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# Crystal Structure and Magnetic Properties of the Magnetically Isolated Zigzag Chain in $KGaCu(PO_4)_2$

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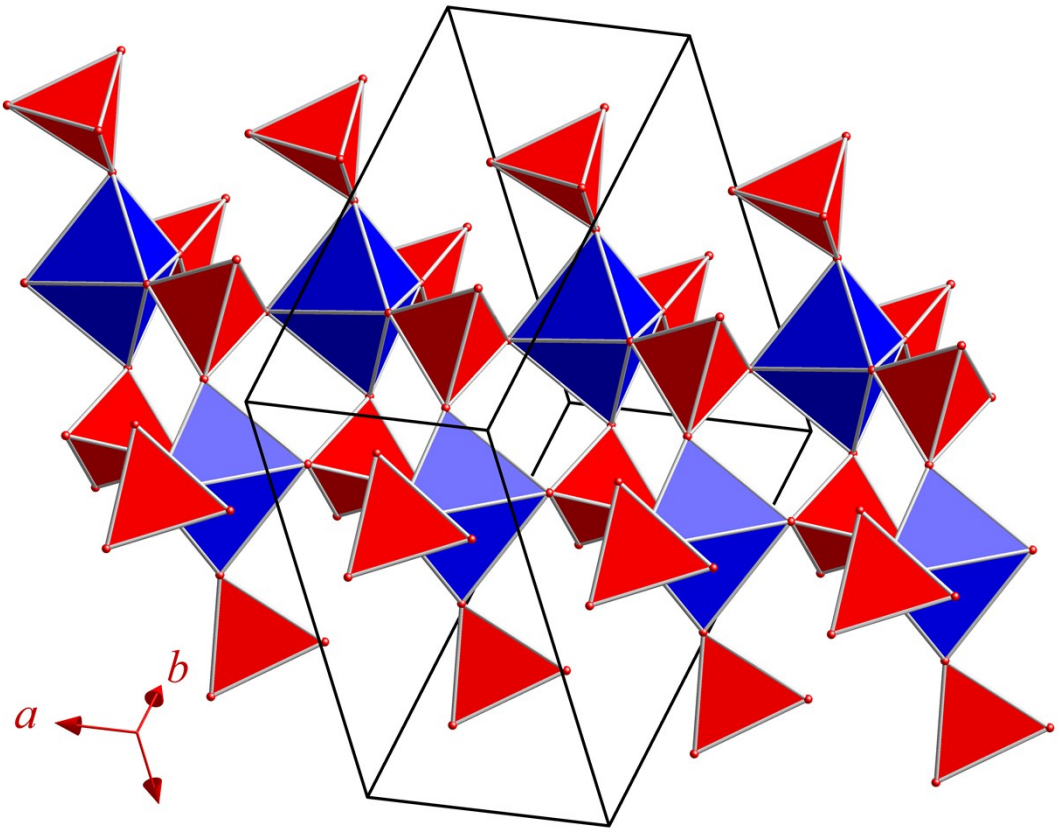


Figure S1 The building unit of a $[Ga_2P_6O_{26}]_\infty$ ribbon built up of $[GaO_5]$ dipyramids (in blue) and $[PO_4]$ tetrahedra (in red) via sharing-corners in $KGaCu(PO_4)_2$

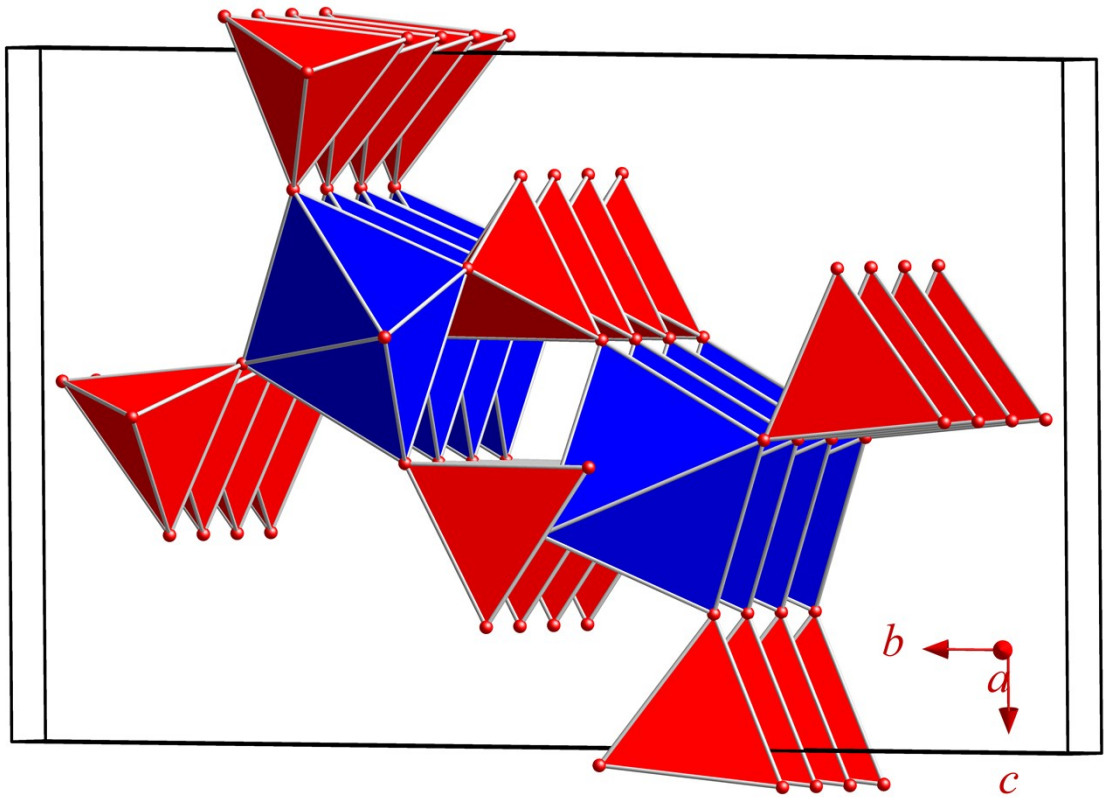


Figure S2 The building unit of a $[Ga_2P_6O_{26}]_\infty$ ribbon in $KGaCu(PO_4)_2$ viewed along *a*-axis.

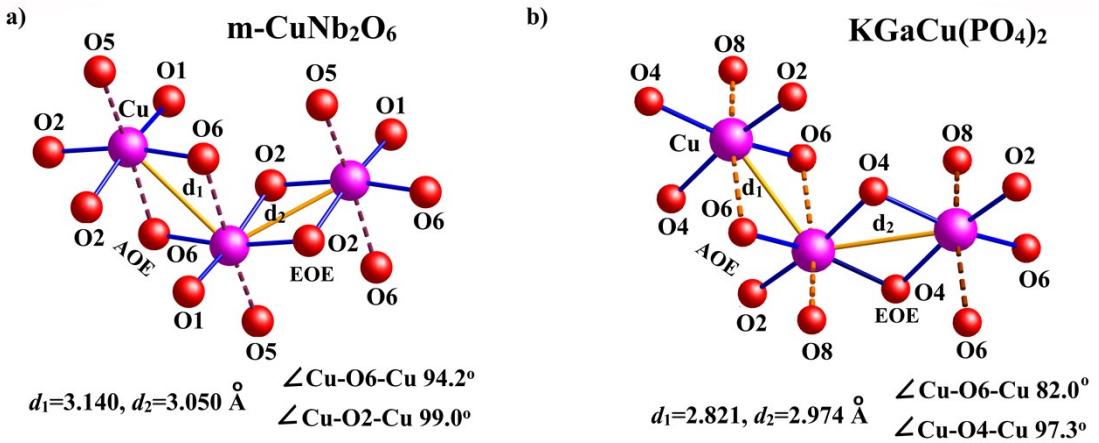


Figure S3 Comparison of copper coordination environments in monoclinic $CuNb_2O_6$(Left) and $KGaCu(PO_4)_2$(Right).

Table S1 Comparison of bond distances and bond angles of $CuO_6$ in $KGaCu(PO_4)_2$ and monoclinic $CuNb_2O_6$

| monoclinic $CuNb_2O_6$ | | $KGaCu(PO_4)_2$ | |
|---|---|---|---|
| Cu1—O6 | 1.942(3) | Cu1—O6 | 1.938 (6) |
| Cu1—O2 | 1.981(2) | Cu1—O4 | 1.948 (6) |
| Cu1—O1 | 2.015(9) | Cu1—O2 | 1.950 (6) |

| | | | |
|---|---|---|---|
| Cu1—O2 | 2.031(5) | Cu1—O4 | 2.012 (6) |
| Cu1—O5 | 2.291(5) | Cu1—O6 | 2.339 (6) |
| Cu1—O6 | 2.329(6) | Cu1—O8 | 2.566(6) |
| Cu-O-Cu | 94.16°(EOA) | Cu-O-Cu | 81.97°(EOA) |
| Cu-O-Cu | 98.95° (EOE) | Cu-O-Cu | 97.34° (EOE) |
| $d_1$(Cu—Cu) | 3.140 Å (EOA) | $d_1$(Cu—Cu) | 2.821 Å (EOA) |
| $d_2$(Cu—Cu) | 3.050 Å (EOE) | $d_2$(Cu—Cu) | 2.974 Å (EOE) |

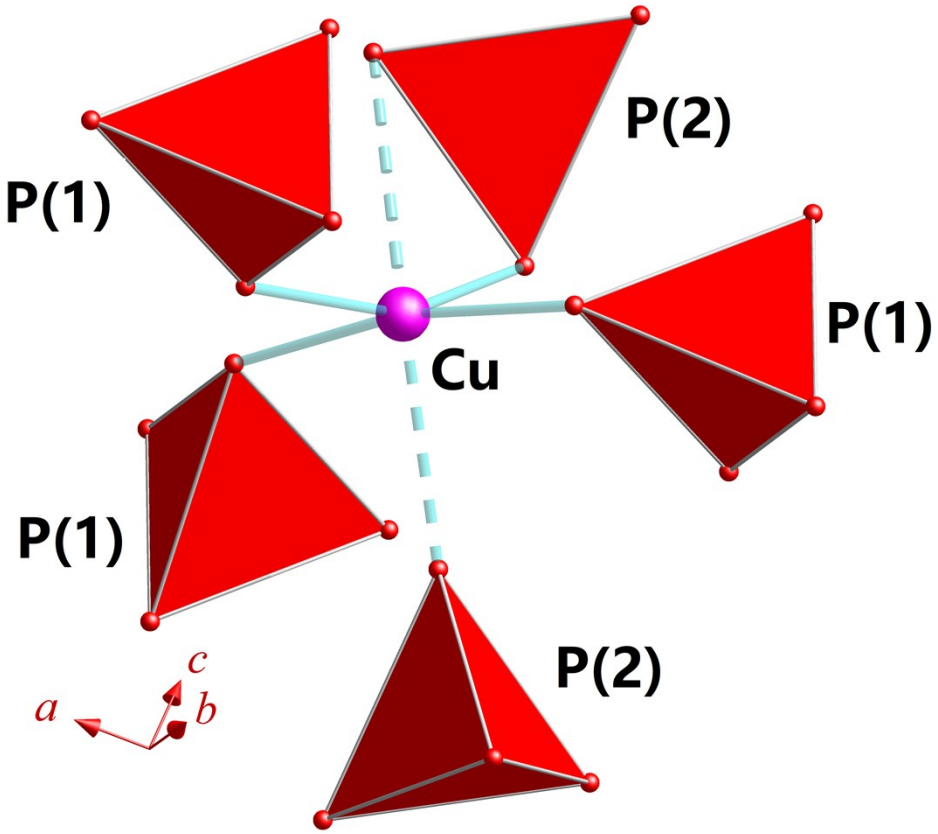


Figure S4 Copper coordination environment in $KGaCu(PO_4)_2$. Each $[CuO_6]$ octahedron links to three $[P(1)O_4]$ and one $[P(2)O_4]$ tetrahedra by sharing O-corners and to one additional $[P(2)O_4]$ by sharing an edge

Table S2 Selected bond distance (Å) of $KGaCu(PO_4)_2$

| Atom - atoms | distance | Atom - atoms | distance |
|---|---|---|---|
| Ga1—O3 | 1.852 (6) | K—O3$^{ii}$ | 2.810 (7) |
| Ga1—O8 | 1.853 (6) | K—O1$^{ii}$ | 2.841 (6) |
| Ga1—O7 | 1.855 (6) | K—O2 | 2.913 (7) |
| Ga1—O1 | 1.955 (6) | K—O7$^{xi}$ | 2.918 (6) |
| Ga1—O5 | 1.984 (6) | K—O5$^{xi}$ | 2.926 (7) |
| Cu1—O6 | 1.938 (6) | K—O4$^{xii}$ | 2.961 (7) |
| Cu1—O4$^{iii}$ | 1.948 (6) | K—O5$^{xii}$ | 2.966 (7) |
| Cu1—O2 | 1.950 (6) | K—O8$^{v}$ | 3.020 (6) |
| Cu1—O4 | 2.012 (6) | O1—K$^{ii}$ | 2.841 (6) |

| | | | |
|---|---|---|---|
| Cu1—O6$^{iv}$ | 2.339 (6) | O2—P1$^{vi}$ | 1.524 (7) |
| P1—O1 | 1.514 (6) | O3—P1$^{xiv}$ | 1.534 (6) |
| P1—O2$^{vi}$ | 1.524 (7) | O3—K$^{ii}$ | 2.810 (7) |
| P1—O3$^{vii}$ | 1.534 (6) | O4—P1$^{xv}$ | 1.548 (6) |
| P1—O4$^{viii}$ | 1.548 (6) | O4—Cu1$^{iii}$ | 1.948 (6) |
| P2—O5 | 1.511 (6) | O4—K$^{x}$ | 2.961 (7) |
| P2—O6 | 1.520 (6) | O5—K$^{i}$ | 2.926 (7) |
| P2—O7$^{vi}$ | 1.534 (6) | O5—K$^{x}$ | 2.966 (7) |
| P2—O8$^{ii}$ | 1.542 (6) | O6—Cu1$^{iv}$ | 2.339 (6) |
| Cu1—Cu1$^{iv}$ | 2.821 (3) | O7—P2$^{vi}$ | 1.534 (6) |
| Cu1—Cu1$^{iii}$ | 2.973 (2) | O7—K$^{i}$ | 2.918 (6) |
| O8—K$^{xvi}$ | 3.021 (6) | O8—P2$^{ii}$ | 1.542 (6) |

Table S3 Selected bond angles (°) of $KGaCu(PO_4)_2$

| Atom - atoms- atoms | Angle | Atom - atoms- atoms | distance |
|---|---|---|---|
| O3—Ga1—O8 | 120.7 (3) | O6—Cu1—O4$^{iii}$ | 156.3 (3) |
| O3—Ga1—O7 | 126.5 (3) | O6—Cu1—O2 | 90.5 (3) |
| O8—Ga1—O7 | 112.6 (3) | O4$^{iii}$—Cu1—O2 | 100.5 (3) |
| O3—Ga1—O1 | 87.2 (3) | O6—Cu1—O4 | 90.4 (2) |
| O8—Ga1—O1 | 92.9 (3) | O4$^{iii}$—Cu1—O4 | 82.7 (3) |
| O7—Ga1—O1 | 95.0 (3) | O2—Cu1—O4 | 169.3 (3) |
| O3—Ga1—O5 | 85.4 (3) | O6—Cu1—O6$^{iv}$ | 98.0 (2) |
| O8—Ga1—O5 | 93.2 (3) | O4$^{iii}$—Cu1—O6$^{iv}$ | 103.6 (2) |
| O7—Ga1—O5 | 87.3 (3) | O2—Cu1—O6$^{iv}$ | 86.3 (2) |
| O1—Ga1—O5 | 172.1 (3) | O4—Cu1—O6$^{iv}$ | 83.1 (2) |
| O1—P1—O2$^{vi}$ | 112.7 (4) | O5—P2—O6 | 109.6 (4) |
| O1—P1—O3$^{vii}$ | 108.0 (3) | O5—P2—O7$^{vi}$ | 113.4 (4) |
| O2$^{vi}$—P1—O3$^{vii}$ | 108.9 (3) | O6—P2—O7$^{vi}$ | 110.9 (3) |
| O1—P1—O4$^{viii}$ | 110.2 (3) | O5—P2—O8$^{ii}$ | 109.0 (4) |
| O2$^{vi}$—P1—O4$^{viii}$ | 112.0 (3) | O6—P2—O8$^{ii}$ | 106.3 (3) |
| O3$^{vii}$—P1—O4$^{viii}$ | 104.6 (3) | O7$^{vi}$—P2—O8$^{ii}$ | 107.3 (3) |
| P1—O1—Ga1 | 143.9 (4) | P2—O5—Ga1 | 138.4 (4) |
| P1$^{vi}$—O2—Cu1 | 123.2 (4) | P2—O6—Cu1 | 106.9 (3) |
| P1$^{xiv}$—O3—Ga1 | 134.5 (4) | P2—O6—Cu1$^{iv}$ | 169.7 (4) |
| P1$^{xv}$—O4—Cu1$^{iii}$ | 122.7 (4) | Cu1—O6—Cu1$^{iv}$ | 82.0 (2) |
| P1$^{xv}$—O4—Cu1 | 125.0 (4) | P2$^{vi}$—O7—Ga1 | 125.0 (4) |
| Cu1$^{iii}$—O4—Cu1 | 97.3 (3) | P2$^{ii}$—O8—Ga1 | 132.0 (4) |

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+3/2; (ii) −*x*, −*y*+1, −*z*+1; (iii) −*x*, −*y*+1, −*z*+2; (iv) −*x*+1, −*y*+1, −*z*+2; (v) *x*, −*y*+1/2, *z*+1/2; (vi) −*x*+1, −*y*+1, −*z*+1; (vii) *x*, −*y*+3/2, *z*−1/2; (viii) *x*, *y*, *z*−1; (ix) −*x*, *y*+1/2, −*z*+1/2; (x) −*x*, *y*+1/2, −*z*+3/2; (xi) −*x*+1, *y*−1/2, −*z*+3/2; (xii) −*x*, *y*−1/2, −*z*+3/2; (xiii) −*x*, *y*−1/2, −*z*+1/2; (xiv) *x*, −*y*+3/2, *z*+1/2; (xv) *x*, *y*, *z*+1; (xvi) *x*, −*y*+1/2, *z*−1/2.

Table S4 Atomic displacement parameters (Å$^2$) of $KGaCu(PO_4)_2$

| | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|
| Ga1 | 0.0052(4) | 0.0038(4) | 0.0054(4) | 0.0005(3) | 0.0008(3) | −0.0005(3) |
| Cu1 | 0.0147(6) | 0.0086(5) | 0.0182(6) | 0.0016(4) | 0.0103(4) | 0.0022(4) |
| P1 | 0.0095(10) | 0.0036(9) | 0.0059(10) | −0.0016(7) | 0.0023(8) | 0.0009(8) |
| P2 | 0.0017(9) | 0.0054(9) | 0.0065(9) | 0.0017(7) | 0.0008(7) | 0.0007(8) |
| K | 0.0182(10) | 0.0169(10) | 0.0208(11) | 0.0022(8) | −0.0045(8) | 0.0014(8) |
| O1 | 0.013(3) | 0.004(3) | 0.006(3) | 0.002(2) | 0.003(2) | 0.003(2) |
| O2 | 0.011(3) | 0.008(3) | 0.018(3) | 0.002(2) | 0.003(3) | −0.001(2) |
| O3 | 0.004(3) | 0.008(3) | 0.015(3) | 0.001(2) | −0.002(2) | −0.003(2) |
| O4 | 0.012(3) | 0.006(3) | 0.009(3) | −0.004(2) | 0.003(2) | −0.001(2) |
| O5 | 0.013(3) | 0.008(3) | 0.013(3) | 0.003(2) | 0.005(2) | 0.003(2) |
| O6 | 0.006(2) | 0.012(3) | 0.004(2) | 0.002(2) | 0.003(2) | 0.001(2) |
| O7 | 0.007(3) | 0.007(3) | 0.012(3) | 0.001(2) | 0.003(2) | −0.001(2) |
| O8 | 0.005(3) | 0.010(3) | 0.015(3) | 0.001(2) | 0.005(2) | −0.005(2) |

Table S5 The bond valence sums (BVS) of $KGaCu(PO_4)_2$

| | K | Cu | Ga | P1 | P2 | BVS |
|---|---|---|---|---|---|---|
| O1 | 0.146 | | 0.543 | 1.276 | | 1.96 |
| O2 | 0.120 | 0.480 | | 1.243 | | 1.84 |
| O3 | 0.053+0.160 | | 0.719 | 1.211 | | 2.14 |
| O4 | 0.106 | 0.483+0.407 | | 1.162 | | 2.16 |
| O5 | 0.116+0.104 | | 0.503 | | 1.284 | 2.00 |
| O6 | 0.041 | 0.497+0.168 | | | 1.255 | 1.96 |
| O7 | 0.119 | | 0.712 | | 1.207 | 2.04 |
| O8 | 0.090 | | 0.718 | | 1.181 | 1.99 |
| BVS | 1.06 | 2.03 | 3.19 | 4.90 | 4.92 | |

Table S6 CHN contents of the title compound $KGaCu(PO_4)_2$

| Number | Weight (mg) | Element | Content (wt. %) |
|---|---|---|---|
| 1 | 7.1320 | N | 0.006 |
| | | C | 0.000 |
| | | H | 0.059 |
| 2 | 5.7740 | N | 0.007 |
| | | C | 0.000 |
| | | H | 0.078 |
| 3 | 3.4990 | N | 0.000 |
| | | C | 0.000 |
| | | H | 0.031 |
| 4 | 2.9630 | N | 0.000 |
| | | C | 0.000 |

| | | |
|---|---|---|
| | H | 0.065 |
| Average | N | 0.003±0.004 |
| | C | 0 |
| | H | 0.058±0.019 |

*The mean H content at ~0.06(2) (wt.%) corresponds to a water content of 0.5(2) wt.%.

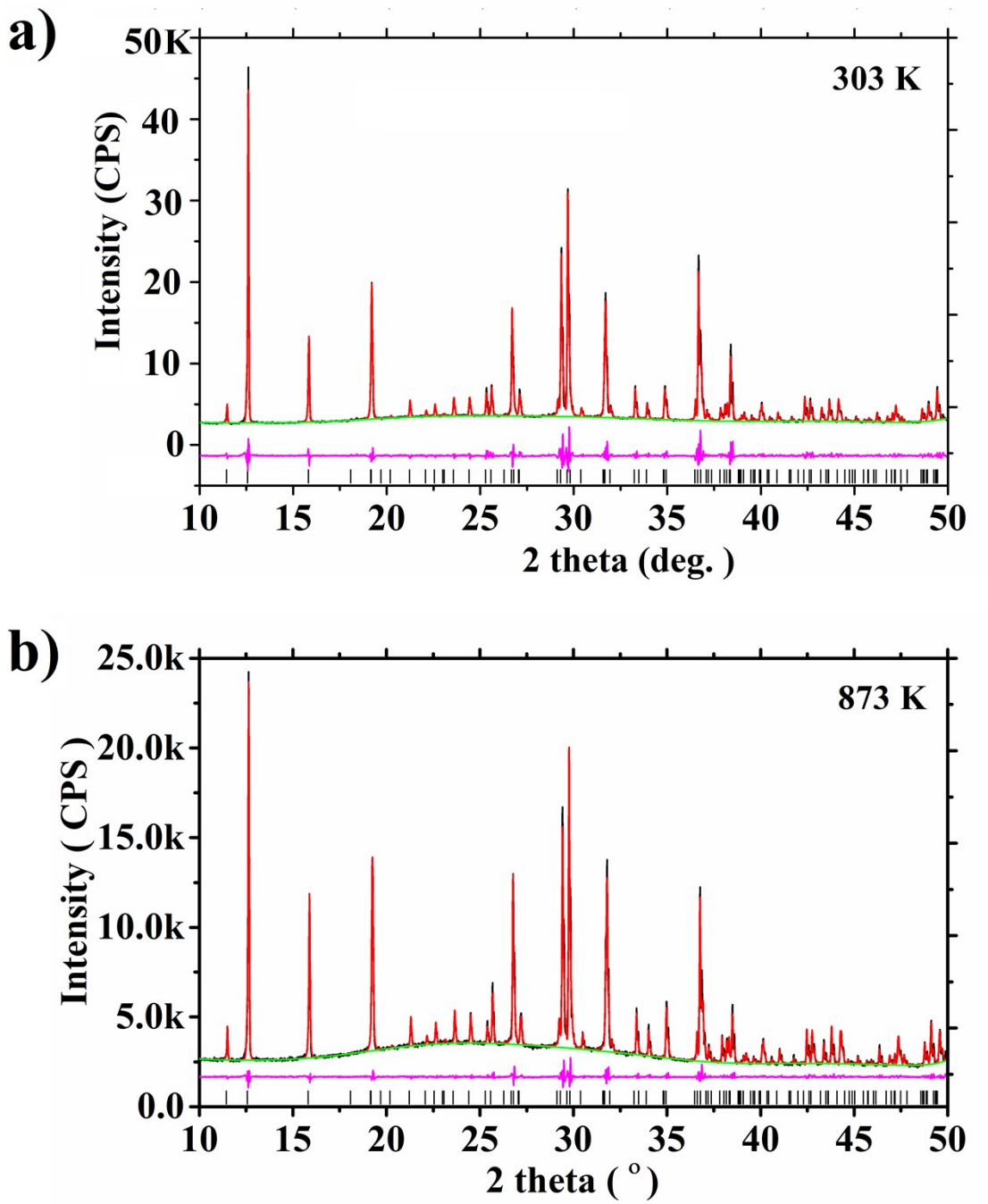


Figure S5 Powder X-ray diffraction patterns of the samples calcined in air for 6 h at 303 and 873 K, respectively. Experimental (black) and calculated (red) X-ray diffraction patterns are shown in an overlapped manner. Their difference profile (pink)

and background (green) from Rietveld refinement are given at the bottom. The Bragg positions are indicated by the vertical bars below the pattern.

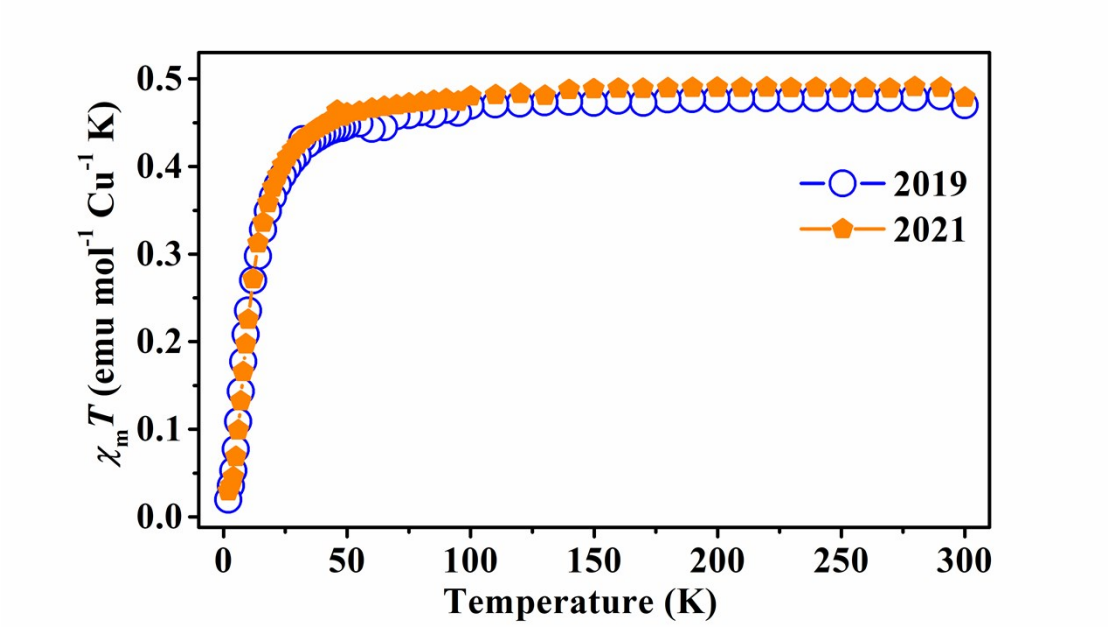


Figure S6 Comparison of the curves of $\chi_m T$ *vs* $T$ of $KGaCu(PO_4)_2$, synthesized in 2019 and 2021, respectively.