 mm vertical
Crystal to Detector Distance	40 cm
Scan Type	ω-2θ
Scan Rate	4.0°/min (in omega) (3 rescans)
Scan Width	(1.26 + 0.30 tanθ)°
$2\theta_{max}$	45.5°
No. of Reflections Measured	Total: 9493 Unique: 8987 (R_{int} = .088)
Corrections	Lorentz-polarization

C. Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares
Function Minimized	Σ w (|Fo| - |Fc|)^2
Least-squares Weights	$4Fo^2/\sigma^2(Fo^2)$
p-factor	0.03
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>2.50σ(I))	6409
No. Variables	833
Reflection/Parameter Ratio	7.69
Residuals: R; R_w	0.062; 0.078
Goodness of Fit Indicator	2.61
Max Shift/Error in Final Cycle	0.83
Maximum Peak in Final Diff. Map	1.97 $e^-/Å^3$
Minimum Peak in Final Diff. Map	-1.78 $e^-/Å^3$

 P-1813-M37

Table S14

Positional parameters and B(eq) for 84sg

atom	x	y	z	B(eq)
Sm(1)	0.95774(6)	1.26091(6)	0.27774(6)	2.98(6)
Sm(2)	0.73418(6)	1.37971(6)	0.28113(6)	2.75(6)
Sm(3)	0.60880(7)	1.18283(6)	0.24660(7)	3.44(7)
Sm(4)	0.80635(7)	1.21103(6)	0.08324(6)	3.20(6)
Cl(1)	0.8094(3)	1.1975(3)	0.2665(3)	3.2(3)
Cl(2)	0.6614(3)	1.3131(3)	0.1458(3)	3.7(3)
Cl(3)	0.6210(3)	1.3072(3)	0.3598(3)	3.8(3)
Cl(4)	0.6875(3)	1.1142(3)	0.1046(3)	4.2(3)
Cl(5)	0.9737(3)	1.1810(3)	0.1244(3)	4.0(3)
Cl(6)	0.8495(3)	1.3614(3)	0.1554(3)	3.5(3)
O(1)	1.0679(8)	1.3151(9)	0.2056(8)	4(1)
O(2)	0.8655(9)	1.0728(8)	0.0391(8)	5(1)
N(1)	0.869(1)	1.3648(9)	0.3579(9)	3(1)
N(2)	1.040(1)	1.182(1)	0.359(1)	4(1)
N(3)	0.483(1)	1.210(1)	0.214(1)	5(1)
N(4)	0.676(1)	1.502(1)	0.266(1)	4(1)
N(5)	0.810(1)	1.257(1)	-0.040(1)	4(1)
N(6)	0.630(1)	1.072(1)	0.324(1)	5(1)
C(1)	1.026(1)	1.103(1)	0.336(1)	4(1)
C(2)	0.981(1)	1.060(1)	0.397(1)	5(1)
C(3)	0.960(2)	0.980(1)	0.364(1)	5(2)
C(4)	1.036(2)	0.924(1)	0.336(2)	6(2)
C(5)	1.080(2)	0.964(1)	0.270(1)	6(2)
C(6)	1.098(1)	1.047(1)	0.298(1)	4(1)
C(7)	0.921(1)	1.425(1)	0.343(1)	3(1)
C(8)	0.882(1)	1.515(1)	0.348(1)	5(1)
C(9)	0.935(2)	1.570(1)	0.317(1)	5(2)
C(10)	1.018(2)	1.558(1)	0.354(1)	5(1)
C(11)	1.062(1)	1.470(1)	0.353(1)	5(2)
C(12)	1.002(1)	1.416(1)	0.382(1)	4(1)
C(13)	0.433(2)	1.357(2)	0.186(2)	10(2)
C(14)	0.420(2)	1.287(2)	0.221(1)	6(2)
C(15)	0.382(1)	1.301(2)	0.306(1)	6(2)
C(16)	0.317(2)	1.378(2)	0.320(2)	9(2)
C(17)	0.334(2)	1.444(2)	0.275(2)	9(3)
C(18)	0.621(1)	1.543(2)	0.327(1)	6(2)
C(19)	0.541(2)	1.535(2)	0.334(3)	13(3)
C(20)	0.648(1)	1.611(1)	0.374(1)	5(1)
C(21)	0.590(2)	1.647(3)	0.436(2)	13(3)
C(22)	0.867(2)	1.287(1)	-0.095(1)	5(2)
C(23)	0.906(2)	1.353(2)	-0.057(1)	8(2)
C(24)	0.971(2)	1.379(2)	-0.110(2)	8(2)
C(25)	1.032(2)	1.310(2)	-0.134(2)	10(3)
C(26)	0.999(2)	1.248(2)	-0.177(2)	8(2)
C(27)	0.934(2)	1.219(2)	-0.126(1)	6(2)
C(28)	1.052(1)	1.373(1)	0.140(1)	6(2)
C(29)	1.133(2)	1.370(2)	0.100(1)	6(2)
C(30)	1.170(1)	1.283(1)	0.104(1)	5(2)
C(31)	1.144(1)	1.262(1)	0.191(1)	5(1)

P-1873-M38

Positional parameters and B(eq) for 84sg

atom	x	y	z	B(eq)
C(32)	0.850(1)	1.359(1)	0.445(1)	3(1)
C(33)	0.774(1)	1.414(1)	0.476(1)	4(1)
C(34)	0.759(1)	1.407(2)	0.567(1)	5(2)
C(35)	0.757(1)	1.324(1)	0.590(1)	5(2)
C(36)	0.843(1)	1.275(1)	0.470(1)	4(1)
C(37)	0.830(1)	1.267(1)	0.562(1)	5(1)
C(38)	1.100(1)	1.178(1)	0.429(1)	3(1)
C(39)	1.063(1)	1.216(1)	0.509(1)	4(1)
C(40)	1.125(1)	1.212(1)	0.575(1)	5(2)
C(41)	1.194(2)	1.250(2)	0.553(1)	6(2)
C(42)	1.237(1)	1.206(2)	0.477(2)	6(2)
C(43)	1.175(1)	1.212(1)	0.409(1)	5(2)
C(44)	0.675(2)	1.544(2)	0.188(2)	8(2)
C(45)	0.740(2)	1.594(1)	0.172(1)	6(2)
C(46)	0.738(2)	1.635(2)	0.092(2)	7(2)
C(47)	0.692(2)	1.612(2)	0.027(2)	10(3)
C(48)	0.628(2)	1.523(1)	0.120(2)	7(2)
C(49)	0.509(2)	1.640(2)	0.437(2)	11(3)
C(50)	0.483(2)	1.575(2)	0.400(2)	7(2)
C(51)	0.628(2)	1.567(2)	0.041(1)	6(2)
C(52)	0.373(2)	1.434(1)	0.194(2)	6(2)
C(53)	0.889(2)	1.012(1)	0.099(2)	6(2)
C(54)	0.844(2)	1.035(2)	-0.034(2)	6.3(6)
C(55)	0.860(2)	0.946(1)	-0.016(2)	9(2)
C(56)	0.374(3)	1.066(3)	0.067(3)	13(1)
C(57)	0.453(2)	1.153(2)	0.159(2)	10(3)
C(58)	0.638(2)	0.994(2)	0.284(1)	6(2)
C(59)	0.642(2)	1.065(2)	0.413(2)	9(3)
C(60)	0.726(1)	1.261(1)	-0.070(1)	4(1)
C(61)	0.719(2)	1.210(2)	-0.151(1)	7(2)
C(62)	0.630(2)	1.207(2)	-0.175(2)	8(2)
C(63)	0.583(2)	1.289(2)	-0.184(2)	9(2)
C(64)	0.587(2)	1.341(2)	-0.108(2)	9(2)
C(65)	0.871(4)	0.938(2)	0.067(3)	18(4)
C(66)	0.389(2)	1.116(2)	0.193(4)	17(4)
C(67)	0.565(3)	1.108(2)	0.458(2)	16(4)
C(68)	0.679(2)	1.343(2)	-0.083(1)	5(2)
C(69)	0.565(3)	0.956(2)	0.300(3)	15(4)
C(70)	0.719(2)	0.945(2)	0.273(2)	8(2)
C(71)	0.719(3)	0.865(2)	0.216(2)	13(3)
C(72)	0.728(2)	1.078(2)	0.440(2)	9(2)
C(73)	0.654(3)	0.829(3)	0.240(2)	12(1)
C(74)	0.575(3)	0.875(3)	0.247(3)	15(1)
C(75)	0.367(3)	1.039(3)	0.145(4)	17(2)
C(76)	0.450(2)	1.180(2)	0.069(2)	12(1)
C(77)	0.425(3)	1.109(3)	0.002(3)	15(1)
C(78)	0.589(2)	1.100(2)	0.558(2)	12(1)
C(79)	0.751(2)	1.065(2)	0.530(2)	10(1)
C(80)	0.678(2)	1.101(2)	0.577(2)	11(1)
H(1)	1.0162	1.0468	0.4430	6.1

P-1873-M39

Positional parameters and B(eq) for 84sg

atom	x	y	z	B(eq)
H(2)	0.9325	1.0945	0.4137	6.1
H(3)	0.9341	0.9530	0.4052	5.9
H(4)	0.9236	0.9916	0.3192	5.9
H(5)	1.0734	0.9114	0.3787	7.0
H(6)	1.0238	0.8757	0.3132	7.0
H(7)	1.1326	0.9297	0.2521	6.8
H(8)	1.0483	0.9736	0.2204	6.8
H(9)	1.1215	1.0732	0.2527	5.4
H(10)	1.1413	1.0354	0.3380	5.4
H(11)	0.9338	1.4202	0.2841	4.0
H(12)	0.8304	1.5260	0.3200	5.9
H(13)	0.8684	1.5284	0.4054	5.9
H(14)	0.9424	1.5635	0.2598	6.1
H(15)	0.9088	1.6263	0.3271	6.1
H(16)	1.0528	1.5909	0.3265	5.0
H(17)	1.0134	1.5751	0.4104	5.0
H(18)	1.0807	1.4561	0.2967	6.5
H(19)	1.1109	1.4631	0.3848	6.5
H(20)	0.9956	1.4232	0.4390	5.3
H(21)	1.0316	1.3595	0.3732	5.3
H(22)	0.4819	1.3694	0.2116	10.5
H(23)	0.4441	1.3501	0.1299	10.5
H(24)	0.3705	1.2778	0.1887	6.6
H(25)	0.3579	1.2544	0.3219	6.7
H(26)	0.4261	1.3033	0.3423	6.7
H(27)	0.2644	1.3655	0.3033	10.1
H(28)	0.3119	1.3889	0.3775	10.1
H(29)	0.2836	1.4837	0.2712	10.8
H(30)	0.3704	1.4704	0.3087	10.8
H(31)	0.6370	1.5030	0.3690	7.4
H(32)	0.5135	1.5584	0.2800	13.6
H(33)	0.5353	1.4782	0.3286	13.6
H(34)	0.7013	1.5926	0.3981	5.7
H(35)	0.6559	1.6544	0.3364	5.7
H(36)	0.6121	1.6246	0.4894	14.1
H(37)	0.5924	1.7048	0.4406	14.1
H(38)	0.8379	1.3085	-0.1444	6.7
H(39)	0.8645	1.3992	-0.0456	8.9
H(40)	0.9299	1.3330	-0.0063	8.9
H(41)	0.9485	1.4026	-0.1594	9.4
H(42)	0.9988	1.4159	-0.0835	9.4
H(43)	1.0782	1.3219	-0.1690	10.6
H(44)	1.0614	1.2805	-0.0872	10.6
H(45)	0.9730	1.2706	-0.2274	9.0
H(46)	1.0390	1.2005	-0.1952	9.0
H(47)	0.9576	1.1893	-0.0798	7.0
H(48)	0.9071	1.1796	-0.1565	7.0
H(49)	1.0141	1.3589	0.1022	6.9
H(50)	1.0335	1.4262	0.1593	6.9
H(51)	1.1281	1.3842	0.0436	7.2

P-1873-M40

Positional parameters and B(eq) for 84sg

atom	x	y	z	B(eq)
H(52)	1.1657	1.4004	0.1264	7.2
H(53)	1.1504	1.2493	0.0649	6.2
H(54)	1.2300	1.2731	0.0981	6.2
H(55)	1.1867	1.2686	0.2275	5.3
H(56)	1.1395	1.2049	0.1924	5.3
H(57)	0.8961	1.3729	0.4752	4.2
H(58)	0.7771	1.4699	0.4638	4.3
H(59)	0.7269	1.4017	0.4495	4.3
H(60)	0.8030	1.4252	0.5956	5.5
H(61)	0.7085	1.4436	0.5835	5.5
H(62)	0.7489	1.3216	0.6503	6.1
H(63)	0.7065	1.3094	0.5691	6.1
H(64)	0.7964	1.2591	0.4440	5.4
H(65)	0.8911	1.2365	0.4536	5.4
H(66)	0.8770	1.2810	0.5889	5.9
H(67)	0.8256	1.2133	0.5769	5.9
H(68)	1.1211	1.1199	0.4407	3.9
H(69)	1.0384	1.2719	0.4964	4.6
H(70)	1.0174	1.1897	0.5251	4.6
H(71)	1.0975	1.2407	0.6239	5.9
H(72)	1.1439	1.1580	0.5908	5.9
H(73)	1.1760	1.3071	0.5386	6.7
H(74)	1.2330	1.2485	0.5949	6.7
H(75)	1.2839	1.2325	0.4593	7.6
H(76)	1.2590	1.1523	0.4892	7.6
H(77)	1.2029	1.1836	0.3590	6.0
H(78)	1.1580	1.2674	0.3908	6.0
H(79)	0.6310	1.5930	0.2059	9.0
H(80)	0.7358	1.6345	0.2157	7.0
H(81)	0.7902	1.5582	0.1770	7.0
H(82)	0.7113	1.6931	0.0997	8.4
H(83)	0.7910	1.6351	0.0715	8.4
H(84)	0.6703	1.6585	-0.0063	10.7
H(85)	0.7326	1.5773	-0.0090	10.7
H(86)	0.6432	1.4673	0.1131	8.4
H(87)	0.5677	1.5312	0.1411	8.4
H(88)	0.4886	1.6420	0.4940	12.3
H(89)	0.4792	1.6883	0.4117	12.3
H(90)	0.4278	1.5906	0.3820	7.9
H(91)	0.4816	1.5329	0.4418	7.9
H(92)	0.5741	1.6041	0.0343	7.6
H(93)	0.6276	1.5267	-0.0029	7.6
H(94)	0.3985	1.4793	0.1815	7.5
H(95)	0.3300	1.4329	0.1559	7.5
H(96)	0.9496	1.0030	0.1086	7.9
H(97)	0.8627	1.0218	0.1499	7.9
H(98)	0.7875	1.0560	-0.0501	8.6
H(99)	0.8773	1.0506	-0.0826	8.6
H(100)	0.8149	0.9241	-0.0409	9.9
H(101)	0.9087	0.9222	-0.0523	9.9