Inorganic Chemistry
including bioinorganic chemistry
Inorg. Chem., 1996, 35(8), 2163-2164, DOI:10.1021/ic950674o

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EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{45}H_{97}N_8Si_6Y_2O_4Li_3$
Formula Weight	1181.46
Crystal Color, Habit	clear, prism
Crystal Dimensions (mm)	0.200 X 0.200 X 0.500
Crystal System	triclinic
No. Reflections Used for Unit Cell Determination (2θ range)	14 (6.9 - 13.4°)
Omega Scan Peak Width at Half-height	0.47
Lattice Parameters:	
	a = 15.90 (1)Å
	b = 17.59 (2)Å
	c = 13.32 (2)Å
	α = 104.27 (8)°
	β = 94.25 (9)°
	γ = 109.84 (7)°
	V = 3343 (6)Å^3
Space Group	$P\bar{1}$ (#2)
Z value	2
D_{calc}	1.173 g/cm^3
F_{000}	1252
$\mu_{(MoK\alpha)}$	18.81 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC6S
Radiation	MoKα (λ = 0.71069 Å)
Temperature	-120°C
Take-off Angle	6.0°

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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) (2 rescans)
Scan Width	(1.31 + 0.30 tanθ)°
$2\theta_{max}$	50.0°
No. of Reflections Measured	Total: 10006 Unique: 9544 (R_{int} = .155)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.92 - 1.00) Decay (-1.30% decline)

C. Structure Solution and Refinement

Structure Solution	Direct Methods
Hydrogen Atom Treatment	Included in calculated positions (d_{C-H} = 0.95Å)
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>5.00σ(I)) No. Variables Reflection/Parameter Ratio	2509 313 8.02
Residuals: R; R_w	0.097; 0.131
Goodness of Fit Indicator	3.38
Max Shift/Error in Final Cycle	1.52
Maximum Peak in Final Diff. Map Minimum Peak in Final Diff. Map	1.63 $e^-/Å^3$ -0.82 $e^-/Å^3$

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Positional parameters for YAMIDE2 M.Tillotson / H.C.Aspinall.

atom	x	y	z	occupancy
Y(1)	0.3155(3)	0.2077(2)	0.2022(3)	
Y(2)	0.5951(2)	0.2230(2)	0.3423(3)	
Si(11)	0.4381(8)	0.4003(8)	0.150(1)	
Si(12)	0.1106(8)	0.2628(8)	0.180(1)	
Si(13)	0.2059(8)	-0.0033(7)	0.237(1)	
Si(21)	0.6665(8)	0.2392(7)	0.0914(9)	
Si(22)	0.5215(7)	0.2373(7)	0.5962(9)	
Si(23)	0.9259(8)	0.4167(8)	0.781(1)	
O(2)	0.465(1)	0.217(1)	0.276(2)	
O(11)	0.329(2)	0.269(1)	0.377(2)	
O(21)	0.713(1)	0.169(1)	0.374(2)	
O(22)	0.514(2)	0.084(2)	0.306(2)	
N(1)	0.273(2)	0.127(2)	0.011(2)	
N(2)	0.726(2)	0.360(2)	0.434(2)	
N(11)	0.413(2)	0.293(2)	0.107(2)	
N(12)	0.174(2)	0.204(2)	0.146(2)	
N(13)	0.285(2)	0.065(2)	0.186(2)	
N(21)	0.647(2)	0.286(2)	0.214(2)	
N(22)	0.561(2)	0.285(2)	0.504(2)	
N(23)	0.924(2)	0.407(2)	0.651(2)	
C(1)	0.773(3)	0.150(2)	0.300(3)	
C(2)	0.815(4)	0.101(3)	0.344(4)	
C(3)	0.780(5)	0.082(4)	0.428(6)	
C(4)	0.719(3)	0.130(2)	0.454(3)	
C(5)	0.517(2)	0.012(3)	0.303(3)	

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Positional parameters for YAMIDE2 M.Tillotson / H.C.Aspinall.

atom	x	y	z	occupancy
C(6)	0.546(3)	-0.035(3)	0.225(3)	
C(7)	0.327(3)	0.366(3)	0.528(3)	
C(8)	0.291(3)	0.290(3)	0.445(3)	
C(11)	0.340(3)	0.164(2)	-0.048(3)	
C(12)	0.383(2)	0.265(2)	-0.005(3)	
C(13)	0.188(3)	0.136(2)	-0.030(3)	
C(14)	0.128(3)	0.137(3)	0.052(3)	
C(15)	0.256(3)	0.033(3)	-0.002(3)	
C(16)	0.311(3)	0.025(2)	0.089(3)	
C(21)	0.774(2)	0.392(2)	0.354(3)	
C(22)	0.711(3)	0.375(2)	0.254(3)	
C(23)	0.682(2)	0.416(2)	0.484(3)	
C(24)	0.625(2)	0.377(2)	0.555(3)	
C(25)	0.788(2)	0.352(2)	0.512(3)	
C(26)	0.863(2)	0.429(2)	0.582(3)	
C(31)	0.986(3)	0.384(3)	0.604(3)	
C(32)	1.009(3)	0.372(3)	0.502(4)	
C(111)	0.352(3)	0.438(3)	0.107(4)	
C(112)	0.542(3)	0.455(2)	0.104(3)	
C(113)	0.460(3)	0.433(3)	0.289(3)	
C(121)	0.171(3)	0.363(3)	0.290(3)	
C(122)	0.068(3)	0.299(3)	0.082(4)	
C(123)	0.010(3)	0.205(3)	0.224(3)	
C(131)	0.164(3)	0.060(3)	0.338(3)	
C(132)	0.258(3)	-0.068(3)	0.298(3)	

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Positional parameters for YAMIDE2 M.Tillotson / H.C.Aspinall.

atom	x	y	z	occupancy
C(133)	0.108(3)	-0.080(2)	0.137(3)	
C(211)	0.784(2)	0.243(2)	0.083(3)	
C(212)	0.644(3)	0.282(3)	-0.013(3)	
C(213)	0.589(3)	0.122(2)	0.052(3)	
C(221)	0.423(3)	0.142(3)	0.529(3)	
C(222)	0.485(3)	0.299(2)	0.700(3)	
C(223)	0.610(3)	0.214(2)	0.671(3)	
C(231)	0.836(3)	0.445(3)	0.821(3)	
C(232)	0.919(4)	0.323(4)	0.817(4)	
C(233)	1.038(4)	0.505(3)	0.853(4)	
Li(1)	0.450(5)	0.274(5)	0.404(6)	
Li(2)	0.420(6)	0.110(6)	0.261(7)	
Li(3)	0.517(5)	0.264(4)	0.170(5)	
H(1)	0.7397	0.1174	0.2310	
H(2)	0.8188	0.1997	0.2955	
H(3)	0.8015	0.0461	0.2957	
H(4)	0.8784	0.1286	0.3638	
H(5)	0.7526	0.0266	0.4204	
H(6)	0.8325	0.1065	0.4889	
H(7)	0.7429	0.1722	0.5203	
H(8)	0.6623	0.0911	0.4558	
H(9)	0.4987	-0.0117	0.3583	
H(10)	0.5475	-0.0891	0.2240	
H(11)	0.5659	-0.0145	0.1650	
H(12)	0.2958	0.3810	0.5814	

Positional parameters for YAMIDE2 M.Tillotson / H.C.Aspinall.

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atom	x	y	z	occupancy
H(13)	0.3875	0.4042	0.5273	
H(14)	0.2300	0.2544	0.4505	
H(15)	0.3872	0.1430	-0.0392	
H(16)	0.3125	0.1463	-0.1179	
H(17)	0.3380	0.2873	-0.0231	
H(18)	0.4333	0.2858	-0.0380	
H(19)	0.2056	0.1863	-0.0529	
H(20)	0.1581	0.0887	-0.0930	
H(21)	0.1103	0.0850	0.0631	
H(22)	0.0791	0.1483	0.0224	
H(23)	0.1930	0.0025	-0.0055	
H(24)	0.2732	0.0107	-0.0671	
H(25)	0.3734	0.0515	0.0869	
H(26)	0.2973	-0.0337	0.0805	
H(27)	0.8074	0.4519	0.3786	
H(28)	0.8182	0.3662	0.3335	
H(29)	0.7461	0.3897	0.2020	
H(30)	0.6772	0.4100	0.2702	
H(31)	0.7240	0.4692	0.5220	
H(32)	0.6426	0.4225	0.4297	
H(33)	0.5891	0.4085	0.5775	
H(34)	0.6645	0.3779	0.6111	
H(35)	0.7534	0.3238	0.5566	
H(36)	0.8177	0.3157	0.4759	
H(37)	0.8365	0.4628	0.6267	

Positional parameters for YAMIDE2 M.Tillotson / H.C.Aspinall.

P-2164-M7

atom	x	y	z	occupancy
H(38)	0.8967	0.4608	0.5403	
H(39)	0.3714	0.4965	0.1367	
H(40)	0.3426	0.4241	0.0321	
H(41)	0.2968	0.4100	0.1283	
H(42)	0.5898	0.4422	0.1278	
H(43)	0.5307	0.4419	0.0296	
H(44)	0.5569	0.5163	0.1319	
H(45)	0.5096	0.4163	0.3131	
H(46)	0.4762	0.4901	0.3171	
H(47)	0.4081	0.4022	0.3156	
H(48)	0.1941	0.3491	0.3476	
H(49)	0.2175	0.3997	0.2664	
H(50)	0.1279	0.3883	0.3107	
H(51)	0.0312	0.3305	0.1133	
H(52)	0.1119	0.3302	0.0547	
H(53)	0.0246	0.2496	0.0283	
H(54)	-0.0261	0.2370	0.2387	
H(55)	-0.0247	0.1542	0.1649	
H(56)	0.0260	0.1876	0.2803	
H(57)	0.2123	0.1003	0.3915	
H(58)	0.1332	0.0893	0.3068	
H(59)	0.1212	0.0241	0.3699	
H(60)	0.2157	-0.1062	0.3229	
H(61)	0.2762	-0.1048	0.2367	
H(62)	0.3107	-0.0351	0.3439	

Positional parameters for YAMIDE2 M.Tillotson / H.C.Aspinall.

P-2164-118

atom	x	y	z	occupancy
H(63)	0.0815	-0.0529	0.1010	
H(64)	0.1319	-0.1156	0.0851	
H(65)	0.0674	-0.1163	0.1670	
H(66)	0.8036	0.2193	0.1312	
H(67)	0.7858	0.2119	0.0124	
H(68)	0.8247	0.3002	0.0950	
H(69)	0.6842	0.3389	0.0018	
H(70)	0.6445	0.2491	-0.0773	
H(71)	0.5820	0.2843	-0.0120	
H(72)	0.5275	0.1184	0.0500	
H(73)	0.5975	0.0944	-0.0133	
H(74)	0.6034	0.0980	0.1047	
H(75)	0.3785	0.1542	0.4935	
H(76)	0.4427	0.1044	0.4750	
H(77)	0.3990	0.1110	0.5756	
H(78)	0.5315	0.3522	0.7367	
H(79)	0.4336	0.3111	0.6726	
H(80)	0.4641	0.2697	0.7513	
H(81)	0.5877	0.1875	0.7209	
H(82)	0.6299	0.1737	0.6198	
H(83)	0.6628	0.2627	0.7003	
H(84)	0.8390	0.4516	0.8954	
H(85)	0.8426	0.4972	0.8090	
H(86)	0.7810	0.4028	0.7844	
H(87)	0.8630	0.2770	0.7811	

Positional parameters for YAMIDE2 M.Tillotson / H.C.Aspinall.

atom	x	y	z	occupancy

P-2164-M9

H(88)	0.9680	0.3066	0.8000	
H(89)	0.9188	0.3319	0.8915	
H(90)	1.0860	0.4866	0.8333	
H(91)	1.0419	0.5536	0.8395	
H(92)	1.0397	0.5106	0.9284	
C(54)	0.080(6)	0.112(6)	0.597(7)	1/2
C(51)	0.212(6)	0.299(6)	0.768(7)	1/2
C(52)	0.150(7)	0.251(7)	0.707(8)	1/2
C(50)	0.211(7)	0.370(7)	0.810(8)	1/2
C(53)	0.125(6)	0.163(7)	0.663(8)	1/2
H(93)	1.0279	0.3738	0.6505	
H(94)	1.0565	0.3555	0.4877	
H(95)	0.9715	0.3815	0.4509	

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P-2164-MID

U values for YAMIDE2 M.Tillotson / H.C.Aspinall.

atom	U11	U22	U33	U12	U13	U23
Y(1)	0.022(3)	0.025(3)	0.017(3)	0.005(2)	-0.004(2)	0.002(2)
Y(2)	0.014(3)	0.022(3)	0.023(3)	0.009(2)	0.003(2)	0.002(2)
Si(11)	0.048(9)	0.037(9)	0.050(9)	0.026(7)	0.017(7)	0.018(7)
Si(12)	0.038(8)	0.042(9)	0.044(9)	0.024(7)	-0.001(7)	0.006(7)
Si(13)	0.028(8)	0.033(8)	0.046(9)	0.008(7)	0.004(7)	0.000(7)
Si(21)	0.038(8)	0.032(8)	0.028(8)	0.014(7)	0.007(6)	0.007(6)
Si(22)	0.026(8)	0.026(8)	0.037(8)	0.010(6)	0.014(6)	0.015(6)
Si(23)	0.042(9)	0.04(1)	0.05(1)	0.002(7)	-0.003(7)	0.020(7)
O(2)	0.021(6)					
O(11)	0.027(7)					
O(21)	0.026(7)					
O(22)	0.032(7)					
N(1)	0.027(8)					
N(2)	0.011(7)					
N(11)	0.026(8)					
N(12)	0.022(8)					
N(13)	0.021(8)					
N(21)	0.021(8)					

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P-21604-M11

U values for YAMIDE2 M.Tillotson / H.C.Aspinall.

atom	U11	U22	U33	U12	U13	U23
N(22)	0.031(9)					
N(23)	0.026(8)					
C(1)	0.04(1)					
C(2)	0.09(2)					
C(3)	0.15(3)					
C(4)	0.04(1)					
C(5)	0.04(1)					
C(6)	0.06(1)					
C(7)	0.06(1)					
C(8)	0.05(1)					
C(11)	0.04(1)					
C(12)	0.03(1)					
C(13)	0.04(1)					
C(14)	0.05(1)					
C(15)	0.05(1)					
C(16)	0.04(1)					
C(21)	0.03(1)					
C(22)	0.04(1)					

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P-2164-M12

U values for YAMIDE2 M.Tillotson / H.C.Aspinall.

atom	U11	U22	U33	U12	U13	U23
C(23)	0.03(1)					
C(24)	0.02(1)					
C(25)	0.03(1)					
C(26)	0.04(1)					
C(31)	0.05(1)					
C(32)	0.08(2)					
C(111)	0.08(2)					
C(112)	0.04(1)					
C(113)	0.05(1)					
C(121)	0.05(1)					
C(122)	0.08(2)					
C(123)	0.07(1)					
C(131)	0.06(1)					
C(132)	0.06(1)					
C(133)	0.04(1)					
C(211)	0.04(1)					
C(212)	0.07(2)					
C(213)	0.04(1)					

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P-2164-M13

U values for YAMIDE2 M.Tillotson / H.C.Aspinall.

atom	U11	U22	U33	U12	U13	U23
C(221)	0.06(1)					
C(222)	0.05(1)					
C(223)	0.05(1)					
C(231)	0.05(1)					
C(232)	0.11(2)					
C(233)	0.10(2)					
Li(1)	0.05(2)					
Li(2)	0.09(3)					
Li(3)	0.05(2)					
H(1)	0.0438					
H(2)	0.0438					
H(3)	0.1112					
H(4)	0.1112					
H(5)	0.1342					
H(6)	0.1342					
H(7)	0.0522					
H(8)	0.0522					
H(9)	0.0375					

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P-2164-M14

U values for YAMIDE2 M.Tillotson / H.C.Aspinall.

atom	U11	U22	U33	U12	U13	U23
H(10)	0.0650					
H(11)	0.0650					
H(12)	0.0664					
H(13)	0.0664					
H(14)	0.0667					
H(15)	0.0437					
H(16)	0.0437					
H(17)	0.0372					
H(18)	0.0372					
H(19)	0.0397					
H(20)	0.0397					
H(21)	0.0574					
H(22)	0.0574					
H(23)	0.0537					
H(24)	0.0537					
H(25)	0.0520					
H(26)	0.0520					
H(27)	0.0376					

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P-2164-M15

U values for YAMIDE2 M.Tillotson / H.C.Aspinall.

atom	U11	U22	U33	U12	U13	U23
H(28)	0.0376					
H(29)	0.0362					
H(30)	0.0362					
H(31)	0.0386					
H(32)	0.0386					
H(33)	0.0271					
H(34)	0.0271					
H(35)	0.0348					
H(36)	0.0348					
H(37)	0.0394					
H(38)	0.0394					
H(39)	0.1004					
H(40)	0.1004					
H(41)	0.1004					
H(42)	0.0503					
H(43)	0.0503					
H(44)	0.0503					
H(45)	0.0545					

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U values for YAMIDE2 M.Tillotson / H.C.Aspinall.

atom	U11	U22	U33	U12	U13	U23
H(46)	0.0545					
H(47)	0.0545					
H(48)	0.0650					
H(49)	0.0650					
H(50)	0.0650					
H(51)	0.0894					
H(52)	0.0894					
H(53)	0.0894					
H(54)	0.0819					
H(55)	0.0819					
H(56)	0.0819					
H(57)	0.0760					
H(58)	0.0760					
H(59)	0.0760					
H(60)	0.0912					
H(61)	0.0912					
H(62)	0.0912					
H(63)	0.0525					

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P-21604-M17

U values for YAMIDE2 M.Tillotson / H.C.Aspinall.

atom	U11	U22	U33	U12	U13	U23
H(64)	0.0525					
H(65)	0.0525					
H(66)	0.0464					
H(67)	0.0464					
H(68)	0.0464					
H(69)	0.0822					
H(70)	0.0822					
H(71)	0.0822					
H(72)	0.0521					
H(73)	0.0521					
H(74)	0.0521					
H(75)	0.0761					
H(76)	0.0761					
H(77)	0.0761					
H(78)	0.0581					
H(79)	0.0581					
H(80)	0.0581					
H(81)	0.0551					

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U values for YAMIDE2 M.Tillotson / H.C.Aspinall.

atom	U11	U22	U33	U12	U13	U23
H(82)	0.0551					
H(83)	0.0551					
H(84)	0.0536					
H(85)	0.0536					
H(86)	0.0536					
H(87)	0.1378					
H(88)	0.1378					
H(89)	0.1378					
H(90)	0.1270					
H(91)	0.1270					
H(92)	0.1270					
C(54)	0.08(2)					
C(51)	0.06(3)					
C(52)	0.06(3)					
C(50)	0.08(3)					
C(53)	0.06(3)					
H(93)	0.0524					
H(94)	0.1057					

U values for YAMIDE2 M.Tillotson / H.C.Aspinall.

atom	U11	U22	U33	U12	U13	U23
H(95)	0.1057					

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P-2164-M19

P-2164-M20

Intramolecular Distances

atom	atom	distance
Y1	O2	2.43(2)
Y1	O11	2.26(2)
Y1	N1	2.51(3)
Y1	N11	2.43(3)
Y1	N12	2.28(3)
Y1	N13	2.35(3)
Y1	LI1	3.01(7)
Y1	LI2	2.95(9)
Y1	LI3	3.11(7)
Y2	O2	2.15(2)
Y2	O21	2.43(2)
Y2	O22	2.25(2)
Y2	N2	2.53(2)
Y2	N21	2.32(3)
Y2	N22	2.35(3)
Y2	LI1	2.84(7)
Y2	LI2	2.76(9)
Y2	LI3	2.89(7)
SI11	N11	1.73(3)
SI11	C111	1.82(5)
SI11	C112	1.84(4)
SI11	C113	1.78(4)
SI12	N12	1.69(3)
SI12	C121	1.88(4)
SI12	C122	1.77(5)
SI12	C123	1.81(4)
SI13	N13	1.73(3)
SI13	C131	1.84(4)
SI13	C132	1.91(4)
SI13	C133	1.85(4)
SI21	N21	1.74(3)
SI21	C211	1.87(4)
SI21	C212	1.81(4)
SI21	C213	1.92(4)
SI21	LI3	2.80(7)
SI22	N22	1.70(3)
SI22	C221	1.83(4)
SI22	C222	1.81(4)
SI22	C223	1.88(4)
SI23	N23	1.70(3)
SI23	C231	1.74(4)
SI23	C232	1.80(6)
SI23	C233	1.91(5)
O2	LI1	1.81(8)
O2	LI2	1.72(9)
O2	LI3	1.92(7)
O11	C8	1.19(4)
O11	LI1	1.90(8)
O21	C1	1.48(4)
O21	C4	1.41(4)
O22	C5	1.28(4)
O22	LI2	1.81(9)

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

Intramolecular Distances (cont)

atom	atom	distance	atom	atom	distance
N1	C11	1.44(4)	C4	H7	0.952
N1	C13	1.49(4)	C4	H8	0.935
N1	C15	1.53(4)	C5	C6	1.37(5)
N2	C21	1.48(4)	C5	H9	0.951
N2	C23	1.46(4)	C6	H10	0.963
N2	C25	1.44(4)	C6	H11	0.979
N11	C12	1.43(4)	C7	C8	1.41(5)
N11	LI3	2.05(7)	C7	H12	0.938
N12	C14	1.43(4)	C7	H13	0.962
N13	C16	1.46(4)	C8	H14	0.981
N13	LI2	2.1(1)	C11	C12	1.60(5)
N21	C22	1.48(4)	C11	H15	0.947
N21	LI3	1.99(7)	C11	H16	0.932
N22	C24	1.54(4)	C12	H17	0.973
N22	LI1	2.04(8)	C12	H18	0.952
N23	C26	1.50(4)	C13	C14	1.49(5)
N23	C31	1.31(4)	C13	H19	0.962
C1	C2	1.46(6)	C13	H20	0.981
C1	H1	0.952	C14	H21	0.918
C1	H2	0.947	C14	H22	0.950
C2	C3	1.35(7)	C15	C16	1.51(5)
C2	H3	0.955	C15	H23	0.962
C2	H4	0.939	C15	H24	0.954
C3	C4	1.50(7)	C16	H25	0.943
C3	H5	0.904	C16	H26	0.962
C3	H6	1.012	C21	C22	1.50(5)

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

P-2164-M22 (cont)

Intramolecular Distances

atom	atom	distance	atom	atom	distance
C21	H27	0.962	C113	H47	0.961
C21	H28	0.977	C121	H48	0.952
C22	H29	0.954	C121	H49	0.936
C22	H30	0.947	C121	H50	0.952
C23	C24	1.48(4)	C122	H51	0.990
C23	H31	0.938	C122	H52	0.892
C23	H32	0.983	C122	H53	0.976
C24	H33	0.937	C123	H54	0.924
C24	H34	0.932	C123	H55	0.993
C25	C26	1.50(5)	C123	H56	0.930
C25	H35	0.955	C131	H57	0.951
C25	H36	0.971	C131	H58	0.956
C26	H37	0.957	C131	H59	0.967
C26	H38	0.951	C132	H60	0.921
C31	C32	1.42(6)	C132	H61	1.027
C31	H93	0.975	C132	H62	0.912
C32	H94	0.913	C133	H63	0.923
C32	H95	0.951	C133	H64	0.997
C111	H39	0.937	C133	H65	0.927
C111	H40	0.960	C211	H66	0.937
C111	H41	0.949	C211	H67	0.966
C112	H42	0.922	C211	H68	0.954
C112	H43	0.943	C212	H69	0.945
C112	H44	0.985	C212	H70	0.915
C113	H45	0.990	C212	H71	0.996
C113	H46	0.916	C213	H72	0.955

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

 P-2164-M23 (cont)

Intramolecular Distances

atom	atom	distance	atom	atom	distance
C213	H73	0.927			
C213	H74	0.957			
C221	H75	0.934			
C221	H76	0.992			
C221	H77	0.940			
C222	H78	0.953			
C222	H79	0.973			
C222	H80	0.967			
C223	H81	0.927			
C223	H82	1.010			
C223	H83	0.941			
C231	H84	0.967			
C231	H85	0.946			
C231	H86	0.932			
C232	H87	0.966			
C232	H88	0.947			
C232	H89	0.961			
C233	H90	0.943			
C233	H91	0.907			
C233	H92	0.983			
LI1	LI2	2.9(1)			
C54	C53	1.1(1)			
C51	C52	1.1(1)			
C51	C50	1.2(1)			
C52	C53	1.4(1)			

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

Intramolecular Bond Angles

atom	atom	atom	angle	atom	atom	atom	angle
O2	Y1	O11	76.0(8)	N12	Y1	N13	101.0(9)
O2	Y1	N1	111.5(8)	N12	Y1	LI1	138(2)
O2	Y1	N11	78.5(9)	N12	Y1	LI2	145(2)
O2	Y1	N12	175.3(9)	N12	Y1	LI3	145(1)
O2	Y1	N13	80.4(8)	N13	Y1	LI1	95(2)
O2	Y1	LI1	37(1)	N13	Y1	LI2	45(2)
O2	Y1	LI2	36(2)	N13	Y1	LI3	100(1)
O2	Y1	LI3	38(1)	LI1	Y1	LI2	58(2)
O11	Y1	N1	170.2(9)	LI1	Y1	LI3	66(2)
O11	Y1	N11	116.5(9)	LI2	Y1	LI3	64(2)
O11	Y1	N12	99.3(9)	O2	Y2	O21	156.2(8)
O11	Y1	N13	104.9(9)	O2	Y2	O22	79.6(9)
O11	Y1	LI1	39(1)	O2	Y2	N2	123.5(9)
O11	Y1	LI2	87(2)	O2	Y2	N21	84.4(9)
O11	Y1	LI3	102(1)	O2	Y2	N22	84.7(9)
N1	Y1	N11	72.1(9)	O2	Y2	LI1	40(2)
N1	Y1	N12	73.2(9)	O2	Y2	LI2	39(2)
N1	Y1	N13	71.1(9)	O2	Y2	LI3	41(1)
N1	Y1	LI1	148(2)	O21	Y2	O22	78.4(8)
N1	Y1	LI2	96(2)	O21	Y2	N2	79.8(8)
N1	Y1	LI3	87(1)	O21	Y2	N21	100.1(8)
N11	Y1	N12	104.0(9)	O21	Y2	N22	109.6(9)
N11	Y1	N13	126.4(9)	O21	Y2	LI1	152(2)
N11	Y1	LI1	96(2)	O21	Y2	LI2	119(2)
N11	Y1	LI2	103(2)	O21	Y2	LI3	137(1)
N11	Y1	LI3	41(1)	O22	Y2	N2	155.0(8)

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

 P-2164-M25 (cont)

Intramolecular Bond Angles

atom	atom	atom	angle	atom	atom	atom	angle
O22	Y2	N21	122.9(9)	N12	SI12	C121	114(2)
O22	Y2	N22	104.8(9)	N12	SI12	C122	118(2)
O22	Y2	LI1	95(2)	N12	SI12	C123	111(2)
O22	Y2	LI2	41(2)	C121	SI12	C122	103(2)
O22	Y2	LI3	102(1)	C121	SI12	C123	106(2)
N2	Y2	N21	73.1(9)	C122	SI12	C123	104(2)
N2	Y2	N22	71.4(9)	N13	SI13	C131	108(2)
N2	Y2	LI1	99(2)	N13	SI13	C132	111(2)
N2	Y2	LI2	160(2)	N13	SI13	C133	113(2)
N2	Y2	LI3	102(1)	C131	SI13	C132	110(2)
N21	Y2	N22	128(1)	C131	SI13	C133	108(2)
N21	Y2	LI1	106(2)	C132	SI13	C133	106(2)
N21	Y2	LI2	107(2)	N21	SI21	C211	117(2)
N21	Y2	LI3	43(1)	N21	SI21	C212	115(2)
N22	Y2	LI1	45(2)	N21	SI21	C213	107(2)
N22	Y2	LI2	95(2)	N21	SI21	LI3	45(2)
N22	Y2	LI3	112(1)	C211	SI21	C212	102(2)
LI1	Y2	LI2	62(2)	C211	SI21	C213	107(2)
LI1	Y2	LI3	71(2)	C211	SI21	LI3	162(2)
LI2	Y2	LI3	69(2)	C212	SI21	C213	108(2)
N11	SI11	C111	117(2)	C212	SI21	LI3	88(2)
N11	SI11	C112	109(2)	C213	SI21	LI3	84(2)
N11	SI11	C113	108(2)	N22	SI22	C221	107(2)
C111	SI11	C112	107(2)	N22	SI22	C222	115(2)
C111	SI11	C113	107(2)	N22	SI22	C223	113(2)
C112	SI11	C113	108(2)	C221	SI22	C222	107(2)

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

P-2164-M26 (cont)

Intramolecular Bond Angles

atom	atom	atom	angle
C221	SI22	C223	112(2)
C222	SI22	C223	102(2)
N23	SI23	C231	110(2)
N23	SI23	C232	115(2)
N23	SI23	C233	106(2)
C231	SI23	C232	108(2)
C231	SI23	C233	110(2)
C232	SI23	C233	108(2)
Y1	O2	Y2	179(1)
Y1	O2	LI1	89(2)
Y1	O2	LI2	89(3)
Y1	O2	LI3	90(2)
Y2	O2	LI1	91(3)
Y2	O2	LI2	90(3)
Y2	O2	LI3	91(2)
LI1	O2	LI2	110(4)
LI1	O2	LI3	128(3)
LI2	O2	LI3	123(4)
Y1	O11	C8	146(3)
Y1	O11	LI1	92(2)
C8	O11	LI1	122(3)
Y2	O21	C1	126(2)
Y2	O21	C4	124(2)
C1	O21	C4	108(3)
Y2	O22	C5	146(2)
Y2	O22	LI2	85(3)
C5	O22	LI2	129(4)
Y1	N1	C11	111(2)
Y1	N1	C13	107(2)
Y1	N1	C15	110(2)
C11	N1	C13	106(3)
C11	N1	C15	112(3)
C13	N1	C15	111(3)
Y2	N2	C21	108(2)
Y2	N2	C23	103(2)
Y2	N2	C25	114(2)
C21	N2	C23	110(3)
C21	N2	C25	111(2)
C23	N2	C25	110(3)
Y1	N11	SI11	117(1)
Y1	N11	C12	114(2)
Y1	N11	LI3	87(2)
SI11	N11	C12	108(2)
SI11	N11	LI3	110(2)
C12	N11	LI3	120(3)
Y1	N12	SI12	138(2)
Y1	N12	C14	113(2)
SI12	N12	C14	109(2)
Y1	N13	SI13	129(1)
Y1	N13	C16	110(2)
Y1	N13	LI2	83(3)
SI13	N13	C16	116(2)

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

P-2164-M27

Intramolecular Bond Angles (cont)

atom	atom	atom	angle	atom	atom	atom	angle
SI13	N13	LI2	117(3)	C3	C2	H3	102.82
C16	N13	LI2	89(3)	C3	C2	H4	108.52
Y2	N21	SI21	128(1)	H3	C2	H4	109.98
Y2	N21	C22	115(2)	C2	C3	C4	107(6)
Y2	N21	LI3	84(2)	C2	C3	H5	114.36
SI21	N21	C22	110(2)	C2	C3	H6	106.48
SI21	N21	LI3	97(2)	C4	C3	H5	113.12
C22	N21	LI3	118(3)	C4	C3	H6	107.05
Y2	N22	SI22	127(2)	H5	C3	H6	108.04
Y2	N22	C24	113(2)	O21	C4	C3	107(4)
Y2	N22	LI1	80(2)	O21	C4	H7	110.17
SI22	N22	C24	111(2)	O21	C4	H8	111.53
SI22	N22	LI1	107(2)	C3	C4	H7	110.17
C24	N22	LI1	113(3)	C3	C4	H8	106.79
SI23	N23	C26	126(2)	H7	C4	H8	110.61
SI23	N23	C31	120(3)	O22	C5	C6	125(4)
C26	N23	C31	114(3)	O22	C5	H9	118.37
O21	C1	C2	105(3)	C6	C5	H9	116.86
O21	C1	H1	111.94	C5	C6	H10	122.85
O21	C1	H2	112.02	C5	C6	H11	121.33
C2	C1	H1	109.46	H10	C6	H11	115.82
C2	C1	H2	109.05	C8	C7	H12	123.07
H1	C1	H2	109.53	C8	C7	H13	116.87
C1	C2	C3	111(5)	H12	C7	H13	120.06
C1	C2	H3	111.41	O11	C8	C7	125(4)
C1	C2	H4	112.19	O11	C8	H14	121.74

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

P-2164-M28
(cont)

Intramolecular Bond Angles

atom	atom	atom	angle	atom	atom	atom	angle
C7	C8	H14	112.74	N1	C15	H23	109.74
N1	C11	C12	113(3)	N1	C15	H24	108.89
N1	C11	H15	106.56	C16	C15	H23	109.54
N1	C11	H16	107.55	C16	C15	H24	110.63
C12	C11	H15	108.29	H23	C15	H24	108.16
C12	C11	H16	110.55	N13	C16	C15	108(3)
H15	C11	H16	111.26	N13	C16	H25	112.65
N11	C12	C11	111(3)	N13	C16	H26	110.53
N11	C12	H17	110.35	C15	C16	H25	108.55
N11	C12	H18	109.10	C15	C16	H26	108.11
C11	C12	H17	109.15	H25	C16	H26	109.04
C11	C12	H18	109.55	N2	C21	C22	113(3)
H17	C12	H18	107.36	N2	C21	H27	111.79
N1	C13	C14	111(3)	N2	C21	H28	111.55
N1	C13	H19	107.81	C22	C21	H27	107.52
N1	C13	H20	106.72	C22	C21	H28	106.45
C14	C13	H19	113.89	H27	C21	H28	106.26
C14	C13	H20	111.48	N21	C22	C21	114(3)
H19	C13	H20	105.92	N21	C22	H29	109.81
N12	C14	C13	111(3)	N21	C22	H30	108.40
N12	C14	H21	111.97	C21	C22	H29	108.99
N12	C14	H22	108.37	C21	C22	H30	106.66
C13	C14	H21	107.37	H29	C22	H30	109.36
C13	C14	H22	105.37	N2	C23	C24	110(3)
H21	C14	H22	112.28	N2	C23	H31	111.89
N1	C15	C16	110(3)	N2	C23	H32	108.82

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

P-2164-MKY

Intramolecular Bond Angles (cont)

atom	atom	atom	angle	atom	atom	atom	angle
C24	C23	H31	109.99	H94	C32	H95	123.88
C24	C23	H32	108.71	SI11	C111	H39	109.96
H31	C23	H32	107.73	SI11	C111	H40	108.38
N22	C24	C23	114(3)	SI11	C111	H41	109.26
N22	C24	H33	107.38	H39	C111	H40	109.76
N22	C24	H34	107.43	H39	C111	H41	110.69
C23	C24	H33	108.89	H40	C111	H41	108.74
C23	C24	H34	107.08	SI11	C112	H42	110.71
H33	C24	H34	112.20	SI11	C112	H43	109.63
N2	C25	C26	120(3)	SI11	C112	H44	107.78
N2	C25	H35	108.06	H42	C112	H43	112.53
N2	C25	H36	107.87	H42	C112	H44	108.84
C26	C25	H35	106.97	H43	C112	H44	107.17
C26	C25	H36	105.81	SI11	C113	H45	108.04
H35	C25	H36	107.30	SI11	C113	H46	112.72
N23	C26	C25	112(3)	SI11	C113	H47	110.04
N23	C26	H37	107.93	H45	C113	H46	108.89
N23	C26	H38	110.29	H45	C113	H47	105.31
C25	C26	H37	108.53	H46	C113	H47	111.50
C25	C26	H38	109.35	SI12	C121	H48	108.46
H37	C26	H38	108.82	SI12	C121	H49	109.29
N23	C31	C32	137(4)	SI12	C121	H50	108.86
N23	C31	H93	113.75	H48	C121	H49	110.53
C32	C31	H93	109.11	H48	C121	H50	109.14
C31	C32	H94	120.89	H49	C121	H50	110.51
C31	C32	H95	115.23	SI12	C122	H51	107.89

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

P-2164-M30

Intramolecular Bond Angles (cont)

atom	atom	atom	angle	atom	atom	atom	angle
SI12	C122	H52	112.96	H63	C133	H64	107.75
SI12	C122	H53	108.11	H63	C133	H65	113.93
H51	C122	H52	110.94	H64	C133	H65	107.44
H51	C122	H53	104.25	SI21	C211	H66	110.66
H52	C122	H53	112.23	SI21	C211	H67	109.13
SI12	C123	H54	110.75	SI21	C211	H68	109.79
SI12	C123	H55	106.52	H66	C211	H67	109.22
SI12	C123	H56	110.00	H66	C211	H68	110.18
H54	C123	H55	108.02	H67	C211	H68	107.80
H54	C123	H56	113.65	SI21	C212	H69	109.99
H55	C123	H56	107.57	SI21	C212	H70	111.65
SI13	C131	H57	111.21	SI21	C212	H71	107.22
SI13	C131	H58	110.74	H69	C212	H70	113.03
SI13	C131	H59	110.31	H69	C212	H71	106.11
H57	C131	H58	108.88	H70	C212	H71	108.51
H57	C131	H59	107.96	SI21	C213	H72	108.31
H58	C131	H59	107.63	SI21	C213	H73	109.80
SI13	C132	H60	111.25	SI21	C213	H74	108.23
SI13	C132	H61	105.75	H72	C213	H73	111.04
SI13	C132	H62	111.79	H72	C213	H74	108.51
H60	C132	H61	105.48	H73	C213	H74	110.88
H60	C132	H62	115.60	SI22	C221	H75	111.30
H61	C132	H62	106.13	SI22	C221	H76	108.36
SI13	C133	H63	110.39	SI22	C221	H77	111.16
SI13	C133	H64	106.64	H75	C221	H76	107.24
SI13	C133	H65	110.36	H75	C221	H77	111.73

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

P-2164-M31 (cont)

Intramolecular Bond Angles

atom	atom	atom	angle	atom	atom	atom	angle
H76	C221	H77	106.81	SI23	C233	H91	110.03
SI22	C222	H78	112.56	SI23	C233	H92	106.64
SI22	C222	H79	111.08	H90	C233	H91	114.01
SI22	C222	H80	111.63	H90	C233	H92	107.31
H78	C222	H79	107.27	H91	C233	H92	110.29
H78	C222	H80	107.78	Y1	LI1	Y2	103(2)
H79	C222	H80	106.19	Y1	LI1	O2	54(2)
SI22	C223	H81	112.48	Y1	LI1	O11	49(2)
SI22	C223	H82	108.01	Y1	LI1	N22	157(3)
SI22	C223	H83	111.80	Y1	LI1	LI2	60(2)
H81	C223	H82	106.40	Y2	LI1	O2	49(2)
H81	C223	H83	112.33	Y2	LI1	O11	151(4)
H82	C223	H83	105.31	Y2	LI1	N22	55(2)
SI23	C231	H84	108.38	Y2	LI1	LI2	58(2)
SI23	C231	H85	108.93	O2	LI1	O11	102(4)
SI23	C231	H86	110.12	O2	LI1	N22	104(4)
H84	C231	H85	108.36	O2	LI1	LI2	34(2)
H84	C231	H86	109.57	O11	LI1	N22	151(4)
H85	C231	H86	111.41	O11	LI1	LI2	96(3)
SI23	C232	H87	110.29	N22	LI1	LI2	98(3)
SI23	C232	H88	111.21	Y1	LI2	Y2	107(3)
SI23	C232	H89	110.82	Y1	LI2	O2	55(3)
H87	C232	H88	108.36	Y1	LI2	O22	161(5)
H87	C232	H89	107.21	Y1	LI2	N13	52(2)
H88	C232	H89	108.83	Y1	LI2	LI1	62(2)
SI23	C233	H90	108.26	Y2	LI2	O2	51(3)

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

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Intramolecular Bond Angles (cont)

atom	atom	atom	angle
Y2	LI2	O22	54(3)
Y2	LI2	N13	159(5)
Y2	LI2	LI1	60(2)
O2	LI2	O22	106(5)
O2	LI2	N13	108(5)
O2	LI2	LI1	36(3)
O22	LI2	N13	146(5)
O22	LI2	LI1	104(4)
N13	LI2	LI1	105(4)
Y1	LI3	Y2	100(2)
Y1	LI3	SI21	154(3)
Y1	LI3	O2	52(2)
Y1	LI3	N11	51(2)
Y1	LI3	N21	152(3)
Y2	LI3	SI21	80(2)
Y2	LI3	O2	48(2)
Y2	LI3	N11	148(3)
Y2	LI3	N21	53(2)
SI21	LI3	O2	123(3)
SI21	LI3	N11	132(3)
SI21	LI3	N21	38(1)
O2	LI3	N11	101(3)
O2	LI3	N21	101(3)
N11	LI3	N21	153(4)
C52	C51	C50	118(11)
C51	C52	C53	130(11)
C54	C53	C52	140(11)

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