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**Ca6.5Pb1.5ZnBi(VO4)7, a novel whitlockite-type vanadate: crystal structure refinement and properties characterization**

**SUPPLEMENTARY MATERIAL**

TABLE I. X-ray powder pattern for Ca6.5Pb1.5ZnBi(VO4)7. The d-spacing values are calculated values from refined lattice parameters, and “I” represents integrated intensity values.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| *dcal* | *Iobs* | *h* | *k* | *l* | *dcal* | *Iobs* | *h* | *k* | *l* | *dcal* | *Iobs* | *h* | *k* | *l* |
| 8.4995 | 46.1 | 1 | -1 | 2 | 1.6085 | 110.9 | 5 | -4 | 15 | 1.2788 | 373.5 | 7 | -1 | 14 |
| 6.7426 | 253.8 | 1 | 0 | 4 | 1.6085 | 110.9 | 5 | -1 | 15 | 1.2785 | 220.4 | 8 | -2 | 7 |
| 6.3940 | 658.4 | 0 | 0 | 6 | 1.6047 | 1118.8 | 6 | -5 | 8 | 1.2772 | 628 | 8 | -5 | 10 |
| 5.4739 | 876 | 2 | -1 | 0 | 1.6015 | 134.3 | 4 | -3 | 19 | 1.2772 | 628 | 7 | 0 | 10 |
| 5.0323 | 4.7 | 2 | -1 | 3 | 1.5985 | 627.5 | 0 | 0 | 24 | 1.2735 | 104.3 | 6 | -5 | 20 |
| 4.6021 | 318.3 | 2 | 0 | 2 | 1.5937 | 13.6 | 6 | -2 | 11 | 1.2694 | 543.7 | 6 | 0 | 18 |
| 4.2792 | 88.6 | 1 | -1 | 8 | 1.5847 | 564 | 6 | -3 | 12 | 1.2694 | 543.7 | 6 | -6 | 18 |
| 4.2498 | 1493 | 2 | -2 | 4 | 1.5802 | 2653.4 | 6 | 0 | 0 | 1.2680 | 221.4 | 8 | -6 | 8 |
| 4.1582 | 36 | 2 | -1 | 6 | 1.5680 | 70.1 | 3 | -1 | 22 | 1.2649 | 62.5 | 5 | -1 | 24 |
| 3.5680 | 42.9 | 3 | -1 | 1 | 1.5661 | 5.8 | 5 | -3 | 17 | 1.2649 | 62.5 | 5 | -4 | 24 |
| 3.5563 | 1596.2 | 1 | 0 | 10 | 1.5593 | 294 | 5 | 0 | 14 | 1.2626 | 120.6 | 8 | -3 | 11 |
| 3.5226 | 494.7 | 3 | -2 | 2 | 1.5574 | 154 | 7 | -3 | 1 | 1.2611 | 5.2 | 4 | -2 | 27 |
| 3.3713 | 157.7 | 2 | 0 | 8 | 1.5564 | 186.2 | 6 | -1 | 10 | 1.2581 | 419.5 | 8 | -4 | 12 |
| 3.3632 | 85.5 | 2 | -1 | 9 | 1.5536 | 240.3 | 7 | -4 | 2 | 1.2558 | 913.2 | 8 | -1 | 0 |
| 3.3569 | 579.7 | 3 | -1 | 4 | 1.5497 | 459.4 | 4 | -1 | 20 | 1.2539 | 28.1 | 5 | -2 | 25 |
| 3.2469 | 7.8 | 3 | -2 | 5 | 1.5385 | 367.9 | 7 | -3 | 4 | 1.2526 | 721.5 | 4 | -4 | 26 |
| 3.1970 | 625.8 | 0 | 0 | 12 | 1.5344 | 102.8 | 2 | -1 | 24 | 1.2498 | 88.1 | 8 | -1 | 3 |
| 3.1604 | 2035.6 | 3 | 0 | 0 | 1.5340 | 111.3 | 6 | -6 | 6 | 1.2498 | 88.1 | 8 | -7 | 3 |
| 2.9993 | 0.1 | 3 | -1 | 7 | 1.5340 | 111.3 | 6 | 0 | 6 | 1.2497 | 78.5 | 6 | -4 | 22 |
| 2.9822 | 10000 | 2 | -2 | 10 | 1.5316 | 49.9 | 6 | -4 | 13 | 1.2453 | 72.4 | 2 | -1 | 30 |
| 2.8706 | 1154.6 | 3 | -2 | 8 | 1.5302 | 199.8 | 6 | -5 | 11 | 1.2438 | 139.3 | 8 | -2 | 10 |
| 2.8332 | 819.5 | 3 | -3 | 6 | 1.5275 | 117.4 | 7 | -4 | 5 | 1.2410 | 34.9 | 3 | -2 | 29 |
| 2.8332 | 819.5 | 3 | 0 | 6 | 1.5195 | 61 | 4 | -2 | 21 | 1.2382 | 278.6 | 7 | -6 | 16 |
| 2.7606 | 101.3 | 2 | -1 | 12 | 1.5182 | 953.2 | 7 | -2 | 0 | 1.2365 | 1039.4 | 7 | -5 | 18 |
| 2.7370 | 8766.4 | 4 | -2 | 0 | 1.5122 | 9.4 | 3 | -2 | 23 | 1.2365 | 1039.4 | 7 | -2 | 18 |
| 2.6763 | 159 | 4 | -2 | 3 | 1.5076 | 19.6 | 7 | -2 | 3 | 1.2338 | 188.9 | 7 | -3 | 19 |
| 2.6325 | 374.9 | 1 | -1 | 14 | 1.5076 | 19.6 | 7 | -5 | 3 | 1.2323 | 18.2 | 8 | -1 | 6 |
| 2.6234 | 133.2 | 4 | -3 | 1 | 1.4996 | 166.3 | 6 | -2 | 14 | 1.2323 | 18.2 | 8 | -7 | 6 |
| 2.6188 | 1627.7 | 3 | -1 | 10 | 1.4992 | 65.3 | 7 | -3 | 7 | 1.2310 | 58.7 | 8 | -5 | 13 |
| 2.6052 | 93.5 | 4 | -1 | 2 | 1.4911 | 3116.6 | 4 | -4 | 20 | 1.2303 | 70.8 | 8 | -6 | 11 |
| 2.5360 | 76.3 | 4 | -3 | 4 | 1.4873 | 854.1 | 5 | -5 | 16 | 1.2211 | 343.6 | 5 | -3 | 26 |
| 2.5161 | 868.5 | 4 | -2 | 6 | 1.4854 | 78.2 | 6 | -3 | 15 | 1.2209 | 45.4 | 6 | -2 | 23 |
| 2.4993 | 18.2 | 3 | -2 | 11 | 1.4845 | 385.8 | 5 | -1 | 18 | 1.2183 | 409.3 | 6 | -1 | 22 |
| 2.4876 | 152.9 | 4 | -1 | 5 | 1.4845 | 385.8 | 5 | -4 | 18 | 1.2174 | 65.8 | 7 | -1 | 17 |
| 2.3724 | 796 | 2 | 0 | 14 | 1.4823 | 860.5 | 7 | -4 | 8 | 1.2151 | 420.7 | 4 | -3 | 28 |
| 2.3708 | 92.5 | 4 | -3 | 7 | 1.4798 | 46.1 | 5 | -2 | 19 | 1.2142 | 81.4 | 7 | -7 | 14 |
| 2.3524 | 3.5 | 4 | -4 | 2 | 1.4771 | 973.6 | 7 | -5 | 6 | 1.2142 | 81.4 | 8 | -3 | 14 |
| 2.3246 | 1252.1 | 1 | 0 | 16 | 1.4771 | 973.6 | 7 | -2 | 6 | 1.2133 | 146.4 | 9 | -4 | 1 |
| 2.3171 | 71.1 | 2 | -1 | 15 | 1.4749 | 159.8 | 6 | -1 | 13 | 1.2115 | 103.6 | 9 | -5 | 2 |
| 2.3057 | 63.7 | 4 | -1 | 8 | 1.4580 | 72.5 | 1 | -1 | 26 | 1.2097 | 199.6 | 7 | -4 | 20 |
| 2.3031 | 33.5 | 4 | -2 | 9 | 1.4533 | 63.3 | 4 | -3 | 22 | 1.2066 | 7.3 | 8 | -4 | 15 |
| 2.3010 | 266.5 | 4 | 0 | 4 | 1.4463 | 0.3 | 6 | -5 | 14 | 1.2046 | 247 | 8 | -1 | 9 |
| 2.2780 | 13.1 | 3 | -1 | 13 | 1.4448 | 583.1 | 7 | -6 | 1 | 1.2046 | 247 | 8 | -7 | 9 |
| 2.2476 | 632.8 | 3 | -3 | 12 | 1.4440 | 889.6 | 7 | -3 | 10 | 1.2043 | 146.5 | 9 | -4 | 4 |
| 2.2476 | 632.8 | 3 | 0 | 12 | 1.4418 | 57.4 | 7 | -1 | 2 | 1.2024 | 83.4 | 6 | -3 | 24 |
| 2.1768 | 140.7 | 3 | -2 | 14 | 1.4387 | 2390 | 5 | -3 | 20 | 1.2010 | 29 | 8 | -2 | 13 |
| 2.1716 | 202.5 | 5 | -2 | 1 | 1.4353 | 81.2 | 6 | -4 | 16 | 1.1990 | 34.9 | 9 | -5 | 5 |
| 2.1690 | 135.5 | 4 | -3 | 10 | 1.4302 | 72.6 | 7 | -5 | 9 | 1.1945 | 46.3 | 9 | -3 | 0 |
| 2.1613 | 460 | 5 | -3 | 2 | 1.4302 | 72.6 | 7 | -2 | 9 | 1.1916 | 108.4 | 6 | -5 | 23 |
| 2.1396 | 238.9 | 2 | -2 | 16 | 1.4297 | 73.7 | 7 | -6 | 4 | 1.1894 | 74 | 1 | -1 | 32 |
| 2.1313 | 1710.4 | 0 | 0 | 18 | 1.4264 | 73 | 3 | 0 | 24 | 1.1893 | 41.1 | 9 | -3 | 3 |
| 2.1249 | 1566.9 | 4 | -4 | 8 | 1.4264 | 73 | 3 | -3 | 24 | 1.1893 | 41.1 | 9 | -6 | 3 |
| 2.1212 | 1191.7 | 5 | -2 | 4 | 1.4230 | 218.7 | 7 | -4 | 11 | 1.1862 | 1067.6 | 4 | 0 | 28 |
| 2.0997 | 74.4 | 4 | -1 | 11 | 1.4208 | 73 | 7 | -1 | 5 | 1.1854 | 244.9 | 3 | -3 | 30 |
| 2.0927 | 14.6 | 5 | -3 | 5 | 1.4166 | 49.5 | 6 | 0 | 12 | 1.1854 | 244.9 | 3 | 0 | 30 |
| 2.0791 | 1021.1 | 4 | -2 | 12 | 1.4166 | 49.5 | 6 | -6 | 12 | 1.1854 | 226.9 | 8 | -6 | 14 |
| 2.0689 | 196.6 | 5 | -1 | 0 | 1.4107 | 26.2 | 3 | -1 | 25 | 1.1852 | 110.7 | 9 | -4 | 7 |
| 2.0424 | 44.7 | 5 | -1 | 3 | 1.4089 | 200.8 | 2 | 0 | 26 | 1.1829 | 460.2 | 8 | 0 | 2 |
| 2.0424 | 44.7 | 5 | -4 | 3 | 1.4085 | 65.4 | 4 | -1 | 23 | 1.1818 | 177.5 | 4 | -1 | 29 |
| 2.0217 | 0.2 | 5 | -2 | 7 | 1.4046 | 218.8 | 4 | 0 | 22 | 1.1793 | 848.7 | 8 | -5 | 16 |
| 2.0164 | 5094.8 | 4 | 0 | 10 | 1.4032 | 35.5 | 6 | -2 | 17 | 1.1793 | 848.7 | 7 | 0 | 16 |
| 1.9928 | 265.9 | 3 | -1 | 16 | 1.3980 | 56.5 | 7 | -6 | 7 | 1.1768 | 452.9 | 9 | -5 | 8 |
| 1.9861 | 0 | 2 | -1 | 18 | 1.3884 | 68.9 | 6 | -1 | 16 | 1.1762 | 85.9 | 8 | -8 | 4 |
| 1.9809 | 2518.4 | 5 | -3 | 8 | 1.3861 | 579.7 | 6 | -3 | 18 | 1.1755 | 55.5 | 7 | -6 | 19 |
| 1.9685 | 744.8 | 5 | -4 | 6 | 1.3843 | 29.7 | 7 | -1 | 8 | 1.1742 | 158.9 | 9 | -3 | 6 |
| 1.9685 | 744.8 | 5 | -1 | 6 | 1.3803 | 174.6 | 4 | -2 | 24 | 1.1742 | 158.9 | 9 | -6 | 6 |
| 1.9633 | 42.3 | 4 | -3 | 13 | 1.3782 | 57.4 | 7 | -3 | 13 | 1.1713 | 2.9 | 5 | -1 | 27 |
| 1.9096 | 3 | 3 | -2 | 17 | 1.3753 | 23.5 | 2 | -1 | 27 | 1.1713 | 2.9 | 5 | -4 | 27 |
| 1.8973 | 87.8 | 4 | -1 | 14 | 1.3714 | 305 | 7 | -5 | 12 | 1.1698 | 117.5 | 3 | -1 | 31 |
| 1.8922 | 863.3 | 5 | -2 | 10 | 1.3714 | 305 | 7 | -2 | 12 | 1.1689 | 632 | 8 | -1 | 12 |
| 1.8870 | 1843.4 | 5 | 0 | 2 | 1.3694 | 230.2 | 5 | -1 | 21 | 1.1689 | 632 | 8 | -7 | 12 |
| 1.8801 | 1778.8 | 1 | -1 | 20 | 1.3694 | 230.2 | 5 | -4 | 21 | 1.1676 | 0.8 | 7 | -5 | 21 |
| 1.8687 | 1.7 | 4 | -2 | 15 | 1.3685 | 1663.4 | 8 | -4 | 0 | 1.1676 | 0.8 | 7 | -2 | 21 |
| 1.8613 | 204.7 | 5 | -4 | 9 | 1.3644 | 985.1 | 3 | -2 | 26 | 1.1655 | 38.8 | 6 | -4 | 25 |
| 1.8613 | 204.7 | 5 | -1 | 9 | 1.3607 | 203 | 8 | -4 | 3 | 1.1645 | 1639.9 | 5 | 0 | 26 |
| 1.8602 | 786.1 | 5 | -5 | 4 | 1.3606 | 161.9 | 5 | -2 | 22 | 1.1623 | 236.6 | 2 | 0 | 32 |
| 1.8456 | 0.9 | 5 | -3 | 11 | 1.3593 | 38.5 | 6 | -5 | 17 | 1.1621 | 69.9 | 7 | -3 | 22 |
| 1.8246 | 608.2 | 6 | -3 | 0 | 1.3560 | 588 | 1 | 0 | 28 | 1.1613 | 0.6 | 8 | -3 | 17 |
| 1.8063 | 23.3 | 6 | -3 | 3 | 1.3548 | 263 | 7 | -4 | 14 | 1.1593 | 2054.3 | 5 | -2 | 28 |
| 1.7927 | 76.5 | 4 | -4 | 14 | 1.3536 | 512.6 | 8 | -5 | 1 | 1.1586 | 2040.2 | 4 | -2 | 30 |
| 1.7898 | 1 | 6 | -4 | 1 | 1.3530 | 95.4 | 7 | -6 | 10 | 1.1578 | 154.9 | 9 | -7 | 1 |
| 1.7840 | 65.5 | 6 | -2 | 2 | 1.3511 | 1055.8 | 7 | -7 | 2 | 1.1574 | 137.1 | 9 | -4 | 10 |
| 1.7781 | 9475.2 | 2 | 0 | 20 | 1.3511 | 1055.8 | 8 | -3 | 2 | 1.1562 | 563.1 | 9 | -2 | 2 |
| 1.7718 | 172.1 | 4 | -3 | 16 | 1.3485 | 600.3 | 5 | 0 | 20 | 1.1546 | 120.6 | 7 | -1 | 20 |
| 1.7670 | 2032.3 | 3 | -3 | 18 | 1.3411 | 262.9 | 8 | -5 | 4 | 1.1528 | 30.5 | 8 | -2 | 16 |
| 1.7670 | 2032.3 | 3 | 0 | 18 | 1.3411 | 262.9 | 7 | 0 | 4 | 1.1515 | 67.9 | 8 | -4 | 18 |
| 1.7634 | 2855.7 | 5 | 0 | 8 | 1.3402 | 65.4 | 6 | -4 | 19 | 1.1505 | 738 | 8 | 0 | 8 |
| 1.7613 | 563.3 | 6 | -4 | 4 | 1.3382 | 81.8 | 8 | -4 | 6 | 1.1502 | 367.3 | 9 | -3 | 9 |
| 1.7591 | 302 | 3 | -1 | 19 | 1.3356 | 11.9 | 7 | -1 | 11 | 1.1502 | 367.3 | 9 | -6 | 9 |
| 1.7546 | 163.7 | 6 | -3 | 6 | 1.3338 | 45.4 | 8 | -3 | 5 | 1.1499 | 213.5 | 9 | -7 | 4 |
| 1.7509 | 48 | 5 | -2 | 13 | 1.3254 | 59.4 | 4 | -3 | 25 | 1.1465 | 62.7 | 9 | -5 | 11 |
| 1.7448 | 39.9 | 6 | -2 | 5 | 1.3236 | 63.3 | 5 | -3 | 23 | 1.1453 | 110.5 | 9 | -2 | 5 |
| 1.7369 | 191.5 | 5 | -1 | 12 | 1.3163 | 526.6 | 2 | -2 | 28 | 1.1400 | 62.9 | 6 | -1 | 25 |
| 1.7369 | 191.5 | 5 | -4 | 12 | 1.3149 | 14.4 | 8 | -5 | 7 | 1.1390 | 37.7 | 6 | -2 | 26 |
| 1.7329 | 36.6 | 2 | -1 | 21 | 1.3140 | 78.3 | 8 | -2 | 1 | 1.1388 | 40.7 | 7 | -4 | 23 |
| 1.7150 | 209.4 | 1 | 0 | 22 | 1.3117 | 645.2 | 8 | -6 | 2 | 1.1372 | 72.8 | 2 | -1 | 33 |
| 1.7125 | 41.1 | 4 | -1 | 17 | 1.3094 | 1643.2 | 6 | -2 | 20 | 1.1369 | 87.1 | 3 | -2 | 32 |
| 1.7037 | 83.1 | 5 | -3 | 14 | 1.3068 | 361.6 | 7 | -3 | 16 | 1.1360 | 33.9 | 8 | -6 | 17 |
| 1.7031 | 33.6 | 6 | -4 | 7 | 1.3055 | 16 | 7 | -5 | 15 | 1.1333 | 88.9 | 9 | -7 | 7 |
| 1.7012 | 104.1 | 6 | -1 | 1 | 1.3055 | 16 | 7 | -2 | 15 | 1.1323 | 536.7 | 8 | -8 | 10 |
| 1.6999 | 2145 | 5 | -5 | 10 | 1.3035 | 866.8 | 7 | -7 | 8 | 1.1303 | 136.2 | 5 | -3 | 29 |
| 1.6962 | 270 | 6 | -5 | 2 | 1.3035 | 866.8 | 8 | -3 | 8 | 1.1272 | 92.2 | 8 | -1 | 15 |
| 1.6912 | 310.5 | 3 | -2 | 20 | 1.3030 | 249.8 | 8 | -4 | 9 | 1.1272 | 92.2 | 8 | -7 | 15 |
| 1.6857 | 315.3 | 4 | 0 | 16 | 1.3026 | 265.1 | 8 | -2 | 4 | 1.1259 | 461.4 | 9 | -2 | 8 |
| 1.6816 | 222.4 | 4 | -2 | 18 | 1.3017 | 420.1 | 6 | -1 | 19 | 1.1248 | 142.2 | 8 | -5 | 19 |
| 1.6784 | 207.2 | 6 | -2 | 8 | 1.2984 | 99 | 7 | -6 | 13 | 1.1238 | 15.8 | 6 | 0 | 24 |
| 1.6774 | 354.3 | 6 | -3 | 9 | 1.2959 | 19.4 | 8 | -6 | 5 | 1.1238 | 15.8 | 6 | -6 | 24 |
| 1.6766 | 637.4 | 6 | -1 | 4 | 1.2910 | 153.2 | 6 | -3 | 21 | 1.1227 | 65.1 | 9 | -4 | 13 |
| 1.6624 | 76.7 | 6 | -5 | 5 | 1.2868 | 75.4 | 4 | -1 | 26 | 1.1211 | 27.3 | 6 | -3 | 27 |
| 1.6366 | 846.8 | 2 | -2 | 22 | 1.2836 | 148.7 | 5 | -5 | 22 | 1.1204 | 141.5 | 1 | 0 | 34 |
| 1.6262 | 0.8 | 6 | -1 | 7 | 1.2825 | 25.4 | 7 | -4 | 17 | 1.1197 | 38.9 | 4 | -3 | 31 |
| 1.6234 | 2834.2 | 6 | -4 | 10 | 1.2798 | 488.5 | 3 | -1 | 28 | 1.1190 | 21.6 | 9 | -3 | 12 |
| 1.6110 | 2143.8 | 5 | -2 | 16 | 1.2788 | 403.7 | 0 | 0 | 30 | 1.1190 | 21.6 | 9 | -6 | 12 |