Electronic Supplementary Material (ESI) for New Journal of Chemistry.


# Syntheses, structures and anti-tumor activity of four organotin(IV) dicarboxylates based on (1,3,4-thiadiazole-2,5-diyldithio)diacetic acid

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Supporting Information

## X-ray crystallography

**Table S1** Selected bond lengths [Å] and angles [°] for complex **1**.

| Complex **1** | | | |
|---|---|---|---|
| Sn(1)-C(6) | 2.118(5) | Sn(1)-C(4) | 2.123(5) |
| Sn(1)-C(5) | 2.124(5) | Sn(1)-O(2) | 2.217(3) |
| Sn(1)-O(1)#1 | 2.372(3) | Sn(1) #2-O(1) | 2.372(3) |
| C(6)-Sn(1)-C(4) | 120.3(3) | C(6)-Sn(1)-C(5) | 123.9(3) |
| C(4)-Sn(1)-C(5) | 115.3(3) | C(6)-Sn(1)-O(2) | 92.26(18) |
| C(4)-Sn(1)-O(2) | 87.50(19) | C(5)-Sn(1)-O(2) | 97.15(17) |
| C(6)-Sn(1)-O(1)#1 | 89.16(18) | C(4)-Sn(1)-O(1)#1 | 85.24(18) |
| C(5)-Sn(1)-O(1)#1 | 88.31(18) | O(2)-Sn(1)-O(1)#1 | 172.29(11) |

Symmetry code for complex **1**: #1 x,-y+1,z-1/2 #2 x,-y+1,z+1/2

**Table S2** Selected bond lengths [Å] and angles [°] for complex **2**.

| Complex **2** | | | |
|---|---|---|---|
| Sn(1)-C(6) | 2.110(10) | Sn(1)-C(5) | 2.102(10) |
| Sn(1)-O(4) | 2.288(6) | Sn(1)-O(3) | 2.011(5) |
| Sn(1)-O(2) | 2.291(8) | Sn(2)-C(8) | 2.101(9) |
| Sn(2)-C(7) | 2.080(10) | Sn(2)-O(4) | 2.577(5) |
| Sn(2)-O(3) | 2.070(5) | Sn(2)-O(2) | 2.903(9) |
| Sn(2)-O(3) #1 | 2.069(5) | C(5)-Sn(1)-C(6) | 139.5(5) |
| C(5)-Sn(1)-O(4) | 89.1(3) | C(6)-Sn(1)-O(4) | 96.2(3) |
| C(5)-Sn(1)-O(2) | 101.5(4) | C(6)-Sn(1)-O(2) | 94.0(4) |
| O(3)-Sn(1)-O(4) | 74.3(2) | O(3)-Sn(1)-O(2) | 75.2(3) |
| O(4)-Sn(1)-O(2) | 149.5(3) | C(7)-Sn(2)-C(8) | 138.9(4) |
| C(7)-Sn(2)-O(2) | 79.0(4) | C(8)-Sn(2)-O(2) | 92.3(3) |
| O(3)-Sn(2)-C(7) | 106.1(3) | O(3)-Sn(2)-C(8) | 104.3(4) |
| O(3)-Sn(2)-O(2) | 61.3(2) | O(3)#1-Sn(2)-O(3) | 75.6(2) |
| O(3)#1-Sn(2)-C(7) | 110.2(4) | O(3)#1-Sn(2)-C(8) | 103.6(3) |
| O(3)#1-Sn(2)-O(2) | 136.6(2) | | |

Symmetry code for complex **2**: #1 -x+1,-y+1, -z+1

**Table S3** Selected bond lengths [Å] and angles [°] for complex **3**.

| Complex **3** | | | |
|---|---|---|---|
| Sn(1)-C(39) | 2.184(14) | Sn(1)-C(35) | 2.088(14) |
| Sn(1)-C(31) | 2.172(14) | Sn(1)-O(6)#1 | 2.219(8) |
| Sn(1)-O(4) | 2.407(9) | Sn(2)-C(51) | 2.131(14) |
| Sn(2)-C(47) | 2.155(14) | Sn(2)-C(43) | 2.131(15) |
| Sn(2)-O(5) | 2.448(10) | Sn(2)-O(3) | 2.199(10) |
| Sn(3)-C(13) | 2.147(16) | Sn(3)-C(9) | 2.127(17) |
| Sn(3)-C(5) | 2.214(15) | Sn(3)-O(8)#2 | 2.421(11) |
| Sn(3)-O(1) | 2.196(10) | Sn(4)-C(25) | 2.244(18) |
| Sn(4)-C(21) | 2.113(17) | Sn(4)-C(17) | 2.122(19) |
| Sn(4)-O(7)#3 | 2.198(11) | Sn(4)-O(2) | 2.446(12) |
| C(39)-Sn(1)-C(31) | 120.0(6) | C(35)-Sn(1)-C(39) | 118.1(6) |
| C(35)-Sn(1)-C(31) | 121.2(6) | O(6)#1-Sn(1)-O(4) | 172.4(3) |
| C(51)-Sn(2)-C(47) | 117.4(6) | C(51)-Sn(2)-C(43) | 121.3(6) |
| C(43)-Sn(2)-C(47) | 120.0(5) | O(3)-Sn(2)-O(5) | 173.9(3) |
| C(9)-Sn(3)-C(13) | 120.2(7) | C(13)-Sn(3)-C(5) | 121.6(7) |
| C(9)-Sn(3)-C(5) | 116.2(7) | O(1)-Sn(3)-O(8)#2 | 173.0(4) |
| C(21)-Sn(4)-C(25) | 119.5(7) | C(17)-Sn(4)-C(25) | 116.3(8) |
| C(17)-Sn(4)-C(21) | 123.0(7) | O(7)#3-Sn(4)-O(2) | 173.3(4) |

Symmetry code for complex **3**: #1 x+1,y,z #2 x,y-1,z #3 x+1,y-1,z

**Table S4** Selected bond lengths [Å] and angles [°] for complex **4**.

| Complex **4** | | | |
|---|---|---|---|
| Sn(1)-C(9) | 2.12(2) | Sn(1)-C(5) | 2.086(19) |
| Sn(1)-O(4) | 2.587(11) | Sn(1)-O(3)#1 | 2.089(11) |
| O(3)-Sn(1)#2 | 2.089(11) | Sn(1)-O(1) | 2.130(11) |
| Sn(1)-O(2) | 2.587(11) | O(3)#1-Sn(1)-O(1) | 80.4(4) |
| O(1)-Sn(1)-O(2) | 55.36(37) | O(4)#1-Sn(1)-O(2) | 169.38(36) |
| O(4)#1-Sn(1)-O(3)#1 | 54.69(39) | C(9)-Sn(1)-O(2) | 84.2(7) |
| C(5)-Sn(1)-O(1) | 102.2(7) | O(3)#1-Sn(1)-C(9) | 105.4(8) |
| C(9)-Sn(1)-O(1) | 102.8(6) | C(5)-Sn(1)-C(9) | 138.3(10) |
| C(5)-Sn(1)-O(3)#1 | 111.3(7) | C(5)-Sn(1)-O(2) | 82.9(7) |
| O(3)#1-Sn(1)-O(2) | 136.0(5) | | |

Symmetry code for complex **4**: #1 x-1,y,z #2 x+1,y,z

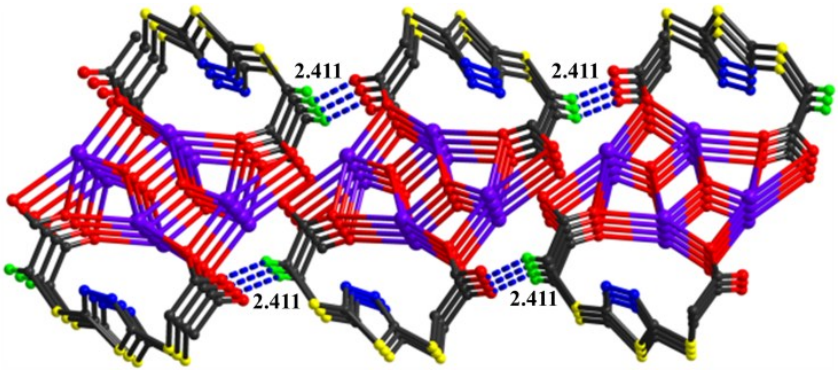


**Figure S1** 2D supramolecular structure of complex **2** constructed by C–H···O (blue dashes) interactions. Methyl groups and hydrogen atoms are omitted for clarity.