Index to Supporting Information

1. Crystal structure of $(Me_5C_5)_2Yb(bipy)$

1.1 Positional Parameters for $(Me_5C_5)_2Yb(bipy)$

atom	x	y	z	atom	x	y	z
YB1	0.19079(2)	0.24016(1)	0.14106(2)	C126	0.3589(5)	0.2896(3)	0.1369(4)
YB2	0.22374(2)	0.00730(1)	-0.10389(2)	C127	0.4172(6)	0.3226(3)	0.1467(5)
N11	0.3097(4)	0.2221(2)	0.0932(3)	C128	0.3998(6)	0.3598(3)	0.1834(5)
N12	0.2840(4)	0.2945(2)	0.1620(3)	C129	0.3241(7)	0.3649(3)	0.2101(5)
N21	0.3086(4)	-0.0528(2)	-0.1061(3)	C130	0.2689(6)	0.3311(3)	0.1976(4)
N22	0.3155(4)	0.0142(2)	-0.0233(3)	C201	0.3181(6)	0.0313(3)	-0.1945(5)
CP10	0.1074	0.2678	0.0624	C202	0.3179(6)	0.0646(3)	-0.1563(4)
CP11	0.1831	0.1952	0.2310	C203	0.2423(8)	0.0847(3)	-0.1565(5)
CP20	0.2645	0.0534	-0.1863	C204	0.1973(6)	0.0591(4)	-0.2017(5)
CP21	0.1082	-0.0169	-0.0555	C200	0.2470(8)	0.0274(4)	-0.2226(4)
C101	0.1634(6)	0.2817(4)	0.0346(5)	C206	0.3896(9)	0.0035(5)	-0.2171(8)
C102	0.1182(6)	0.3038(3)	0.0798(5)	C207	0.392(1)	0.0825(6)	-0.1227(7)
C103	0.0590(6)	0.2760(4)	0.1011(5)	C208	0.222(1)	0.1263(5)	-0.1206(7)
C104	0.0660(6)	0.2369(3)	0.0685(5)	C209	0.1225(8)	0.0747(6)	-0.2269(8)
C105	0.1305(7)	0.2406(3)	0.0278(4)	C210	0.226(2)	-0.0062(6)	-0.2756(6)
C106	0.2307(8)	0.3020(6)	-0.0014(6)	C211	0.0821(6)	-0.0254(5)	-0.1045(5)
C107	0.129(1)	0.3537(5)	0.0969(8)	C212	0.0758(6)	0.0140(4)	-0.0752(6)
C108	-0.0082(8)	0.2908(6)	0.1429(6)	C213	0.1143(6)	0.0115(3)	-0.0177(5)
C109	0.0036(8)	0.1987(4)	0.0670(7)	C214	0.1444(5)	-0.0315(4)	-0.0133(5)
C110	0.149(1)	0.2024(5)	-0.0180(6)	C215	0.1243(6)	-0.0533(3)	-0.0666(6)
C111	0.2336(6)	0.2169(3)	0.2559(4)	C216	0.0427(9)	-0.0411(7)	-0.1679(7)
C112	0.1522(6)	0.2249(3)	0.2584(4)	C217	0.0212(8)	0.0517(5)	-0.0956(9)
C113	0.1130(5)	0.1917(3)	0.2233(4)	C218	0.1122(9)	0.0481(5)	0.0321(7)
C114	0.1716(6)	0.1632(3)	0.1982(4)	C219	0.1847(8)	-0.0523(6)	0.0450(6)

C115	0.2452(5)	0.1790(3)	0.2194(4)	C220	0.138(1)	-0.1039(5)	-0.075(1)
C116	0.2961(7)	0.2417(4)	0.2946(6)	C221	0.3026(6)	-0.0864(3)	-0.1486(4)
C117	0.1075(9)	0.2596(4)	0.2984(6)	C222	0.3516(6)	-0.1227(3)	-0.1522(5)
C118	0.0243(6)	0.1813(5)	0.2269(6)	C223	0.4141(7)	-0.1239(3)	-0.1063(5)
C119	0.1577(8)	0.1202(3)	0.1621(5)	C224	0.4221(6)	-0.0912(3)	-0.0608(5)
C120	0.3252(6)	0.1558(4)	0.2112(5)	C225	0.3670(5)	-0.0551(3)	-0.0609(4)
C121	0.3207(5)	0.1844(3)	0.0588(4)	C226	0.3690(5)	-0.0204(3)	-0.0148(4)
C122	0.3926(6)	0.1741(3)	0.0298(4)	C227	0.4203(5)	-0.0208(3)	0.0372(4)
C123	0.4555(6)	0.2038(3)	0.0361(4)	C228	0.4196(6)	0.0148(4)	0.0799(4)
C124	0.4461(5)	0.2418(3)	0.0705(4)	C229	0.3662(6)	0.0509(3)	0.0703(4)
C125	0.3723(5)	0.2505(3)	0.0995(4)	C230	0.3162(6)	0.0487(3)	0.0174(4)

CP10, CP11, CP20 and CP21 are the calculated centroids of the rings C101 - C105, C111 - C115, C201 - C205 and C211 - C215, respectively.

1.2 Thermal Parameters for $(Me_5C_5)_2Yb(bipy)$

atom	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)
YB1	0.00218(1)	0.00080(0)	0.00176(1)	-0.00016(1)	0.00012(2)	0.00009(1)
YB2	0.00241(1)	0.00084(0)	0.00181(1)	-0.00004(2)	0.00005(2)	0.00007(1)
N11	0.0025(3)	0.00092(9)	0.0022(2)	-0.0002(3)	0.0011(4)	-0.0001(2)
N12	0.0032(3)	0.00082(8)	0.0019(2)	-0.0005(3)	0.0006(4)	-0.0005(2)
N21	0.0030(3)	0.0012(1)	0.0019(2)	0.0003(3)	-0.0002(5)	-0.0003(2)
N22	0.0036(3)	0.00099(9)	0.0018(2)	-0.0003(3)	-0.0003(4)	-0.0004(2)
C101	0.0036(4)	0.0022(2)	0.0032(3)	0.0007(5)	-0.0002(6)	0.0027(4)
C102	0.0068(5)	0.0007(1)	0.0039(3)	0.0004(4)	-0.0064(6)	0.0005(3)
C103	0.0038(4)	0.0022(2)	0.0027(3)	0.0021(5)	0.0008(6)	0.0019(4)
C104	0.0054(4)	0.0014(1)	0.0039(3)	-0.0018(4)	-0.0054(6)	0.0022(4)
C105	0.0071(5)	0.0018(1)	0.0018(2)	0.0040(5)	-0.0024(6)	-0.0010(4)
C106	0.0049(6)	0.0067(3)	0.0065(4)	-0.0019(8)	0.0004(9)	0.0101(5)
C107	0.025(1)	0.0014(2)	0.0104(6)	0.0038(9)	-0.024(1)	-0.0019(6)

C108	0.0082(6)	0.0066(4)	0.0041(4)	0.0107(7)	0.0042(9)	0.0029(7)
C109	0.0128(7)	0.0033(2)	0.0093(5)	-0.0102(6)	-0.015(1)	0.0070(6)
C110	0.017(1)	0.0043(2)	0.0044(4)	0.0114(8)	-0.011(1)	-0.0063(5)
C111	0.0042(4)	0.0014(1)	0.0018(2)	-0.0014(4)	-0.0007(6)	0.0008(3)
C112	0.0054(4)	0.0011(1)	0.0019(2)	0.0017(4)	0.0017(6)	0.0008(3)
C113	0.0030(4)	0.0015(1)	0.0027(3)	-0.0001(4)	0.0006(6)	0.0018(3)
C114	0.0054(5)	0.0007(1)	0.0021(2)	-0.0006(4)	-0.0013(6)	0.0006(3)
C115	0.0033(4)	0.0014(1)	0.0017(2)	0.0006(4)	-0.0002(5)	0.0010(3)
C116	0.0085(6)	0.0027(2)	0.0036(3)	-0.0042(6)	-0.0057(8)	0.0013(5)
C117	0.0132(8)	0.0020(2)	0.0039(4)	0.0048(7)	0.0071(9)	0.0003(5)
C118	0.0021(4)	0.0041(2)	0.0060(4)	-0.0024(5)	-0.0013(7)	0.0060(5)
C119	0.0111(8)	0.0008(1)	0.0036(3)	-0.0022(5)	-0.0026(9)	-0.0001(4)
C120	0.0044(5)	0.0027(2)	0.0033(3)	0.0034(5)	0.0020(7)	0.0022(4)
C121	0.0041(4)	0.0010(1)	0.0023(3)	0.0010(4)	0.0005(6)	-0.0003(3)
C122	0.0052(5)	0.0015(1)	0.0021(3)	0.0008(5)	0.0001(6)	0.0001(4)
C123	0.0045(4)	0.0014(1)	0.0021(3)	0.0011(4)	0.0013(6)	0.0005(3)
C124	0.0035(4)	0.0013(1)	0.0021(2)	0.0002(4)	0.0015(6)	0.0009(3)
C125	0.0028(3)	0.0009(1)	0.0017(2)	0.0001(3)	0.0003(5)	0.0004(3)
C126	0.0028(3)	0.0011(1)	0.0019(2)	0.0000(3)	0.0002(5)	0.0002(3)
C127	0.0040(4)	0.0011(1)	0.0036(3)	-0.0017(4)	0.0002(7)	-0.0002(4)
C128	0.0046(5)	0.0016(2)	0.0039(4)	-0.0020(5)	-0.0005(7)	-0.0001(4)
C129	0.0058(5)	0.0012(1)	0.0040(4)	-0.0017(5)	0.0005(8)	-0.0009(4)
C130	0.0049(4)	0.0011(1)	0.0020(2)	-0.0001(4)	0.0009(6)	-0.0004(3)
C201	0.0037(4)	0.0018(2)	0.0036(3)	0.0010(5)	0.0027(6)	0.0024(4)
C202	0.007(5)	0.0019(1)	0.0019(3)	-0.0046(4)	-0.0014(6)	0.0012(3)
C203	0.0114(7)	0.0006(1)	0.0036(3)	0.0004(5)	0.0093(7)	0.0004(3)
C204	0.0026(4)	0.0022(2)	0.0050(3)	0.0005(4)	0.0005(7)	0.0041(4)
C200	0.0091(7)	0.0016(1)	0.0019(3)	-0.0028(6)	-0.0003(7)	0.0002(4)
C206	0.0112(8)	0.0041(3)	0.0097(6)	0.0075(8)	0.014(1)	0.0062(7)

C207	0.0137(8)	0.0072(3)	0.0066(5)	-0.0153(8)	-0.009(1)	0.0078(7)
C208	0.037(2)	0.0014(2)	0.0075(5)	0.004(1)	0.025(1)	0.0003(6)
C209	0.0035(6)	0.0116(4)	0.0158(5)	-0.0002(8)	-0.003(1)	0.0246(5)
C210	0.048(3)	0.0031(3)	0.0024(4)	-0.013(1)	-0.002(2)	-0.0005(6)
C211	0.0030(4)	0.0039(3)	0.0029(3)	-0.0031(5)	0.0004(6)	0.0012(5)
C212	0.0028(4)	0.0019(2)	0.0064(4)	0.0016(4)	0.0039(7)	0.0039(4)
C213	0.0054(4)	0.0017(1)	0.0044(3)	-0.0029(4)	0.0074(6)	-0.0024(4)
C214	0.0026(4)	0.0022(2)	0.0035(3)	-0.0014(4)	0.0006(6)	0.0025(4)
C215	0.0041(4)	0.0013(1)	0.0056(4)	-0.0021(4)	0.0040(7)	-0.0004(4)
C216	0.0092(8)	0.0087(5)	0.0037(4)	-0.0110(9)	-0.002(1)	-0.0005(9)
C217	0.0073(6)	0.0057(3)	0.0182(8)	0.0091(7)	0.015(1)	0.0168(6)
C218	0.0132(8)	0.0044(3)	0.0099(5)	-0.0081(8)	0.0184(9)	-0.0092(6)
C219	0.0050(6)	0.0064(3)	0.0055(4)	-0.0018(8)	-0.0010(9)	0.0089(5)
C220	0.0114(8)	0.0014(2)	0.018(1)	-0.0026(7)	0.017(1)	-0.0012(8)
C221	0.0051(4)	0.0010(1)	0.0021(2)	-0.0005(4)	0.0013(6)	-0.0007(3)
C222	0.0050(5)	0.0013(1)	0.0031(3)	0.0016(4)	0.0001(7)	0.0004(4)
C223	0.0064(5)	0.0013(1)	0.0035(3)	0.0019(5)	0.0013(8)	0.0001(4)
C224	0.0041(4)	0.0012(1)	0.0034(3)	0.0013(4)	0.0005(7)	-0.0000(4)
C225	0.0026(3)	0.0012(1)	0.0020(2)	-0.0001(4)	0.0008(5)	0.0003(3)
C226	0.0025(3)	0.0010(1)	0.0018(2)	-0.0004(3)	0.0003(5)	0.0003(3)
C227	0.0036(4)	0.0015(1)	0.0023(3)	-0.0007(4)	-0.0005(6)	0.0004(3)
C228	0.0043(4)	0.0018(2)	0.0023(3)	-0.0007(5)	0.0001(6)	0.0001(4)
C229	0.0044(4)	0.0016(2)	0.0023(3)	-0.0014(4)	-0.0001(6)	-0.0002(4)
C230	0.0050(4)	0.0012(1)	0.0023(3)	-0.0006(4)	0.0014(6)	-0.0007(3)

The form of the anisotropic thermal parameter is:

$\exp[-\{B(1,1)h^2 + B(2,2)k^2 + B(3,3)l^2 + B(1,2)hk + B(1,3)hl + B(2,3)kl\}]$.

1.3 Bond Lengths of $(Me_5C_5)_2Yb(bipy)$

atom	atom	distance	atom	atom	distance
YB1	C101	2.625(9)	YB2	C201	2.607(8)
YB1	C102	2.621(8)	YB2	C202	2.602(8)
YB1	C103	2.625(8)	YB2	C203	2.599(8)
YB1	C104	2.623(8)	Y82	C204	2.635(9)
YB1	C105	2.616(8)	YB2	C205	2.625(9)
YB1	CP10	2.343	YB2	CP20	2.339
YB1	C111	2.640(7)	YB2	C211	2.597(9)
YB1	C112	2.619(8)	YB2	C212	2.592(9)
YB1	C113	2.631(7)	YB2	C213	2.612(8)
YB1	C114	2.634(7)	YB2	C214	2.623(8)
YB1	C115	2.647(7)	YB2	C215	2.606(8)
YB1	CP11	2.346	YB2	CP21	2.332
YB1	N11	2.324(6)	YB2	N21	2.310(6)
YB1	N12	2.318(5)	YB2	N22	2.324(6)
N11	C121	1.361(9)	N21	C221	1.359(9)
N11	C125	1.371(8)	N21	C225	1.383(9)
C121	C122	1.40(1)	C221	C222	1.37(1)
C122	C123	1.40(1)	C222	C223	1.44(1)
C123	C124	1.36(1)	C223	C224	1.39(1)
C124	C125	1.421(9)	C224	C225	1.43(1)
C125	C126	1.436(9)	C225	C226	1.433(9)
C126	C127	1.42(1)	C226	C227	1.41(1)
C127	C128	1.39(1)	C227	C228	1.40(1)
C128	C129	1.41(1)	C228	C229	1.43(1)
C129	C130	1.41(1)	C229	C230	1.41(1)
N12	C126	1.385(9)	N22	C226	1.394(9)

N12	C130	1.360(9)	N22	C230	1.351(9)
C101	C102	1.40(1)	C201	C202	1.29(1)
C102	C103	1.38(1)	C202	C203	1.42(1)
C103	C104	1.37(1)	C203	C204	1.45(1)
C104	C105	1.40(1)	C204	C205	1.35(1)
C105	C101	1.36(1)	C205	C201	1.35(1)
C101	C106	1.50(1)	C201	C206	1.55(1)
C102	C107	1.55(1)	C202	C207	1.55(1)
C103	C108	1.51(1)	C203	C208	1.50(1)
C104	C109	1.56(1)	C204	C209	1.46(1)
C105	C110	1.54(1)	C205	C210	1.55(1)
C111	C112	1.40(1)	C211	C212	1.34(1)
C112	C113	1.41(1)	C212	C213	1.39(1)
C113	C114	1.42(1)	C213	C214	1.39(1)
C114	C115	1.41(1)	C214	C215	1.35(1)
C115	C111	1.39(1)	C215	C211	1.37(1)
C111	C116	1.54(1)	C211	C216	1.58(1)
C112	C117	1.54(1)	C212	C217	1.53(1)
C113	C118	1.54(1)	C213	C218	1.53(1)
C114	C119	1.52(1)	C214	C219	1.55(1)
C115	C120	1.54(1)	C215	C202	1.55(1)

1.4 Bond Angles of $(Me_5C_5)_2Yb(bipy)$

atom	atom	atom	angle	atom	atom	atom	angle
N11	YB1	N12	69.9(2)	N21	YB2	N22	70.5(2)
N11	YB1	CP10	107.1	N21	YB2	CP20	105.3
N11	YB1	CP11	105.7	N21	YB2	CP21	106.8
N12	YB1	CP10	107.4	N22	YB2	CP20	107.5
N12	YB1	CP11	106.7	N22	YB2	CP21	105.5

CP10	YB1	CP11	138.8	CP20	YB2	CP21	139.9
YB1	N11	C121	123.4(5)	YB2	N21	C221	123.2(5)
YB1	N11	C125	119.0(4)	YB2	N21	C225	118.3(5)
C121	N11	C125	117.7(6)	C221	N21	C225	118.5(6)
YB1	N12	C126	118.5(4)	YB2	N22	C226	117.8(4)
YB1	N12	C130	123.2(5)	YB2	N22	C230	123.1(5)
C126	N12	C130	118.3(6)	C126	N22	C230	118.9(6)
N11	C121	C122	122.7(8)	N21	C221	C222	125.6(8)
C121	C122	C123	118.7(8)	C221	C222	C223	115.5(8)
C122	C123	C124	119.8(8)	C222	C223	C224	121.6(8)
C123	C124	C125	119.3(7)	C223	C224	C225	118.2(8)
C124	C125	N11	121.7(7)	C224	C225	N21	120.6(7)
C124	C125	C126	122.1(7)	C224	C225	C226	122.4(7)
N11	C125	C126	116.2(6)	N21	C225	C226	117.1(7)
C125	C126	N12	116.5(6)	C225	C226	N22	116.0(6)
C125	C126	C127	122.9(7)	C225	C226	C227	123.1(7)
N12	C126	C127	120.6(7)	N22	C226	C227	120.8(7)
C126	C127	C128	119.8(8)	C226	C227	C228	119.8(8)
C127	C128	C129	120.2(8)	C227	C228	C229	119.5(8)
C128	C129	C130	116.9(8)	C228	C229	C230	117.4(8)
C129	C130	N12	124.2(8)	C229	C230	N22	123.5(8)
C105	C101	C102	106.1(9)	C205	C201	C202	110(1)
C101	C102	C103	109.7(9)	C201	C202	C203	109.3(9)
C102	C103	C104	106.9(9)	C202	C203	C204	104.6(8)
C103	C104	C105	108.1(9)	C203	C204	C205	105.4(9)
C104	C105	C101	109.2(9)	C204	C205	C201	110.5(9)
C106	C101	C102	125(1)	C206	C201	C202	128(1)
C106	C101	C105	129(1)	C206	C201	C205	121(1)
C107	C102	C101	124(1)	C207	C202	C201	124(1)

C107	C102	C103	126(1)	C207	C202	C203	126(1)
C108	C103	C102	124(1)	C208	C203	C202	124(2)
C108	C103	C104	128(1)	C208	C203	C204	131(2)
C109	C104	C103	126(1)	C209	C204	C203	122(2)
C109	C104	C105	125(1)	C209	C204	C205	131(2)
C110	C105	C101	131(1)	C210	C205	C201	125(2)
C110	C105	C104	119(1)	C210	C205	C204	124(2)
C115	C111	C112	107.6(7)	C215	C211	C212	108(1)
C111	C112	C113	108.8(7)	C211	C212	C213	109(1)
C112	C113	C114	107.2(7)	C212	C213	C214	106(1)
C113	C114	C115	107.3(7)	C213	C214	C215	107(1)
C114	C115	C111	109.1(7)	C214	C215	C211	109(1)
C116	C111	C112	125.2(9)	C216	C211	C212	129(2)
C116	C111	C115	126.6(9)	C216	C211	C215	123(2)
C117	C112	C111	128(1)	C217	C212	C211	125(2)
C117	C112	C113	122.5(9)	C217	C212	C213	125(2)
C118	C113	C112	125.3(9)	C218	C213	C212	124(2)
C118	C113	C114	125.7(9)	C218	C213	C214	129(2)
C119	C114	C113	126.5(8)	C219	C214	C213	126(1)
C119	C114	C115	125.8(8)	C219	C214	C215	126(1)
C120	C115	C111	124.1(8)	C220	C215	C211	128(2)
C120	C115	C114	126.4(8)	C220	C215	C214	122(2)

Plane 1

Atoms defining plane	Distance
C101	0.004
C102	-0.006
C103	0.006
C104	-0.003
C105	-0.001

Plane 2

Atoms defining plane	Distance
C111	-0.002
C112	-0.003
C113	0.005
C114	-0.006
C115	0.005

Additional atoms	Distance	Additional atoms	Distance
YB1	2.343	YB1	-2.346
C106	-0.069	C116	0.171
C107	-0.169	C117	0.145
C108	-0.204	C118	0.349
C109	-0.260	C119	0.124
C110	-0.105	C120	0.171
Plane 3		Plane 4	
Atoms defining plane	Distance	Atoms defining plane	Distance
N11	-0.005	N12	-0.001
C121	-0.001	C126	0.010
C122	0.004	C127	-0.006
C123	-0.003	C128	-0.007
C124	-0.003	C129	0.004
C125	0.006	C130	0.000
Additional atoms	Distance	Additional atoms	Distance
YB1	-0.029	YB1	-0.050
C126	0.022	C125	0.000
N12	0.013	N11	-0.013
Plane 5		Plane 6	
Atoms defining plane	Distance	Atoms defining plane	Distance
C201	0.005	C211	-0.001
C202	-0.007	C212	0.000
C203	0.006	C213	0.001
C204	-0.003	C214	-0.001
C205	-0.001	C215	0.001
Additional atoms	Distance	Additional atoms	Distance
YB2	2.338	YB2	2.332
C206	-0.202	C216	-0.127

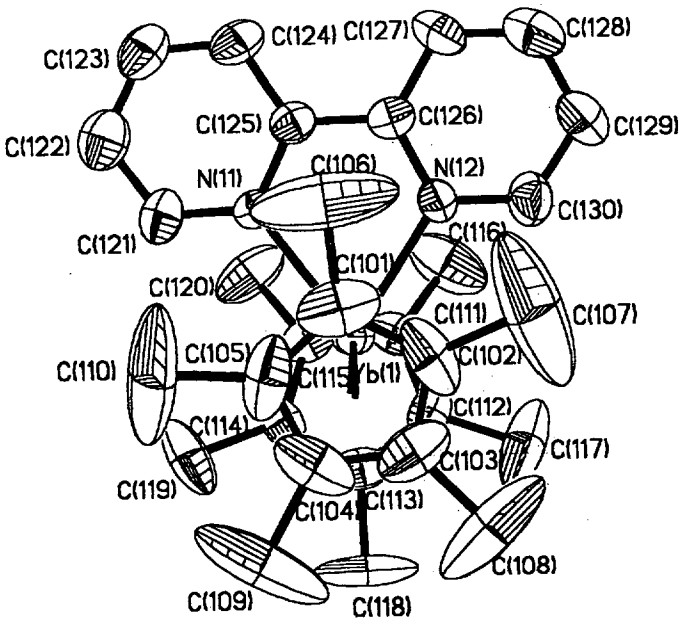
C207	-0.188	C217	-0.252
C208	-0.094	C218	-0.153
C209	-0.302	C219	-0.150
C210	-0.109	C220	-0.188

Plane 7		Plane 8	
Atoms defining plane	Distance	Atoms defining plane	Distance
N21	0.015	N22	-0.016
C221	-0.003	C226	0.013
C222	-0.010	C227	-0.003
C223	0.012	C228	-0.004
C224	-0.001	C229	0.002
C225	-0.013	C230	0.008
Additional atoms	Distance	Additional atoms	Distance
YB2	0.036	YB2	-0.238
C226	-0.065	C225	0.035
N22	0.028	N21	-0.083

Dihedral angles between planes:

	1	2	3		5	6	7
2	41.8			6	40.7		
3	20.2	21.6		7	19.7	21.1	
4	20	21.8	0.3	8	25.9	15.1	6.3

1.6 ORTEP diagram of molecule 1 of $(Me_5C_5)_2Yb(bipy)$ (50% probability ellipsoids) showing atom labelling scheme (the labelling scheme for molecule 2 is the same with the first digit 2 in each atom number)



2. Crystal Structure of $[(Me_5C_5)_2Yb(bipy)]^+[(Me_5C_5)_2YbCl_2]^-$

2.1 Positional Parameters for $[(Me_5C_5)_2Yb(bipy)]^+[(Me_5C_5)_2YbCl_2]^-$

2.1.1 Positional Parameters for Non-Hydrogen Atoms of $[(Me_5C_5)_2Yb(bipy)]^+[(Me_5C_5)_2YbCl_2]^-$

atom	x	y	z	atom	x	y	z
YB1	0.55087(2)	-0.22087(1)	0.23286(1)	C21	-0.0021(4)	0.4440(3)	0.1964(3)
YB2	0.06735(2)	0.28429(1)	0.26417(1)	C22	-0.0676(4)	0.3628(3)	0.1496(3)
Cl1	0.7467(1)	-0.1611(1)	0.32438(8)	C23	-0.1519(4)	0.3116(4)	0.2006(3)
Cl2	0.5014(1)	-0.38895(9)	0.30119(8)	C24	-0.1422(4)	0.3624(3)	0.2766(3)
N1	0.1699(3)	0.3629(2)	0.3827(2)	C25	-0.0495(4)	0.4436(3)	0.2740(3)
N2	-0.0034(3)	0.2058(2)	0.3837(2)	C26	0.0885(5)	0.5233(4)	0.1646(3)

C111	0.6265	-0.2653	0.1080	C27	-0.0666(6)	0.3480(4)	0.0594(3)
C112	0.3995	-0.1187	0.2744	C28	-0.2472(5)	0.2257(5)	0.1747(4)
C113	-0.0827	0.3849	0.2194	C29	-0.2276(5)	0.3433(4)	0.3442(3)
C114	0.2040	0.1807	0.2165	C30	-0.0226(5)	0.5246(4)	0.3381(3)
C1	0.5467(4)	-0.2221(3)	0.0740(3)	C31	0.2889(4)	0.2397(4)	0.2389(3)
C2	0.5363(4)	-0.3238(3)	0.0951(3)	C32	0.2236(4)	0.2378(3)	0.1614(3)
C3	0.6520(4)	-0.3450(3)	0.1330(3)	C33	0.1322(5)	0.1557(4)	0.1611(3)
C4	0.7311(4)	-0.2555(3)	0.1366(3)	C34	0.1405(5)	0.1099(3)	0.2362(3)
C5	0.6663(4)	-0.1803(3)	0.1013(3)	C35	0.2350(5)	0.1606(4)	0.2848(3)
C6	0.4583(5)	-0.1770(4)	0.0136(3)	C36	0.4059(5)	0.3060(5)	0.2616(5)
C7	0.4271(5)	-0.3999(4)	0.0732(3)	C37	0.2611(6)	0.2995(4)	0.0905(4)
C8	0.6868(5)	-0.4461(4)	0.1574(4)	C38	0.0508(6)	0.1118(5)	0.0883(4)
C9	0.8679(4)	-0.2466(4)	0.1630(4)	C39	0.0706(7)	0.0113(4)	0.2573(4)
C10	0.7207(5)	-0.0742(4)	0.0880(4)	C40	0.2815(6)	0.1274(5)	0.3681(4)
C11	0.4148(4)	-0.0667(3)	0.2169(3)	C50	-0.0932(4)	0.1301(3)	0.3821(3)
C12	0.3282(4)	-0.1521(3)	0.2193(3)	C51	-0.1349(5)	0.0853(4)	0.4507(3)
C13	0.3393(4)	-0.1898(3)	0.2982(3)	C52	-0.0830(5)	0.1204(4)	0.5248(3)
C14	0.4344(4)	-0.1309(3)	0.3445(3)	C53	0.0105(4)	0.1978(4)	0.5286(3)
C15	0.4807(4)	-0.0539(3)	0.2931(3)	C54	0.0494(4)	0.2386(3)	0.4564(3)
C16	0.4180(5)	0.0116(4)	0.1519(3)	C55	0.1511(4)	0.3218(3)	0.4556(2)
C17	0.2272(5)	-0.1876(4)	0.1563(4)	C56	0.2217(4)	0.3554(3)	0.5254(3)
C18	0.2527(5)	-0.2729(4)	0.3309(4)	C57	0.3109(4)	0.4356(4)	0.5210(3)
C19	0.4732(6)	-0.1432(5)	0.4324(3)	C58	0.3273(4)	0.4800(3)	0.4472(3)
C20	0.5737(5)	0.0337(4)	0.3185(4)	C59	0.2564(4)	0.4411(3)	0.3799(3)

C111, C112, C113 and C114 are the calculated centroids of the rings C1 - C5, C11 - C15, C21 -C25 and C31 - C35, respectively.

2.1.2 Positional Parameters for Hydrogen Atoms of $[(Me_5C_5)_2Yb(bipy)]^+[(Me_5C_5)_2YbCl_2]^-$

atom	x	y	z	atom	x	y	z
H61	0.4804	-0.1898	-0.4010	H272	0.0137	0.3692	0.0426
H62	0.3761	-0.2060	0.0197	H273	-0.0868	0.2792	0.0458
H63	0.4628	-0.1068	0.0232	H281	-0.3210	0.2512	0.1530
H71	0.4367	-0.4299	0.0218	H282	-0.2154	0.1862	0.1343
H72	0.4230	-0.4500	0.1135	H283	-0.2650	0.1857	0.2205
H73	0.3527	-0.3678	0.0706	H291	-0.2975	0.3802	0.3351
H81	0.7208	-0.4770	0.1131	H292	-0.2546	0.2739	0.3455
H82	0.7466	-0.4392	0.2026	H293	-0.1845	0.3638	0.3948
H83	0.6150	-0.4862	0.1721	H301	-0.0779	0.5746	0.3285
H91	0.9136	-0.2626	0.1183	H302	-0.0336	0.4969	0.3903
H92	0.8938	-0.1801	0.1814	H303	0.0606	0.5536	0.3361
H93	0.8823	-0.2916	0.2060	H361	0.4754	0.2740	0.2464
H101	0.7594	-0.0712	0.0379	H362	0.4034	0.3676	0.2341
H102	0.6563	-0.0310	0.0862	H363	0.4129	0.3183	0.3188
H103	0.7804	-0.0539	0.1314	H371	0.3193	0.2670	0.0619
H161	0.3592	0.0575	0.1615	H372	0.1899	0.3075	0.0551
H162	0.4987	0.0463	0.1532	H373	0.2979	0.3633	0.1096
H163	0.3981	-0.0198	0.1000	H381	0.0946	0.0664	0.0596
H171	0.1565	-0.1526	0.1631	H382	-0.0227	0.0773	0.1065
H172	0.2553	-0.1754	0.1036	H383	0.0294	0.1641	0.0532
H173	0.2056	-0.2573	0.1621	H391	0.1151	-0.0424	0.2413
H181	0.1833	-0.2454	0.3513	H392	0.0625	0.0093	0.3143
H182	0.2250	-0.3199	0.2884	H393	-0.0095	0.0051	0.2293
H183	0.2957	-0.3055	0.3736	H401	0.3425	0.0822	0.3623
H191	0.4235	-0.1069	0.4650	H402	0.3170	0.1841	0.3995
H192	0.4628	-0.2120	0.4455	H403	0.2141	0.0951	0.3948

H193	0.5580	-0.1184	0.4425	H501	-0.1300	0.1061	0.3307
H201	0.5315	0.0866	0.3385	H511	-0.1984	0.0312	0.4469
H202	0.6309	0.0137	0.3600	H521	-0.1113	0.0915	0.5734
H203	0.6172	0.0560	0.2729	H531	0.0478	0.2228	0.5796
H261	0.0448	0.5757	0.1421	H561	0.2091	0.3236	0.5758
H262	0.1453	0.5494	0.2079	H571	0.3602	0.4598	0.5683
H263	0.1327	0.4951	0.1237	H581	0.3864	0.5364	0.4428
H271	-0.1260	0.3862	0.0326	H591	0.2693	0.4710	0.3288

2.2 Thermal Parameters for Non-Hydrogen Atoms of $[(Me_5C_5)_2Yb(bipy)]^+[(Me_5C_5)_2YbCl_2]^-$

atom	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)
YB1	3.333(8)	3.639(8)	2.983(8)	0.025(7)	-0.148(6)	0.658(6)
YB2	3.366(8)	3.543(8)	2.974(8)	0.297(7)	0.080(6)	0.364(6)
Cl1	4.86(5)	6.90(7)	5.21(6)	-0.12(5)	-1.76(5)	0.37(5)
Cl2	7.59(7)	4.78(5)	5.65(6)	-0.02(5)	0.90(5)	2.11(4)
N1	3.5(1)	3.9(1)	3.3(1)	0.2(1)	-0.1(1)	0.6(1)
N2	3.4(1)	4.4(2)	3.7(2)	0.1(1)	-0.1(1)	0.5(1)
C1	4.0(2)	5.5(2)	3.3(2)	1.4(2)	0.1(2)	0.5(2)
C2	3.4(2)	5.3(2)	4.4(2)	0.3(2)	0.3(2)	-0.4(2)
C3	4.5(2)	4.7(2)	4.5(2)	1.5(2)	-0.1(2)	0.0(2)
C4	3.3(2)	6.0(2)	4.0(2)	0.9(2)	0.2(2)	-0.1(2)
C5	4.2(2)	4.8(2)	3.7(2)	0.3(2)	1.0(2)	0.6(2)
C6	7.0(3)	9.1(3)	3.9(2)	3.2(2)	-0.8(2)	1.1(2)
C7	6.0(3)	7.1(3)	6.5(3)	-0.4(2)	0.2(2)	-2.2(2)
C8	7.4(3)	6.2(3)	8.4(3)	2.9(2)	0.5(3)	0.2(2)
C9	3.4(2)	9.1(3)	8.1(3)	0.9(2)	0.1(2)	-0.2(3)
C10	7.0(3)	6.8(3)	7.4(3)	-0.5(2)	2.7(2)	1.5(2)
C11	4.1(2)	3.8(2)	5.0(2)	0.9(2)	0.6(2)	0.2(2)
C12	3.3(2)	4.8(2)	5.1(2)	0.5(2)	0.2(2)	-0.8(2)

C13	4.4(2)	4.4(2)	5.8(2)	-0.8(2)	1.8(2)	-0.6(2)
C14	5.5(2)	5.2(2)	4.2(2)	-0.1(2)	0.8(2)	-0.6(2)
C15	4.3(2)	3.8(2)	5.3(2)	-0.2(2)	0.8(2)	-0.4(2)
C16	7.5(3)	5.9(2)	7.1(3)	2.5(2)	1.7(2)	2.1(2)
C17	4.2(2)	7.7(3)	8.3(3)	1.2(2)	-0.3(2)	-2.3(3)
C18	6.4(3)	6.4(3)	10.2(4)	-1.2(2)	4.0(2)	0.2(3)
C19	10.4(4)	8.5(3)	4.8(3)	0.0(3)	0.9(3)	-0.2(3)
C20	5.5(3)	4.9(2)	10.3(4)	-1.0(2)	0.3(3)	-0.6(3)
C21	3.9(2)	4.4(2)	4.5(2)	0.8(2)	-0.2(2)	1.2(2)
C22	4.7(2)	5.4(2)	3.8(2)	0.7(2)	-0.7(2)	0.7(2)
C23	3.8(2)	5.6(2)	4.6(2)	-0.5(2)	-1.0(2)	0.9(2)
C24	3.0(2)	5.3(2)	4.7(2)	0.8(2)	-0.0(2)	1.1(2)
C25	4.0(2)	4.3(2)	4.5(2)	1.2(2)	-0.4(2)	0.6(2)
C26	5.7(3)	5.2(2)	6.9(3)	0.1(2)	0.7(2)	2.0(2)
C27	8.2(3)	9.0(3)	3.6(2)	1.0(3)	-1.0(2)	1.1(2)
C28	5.6(3)	8.5(3)	7.7(3)	-1.7(3)	-1.4(3)	0.0(3)
C29	4.5(2)	7.1(3)	7.1(3)	1.0(2)	1.6(2)	1.0(2)
C30	5.9(2)	5.3(2)	6.1(3)	1.4(2)	0.4(2)	-0.5(2)
C31	4.1(2)	5.6(2)	7.7(3)	1.2(2)	1.4(2)	-1.6(2)
C32	5.2(2)	5.3(2)	4.8(2)	1.0(2)	2.2(2)	0.0(2)
C33	5.8(2)	5.3(2)	5.5(2)	0.5(2)	1.4(2)	-0.8(2)
C34	7.0(3)	4.1(2)	5.7(2)	0.9(2)	1.7(2)	0.1(2)
C35	6.4(2)	5.3(2)	6.4(3)	2.7(2)	1.3(2)	0.7(2)
C36	4.1(3)	9.9(4)	15.2(5)	0.9(3)	1.4(3)	-4.0(4)
C37	9.4(3)	7.6(3)	8.4(3)	1.5(3)	5.1(2)	2.0(3)
C38	10.1(4)	8.0(3)	7.6(3)	-0.0(3)	0.7(3)	-3.3(3)
C39	12.7(4)	4.1(3)	11.6(4)	-0.1(3)	5.5(3)	0.2(3)
C40	10.0(3)	10.2(3)	7.0(3)	6.0(2)	0.4(3)	1.4(3)
C50	4.6(2)	5.0(2)	5.2(2)	-0.7(2)	-0.4(2)	0.7(2)

C51	4.8(2)	5.7(2)	7.0(3)	-1.0(2)	0.2(2)	2.5(2)
C52	6.0(3)	7.2(3)	5.3(2)	-1.1(2)	0.7(2)	2.8(2)
C53	5.3(2)	5.8(2)	4.0(2)	-0.4(2)	0.2(2)	1.2(2)
C54	3.7(2)	3.8(2)	3.6(2)	0.6(1)	0.3(2)	1.0(1)
C55	3.0(2)	4.0(2)	3.3(2)	0.4(1)	-0.0(1)	0.5(1)
C56	4.9(2)	5.1(2)	3.3(2)	0.7(2)	0.0(2)	0.9(2)
C57	4.9(2)	5.4(2)	4.3(2)	0.0(2)	-1.2(2)	0.1(2)
C58	4.2(2)	5.2(2)	5.0(2)	-1.0(2)	-0.6(2)	0.6(2)
C59	4.0(2)	4.4(2)	4.3(2)	-0.1(2)	0.0(2)	0.9(2)

The form of the anisotropic thermal parameter is:

$\exp[-0.25\{h^2a^{*2}B(1,1) + k^2b^{*2}B(2,2) + l^2c^{*2}B(3,3) + 2hka^*b^*B(1,2) + 2hla^*c^*B(1,3) + 2klb^*c^*B(2,3)\}]$, where a^*, b^* and c^* are reciprocal lattice constants.

2.3 Bond Lengths Involving Non-Hydrogen Atoms of $[(Me_5C_5)_2Yb(bipy)]^+[(Me_5C_5)_2YbCl_2]^-$

atom	atom	distance	atom	atom	distance
Yb1	Cl1	2.573(1)	C5	C10	1.512(5)
Yb1	Cl2	2.560(1)	C11	C12	1.412(5)
Yb1	C1	2.612(3)	C11	C15	1.400(5)
Yb1	C2	2.631(4)	C11	C16	1.508(5)
Yb1	C3	2.689(4)	C12	C13	1.401(5)
Yb1	C4	2.672(3)	C12	C17	1.495(5)
Yb1	C5	2.612(3)	C13	C14	1.411(5)
Yb1	C11	2.663(3)	C13	C18	1.516(5)
Yb1	C12	2.665(3)	C14	C15	1.419(5)
Yb1	C13	2.667(4)	C14	C19	1.493(6)
Yb1	C14	2.647(4)	C15	C20	1.509(5)
Yb1	C15	2.642(3)	C21	C22	1.429(5)
Yb1	C111	2.358	C21	C25	1.411(5)
Yb1	C112	2.371	C21	C26	1.501(5)

Yb2	N1	2.363(3)	C22	C23	1.418(5)
Yb2	N2	2.381(3)	C22	C27	1.497(5)
Yb2	C21	2.582(3)	C23	C24	1.412(5)
Yb2	C22	2.602(3)	C23	C28	1.509(5)
Yb2	C23	2.592(3)	C24	C25	1.413(5)
Yb2	C24	2.614(3)	C24	C29	1.505(5)
Yb2	C25	2.601(3)	C25	C30	1.500(5)
Yb2	C31	2.592(4)	C31	C32	1.414(6)
Yb2	C32	2.591(3)	C31	C35	1.414(6)
Yb2	C33	2.588(4)	C31	C36	1.500(6)
Yb2	C34	2.592(4)	C32	C33	1.409(5)
Yb2	C35	2.587(4)	C32	C37	1.495(6)
Yb2	C113	2.302	C33	C34	1.387(6)
Yb2	C114	2.300	C33	C38	1.517(7)
N1	C55	1.347(4)	C34	C35	1.376(6)
N1	C59	1.342(4)	C34	C39	1.517(6)
N2	C50	1.336(4)	C35	C40	1.516(6)
N2	C54	1.340(4)	C50	C51	1.369(5)
C1	C2	1.408(5)	C51	C52	1.366(6)
C1	C5	1.404(5)	C52	C53	1.378(5)
C1	C6	1.506(5)	C53	C54	1.389(5)
C2	C3	1.419(5)	C54	C55	1.492(4)
C2	C7	1.508(5)	C55	C56	1.381(5)
C3	C4	1.404(5)	C56	C57	1.383(5)
C3	C8	1.496(5)	C57	C58	1.374(5)
C4	C5	1.394(5)	C58	C59	1.371(5)
C4	C9	1.510(5)			

2.4 Bond Angles Involving Non-Hydrogen Atoms of $[(Me_5C_5)_2Yb(bipy)]^+[(Me_5C_5)_2YbCl_2]^-$

atom	atom	atom	angle	atom	atom	atom	angle
Cl1	Yb1	Cl2	97.25(3)	C11	C15	C20	125.4(4)
Cl1	Yb1	C111	104.6	C14	C15	C20	126.1(4)
Cl1	Yb1	C112	103.9	C22	C21	C25	107.8(3)
Cl2	Yb1	C111	103.8	C22	C21	C26	125.6(3)
Cl2	Yb1	C112	105.1	C25	C21	C26	126.1(4)
C111	Yb1	C112	135.9	C21	C22	C23	107.4(3)
N1	Yb2	N2	68.96(9)	C21	C22	C27	125.7(4)
N1	Yb2	C113	106.5	C23	C22	C27	125.8(4)
N1	Yb2	C114	105.5	C22	C23	C24	108.3(3)
N2	Yb2	C113	106.4	C22	C23	C28	125.7(4)
N2	Yb2	C114	104.7	C24	C23	C28	125.5(4)
C113	Yb2	C114	141.5	C23	C24	C25	108.0(3)
Yb2	N1	C55	119.1(2)	C23	C24	C29	126.1(3)
Yb2	N1	C59	122.6(2)	C25	C24	C29	125.3(4)
C55	N1	C59	118.0(3)	C21	C25	C24	108.4(3)
Yb2	N2	C50	123.2(2)	C21	C25	C30	126.0(3)
Yb2	N2	C54	118.7(2)	C24	C25	C30	124.9(3)
C50	N2	C54	118.1(3)	C32	C31	C35	108.2(4)
C2	C1	C5	107.7(3)	C32	C31	C36	124.2(5)
C2	C1	C6	124.9(4)	C35	C31	C36	127.0(5)
C5	C1	C6	126.3(4)	C31	C32	C33	106.2(4)
C1	C2	C3	107.8(3)	C31	C32	C37	125.5(4)
C1	C2	C7	126.4(3)	C33	C32	C37	127.5(4)
C3	C2	C7	125.5(4)	C32	C33	C34	108.9(4)
C2	C3	C4	107.5(3)	C32	C33	C38	126.9(4)
C2	C3	C8	125.9(4)	C34	C33	C38	123.6(4)
C4	C3	C8	126.4(3)	C33	C34	C35	109.0(4)

C3	C4	C5	108.4(3)	C33	C34	C39	125.6(5)
C3	C4	C9	125.1(3)	C35	C34	C39	124.8(4)
C5	C4	C9	125.9(4)	C31	C35	C34	107.7(4)
C1	C5	C4	108.5(3)	C31	C35	C40	127.1(5)
C1	C5	C10	126.0(3)	C34	C35	C40	124.8(5)
C4	C5	C10	125.2(3)	N2	C50	C51	123.5(4)
C12	C11	C15	108.5(3)	C50	C51	C52	118.4(4)
C12	C11	C16	126.4(4)	C51	C52	C53	119.6(4)
C15	C11	C16	123.7(3)	C52	C53	C54	118.8(4)
C11	C12	C13	107.3(3)	N2	C54	C53	121.6(3)
C11	C12	C17	127.7(4)	N2	C54	C55	116.5(3)
C13	C12	C17	124.2(4)	C53	C54	C55	121.8(3)
C12	C13	C14	109.1(3)	N1	C55	C54	116.0(3)
C12	C13	C18	125.0(4)	N1	C55	C56	121.7(3)
C14	C13	C18	125.5(4)	C54	C55	C56	122.3(3)
C13	C14	C15	106.9(3)	C55	C56	C57	119.3(3)
C13	C14	C19	126.5(4)	C56	C57	C58	119.1(3)
C15	C14	C19	126.5(4)	C57	C58	C59	119.5(3)
C11	C15	C14	108.2(3)	N1	C59	C58	123.3(3)

2.5 Least Squares Planes of $[(Me_5C_5)_2Yb(bipy)]^+[(Me_5C_5)_2YbCl_2]^-$

Plane 1		Plane 2	
Atoms defining plane	Distance	Atoms defining plane	Distance
C1	-0.011	C11	-0.007
C2	0.010	C12	0.010
C3	-0.005	C13	-0.009
C4	-0.002	C14	0.005
C5	0.008	C15	0.001
Additional Atoms	Distance	Additional Atoms	Distance
YB1	2.356	YB1	2.371
C6	-0.374	C16	-0.301
C7	-0.089	C17	-0.164
C8	-0.132	C18	-0.181
C9	-0.182	C19	-0.057
C10	-0.077	C20	-0.136
Plane 3		Plane 4	
Atoms defining plane	Distance	Atoms defining plane	Distance
C21	0.008	C31	-0.007
C22	-0.012	C32	0.006
C23	0.011	C33	-0.002
C24	-0.006	C34	-0.003
C25	-0.001	C35	0.006
Additional Atoms	Distance	Additional Atoms	Distance
YB2	2.302	YB2	2.300
C26	-0.124	C36	-0.201
C27	-0.296	C37	-0.189
C28	-0.107	C38	-0.206
C29	-0.199	C39	-0.192

C30	-0.206

Plane 5

Atoms defining plane	Distance
N1	-0.011
C55	0.016
C56	0.000
C57	-0.008
C58	0.013
C59	-0.003
Additional Atoms	**Distance**
YB2	-0.318
C54	0.080
N2	-0.047

C40	-0.133

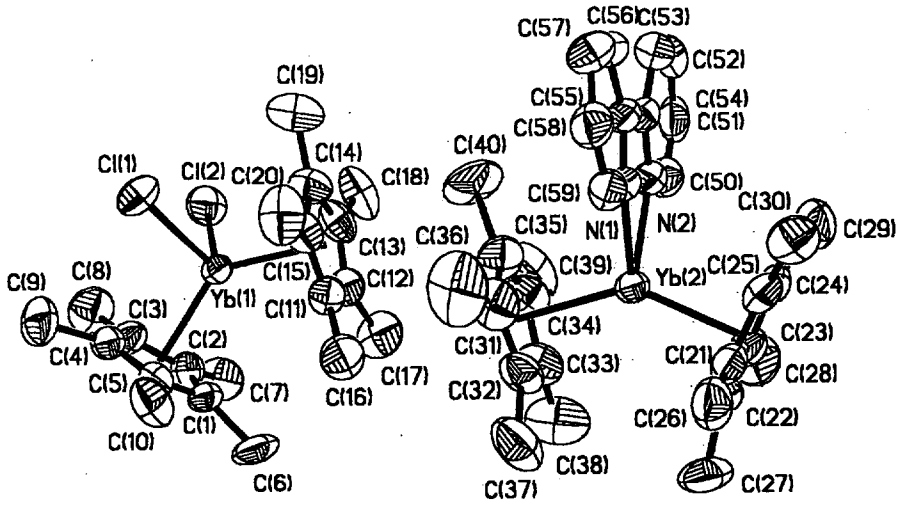
Plane 6

Atoms defining plane	Distance
N2	0.008
C50	0.001
C51	-0.008
C52	0.006
C53	0.003
C54	-0.010
Additional Atoms	**Distance**
YB2	0.043
C55	-0.030
N2	0.124

Dihedral angles between planes:

	1	3	4	5
2	134.0	4	140.9	
		5	151.0	10.1
		6	158.7	18.0	8.0

2.6 ORTEP diagram of $[(Me_5C_5)_2Yb(bipy)]^+[(Me_5C_5)_2YbCl_2]^-$ (50% probability ellipsoids) showing atom labelling scheme



3. Crystal structure of $[1,3\text{-}(Me_3C)_2C_5H_3]_2Yb(bipy).toluene$

3.1 Positional Parameters for $[1,3\text{-}(Me_3C)_2C_5H_3]_2Yb(bipy).toluene$

3.1.1 Positional Parameters for Non-Hydrogen Atoms of $[1,3\text{-}(Me_3C)_2C_5H_3]_2Yb(bipy).toluene$

atom	x	y	z	atom	x	y	z
Yb(1)	0.6250	0.1250	0.38867(1)	C(11)	0.4760(4)	0.3001(3)	0.3678(3)
N(1)	0.5695(2)	0.0913(2)	0.3188(1)	C(12)	0.5194(6)	0.2391(4)	0.3093(3)
C(1)	0.5194(3)	0.0535(3)	0.3189(2)	C(13)	0.5994(4)	0.2988(3)	0.3502(3)
C(2)	0.4973(3)	0.0253(2)	0.2822(2)	C(14)	0.4663(3)	0.1124(3)	0.4650(2)
C(3)	0.5274(4)	0.0371(3)	0.2419(2)	C(15)	0.4489(4)	0.0628(3)	0.4365(2)
C(4)	0.5778(3)	0.0773(3)	0.2402(2)	C(16)	0.3982(4)	0.1406(3)	0.4763(3)
C(5)	0.5976(3)	0.1039(2)	0.2790(2)	C(17)	0.4993(5)	0.0931(4)	0.5077(2)
C(6)	0.5120(3)	0.1526(3)	0.4403(2)	C(18)	0.5704(3)	0.1801(2)	0.4569(2)
C(7)	0.4966(3)	0.1767(3)	0.3985(2)	C(19)	0.8750	0.4291(8)	0.3750
C(8)	0.5438(3)	0.2193(2)	0.3898(2)	C(20)	0.8114(7)	0.4041(6)	0.3746(5)
C(9)	0.5902(3)	0.2212(2)	0.4262(2)	C(21)	0.753(2)	0.336(1)	0.375(1)

C(10)	0.5347(4)	0.2628(3)	0.3538(2)	C(100)	0.5426	0.1900	0.4223

C(100) is the calculated centroid of the ring C(6), C(7), C(8), C(9), C(18).

3.1.2 Positional Parameters for Hydrogen Atoms of [1,3-(Me$_3$C)$_2$C$_5$H$_3$]$_2$Yb(bipy).toluene

atom	x	y	z	atom	x	y	z
H(1)	0.5163	0.1244	0.5248	H(14)	0.4321	0.2814	0.3646
H(2)	0.3692	0.1189	0.4963	H(15)	0.5221	0.2672	0.2865
H(3)	0.4206	0.0382	0.4501	H(16)	0.5500	0.2107	0.3015
H(4)	0.4725	0.2249	0.3080	H(17)	0.6386	0.2783	0.3404
H(5)	0.4753	0.3321	0.3510	H(18)	0.5922	0.3280	0.3288
H(6)	0.4955	0.0467	0.3471	H(19)	0.6100	0.3153	0.3780
H(7)	0.4617	-0.0019	0.2842	H(20)	0.4226	0.0773	0.4096
H(8)	0.5125	0.0184	0.2153	H(21)	0.4891	0.0469	0.4243
H(9)	0.5993	0.0849	0.2110	H(22)	0.4075	0.1746	0.4945
H(10)	0.4585	0.1654	0.3790	H(23)	0.3721	0.1517	0.4522
H(11)	0.6284	0.2476	0.4289	H(24)	0.4720	0.0716	0.5253
H(12)	0.5939	0.1737	0.4855	H(25)	0.5425	0.0723	0.5008
H(13)	0.4810	0.3088	0.3988				

3.2 Thermal Parameters for Non-Hydrogen Atoms of [1,3-(Me$_3$C)$_2$C$_5$H$_3$]$_2$Yb(bipy).toluene

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Yb(1)	0.0302(2)	0.0247(2)	0.0205(2)	0.0014(3)	0.0000	0.0000
N(1)	0.028(3)	0.026(3)	0.025(3)	0.001(3)	-0.001(2)	-0.005(2)
C(1)	0.035(4)	0.032(4)	0.030(3)	0.000(3)	0.006(3)	0.005(3)
C(2)	0.033(4)	0.037(4)	0.039(4)	-0.008(3)	-0.001(3)	-0.002(3)
C(3)	0.049(4)	0.045(4)	0.026(3)	-0.002(4)	-0.010(3)	-0.004(3)
C(4)	0.047(4)	0.039(4)	0.028(3)	-0.011(3)	0.002(3)	-0.004(3)
C(5)	0.032(3)	0.028(3)	0.024(3)	0.001(3)	-0.002(3)	0.004(2)
C(6)	0.035(4)	0.031(3)	0.029(3)	0.004(3)	0.006(3)	-0.003(3)
C(7)	0.031(4)	0.042(4)	0.027(3)	0.008(3)	0.002(3)	-0.011(3)

C(8)	0.040(4)	0.036(4)	0.027(3)	0.013(3)	0.005(3)	-0.001(3)
C(9)	0.029(3)	0.026(3)	0.030(3)	0.001(3)	0.002(3)	-0.004(3)
C(10)	0.062(5)	0.045(4)	0.032(3)	0.026(4)	0.008(3)	0.004(3)
C(11)	0.075(5)	0.067(5)	0.073(6)	0.043(4)	0.020(5)	0.030(5)
C(12)	0.21(1)	0.065(6)	0.044(5)	0.048(7)	-0.032(6)	-0.002(4)
C(13)	0.083(8)	0.070(6)	0.101(7)	0.013(5)	0.025(5)	0.055(5)
C(14)	0.045(4)	0.046(5)	0.039(3)	-0.006(3)	0.018(3)	-0.004(3)
C(15)	0.057(5)	0.050(5)	0.057(4)	-0.010(4)	0.021(4)	-0.002(4)
C(16)	0.068(6)	0.067(6)	0.104(6)	-0.016(4)	0.055(5)	-0.013(5)
C(17)	0.091(7)	0.094(7)	0.057(5)	-0.038(6)	0.014(5)	0.033(5)
C(18)	0.035(4)	0.031(4)	0.022(3)	0.013(3)	0.002(3)	-0.004(3)
C(19)	0.24(3)	0.13(2)	0.053(8)	0.0000	-0.06(2)	0.0000
C(20)	0.21(2)	0.21(2)	0.046(5)	0.03(1)	-0.02(1)	-0.05(1)

The general temperature factor expression:

$\exp[-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl)]$

3.3 Bond Lengths of $[1,3\text{-}(Me_3C)_2C_5H_3]_2Yb(bipy)$.toluene

3.3.1 Bond Lengths Involving Non-Hydrogen Atoms of $[1,3\text{-}(Me_3C)_2C_5H_3]_2Yb(bipy)$.toluene

atom	atom	distance	atom	atom	distance
Yb(1)	N(1)	2.503(4)	C(6)	C(18)	1.406(9)
Yb(1)	C(6)	2.766(6)	C(7)	C(8)	1.411(9)
Yb(1)	C(7)	2.803(6)	C(8)	C(9)	1.419(8)
Yb(1)	C(8)	2.791(6)	C(8)	C(10)	1.527(9)
Yb(1)	C(9)	2.696(6)	C(9)	C(18)	1.417(8)
Yb(1)	C(18)	2.674(6)	C(10)	C(11)	1.52(1)
Yb(1)	C(100)	2.468	C(10)	C(12)	1.49(1)
N(1)	C(1)	1.338(8)	C(10)	C(13)	1.53(1)
N(1)	C(5)	1.351(7)	C(14)	C(15)	1.52(1)
C(1)	C(2)	1.369(8)	C(14)	C(16)	1.53(1)

C(2)	C(3)	1.376(8)	C(14)	C(17)	1.51(1)
C(3)	C(4)	1.39(1)	C(19)	C(20)	1.37(2)
C(4)	C(5)	1.392(8)	C(19)	C(20)	1.37(2)
C(5)	C(5)	1.48(1)	C(20)	C(20)	1.43(3)
C(6)	C(7)	1.423(8)	C(20)	C(21)	1.15(4)
C(6)	C(14)	1.516(9)			

3.3.2 Bond Lengths Involving Hydrogen Atoms of [1,3-(Me$_3$C)$_2$C$_5$H$_3$]$_2$Yb(bipy).toluene

atom	atom	distance	atom	atom	distance
C(1)	H(6)	0.98	C(13)	H(18)	0.97
C(2)	H(7)	0.96	C(13)	H(19)	0.95
C(3)	H(8)	0.97	C(15)	H(3)	0.91
C(4)	H(9)	0.99	C(15)	H(20)	1.02
C(7)	H(10)	0.98	C(15)	H(21)	0.94
C(9)	H(11)	0.99	C(16)	H(2)	0.98
C(11)	H(5)	0.93	C(16)	H(22)	1.01
C(11)	H(13)	0.96	C(16)	H(23)	0.92
C(11)	H(14)	0.97	C(17)	H(1)	0.98
C(12)	H(4)	0.97	C(17)	H(24)	0.91
C(12)	H(15)	0.97	C(17)	H(25)	1.00
C(12)	H(16)	0.94	C(18)	H(12)	0.99
C(13)	H(17)	0.96			

3.4 Bond Angles of [1,3-(Me$_3$C)$_2$C$_5$H$_3$]$_2$Yb(bipy).toluene

3.4.1 Bond Angles Involving Non-Hydrogen Atoms of [1,3-(Me$_3$C)$_2$C$_5$H$_3$]$_2$Yb(bipy).toluene

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	Yb(1)	N(1)	65.5(2)	C(9)	C(8)	C(10)	126.7(5)
N(1)	Yb(1)	C(100)	106.3	C(8)	C(9)	C(18)	108.1(5)
N(1)	Yb(1)	C(100)	114.2	C(8)	C(10)	C(11)	108.0(5)

C(100)	Yb(1)	C(100)	131.6	C(8)	C(10)	C(12)	112.9(6)
Yb(1)	N(1)	C(1)	122.4(3)	C(8)	C(10)	C(13)	110.9(6)
Yb(1)	N(1)	C(5)	119.8(4)	C(11)	C(10)	C(12)	109.6(7)
C(1)	N(1)	C(5)	116.8(5)	C(11)	C(10)	C(13)	106.6(6)
N(1)	C(1)	C(2)	124.8(5)	C(12)	C(10)	C(13)	108.7(6)
C(1)	C(2)	C(3)	118.3(6)	C(6)	C(14)	C(15)	111.7(5)
C(2)	C(3)	C(4)	118.6(5)	C(6)	C(14)	C(16)	108.6(5)
C(3)	C(4)	C(5)	119.6(5)	C(6)	C(14)	C(17)	111.9(6)
N(1)	C(5)	C(4)	121.8(4)	C(15)	C(14)	C(16)	107.1(6)
N(1)	C(5)	C(5)	116.6(3)	C(15)	C(14)	C(17)	109.0(6)
C(4)	C(5)	C(5)	121.6(4)	C(16)	C(14)	C(17)	108.4(6)
C(7)	C(6)	C(14)	125.4(5)	C(6)	C(18)	C(9)	109.0(5)
C(7)	C(6)	C(18)	106.5(5)	C(20)	C(19)	C(20)	127(2)
C(14)	C(6)	C(18)	127.2(5)	C(20)	C(19)	C(21)	112(1)
C(6)	C(7)	C(8)	109.6(5)	C(20)	C(19)	C(21)	112(1)
C(7)	C(8)	C(9)	106.8(5)	C(19)	C(20)	C(20)	116(1)
C(7)	C(8)	C(10)	125.0(5)	C(20)	C(20)	C(21)	124(1)

3.4.2 Bond Angles Involving Hydrogen Atoms of [1,3-$(Me_3C)_2C_5H_3]_2$Yb(bipy).toluene

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	C(1)	H(6)	117.4	C(10)	C(13)	H(18)	110.7
C(2)	C(1)	H(6)	117.7	C(10)	C(13)	H(19)	110.9
C(1)	C(2)	H(7)	121.5	H(17)	C(13)	H(18)	107.2
C(3)	C(2)	H(7)	120.2	H(17)	C(13)	H(19)	108.8
C(2)	C(3)	H(8)	120.5	H(18)	C(13)	H(19)	107.6
C(4)	C(3)	H(8)	120.9	C(14)	C(15)	H(3)	113.9
C(3)	C(4)	H(9)	117.6	C(14)	C(15)	H(20)	106.3
C(5)	C(4)	H(9)	122.8	C(14)	C(15)	H(21)	111.4
C(6)	C(7)	H(10)	124.8	H(3)	C(15)	H(20)	106.8

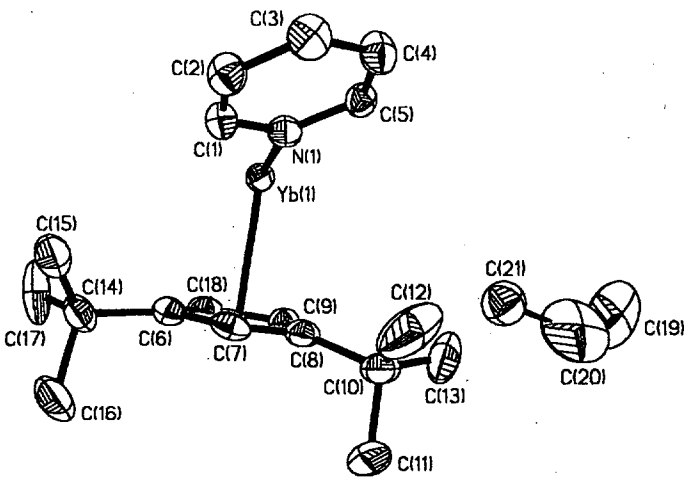
C(8)	C(7)	H(10)	125.6	H(3)	C(15)	H(21)	113.4
C(8)	C(9)	H(11)	124.0	H(20)	C(15)	H(21)	104.3
C(18)	C(9)	H(11)	127.9	C(14)	C(16)	H(2)	112.7
C(10)	C(11)	H(5)	111.4	C(14)	C(16)	H(22)	109.7
C(10)	C(11)	H(13)	109.0	C(14)	C(16)	H(23)	115.4
C(10)	C(11)	H(14)	110.1	H(2)	C(16)	H(22)	102.4
H(5)	C(11)	H(13)	110.0	H(2)	C(16)	H(23)	109.2
H(5)	C(11)	H(14)	109.2	H(22)	C(16)	H(23)	106.3
H(13)	C(11)	H(14)	107.0	C(14)	C(17)	H(1)	110.3
C(10)	C(12)	H(4)	111.1	C(14)	C(17)	H(24)	115.5
C(10)	C(12)	H(15)	110.4	C(14)	C(17)	H(25)	109.5
C(10)	C(12)	H(16)	112.7	H(1)	C(17)	H(24)	109.8
H(4)	C(12)	H(15)	105.8	H(1)	C(17)	H(25)	103.0
H(4)	C(12)	H(16)	108.2	H(24)	C(17)	H(25)	108.0
H(15)	C(12)	H(16)	108.3	C(6)	C(18)	H(12)	127.1
C(10)	C(13)	H(17)	111.7	C(9)	C(18)	H(12)	123.9

3.5 Least Squares Planes of $[1,3\text{-}(Me_3C)_2C_5H_3]_2Yb(bipy)$.toluene

Plane 1.	χ^2 = 4.1	Plane 2.	χ^2 = 33.8
Atoms defining plane	Distance	Atoms defining plane	Distance
C(6)	-0.0078	N(1)	0.0135
C(7)	0.0077	C(1)	-0.0154
C(8)	-0.0045	C(2)	-0.0023
C(9)	0.0000	C(3)	0.0120
C(18)	0.0021	C(4)	-0.0041
Additional atoms	Distance	C(5)	-0.0099
Yb(1)	2.4625	Additional atoms	Distance
C(10)	-0.3075	Yb(1)	0.5131
C(14)	-0.2367		

Dihedral angle between planes: 36.4°

3.6 ORTEP diagram of [1,3-(Me$_3$C)$_2$C$_5$H$_3$]$_2$Yb(bipy).toluene (50% probability ellipsoids) showing atom labelling scheme (only the assymetric unit, which consists of half the molecule, is shown)



4. Crystal structure of [1,3-(Me$_3$Si)$_2$C$_5$H$_3$]$_2$Yb(phen)

4.1 Positional Parameters for [1,3-(Me$_3$Si)$_2$C$_5$H$_3$]$_2$Yb(phen)

4.1.1 Positional Parameters for Non-Hydrogen Atoms of [1,3-(Me$_3$Si)$_2$C$_5$H$_3$]$_2$Yb(phen)

atom	x	y	z	atom	x	y	z
Yb(1)	1.03728(2)	0.19296(1)	0.75747(2)	C(16)	1.2060(5)	0.1904(3)	0.6710(3)
Si(1)	0.6579(2)	0.2253(1)	0.7313(1)	C(17)	1.4637(6)	0.0258(4)	0.8496(4)
Si(2)	1.1065(2)	0.37359(9)	0.8749(1)	C(18)	1.2021(6)	-0.0100(3)	0.8455(4)
Si(3)	1.3150(2)	0.0622(1)	0.8600(1)	C(19)	1.3383(6)	0.0987(4)	0.9595(4)
Si(4)	1.1760(1)	0.21223(8)	0.5660(1)	C(20)	1.2964(6)	0.1723(3)	0.5259(3)
N(1)	0.9302(4)	0.0834(2)	0.7061(3)	C(21)	1.1790(6)	0.3078(4)	0.5548(3)
N(2)	0.9724(4)	0.1217(2)	0.8578(3)	C(22)	1.0254(6)	0.1813(4)	0.5054(4)
C(1)	0.8938(5)	0.2846(3)	0.8122(3)	C(23)	0.9137(6)	0.0619(3)	0.6338(4)
C(2)	0.8162(5)	0.2606(3)	0.7416(3)	C(24)	0.8529(6)	0.0011(4)	0.6042(4)
C(3)	0.8688(5)	0.2865(3)	0.6825(3)	C(25)	0.8058(6)	-0.0394(3)	0.6522(4)
C(4)	0.9749(5)	0.3254(3)	0.7169(3)	C(26)	0.8178(5)	-0.0195(3)	0.7287(3)
C(5)	0.9945(5)	0.3237(3)	0.7995(3)	C(27)	0.8835(5)	0.0423(3)	0.7542(3)

C(6)	0.6327(6)	0.2144(4)	0.8289(4)	C(28)	0.9013(5)	0.0638(3)	0.8322(3)
C(7)	0.6219(6)	0.1408(4)	0.6803(4)	C(29)	0.8473(5)	0.0243(3)	0.8813(3)
C(8)	0.5460(6)	0.2880(3)	0.6747(5)	C(30)	0.8655(6)	0.0467(3)	0.9577(4)
C(9)	1.1584(6)	0.3196(3)	0.9638(4)	C(31)	0.9366(6)	0.1042(3)	0.9834(4)
C(10)	1.0319(7)	0.4522(4)	0.9031(5)	C(32)	0.9894(5)	0.1398(3)	0.9309(4)
C(11)	1.2437(6)	0.4021(3)	0.8430(4)	C(33)	0.7652(5)	-0.0576(3)	0.7805(4)
C(12)	1.2166(5)	0.1254(3)	0.7077(3)	C(34)	0.7771(6)	-0.0359(3)	0.8526(4)
C(13)	1.2626(5)	0.1322(3)	0.7882(3)	C(100)	0.910	0.296	0.751
C(14)	1.2825(5)	0.2048(3)	0.8024(3)	C(101)	1.243	0.179	0.740
C(15)	1.2493(5)	0.2397(3)	0.7310(4)				

C(100) and C(101) are the calculated centroids of the rings C(1) - C(5) and C(12) - C(16), respectively.

4.1.2 Positional Parameters for Hydrogen Atoms of $[1,3\text{-}(Me_3Si)_2C_5H_3]_2Yb(phen)$

atom	x	y	z	atom	x	y	z
H(1)	0.881	0.272	0.866	H(26)	1.470	-0.022	0.865
H(2)	0.840	0.280	0.622	H(27)	1.466	0.028	0.797
H(3)	1.029	0.348	0.687	H(28)	1.124	0.005	0.850
H(4)	0.674	0.172	0.853	H(29)	1.192	-0.031	0.795
H(5)	0.666	0.252	0.861	H(30)	1.231	-0.047	0.882
H(6)	0.548	0.210	0.826	H(31)	1.261	0.112	0.969
H(7)	0.640	0.143	0.631	H(32)	1.375	0.064	0.998
H(8)	0.536	0.130	0.672	H(33)	1.391	0.138	0.967
H(9)	0.669	0.105	0.710	H(34)	1.371	0.197	0.540
H(10)	0.522	0.321	0.706	H(35)	1.312	0.125	0.545
H(11)	0.579	0.311	0.637	H(36)	1.269	0.170	0.471
H(12)	0.472	0.264	0.646	H(37)	1.256	0.327	0.585
H(13)	1.201	0.279	0.954	H(38)	1.172	0.321	0.502
H(14)	1.091	0.305	0.983	H(39)	1.114	0.330	0.571
H(15)	1.215	0.345	1.004	H(40)	0.958	0.206	0.517

H(16)	1.008	0.445	0.950	H(41)	1.019	0.189	0.451
H(17)	1.086	0.492	0.910	H(42)	1.014	0.133	0.512
H(18)	0.958	0.464	0.864	H(43)	0.944	0.092	0.599
H(19)	1.289	0.362	0.832	H(44)	0.842	-0.010	0.551
H(20)	1.220	0.429	0.797	H(45)	0.763	-0.084	0.631
H(21)	1.298	0.428	0.882	H(46)	0.829	0.021	0.994
H(22)	1.186	0.081	0.674	H(47)	0.947	0.121	1.036
H(23)	1.330	0.233	0.854	H(48)	1.042	0.180	0.950
H(24)	1.253	0.289	0.722	H(49)	0.720	-0.101	0.763
H(25)	1.530	0.051	0.881	H(50)	0.736	-0.060	0.885

4.2 Thermal Parameters for Non-Hydrogen Atoms of [1,3-$(Me_3Si)_2C_5H_3]_2$Yb(phen)

atom	U11	U22	U33	U12	U13	U23
Yb(1)	0.0182(1)	0.0182(1)	0.0275(1)	-0.0004(2)	0.0086(1)	0.0013(2)
Si(1)	0.019(1)	0.033(1)	0.030(1)	-0.0000(8)	0.0054(8)	0.0008(9)
Si(2)	0.026(1)	0.030(1)	0.041(1)	-0.0041(9)	0.008(1)	-0.011(1)
Si(3)	0.030(1)	0.040(1)	0.037(1)	0.013(1)	0.013(1)	0.015(1)
Si(4)	0.024(1)	0.033(1)	0.024(1)	0.0002(8)	0.0066(8)	0.0033(8)
N(1)	0.024(3)	0.029(3)	0.023(3)	-0.003(2)	0.007(2)	-0.004(3)
N(2)	0.021(3)	0.020(3)	0.027(3)	0.008(2)	0.003(2)	0.004(2)
C(1)	0.023(3)	0.024(4)	0.026(4)	0.004(3)	0.011(3)	-0.003(3)
C(2)	0.018(3)	0.018(4)	0.028(4)	0.004(3)	0.007(3)	0.002(3)
C(3)	0.022(3)	0.025(4)	0.023(4)	0.009(3)	0.005(3)	0.003(3)
C(4)	0.025(4)	0.013(4)	0.038(4)	0.002(3)	0.014(3)	0.007(3)
C(5)	0.029(4)	0.017(4)	0.031(4)	0.009(3)	0.011(3)	0.003(3)
C(6)	0.041(5)	0.101(7)	0.049(5)	-0.023(4)	0.019(4)	-0.008(4)
C(7)	0.037(5)	0.050(5)	0.057(5)	-0.010(4)	0.000(4)	-0.010(4)
C(8)	0.029(4)	0.042(5)	0.108(7)	-0.000(3)	0.006(4)	0.019(4)
C(9)	0.039(4)	0.061(5)	0.039(4)	-0.018(4)	0.013(3)	-0.009(4)

C(10)	0.059(6)	0.052(5)	0.097(7)	0.005(4)	-0.002(5)	-0.055(5)
C(11)	0.047(5)	0.036(4)	0.042(5)	-0.019(3)	0.004(4)	-0.003(3)
C(12)	0.024(4)	0.025(4)	0.025(4)	0.000(3)	0.009(3)	-0.002(3)
C(13)	0.018(3)	0.033(4)	0.026(4)	0.005(3)	0.008(3)	0.009(3)
C(14)	0.016(3)	0.027(4)	0.026(4)	-0.002(3)	0.007(3)	-0.003(3)
C(15)	0.016(3)	0.020(4)	0.031(4)	-0.002(3)	0.010(3)	0.001(3)
C(16)	0.017(3)	0.026(3)	0.026(3)	-0.000(3)	0.005(3)	0.004(4)
C(17)	0.035(5)	0.066(6)	0.085(6)	0.022(4)	0.014(4)	0.036(5)
C(18)	0.052(5)	0.034(4)	0.054(5)	0.017(4)	0.026(4)	0.016(4)
C(19)	0.047(5)	0.061(5)	0.038(4)	0.005(4)	0.006(4)	0.013(4)
C(20)	0.051(4)	0.051(5)	0.026(4)	0.007(3)	0.011(3)	0.000(3)
C(21)	0.056(5)	0.045(4)	0.038(4)	0.010(4)	0.020(3)	0.013(4)
C(22)	0.042(4)	0.085(6)	0.035(4)	-0.023(4)	0.007(3)	0.018(4)
C(23)	0.043(5)	0.041(4)	0.033(4)	-0.014(4)	0.013(4)	-0.004(4)
C(24)	0.052(5)	0.058(5)	0.033(5)	-0.009(4)	0.017(4)	-0.014(4)
C(25)	0.038(4)	0.035(4)	0.047(5)	-0.008(3)	0.007(4)	-0.013(4)
C(26)	0.024(4)	0.026(4)	0.028(4)	0.001(3)	0.006(3)	-0.005(3)
C(27)	0.017(3)	0.019(3)	0.030(4)	0.002(3)	0.004(3)	-0.001(3)
C(28)	0.015(3)	0.019(4)	0.026(4)	0.003(3)	0.008(3)	-0.000(3)
C(29)	0.025(4)	0.027(4)	0.026(4)	0.003(3)	0.009(3)	0.001(3)
C(30)	0.042(4)	0.040(4)	0.039(5)	0.003(3)	0.021(4)	0.010(4)
C(31)	0.049(5)	0.041(4)	0.029(4)	0.004(4)	0.019(4)	0.004(3)
C(32)	0.031(4)	0.027(4)	0.032(4)	-0.002(3)	0.004(3)	-0.006(3)
C(33)	0.029(4)	0.022(4)	0.057(5)	-0.002(3)	0.017(4)	0.005(4)
C(34)	0.033(4)	0.030(4)	0.041(5)	-0.003(3)	0.017(3)	0.007(4)

The general temperature factor expression:

$$\exp[-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl)]$$

4.3 Bond Lengths of $[1,3\text{-}(Me_3Si)_2C_5H_3]_2Yb(phen)$

4.3.1 Bond Lengths Involving Non-Hydrogen Atoms of $[1,3\text{-}(Me_3Si)_2C_5H_3]_2Yb(phen)$

atom	atom	distance	atom	atom	distance
Yb(1)	N(1)	2.487(5)	C(31)	C(32)	1.412(8)
Yb(1)	N(2)	2.514(5)	C(33)	C(34)	1.333(8)
Yb(1)	C(1)	2.735(5)	Si(4)	C(16)	1.872(5)
Yb(1)	C(2)	2.752(5)	Si(4)	C(20)	1.853(6)
Yb(1)	C(3)	2.707(5)	Si(4)	C(21)	1.854(7)
Yb(1)	C(4)	2.696(5)	Si(4)	C(22)	1.859(7)
Yb(1)	C(5)	2.708(5)	N(1)	C(23)	1.327(7)
Yb(1)	C(12)	2.731(5)	N(1)	C(27)	1.370(7)
Yb(1)	C(13)	2.712(5)	N(2)	C(28)	1.380(7)
Yb(1)	C(14)	2.672(5)	N(2)	C(32)	1.321(7)
Yb(1)	C(15)	2.697(5)	C(1)	C(2)	1.419(7)
Yb(1)	C(16)	2.737(5)	C(1)	C(5)	1.424(7)
Yb(1)	C(100)	2.436	C(2)	C(3)	1.428(7)
Yb(1)	C(101)	2.427	C(3)	C(4)	1.409(7)
Si(1)	C(2)	1.866(6)	C(4)	C(5)	1.442(8)
Si(1)	C(6)	1.853(7)	C(12)	C(13)	1.410(7)
Si(1)	C(7)	1.861(7)	C(12)	C(16)	1.406(7)
Si(1)	C(8)	1.848(7)	C(13)	C(14)	1.429(8)
Si(2)	C(5)	1.859(6)	C(14)	C(15)	1.410(7)
Si(2)	C(9)	1.868(7)	C(15)	C(16)	1.425(8)
Si(2)	C(10)	1.862(7)	C(23)	C(24)	1.390(9)
Si(2)	C(11)	1.857(7)	C(24)	C(25)	1.364(9)
Si(3)	C(13)	1.853(6)	C(25)	C(26)	1.399(8)
Si(3)	C(17)	1.863(7)	C(26)	C(27)	1.413(7)
Si(3)	C(18)	1.855(7)	C(26)	C(33)	1.424(8)

Si(3)	C(19)	1.872(7)	C(27)	C(28)	1.422(7)
C(29)	C(34)	1.423(8)	C(28)	C(29)	1.411(7)
C(30)	C(31)	1.374(8)	C(29)	C(30)	1.400(8)

4.3.2 Bond Lengths Involving Hydrogen Atoms of $[1,3\text{-}(Me_3Si)_2C_5H_3]_2Yb(phen)$

atom	atom	distance	atom	atom	distance
C(1)	H(1)	1.03	C(17)	H(26)	0.96
C(3)	H(2)	1.05	C(17)	H(27)	0.95
C(4)	H(3)	1.01	C(18)	H(28)	0.94
C(6)	H(4)	0.98	C(18)	H(29)	0.97
C(6)	H(5)	0.95	C(18)	H(30)	0.97
C(6)	H(6)	0.95	C(19)	H(31)	0.95
C(7)	H(7)	0.96	C(19)	H(32)	0.97
C(7)	H(8)	0.95	C(19)	H(33)	0.95
C(7)	H(9)	0.95	C(20)	H(34)	0.94
C(8)	H(10)	0.94	C(20)	H(35)	0.97
C(8)	H(11)	0.96	C(20)	H(36)	0.96
C(8)	H(12)	0.98	C(21)	H(37)	0.97
C(9)	H(13)	0.97	C(21)	H(38)	0.96
C(9)	H(14)	0.95	C(21)	H(39)	0.95
C(9)	H(15)	0.97	C(22)	H(40)	0.96
C(10)	H(16)	0.96	C(22)	H(41)	0.97
C(10)	H(17)	0.96	C(22)	H(42)	0.95
C(10)	H(18)	0.97	C(23)	H(43)	0.98
C(11)	H(19)	0.97	C(24)	H(44)	0.96
C(11)	H(20)	0.95	C(25)	H(45)	1.00
C(11)	H(21)	0.95	C(30)	H(46)	0.98
C(12)	H(22)	1.04	C(31)	H(47)	0.98
C(14)	H(23)	1.08	C(32)	H(48)	0.99

C(15)	H(24)	0.97	C(33)	H(49)	0.99
C(17)	H(25)	0.94	C(34)	H(50)	0.96

4.4 Bond Angles of $[1,3\text{-}(Me_3Si)_2C_5H_3]_2Yb(phen)$

4.4.1 Bond Angles Involving Non-Hydrogen Atoms of $[1,3\text{-}(Me_3Si)_2C_5H_3]_2Yb(phen)$

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	Yb(1)	N(2)	66.5(2)	Si(1)	C(2)	C(1)	124.0(4)
N(1)	Yb(1)	C(100)	116.9	Si(1)	C(2)	C(3)	128.1(4)
N(1)	Yb(1)	C(101)	104.0	C(1)	C(2)	C(3)	105.8(5)
N(2)	Yb(1)	C(100)	102.1	C(2)	C(3)	C(4)	108.9(5)
N(2)	Yb(1)	C(101)	119.2	C(3)	C(4)	C(5)	109.2(5)
C(100)	Yb(1)	C(101)	130.9	Si(2)	C(5)	C(1)	125.0(4)
C(2)	Si(1)	C(6)	108.6(3)	Si(2)	C(5)	C(4)	129.2(4)
C(2)	Si(1)	C(7)	116.7(3)	C(1)	C(5)	C(4)	104.9(5)
C(2)	Si(1)	C(8)	108.2(3)	C(13)	C(12)	C(16)	111.2(5)
C(6)	Si(1)	C(7)	107.4(3)	Si(3)	C(13)	C(12)	127.7(5)
C(6)	Si(1)	C(8)	110.3(4)	Si(3)	C(13)	C(14)	125.5(5)
C(7)	Si(1)	C(8)	105.7(3)	C(12)	C(13)	C(14)	105.9(5)
C(5)	Si(2)	C(9)	109.7(3)	C(13)	C(14)	C(15)	108.2(5)
C(5)	Si(2)	C(10)	110.5(3)	C(14)	C(15)	C(16)	109.2(5)
C(5)	Si(2)	C(11)	112.9(3)	Si(4)	C(16)	C(12)	130.0(5)
C(9)	Si(2)	C(10)	106.5(3)	Si(4)	C(16)	C(15)	123.3(5)
C(9)	Si(2)	C(11)	109.0(3)	C(12)	C(16)	C(15)	105.6(5)
C(10)	Si(2)	C(11)	108.0(3)	N(1)	C(23)	C(24)	124.6(6)
C(13)	Si(3)	C(17)	109.8(3)	C(23)	C(24)	C(25)	118.2(6)
C(13)	Si(3)	C(18)	111.4(3)	C(24)	C(25)	C(26)	120.4(6)
C(13)	Si(3)	C(19)	109.3(3)	C(25)	C(26)	C(27)	117.4(6)
C(17)	Si(3)	C(18)	107.5(3)	C(25)	C(26)	C(33)	123.1(6)
C(17)	Si(3)	C(19)	109.0(3)	C(27)	C(26)	C(33)	119.5(6)

C(18)	Si(3)	C(19)	109.8(3)	N(1)	C(27)	C(26)	122.4(5)
C(16)	Si(4)	C(20)	109.6(3)	N(1)	C(27)	C(28)	118.1(5)
C(16)	Si(4)	C(21)	109.2(3)	C(26)	C(27)	C(28)	119.6(5)
C(16)	Si(4)	C(22)	114.7(3)	N(2)	C(28)	C(27)	119.1(5)
C(20)	Si(4)	C(21)	109.6(3)	N(2)	C(28)	C(29)	122.1(5)
C(20)	Si(4)	C(22)	106.5(3)	C(27)	C(28)	C(29)	118.8(5)
C(21)	Si(4)	C(22)	107.1(3)	C(28)	C(29)	C(30)	117.8(5)
Yb(1)	N(1)	C(23)	124.0(4)	C(28)	C(29)	C(34)	120.0(5)
Yb(1)	N(1)	C(27)	118.9(4)	C(30)	C(29)	C(34)	122.2(6)
C(23)	N(1)	C(27)	117.0(5)	C(29)	C(30)	C(31)	120.2(6)
Yb(1)	N(2)	C(28)	116.8(4)	C(30)	C(31)	C(32)	118.4(6)
Yb(1)	N(2)	C(32)	124.8(4)	N(2)	C(32)	C(31)	123.6(6)
C(28)	N(2)	C(32)	117.9(5)	C(26)	C(33)	C(34)	121.0(6)
C(2)	C(1)	C(5)	111.2(5)	C(29)	C(34)	C(33)	121.0(6)

4.4.2 Bond Angles Involving Hydrogen Atoms of $[1,3\text{-}(Me_3Si)_2C_5H_3]_2Yb(phen)$

atom	atom	atom	angle	atom	atom	atom	angle
C(2)	C(1)	H(1)	123.7	H(37)	C(21)	H(39)	108.0
C(5)	C(1)	H(1)	125.0	H(38)	C(21)	H(39)	108.3
C(2)	C(3)	H(2)	130.2	Si(2)	C(9)	H(15)	110.8
C(4)	C(3)	H(2)	120.9	H(13)	C(9)	H(14)	108.2
C(3)	C(4)	H(3)	123.7	H(13)	C(9)	H(15)	107.0
C(5)	C(4)	H(3)	127.0	H(14)	C(9)	H(15)	108.2
Si(1)	C(6)	H(4)	109.6	Si(2)	C(10)	H(16)	111.7
Si(1)	C(6)	H(5)	111.1	Si(2)	C(10)	H(17)	111.7
Si(1)	C(6)	H(6)	111.0	Si(2)	C(10)	H(18)	111.1
H(4)	C(6)	H(5)	107.6	H(16)	C(10)	H(17)	108.1
H(4)	C(6)	H(6)	107.5	H(16)	C(10)	H(18)	107.0
H(5)	C(6)	H(6)	109.9	H(17)	C(10)	H(18)	107.0

Si(1)	C(7)	H(7)	110.0	Si(2)	C(11)	H(19)	110.0
Si(1)	C(7)	H(8)	110.2	Si(2)	C(11)	H(20)	111.3
Si(1)	C(7)	H(9)	110.5	Si(2)	C(11)	H(21)	111.1
H(7)	C(7)	H(8)	108.5	H(19)	C(11)	H(20)	107.5
H(7)	C(7)	H(9)	108.7	H(19)	C(11)	H(21)	107.5
H(8)	C(7)	H(9)	109.0	H(20)	C(11)	H(21)	109.4
Si(1)	C(8)	H(10)	111.9	C(13)	C(12)	H(22)	130.1
Si(1)	C(8)	H(11)	110.9	C(16)	C(12)	H(22)	118.6
Si(1)	C(8)	H(12)	110.0	C(13)	C(14)	H(23)	131.7
H(10)	C(8)	H(11)	109.2	C(15)	C(14)	H(23)	119.1
H(10)	C(8)	H(12)	107.9	C(14)	C(15)	H(24)	127.0
H(11)	C(8)	H(12)	106.7	C(16)	C(15)	H(24)	123.8
Si(2)	C(9)	H(13)	110.9	Si(3)	C(17)	H(25)	110.3
Si(2)	C(9)	H(14)	111.7	Si(3)	C(17)	H(26)	109.4
H(25)	C(17)	H(27)	110.1	Si(3)	C(17)	H(27)	109.8
H(26)	C(17)	H(27)	108.0	H(25)	C(17)	H(26)	109.2
Si(3)	C(18)	H(28)	112.2	Si(4)	C(22)	H(40)	111.3
Si(3)	C(18)	H(29)	110.6	Si(4)	C(22)	H(41)	110.9
Si(3)	C(18)	H(30)	110.9	Si(4)	C(22)	H(42)	112.0
H(28)	C(18)	H(29)	108.2	H(40)	C(22)	H(41)	106.7
H(28)	C(18)	H(30)	108.7	H(40)	C(22)	H(42)	108.3
H(29)	C(18)	H(30)	106.0	H(41)	C(22)	H(42)	107.5
Si(3)	C(19)	H(31)	110.8	N(1)	C(23)	H(43)	116.7
Si(3)	C(19)	H(32)	110.2	C(24)	C(23)	H(43)	118.7
Si(3)	C(19)	H(33)	110.9	C(23)	C(24)	H(44)	119.9
H(31)	C(19)	H(32)	107.6	C(25)	C(24)	H(44)	121.8
H(31)	C(19)	H(33)	109.3	C(24)	C(25)	H(45)	118.5
H(32)	C(19)	H(33)	108.1	C(26)	C(25)	H(45)	121.1
Si(4)	C(20)	H(34)	111.3	C(29)	C(30)	H(46)	120.5

Si(4)	C(20)	H(35)	109.8	C(31)	C(30)	H(46)	119.3
Si(4)	C(20)	H(36)	110.5	C(30)	C(31)	H(47)	120.8
H(34)	C(20)	H(35)	108.6	C(32)	C(31)	H(47)	120.8
H(34)	C(20)	H(36)	109.5	N(2)	C(32)	H(48)	118.5
H(35)	C(20)	H(36)	107.2	C(31)	C(32)	H(48)	117.9
Si(4)	C(21)	H(37)	110.7	C(26)	C(33)	H(49)	119.9
Si(4)	C(21)	H(38)	111.1	C(34)	C(33)	H(49)	119.1
Si(4)	C(21)	H(39)	111.7	C(29)	C(34)	H(50)	119.3
H(37)	C(21)	H(38)	107.0	C(33)	C(34)	H(50)	119.6

4.5 Least Squares Planes of $[1,3\text{-}(Me_3Si)_2C_5H_3]_2Yb(phen)$

Plane 1.	$\chi^2 = 11$	Plane 2.	$\chi^2 = 4.9$
Atoms defining plane	Distance	Atoms defining plane	Distance
C(1)	-0.0087	C(12)	0.0046
C(2)	0.0019	C(13)	0.0000
C(3)	0.0060	C(14)	-0.0042
C(4)	-0.0102	C(15)	0.0070
C(5)	0.0108	C(16)	-0.0062
Additional atoms	Distance	Additional atoms	Distance
Yb(1)	2.4341	Yb(1)	-2.4262
Si(1)	-0.4005	Si(3)	0.2656
Si(2)	-0.2069	Si(4)	0.2737
Plane 3.	$\chi^2 = 10.8$	Plane 4.	$\chi^2 = 8.5$
Atoms defining plane	Distance	Atoms defining plane	Distance
C(23)	-0.0085	C(28)	-0.0076
C(24)	0.0035	C(29)	0.0110
C(25)	0.0093	C(30)	-0.0065
C(26)	-0.0122	C(31)	-0.0040
C(27)	0.0079	C(32)	0.0066