**TABLE S1.** X-ray powder diffraction data of the title compound[*P*, Z=2], a = 5.5866(6) Å, b = 9.300(1) Å, c = 19.470(7) Å, α = 99.259(15)°, β = 92.001(15)°, γ = 98.159(11)° and V = 986.6(4) Å3. The particular peak that has the strongest intensity in the entire pattern is assigned an intensity of 100 and other lines are scaled relative to this value. The *d*obs values come directly from the observed PXRD data and are used to determine the lattice parameters and from them the *d*cal values. ‘‘*Iobs*’’ represents integrated intensity values and Mult represents ‘‘Multiplicity’’.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 2*θ*obs (°) | *d*obs (Å) | Iobs (%) | *h* | *k* | *l* | M | 2*θ*cal (°) | *d*cal (Å) | Δ2*θ* (°) |
| 2.1445 | 18.9914 | 28 | 0 | 0 | 1 | 2 | 2.1187 | 19.1829 | 0.0258 |
| 4.5003 | 9.0516 | 6 | 0 | 1 | 0 | 2 | 4.479 | 9.0757 | 0.0213 |
| 5.2921 | 7.6982 | 8 | 0 | 1 | 1 | 2 | 5.2669 | 7.7189 | 0.0252 |
| 7.3957 | 5.5104 | 15 | 1 | 0 | 0 | 2 | 7.3669 | 5.5204 | 0.0288 |
| 7.8137 | 5.216 | 23 | 1 | 0 | 1 | 2 | 7.786 | 5.2237 | 0.0277 |
| 8.0565 | 5.0591 | 31 | 1 | -1 | 0 | 2 | 8.0306 | 5.0648 | 0.0259 |
| 8.2485 | 4.9415 | 29 | 1 | -1 | 1 | 2 | 8.2251 | 4.9452 | 0.0234 |
| 8.2923 | 4.9155 | 8 | 1 | 0 | -2 | 2 | 8.2814 | 4.9117 | 0.0109 |
| 8.3933 | 4.8564 | 11 | 0 | 1 | 3 | 2 | 8.3734 | 4.8578 | 0.0199 |
| 8.8955 | 4.5827 | 8 | 0 | -2 | 1 | 2 | 8.8593 | 4.5918 | 0.0362 |
|  |  | 6 | 1 | -1 | 2 | 2 | 8.9345 | 4.5533 |  |
| 8.9887 | 4.5353 | 96 | 0 | 2 | 0 | 2 | 8.9649 | 4.5379 | 0.0238 |
| 9.1975 | 4.4326 | 13 | 1 | 1 | 0 | 2 | 9.1809 | 4.4313 | 0.0166 |
| 9.2322 | 4.416 | 17 | 1 | -1 | -2 | 2 | 9.2302 | 4.4077 | 0.002 |
| 9.2532 | 4.4059 | 14 | 0 | -2 | 2 | 2 | 9.2531 | 4.3968 | 0.0001 |
| 9.4844 | 4.2988 | 16 | 1 | 0 | -3 | 2 | 9.4478 | 4.3064 | 0.0366 |
| 9.6277 | 4.235 | 29 | 1 | 1 | -2 | 2 | 9.6036 | 4.2367 | 0.0241 |
| 9.6844 | 4.2102 | 16 | 1 | 1 | 1 | 2 | 9.6874 | 4.2001 | -0.003 |
|  |  | 7 | 1 | -1 | -3 | 2 | 10.4448 | 3.8963 |  |
| 10.499 | 3.8843 | 17 | 1 | 1 | -3 | 2 | 10.4754 | 3.8850 | 0.0236 |
| 10.7101 | 3.808 | 33 | 1 | -2 | 1 | 2 | 10.723 | 3.7955 | -0.0129 |
| 10.8051 | 3.7746 | 9 | 0 | -1 | 5 | 2 | 10.8027 | 3.7676 | 0.0024 |
| 11.1589 | 3.6554 | 66 | 1 | -2 | 2 | 2 | 11.1348 | 3.6556 | 0.0241 |
| 11.7183 | 3.4814 | 9 | 1 | 1 | -4 | 2 | 11.6744 | 3.4871 | 0.0439 |
| 11.8648 | 3.4386 | 100 | 1 | -2 | 3 | 2 | 11.9176 | 3.4162 | -0.0528 |
| 11.9264 | 3.4209 | 35 | 1 | -2 | -2 | 2 | 11.9239 | 3.4144 | 0.0025 |
| 12.3173 | 3.3127 | 31 | 1 | 2 | -1 | 2 | 12.2876 | 3.3138 | 0.0297 |
| 12.7589 | 3.1985 | 10 | 0 | 0 | 6 | 2 | 12.7375 | 3.1972 | 0.0214 |
|  |  | 6 | 1 | -2 | 4 | 2 | 13.0054 | 3.1316 |  |
|  |  | 6 | 1 | 2 | -3 | 2 | 13.0629 | 3.1178 |  |
| 13.0903 | 3.1179 | 17 | 1 | -1 | 5 | 2 | 13.063 | 3.1178 | 0.0273 |
|  |  | 7 | 1 | 0 | 5 | 2 | 13.2819 | 3.0667 |  |
|  |  | 6 | 0 | 3 | 0 | 2 | 13.4645 | 3.0253 |  |
| 13.5751 | 3.007 | 7 | 1 | -1 | -5 | 2 | 13.5697 | 3.0019 | 0.0054 |
|  |  | 10 | 1 | 2 | 2 | 2 | 13.7622 | 2.9601 |  |
|  |  | 14 | 0 | -3 | 3 | 2 | 13.8986 | 2.9312 |  |
| 13.9534 | 2.9259 | 27 | 1 | 2 | -4 | 2 | 13.9308 | 2.9245 | 0.0226 |
|  |  | 14 | 0 | 3 | 1 | 2 | 13.9807 | 2.9141 |  |
|  |  | 6 | 0 | 1 | 6 | 2 | 14.2037 | 2.8686 |  |
|  |  | 15 | 0 | -2 | 6 | 2 | 14.3063 | 2.8481 |  |
| 14.3345 | 2.8485 | 14 | 1 | -2 | 5 | 2 | 14.3304 | 2.8433 | 0.0041 |
| 14.3438 | 2.8467 | 17 | 1 | 0 | -6 | 2 | 14.3451 | 2.8404 | -0.0013 |
| 14.366 | 2.8422 | 7 | 1 | -3 | 0 | 2 | 14.3579 | 2.8379 | 0.0081 |
|  |  | 10 | 1 | -3 | 2 | 2 | 14.4475 | 2.8204 |  |
|  |  | 7 | 0 | -3 | 4 | 2 | 14.6722 | 2.7774 |  |
|  |  | 22 | 2 | 0 | 0 | 2 | 14.7644 | 2.7602 |  |
|  |  | 8 | 2 | -1 | 0 | 2 | 14.7756 | 2.7581 |  |
| 14.8022 | 2.7589 | 27 | 0 | -1 | 7 | 2 | 14.796 | 2.7543 | 0.0062 |
| 14.8798 | 2.7446 | 7 | 0 | 0 | 7 | 2 | 14.8715 | 2.7404 | 0.0083 |
|  |  | 6 | 1 | 1 | 5 | 2 | 14.9229 | 2.7310 |  |
|  |  | 7 | 0 | 2 | 5 | 2 | 15.0169 | 2.7140 |  |
|  |  | 6 | 2 | 0 | 1 | 2 | 15.0418 | 2.7096 |  |
| 15.0572 | 2.7125 | 6 | 1 | 2 | -5 | 2 | 15.0533 | 2.7075 | 0.0039 |
|  |  | 8 | 2 | 0 | -2 | 2 | 15.1224 | 2.6952 |  |
|  |  | 11 | 1 | -1 | -6 | 2 | 15.3424 | 2.6568 |  |
| 15.4704 | 2.6405 | 8 | 1 | -3 | -2 | 2 | 15.4881 | 2.6320 | -0.0177 |
| 15.7990 | 2.5859 | 6 | 0 | -3 | 5 | 2 | 15.7 | 2.5966 | 0.099 |
|  |  | 7 | 2 | -1 | -3 | 2 | 16.052 | 2.5401 |  |
|  |  | 11 | 2 | 1 | 0 | 2 | 16.0701 | 2.5372 |  |
|  |  | 10 | 1 | 3 | -1 | 2 | 16.0948 | 2.5334 |  |
| 16.1167 | 2.5352 | 10 | 2 | -2 | 0 | 2 | 16.1011 | 2.5324 | 0.0156 |
| 16.4681 | 2.4815 | 8 | 1 | 0 | 7 | 2 | 17.0042 | 2.3988 |  |
| 17.0299 | 2.4002 | 7 | 0 | 0 | 8 | 2 | 17.0108 | 2.3979 | 0.0191 |
|  |  | 15 | 1 | 1 | -8 | 2 | 18.2751 | 2.2332 |  |
| 18.3184 | 2.2327 | 7 | 2 | -1 | 5 | 2 | 18.2944 | 2.2309 | 0.024 |
| 18.3623 | 2.2274 | 8 | 2 | 1 | -5 | 2 | 18.3657 | 2.2223 | -0.0034 |
| 18.5501 | 2.205 | 8 | 1 | -1 | 8 | 2 | 18.5453 | 2.2010 | 0.0048 |
| 18.7023 | 2.1872 | 10 | 2 | 2 | -3 | 2 | 18.7023 | 2.1827 | 0 |
| 18.9463 | 2.1593 | 37 | 0 | -1 | 9 | 2 | 18.9266 | 2.1570 | 0.0197 |
| 19.2865 | 2.1216 | 8 | 2 | -3 | -2 | 2 | 19.2672 | 2.1193 | 0.0193 |
| 19.4921 | 2.0994 | 11 | 1 | 2 | -8 | 2 | 19.4773 | 2.0966 | 0.0148 |
| 20.1858 | 2.028 | 16 | 1 | 1 | -9 | 2 | 20.1647 | 2.0258 | 0.0211 |
|  |  | 7 | 2 | 0 | -7 | 2 | 20.3778 | 2.0049 |  |
| 20.4171 | 2.0052 | 14 | 1 | 1 | 8 | 2 | 20.3943 | 2.0033 | 0.0228 |
| 20.5315 | 1.9942 | 6 | 1 | -4 | 6 | 2 | 20.897 | 1.9556 | -0.3655 |
| 20.9947 | 1.9507 | 7 | 2 | -2 | -6 | 2 | 20.9776 | 1.9482 | 0.0171 |
|  |  | 7 | 0 | -1 | 10 | 2 | 21.0238 | 1.9439 |  |
| 21.324 | 1.921 | 23 | 0 | 0 | 10 | 2 | 21.308 | 1.9183 | 0.016 |
|  |  | 6 | 2 | 3 | 0 | 2 | 21.4896 | 1.9023 |  |
| 21.5055 | 1.9049 | 16 | 0 | -3 | 9 | 2 | 21.5302 | 1.8987 | -0.0247 |
|  |  | 6 | 2 | 3 | -4 | 2 | 21.9352 | 1.8641 |  |
|  |  | 6 | 1 | 3 | 6 | 2 | 22.371 | 1.8282 |  |
| 21.6522 | 1.8921 | 6 | 1 | -3 | 9 | 2 | 22.4897 | 1.8187 | -0.8375 |
| 22.5248 | 1.8197 | 7 | 1 | -1 | 10 | 2 | 22.5013 | 1.8178 | 0.0235 |
| 22.6540 | 1.8095 | 10 | 1 | -5 | 3 | 2 | 22.6047 | 1.8096 | 0.0493 |
|  |  | 8 | 2 | -3 | 7 | 2 | 22.8898 | 1.7873 |  |
| 23.2960 | 1.7603 | 11 | 2 | 0 | 8 | 2 | 23.2576 | 1.7594 | 0.0384 |
|  |  | 6 | 3 | 1 | 1 | 2 | 23.632 | 1.7320 |  |
| 23.6793 | 1.7322 | 6 | 0 | -2 | 11 | 2 | 23.6907 | 1.7277 | -0.0114 |
|  |  | 7 | 0 | -5 | 6 | 2 | 23.9957 | 1.7061 |  |
| 24.0297 | 1.7073 | 6 | 0 | -4 | 9 | 2 | 24.0477 | 1.7024 | -0.018 |
| 24.2049 | 1.6951 | 6 | 1 | 1 | 10 | 2 | 24.3315 | 1.6829 | -0.1266 |
| 24.4787 | 1.6764 | 7 | 0 | 1 | 11 | 2 | 24.646 | 1.6617 | -0.1673 |
| 24.8181 | 1.6538 | 11 | 1 | 2 | -11 | 2 | 24.83 | 1.6496 | -0.0119 |
|  |  | 8 | 2 | 0 | 9 | 2 | 24.9663 | 1.6407 |  |
|  |  | 10 | 2 | -5 | 0 | 2 | 25.0887 | 1.6329 |  |
|  |  | 7 | 3 | 2 | -1 | 2 | 25.0946 | 1.6325 |  |
| 25.2260 | 1.6275 | 7 | 0 | -1 | 12 | 2 | 25.2679 | 1.6215 | -0.0419 |
|  |  | 8 | 3 | -3 | 4 | 2 | 25.4116 | 1.6125 |  |
| 25.5755 | 1.6057 | 10 | 0 | -4 | 10 | 2 | 25.557 | 1.6034 | 0.0185 |
|  |  | 12 | 1 | 4 | -9 | 2 | 25.6478 | 1.5978 |  |
|  |  | 7 | 0 | -5 | 8 | 2 | 25.9364 | 1.5804 |  |
| 25.9687 | 1.5817 | 8 | 2 | -5 | -2 | 2 | 25.9474 | 1.5797 | 0.0213 |
|  |  | 8 | 1 | 1 | -12 | 2 | 26.112 | 1.5699 |  |
|  |  | 14 | 1 | 0 | -12 | 2 | 26.2753 | 1.5603 |  |
|  |  | 7 | 3 | 0 | 6 | 2 | 26.357 | 1.5556 |  |
|  |  | 10 | 0 | 2 | 11 | 2 | 26.5672 | 1.5435 |  |
| 26.6132 | 1.5441 | 7 | 1 | -1 | 12 | 2 | 26.5942 | 1.5420 | 0.019 |
|  |  | 9 | 3 | -1 | 7 | 2 | 26.9807 | 1.5203 |  |
|  |  | 8 | 2 | -3 | 10 | 2 | 27.2438 | 1.5059 |  |
|  |  | 6 | 3 | 0 | 7 | 2 | 27.5861 | 1.4875 |  |
|  |  | 8 | 2 | -5 | 7 | 2 | 27.7261 | 1.4802 |  |
|  |  | 7 | 2 | 2 | -11 | 2 | 28.0083 | 1.4655 |  |
|  |  | 7 | 3 | -1 | 8 | 2 | 28.2915 | 1.4512 |  |
| 28.9221 | 1.4232 | 10 | 0 | 2 | 12 | 2 | 28.6317 | 1.4343 | 0.2904 |
|  |  | 7 | 1 | -1 | -13 | 2 | 29.306 | 1.4020 |  |
| 29.8833 | 1.3784 | 7 | 1 | -4 | 12 | 2 | 29.5021 | 1.3929 | 0.3812 |
|  |  | 6 | 1 | 2 | 12 | 2 | 30.3347 | 1.3555 |  |
|  |  | 8 | 4 | -2 | 3 | 2 | 30.5583 | 1.3458 |  |
|  |  | 9 | 3 | 4 | 0 | 2 | 30.8155 | 1.3349 |  |
|  |  | 8 | 2 | 3 | -12 | 2 | 31.1044 | 1.3228 |  |
|  |  | 9 | 2 | 4 | 7 | 2 | 31.2282 | 1.3176 |  |
| 31.6445 | 1.3035 | 28 | 1 | -3 | 14 | 2 | 31.6578 | 1.3002 | -0.0133 |
|  |  | 6 | 0 | -1 | 15 | 2 | 31.7443 | 1.2968 |  |
|  |  | 6 | 2 | -1 | 13 | 2 | 31.7447 | 1.2967 |  |
|  |  | 9 | 4 | 1 | 3 | 2 | 32.0171 | 1.2860 |  |
|  |  | 18 | 3 | -6 | 2 | 2 | 32.414 | 1.2707 |  |
| 32.7493 | 1.2606 | 28 | 0 | 2 | 14 | 2 | 32.8352 | 1.2548 | -0.0859 |