Synthesis, characterization and crystal structure of two zinc linear dicarboxilates

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# INFRARED SPECTRA



FIGURE S1. IR spectra for ZnAdp and ZnSc samples.

# THERMOGRAVIMETRIC ANALYSIS



FIGURE S2. Thermogravimetric curve (green) and it temperature derivative (blue) of ZnAdp.



FIGURE S3. Thermogravimetric curve (green) and it temperature derivative (blue) of ZnSc.



FIGURE S4. Inorganic sheets of ZnO4 distorted octahedra pillared by adipate ligands in a 2×2×2 supercell of ZnAdp shown in **b** direction.

# CRYSTAL STRUCTURE

TABLE S1. Atomic positions, temperature and occupation factors derived from the Rietveld refined crystal structure for: ZnAdp and ZnSc.

| Atom | site |  x |  y |  z | Biso | Occ |
| --- | --- | --- | --- | --- | --- | --- |
| Zn2(C6H8O4)2 (ZnAdp) |
| Zn1 | 2a | 0.753(2) | 1.047(1) | 0.277(3) | 1.85(2) | 1 |
| Oc1 | 2a | 0.651(2) | 0.861(3) | 0.209(4) | 2.38(3) | 1 |
| Oc2 | 2a | 0.721(4) | 0.479(2) | 0.262(3) | 2.38(3) | 1 |
| Oc3 | 2a | 0.850(3) | 0.930(3) | 0.168(4) | 2.38(3) | 1 |
| Oc4 | 2a | 0.781(2) | 1.027(2) | 0.482(5) | 2.38(3) | 1 |
| C1 | 2a | 0.660(3) | 0.598(4) | 0.201(1) | 2.38(3) | 1 |
| C2 | 2a | 0.597(3) | 0.428(3) | 0.119(5) | 2.38(3) | 1 |
| C3 | 2a | 0.529(1) | 0.599(2) | 0.044(4) | 2.38(3) | 1 |
| C4 | 2a | 0.840(4) | 0.886(2) | 0.035(3) | 2.38(3) | 1 |
| C5 | 2a | 0.902(3) | 0.699(4) | -0.040(4) | 2.38(3) | 1 |
| C6 | 2a | 0.964(2) | 0.553(3) | 0.058(4) | 2.38(3) | 1 |
| Zn2(OH)2(C4H4O4) (ZnSc) |
| Zn | 2d | 0.9600(1) | 0.6676(1) | 0 | 0.0159(2) | 1 |
| Oc1 | 2d | 0.1683(7) | 0.5879(2) | 0 | 0.0266(8) | 1 |
| Oc2 | 2d | 0.5597(6) | 0.6423(2) | 0 | 0.0238(8) | 1 |
| Oh | 2d | 0 | 0.7128(2) | 0.75 | 0.0190(7) | 1 |
| H3 | 1d | 0.857(10) | 0.736(3) | -0.253(10) | 0.029 | 0.5 |
| H3A | 1d | 0.7091 | 0.5282 | 0.1159 | 0.022 | 0.5 |
| C1 | 2d | 0.4328(8) | 0.5906(2) | 0 | 0.016(1) | 1 |
| C2 | 2d | 0.5913(9) | 0.5295(2) | 0 | 0.018(1) | 1 |

TABLE S2. Calculated Bond lengths (Å) and angles (°) from the refined structure for samples studied

|  | Bond lengths (Å) | Angles (°) |
| --- | --- | --- |
| ZnAdp | Zn-Oc1= 1.970(2) | Oc1-Zn-Oc2= 102.19(1)  | Oc1-C1-C2= 119.44(2) |
| Zn-Oc2= 2.138(1) | Oc1-Zn-Oc3= 112.43(3) | Oc2-C1-C2= 120.33(2) |
| Zn-Oc3= 1.958(1) | Oc1-Zn-Oc4= 118.37(2) | Oc3-C4-C5= 118.04(2) |
| Zn-Oc4= 1.955(1) | Oc2-Zn-Oc3= 116.24(1) | Oc4-C4-C5= 124.43(2) |
| Oc1-C1= 1.266(1) | Oc2-Zn-Oc4= 99.32(2) | C1-C2-C3= 114.83(3) |
| Oc2-C1= 1.268(1) | Oc3-Zn-Oc4= 107.88(2) | C4-C5-C6= 115.06(2) |
| Oc3-C4= 1.244(1) | Zn-Oc1-C1= 112.08(2) |  |
| Oc4-C4= 1.158(1) | Zn-Oc2-C1= 130.62(2) |  |
| C1-C2= 1.506(1) | Zn-Oc3-C4= 116.74(2) |  |
| C2-C3= 1.527(1) | Zn-Oc4-C4= 125.34(2) |  |
| C4-C5= 1.516(1) | Oc1-C1-Oc2= 120.21(3) |  |
| C5-C6= 1.525(2) | Oc3-C4-Oc4= 117.16(3) |  |
| ZnSc | Zn-Oh= 1.937(2) | Oh-Zn-Oc2= 103.2(1) | Oc1-Zn-Oc2= 105.0(1) |
| Zn-Oc1= 1.962(3) | Oh-Zn-Oc1= 112.1(1) | Oh’-Zn-Oh= 119.4(2) |
| Zn-Oc2= 1.992(3) |  |  |

# CRYSTALLOGRAPHIC DATA FOR ZnAdp

TABLE S3. Miller indices, calculated and observed angles, d spacing in Angstroms and relative intensities for reflections for ZnAdp.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| h | k | l | 2thetaobs | 2thetacalc | dhkl | I/Io | Δ2theta |
| 2 | 0 | 0 | 10.921 | 10.911 | 8.101 | 100 | 0.01 |
| 0 | 1 | 0 | 18.547 | 18.543 | 4.781 | 9 | 0.004 |
| 0 | 0 | 2 | 19.136 | 19.134 | 4.634 | 11 | 0.002 |
| 1 | 1 | 0 | 19.337 | 19.341 | 4.585 | 5 | -0.004 |
| -1 | 0 | 2 | 19.918 | 19.879 | 4.462 | 4 | 0.039 |
| 1 | 0 | 2 | 19.940 | 4.449 | -0.022 |
| 2 | 1 | 0 | 21.575 | 21.564 | 4.117 | 67 | 0.011 |
| -1 | 1 | 1 | 21.590 | 4.113 | -0.015 |
| -2 | 0 | 2 | 22.043 | 22.023 | 4.032 | 40 | 0.02 |
| 2 | 0 | 2 | 22.145 | 22.133 | 4.012 | 21 | 0.012 |
| -2 | 1 | 1 | 23.623 | 23.598 | 3.767 | 9 | 0.025 |
| 2 | 1 | 1 | 23.650 | 3.758 | -0.027 |
| 3 | 1 | 0 | 24.862 | 24.851 | 3.579 | 10 | 0.011 |
| -3 | 0 | 2 | 25.242 | 25.228 | 3.527 | 18 | 0.014 |
| 3 | 1 | 1 | 26.751 | 26.706 | 3.335 | 8 | 0.045 |
| 0 | 1 | 2 | 26.768 | 3.327 | -0.017 |
| -1 | 1 | 2 | 27.333 | 27.315 | 3.262 | 1 | 0.018 |
| 1 | 1 | 2 | 27.360 | 3.257 | -0.027 |
| 4 | 1 | 0 | 28.914 | 28.864 | 3.090 | 8 | 0.05 |
| -2 | 1 | 2 | 28.941 | 3.083 | -0.027 |
| 2 | 1 | 2 | 29.011 | 29.027 | 3.073 | 5 | -0.016 |
| 4 | 0 | 2 | 29.366 | 29.342 | 3.041 | 5 | 0.024 |
| 4 | 1 | 1 | 30.492 | 30.504 | 2.928 | 4 | -0.012 |
| 3 | 1 | 2 | 31.609 | 31.612 | 2.828 | < 1 | -0.003 |
| 5 | 1 | 0 | 33.363 | 33.375 | 2.682 | 2 | -0.012 |
| -5 | 0 | 2 | 33.641 | 33.627 | 2.663 | 4 | 0.014 |
| 4 | 1 | 2 | 34.942 | 34.936 | 2.566 | 4 | 0.006 |
| -1 | 1 | 3 | 34.962 | 2.564 | -0.02 |
| 2 | 1 | 3 | 36.359 | 36.375 | 2.468 | < 1 | -0.016 |
| 0 | 2 | 0 | 37.561 | 37.595 | 2.390 | 7 | -0.034 |
| 6 | 1 | 0 | 38.269 | 38.245 | 2.351 | 2 | 0.024 |
| -3 | 1 | 3 | 38.369 | 38.379 | 2.343 | 2 | -0.01 |
| 0 | 0 | 4 | 38.798 | 38.831 | 2.317 | 6 | -0.033 |
| 5 | 1 | 2 | 38.838 | 2.316 | -0.04 |
| -1 | 0 | 4 | 39.214 | 39.208 | 2.296 | 11 | 0.006 |
| 1 | 0 | 4 | 39.297 | 39.274 | 2.292 | 3 | 0.023 |
| -1 | 2 | 1 | 39.277 | 2.292 | 0.02 |
| 6 | 1 | 1 | 39.569 | 39.556 | 2.276 | 6 | 0.013 |
| -2 | 0 | 4 | 40.385 | 40.391 | 2.231 | 4 | -0.006 |
| -2 | 2 | 1 | 40.475 | 40.480 | 2.226 | 3 | -0.005 |
| 4 | 1 | 3 | 41.366 | 41.378 | 2.180 | 3 | -0.012 |
| -3 | 2 | 1 | 42.441 | 42.428 | 2.129 | 2 | 0.013 |
| 0 | 2 | 2 | 42.530 | 42.517 | 2.124 | 2 | 0.013 |
| 6 | 1 | 2 | 43.207 | 43.195 | 2.092 | 4 | 0.012 |
| 4 | 2 | 0 | 43.935 | 43.945 | 2.058 | 6 | -0.01 |
| 2 | 1 | 4 | 44.896 | 44.905 | 2.016 | 4 | -0.009 |
| -4 | 0 | 4 | 44.917 | 2.016 | -0.021 |
| -4 | 2 | 1 | 45.022 | 45.044 | 2.011 | 3 | -0.022 |
| -3 | 2 | 2 | 45.796 | 45.818 | 1.978 | < 1 | -0.022 |
| 3 | 1 | 4 | 46.725 | 46.740 | 1.941 | 1 | -0.015 |
| 0 | 2 | 3 | 48.109 | 48.086 | 1.890 | 3 | 0.023 |
| -5 | 0 | 4 | 48.101 | 1.890 | 0.008 |
| 5 | 0 | 4 | 48.364 | 48.380 | 1.879 | 2 | -0.016 |
| 4 | 2 | 2 | 48.392 | 1.879 | -0.028 |
| -8 | 0 | 2 | 48.917 | 48.934 | 1.859 | 3 | -0.017 |
| 8 | 0 | 2 | 49.137 | 49.154 | 1.852 | 2 | -0.017 |
| 6 | 2 | 0 | 50.988 | 50.978 | 1.789 | 2 | 0.01 |
| -5 | 1 | 4 | 51.978 | 51.982 | 1.757 | 1 | -0.004 |
| 6 | 0 | 4 | 52.119 | 52.113 | 1.753 | 1 | 0.006 |
| -7 | 1 | 3 | 52.868 | 52.829 | 1.731 | 2 | 0.039 |
| 7 | 1 | 3 | 53.097 | 53.101 | 1.723 | 2 | -0.004 |
| 6 | 2 | 2 | 55.015 | 55.021 | 1.667 | 2 | -0.006 |
| 6 | 1 | 4 | 55.765 | 55.793 | 1.646 | 1 | -0.028 |
| 7 | 0 | 4 | 56.306 | 56.290 | 1.632 | 2 | 0.016 |
| 2 | 2 | 4 | 56.459 | 56.459 | 1.628 | 1 | 0 |
| 10 | 0 | 0 | 56.746 | 56.769 | 1.620 | < 1 | -0.023 |
| 8 | 1 | 3 | 57.834 | 57.837 | 1.592 | < 1 | -0.003 |
| -4 | 1 | 5 | 57.840 | 1.592 | -0.006 |
| -7 | 2 | 2 | 58.898 | 58.876 | 1.567 | < 1 | 0.022 |
| 8 | 2 | 0 | 59.803 | 59.797 | 1.545 | 2 | 0.006 |
| 7 | 1 | 4 | 59.797 | 1.545 | 0.006 |
| 0 | 0 | 6 | 59.818 | 1.544 | -0.015 |
| -1 | 0 | 6 | 60.062 | 60.081 | 1.538 | 1 | -0.019 |
| 5 | 1 | 5 | 60.840 | 60.822 | 1.522 | < 1 | 0.018 |
| 4 | 3 | 0 | 62.584 | 62.585 | 1.483 | < 1 | -0.001 |
| 3 | 0 | 6 | 62.584 | 1.483 | 0 |
| -9 | 1 | 3 | 62.606 | 1.482 | -0.022 |
| -5 | 2 | 4 | 62.603 | 1.482 | -0.019 |
| -4 | 3 | 1 | 63.441 | 63.450 | 1.464 | 1 | -0.009 |
| 0 | 2 | 5 | 63.447 | 1.464 | -0.006 |
| -1 | 1 | 6 | 63.457 | 1.464 | -0.016 |
| 4 | 3 | 1 | 63.503 | 63.496 | 1.463 | < 1 | 0.007 |
| 1 | 1 | 6 | 63.527 | 1.463 | -0.024 |
| 3 | 3 | 2 | 64.116 | 64.133 | 1.451 | < 1 | -0.017 |
| 6 | 2 | 4 | 66.019 | 66.018 | 1.413 | < 1 | 0.001 |
| -5 | 3 | 1 | 66.021 | 1.413 | -0.002 |
| -5 | 0 | 6 | 66.893 | 66.891 | 1.397 | < 1 | 0.002 |
| 4 | 2 | 5 | 68.115 | 68.106 | 1.375 | < 1 | 0.009 |
| -9 | 2 | 2 | 68.122 | 1.375 | -0.007 |
| -6 | 3 | 1 | 69.091 | 69.098 | 1.358 | < 1 | -0.007 |
| -5 | 1 | 6 | 70.122 | 70.088 | 1.341 | < 1 | 0.034 |
| 10 | 2 | 0 | 70.102 | 1.341 | 0.02 |
| 10 | 0 | 4 | 71.178 | 71.132 | 1.324 | < 1 | 0.046 |
| -2 | 3 | 4 | 72.912 | 72.877 | 1.296 | < 1 | 0.035 |
| 5 | 3 | 3 | 72.896 | 1.296 | 0.016 |
| -11 | 1 | 3 | 73.761 | 73.747 | 1.284 | < 1 | 0.014 |
| -4 | 3 | 4 | 76.064 | 76.060 | 1.250 | < 1 | 0.004 |
| -9 | 1 | 5 | 76.068 | 1.250 | -0.004 |
| 8 | 3 | 1 | 76.759 | 76.765 | 1.240 | < 1 | -0.006 |
| -7 | 2 | 5 | 76.777 | 1.240 | -0.018 |
| 3 | 1 | 7 | 76.779 | 1.240 | -0.02 |
| 0 | 3 | 5 | 79.205 | 79.195 | 1.208 | < 1 | 0.01 |
| 8 | 3 | 2 | 79.234 | 1.208 | -0.029 |
| -12 | 1 | 3 | 79.854 | 79.851 | 1.200 | < 1 | 0.003 |
| 11 | 1 | 4 | 79.851 | 1.200 | 0.003 |
| 0 | 4 | 1 | 81.062 | 81.052 | 1.185 | < 1 | 0.01 |
| -10 | 1 | 5 | 81.063 | 1.185 | -0.001 |
| 5 | 1 | 7 | 81.076 | 1.185 | -0.014 |
| 8 | 3 | 3 | 83.276 | 83.280 | 1.159 | < 1 | -0.004 |
| -4 | 3 | 5 | 83.284 | 1.159 | -0.008 |
| 10 | 3 | 0 | 85.373 | 85.366 | 1.136 | < 1 | 0.007 |
| -12 | 1 | 4 | 85.378 | 1.136 | -0.005 |
| 9 | 1 | 6 | 85.421 | 1.136 | -0.048 |
| -2 | 4 | 3 | 88.459 | 88.425 | 1.104 | < 1 | 0.034 |
| -6 | 3 | 5 | 88.426 | 1.104 | 0.033 |
| -10 | 3 | 2 | 88.433 | 1.104 | 0.026 |