Supplementary Material (ESI) for Dalton Transactions


# Supplementary Material for

## Metal Based Synthetic Routes to Heavy Alkaline Earth Aryloxo Complexes Involving Ligands of Moderate Steric Bulk

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### Selected Bond Angles for Compounds 1, 3, 4, 5, 7, 8

Table S2: Bond angles (°) for compounds **1** and **3**.

| | **1** Ae = Ca | **3** Ae = Sr | | **1** Ae = Ca | **3** Ae = Sr |
|---|---|---|---|---|---|
| *Bond angles* | | | | | |
| O(1) - Ae(1) - O(2) | 109.3(1) | 110.95(5) | O(2) - Ae(2) - O(3) | 75.7(1) | 75.65(4) |
| O(1) - Ae(1) - O(3) | 113.7(1) | 113.83(5) | O(2) - Ae(2) - O(4) | 114.2(1) | 113.98(5) |
| O(1) - Ae(1) - O(5) | 89.7(1) | 92.52(5) | O(2) - Ae(2) - O(9) | 154.2(1) | 152.29(5) |
| O(1) - Ae(1) - O(7) | 86.0(1) | 87.66(5) | O(2) - Ae(2) - O(11) | 87.7(1) | 86.56(5) |
| O(1) - Ae(1) - O(8) | 145.7(1) | 146.00(5) | O(2) - Ae(2) - O(12) | 94.5(1) | 95.37(4) |
| O(2) - Ae(1) - O(3) | 75.8(1) | 75.62(4) | O(3) - Ae(2) - O(4) | 108.1(1) | 109.38(5) |
| O(2) - Ae(1) - O(5) | 91.7(1) | 89.05(5) | O(3) - Ae(2) - O(9) | 89.6(1) | 88.13(5) |
| O(2) - Ae(1) - O(7) | 164.4(1) | 161.34(5) | O(3) - Ae(2) - O(11) | 104.6(1) | 104.16(4) |
| O(2) - Ae(1) - O(8) | 102.3(1) | 100.83(5) | O(3) - Ae(2) - O(12) | 165.7(1) | 164.13(4) |
| O(3) - Ae(1) - O(5) | 156.0(1) | 152.78(5) | O(4) - Ae(2) - O(9) | 90.3(1) | 92.42(5) |
| O(3) - Ae(1) - O(7) | 95.5(1) | 96.06(4) | O(4) - Ae(2) - O(11) | 144.2(1) | 143.96(5) |
| O(3) - Ae(1) - O(8) | 86.4(1) | 85.00(5) | O(4) - Ae(2) - O(12) | 85.4(1) | 86.15(5) |
| O(5) - Ae(1) - O(7) | 91.6(1) | 91.53(5) | O(9) - Ae(2) - O(11) | 75.5(1) | 75.65(5) |
| O(5) - Ae(1) - O(8) | 76.1(1) | 75.81(5) | O(9) - Ae(2) - O(12) | 95.4(1) | 94.64(5) |
| O(7) - Ae(1) - O(8) | 63.8(1) | 61.38(4) | O(11) - Ae(2) - O(12) | 63.97(9) | 61.70(4) |

Table S3: Bond angles (°) for compound **4**.

| *Bond angles* | | | |
|---|---|---|---|
| O(1) - Sr(1) - O(2) | 71.8(1) | O(1) - Sr(3) - O(5) | 76.7(1) |
| O(1) - Sr(1) - O(3) | 71.4(1) | O(1) - Sr(3) - O(9) | 144.7(2) |
| O(1) - Sr(1) - O(4) | 76.9(1) | O(1) - Sr(3) - O(10) | 152.8(2) |
| O(1) - Sr(1) - O(5)#1 | 77.6(1) | O(2)#1 - Sr(3) - O(3) | 77.1(1) |
| O(1) - Sr(1) - O(7) | 149.8(2) | O(2)#1 - Sr(3) - O(4) | 143.7(1) |
| O(1) - Sr(1) - O(8) | 146.9(2) | O(2)#1 - Sr(3) - O(5) | 74.3(1) |
| O(2) - Sr(1) - O(3) | 76.7(1) | O(3) - Sr(3) - O(4) | 75.8(1) |
| O(2) - Sr(1) - O(4) | 142.9(1) | O(3) - Sr(3) - O(5) | 142.5(1) |
| O(2) - Sr(1) - O(5)#1 | 75.2(1) | O(4) - Sr(3) - O(5) | 116.2(1) |
| O(3) - Sr(1) - O(4) | 74.7(1) | O(9) - Sr(3) - O(10) | 61.2(2) |
| O(3) - Sr(1) - O(5)#1 | 143.2(1) | Sr(1) - O(1) - Sr(1)#1 | 167.1(3) |
| O(4) - Sr(1) - O(5)#1 | 117.2(1) | Sr(1) - O(1) - Sr(2) | 83.6(1) |
| O(7) - Sr(1) - O(8) | 62.0(1) | Sr(1) - O(1) - Sr(3) | 89.0(1) |
| O(2) - Sr(2) - O(2)#1 | 129.8(2) | Sr(1) - O(1) - Sr(3)#1 | 89.5(1) |
| O(2) - Sr(2) - O(3) | 79.5(1) | Sr(1)#1 - O(1) - Sr(3) | 89.5(1) |
| O(2) - Sr(2) - O(3)#1 | 79.5(1) | Sr(1)#1 - O(1) - Sr(3)#1 | 89.0(1) |
| O(2)#1 - Sr(2) - O(3) | 79.5(1) | Sr(2) - O(1) - Sr(3) | 83.2(1) |
| O(2) - Sr(2) - O(6) | 115.1(1) | Sr(3) - O(1) - Sr(3)#1 | 166.3(3) |
| O(2)#1 - Sr(2) - O(6) | 115.1(1) | Sr(1) - O(2) - Sr(2) | 98.2(1) |
| O(3) - Sr(2) - O(6) | 115.4(1) | Sr(1) - O(2) - Sr(3)#1 | 92.0(1) |
| O(3)#1 - Sr(2) - O(3) | 129.3(2) | Sr(2) - O(2) - Sr(3)#1 | 97.8(1) |
| O(3)#1 - Sr(2) - O(6) | 115.4(1) | Sr(1) - O(3) - Sr(2) | 98.4(1) |
| O(1) - Sr(3) - O(2)#1 | 71.5(1) | Sr(1) - O(3) - Sr(3) | 92.1(1) |
| O(1) - Sr(3) - O(3) | 71.6(1) | Sr(2) - O(3) - Sr(3) | 98.8(1) |
| O(1) - Sr(3) - O(4) | 77.4(1) | Sr(2) - O(6) - C(22) | 180.0(1) |

Symmetry operation used to generate equivalent atoms: #1: -x, y, -z + 1/2

Table S4: Bond angles (°) for compound **7**.

*Bond angles*

| | | | | | |
|---|---|---|---|---|---|
| O(1) - Ba(1) - O(2) | 68.7(2) | O(1) - Ba(3) - O(13) | 141.7(2) | O(1) - Ba(5) - O(18) | 134.0(2) |
| O(1) - Ba(1) - O(3) | 69.5(1) | O(1) - Ba(3) - O(14) | 160.7(2) | O(4) - Ba(5) - O(5) | 73.2(2) |
| O(1) - Ba(1) - O(7) | 75.1(2) | O(3) - Ba(3) - O(4) | 78.2(2) | O(4) - Ba(5) - O(6) | 75.7(2) |
| O(1) - Ba(1) - O(8) | 76.3(2) | O(3) - Ba(3) - O(6) | 138.7(2) | O(4) - Ba(5) - O(9) | 139.3(2) |
| O(1) - Ba(1) - O(11) | 152.6(2) | O(3) - Ba(3) - O(7) | 75.4(2) | O(5) - Ba(5) - O(6) | 138.8(2) |
| O(1) - Ba(1) - O(12) | 148.9(2) | O(4) - Ba(3) - O(6) | 75.9(2) | O(5) - Ba(5) - O(9) | 73.1(1) |
| O(2) - Ba(1) - O(3) | 74.1(2) | O(4) - Ba(3) - O(7) | 140.0(2) | O(6) - Ba(5) - O(9) | 118.6(2) |
| O(2) - Ba(1) - O(7) | 138.1(2) | O(6) - Ba(3) - O(7) | 105.9(2) | O(17) - Ba(5) - O(18) | 56.3(2) |
| O(2) - Ba(1) - O(8) | 74.8(1) | O(13) - Ba(3) - O(14) | 57.5(2) | Ba(1) - O(1) - Ba(3) | 88.8(1) |
| O(3) - Ba(1) - O(7) | 74.1(2) | O(1) - Ba(4) - O(2) | 69.1(2) | Ba(1) - O(1) - Ba(4) | 89.4(1) |
| O(3) - Ba(1) - O(8) | 140.1(2) | O(1) - Ba(4) - O(5) | 68.9(2) | Ba(1) - O(1) - Ba(5) | 173.2(2) |
| O(7) - Ba(1) - O(8) | 116.4(2) | O(1) - Ba(4) - O(8) | 75.7(2) | Ba(3) - O(1) - Ba(4) | 166.0(2) |
| O(11) - Ba(1) - O(12) | 57.4(2) | O(1) - Ba(4) - O(9) | 77.1(2) | Ba(3) - O(1) - Ba(5) | 89.6(1) |
| O(2) - Ba(2) - O(3) | 77.5(2) | O(1) - Ba(4) - O(15) | 144.9(2) | Ba(4) - O(1) - Ba(5) | 90.6(1) |
| O(2) - Ba(2) - O(4) | 127.4(1) | O(1) - Ba(4) - O(16) | 156.2(2) | Ba(1) - O(2) - Ba(2) | 100.9(2) |
| O(2) - Ba(2) - O(5) | 80.2(2) | O(2) - Ba(4) - O(5) | 77.5(1) | Ba(1) - O(2) - Ba(4) | 94.5(1) |
| O(2) - Ba(2) - O(10) | 109.7(2) | O(2) - Ba(4) - O(8) | 75.0(1) | Ba(2) - O(2) - Ba(4) | 99.5(2) |
| O(3) - Ba(2) - O(4) | 80.8(2) | O(2) - Ba(4) - O(9) | 142.4(2) | Ba(1) - O(3) - Ba(2) | 100.7(2) |
| O(3) - Ba(2) - O(5) | 128.3(2) | O(5) - Ba(4) - O(8) | 140.9(1) | Ba(1) - O(3) - Ba(3) | 94.9(1) |
| O(3) - Ba(2) - O(10) | 117.2(2) | O(5) - Ba(4) - O(9) | 75.3(1) | Ba(2) - O(3) - Ba(3) | 99.1(2) |
| O(4) - Ba(2) - O(5) | 76.9(2) | O(8) - Ba(4) - O(9) | 112.6(2) | Ba(2) - O(4) - Ba(3) | 98.1(2) |
| O(4) - Ba(2) - O(10) | 122.8(2) | O(15) - Ba(4) - O(16) | 58.3(2) | Ba(2) - O(4) - Ba(5) | 100.8(2) |
| O(5) - Ba(2) - O(10) | 114.1(2) | O(1) - Ba(5) - O(4) | 70.3(2) | Ba(3) - O(4) - Ba(5) | 93.6(1) |
| O(1) - Ba(3) - O(3) | 68.7(1) | O(1) - Ba(5) - O(5) | 69.6(2) | Ba(2) - O(5) - Ba(4) | 98.3(2) |
| O(1) - Ba(3) - O(4) | 68.2(1) | O(1) - Ba(5) - O(6) | 74.9(2) | Ba(2) - O(5) - Ba(5) | 100.4(2) |
| O(1) - Ba(3) - O(6) | 72.0(2) | O(1) - Ba(5) - O(9) | 77.1(2) | Ba(4) - O(5) - Ba(5) | 92.1(1) |
| O(1) - Ba(3) - O(7) | 74.4(2) | O(1) - Ba(5) - O(17) | 169.5(2) | Ba(2) - O(10) - C(42) | 167.7(5) |

Table S5: Bond angles (°) for compounds **5** and **8**.

| | **5** Ae = Sr | **8** Ae = Ba | | **5** Ae = Sr | **8** Ae = Ba |
|---|---|---|---|---|---|
| *Bond angles* | | | | | |
| O(1) - Ae(1) - O(1)#1 | 180.0(1) | 180.0(1) | O(1) - Ae(2) - O(2) | 78.4(1) | 75.1(1) |
| O(1) - Ae(1) - O(2) | 73.1(1) | 70.8(1) | O(1) - Ae(2) - O(3) | 76.1(1) | 77.4(1) |
| O(1) - Ae(1) - O(2)#1 | 106.9(1) | 109.2(1) | O(1) - Ae(2) - O(4) | 85.8(1) | 87.6(1) |
| O(1) - Ae(1) - O(3) | 71.5(1) | 71.8(1) | O(1) - Ae(2) - O(5) | 123.6(1) | 118.9(1) |
| O(1) - Ae(1) - O(3)#1 | 108.5(1) | 108.2(1) | O(1) - Ae(2) - O(6) | 147.5(1) | 152.2(1) |
| O(1)#1 - Ae(1) - O(2) | 106.9(1) | 109.2(1) | O(2) - Ae(2) - O(3) | 77.4(1) | 77.8(1) |
| O(1)#1 - Ae(1) - O(2)#1 | 73.1(1) | 70.8(1) | O(2) - Ae(2) - O(4) | 142.8(1) | 131.2(1) |
| O(1)#1 - Ae(1) - O(3) | 108.5(1) | 108.2(1) | O(2) - Ae(2) - O(5) | 82.5(1) | 151.0(1) |
| O(1)#1 - Ae(1) - O(3)#1 | 71.5(1) | 71.8(1) | O(2) - Ae(2) - O(6) | 128.8(1) | 93.9(1) |
| O(2) - Ae(1) - O(2)#1 | 180.0(1) | 180.0(1) | O(3) - Ae(2) - O(4) | 131.0(1) | 142.7(1) |
| O(2) - Ae(1) - O(3) | 74.9(1) | 75.2(1) | O(3) - Ae(2) - O(5) | 148.2(1) | 80.7(1) |
| O(2) - Ae(1) - O(3)#1 | 105.2(2) | 104.8(1) | O(3) - Ae(2) - O(6) | 91.6(1) | 125.9(1) |
| O(2)#1 - Ae(1) - O(3) | 105.2(1) | 104.8(1) | O(4) - Ae(2) - O(5) | 78.6(1) | 77.0(1) |
| O(2)#1 - Ae(1) - O(3)#1 | 74.9(1) | 75.2(1) | O(4) - Ae(2) - O(6) | 80.0(1) | 80.7(1) |
| O(3) - Ae(1) - O(3)#1 | 180.0(2) | 180.0(2) | O(5) - Ae(2) - O(6) | 82.0(1) | 83.0(1) |

Symmetry operation used to generate equivalent atoms: #1: -x + 1, -y, -z + 1