Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


Supporting Information

# Luminescence-structure relationships in solids doped with $Bi^{3+}$

Philippe Boutinaud
*Université Clermont Auvergne, Clermont Auvergne INP, CNRS, ICCF, F-63000 Clermont–Ferrand, France*
*philippe.boutinaud@sigma-clermont.fr*

We illustrate here the handmade step-by-step calculation of *he* for several representative compounds of interest in the field of spectroscopy.

A.1. $CaF_2$

With its single cation and anion sites, the cubic fluorine is among the simplest case to start with. Its crystal structure is represented in Fig. S1.

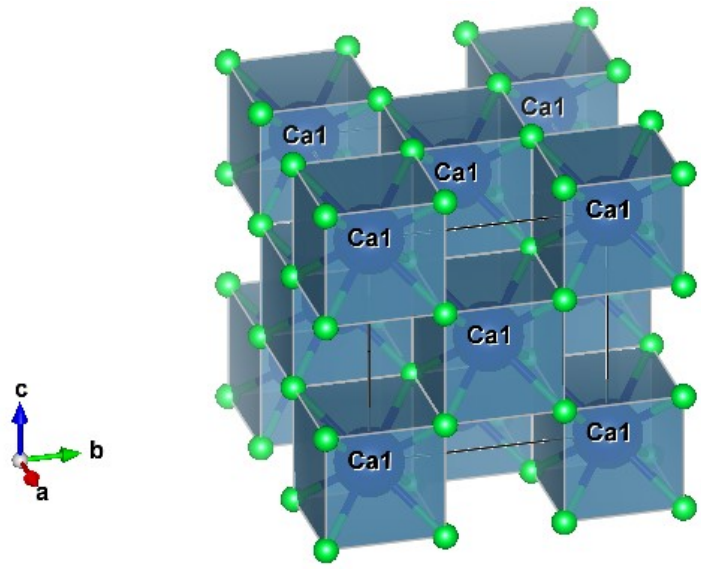


Figure S1. The crystal structure of $CaF_2$. The fluoride atoms appear in green.

Matrices I and II are reproduced below.

| Matrix I – source ICSD - 2300449<br>Space group n°225, V = 163 Å$^3$, Z = 4 | Ca | F |
|---|---|---|
| Ca | | N(F-Ca) = 4 |
| F | N(Ca-F)=8 | |
| Total coordination | N(Ca) = 8 | N(F) = 4 |
| Site multiplicity | w(Ca) = 4 | w(F) = 8 |
| Kappa values (from Eqn. (3)) | $K(Ca-F) =$ 1 | $K(F-Ca) =$ 2 |

| Matrix II – source ICSD - 2300449 | Ca |
|---|---|
| F | d(Ca-F) = 2.365 Å |
| Bond Valence Parameter | 1.842 |

The very simple $CaF_2$ is not decomposable into binary units. The value of *he* at Ca site is given by: $he(Ca) = [N(Ca-F)f_c(Ca-F)\alpha(Ca-F)Q(F)^2]^{1/2}$. The different steps of the calculation are detailed in Table A1.

Table A1 : The step-by-step calculation of *he(Ca)* in $CaF_2$

| Compound $CaF_2$ | Site Ca | Eqn. number |
|---|---|---|
| Q(Ca) | 1.943 | from VESTA |
| Q(F) | 0.971 | (5) |
| $\Gamma_1(Ca-F)$ | 30.79 | (7) |
| $\Gamma_2(Ca-F)$ | 11.66 | (8) |
| $N^*(Ca-F)$ | 0.382 | (10) |
| $\upsilon(Ca-F)$ | 5.090 | (11) |
| $\Gamma_3(Ca-F)$ | 0.064 | (9) |
| $f_c(Ca-F)$ | 0.040 | (6) |
| $\alpha(Ca-F)$ | 0.278 | (11) |
| $he(Ca)$ | 0.294 | (4) |

A.2. $YPO_4$

With two cation sites and single anion site, $YPO_4$ constitutes a representative member of all zircon-structured lattices (YVO4, etc…). Its crystal structure is represented in Fig. S2. Y is considered as the doping site for the luminescent activator.

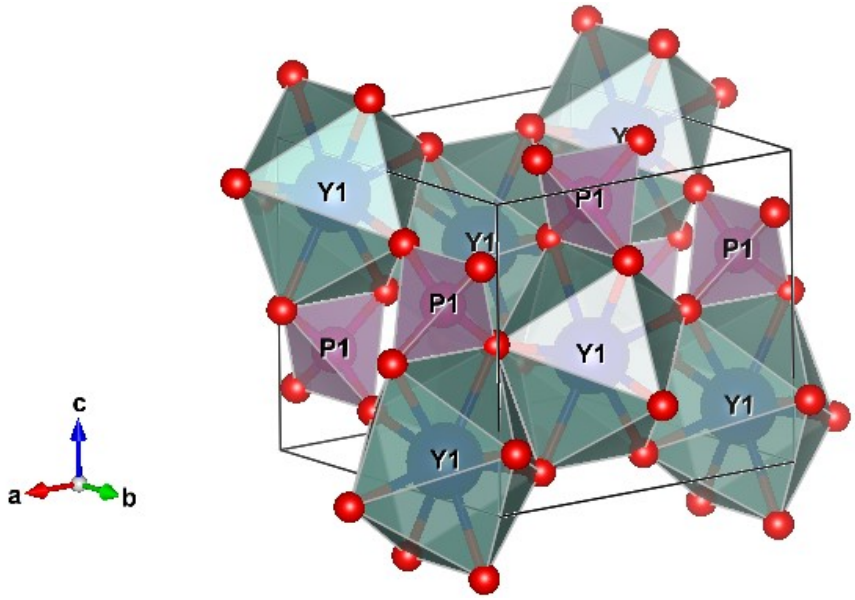


Figure S2. The crystal structure of $YPO_4$. The oxygen atoms appear in red.

Matrices I and II for this compound are reproduced below.

| Matrix I – source ICSD - 79754<br>Space group n°141, V = 286.5 Å$^3$, Z = 4 | Y | P | O |
|---|---|---|---|
| Y | | | N(O-Y) = 2 |
| P | | | N(O-P) = 1 |
| O | N(Y-O)=8 | N(P-O) = 4 | |
| Total coordination | N(Y) = 8 | N(P) = 4 | N(O) = 3 |
| Site multiplicity | w(Y) = 4 | w(P) = 4 | w(O) = 16 |
| Kappa values (from Eqn. (3)) | K$(Y-O) = 1$ | K$(P-O) = 1$ | K$(O-Y) = 8/3$<br>K$(O-P) = 4/3$ |

| Matrix II – source ICSD - 79754 | Y | P |
|---|---|---|
| O | d(Y-O) = 2.345 Å | d(P-O) = 1.540 Å |
| Bond Valence Parameter | 2.014 | 1.604 |

Eqn. (2) gives $YPO_4 = YO_{8/3} + PO_{4/3}$. The value of *he* at Y site is given by:
$he(Y) = [N(Y-O)f_c(Y-O)\alpha(Y-O)Q(O)^2]^{1/2}$. The different steps of the calculation are detailed in Table A2.

Table A2: The step-by-step calculation of *he(Y)* in $YPO_4$

| Compound $YPO_4$ | Site Y | Eqn. number |
|---|---|---|
| Q(Y) | 3.286 | from VESTA |
| Q(O) | 1.232 | (5) |
| $\Gamma_1(Y-O)$ | 20.79 | (7) |
| $\Gamma_2(Y-O)$ | 6.572 | (8) |
| $N^*(Y-O)$ | 1.643 | (10) |
| $\upsilon(Y-O)$ | 7.843 | (11) |
| $\Gamma_3(Y-O)$ | 0.085 | (9) |
| $f_c(Y-O)$ | 0.146 | (6) |
| $\alpha(Y-O)$ | 0.707 | (11) |
| $he(Y)$ | 1.120 | (4) |

A.3. $Y_2O_3$

$Y_2O_3$ is representative of sesquioxides. The corresponding crystal structure is represented in Fig. S3. Considering the presence of two sites for yttrium, $Y_2O_3$ should be written as $Y1_{1/2}Y2_{3/2}O_3$. Since Y1 and Y2 are both available for a luminescent activator, we will calculate he(Y1) and he(Y2).

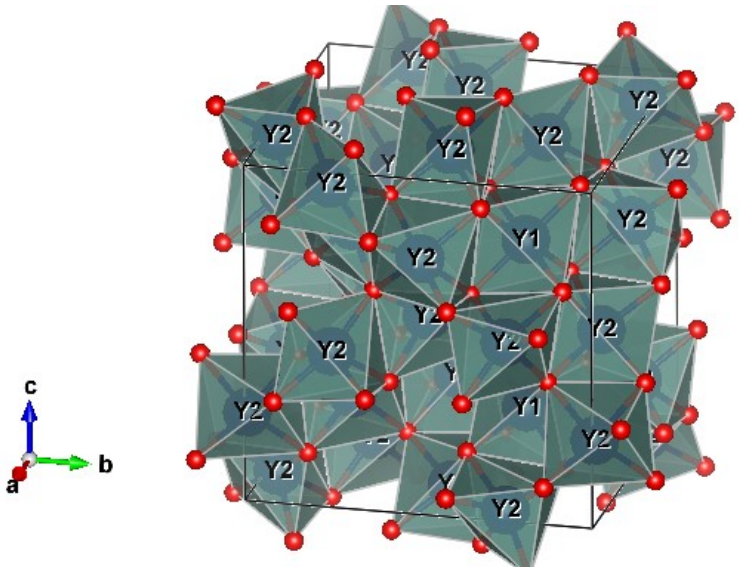


Figure S3. The crystal structure of $Y_2O_3$. The oxygen atoms appear in red.

Matrices I and II for this compound are reproduced below.

| Matrix I – source ICSD - 192862<br>Space group n°206, V = 1191 Å$^3$, Z = 16 | Y1 | Y2 | O |
|---|---|---|---|
| Y1 | | | N(O-Y1) = 1 |
| Y2 | | | N(O-Y2) = 3 |
| O | N(Y1-O)=6 | N(Y2-O) = 6 | |
| Total coordination | N(Y1) = 6 | N(Y2) = 6 | N(O) = 4 |
| Site multiplicity | w(Y1) = 8 | w(Y2) = 24 | w(O) = 48 |
| Kappa values (from Eqn. (3)) | $K(Y1-O) = 1/2$ | $K(Y2-O) = 3/2$ | $K(O-Y1) = 3/4$<br>$K(O-Y2) = 9/4$ |

| Matrix II – source ICSD - 192862 | Y1 | Y2 |
|---|---|---|
| O | d(Y1-O) = 2.279 Å | d(Y2-O) = 2.281 Å |
| Bond Valence Parameter | 2.014 | 2.014 |

Eqn. (2) gives $Y1_{1/2}Y2_{3/2}O_3 = Y1_{1/2}O_{3/4} + Y2_{3/2}O_{9/4}$. The value of *he* at Y1 and Y2 sites is given by: $he(Yi) = [N(Yi-O)f_c(Yi-O)\alpha(Yi-O)Q(O_{Yi})^2]^{1/2}$ with I = 1 or 2, respectively. Note that the Q(O) value may depend on the nearby cation Y1 or Y2. This is noted as $Q(O_{Yi})$ in the above equation. In the present case, however, we have $Q(O_{Y1}) = Q(O_{Y2}) = Q(O)$. The different steps of the calculation are detailed in Table A3.

Table A3 : The step-by-step calculation of *he(Y1)* and he(Y2) in $Y_2O_3$

| Compound $Y_2O_3$ | Site Y1 (i = 1) | Site Y2 (i = 2) | Eqn. number |
|---|---|---|---|
| Q(Yi) | 2.933 | 2.933 | from VESTA |
| $Q(O_{Yi})$ | 1.955 | 1.955 | (5) |
| $\Gamma_1(Yi-O)$ | 25.88 | 25.86 | (7) |
| $\Gamma_2(Yi-O)$ | 5.866 | 5.866 | (8) |
| $N^*(Yi-O)$ | 1.955 | 1.955 | (10) |
| $\upsilon(Yi-O)$ | 6.191 | 6.207 | (11) |
| $\Gamma_3(Yi-O)$ | 0.077 | 0.077 | (9) |
| $f_c(Yi-O)$ | 0.162 | 0.162 | (6) |
| $\alpha(Yi-O)$ | 0.692 | 0.695 | (11) |
| $he(Yi)$ | 1.603 | 1.607 | (4) |

A.4. $Cs_2NaYX_6$ (X = Cl, Br)

$Cs_2NaYCl_6$ and $Cs_2NaYBr_6$ are representative of double halide perovskites with cubic structure. This crystal structure is represented in Fig. S4. Y is the doping site of interest. We will calculate he(Y) in both cases.

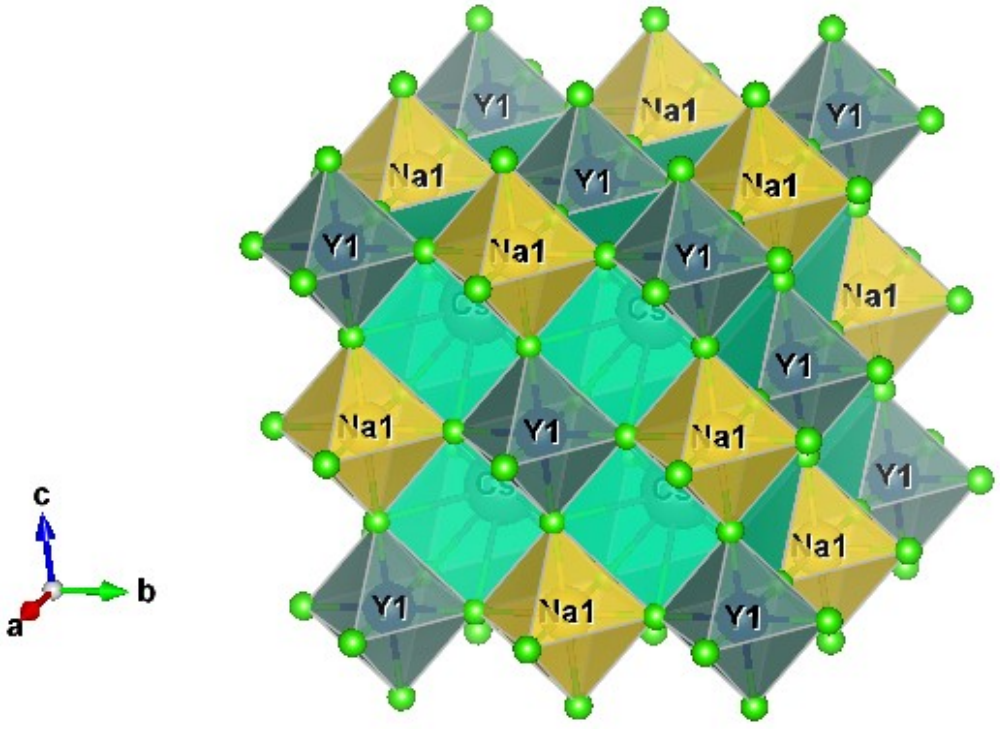


Figure S4. The crystal structure of $Cs_2NaYX_6$ (X = Cl, Br). The halogen atoms appear in green.

Matrices I and II for these compounds are reproduced below.

| Matrix I – source ICSD - 245353 (X = Cl) and 65733 (X = Br). Space group n°225, V = 1234. 5 Å$^3$ (X = Cl) and 1444.7 Å$^3$ (X = Br), Z = 4 | Cs | Na | Y | X |
|---|---|---|---|---|
| Cs | | | | N(X-Cs) = 4 |
| Na | | | | N(X-Na) = 1 |
| Y | | | | N(X-Y) = 1 |
| X | N(Cs-X) = 12 | N(Na-X) = 6 | N(Y-X) = 6 | |
| Total coordination | N(Cs) = 12 | N(Na) = 6 | N(Y) = 6 | N(X) = 6 |
| Site multiplicity | w(Cs) = 8 | w(Na) = 4 | w(Y) = 4 | w(X) = 24 |
| Kappa values (from Eqn. (3)) | $K(Cs-X) = 2$ | $K(Na-X) = 1$ | $K(Y-X) = 1$ | $K(X-Cs) = 4$<br>$K(X-Na) = 1$<br>$K(X-Y) = 1$ |

| Matrix II – source ICSD - 245353 (X = Cl) and 65733 (X = Br) | Cs | Na | Y |
|---|---|---|---|
| X = Cl | d(Cs-Cl) = 3.793 Å | d(Na-Cl) = 2.744 Å | d(Y-Cl) = 2.619 Å |
| Bond Valence Parameter | 2.79 | 2.15 | 2.40 |
| X = Br | d(Cs-Br) = 3.997 Å | d(Na-Br) = 2.887 Å | d(Y-Br) = 2.765 Å |
| Bond Valence Parameter | 2.95 | 2.33 | 2.55 |

The lattice decomposition (Eqn. (2)) gives $Cs_2NaYX_6 = Cs_2X_4 + Na_1X_1 + Y_1X_1$.We have:
$he(Y) = [N(Y-X)f_c(Y-X)\alpha(Y-X)Q(X)^2]^{1/2}$ . The different steps of the calculation are detailed in Table A4.

Table A4: The step-by-step calculation of *he(Y)* in $Cs_2NaYX_6$ (X = Cl, Br)

| Compound | $Cs_2NaYCl_6$ | $Cs_2NaYBr_6$ | Eqn. number |
|---|---|---|---|
| Q(Y) | 3.31 | 3.35 | from VESTA |
| Q(X) | 3.31 | 3.35 | (5) |
| $\Gamma_1(Y-X)$ | 35.18 | 33.33 | (7) |
| $\Gamma_2(Y-X)$ | 19.86 | 20.1 | (8) |
| $N^*(Y-X)$ | 4.413 | 4.473 | (10) |
| $\upsilon(Y-X)$ | 3.598 | 4.232 | (11) |
| $\Gamma_3(Y-X)$ | 0.0248 | 0.0222 | (9) |
| $f_c(Y-X)$ | 0.042 | 0.044 | (6) |
| $\alpha(Y-X)$ | 0.551 | 0.683 | (11) |
| $he(Y)$ | 1.24 | 1.42 | (4) |

A.5. $Y_3Al_5O_{12}$

$Y_3Al_5O_{12}$ is representative of garnets. Its input matrix is like that of double halide perovskites but here, three cation sites are potentially available for luminescent dopants; the Y site for e. g. lanthanides and the Al sites for e. g. transition metals. The compound is written as $Y_3Al1_2Al2_3O_{12}$. The corresponding crystal structure is represented in Fig. S5.

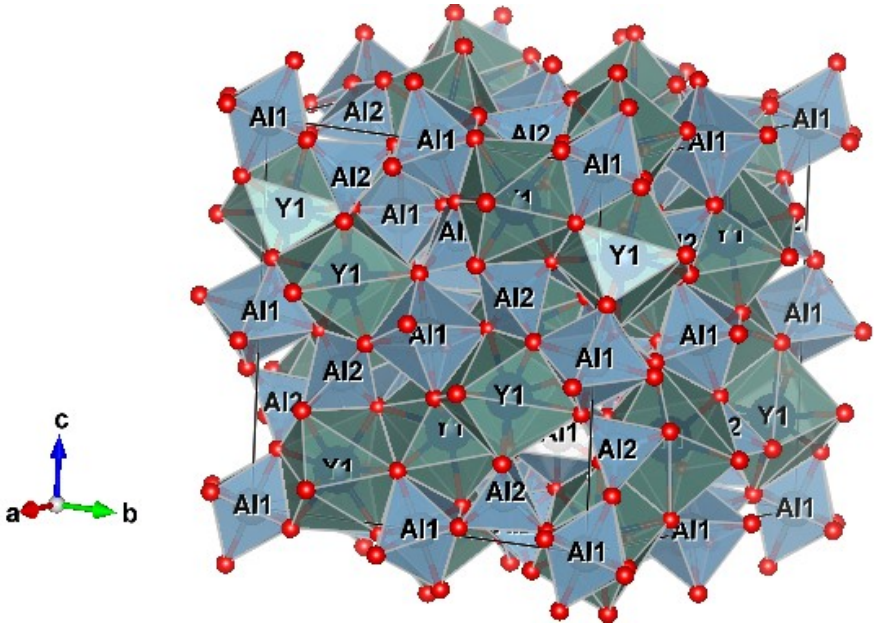


Figure S5. The crystal structure of $Y_3Al_5O_{12}$. The oxygen atoms appear in red.

We will calculate he(Y), he(Al1) and he(Al2). Matrices I and II for this compound are reproduced below.

| Matrix I – source ICSD - 280104 Space group n°230, V = 1730.7 Å$^3$, Z = 8 | Y | Al1 | Al2 | O |
|---|---|---|---|---|
| Y | | | | N(O-Y) = 2 |
| Al1 | | | | N(O-Al1) = 1 |
| Al2 | | | | N(O-Al2) = 1 |
| O | N(Y-O) = 8 | N(Al1-O) = 6 | N(Al2-O) = 4 | |
| Total coordination | N(Y) = 8 | N(Al1) = 6 | N(Al2) = 4 | N(O) = 4 |
| Site multiplicity | w(Y) = 24 | w(Al1) = 16 | w(Y2) = 24 | w(O) = 96 |
| Kappa values (from Eqn. (3)) | $K(Y-O) = 3$ | $K(Al1-O) = 2$ | $K(Al2-O) = 3$ | $K(O-Y) = 6$<br>$K(O-Al1) = 3$<br>$K(O-Al2) = 3$ |

| Matrix II – source ICSD - 280104 | Y | Al1 | Al2 |
|---|---|---|---|
| O | d(Y-O) = 2.377 Å | d(Al1-O) = 1.938 Å | d(Al2-O) = 1.754 Å |
| Bond Valence Parameter | 2.014 | 1.651 | 1.651 |

The lattice decomposition (Eqn. (2)) gives $Y_3Al1_2Al2_3O_{12} = Y_3O_6 + Al1_2O_3 + Al2_3O_3$. We have: $he(Y) = [N(Y-O)f_c(Y-O)\alpha(Y-O)Q(O)^2]^{1/2}$ and $he(Ali) = [N(Ali-O)f_c(Ali-O)\alpha(Ali-O)Q(O_{Ali})^2]^{1/2}$ with I = 1 or 2, respectively. Note that the Q(O) value may depend on the nearby cation Al1 or Al2. This is noted as $Q(O_{Ali})$ in the above equation. The different steps of the calculation are detailed in Table A5.

Table A5: The step-by-step calculation of *he(Y), he(Al1)* and *he(Al2)* in $Y_3Al_5O_{12}$

| Compound $Y_3Al_5O_{12}$ | Site Y | Compound $Y_3Al_5O_{12}$ | Site Al1 (i = 1) | Site Al2 (i = 2) | Eqn. number |
|---|---|---|---|---|---|
| Q(Y) | 3.04 | Q(Ali) | 2.76 | 3.03 | from VESTA |
| Q(O) | 1.52 | $Q(O_{Ali})$ | 1.84 | 3.03 | (5) |
| $\Gamma_1(Y-O)$ | 30.63 | $\Gamma_1(Ali-O)$ | 30.43 | 23.35 | (7) |
| $\Gamma_2(Y-O)$ | 6.08 | $\Gamma_2(Ali-O)$ | 5.52 | 6.06 | (8) |
| $N^*(Y-O)$ | 1.52 | $N^*(Ali-O)$ | 1.38 | 3.03 | (10) |

| | | | | | |
|---|---|---|---|---|---|
| $\upsilon(Y-O)$ | 6.124 | $\upsilon(Ali-O)$ | 3.319 | 2.460 | (11) |
| $\Gamma_3(Y-O)$ | 0.076 | $\Gamma_3(Ali-O)$ | 0.102 | 0.081 | (9) |
| $f_c(Y-O)$ | 0.097 | $f_c(Ali-O)$ | 0.168 | 0.425 | (6) |
| $\alpha(Y-O)$ | 0.495 | $\alpha(Ali-O)$ | 0.277 | 0.417 | (11) |
| $he(Y)$ | 0.942 | $he(Ali)$ | 0.972 | 2.551 | (4) |

A.6. $YAlO_3$

$YAlO_3$ is representative of orthorhombically-distorted perovskites ($CaTiO_3$, $CaZrO_3$, $CaSnO_3$, etc…). Its crystal structure is represented in Fig. S6. This is a case where the oxygen atoms occupy two different sites and cation sites are both available for luminescent dopants.

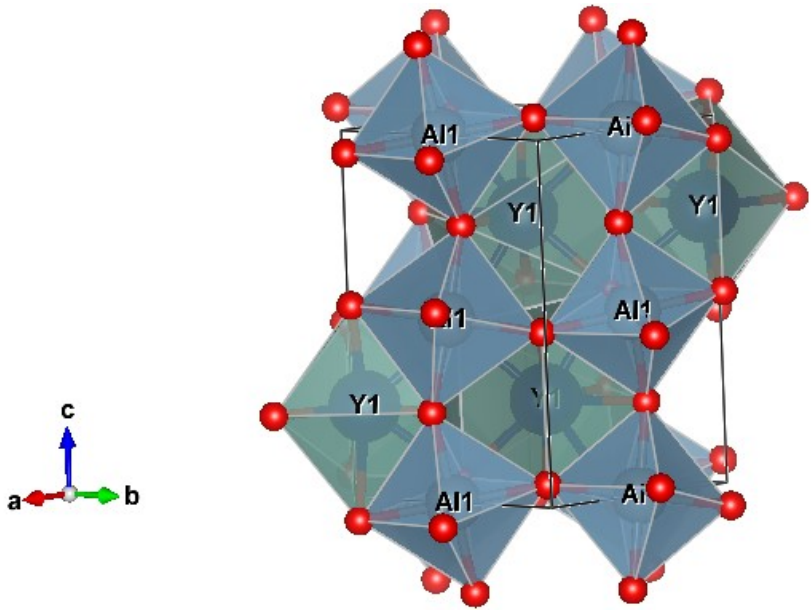


Figure S6. The crystal structure of $YAlO_3$. The oxygen atoms appear in red.

We will calculate *he(Y)* and *he(Al)*. Matrices I and II for this compound are reproduced below.

| Matrix I – source ICSD - 191383<br>Space group n°62,<br>V = 203.9 Å$^3$, Z = 4 | Y | Al | O1 | O2 |
|---|---|---|---|---|
| Y | | | N(O1-Y) = 2 | N(O2-Y) = 3 |
| Al | | | N(O1-Al) = 2 | N(O2-Al) = 2 |
| O1 | N(Y-O1) = 2 | N(Al-O1) = 2 | | |
| O2 | N(Y-O2) = 6 | N(Al-O2) = 4 | | |
| Total coordination | N(Y) = 8 | N(Al) = 6 | N(O1) = 4 | N(O2) = 5 |
| Site multiplicity | w(Y) = 4 | w(Al) = 4 | w(O1) = 4 | w(O2) = 8 |
| Kappa values<br>(from Eqn. (3)) | $K(Y-O1) = 1/4$<br>$K(Y-O2) = 3/4$ | $K(Al-O1) = 1/3$<br>$K(Al-O2) = 2/3$ | $K(O1-Y) = 1/2$<br>$K(O1-Al) = 1/2$ | $K(O2-Y) = 6/5$<br>$K(O2-Al) = 4/5$ |

| Matrix II – source ICSD - 191383 | Y | Al |
|---|---|---|
| O1 | d(Y-O1) = 2.300 Å* | d(Al-O1) = 1.893 Å |
| O2 | d(Y-O2) = 2.444 Å* | d(Al-O2) = 1.913 Å * |
| Bond Valence Paramater | 2.014 | 1.651 |

* Averaged values

The lattice decomposition (Eqn. (2)) gives $YAlO1_1O2_2 = Y_{1/4}O1_{1/2} + Y_{3/4}O2_{6/5} + Al_{1/3}O1_{1/2} + Al_{2/3}O2_{4/5}$. We have: $he(Y) = [N(Y-O1)f_c(Y-O1)\alpha(Y-O1)Q(O1)^2 + N(Y-O2)f_c(Y-O2)\alpha(Y-O2)Q(O2)^2]^{1/2}$ and

$he(Al) = [N(Al-O1)f_c(Al-O1)\alpha(Al-O1)Q(O1)^2 + N(Al-O2)f_c(Al-O2)\alpha(Al-O2)Q(O2)^2]^{1/2}$ . The different steps of the calculation are detailed in Table A6.

Table A6: The step-by-step calculation of *he(Y)* and *he(Al)* in $YAlO_3$

| Compound $YAlO_3$ | Site Y | Compound $YAlO_3$ | Site Al | Eqn. number |
|---|---|---|---|---|
| Q(Y) | 2.895 | Q(Al) | 3.012 | from VESTA |
| Q(O1) | 1.447 | Q(O1) | 2.008 | (5) |
| Q(O2) | 1.809 | Q(O2) | 2.510 | |
| $\Gamma_1(Y-O1)$ | 31.66 | $\Gamma_1(Al-O1)$ | 31.16 | (7) |
| $\Gamma_1(Y-O2)$ | 39.67 | $\Gamma_1(Al-O2)$ | 39.81 | |
| $\Gamma_2(Y-O1)$ | 5.79 | $\Gamma_2(Al-O1)$ | 6.024 | (8) |
| $\Gamma_2(Y-O2)$ | 5.79 | $\Gamma_2(Al-O2)$ | 6.024 | |
| $N^*(Y-O1)$ | 1.447 | $N^*(Al-O1)$ | 2.008 | (10) |
| $N^*(Y-O2)$ | 1.447 | $N^*(Al-O2)$ | 2.008 | |
| $\upsilon(Y-O1)$ | 4.041 | $\upsilon(Al-O1)$ | 2.253 | (11) |
| $\upsilon(Y-O2)$ | 4.848 | $\upsilon(Al-O2)$ | 2.325 | |
| $\Gamma_3(Y-O1)$ | 0.071 | $\Gamma_3(Al-O1)$ | 0.079 | (9) |
| $\Gamma_3(Y-O2)$ | 0.065 | $\Gamma_3(Al-O2)$ | 0.078 | |
| $f_c(Y-O1)$ | 0.130 | $f_c(Al-O1)$ | 0.232 | (6) |
| $f_c(Y-O2)$ | 0.077 | $f_c(Al-O2)$ | 0.153 | |
| $\alpha(Y-O1)$ | 0.440 | $\alpha(Al-O1)$ | 0.315 | (11) |
| $\alpha(Y-O2)$ | 0.416 | $\alpha(Al-O2)$ | 0.271 | |
| $he(Y)$ | 0.932 | $he(Al)$ | 1.278 | (4) |

A.7. β-$NaYF_4$

β-$NaYF_4$ is an important up-conversion crystal when doped with $Er^{3+}$ and $Yb^{3+}$ where the occupancy factor (occ.) of some atoms differs from unity. The corresponding crystal structure is represented in Fig. S7.

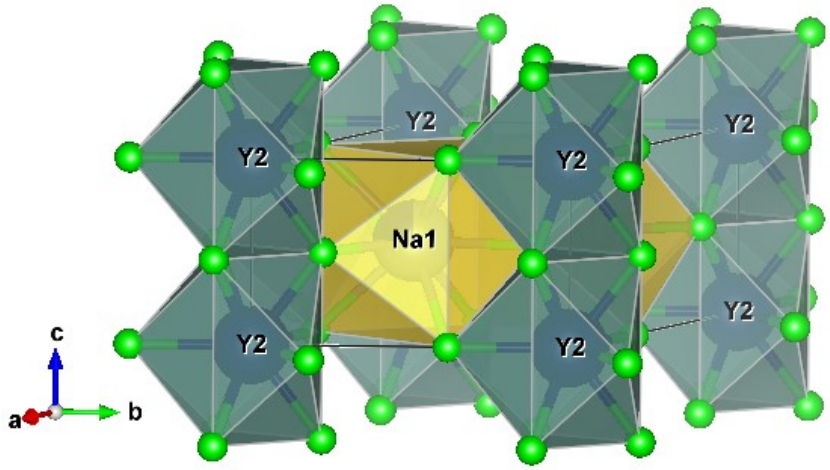


Figure S7. The crystal structure of β-$NaYF_4$. The fluoride atoms appear in green. The Na1 sites are occupied at 25% by Y1 atoms.

The doping sites are (Na1,Y1) and Y2. Matrices I and II for this compound are reproduced below.

| Matrix I – source ICSD - 51917 Space group n°189, V = 105.9 Å$^3$, Z = 1.5 | Na1,Y1 (occ. 0.75,0.25) | Y2 (occ. 1) | F1 (occ. 1) | F2 (occ. 1) |
|---|---|---|---|---|
| Y1,Na1 | | | N(F1-Na1,Y1) = 4 | N(F2-Na1,Y1) = 2 |
| Y2 | | | N(F1-Y2) = 1 | N(F2-Y2) = 2 |

| | | | | |
|---|---|---|---|---|
| Na2 | | | | |
| F1 | N(Na1,Y1-F1) = 6 | N(Y2-F1) = 3 | | |
| F2 | N(Na1,Y1-F2) = 3 | N(Y2-F2) = 6 | | |
| Total coordination | N(Na1,Y1) = 9 | N(Y2) = 9 | N(F1) = 5 | N(F2) = 4 |
| Site multiplicity | w(Na1,Y1) = 2 | w(Y2) = 1 | w(F1) = 3 | w(F2) = 3 |
| Kappa values (from Eqn. (3)) | $K(Na1,Y1-F1) = 2/3$<br>$K(Na1,Y1-F2) = 1/3$ | $K(Y2-F1) = 1/6$<br>$K(Y2-F2) = 1/3$ | $K(F1-Na1,Y1) = 6/5$<br>$K(F1-Y2) = 3/10$ | $K(F2-Na1,Y1) = 3/4$<br>$K(F2-Y2) = 3/4$ |

| Matrix II – source ICSD - 51917 | Na1,Y1 | Y2 |
|---|---|---|
| F1 | d(Na1,Y1-F1) = 2.541 Å | d(Y2-F1) = 2.259 Å |
| F2 | d(Na1,Y1-F2) = 2.366 Å | d(Y2-F2) = 2.190 Å |
| Bond Valence Parameter | 1.734 | 1.904 |

* Averaged values

The compound is written as $(Na1,Y1)_1Y2_{1/2}F1_{3/2}F2_{3/2}$. The lattice decomposition (Eqn. (2)) gives $(Na1,Y1)_1Y2_{1/2}F1_{3/2}F2_{3/2} = (Na1,Y1)_{2/3}F1_{6/5} + (Na1,Y1)_{1/3}F2_{3/4} + Y2_{1/6}F1_{3/10} + Y2_{1/3}F2_{3/4}$.

We have:

$$he(Na1,Y1) = [N(Na1,Y1-F1)f_c(Na1,Y1-F1)\alpha(Na1,Y1-F1)Q(F1)^2 + N(Na1,Y1-F2)f_c(Na1,Y1-F2)\alpha(Na1,Y1-F2)Q(F2)^2]^{1/2}$$

and $he(Y2) = [N(Y2-F1)f_c(Y2-F1)\alpha(Y2-F1)Q(F1)^2 + N(Y2-F2)f_c(Y2-F2)\alpha(Y2-F2)Q(F2)^2]^{1/2}$. The different steps of the calculation are detailed in Table A7.

Table A7: The step-by-step calculation of *he(Na1,Y1)* and *he(Y2)* in $NaYF_4$

| Compound $NaYF_4$ | Site Na1,Y1 | Compound $NaYF_4$ | Site Y2 | Eqn. number |
|---|---|---|---|---|
| Q(Na1,Y1) | 1.220 | Q(Y2) | 3.919 | from VESTA |
| Q(F1) | 0.678 | Q(F1) | 2.177 | (5) |
| Q(F2) | 0.542 | Q(F2) | 1.742 | |
| $\Gamma_1(Na1,Y1-F1)$ | 41.63 | $\Gamma_1(Y2-F1)$ | 46.83 | (7) |
| $\Gamma_1(Na1,Y1-F2)$ | 33.19 | $\Gamma_1(Y2-F2)$ | 35.86 | |
| $\Gamma_2(Na1,Y1-F1)$ | 7.32 | $\Gamma_2(Y2-F1)$ | 23.51 | (8) |
| $\Gamma_2(Na1,Y1-F2)$ | 7.32 | $\Gamma_2(Y2-F2)$ | 23.51 | |
| $N^*(Na1,Y1-F1)$ | 1.084 | $N^*(Y2-F1)$ | 3.483 | (10) |
| $N^*(Na1,Y1-F2)$ | 1.084 | $N^*(Y2-F2)$ | 3.483 | |
| $\upsilon(Na1,Y1-F1)$ | 4.646 | $\upsilon(Y2-F1)$ | 3.265 | (11) |
| $\upsilon(Na1,Y1-F2)$ | 3.751 | $\upsilon(Y2-F2)$ | 2.974 | |
| $\Gamma_3(Na1,Y1-F1)$ | 0.066 | $\Gamma_3(Y2-F1)$ | 0.044 | (9) |
| $\Gamma_3(Na1,Y1-F2)$ | 0.072 | $\Gamma_3(Y2-F2)$ | 0.046 | |
| $f_c(Na1,Y1-F1)$ | 0.037 | $f_c(Y2-F1)$ | 0.011 | (6) |
| $f_c(Na1,Y1-F2)$ | 0.067 | $f_c(Y2-F2)$ | 0.021 | |
| $\alpha(Na1,Y1-F1)$ | 0.226 | $\alpha(Y2-F1)$ | 0.127 | (11) |
| $\alpha(Na1,Y1-F2)$ | 0.257 | $\alpha(Y2-F2)$ | 0.183 | |
| $he(Na1,Y1)$ | 0.195 | $he(Y2)$ | 0.299 | (4) |