**Electronic supplementary materials** *Mendeleev Commun.*, 2021, **31**, 113-115

# Upconversion luminescence and ratiometric temperature sensing behavior of $Er^{3+}/Yb^{3+}$-codoped $CaY_2Ge_3O_{10}$ germanate

**Olga A. Lipina, Ludmila L. Surat, Alexander Yu. Chufarov, Alexander P. Tyutyunnik and Vladimir G. Zubkov**

(*a*) (*b*)

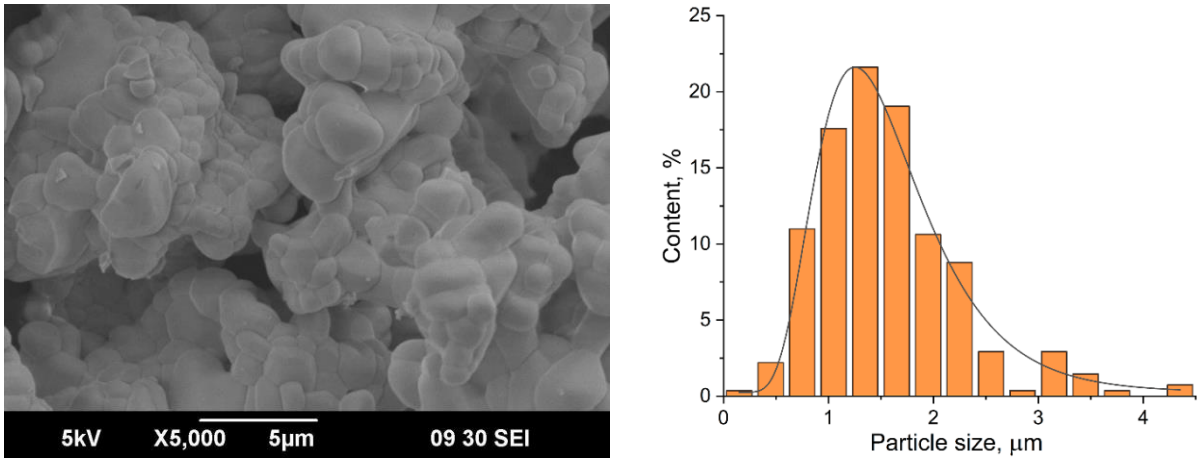


**Figure S1** SEM image of $CaY_{1.5}Yb_{0.45}Er_{0.05}Ge_3O_{10}$ powder (*a*) and the particle size distribution histogram with log-normal distribution fit (*b*).

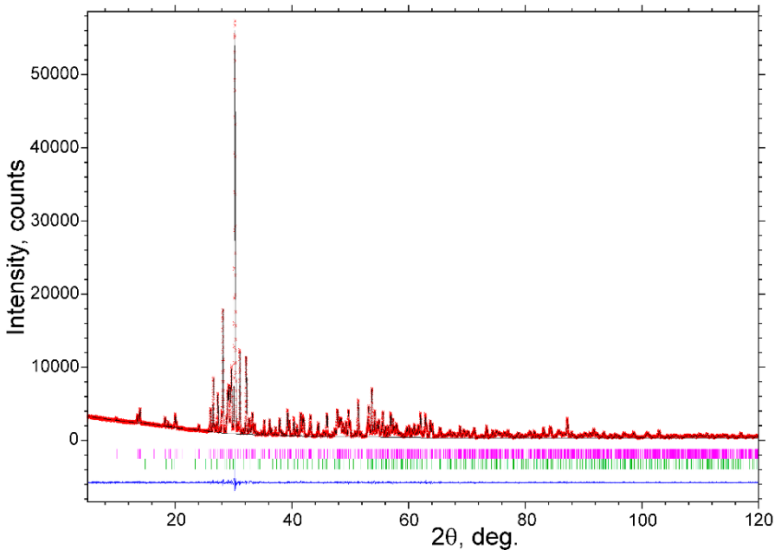


**Figure S2** Experimental (red crosses), calculated (black line) and difference (blue line) X-ray diffraction profiles of $CaY_{1.5}Yb_{0.45}Er_{0.05}Ge_3O_{10}$ germanate. Short vertical pink and green lines indicate the Bragg reflection positions of the main phase and impurity phase, ($Y_2Ge_2O_7$), respectively.

**Table S1** Crystallographic data and refinement parameters for $CaY_{1.5}Yb_{0.45}Er_{0.05}Ge_3O_{10}$ [a]

| *Crystallographic data* | |
|---|---|
| Monoclinic, $P2_1/c$, Z = 4 | Cu $K\alpha_1$ radiation |
| $a$ = 6.89311(3) Å | T = 298 K |
| $b$ = 6.82566(3) Å | |
| $c$ = 18.72812(9) Å | *Refinement parameters* |
| $\beta$ = 108.9708(3) ° | $wRp$ = 3.38 % |
| $V$ = 833.298(8) Å$^3$ | $Rp$ = 2.52 % |
| $M_r$ = 637.43 | $R(F^2)$ = 1.37 % |
| $D_x$ = 5.081 g/cm$^3$ | $\chi^2$ = 1.601 |

[a] Content of impurity 2.4 mass % $Y_2Ge_2O_7$.

**Table S2** Atomic coordinates, thermal parameters[a] ($U_{iso}\times100$, Å$^2$) and fractions for $CaY_{1.5}Yb_{0.45}Er_{0.05}Ge_3O_{10}$

| Atoms | *x* | *y* | *z* | $U_{iso}\times100$, Å$^2$ | Fractions |
|---|---|---|---|---|---|
| Ca/Y/Yb/Er(1) | 0.02523(15) | 0.89994(13) | 0.41507(5) | 2.33(3) | 0.445/0.416/0.125/0.014 |
| Ca/Y/Yb/Er(2) | 0.58068(16) | 0.23285(15) | 0.41463(6) | 2.17(3) | 0.535/0.349/0.105/0.011 |
| Ca/Y/Yb/Er(3) | 0.12854(10) | 0.12729(10) | 0.25315(4) | 1.91(2) | 0.020/0.735/0.220/0.025 |
| Ge(1) | 0.09745(15) | 0.37018(15) | 0.42415(6) | 2.10(3) | 1.000 |
| Ge(2) | 0.45284(16) | 0.22587(14) | 0.07179(6) | 1.89(3) | 1.000 |
| Ge(3) | 0.65546(15) | 0.11634(15) | 0.24056(6) | 1.86(3) | 1.000 |
| O(1) | 0.0149(7) | 0.0768(7) | 0.12730(30) | 1.92(4) | 1.000 |
| O(2) | 0.0651(7) | 0.7171(7) | 0.04493(28) | 1.92(4) | 1.000 |
| O(3) | 0.1466(7) | 0.4476(6) | 0.21617(27) | 1.92(4) | 1.000 |
| O(4) | 0.1872(7) | 0.8122(6) | 0.26827(27) | 1.92(4) | 1.000 |
| O(5) | 0.2119(8) | 0.2010(7) | 0.37857(28) | 1.92(4) | 1.000 |
| O(6) | 0.3032(7) | 0.0560(7) | 0.00455(30) | 1.92(4) | 1.000 |
| O(7) | 0.3033(7) | 0.4108(7) | 0.08646(25) | 1.92(4) | 1.000 |
| O(8) | 0.4767(7) | 0.1599(6) | 0.28559(27) | 1.92(4) | 1.000 |
| O(9) | 0.5273(8) | 0.0448(6) | 0.14526(29) | 1.92(4) | 1.000 |
| O(10) | 0.6410(7) | 0.3256(7) | 0.03966(28) | 1.92(4) | 1.000 |

[a] The thermal vibration parameters of oxygen atoms have been constrained as a single variable.

**Table S3** Selected interatomic distances (Å) and angles (°) for $CaY_{1.5}Yb_{0.45}Er_{0.05}Ge_3O_{10}$

| *Interatomic distances* | | | |
|---|---|---|---|
| Ca(1)/*RE*(1)–O(1) | 2.330(5) | Ge(1)–O(1) | 1.741(5) |
| Ca(1)/*RE*(1)–O(2) | 2.437(5) | Ge(1)–O(2) | 1.762(5) |
| Ca(1)/*RE*(1)–O(2) | 2.489(5) | Ge(1)–O(5) | 1.767(5) |
| Ca(1)/*RE*(1)–O(3) | 2.378(5) | Ge(1)–O(6) | 1.773(5) |
| Ca(1)/*RE*(1)–O(5) | 2.630(5) | **Ge(1)–O** | **1.761** |
| Ca(1)/*RE*(1)–O(7) | 2.257(4) | | |
| Ca(1)/*RE*(1)–O(10) | 2.236(5) | Ge(2)–O(6) | 1.775(5) |
| **Ca(1)/*RE*(1)–O** | **2.394** | Ge(2)–O(7) | 1.707(4) |
| | | Ge(2)–O(9) | 1.796(5) |
| Ca(2)/*RE*(2)–O(2) | 2.312(5) | Ge(2)–O(10) | 1.736(5) |
| Ca(2)/*RE*(2)–O(5) | 2.418(5) | **Ge(2)–O** | **1.754** |
| Ca(2)/*RE*(2)–O(6) | 2.647(5) | | |
| Ca(2)/*RE*(2)–O(7) | 2.342(5) | Ge(3)–O(3) | 1.768(4) |
| Ca(2)/*RE*(2)–O(8) | 2.340(5) | Ge(3)–O(4) | 1.763(4) |
| Ca(2)/*RE*(2)–O(9) | 2.409(5) | Ge(3)–O(8) | 1.730(4) |
| Ca(2)/*RE*(2)–O(10) | 2.276(5) | Ge(3)–O(9) | 1.783(5) |
| **Ca(2)/*RE*(2)–O** | **2.392** | **Ge(3)–O** | **1.761** |
| | | | |
| Ca(3)/*RE*(3)–O(1) | 2.256(5) | Ge(1)–Ge(2) | 3.1100(14) |
| Ca(3)/*RE*(3)–O(3) | 2.309(4) | Ge(2)–Ge(3) | 3.1031(14) |
| Ca(3)/*RE*(3)–O(3) | 2.478(4) | **Ge-Ge** | 3.1066 |
| Ca(3)/*RE*(3)–O(4) | 2.190(4) | | |
| Ca(3)/*RE*(3)–O(4) | 2.434(5) | *Bond angles* | |
| Ca(3)/*RE*(3)–O(5) | 2.285(5) | Ge(1)-O(6)-Ge(2) | 122.47(26) |
| Ca(3)/*RE*(3)–O(8) | 2.287(5) | Ge(2)-O(9)-Ge(3) | 120.25(26) |
| **Ca(3)/*RE*(3)–O** | **2.320** | Ge(1)-Ge(2)-Ge(3) | 144.92(5) |