Appendix

Table A 3.1 Infrared spectroscopic data for carboxylic acids

Code	Compounds	Frequencies (cm^{-1})
A1	$C_6H_5CH=CHCO_2H$	1681.6(s), 1626.8(m), 1576.4(w), 1493.5(w), 1452.1(s), 1417.6(m), 1330.0(w), 1312.0(m), 1285.4(m), 1266.1(m), 1221.0(w), 1205.5(w), 1173.6(w), 1158.2(w), 1073.5(w), 1025.7(w), 978.2(m), 943.2(m), 913.8(m), 943.2(m), 874.1(w), 846.6(w), 768.1(w), 710.6(w), 697(w),682.2(w), 589.6(w), 541.9(w), 485.1(w)
A2	*p*-$CH_3C_6H_4CH=CHCO_2H$	1681.7(s), 1621.8(m), 1605.5(m), 1511.9(w), 1503.9(w), 1455.0(s), 1310.5(m), 1284.5(m), 1223.6(m), 1209.6(m), 1117.1(w),1042.2(w), 987.8(m), 942.8(m), 878.3(m), 855.8(w), 814(m), 771.2(w), 733.9(w), 723(w), 684.9(w), 548(w), 516.5(w), 496.0(w)
A3	*p*-$CH_3OC_6H_4CH=CHCO_2H$	1681.8(s), 1622.0(m), 1595.1(s), 1510.9(s), 1455.0(s), 1336.1(m), 1309.1(m), 1289.2(m), 1253.5(s), 1217.6(m), 1115.9(w), 1027.6(m), 975(w), 935.8(w), 861.8(w), 824(m), 773.6(w), 722.3(w), 686.2(w), 638.1(w), 566.6(w), 528.0(w), 512.4(w), 478.4(w)
A4	*p*-$NO_2C_6H_4CH=CHCO_2H$	1681.2(s), 1630.3(m), 1604.0(m), 1593.7(m), 1536.9(m), 1494.8(m), 1426.3(s), 1409.9(w), 1352.1(s), 1340.6(s), 1303.0(s), 1281.9(s), 1263.4(m), 1226.6(m), 1181.7(w), 1108.0(w), 1012.5(w), 987.5(w), 932.4(w), 882.5(w), 868.1(w), 849.1(w), 832.3(w), 759.6(w), 713.2(w), 671.5(w), 644.1(w), 632(w), 551.1(w), 521.8(w), 480.5(w), 435.7(w), 416.3(w)
A5	*p*-$ClC_6H_4CH=CHCO_2H$	1678.3(s), 1626.1(s), 1591.8(w), 1569.7(w), 1490.0(m), 1453.2(s), 1405.2(m), 1339.5(m), 1305.6(m), 1232.8(w), 1206.0(w), 1176.1(w), 1108.5(w), 1086.1(w), 1012.0(w), 958.2(m), 941.8(m), 873.9(w), 820.7(m), 734.9(w), 719(w), 656(w), 546.2(w), 492.2(w), 450.1(w)
A6	$C_6H_5CH(Br)CH(Br)CO_2H$	1705.9(s), 1493.88(m), 1455.9(s), 1317.77(w), 1298.9(m), 1278.0(m), 1221.8(m), 1197.5(m), 1163.5(w), 1145.5(m), 1088.2(w), 1062.7(w), 1029.8(w), 559.7(w), 527.4(w), 474.8(w)
A7	*p*-$CH_3C_6H_4CH(Br)CH(Br)CO_2H$	1701.7(s), 1458.6(s), 1413.4 (m), 1305.82(m), 1267.8(m), 1224.3(w), 1203.7(m), 1178.2(m), 974.2(w), 680.9(w), 576.9(w), 556.8(w), 517.1(w), 494.0(w)
A8	*p*-$CH_3OC_6H_4CH(Br)CH(OCH_3)CO_2H$	1706.3(s), 1588.4(w), 1516.1(m), 1464.3(S), 1421.3(m), 1309.5(w), 1280.1(m), 1253.7(s), 1204.2(w), 1183.4(s), 1095.8(m), 1077.09(w), 1034.3(m), 961.4(w), 914.5(w), 675.45(w), 580.4(m), 560.1(m), 518.3(w)

b=[s=strong, m=medium, w=weak, b=broad]

Table A3.1 continued

A9	[*p*-$ClC_6H_4CH(Br)CH(Br)COO^-$][$(CH_3)_2NC_5H_4NH]^+Br^-$	1700.4(s), 1626.3(s), 1518.1(m), 1462.3(s), 1420.4(m), 1305.7(m), 1279.1(m), 1252.8(m), 1176.2(m), 1085.9(m), 962.1(w), 881.2(w), 821.8(m), 715.7(m), 543.4(w), 491.0(w)
A10	$(CH_3)_2NCS_2CH_2CO_2H$	1697.1(s), 1497.2(m), 1458.9(s), 1354.7(m), 1305.3(m), 1253.9(m), 1213.3(m), 1186.6(m), 1145.3(w), 1050.3(w), 1001.0(w), 984(w), 912.8(w), 881.4(w), 792.3(w), 722.1(w), 675.1(w).
A11	$(CH_3CH_2)_2NCS_2CH_2CO_2H$	1712.4(s), 1493.6(s), 1459.0(s), 1424(s), 1352.3(s), 1313.2(s), 1279.9(m), 1269.5(s), 1214.2(m), 1199.7(s), 1176.4(m), 1142.9(w), 1083.7(w), 1073.3(w), 981.8 (w), 915.3(w), 880.6(w), 829.1(w), 772.9(w), 722.3(w), 668.1(w)
A12	$CH_3CH_2CH_2CH_2(CH_3)$ $NCS_2CH_2CO_2H$6	1701.5(s), 1459.1(s), 1318.2(s), 1287.4(m), 1205.5(m), 1181.2(m), 1140.5(m), 1032.6(m), 959.6(w), 943.4(w), 899.3(w), 852(w), 794.4(w), 776.9(w), 722.2(w), 663.9(w)
A13	$((CH_3)_2C)_2NCS_2CH_2CO_2H$	1695.8(s), 1456.2(s), 1395.1(m), 1353(m), 1298(m), 1251.4(m), 1217.9(s), 1186.9(s), 1145.6(m), 1112.7(w), 1069.8(w), 989.8(m), 904.9(w), 880(w), 786.2(w), 727.5(w), 674.4(w)
A14	 $CS_2CH_2CO_2H$	1700.6(s), 1456.0(s), 1431.0(s), 1352.8(m), 1308.4(m), 1274.8(m), 1240.8(s), 1226.2(s), 1212.9(s), 1181.1(s), 1129.6(w), 1110.6(w), 1068.7(w), 1005.9(w), 980.5(w), 945.4(w), 909.1(w), 892.5(w), 873.4(w), 850.4(w), 789.7(w), 722.4(w), 671.2(w), 605.6(w)
A15	 $CS_2CH_2CO_2H$	1697.0(s), 1435.9(s), 1360.1(m), 1302.2(m), 1267.6(m), 1243.4(s), 1211.0(m), 1176.2(s), 1109.8(m), 1059.5(w), 1029.4(m), 997.5(m), 908.7(w), 877.1(w), 862.9(w), 817.8(w), 793.3(w), 722.2(w), 678.8(w), 636.4(w)

b=[s=strong, m=medium, w=weak, b=broad]

Table A 3.2 Infrared spectroscopic data for triorganotin *p*-substituted cinnamate

Code	Compounds	Frequencies (cm^{-1})
C1	$(CH_3CH_2CH_2CH_2)_3SnO_2CCH=CHC_6H_5$	1641.4(s), 1608.2(m), 1588.0(w), 1578.1(m), 1544.3(s), 1527.3(s), 1494.5(m), 1451.8(s), 1380.1(s), 1342.9(s), 1289.5(w), 1254.4(w), 1218.0(w),1200.7(w), 1157.7(w), 1179.3(w), 1072.5(w), 1050.0(w), 1029.8(w), 986.0(w), 977.8(w), 870.5(w), 849.9(w), 772.2(w), 736.6(w), 714.2(w), 700.2(w), 684.7(w), 610.73(w), 589.3(w), 548.0(w), 510.2(w), 483.0(w), 449.2(w)
C2	$(CH_3CH_2CH_2CH_2)_3SnO_2CCH=CHC_6H_4(CH_3$-*p*)	1641.5(s), 1612.5(m), 1570.0(m), 1543.6(s), 1527.7(s), 1512.0(s), 1443.1(s), 1341.6(s),1288.1(m), 1222.0(w), 1210.5(w), 1178.4(w), 1157.3(w), 1116.0(w), 1046.8(w), 1019.9(w), 981.6(w), 873.5(w), 813.8(w), 778.2(w), 721.7(m), 701.7(w), 668.9(w), 601.2(w), 548.9(w), 528.6(w), 494.0(w)
C3	$(CH_3CH_2CH_2CH_2)_3SnO_2CCH=CHC_6H_4(OCH_3$-*p*)	1634.8(m), 1605.8(s), 1576.9(m), 1542.0(m),1524.2(m), 1511.6(s), 1455.0(s), 1349.9(m), 1291.7(m), 1247.6(s), 1172.0(s), 1108.4(w), 1074.6(w), 1038.5(m), 981.6(m), 930.6(w), 869.5(m), 827.6(m), 804.4(w), 722.3(w), 699.8(w), 669.8(w), 639.1(w), 605.3(w), 557(w), 514.7(w), 458.1(w), 416.6(w)
C4	$(CH_3CH_2CH_2CH_2)_3SnO_2CCH=CHC_6H_4(NO_2$-*p*)	1641.0(m), 1600.8(m), 1590.0(s), 1553.5(s), 1521.0(s). 1491.6(m), 1455.2(s),1416.1(m), 1342.0(s), 1320.0(m), 1251.6(m), 1221.8(w), 1197.5(w), 1177.8(w), 1157.3(w), 1108.3(w), 1078.4(w)1012.6(w), 979.8(w), 956.4(w), 865.9(w), 848.0(w), 762.2(w), 736.2(m), 719.7(m), 701.2(w), 647.4(w), 513.0(w), 551.1(w), 480.2(w), 437.0(w), 413.0(w)
C5	$(CH_3CH_2CH_2CH_2)_3SnO_2CCH=CHC_6H_4(Cl$-*p*)	1640.6(s),1605.2(m), 1593.9(m), 1546.6(s),1527.0(s),1489.8(s), 1453.2(s), 1405.3(s), 1370.1(s), 1291.5(m), 1217.5(w), 1197.9(w), 1178.8(w), 1158.0(w), 1120.0(w), 1107.9(w),1088.2(s), 1012.5(w), 979.9(w), 940.0(w), 875.9(w), 852.4(w), 823.9(m), 771.3(w), 747.8(w), 736.1(w), 701.2(w), 672.1(w), 662.2(w), 603.3(w), 547.2(w), 511.5(w), 493.9(w), 454.4(w), 426.3(w), 408.0(w)
C6	$(C_6H_{11})_3SnO_2CCH=CHC_6H_5$	1651.4(s), 1625.3(m), 1574.7(w), 1558.0(s), 1495.6(w), 1448.0(s), 1411.3(m), 1341.3(s), 1287.5(s), 1269.5(w), 1258.2(w), 1218.3(m), 1170.3(w), 1071.5(w), 1040.0(w), 1025.4(w), 991.9(w), 975.9(w), 965.0(w), 908.1(w), 876.1(w), 840.6(w), 803.6(w), 770.3(m), 738.1(w), 724.7(w), 712.3(w), 685.6(w), 666.3(w), 623.4(w), 612.5(w), 592.0(w), 558.1(w), 530.0(w), 486.0(w), 415.8(w), 403.9(w)
C7	$(C_6H_{11})_3SnO_2CCH=CHC_6H_4(CH_3$-*p*)	1649.0(s), 1618.7(m), 1604.9(m), 1571.4(w), 1513.6(w), 1449.0(s), 1411.6(w), 1366.0(s), 1344.8(s), 1285.5(w), 1222.2(s), 1209.7(m), 1197.4(w), 1170.6(w), 1116.0(w), 1083.9(w), 1040.9(w), 986.4(w), 907.9(w), 875.4(w),

b=[s=strong, m=medium, w=weak, b=broad]

Table A 3.2 continued

		840.4(w), 815.9(w), 779.6(w), 722.7(w), 664.7(w), 588.3(w), 532.5(w), 518.9(w), 496.7(w), 422.8(w)
C8	$(C_6H_{11})_3SnO_2CCH{=}CHC_6H_4(OCH_3$-*p*)	1648.3(s), 1613.2(m), 1589.2(m), 1513.0(s), 1448.5(s), 1350.0(w), 1291.4(w), 1248.2(s), 1170.8(m), 1151.9(w), 1099.4(w), 1083.9(w), 1038.1(m), 993.3(w), 972.6(w), 829.8(w), 777.6(w), 722.3(w), 698.3(w), 572.0(w), 558.2(w), 492.2(w)
C9	$(C_6H_{11})_3\ SnO_2CCH{=}CHC_6H_4(NO_2$-*p*)	1687.8(s), 1629.9(m), 1606.1(m), 1597.1(m), 1520.8(s), 1495.9(m), 1447.1(s), 1349.7(s), 1308.3(s), 1284.4(m), 1227.8(w), 1209.6(w), 1184.1(w), 1116.1(w), 1014.2(w), 987.6(w), 960.5(w), 919.2(w), 848,1(w), 833.7(w), 760.0(w), 717.3(w), 673.0(w), 552.9(w), 524.1(w), 479.4(w), 435.7(w)
C10	$(C_6H_{11})_3\ SnO_2CCH{=}CHC_6H_4$(Cl-*p*)	1714.4(s), 1604.5(w), 1591.0(w), 1569.1(w),1495.7(w), 1429.9(s), 1317.9(w), 1297.9(w), 1279.4(m), 1220.0(w), 1146.7(w), 1076.0(w), 1023.9(w), 998.0(w), 911.2(w), 820.0(m),766.5(w), 725.1(m), 697.5(m), 658.9 (w), 622.0(w), 600.3(w), 559.9(w), 526.2(w), 446.51(w)
C11	$(C_6H_5CH_2)_3SnO_2CCH{=}CHC_6H_5$	1635.8(s), 1597.9(m), 1578.0(m), 1547.9(s), 1518.1(s), 1491.2(s), 1450.3(s), 1398.2(s), 1252.2(m), 1206.7(m), 1179.4(w), 1123.7(w),1095.8(w), 1070.6(w), 1052.6(m), 904.1(w), 868.3(w), 797.9(w), 771.9 (w), 760.2(m), 734.5(w), 726.0(w), 711.7(w), 588.7(w), 552.0(w), 477.9(w), 448.0(w)
C12	$(C_6H_5CH_2)_3SnO_2CCH{=}CHC_6H_4(-CH_3$-*p*)	1636.4(s), 1597.7(s), 1491.3(m), 1451.3(s), 1255.4(w), 1210.0(w), 1179.8(w), 1117.8(w), 1055.1(w), 1029.9(w), 906.6(w), 815.8(w), 755.6(m), 723.0(w), 696.3(m), 623.5(w), 587.5(w), 559.8(w), 550.1(w), 526.0(w), 494.9(w), 453.9(w)
C13	$(C_6H_5CH_2)_3SnO_2CCH{=}CHC_6H_4(OCH_3$-*p*)	1638.2(s), 1594.7(s), 1579.2(s), 1513.5(m), 1491.9(m), 1455.4(s), 1305.6(w), 1294.0(m), 1248.2(m),1207.1(m), 1173.8(s), 1159.6(m), 1072.0(s), 1055.7(m), 1033.4(m), 969.9(w), 831.8(w), 757.3(w), 736.0(w), 698.0(w), 582.1(w), 448.2(w)
C14	$(C_6H_5CH_2)_3\ SnO_2CCH{=}CHC_6H_4(NO_2$-*p*)	1639.9(s), 1597.7(s), 1548.2(s), 1519.8(s), 1490.4(s), 1452.3(s), 1414.8(m), 1380.0(s), 1343.5(s), 1253.3(w), 1202.2(m), 1118.7(w), 1110.3(m), 1052.7(m), 987.3(w), 846.4(w), 796.1(w), 758.4(m), 724.7(m), 697.3(m), 556.0(w), 450.0(w)
C15	$(C_6H_5CH_2)_3\ SnO_2CCH{=}CHC_6H_4$(Cl-*p*)	1635.7(s), 1597.0(m),1546.8(s), 1514.0(s), 1489.9(s), 1453.2(s), 1407.0(s), 1251.8(m), 1202.7(m), 1174.3(w), 1110.1(w), 1087.5(m), 1052.1(m), 1012.2(w), 987.8(w), 872.6(w), 823.6(m), 493.3(w), 453.3(w), 796.5(w), 756.5(m), 724.8(m), 697.0(m), 664.3(w), 544.9(w), 493.3(w), 455.3(w)

b=[s=strong, m=medium, w=weak, b=broad]

Table A 3.3 Infrared spectroscopic data for triorganotin carboxylate complexes

Code	Compounds	Frequencies (cm^{-1})
P1	$(CH_3CH_2CH_2CH_2)_3SnO_2CCH(Br)CH(Br)C_6H_5$	1639.7(s), 1490.3(m), 1453.0(s), 1408.9(m), 1351.5(m), 1312.8(w), 1229.6(w), 1206.2(w), 1166.8(w), 1151.9(w), 1058.9(w), 1028.4(w), 721.3(w), 695.8(w), 623.7(w), 603.5(w), 566.8(w), 453.0(w)
P2	$(CH_3CH_2CH_2CH_2)_3SnO_2CCH(Br)CH(Br)C_6H_4(CH_3$-*p*$)$	1640.7(m), 1491.2(m), 1458.5(s), 1413.5 (m), 1352.4(m),1305.8(m), 1268.8(m), 1225.3(w), 1203.7(m), 1175.2(m), 1057.7(m), 1028.5(w), 978.2(w), 723.5(w), 692.9(w), 632.0(w), 556.8(w), 517.1(w), 494.0(w)
P3	$(CH_3CH_2CH_2CH_2)_3SnO_2C$	1639.2(m), 1490.8(m), 1456.8(s), 1412.3(m), 1352.0(m), 1308.7(m), 1292.1(m), 1248.5(m), 1225.3(m),
	$CH(Br)CH(OCH_3)C_6H_4(OCH_3$-*p*$)$	1180.1(m), 1171.2(m), 1160.5(m), 1092.0(w), 1068.9(w), 1040.1(m), 989.8(w), 968.2(w), 938.9(w), 964.5(w), 938.2(w),719.3(w), 654.8(w), 638.1(w), 568.6(w), 528.3(w), 515.4(w), 472.6(w)
P4	$(C_6H_{11})_3SnO_2CCH(Br)CH(Br)C_6H_5$	1660.3(m), 1490.1(m), 1456.1(s),1408.7(m), 1349.1(m), 1309.2(m), 1290.1(m), 1248.8(m), 1228.8(m), 1207.5(w), 1170.1(m), 1148.2(m), 1028.9(w), 678.0(w), 560.7(w), 526.5(w), 473.9(w)
P5	$(C_6H_{11})_3SnO_2CCH(Br)CH(Br)C_6H_4(CH_3$-*p*$)$	1659.7(m), 1491.0(m), 1458.5(s), 1413.4 (m), 1305.2(m), 1267.8(m), 1223.3(w), 1200.7(m), 1176.2(m), 973.2(w), 680.9(w), 576.9(w), 556.8(w), 517.1(w), 494.0(w)
P6	$(C_6H_{11})_3SnO_2CCH(Br)CH(OCH_3)C_6H_4(OCH_3$-*p*$)$	1661.3(m), 1492.3(m), 1458.0(s),1325.8(m), 1290.3(m), 1250.6(m), 1222.8(w), 1182.0(w), 1170.9(w), 1159.4(w), 1094.0(m), 1072.4(w), 1032.1(w), 991.8(w), 965.8(w), 940.6(w), 655.5(w), 638.1(w), 584.4(w), 572.3(w), 492.3(w), 445.43(w), 416.2(w)
P7	$(C_6H_5CH_2)_3SnO_2CCH(Br)CH(Br)C_6H_5$	1614.8(s), 1492.0(m), 1455.0(s), 1409.4(s), 1351.5(m), 1311.8(w), 1229.0(w), 1208.2(w), 1168.9(w), 1151.9(w), 1057.9(w), 1028.4(w), 697.0(w), 624.2(w), 606.6(w), 565.9(w), 454.0(w)
P8	$(C_6H_5CH_2)_3SnO_2CCH(Br)CH(Br)C_6H_4(CH_3$-*p*$)$	1616.8(s), 1490.2(m), 1456.7(s), 1417.5(m), 1352.7(m), 1310.2(m), 1292.2(m), 1250.2(m), 1227.5(m), 1205.3(w), 1175.3(m), 1149.2(m), 1025.3(w), 678.2(w), 568.5(w), 518.3(w), 478.2(w)
P9	$(C_6H_5CH_2)_3SnO_2CCH(Br)CH(OCH_3)C_6H_4(OCH_3$-*p*$)$	1620.3(m), 1490.8(m), 1459.3(s), 1418.3(m), 1350.9(m), 1307.9(m), 1291.3(m), 1245.8(m), 1225.8(m), 1206.8(w), 1168.3(m), 1092.0(w), 1068.9(w), 1041.3(m), 992.8(w), 970.2(w), 940.7(w), 963.6(w), 939.5(w), 657.9(w), 639.7(w), 570.1(w), 527.6(w), 518.3(w), 473.0(w)

b=[s=strong, m=medium, w=weak, b=broad]

Table A 3.4 Infrared spectroscopic data for triorganotin diorganodithiocarbamylacetates

Code	Compounds	Frequencies (cm^{-1})
D1	$(C_6H_{11})_3SnO_2CH_2CS_2N(CH_3)_2$	1661.7(m), 1589.4(w), 1456.8(s), 1326.9(m), 1266.5(m), 1260.1(m), 1170.0(m), 1112.8(m), 1029.6(m), 992.4(m), 875.5(w), 722.1(w), 539.4(w)
D2	$(C_6H_{11})_3SnO_2CH_2CS_2N(CH_3CH_2)_2$	1661.2(m), 1456.1(s), 1312.1(m), 1265.1(m), 1170.0(m), 1112.2(m), 1025.3(w), 992.2(w), 876.0(w), 722.0(w), 540.0(w)
D3	$(C_6H_{11})_3SnO_2CH_2CS_2N(CH_3)CH_2CH_2CH_2CH_3$	1660.8(m), 1458.2(s), 1310.0(m), 1192.7(m), 1170.2(m), 1143.3(m), 1035.1(m), 992.0(w), 877.2(w), 721.8(w)
D4	$(C_6H_{11})_3SnO_2CH_2CS_2N(C(CH_3)_2)_2$	1662.3(m), 1575.5(m), 1458.8(s), 1254.6(m), 1168.4(m), 1078.0(m), 991.1(w), 875.2(w), 722.1(w)
D5	$(C_6H_{11})_3SnO_2CH_2CS_2$ 	1673.8(m), 1456.0(s), 1322.4(m), 1285.0(w), 1244.1(w), 1229.9(w), 1170.7(w), 1109.9(w), 990.5(w), 973.3(w), 881.8(w), 857.8(w), 793.9(w), 722.2(w), 684.9(w), 566.3(w)
D6	$(C_6H_{11})_3SnO_2CH_2CS_2$ 	1670.2(m), 1455.9(s), 1320.8(m), 1267.5(m), 1243.2(s), 1176.0(m), 1109.7(m), 1029.3(m), 990.5(w), 908.5(w), 877.0(w), 862.7(w),817.7(w), 793.0(w), 722.2(w), 678.7(w), 636.3(w)

b=[s=strong, m=medium, w=weak, b=broad]

Table A 3.5 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **A4**. $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	$U_{(eq)}$
O(1)	7559(2)	3342(2)	5002(1)	25(1)
O(2)	4635(2)	2685(2)	5448(1)	23(1)
O(3)	10778(2)	-10844(2)	7395(1)	22(1)
O(4)	13451(2)	-10452(2)	6910(1)	23(1)
N(1)	11653(2)	-9791(2)	7048(1)	16(1)
C(1)	6516(2)	2089(3)	5342(1)	18(1)
C(2)	7780(2)	-97(3)	5590(1)	19(1)
C(3)	7060(2)	-1445(3)	5975(1)	17(1)
C(4)	8265(2)	-3585(3)	6250(1)	16(1)
C(5)	7355(2)	-4790(3)	6658(1)	17(1)
C(6)	8450(2)	-6821(3)	6924(1)	17(1)
C(7)	10477(2)	-7613(3)	6776(1)	15(1)
C(8)	11435(2)	-6467(3)	6375(1)	19(1)
C(9)	10325(2)	-4454(3)	6113(1)	19(1)

Table A 3.6 Bond lengths (Å) for **A4**

O(1)-C(1)	1.3063(16)
O(2)-C(1)	1.2405(16)
O(3)-N(1)	1.2252(14)
O(4)-N(1)	1.2291(14)
N(1)-C(7)	1.4704(16)
C(1)-C(2)	1.4709(18)
C(2)-C(3)	1.3329(19)
C(3)-C(4)	1.4696(17)
C(4)-C(5)	1.3975(18)
C(4)-C(9)	1.4042(18)
C(5)-C(6)	1.3881(18)
C(6)-C(7)	1.3847(17)
C(7)-C(8)	1.3849(18)
C(8)-C(9)	1.3798(18)

Table A 3.7 Bond angles (^{o}) for **A4**

O(3)-N(1)-O(4)	123.97(11)
O(3)-N(1)-C(7)	118.12(10)
O(4)-N(1)-C(7)	117.90(11)
O(2)-C(1)-O(1)	123.27(12)
O(2)-C(1)-C(2)	122.95(12)
O(1)-C(1)-C(2)	113.78(11)
C(3)-C(2)-C(1)	22.31(12)
C(2)-C(3)-C(4)	125.19(12)
C(5)-C(4)-C(9)	118.85(12)
C(5)-C(4)-C(3)	119.63(12)
C(9)-C(4)-C(3)	121.52(12)
C(6)-C(5)-C(4)	121.01(12)
C(7)-C(6)-C(5)	118.18(12)
C(6)-C(7)-C(8)	122.55(12)
C(6)-C(7)-N(1)	119.17(11)
C(8)-C(7)-N(1)	118.27(11)
C(9)-C(8)-C(7)	118.58(12)
C(8)-C(9)-C(4)	120.83(12)

Symmetry transformations used to generate equivalent atoms: -x –y -z

Table A 3.8 Anisotropic displacement parameters ($Å^2$ x 10^3) for **A4.** The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2a^2U_{11} + ... + 2hkabU_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O(1)	28(1)	24(1)	24(1)	9(1)	7(1)	7(1)
O(2)	23(1)	25(1)	22(1)	6(1)	4(1)	7(1)
O(3)	24(1)	21(1)	22(1)	7(1)	2(1)	1(1)
O(4)	22(1)	23(1)	25(1)	0(1)	3(1)	9(1)
N(1)	18(1)	14(1)	17(1)	-1(1)	-1(1)	1(1)
C(1)	23(1)	17(1)	14(1)	1(1)	0(1)	2(1)
C(2)	20(1)	19(1)	19(1)	1(1)	1(1)	5(1)
C(3)	18(1)	16(1)	17(1)	-1(1)	0(1)	3(1)
C(4)	18(1)	14(1)	15(1)	0(1)	-1(1)	1(1)
C(5)	16(1)	18(1)	19(1)	-1(1)	3(1)	3(1)
C(6)	19(1)	17(1)	15(1)	1(1)	3(1)	0(1)
C(7)	17(1)	12(1)	16(1)	-1(1)	-2(1)	1(1)
C(8)	16(1)	20(1)	20(1)	1(1)	3(1)	2(1)
C(9)	19(1)	20(1)	17(1)	4(1)	4(1)	1(1)

Table A 3.9 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **A4.**

	x	y	z	$U_{(eq)}$
H(1)	6780(40)	4590(40)	4867(9)	88(9)
H(2)	9159	-563	5471	23
H(3)	5656	-986	6080	21
H(5)	5965	-4211	6754	21
H(6)	7826	-7644	7200	20
H(8)	12827	-7055	6281	22
H(9)	10961	-3644	5837	23

Table A 3.10 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **A6**. $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	$U_{(eq)}$
Br(1)	-636(1)	4558(1)	5633(1)	34(1)
Br(2)	4836(1)	3105(1)	6358(1)	24(1)
O(1)	4014(11)	3337(6)	5151(2)	64(2)
O(2)	4075(8)	5364(5)	5501(2)	35(1)
C(1)	3614(15)	4173(9)	5480(3)	51(3)
C(2)	2690(20)	3443(10)	5884(3)	92(5)
C(3)	1539(16)	4162(9)	6154(3)	63(3)
C(4)	497(11)	3526(8)	6550(2)	30(2)
C(5)	218(9)	4319(7)	6936(2)	23(2)
C(6)	-774(10)	3780(7)	7301(2)	22(2)
C(7)	-1448(9)	2464(7)	7288(2)	24(2)
C(8)	-1166(9)	1668(7)	6905(2)	23(2)
C(9)	-201(10)	2205(8)	6534(3)	29(2)

Table A 3.11 Bond lengths (Å) **A6**

Br(1)-C(3)	2.195(13)
Br(2)-C(2)	2.077(16)
O(1)-C(1)	1.292(9)
O(2)-C(1)	1.203(9)
C(1)-C(2)	1.527(11)
C(2)-C(3)	1.328(13)
C(3)-C(4)	1.505(10)
C(4)-C(9)	1.375(10)
C(4)-C(5)	1.383(10)
C(5)-C(6)	1.380(9)
C(6)-C(7)	1.365(10)
C(7)-C(8)	1.377(9)
C(8)-C(9)	1.383(9)

Table A 3.12 Bond angles (^{o}) for **A6**

O(2)-C(1)-O(1)	125.7(7)
O(2)-C(1)-C(2)	121.6(7)
O(1)-C(1)-C(2)	112.2(7)
C(3)-C(2)-C(1)	118.4(9)
C(3)-C(2)-Br(2)	97.4(8)
C(1)-C(2)-Br(2)	106.2(9)
C(2)-C(3)-C(4)	122.5(8)
C(2)-C(3)-Br(1)	95.9(9)
C(4)-C(3)-Br(1)	105.5(7)
C(9)-C(4)-C(5)	119.9(6)
C(9)-C(4)-C(3)	122.1(7)
C(5)-C(4)-C(3)	118.0(7)
C(6)-C(5)-C(4)	119.6(7)
C(7)-C(6)-C(5)	120.6(6)
C(6)-C(7)-C(8)	120.0(6)
C(7)-C(8)-C(9)	119.9(6)
C(4)-C(9)-C(8)	120.1(7)

Symmetry transformations used to generate equivalent atoms: -x –y -z

Table A 3.13 Anisotropic displacement parameters ($Å^2$ x 10^3) for **A6.** The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^2 U_{11} + ... + 2hkabU_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br(1)	36(1)	43(1)	22(1)	10(1)	-4(1)	1(1)
Br(2)	24(1)	25(1)	24(1)	5(1)	2(1)	-3(1)
O(1)	136(7)	22(3)	35(3)	-13(2)	48(4)	-30(4)
O(2)	59(4)	24(3)	21(2)	-1(2)	0(2)	-5(3)
C(1)	97(8)	26(5)	31(4)	-14(4)	34(5)	-28(5)
C(2)	182(13)	37(5)	57(6)	-26(5)	84(8)	-59(7)
C(3)	104(9)	19(4)	67(6)	-11(4)	67(6)	-24(5)
C(4)	37(4)	22(4)	29(4)	6(3)	15(3)	-5(3)
C(5)	21(4)	17(3)	29(4)	2(3)	7(3)	1(3)
C(6)	24(4)	25(4)	18(3)	5(3)	-3(3)	6(3)
C(7)	20(3)	32(4)	20(3)	9(3)	4(3)	2(3)
C(8)	18(3)	20(4)	30(4)	8(3)	9(3)	-3(3)
C(9)	34(4)	23(4)	28(4)	-3(3)	12(3)	-5(3)

Table A 3.14 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **A6.**

	x	*y*	*z*	$U_{(eq)}$
H(1)	4649	3613	4926	97
H(2)	2082	2559	5788	110
H(3)	1370	5115	6095	76
H(5)	707	5229	6950	27
H(6)	-991	4330	7564	27
H(7)	-2112	2097	7543	29
H(8)	-1633	752	6895	27
H(9)	-20	1661	6268	35

Table A 3.15 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **A8**. $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	$U_{(eq)}$
Br(1)	7512(1)	5333(1)	7918(1)	23(1)
O(1)	5319(2)	5584(4)	6912(3)	30(1)
O(2)	5870(1)	5985(3)	5127(2)	24(1)
O(3)	6103(2)	9733(3)	6595(3)	29(1)
O(4)	9618(1)	12499(3)	10191(2)	24(1)
C(1)	5890(2)	6148(4)	6367(3)	21(1)
C(2)	6613(2)	7057(4)	7426(3)	19(1)
C(3)	6847(2)	8733(4)	6807(3)	19(1)
C(4)	6053(2)	11207(5)	5676(4)	36(1)
C(5)	7603(2)	9682(4)	7716(3)	17(1)
C(6)	8290(2)	9989(4)	7223(3)	19(1)
C(7)	8978(2)	10929(5)	8002(3)	19(1)
C(8)	8981(2)	11553(4)	9325(3)	16(1)
C(9)	8298(2)	11247(4)	9847(3)	20(1)
C(10)	7613(2)	10322(5)	9048(3)	20(1)
C(11)	10318(2)	12903(5)	9659(4)	27(1)

Table A 3.16 Bond lengths (Å) for **A8**

Br(1)-C(2)	1.945(3)
O(1)-C(1)	1.288(4)
O(2)-C(1)	1.221(4)
O(3)-C(3)	1.418(4)
O(3)-C(4)	1.427(5)
O(4)-C(8)	1.367(4)
O(4)-C(11)	1.438(4)
C(1)-C(2)	1.524(4)
C(2)-C(3)	1.506(5)
C(3)-C(5)	1.510(4)
C(5)-C(6)	1.383(5)
C(5)-C(10)	1.396(4)
C(6)-C(7)	1.387(5)
C(7)-C(8)	1.387(4)
C(8)-C(9)	1.391(4)
C(9)-C(10)	1.384(4)

Table A 3.17 Bond angle (^{o}) for **A8**

C(3)-O(3)-C(4)	114.0(3)
C(8)-O(4)-C(11)	116.8(3)
O(2)-C(1)-O(1)	124.5(3)
O(2)-C(1)-C(2)	121.9(3)
O(1)-C(1)-C(2)	113.6(3)
C(3)-C(2)-C(1)	110.3(3)
C(3)-C(2)-Br(1)	113.5(2)
C(1)-C(2)-Br(1)	106.0(2)
O(3)-C(3)-C(2)	101.3(3)
O(3)-C(3)-C(5)	112.6(3)
C(2)-C(3)-C(5)	115.3(3)
C(6)-C(5)-C(10)	118.4(3)
C(6)-C(5)-C(3)	120.5(3)
C(10)-C(5)-C(3)	121.1(3)
C(5)-C(6)-C(7)	122.0(3)
C(6)-C(7)-C(8)	118.9(3)
O(4)-C(8)-C(7)	124.5(3)
O(4)-C(8)-C(9)	115.4(3)
C(7)-C(8)-C(9)	120.1(3)
C(10)-C(9)-C(8)	120.2(3)
C(9)-C(10)-C(5)	120.4(3)

Table A 3.18 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **A8.** The anisotropic displacement factor exponent takes the form: $-2\pi^2 [\ h^2a^2U_{11} + ... + 2hkabU_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br(1)	19(1)	19(1)	26(1)	-2(1)	-4(1)	3(1)
O(1)	21(1)	41(2)	25(1)	-5(1)	5(1)	-6(1)
O(2)	15(1)	28(1)	26(1)	1(1)	2(1)	-6(1)
O(3)	19(1)	23(1)	39(1)	3(1)	0(1)	1(1)
O(4)	16(1)	26(1)	28(1)	-6(1)	6(1)	-9(1)
C(1)	18(2)	16(2)	27(2)	0(1)	0(1)	1(1)
C(2)	17(2)	21(2)	19(2)	-1(1)	3(1)	3(1)
C(3)	15(1)	19(2)	21(2)	-2(1)	-2(1)	0(1)
C(4)	29(2)	29(2)	40(2)	7(2)	-6(2)	4(2)
C(5)	17(2)	14(2)	17(1)	1(1)	1(1)	0(1)
C(6)	22(2)	21(2)	15(1)	-1(1)	5(1)	-1(1)
C(7)	18(2)	20(2)	21(2)	0(1)	10(1)	-2(1)
C(8)	15(1)	14(2)	19(1)	1(1)	2(1)	-2(1)
C(9)	20(2)	22(2)	18(2)	-7(1)	6(1)	-5(1)
C(10)	16(2)	23(2)	22(2)	-5(1)	8(1)	-2(1)
C(11)	18(2)	26(2)	38(2)	0(2)	9(1)	-6(1)

Table A 3.19 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **A8**

	x	*y*	*z*	$U_{(eq)}$
H(1)	5368	5737	7774	44
H(2)	6438	7356	8290	23
H(3)	6942	8464	5870	23
H(4A)	5517	11811	5557	54
H(4B)	6095	10796	4756	54
H(4C)	6511	12027	6083	54
H(6)	8292	9544	6323	23
H(7)	9440	11142	7635	23
H(9)	10754	11674	10754	24
H(10)	7148	10122	9408	24
H(11A)	10732	13579	10367	40
H(11B)	10127	13603	8793	40
H(11C)	10571	11803	9453	40

Table A 3.20 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **A9**. $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	$U_{(eq)}$
Br(1)	2635(2)	1572(1)	1165(1)	23(1)
Br(2)	860(2)	988(1)	5821(1)	33(1)
Br(3)	-3975(2)	1245(1)	3251(1)	41(1)
Cl(1)	-6366(4)	1316(2)	8423(3)	34(1)
C(10)	-1830(15)	1283(5)	9547(10)	23(2)
C(11)	-857(15)	1048(6)	8716(9)	24(2)
N(2)	-1930(13)	1903(5)	9759(8)	25(2)
C(3)	-4300(17)	1711(6)	6963(9)	26(2)
N(1)	-1687(15)	-26(5)	9011(9)	33(3)
O(2)	-10(16)	669(4)	3080(8)	43(3)
O(1)	515(15)	1725(4)	3102(9)	43(3)
C(4)	-5105(15)	1188(6)	7378(9)	24(2)
C(5)	-4905(16)	564(6)	6993(9)	25(2)
C(14)	-2706(15)	792(6)	10104(10)	25(2)
C(12)	-845(16)	411(6)	8472(11)	30(3)
C(6)	-3830(18)	469(6)	6195(10)	30(3)
C(2)	-3270(20)	1619(6)	6169(10)	34(3)
C(16)	-954(18)	2375(6)	9210(11)	32(3)
C(1)	-3000(20)	998(6)	5775(11)	37(3)
C(7)	-1880(40)	887(7)	4900(18)	87(9)
C(13)	-2596(17)	163(6)	9817(11)	33(3)
C(15)	-2880(20)	2135(7)	10629(13)	42(3)
C(9)	-230(20)	1199(6)	3408(12)	36(3)
C(8)	-1320(40)	1332(8)	4310(20)	105(12)

Table A 3.21 Bond lengths (Å) for **A9**

Br(2)-C(7)	2.29(3)	N(1)-C(13)	1.351(19)
Br(3)-C(8)	2.30(3)	O(2)-C(9)	1.185(16)
Cl(1)-C(4)	1.740(12)	O(1)-C(9)	1.309(16)
C(10)-N(2)	1.310(15)	C(4)-C(5)	1.389(17)
C(10)-C(11)	1.438(16)	C(5)-C(6)	1.388(17)
C(10)-C(14)	1.445(16)	C(14)-C(13)	1.351(19)
C(11)-C(12)	1.348(17)	C(6)-C(1)	1.406(18)
N(2)-C(16)	1.458(15)	C(2)-C(1)	1.393(17)
N(2)-C(15)	1.464(16)	C(1)-C(7)	1.493(19)
C(3)-C(2)	1.363(17)	C(7)-C(8)	1.28(2)
C(3)-C(4)	1.381(17)	C(9)-C(8)	1.51(2)
N(1)-C(12)	1.343(18)		

Table A 3.22 Bond angles (°) for **A9**

N(2)-C(10)-C(11)	121.4(10)	C(5)-C(6)-C(1)	120.3(11)
N(2)-C(10)-C(14)	123.1(11)	C(3)-C(2)-C(1)	120.6(12)
C(11)-C(10)-C(14)	115.5(11)	C(2)-C(1)-C(6)	119.2(12)
C(12)-C(11)-C(10)	120.4(12)	C(2)-C(1)-C(7)	121.4(12)
C(10)-N(2)-C(16)	120.8(10)	C(6)-C(1)-C(7)	119.4(11)
C(10)-N(2)-C(15)	121.0(10)	C(8)-C(7)-C(1)	125.2(15)
C(16)-N(2)-C(15)	117.9(10)	C(8)-C(7)-Br(2)	81.0(2)
C(2)-C(3)-C(4)	120.0(11)	C(1)-C(7)-Br(2)	103.5(14)
C(12)-N(1)-C(13)	120.7(11)	C(14)-C(13)-N(1)	121.7(12)
C(3)-C(4)-C(5)	121.4(11)	O(2)-C(9)-O(1)	125.2(13)
C(3)-C(4)-Cl(1)	119.1(9)	O(2)-C(9)-C(8)	122.5(13)
C(5)-C(4)-Cl(1)	119.5(9)	O(1)-C(9)-C(8)	112.1(11)
C(6)-C(5)-C(4)	118.5(11)	C(7)-C(8)-C(9)	123.7(15)
C(13)-C(14)-C(10)	119.9(12)	C(7)-C(8)-Br(3)	85.0(2)
N(1)-C(12)-C(11)	121.7(12)	C(9)-C(8)-Br(3)	97.6(16)

Table A 3.23 Anisotropic displacement parameters ($Å^2$ x 10^3) for **A9**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2a^2U_{11} + ... + 2hkabU_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br(1)	25(1)	30(1)	16(1)	0(1)	7(1)	-3(1)
Br(2)	24(1)	52(1)	22(1)	4(1)	0(1)	5(1)
Br(3)	36(1)	66(1)	17(1)	-17(1)	-6(1)	18(1)
Cl(1)	23(2)	55(2)	24(2)	-1(1)	12(1)	3(1)
C(10)	17(5)	27(6)	24(6)	5(4)	0(4)	0(4)
C(11)	15(5)	37(6)	19(5)	-3(4)	-3(4)	6(4)
N(2)	20(5)	28(5)	29(5)	3(4)	10(4)	-2(4)
C(3)	33(7)	33(6)	13(5)	-1(4)	5(5)	0(5)
N(1)	36(6)	30(5)	28(6)	-3(4)	-19(5)	5(4)
O(2)	69(8)	31(5)	38(5)	-5(4)	35(5)	1(4)
O(1)	62(7)	25(5)	49(6)	-4(4)	36(5)	-5(4)
C(4)	19(5)	39(6)	14(5)	2(4)	4(4)	3(4)
C(5)	25(6)	34(6)	14(5)	2(4)	1(4)	-1(5)
C(14)	19(5)	34(6)	22(6)	6(4)	0(4)	-1(4)
C(12)	21(6)	34(6)	32(7)	-3(5)	-9(5)	2(5)
C(6)	38(7)	33(6)	19(6)	5(4)	4(5)	0(5)
C(2)	58(9)	31(7)	17(6)	1(5)	18(6)	6(6)
C(16)	31(7)	31(6)	36(7)	4(5)	10(6)	-5(5)
C(1)	68(10)	19(6)	33(7)	-1(5)	37(7)	4(6)
C(7)	180(20)	24(8)	86(14)	-14(8)	113(17)	-16(10)
C(13)	25(6)	34(7)	37(7)	12(5)	-9(6)	-6(5)
C(15)	44(9)	40(8)	47(9)	-11(6)	24(7)	2(6)
C(9)	45(8)	27(7)	39(8)	-3(5)	17(6)	-3(5)
C(8)	180(30)	21(8)	150(20)	-27(10)	140(20)	-21(11)

Table A 3.24 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **C6.** $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	$U_{(eq)}$
Sn(1)	4796(2)	855(1)	8516(1)	57(1)
Sn(2)	6862(2)	2003(1)	5225(1)	64(1)
O(1)	2859(12)	645(2)	7170(10)	51(3)
O(2)	2389(13)	632(2)	9074(13)	66(3)
O(3)	8016(16)	1685(2)	5187(15)	79(4)
O(4)	6957(16)	1749(2)	2959(14)	69(4)
C(1)	5620(20)	910(7)	6950(30)	155(16)
C(2)	7170(40)	806(9)	7140(30)	290(30)
C(3)	7610(20)	846(4)	5935(18)	85(7)
C(4)	6270(40)	928(7)	4610(20)	230(20)
C(5)	5210(40)	1124(6)	4710(30)	190(20)
C(6)	4490(20)	1038(6)	5670(20)	139(13)
C(7)	3890(20)	1202(4)	8870(20)	85(7)
C(8)	2230(20)	1242(4)	7800(20)	88(7)
C(9)	1790(30)	1506(6)	7990(30)	143(13)
C(10)	1860(30)	1524(6)	9430(30)	170(15)
C(11)	3540(30)	1488(4)	10460(30)	139(13)
C(12)	4120(40)	1235(4)	10360(20)	156(14)
C(13)	6203(18)	611(2)	10117(13)	46(4)
C(14)	6010(20)	623(3)	11459(12)	62(5)
C(15)	7090(17)	446(2)	12528(14)	46(4)
C(16)	6940(20)	189(2)	11997(14)	57(5)
C(17)	7152(19)	177(3)	10666(13)	58(5)
C(18)	6112(16)	354(2)	9584(14)	47(4)

Table A 3.24 continued

C(19)	2070(20)	576(3)	7848(18)	52(4)
C(20)	786(17)	393(3)	7063(16)	47(4)
C(21)	-26(17)	282(3)	7613(16)	45(4)
C(22)	-1190(11)	99(2)	7077(10)	50(4)
C(23)	-1738(13)	33(2)	5689(10)	54(4)
C(24)	-2944(13)	-135(2)	5128(8)	60(5)
C(25)	-3603(12)	-238(2)	5955(12)	72(6)
C(26)	-3056(13)	-172(2)	7343(11)	61(5)
C(27)	-1849(12)	-4(2)	7904(8)	61(5)
C(28)	7830(20)	2308(3)	4567(16)	79(6)
C(29)	7150(30)	2337(4)	3016(17)	128(11)
C(30)	7790(30)	2558(3)	2570(30)	122(10)
C(31)	7610(20)	2792(4)	3224(16)	84(7)
C(32)	8330(30)	2755(4)	4774(17)	120(10)
C(33)	7590(30)	2543(3)	5180(30)	143(13)
C(34)	7690(40)	1977(3)	7460(30)	161(15)
C(35)	7370(30)	2202(4)	8100(20)	133(11)
C(36)	8110(40)	2146(6)	9641(18)	210(20)
C(37)	7200(30)	1948(4)	9960(30)	115(10)
C(38)	7680(40)	1722(5)	9427(19)	163(14)
C(39)	7020(30)	1757(4)	7873(18)	112(9)
C(40)	4800(40)	1961(3)	4320(30)	250(30)
C(41)	3660(20)	2142(4)	4480(30)	104(9)
C(42)	1890(20)	2135(5)	3710(30)	145(13)
C(43)	1320(40)	1887(5)	3900(40)	200(20)
C(44)	2070(20)	1701(4)	3310(30)	130(11)
C(45)	3840(20)	1729(4)	4010(30)	142(12)

Table A 3.24 continued

C(46)	7740(20)	1626(4)	3910(20)	62(5)
C(47)	8650(20)	1404(3)	3830(30)	75(6)
C(48)	8600(20)	1340(4)	2590(30)	84(7)
C(49)	9432(13)	1128(2)	2301(16)	86(8)
C(50)	9465(13)	1116(2)	1007(14)	95(8)
C(51)	10247(15)	926(3)	704(15)	90(8)
C(52)	10995(13)	749(2)	1690(20)	114(11)
C(53)	10962(13)	762(2)	2988(17)	100(9)
C(54)	10180(15)	951(3)	3292(13)	89(7)

Table A 3.25 Bond lengths (Å) for **C6**

Sn(1)-C(1)	2.128(19)	C(14)-C(15)	1.516(8)
Sn(1)-O(1)	2.125(10)	C(15)-C(16)	1.511(8)
Sn(1)-C(13)	2.135(13)	C(16)-C(17)	1.509(8)
Sn(1)-C(7)	2.193(19)	C(17)-C(18)	1.513(8)
Sn(2)-C(40)	1.78(3)	C(19)-C(20)	1.53(2)
Sn(2)-O(3)	2.066(14)	C(20)-C(21)	1.29(2)
Sn(2)-C(28)	2.162(17)	C(21)-C(22)	1.422(18)
Sn(2)-C(34)	2.17(2)	C(22)-C(23)	1.3900
O(1)-C(19)	1.289(17)	C(22)-C(27)	1.3900
O(2)-C(19)	1.245(19)	C(23)-C(24)	1.3900
O(3)-C(46)	1.31(2)	C(24)-C(25)	1.3900
O(4)-C(46)	1.19(2)	C(25)-C(26)	1.3900
C(1)-C(2)	1.503(8)	C(26)-C(27)	1.3900
C(1)-C(6)	1.508(8)	C(28)-C(29)	1.505(8)
C(2)-C(3)	1.515(8)	C(28)-C(33)	1.510(8)
C(3)-C(4)	1.509(8)	C(29)-C(30)	1.513(8)
C(4)-C(5)	1.505(8)	C(30)-C(31)	1.512(8)
C(5)-C(6)	1.514(8)	C(31)-C(32)	1.509(8)
C(7)-C(12)	1.512(8)	C(32)-C(33)	1.515(8)
C(7)-C(8)	1.515(8)	C(34)-C(35)	1.505(8)
C(8)-C(9)	1.55(3)	C(34)-C(39)	1.512(8)
C(9)-C(10)	1.508(8)	C(35)-C(36)	1.515(8)
C(10)-C(11)	1.512(8)	C(36)-C(37)	1.513(8)
C(11)-C(12)	1.514(8)	C(37)-C(38)	1.511(8)
C(13)-C(14)	1.513(8)	C(38)-C(39)	1.513(8)
C(13)-C(18)	1.512(8)	C(40)-C(45)	1.517(8)

Table A 3.25 continued

C(40)-C(41)	1.524(8)	C(49)-C(50)	1.3900
C(42)-C(43)	1.510(8)	C(49)-C(54)	1.3900
C(43)-C(44)	1.515(8)	C(50)-C(51)	1.3900
C(44)-C(45)	1.519(8)	C(51)-C(52)	1.3900
C(46)-C(47)	1.52(3)	C(52)-C(53)	1.3900
C(47)-C(48)	1.34(3)	C(53)-C(54)	1.3900
C(48)-C(49)	1.50(2)		

Table A 3.26 Bond angles (°) for **C6**

C(1)-Sn(1)-O(1)	92.4(10)	C(10)-C(9)-C(8)	107(2)
C(1)-Sn(1)-C(13)	113.9(6)	C(9)-C(10)-C(11)	108(2)
O(1)-Sn(1)-C(13)	105.3(5)	C(10)-C(11)-C(12)	112(2)
C(1)-Sn(1)-C(7)	107.8(11)	C(7)-C(12)-C(11)	106(2)
O(1)-Sn(1)-C(7)	107.8(6)	C(14)-C(13)-C(18)	112.5(11)
C(13)-Sn(1)-C(7)	124.5(6)	C(14)-C(13)-Sn(1)	116.4(9)
C(40)-Sn(2)-O(3)	110.0(6)	C(18)-C(13)-Sn(1)	111.8(8)
C(40)-Sn(2)-C(28)	115.9(8)	C(13)-C(14)-C(15)	111.7(11)
O(3)-Sn(2)-C(28)	110.8(7)	C(16)-C(15)-C(14)	113.2(13)
C(40)-Sn(2)-C(34)	113.0(11)	C(17)-C(16)-C(15)	111.3(12)
O(3)-Sn(2)-C(34)	90.9(8)	C(16)-C(17)-C(18)	112.8(12)
C(28)-Sn(2)-C(34)	113.4(7)	C(17)-C(18)-C(13)	113.7(12)
C(19)-O(1)-Sn(1)	108.4(10)	O(2)-C(19)-O(1)	124.8(16)
C(46)-O(3)-Sn(2)	110.7(12)	O(2)-C(19)-C(20)	121.5(14)
C(2)-C(1)-C(6)	124.9(18)	O(1)-C(19)-C(20)	113.4(14)
C(2)-C(1)-Sn(1)	119.7(11)	C(21)-C(20)-C(19)	123.2(14)
C(6)-C(1)-Sn(1)	115.3(12)	C(20)-C(21)-C(22)	131.1(14)
C(1)-C(2)-C(3)	115.4(18)	C(23)-C(22)-C(27)	120.0
C(4)-C(3)-C(2)	114.5(17)	C(23)-C(22)-C(21)	119.3(9)
C(5)-C(4)-C(3)	118(2)	C(27)-C(22)-C(21)	120.6(9)
C(4)-C(5)-C(6)	109(2)	C(22)-C(23)-C(24)	120.0
C(1)-C(6)-C(5)	114.3(17)	C(25)-C(24)-C(23)	120.0
C(12)-C(7)-C(8)	114.9(19)	C(24)-C(25)-C(26)	120.0
C(12)-C(7)-Sn(1)	112.9(11)	C(27)-C(26)-C(25)	120.0
C(8)-C(7)-Sn(1)	110.5(13)	C(26)-C(27)-C(22)	120.0
C(7)-C(8)-C(9)	106.7(16)	C(29)-C(28)-C(33)	108.1(17)

Table A 3.26 continued

C(29)-C(28)-Sn(2)	113.3(11)	C(43)-C(42)-C(41)	109(2)
C(33)-C(28)-Sn(2)	111.4(12)	C(42)-C(43)-C(44)	108(2)
C(28)-C(29)-C(30)	112.9(17)	C(43)-C(44)-C(45)	109(2)
C(31)-C(30)-C(29)	114.1(18)	C(40)-C(45)-C(44)	129(2)
C(32)-C(31)-C(30)	107.4(19)	O(4)-C(46)-O(3)	121.5(19)
C(31)-C(32)-C(33)	111.6(18)	O(4)-C(46)-C(47)	125(2)
C(35)-C(34)-C(39)	110(2)	O(3)-C(46)-C(47)	113.1(19)
C(35)-C(34)-Sn(2)	113.1(16)	C(48)-C(47)-C(46)	119(2)
C(39)-C(34)-Sn(2)	111.4(16)	C(47)-C(48)-C(49)	126(2)
C(34)-C(35)-C(36)	103(2)	C(50)-C(49)-C(54)	120.0
C(37)-C(36)-C(35)	110.2(19)	C(50)-C(49)-C(48)	117.9(14)
C(38)-C(37)-C(36)	103(2)	C(54)-C(49)-C(48)	122.1(14)
C(37)-C(38)-C(39)	105(2)	C(49)-C(50)-C(51)	120.0
C(34)-C(39)-C(38)	112.7(19)	C(52)-C(51)-C(50)	120.0
C(45)-C(40)-C(41)	101(2)	C(53)-C(52)-C(51)	120.0
C(45)-C(40)-Sn(2)	129.8(19)	C(52)-C(53)-C(54)	120.0
C(41)-C(40)-Sn(2)	120.8(15)	C(53)-C(54)-C(49)	120.0
C(42)-C(41)-C(40)	126(2)		

Table A 3.27 Anisotropic displacement parameters ($Å^2$ x 10^3) for **C6.** The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$h^2 a^2 U_{11}$ + ... + 2hkabU_{12}]

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sn(1)	72(1)	43(1)	66(1)	14(1)	39(1)	12(1)
Sn(2)	89(1)	56(1)	58(1)	5(1)	43(1)	1(1)
O(1)	51(7)	59(8)	33(7)	-6(5)	9(6)	-3(5)
O(2)	54(8)	87(10)	67(9)	-29(7)	36(7)	-20(6)
O(3)	102(11)	43(8)	89(11)	18(7)	37(10)	-2(7)
O(4)	94(10)	47(8)	76(10)	21(7)	47(9)	20(7)
C(1)	89(19)	280(40)	130(20)	130(30)	72(19)	30(20)
C(2)	340(50)	460(80)	170(30)	200(40)	220(40)	300(60)
C(3)	95(16)	110(19)	63(14)	38(12)	47(14)	45(13)
C(4)	420(60)	230(50)	130(30)	100(30)	210(40)	140(40)
C(5)	200(40)	320(60)	90(20)	110(30)	90(30)	110(40)
C(6)	100(20)	240(40)	82(19)	90(20)	45(17)	10(20)
C(7)	79(15)	51(12)	120(20)	27(13)	43(16)	23(10)
C(8)	120(20)	70(15)	76(15)	9(11)	37(16)	45(13)
C(9)	51(15)	180(30)	110(20)	10(20)	-45(18)	74(18)
C(10)	160(30)	140(30)	260(40)	0(30)	140(30)	80(20)
C(11)	85(18)	90(20)	180(30)	-72(19)	0(20)	34(14)
C(12)	240(40)	110(30)	130(30)	-22(19)	80(30)	70(20)
C(13)	52(10)	27(8)	58(11)	14(7)	24(9)	4(6)
C(14)	91(14)	56(12)	58(12)	-7(9)	51(12)	-1(9)
C(15)	38(10)	59(11)	30(10)	7(7)	3(9)	9(7)
C(16)	94(14)	35(9)	67(12)	3(8)	58(12)	13(8)
C(17)	78(13)	48(10)	68(12)	17(8)	48(11)	18(9)
C(18)	55(10)	37(9)	68(12)	-11(8)	44(10)	-1(7)

Table A 3.27 continued

C(19)	56(12)	60(11)	52(12)	0(8)	33(11)	9(8)
C(20)	37(10)	71(12)	31(10)	-9(8)	12(9)	8(8)
C(21)	46(10)	56(10)	42(10)	0(8)	27(9)	13(8)
C(22)	56(11)	43(10)	64(12)	21(8)	38(10)	31(8)
C(23)	41(11)	73(13)	35(11)	3(8)	4(10)	-3(9)
C(24)	92(15)	34(9)	44(11)	16(8)	18(11)	14(9)
C(25)	121(17)	26(9)	92(15)	-22(9)	68(14)	-1(9)
C(26)	62(12)	54(11)	85(14)	6(10)	49(12)	2(9)
C(27)	65(12)	67(13)	70(13)	1(9)	46(11)	10(9)
C(28)	57(13)	76(15)	77(15)	33(11)	0(12)	-17(10)
C(29)	270(40)	62(16)	101(19)	1(13)	120(20)	-42(18)
C(30)	190(30)	78(19)	140(20)	41(17)	120(20)	26(17)
C(31)	39(12)	95(18)	67(16)	33(12)	-27(12)	15(10)
C(32)	110(20)	80(18)	100(20)	47(14)	-28(17)	-28(14)
C(33)	260(40)	58(17)	90(19)	3(14)	50(20)	-30(19)
C(34)	360(50)	61(18)	120(20)	36(15)	160(30)	10(20)
C(35)	210(30)	110(30)	130(20)	9(18)	130(30)	-20(20)
C(36)	380(60)	170(40)	23(16)	-24(16)	30(20)	-80(40)
C(37)	120(20)	130(30)	130(20)	71(19)	83(19)	34(17)
C(38)	300(50)	90(30)	130(20)	41(19)	120(30)	30(30)
C(39)	160(30)	110(20)	64(16)	23(13)	48(17)	-28(17)
C(40)	640(80)	13(10)	380(50)	-54(17)	490(60)	-80(20)
C(41)	86(17)	87(18)	120(20)	-19(15)	21(17)	-66(14)
C(42)	210(40)	100(20)	200(30)	-20(20)	150(30)	-10(20)
C(43)	200(30)	190(40)	340(50)	-140(40)	240(40)	-90(30)
C(44)	57(16)	110(20)	180(30)	0(20)	0(20)	-30(14)
C(45)	140(30)	100(20)	210(30)	20(20)	100(30)	54(19)

Table A 3.27 continued

C(46)	39(11)	74(14)	73(16)	8(12)	24(12)	1(9)
C(47)	52(12)	46(12)	121(19)	13(12)	31(14)	-6(9)
C(48)	69(14)	46(12)	160(20)	4(13)	67(16)	-6(9)
C(49)	30(10)	35(10)	180(20)	10(13)	28(14)	-6(7)
C(50)	76(15)	77(16)	160(20)	-58(16)	81(17)	-32(11)
C(51)	42(12)	62(14)	160(20)	-42(15)	36(15)	-33(10)
C(52)	35(12)	58(14)	250(40)	-30(20)	60(19)	-5(10)
C(53)	58(14)	56(14)	180(30)	12(16)	48(17)	11(10)
C(54)	61(14)	67(15)	140(20)	14(14)	42(15)	9(10)

Table A 3.28 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2} x 10^3) for **C6.**

	x	*y*	*z*	$U_{(eq)}$
H(1A)	6118	1067	7381	186
H(2A)	7832	721	7953	347
H(3A)	8452	969	6209	102
H(3B)	8039	693	5752	102
H(4A)	6723	985	3971	273
H(4B)	5621	784	4178	273
H(5A)	4377	1159	3778	233
H(5B)	5816	1275	5078	233
H(6A)	4048	1180	5947	167
H(6B)	3615	926	5144	167
H(7A)	4537	1331	8702	102
H(8A)	1505	1126	7939	106
H(8B)	2167	1220	6854	106
H(9A)	2531	1622	7883	171
H(9B)	718	1545	7294	171
H(10A)	1183	1398	9570	203
H(10B)	1480	1685	9574	203
H(11A)	3631	1515	11409	167
H(11B)	4208	1609	10275	167
H(12A)	5244	1219	10998	188
H(12B)	3521	1111	10611	188
H(13A)	7307	663	10368	55
H(14A)	4909	584	11271	74
H(14B)	6233	790	11835	74
H(15A)	8185	501	12823	56

Table A 3.28 continued

H(15B)	6854	449	13352	56
H(16A)	7744	86	12707	69
H(16B)	5898	124	11836	69
H(17A)	6914	10	10287	70
H(17B)	8259	212	10869	70
H(18A)	5014	297	9233	57
H(18B)	6411	355	8795	57
H(20A)	571	359	6124	56
H(21A)	194	332	8533	54
H(23A)	-1288	103	5124	64
H(24A)	-3318	-179	4179	72
H(25A)	-4427	-352	5571	86
H(26A)	-3506	-242	7908	73
H(27A)	-1475	41	8852	73
H(28A)	8983	2281	4908	95
H(29A)	6001	2351	2654	154
H(29B)	7391	2190	2604	154
H(30A)	8909	2531	2803	146
H(30B)	7234	2573	1547	146
H(31A)	8151	2926	2977	100
H(31B)	6489	2835	2893	100
H(32A)	8202	2904	5233	143
H(32B)	9469	2724	5100	143
H(33A)	8050	2529	6206	172
H(33B)	6451	2573	4858	172
H(34A)	8857	1955	7861	194
H(35A)	6231	2230	7763	159

Table A 3.28 continued

H(35B)	7861	2346	7894	159
H(36A)	9205	2094	9927	249
H(36B)	8109	2295	10168	249
H(37A)	7499	1936	10974	138
H(37B)	6057	1976	9479	138
H(38A)	7233	1575	9660	195
H(38B)	8832	1707	9830	195
H(39A)	7246	1610	7449	135
H(39B)	5869	1775	7500	135
H(40A)	4660	2003	3362	300
H(41A)	3889	2143	5479	125
H(41B)	3982	2304	4281	125
H(42A)	1413	2261	4078	174
H(42B)	1569	2167	2711	174
H(43A)	166	1878	3406	242
H(43B)	1624	1855	4896	242
H(44A)	1686	1724	2301	156
H(44B)	1776	1535	3480	156
H(45A)	4173	1645	4912	171
H(45B)	4232	1629	3449	171
H(47A)	9247	1311	4633	90
H(48A)	7980	1438	1819	100
H(50A)	8954	1237	330	114
H(51A)	10270	918	-181	108
H(52A)	11530	620	1487	137
H(53A)	11473	641	3666	120
H(54A)	10157	960	4176	106

Table A 3.29 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2} x 10^3) for **C5**. $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	$U_{(eq)}$
Sn(1)	2137(1)	5426(1)	4841(1)	21(1)
Br(1)	4378(1)	3723(1)	4401(1)	35(1)
Br(2)	2584(1)	600(1)	3299(1)	31(1)
O(1)	2659(2)	4358(3)	4077(2)	39(1)
O(2)	3143(2)	2973(3)	5299(2)	45(1)
C(1)	1569(2)	6666(4)	3632(2)	22(1)
C(2)	1216(2)	7996(4)	3873(3)	26(1)
C(3)	854(2)	8880(4)	3002(3)	28(1)
C(4)	377(2)	7926(4)	2262(3)	28(1)
C(5)	726(2)	6598(4)	2018(2)	28(1)
C(6)	1087(2)	5702(4)	2895(3)	28(1)
C(7)	1627(2)	3824(4)	5421(2)	23(1)
C(8)	1404(2)	2437(4)	4836(3)	29(1)
C(9)	1064(2)	1361(4)	5322(3)	34(1)
C(10)	487(2)	2078(4)	5554(3)	29(1)
C(11)	710(2)	3462(4)	6139(3)	31(1)
C(12)	1040(2)	4543(4)	5642(3)	26(1)
C(13)	2833(2)	6755(4)	5863(2)	23(1)
C(14)	2482(2)	7634(4)	6445(3)	30(1)
C(15)	2972(2)	8594(5)	7173(3)	40(1)
C(16)	3352(2)	9610(5)	6714(3)	40(1)
C(17)	3701(2)	8748(5)	6152(3)	35(1)
C(18)	3220(2)	7777(5)	5415(3)	33(1)
C(19)	3064(2)	3375(5)	4512(4)	43(1)

Table A 3.29 continued

C(20)	3465(4)	2732(7)	3902(6)	86(2)
C(21)	3511(4)	1324(10)	3833(6)	103(3)
C(22)	3980(3)	619(6)	3377(4)	59(2)
C(23)	4391(3)	-514(6)	3837(4)	60(2)
C(24)	4791(3)	-1224(6)	3434(3)	49(1)
C(25)	4800(2)	-820(5)	2563(3)	36(1)
C(26)	4408(2)	312(5)	2089(3)	35(1)
C(27)	3996(2)	1048(5)	2490(3)	44(1)

Table A 3.30 Bond lengths (Å) **C5**

Sn(1)-O(1)	2.072(3)	C(9)-C(10)	1.521(5)
Sn(1)-C(13)	2.141(4)	C(10)-C(11)	1.523(5)
Sn(1)-C(7)	2.157(3)	C(11)-C(12)	1.531(5)
Sn(1)-C(1)	2.158(3)	C(13)-C(18)	1.530(5)
Br(1)-C(20)	2.054(8)	C(13)-C(14)	1.539(5)
Br(2)-C(21)	1.990(7)	C(14)-C(15)	1.526(6)
O(1)-C(19)	1.271(5)	C(15)-C(16)	1.526(6)
O(2)-C(19)	1.201(6)	C(16)-C(17)	1.507(6)
C(1)-C(6)	1.528(5)	C(17)-C(18)	1.530(6)
C(1)-C(2)	1.525(5)	C(19)-C(20)	1.548(7)
C(2)-C(3)	1.525(5)	C(20)-C(21)	1.290(10)
C(3)-C(4)	1.520(5)	C(21)-C(22)	1.517(7)
C(4)-C(5)	1.519(5)	C(22)-C(23)	1.387(8)
C(5)-C(6)	1.536(5)	C(22)-C(27)	1.402(7)
C(7)-C(12)	1.531(5)	C(23)-C(24)	1.351(7)
C(7)-C(8)	1.525(5)	C(24)-C(25)	1.369(6)
C(7)-H(7)	1.0000	C(25)-C(26)	1.374(6)
C(8)-C(9)	1.531(5)	C(26)-C(27)	1.381(6)

Table A 3.31 Bond angles (°) for **C5**

O(1)-Sn(1)-C(13)	107.13(13)	C(18)-C(13)-Sn(1)	111.7(2)
O(1)-Sn(1)-C(7)	109.48(13)	C(14)-C(13)-Sn(1)	110.7(2)
C(13)-Sn(1)-C(7)	114.25(13)	C(15)-C(14)-C(13)	111.2(3)
O(1)-Sn(1)-C(1)	91.76(12)	C(16)-C(15)-C(14)	111.0(3)
C(13)-Sn(1)-C(1)	112.88(13)	C(17)-C(16)-C(15)	111.2(4)
C(7)-Sn(1)-C(1)	118.36(14)	C(16)-C(17)-C(18)	111.9(4)
C(19)-O(1)-Sn(1)	115.9(3)	C(17)-C(18)-C(13)	111.0(3)
C(6)-C(1)-C(2)	111.1(3)	O(2)-C(19)-O(1)	125.8(4)
C(6)-C(1)-Sn(1)	112.5(2)	O(2)-C(19)-C(20)	122.6(5)
C(2)-C(1)-Sn(1)	113.5(2)	O(1)-C(19)-C(20)	111.6(5)
C(3)-C(2)-C(1)	111.4(3)	C(21)-C(20)-C(19)	119.5(6)
C(4)-C(3)-C(2)	111.7(3)	C(21)-C(20)-Br(1)	112.1(6)
C(3)-C(4)-C(5)	111.5(3)	C(19)-C(20)-Br(1)	104.4(4)
C(4)-C(5)-C(6)	111.3(3)	C(20)-C(21)-C(22)	122.2(7)
C(1)-C(6)-C(5)	111.1(3)	C(20)-C(21)-Br(2)	105.6(6)
C(12)-C(7)-C(8)	110.6(3)	C(22)-C(21)-Br(2)	112.6(4)
C(12)-C(7)-Sn(1)	110.2(2)	C(23)-C(22)-C(27)	118.8(4)
C(8)-C(7)-Sn(1)	115.3(2)	C(23)-C(22)-C(21)	119.1(6)
C(9)-C(8)-C(7)	111.0(3)	C(27)-C(22)-C(21)	122.0(6)
C(10)-C(9)-C(8)	111.8(3)	C(24)-C(23)-C(22)	121.1(5)
C(9)-C(10)-C(11)	111.1(3)	C(23)-C(24)-C(25)	120.1(5)
C(10)-C(11)-C(12)	110.7(3)	C(24)-C(25)-C(26)	120.6(4)
C(7)-C(12)-C(11)	111.1(3)	C(25)-C(26)-C(27)	120.0(4)
C(18)-C(13)-C(14)	111.1(3)	C(26)-C(27)-C(22)	119.4(5)

Table A 3.32 Anisotropic displacement parameters ($Å^2$ x 10^3) for **C14.** The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^2 U_{11} + ... + 2hkabU_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sn(1)	22(1)	20(1)	21(1)	1(1)	10(1)	2(1)
Br(1)	36(1)	41(1)	30(1)	-10(1)	14(1)	-17(1)
Br(2)	25(1)	33(1)	36(1)	-5(1)	10(1)	-7(1)
O(1)	47(2)	44(2)	34(2)	2(1)	26(1)	14(2)
O(2)	36(2)	35(2)	62(2)	11(2)	12(2)	10(1)
C(1)	20(2)	22(2)	24(2)	1(1)	7(1)	1(1)
C(2)	28(2)	25(2)	25(2)	-1(2)	8(2)	3(2)
C(3)	31(2)	24(2)	28(2)	-1(2)	8(2)	1(2)
C(4)	26(2)	32(2)	23(2)	5(2)	4(2)	-2(2)
C(5)	32(2)	29(2)	21(2)	-3(2)	4(2)	-8(2)
C(6)	35(2)	22(2)	25(2)	-1(2)	7(2)	-3(2)
C(7)	26(2)	22(2)	23(2)	1(1)	9(2)	-1(2)
C(8)	34(2)	25(2)	34(2)	-6(2)	18(2)	-2(2)
C(9)	42(2)	21(2)	45(2)	-4(2)	23(2)	0(2)
C(10)	32(2)	25(2)	33(2)	-2(2)	15(2)	-4(2)
C(11)	38(2)	28(2)	34(2)	-5(2)	22(2)	-4(2)
C(12)	31(2)	19(2)	35(2)	-5(2)	19(2)	-3(2)
C(13)	23(2)	24(2)	21(2)	3(1)	5(1)	4(2)
C(14)	33(2)	32(2)	29(2)	-3(2)	14(2)	-1(2)
C(15)	49(3)	43(3)	32(2)	-13(2)	19(2)	-10(2)
C(16)	47(3)	30(2)	42(2)	-7(2)	12(2)	-10(2)
C(17)	37(2)	36(2)	32(2)	2(2)	11(2)	-12(2)
C(18)	35(2)	39(2)	29(2)	-4(2)	15(2)	-11(2)
C(19)	43(3)	36(2)	58(3)	-2(2)	28(2)	8(2)

Table A 3.32 continued

C(20)	89(5)	67(4)	129(6)	-14(4)	73(5)	24(4)
C(21)	88(5)	115(6)	29(7)	-69(6)	69(5)	-17(5)
C(22)	73(4)	64(4)	59(3)	-26(3)	48(3)	-2(3)
C(23)	96(5)	57(3)	39(3)	-4(3)	39(3)	-1(3)
C(24)	58(3)	49(3)	36(3)	-4(2)	8(2)	5(2)
C(25)	28(2)	43(2)	41(2)	-17(2)	16(2)	-3(2)
C(26)	45(2)	35(2)	30(2)	-10(2)	21(2)	-12(2)
C(27)	48(3)	33(2)	50(3)	-12(2)	16(2)	6(2)

Table A 3.33 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2} x 10^3) for **C14**

	x	*y*	*z*	$U_{(eq)}$
H(1)	1895	7061	3336	26
H(2A)	894	7659	4183	32
H(2B)	1545	8636	4318	32
H(3A)	604	9690	3177	33
H(3B)	1183	9324	2739	33
H(4A)	178	8519	1691	33
H(4B)	15	7587	2494	33
H(5A)	1051	6933	1711	34
H(5B)	396	5964	1571	34
H(6A)	757	5270	3161	33
H(6B)	1333	4885	2721	33
H(7)	1946	3502	6033	28
H(8A)	1093	2709	4217	35
H(8B)	1794	1954	4735	35
H(9A)	899	502	4909	41
H(9B)	1392	1000	5905	41
H(10A)	300	1371	5903	35
H(10B)	135	2334	4967	35
H(11A)	1028	3193	6754	37
H(11B)	322	3939	6248	37
H(12A)	711	4879	5053	32
H(12B)	1198	5415	6044	32
H(13)	3158	6080	6299	28
H(14A)	2135	8265	6024	36
H(14B)	2263	6943	6764	36

Table A 3.33 continued

H(15A)	2729	9192	7509	48
H(15B)	3290	7957	7637	48
H(16A)	3039	10314	6299	48
H(16B)	3682	10182	7203	48
H(17A)	4047	8121	6579	42
H(17B)	3923	9440	5839	42
H(18A)	3472	7180	5092	40
H(18B)	2906	8407	4944	40
H(20)	3254	3114	3254	103
H(21)	3661	957	4493	123
H(23)	4393	-795	4445	72
H(24)	5066	-2006	3757	59
H(25)	5080	-1328	2282	43
H(26)	4420	589	1486	41
H(27)	3727	1837	2167	52

Table A 3.34 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2} x 10^3) for **P4.** $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	$U_{(eq)}$
Sn(1)	2137(1)	5426(1)	4841(1)	21(1)
Br(1)	4378(1)	3723(1)	4401(1)	35(1)
Br(2)	2584(1)	600(1)	3299(1)	31(1)
O(1)	2659(2)	4358(3)	4077(2)	39(1)
O(2)	3143(2)	2973(3)	5299(2)	45(1)
C(1)	1569(2)	6666(4)	3632(2)	22(1)
C(2)	1216(2)	7996(4)	3873(3)	26(1)
C(3)	854(2)	8880(4)	3002(3)	28(1)
C(4)	377(2)	7926(4)	2262(3)	28(1)
C(5)	726(2)	6598(4)	2018(2)	28(1)
C(6)	1087(2)	5702(4)	2895(3)	28(1)
C(7)	1627(2)	3824(4)	5421(2)	23(1)
C(8)	1404(2)	2437(4)	4836(3)	29(1)
C(9)	1064(2)	1361(4)	5322(3)	34(1)
C(10)	487(2)	2078(4)	5554(3)	29(1)
C(11)	710(2)	3462(4)	6139(3)	31(1)
C(12)	1040(2)	4543(4)	5642(3)	26(1)
C(13)	2833(2)	6755(4)	5863(2)	23(1)
C(14)	2482(2)	7634(4)	6445(3)	30(1)
C(15)	2972(2)	8594(5)	7173(3)	40(1)
C(16)	3352(2)	9610(5)	6714(3)	40(1)
C(17)	3701(2)	8748(5)	6152(3)	35(1)
C(18)	3220(2)	7777(5)	5415(3)	33(1)
C(19)	3064(2)	3375(5)	4512(4)	43(1)

Table A 3.34 continued

C(20)	3465(4)	2732(7)	3902(6)	86(2)
C(21)	3511(4)	1324(10)	3833(6)	103(3)
C(22)	3980(3)	619(6)	3377(4)	59(2)
C(23)	4391(3)	-514(6)	3837(4)	60(2)
C(24)	4791(3)	-1224(6)	3434(3)	49(1)
C(25)	4800(2)	-820(5)	2563(3)	36(1)
C(26)	4408(2)	312(5)	2089(3)	35(1)
C(27)	3996(2)	1048(5)	2490(3)	44(1)

Table A 3.35 Bond lengths (Å) for **P4**

Sn(1)-O(1)	2.072(3)	C(9)-C(10)	1.521(5)
Sn(1)-C(13)	2.141(4)	C(10)-C(11)	1.523(5)
Sn(1)-C(7)	2.157(3)	C(11)-C(12)	1.531(5)
Sn(1)-C(1)	2.158(3)	C(13)-C(18)	1.530(5)
Br(1)-C(20)	2.054(8)	C(13)-C(14)	1.539(5)
Br(2)-C(21)	1.990(7)	C(14)-C(15)	1.526(6)
O(1)-C(19)	1.271(5)	C(15)-C(16)	1.526(6)
O(2)-C(19)	1.201(6)	C(16)-C(17)	1.507(6)
C(1)-C(6)	1.528(5)	C(17)-C(18)	1.530(6)
C(1)-C(2)	1.525(5)	C(19)-C(20)	1.548(7)
C(2)-C(3)	1.525(5)	C(20)-C(21)	1.290(10)
C(3)-C(4)	1.520(5)	C(21)-C(22)	1.517(7)
C(4)-C(5)	1.519(5)	C(22)-C(23)	1.387(8)
C(5)-C(6)	1.536(5)	C(22)-C(27)	1.402(7)
C(7)-C(12)	1.531(5)	C(23)-C(24)	1.351(7)
C(7)-C(8)	1.525(5)	C(24)-C(25)	1.369(6)
C(7)-H(7)	1.0000	C(25)-C(26)	1.374(6)
C(8)-C(9)	1.531(5)	C(26)-C(27)	1.381(6)

Table A 3.36 Bond angles (°) for **P4**

O(1)-Sn(1)-C(13)	107.13(13)	C(18)-C(13)-Sn(1)	111.7(2)
O(1)-Sn(1)-C(7)	109.48(13)	C(14)-C(13)-Sn(1)	110.7(2)
C(13)-Sn(1)-C(7)	114.25(13)	C(15)-C(14)-C(13)	111.2(3)
O(1)-Sn(1)-C(1)	91.76(12)	C(16)-C(15)-C(14)	111.0(3)
C(13)-Sn(1)-C(1)	112.88(13)	C(17)-C(16)-C(15)	111.2(4)
C(7)-Sn(1)-C(1)	118.36(14)	C(16)-C(17)-C(18)	111.9(4)
C(19)-O(1)-Sn(1)	115.9(3)	C(17)-C(18)-C(13)	111.0(3)
C(6)-C(1)-C(2)	111.1(3)	O(2)-C(19)-O(1)	125.8(4)
C(6)-C(1)-Sn(1)	112.5(2)	O(2)-C(19)-C(20)	122.6(5)
C(2)-C(1)-Sn(1)	113.5(2)	O(1)-C(19)-C(20)	111.6(5)
C(3)-C(2)-C(1)	111.4(3)	C(21)-C(20)-C(19)	119.5(6)
C(4)-C(3)-C(2)	111.7(3)	C(21)-C(20)-Br(1)	112.1(6)
C(3)-C(4)-C(5)	111.5(3)	C(19)-C(20)-Br(1)	104.4(4)
C(4)-C(5)-C(6)	111.3(3)	C(20)-C(21)-C(22)	122.2(7)
C(1)-C(6)-C(5)	111.1(3)	C(20)-C(21)-Br(2)	105.6(6)
C(12)-C(7)-C(8)	110.6(3)	C(22)-C(21)-Br(2)	112.6(4)
C(12)-C(7)-Sn(1)	110.2(2)	C(23)-C(22)-C(27)	118.8(4)
C(8)-C(7)-Sn(1)	115.3(2)	C(23)-C(22)-C(21)	119.1(6)
C(9)-C(8)-C(7)	111.0(3)	C(27)-C(22)-C(21)	122.0(6)
C(10)-C(9)-C(8)	111.8(3)	C(24)-C(23)-C(22)	121.1(5)
C(9)-C(10)-C(11)	111.1(3)	C(23)-C(24)-C(25)	120.1(5)
C(10)-C(11)-C(12)	110.7(3)	C(24)-C(25)-C(26)	120.6(4)
C(7)-C(12)-C(11)	111.1(3)	C(25)-C(26)-C(27)	120.0(4)
C(18)-C(13)-C(14)	111.1(3)	C(26)-C(27)-C(22)	119.4(5)

Table A 3.37 Anisotropic displacement parameters ($Å^2$ x 10^3) for **P4.** The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^2 U_{11} + ... + 2hkabU_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sn(1)	22(1)	20(1)	21(1)	1(1)	10(1)	2(1)
Br(1)	36(1)	41(1)	30(1)	-10(1)	14(1)	-17(1)
Br(2)	25(1)	33(1)	36(1)	-5(1)	10(1)	-7(1)
O(1)	47(2)	44(2)	34(2)	2(1)	26(1)	14(2)
O(2)	36(2)	35(2)	62(2)	11(2)	12(2)	10(1)
C(1)	20(2)	22(2)	24(2)	1(1)	7(1)	1(1)
C(2)	28(2)	25(2)	25(2)	-1(2)	8(2)	3(2)
C(3)	31(2)	24(2)	28(2)	-1(2)	8(2)	1(2)
C(4)	26(2)	32(2)	23(2)	5(2)	4(2)	-2(2)
C(5)	32(2)	29(2)	21(2)	-3(2)	4(2)	-8(2)
C(6)	35(2)	22(2)	25(2)	-1(2)	7(2)	-3(2)
C(7)	26(2)	22(2)	23(2)	1(1)	9(2)	-1(2)
C(8)	34(2)	25(2)	34(2)	-6(2)	18(2)	-2(2)
C(9)	42(2)	21(2)	45(2)	-4(2)	23(2)	0(2)
C(10)	32(2)	25(2)	33(2)	-2(2)	15(2)	-4(2)
C(11)	38(2)	28(2)	34(2)	-5(2)	22(2)	-4(2)
C(12)	31(2)	19(2)	35(2)	-5(2)	19(2)	-3(2)
C(13)	23(2)	24(2)	21(2)	3(1)	5(1)	4(2)
C(14)	33(2)	32(2)	29(2)	-3(2)	14(2)	-1(2)
C(15)	49(3)	43(3)	32(2)	-13(2)	19(2)	-10(2)
C(16)	47(3)	30(2)	42(2)	-7(2)	12(2)	-10(2)
C(17)	37(2)	36(2)	32(2)	2(2)	11(2)	-12(2)
C(18)	35(2)	39(2)	29(2)	-4(2)	15(2)	-11(2)
C(19)	43(3)	36(2)	58(3)	-2(2)	28(2)	8(2)

Table A 3.37 continued

C(20)	89(5)	67(4)	129(6)	-14(4)	73(5)	24(4)
C(21)	88(5)	115(6)	29(7)	-69(6)	69(5)	-17(5)
C(22)	73(4)	64(4)	59(3)	-26(3)	48(3)	-2(3)
C(23)	96(5)	57(3)	39(3)	-4(3)	39(3)	-1(3)
C(24)	58(3)	49(3)	36(3)	-4(2)	8(2)	5(2)
C(25)	28(2)	43(2)	41(2)	-17(2)	16(2)	-3(2)
C(26)	45(2)	35(2)	30(2)	-10(2)	21(2)	-12(2)
C(27)	48(3)	33(2)	50(3)	-12(2)	16(2)	6(2)

Table A 3.38 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2} x 10^3) for **P4.**

	x	*y*	*z*	$U_{(eq)}$
H(1)	1895	7061	3336	26
H(2A)	894	7659	4183	32
H(2B)	1545	8636	4318	32
H(3A)	604	9690	3177	33
H(3B)	1183	9324	2739	33
H(4A)	178	8519	1691	33
H(4B)	15	7587	2494	33
H(5A)	1051	6933	1711	34
H(5B)	396	5964	1571	34
H(6A)	757	5270	3161	33
H(6B)	1333	4885	2721	33
H(7)	1946	3502	6033	28
H(8A)	1093	2709	4217	35
H(8B)	1794	1954	4735	35
H(9A)	899	502	4909	41
H(9B)	1392	1000	5905	41
H(10A)	300	1371	5903	35
H(10B)	135	2334	4967	35
H(11A)	1028	3193	6754	37
H(11B)	322	3939	6248	37
H(12A)	711	4879	5053	32
H(12B)	1198	5415	6044	32
H(13)	3158	6080	6299	28
H(14A)	2135	8265	6024	36
H(14B)	2263	6943	6764	36

Table A 3.38 continued

H(15A)	2729	9192	7509	48
H(15B)	3290	7957	7637	48
H(16A)	3039	10314	6299	48
H(16B)	3682	10182	7203	48
H(17A)	4047	8121	6579	42
H(17B)	3923	9440	5839	42
H(18A)	3472	7180	5092	40
H(18B)	2906	8407	4944	40
H(20)	3254	3114	3254	103
H(21)	3661	957	4493	123
H(23)	4393	-795	4445	72
H(24)	5066	-2006	3757	59
H(25)	5080	-1328	2282	43
H(26)	4420	589	1486	41
H(27)	3727	1837	2167	52

Table A 3.39 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2} x 10^3) for **D1**. $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	$U_{(eq)}$
Sn(1)	7406(1)	6245(1)	7736(1)	16(1)
Sn(2)	2406(1)	5275(1)	7743(1)	17(1)
O(1)	7257(1)	4652(2)	8239(1)	21(1)
O(2)	7481(1)	3133(2)	7718(1)	29(1)
O(3)	5986(4)	-1699(6)	10109(5)	36(2)
O(4)	6223(5)	-96(19)	10718(4)	63(2)
O(3')	6225(4)	-1780(6)	10239(5)	36(2)
O(4')	5957(5)	-86(19)	10602(4)	63(2)
O(5)	2269(1)	3674(2)	8256(1)	24(1)
O(6)	2471(1)	2147(2)	7726(1)	27(1)
O(7)	1482(10)	-2711(10)	10365(13)	39(2)
O(8)	768(8)	-1190(30)	10434(7)	47(3)
O(7')	1347(10)	-2814(10)	10294(13)	39(2)
O(8')	890(8)	-1250(30)	10558(7)	47(3)
N(1)	6176(1)	-592(3)	10271(1)	37(1)
N(2)	1189(1)	-1650(3)	10265(1)	35(1)
C(1)	7150(2)	7671(3)	8232(1)	23(1)
C(2)	6969(1)	7136(2)	8696(1)	19(1)
C(3)	6317(1)	6732(2)	8599(1)	31(1)
C(4)	6163(1)	6204(2)	9031(1)	48(1)
C(5)	6661(2)	6082(2)	9558(1)	54(1)
C(6)	7313(1)	6487(3)	9655(1)	50(1)
C(7)	7467(1)	7014(2)	9224(1)	32(1)
C(8)	8458(2)	5814(3)	7962(1)	23(1)

Table A 3.39 continued

C(9)	8840(1)	6165(2)	8568(1)	20(1)
C(10)	8892(1)	5266(1)	8984(1)	23(1)
C(11)	9235(1)	5598(2)	9539(1)	26(1)
C(12)	9526(1)	6829(2)	9678(1)	28(1)
C(13)	9474(1)	7728(2)	9262(1)	27(1)
C(14)	9131(1)	7396(2)	8707(1)	22(1)
C(15)	6609(2)	5625(3)	6983(1)	22(1)
C(16)	5933(1)	5861(2)	7020(1)	23(1)
C(17)	5672(1)	4951(2)	7283(1)	27(1)
C(18)	5061(1)	5189(2)	7335(1)	36(1)
C(19)	4711(1)	6337(3)	7124(1)	44(1)
C(20)	4971(1)	7247(2)	6860(1)	47(1)
C(21)	5582(1)	7009(2)	6809(1)	35(1)
C(22)	7304(2)	3466(3)	8115(1)	19(1)
C(23)	7142(2)	2458(3)	8452(1)	20(1)
C(24)	6978(2)	2774(3)	8881(1)	22(1)
C(25)	6786(1)	1866(2)	9237(1)	22(1)
C(26)	6623(1)	2405(1)	9662(1)	27(1)
C(27)	6419(1)	1598(2)	10000(1)	30(1)
C(28)	6378(1)	252(2)	9914(1)	26(1)
C(29)	6541(1)	-287(1)	9489(1)	29(1)
C(30)	6745(1)	520(2)	9150(1)	28(1)
C(31)	3437(2)	4752(3)	7897(1)	23(1)
C(32)	3878(1)	5362(2)	8444(1)	26(1)
C(33)	3923(1)	4797(2)	8944(1)	35(1)
C(34)	4287(1)	5415(3)	9444(1)	46(1)
C(35)	4607(1)	6599(3)	9445(1)	48(1)

Table A 3.39 continued

C(36)	4562(1)	7164(2)	8945(1)	43(1)
C(37)	4198(1)	6546(2)	8445(1)	33(1)
C(38)	2317(2)	6679(3)	8328(1)	21(1)
C(39)	1766(1)	6429(2)	8546(1)	21(1)
C(40)	1874(1)	5606(2)	8998(1)	26(1)
C(41)	1361(1)	5380(2)	9189(1)	33(1)
C(42)	739(1)	5977(2)	8929(1)	35(1)
C(43)	631(1)	6800(2)	8477(1)	38(1)
C(44)	1144(1)	7026(2)	8285(1)	29(1)
C(45)	1567(2)	4719(3)	7011(1)	25(1)
C(46)	909(1)	5305(2)	6984(1)	26(1)
C(47)	541(1)	4697(2)	7257(1)	37(1)
C(48)	-56(1)	5252(3)	7243(1)	52(1)
C(49)	-285(1)	6416(3)	6956(1)	56(1)
C(50)	83(1)	7024(2)	6684(1)	51(1)
C(51)	680(1)	6469(2)	6698(1)	35(1)
C(52)	2322(2)	2495(3)	8130(1)	20(1)
C(53)	2186(2)	1483(3)	8485(1)	21(1)
C(54)	1910(2)	1782(3)	8853(1)	25(1)
C(55)	1722(1)	857(2)	9202(1)	26(1)
C(56)	1340(2)	1327(2)	9492(1)	54(1)
C(57)	1160(1)	494(2)	9836(1)	57(1)
C(58)	1362(1)	-808(2)	9891(1)	28(1)
C(59)	1744(1)	-1278(2)	9602(1)	29(1)
C(60)	1924(1)	-446(2)	9257(1)	26(1)

Table A 3.40 Bond lengths (Å) for **D1**

Sn(1)-C(1)	2.149(3)	C(1)-C(2)	1.499(3)
Sn(1)-C(15)	2.153(3)	C(2)-C(3)	1.3900
Sn(1)-C(8)	2.156(3)	C(2)-C(7)	1.3900
Sn(1)-O(1)	2.182(2)	C(3)-C(4)	1.3900
Sn(1)-O(2)	2.320(2)	C(4)-C(5)	1.3900
Sn(2)-C(45)	2.144(3)	C(5)-C(6)	1.3900
Sn(2)-C(38)	2.149(3)	C(6)-C(7)	1.3900
Sn(2)-C(31)	2.164(3)	C(8)-C(9)	1.518(3)
Sn(2)-O(5)	2.199(2)	C(9)-C(10)	1.3900
Sn(2)-O(6)#2	2.334(2)	C(9)-C(14)	1.3900
O(1)-C(22)	1.267(3)	C(10)-C(11)	1.3900
O(2)-C(22)	1.272(3)	C(11)-C(12)	1.3900
O(2)-Sn(1)#3	2.320(2)	C(12)-C(13)	1.3900
O(3)-N(1)	1.222(6)	C(13)-C(14)	1.3900
O(4)-N(1)	1.235(7)	C(15)-C(16)	1.512(3)
O(3')-N(1)	1.223(6)	C(16)-C(17)	1.3900
O(4')-N(1)	1.238(7)	C(16)-C(21)	1.3900
O(5)-C(52)	1.264(3)	C(17)-C(18)	1.3900
O(6)-C(52)	1.259(3)	C(18)-C(19)	1.3900
O(6)-Sn(2)#4	2.334(2)	C(19)-C(20)	1.3900
O(7)-N(2)	1.231(7)	C(20)-C(21)	1.3900
O(8)-N(2)	1.240(7)	C(22)-C(23)	1.476(4)
O(7')-N(2)	1.230(7)	C(23)-C(24)	1.327(4)
O(8')-N(2)	1.235(7)	C(24)-C(25)	1.473(3)
N(1)-C(28)	1.447(3)	C(25)-C(26)	1.3900
N(2)-C(58)	1.446(3)	C(25)-C(30)	1.3900

Table A 3.40 continued

C(26)-C(27)	1.3900	C(43)-C(44)	1.3900
C(27)-C(28)	1.3900	C(45)-C(46)	1.513(3)
C(28)-C(29)	1.3900	C(46)-C(47)	1.3900
C(29)-C(30)	1.3900	C(46)-C(51)	1.3900
C(31)-C(32)	1.513(4)	C(47)-C(48)	1.3900
C(32)-C(33)	1.3900	C(48)-C(49)	1.3900
C(32)-C(37)	1.3900	C(49)-C(50)	1.3900
C(33)-C(34)	1.3900	C(50)-C(51)	1.3900
C(34)-C(35)	1.3900	C(52)-C(53)	1.485(4)
C(35)-C(36)	1.3900	C(53)-C(54)	1.334(4)
C(36)-C(37)	1.3900	C(54)-C(55)	1.468(3)
C(38)-C(39)	1.513(3)	C(55)-C(56)	1.3900
C(39)-C(40)	1.3900	C(55)-C(60)	1.3900
C(39)-C(44)	1.3900	C(56)-C(57)	1.3900
C(40)-C(41)	1.3900	C(57)-C(58)	1.3900
C(41)-C(42)	1.3900	C(58)-C(59)	1.3900
C(42)-C(43)	1.3900	C(59)-C(60)	1.3900

Table A 3.41 Bond angles (°) for **D1**

C(1)-Sn(1)-C(15)	116.64(12)	O(3')-N(1)-O(4)	119.4(11)
C(1)-Sn(1)-C(8)	117.02(13)	O(3)-N(1)-O(4')	117.3(11)
C(15)-Sn(1)-C(8)	125.49(12)	O(3')-N(1)-O(4')	121.7(12)
C(1)-Sn(1)-O(1)	91.07(9)	O(4)-N(1)-O(4')	25.1(7)
C(15)-Sn(1)-O(1)	94.51(10)	O(3)-N(1)-C(28)	118.3(7)
C(8)-Sn(1)-O(1)	93.42(10)	O(3')-N(1)-C(28)	119.6(7)
C(1)-Sn(1)-O(2)	80.82(10)	O(4)-N(1)-C(28)	114.8(10)
C(15)-Sn(1)-O(2)	89.00(10)	O(4')-N(1)-C(28)	118.7(11)
C(8)-Sn(1)-O(2)	90.47(10)	O(7')-N(2)-O(7)	14.0(17)
O(1)-Sn(1)-O(2)	171.89(8)	O(7')-N(2)-O(8')	118(3)
C(45)-Sn(2)-C(38)	122.28(12)	O(7)-N(2)-O(8')	120(2)
C(45)-Sn(2)-C(31)	123.99(12)	O(7')-N(2)-O(8)	125(2)
C(38)-Sn(2)-C(31)	112.99(12)	O(7)-N(2)-O(8)	130(2)
C(45)-Sn(2)-O(5)	94.59(11)	O(8')-N(2)-O(8)	15.6(18)
C(38)-Sn(2)-O(5)	89.97(9)	O(7')-N(2)-C(58)	118.8(18)
C(31)-Sn(2)-O(5)	93.75(10)	O(7)-N(2)-C(58)	115.1(18)
C(45)-Sn(2)-O(6)	88.74(10)	O(8')-N(2)-C(58)	122.7(16)
C(38)-Sn(2)-O(6)	83.09(10)	O(8)-N(2)-C(58)	114.7(15)
C(31)-Sn(2)-O(6)	89.43(10)	C(2)-C(1)-Sn(1)	115.87(18)
O(5)-Sn(2)-O(6)	173.04(8)	C(3)-C(2)-C(7)	120.0
C(22)-O(1)-Sn(1)	121.17(19)	C(3)-C(2)-C(1)	120.75(19)
C(22)-O(2)-Sn(1)	139.0(2)	C(7)-C(2)-C(1)	119.23(19)
C(52)-O(5)-Sn(2)	120.44(19)	C(2)-C(3)-C(4)	120.0
C(52)-O(6)-Sn(2)	141.3(2)	C(5)-C(4)-C(3)	120.0
O(3)-N(1)-O(3')	23.8(6)	C(4)-C(5)-C(6)	120.0
O(3)-N(1)-O(4)	126.9(12)	C(5)-C(6)-C(7)	120.0

Table A 3.41 continued

C(6)-C(7)-C(2)	120.0	C(30)-C(25)-C(24)	122.48(17)
C(9)-C(8)-Sn(1)	109.68(17)	C(25)-C(26)-C(27)	120.0
C(10)-C(9)-C(14)	120.0	C(26)-C(27)-C(28)	120.0
C(10)-C(9)-C(8)	120.19(17)	C(29)-C(28)-C(27)	120.0
C(14)-C(9)-C(8)	119.81(17)	C(29)-C(28)-N(1)	119.86(17)
C(9)-C(10)-C(11)	120.0	C(27)-C(28)-N(1)	120.13(17)
C(12)-C(11)-C(10)	120.0	C(28)-C(29)-C(30)	120.0
C(11)-C(12)-C(13)	120.0	C(29)-C(30)-C(25)	120.0
C(14)-C(13)-C(12)	120.0	C(32)-C(31)-Sn(2)	107.96(18)
C(13)-C(14)-C(9)	120.0	C(33)-C(32)-C(37)	120.0
C(16)-C(15)-Sn(1)	110.42(18)	C(33)-C(32)-C(31)	120.21(19)
C(17)-C(16)-C(21)	120.0	C(37)-C(32)-C(31)	119.60(18)
C(17)-C(16)-C(15)	119.98(18)	C(32)-C(33)-C(34)	120.0
C(21)-C(16)-C(15)	119.98(18)	C(33)-C(34)-C(35)	120.0
C(18)-C(17)-C(16)	120.0	C(36)-C(35)-C(34)	120.0
C(17)-C(18)-C(19)	120.0	C(35)-C(36)-C(37)	120.0
C(20)-C(19)-C(18)	120.0	C(36)-C(37)-C(32)	120.0
C(19)-C(20)-C(21)	120.0	C(39)-C(38)-Sn(2)	116.21(18)
C(20)-C(21)-C(16)	120.0	C(40)-C(39)-C(44)	120.0
O(1)-C(22)-O(2)	122.5(3)	C(40)-C(39)-C(38)	120.74(17)
O(1)-C(22)-C(23)	117.2(3)	C(44)-C(39)-C(38)	119.26(17)
O(2)-C(22)-C(23)	120.2(3)	C(39)-C(40)-C(41)	120.0
C(24)-C(23)-C(22)	121.6(3)	C(42)-C(41)-C(40)	120.0
C(23)-C(24)-C(25)	126.7(3)	C(41)-C(42)-C(43)	120.0
C(26)-C(25)-C(30)	120.0	C(44)-C(43)-C(42)	120.0
C(26)-C(25)-C(24)	117.50(17)	C(43)-C(44)-C(39)	120.0

Table A 3.41 continued

C(46)-C(45)-Sn(2)	113.29(19)	C(54)-C(53)-C(52)	121.9(3)
C(47)-C(46)-C(51)	120.0	C(53)-C(54)-C(55)	126.4(3)
C(47)-C(46)-C(45)	120.02(19)	C(56)-C(55)-C(60)	120.0
C(51)-C(46)-C(45)	119.97(19)	C(56)-C(55)-C(54)	117.85(18)
C(46)-C(47)-C(48)	120.0	C(60)-C(55)-C(54)	122.14(18)
C(47)-C(48)-C(49)	120.0	C(57)-C(56)-C(55)	120.0
C(50)-C(49)-C(48)	120.0	C(56)-C(57)-C(58)	120.0
C(49)-C(50)-C(51)	120.0	C(57)-C(58)-C(59)	120.0
C(50)-C(51)-C(46)	120.0	C(57)-C(58)-N(2)	119.3(2)
O(6)-C(52)-O(5)	124.0(3)	C(59)-C(58)-N(2)	120.7(2)
O(6)-C(52)-C(53)	119.5(3)	C(59)-C(60)-C(55)	120.0
O(5)-C(52)-C(53)	116.4(3)		

Symmetry transformations used to generate equivalent atoms:

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

#3 -x+3/2,y-1/2,-z+3/2 #4 -x+1/2,y-1/2,-z+3/2

Table A 3.42 Anisotropic displacement parameters ($Å^2 \times 10^3$) for **D1.** The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^2 U_{11} + ... + 2hkabU_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sn(1)	21(1)	13(1)	18(1)	-1(1)	11(1)	0(1)
Sn(2)	19(1)	14(1)	22(1)	0(1)	13(1)	1(1)
O(1)	31(1)	13(1)	23(1)	-2(1)	15(1)	-1(1)
O(2)	39(1)	24(1)	30(1)	0(1)	20(1)	3(1)
O(3)	46(5)	26(2)	41(4)	2(2)	23(4)	-9(2)
O(4)	120(7)	45(2)	49(4)	-8(3)	60(4)	-19(6)
O(3')	46(5)	26(2)	41(4)	2(2)	23(4)	-9(2)
O(4')	120(7)	45(2)	49(4)	-8(3)	60(4)	-19(6)
O(5)	39(1)	13(1)	31(1)	1(1)	25(1)	1(1)
O(6)	36(1)	24(1)	32(1)	-2(1)	23(1)	2(1)
O(7)	35(7)	39(2)	37(6)	13(2)	8(5)	-14(3)
O(8)	84(5)	43(3)	29(6)	-4(6)	40(5)	-18(4)
O(7')	35(7)	39(2)	37(6)	13(2)	8(5)	-14(3)
O(8')	84(5)	43(3)	29(6)	-4(6)	40(5)	-18(4)
N(1)	63(2)	26(2)	31(2)	-1(1)	30(2)	-7(2)
N(2)	50(2)	32(2)	26(2)	-2(1)	17(1)	-18(2)
C(1)	38(2)	8(1)	27(2)	-3(1)	17(1)	-1(1)
C(2)	24(2)	13(1)	25(2)	-2(1)	14(1)	3(1)
C(3)	28(2)	28(2)	43(2)	-15(2)	19(2)	-3(1)
C(4)	57(3)	26(2)	91(4)	-22(2)	62(3)	-16(2)
C(5)	108(4)	23(2)	66(3)	10(2)	70(3)	13(2)
C(6)	75(3)	51(3)	33(2)	17(2)	30(2)	32(2)
C(7)	29(2)	42(2)	26(2)	0(2)	11(1)	10(2)
C(8)	26(2)	22(2)	25(2)	3(1)	15(1)	4(1)

Table A 3.42 continued

C(9)	19(2)	21(2)	25(2)	3(1)	13(1)	4(1)
C(10)	22(2)	20(2)	29(2)	6(1)	13(1)	4(1)
C(11)	25(2)	29(2)	28(2)	10(1)	14(1)	8(1)
C(12)	26(2)	34(2)	23(2)	-3(1)	10(1)	5(1)
C(13)	25(2)	22(2)	34(2)	-3(1)	12(1)	2(1)
C(14)	22(2)	19(2)	29(2)	6(1)	15(1)	4(1)
C(15)	24(2)	21(2)	22(2)	-3(1)	12(1)	-2(1)
C(16)	21(2)	25(2)	23(2)	-6(1)	7(1)	-2(1)
C(17)	29(2)	28(2)	26(2)	-8(1)	11(1)	-8(1)
C(18)	29(2)	49(2)	32(2)	-11(2)	13(2)	-13(2)
C(19)	23(2)	69(3)	43(2)	-10(2)	14(2)	-3(2)
C(20)	31(2)	54(3)	54(3)	2(2)	14(2)	16(2)
C(21)	32(2)	34(2)	40(2)	3(2)	13(2)	6(2)
C(22)	21(2)	16(1)	22(2)	-2(1)	9(1)	1(1)
C(23)	24(2)	12(1)	25(2)	1(1)	10(1)	-1(1)
C(24)	28(2)	14(1)	28(2)	-1(1)	14(1)	-2(1)
C(25)	28(2)	18(1)	23(2)	1(1)	13(1)	-1(1)
C(26)	41(2)	18(2)	29(2)	-1(1)	20(2)	2(1)
C(27)	46(2)	27(2)	27(2)	-4(1)	26(2)	1(2)
C(28)	38(2)	22(2)	23(2)	1(1)	16(2)	-2(1)
C(29)	48(2)	18(2)	30(2)	-2(1)	24(2)	-3(1)
C(30)	44(2)	21(2)	28(2)	-4(1)	24(2)	-5(1)
C(31)	23(2)	21(2)	31(2)	0(1)	15(1)	5(1)
C(32)	18(2)	26(2)	33(2)	2(1)	10(1)	7(1)
C(33)	25(2)	48(2)	31(2)	6(2)	11(2)	6(2)
C(34)	28(2)	76(3)	31(2)	3(2)	10(2)	10(2)
C(35)	26(2)	68(3)	43(2)	-20(2)	4(2)	8(2)

Table A 3.42 continued

C(36)	27(2)	35(2)	58(3)	-12(2)	8(2)	4(2)
C(37)	24(2)	28(2)	44(2)	4(2)	11(2)	8(1)
C(38)	28(2)	14(1)	25(2)	-1(1)	16(1)	1(1)
C(39)	26(2)	18(2)	21(2)	-2(1)	13(1)	3(1)
C(40)	31(2)	25(2)	27(2)	4(1)	16(1)	9(1)
C(41)	50(2)	23(2)	35(2)	6(1)	29(2)	6(2)
C(42)	34(2)	42(2)	41(2)	-4(2)	28(2)	0(2)
C(43)	27(2)	56(2)	34(2)	1(2)	17(2)	13(2)
C(44)	31(2)	36(2)	25(2)	4(1)	16(1)	11(2)
C(45)	26(2)	22(2)	28(2)	-5(1)	13(1)	-3(1)
C(46)	21(2)	27(2)	28(2)	-9(1)	8(1)	-4(1)
C(47)	33(2)	34(2)	51(2)	-10(2)	23(2)	-9(2)
C(48)	29(2)	66(3)	66(3)	-22(2)	24(2)	-12(2)
C(49)	24(2)	79(3)	56(3)	-26(3)	5(2)	12(2)
C(50)	43(2)	47(3)	43(2)	-11(2)	-5(2)	19(2)
C(51)	33(2)	33(2)	34(2)	-5(2)	6(2)	3(2)
C(52)	22(2)	12(1)	30(2)	1(1)	15(1)	0(1)
C(53)	28(2)	11(1)	26(2)	1(1)	13(1)	-1(1)
C(54)	35(2)	15(1)	30(2)	-3(1)	17(2)	-1(1)
C(55)	37(2)	21(2)	25(2)	-1(1)	19(2)	-5(1)
C(56)	106(4)	20(2)	75(3)	6(2)	78(3)	8(2)
C(57)	110(4)	27(2)	73(3)	2(2)	80(3)	3(2)
C(58)	41(2)	25(2)	22(2)	-3(1)	16(2)	-13(2)
C(59)	33(2)	24(2)	31(2)	3(1)	13(2)	-2(1)
C(60)	33(2)	22(2)	30(2)	1(1)	17(2)	-1(1)

List of Publication:

1. **Tricyclo-hexyl(2,3-dibromo-3-phenyl-propionato-κO)tin(IV)** Thong, P.Y., Lo, K.M., Ng, S.W. (2009) Acta Crystallographica Section E: Structure Reports Online 65 (5), pp. m490.

2. **catena-Poly[[tribenzyl-tin(IV)]-μ-4-nitro-cinnamato-κ2 O:O′]** Thong, P.Y., Lo, K.M., Ng, S.W. (2008) Acta Crystallographica Section E: Structure Reports Online 64 (11), pp. m1390.
3. **2,3-Dibromo-3-phenylpropionic acid** Thong, P.Y., Lo, K.M., Ng, S.W. (2008) Acta Crystallographica Section E: Structure Reports Online 64 (10), pp. o1946