

Supporting Information

Structural, thermal and functional properties of a hybrid dicyanamide-perovskite solid solution.

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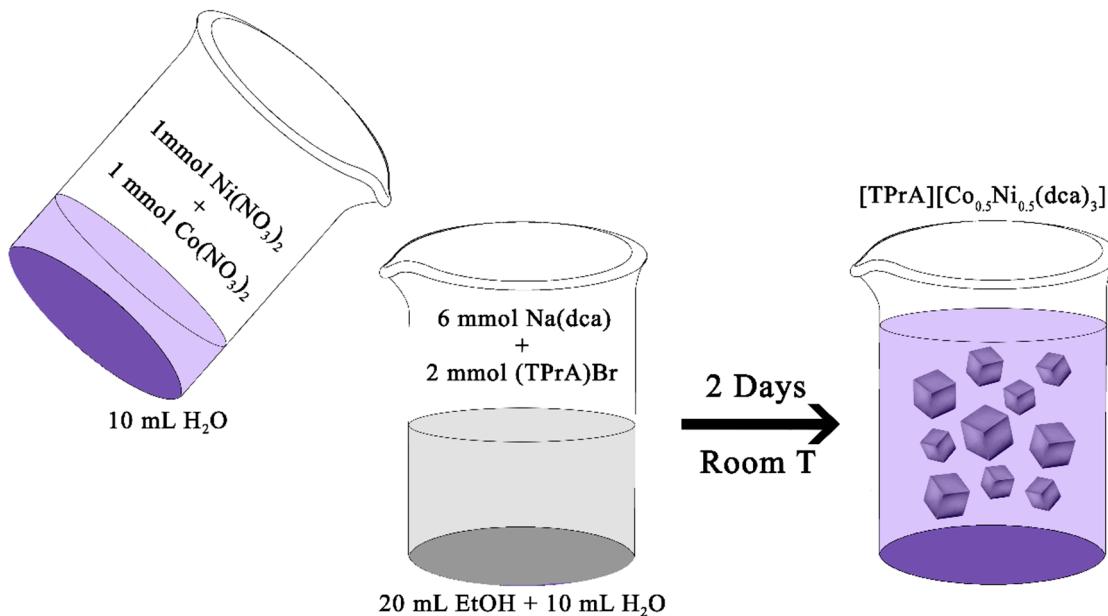
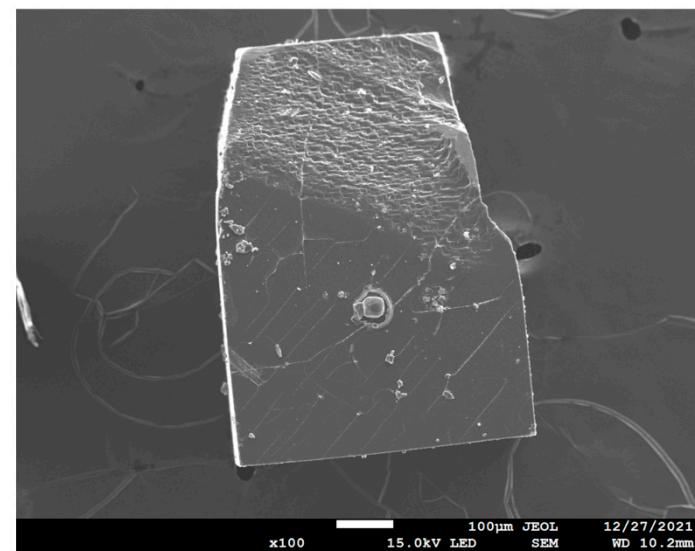
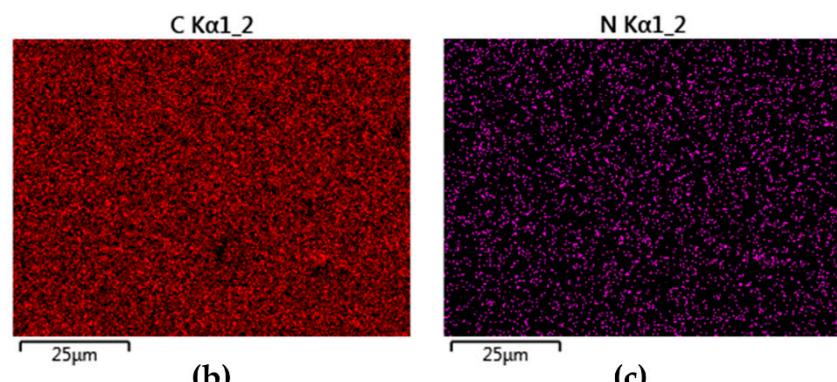


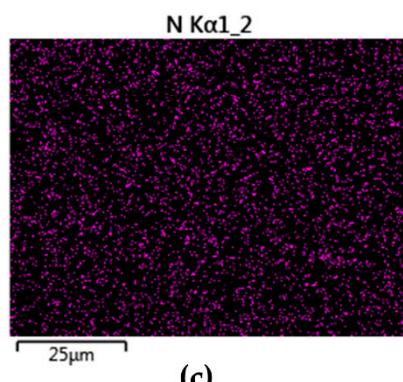
Figure S1. Synthesis scheme of $[TPrA][Co_{0.5}Ni_{0.5}(dca)_3]$ by slow evaporation.



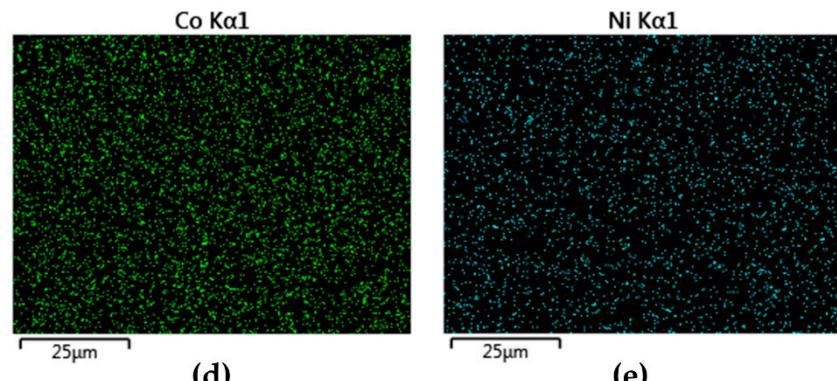
(a)



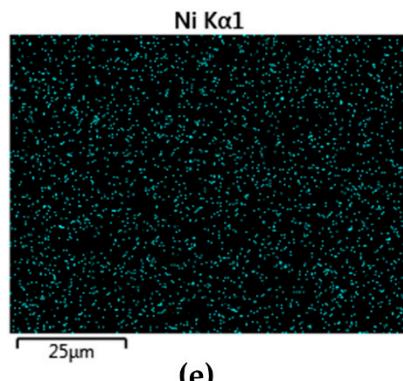
(b)



(c)



(d)



(e)

Figure S2. (a) Scanning Electron Microscopy image of the $[\text{TPrA}][\text{Co}_{0.5}\text{Ni}_{0.5}(\text{dca})_3]$, X-ray map of (b) carbon, (c) nitrogen, (d) cobalt and (e) nickel.

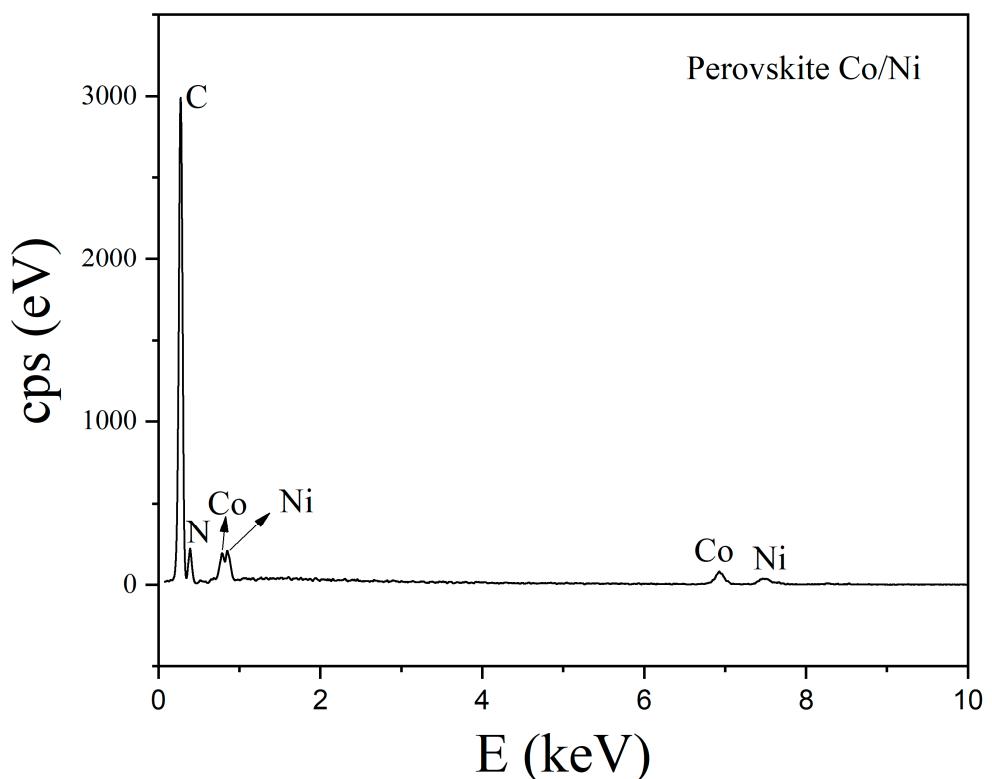


Figure S3. EDS spectrum of the [TPrA][Co_{0.5}Ni_{0.5}(dca)₃].

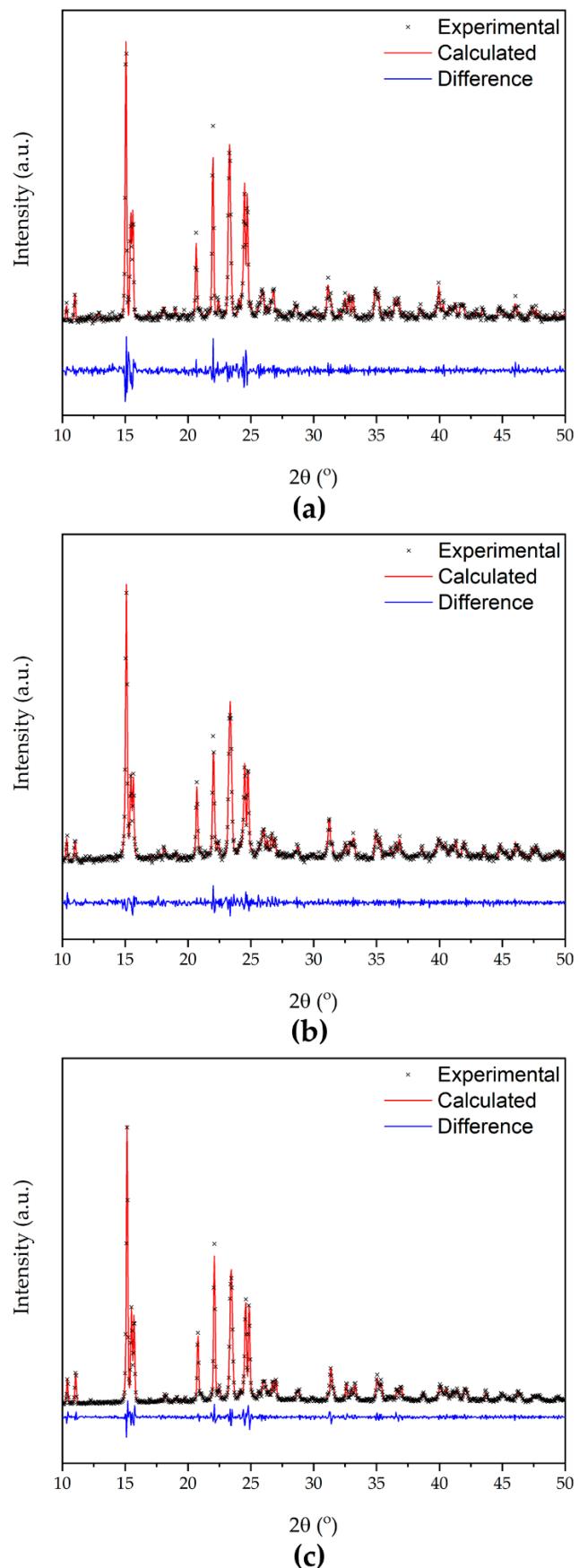


Figure S4. Le Bail refinements of the (a) [TPrA][Co(dca)₃], (b) [TPrA][Co_{0.5}Ni_{0.5}(dca)₃] and (c) [TPrA][Ni(dca)₃].

Table S1. Crystal data and structure refinement for [TPrA][Co_{0.5}Ni_{0.5}(dca)₃].

Empirical formula	C ₃₆ H ₂₈ CoN ₂₀ Ni
Formula weight	73.06
Temperature/K	100
Crystal system	tetragonal
Space group	P-42 ₁ C
a/Å	16.0652(12)
b/Å	16.0652(12)
c/Å	17.0550(12)
α/°	90
β/°	90
γ/°	90
Volume/Å ³	4401.7(7)
Z	4
Q _{calc} g/cm ³	1.295
μ/mm ⁻¹	0.855
F(000)	1756.0
Crystal size/mm ³	0.485 × 0.236 × 0.19
Radiation	MoKα ($\lambda = 0.71073$)
2Θ range for data collection/°	2.388 to 52.766
Index ranges	-20 ≤ h ≤ 20, -20 ≤ k ≤ 18, -21 ≤ l ≤ 21
Reflections collected	65896
Independent reflections	4494 [$R_{\text{int}} = 0.0430$, $R_{\text{sigma}} = 0.0189$]
Data/restraints/parameters	4494/11/285
Goodness-of-fit on F ²	1.337
Final R indexes [I>=2σ (I)]	$R_1 = 0.0750$, $wR_2 = 0.1798$
Final R indexes [all data]	$R_1 = 0.0759$, $wR_2 = 0.1823$
Largest diff. peak/hole / e Å ⁻³	0.69/-1.19
Flack parameter	0.008(4)

Table S2. Bond lengths of M-N.

	Bond length (\AA)
M-N1	2.12 (1)
M-N4	2.12(1)
M-N7	2.13(1)
M-N8	2.07(1)
M-N11	2.12(1)
M-N12	2.06(1)

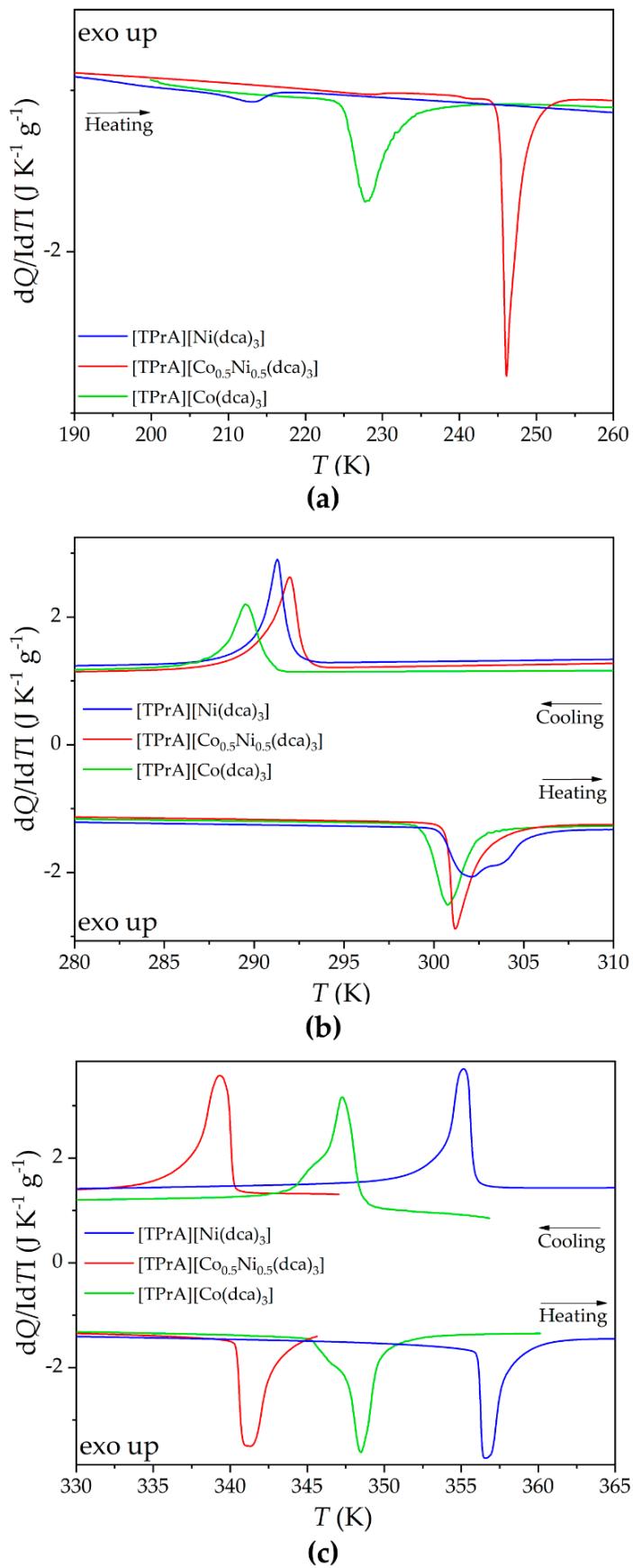


Figure S5. Detail of the DSC of the [TPrA][Co(dca)₃], [TPrA][Co_{0.5}Ni_{0.5}(dca)₃] and [TPrA][Ni(dca)₃] from (a) 200 K to 260 K, (b) 280 K to 310 K and (c) 330 K to 365 K.

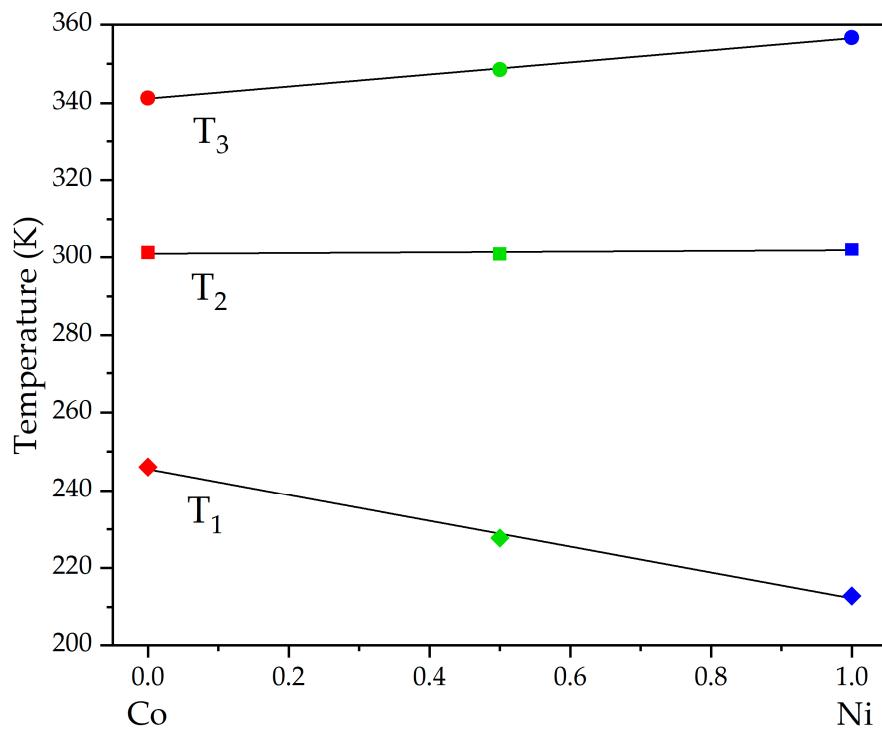


Figure S6. Dependence of the transition temperature observed by DSC (by heating) on the metal proportion, for the samples [TPrA][Co(dca)₃], [TPrA][Co_{0.5}Ni_{0.5}(dca)₃] and [TPrA][Ni(dca)₃].

Table S3. UV-Vis bands of the [TPrA][Co_xNi_{1-x}(dca)₃] ($x = 1.0, 0.5, 0.0$).

Co(II) ground state $^4\text{T}_1(\text{F})$	λ (nm)	
$^4\text{T}_1(\text{P})$	484	Intense and wide band. Overlapping with $^2\text{T}_2(\text{G})$ band
$^2\text{T}_2(\text{G})$	523	Intense and wide band. Overlapping with $^4\text{T}_1(\text{P})$ band
^2E , $^2\text{T}_1(\text{G})$	613	Weak band. Overlapping and partially concealed by previous signals.
Ni(II) ground state $^3\text{A}_{2g}(\text{F})$	λ (nm)	
$^3\text{T}_{1g}(\text{P})$	388 and 458	Intense narrow band with a shoulder (symmetry loss)
$^4\text{T}_{1g}(\text{F})$	635 and 723	Intense wide band with a shoulder (symmetry loss)
Ni(II) + Co(II) solid solution ground states $^4\text{T}_1(\text{F})$ (from Co(II)) and $^3\text{A}_{2g}(\text{F})$ (from Ni(II))	λ (nm)	
$^3\text{T}_{1g}(\text{P})$	388	Intense narrow band
$^4\text{T}_1(\text{P})$	480	Intense and wide band. Overlapping with $^2\text{T}_2(\text{G})$ band
$^2\text{T}_2(\text{G})$	518	Intense and wide band. Overlapping with $^4\text{T}_1(\text{P})$ band
$^4\text{T}_{1g}(\text{F})$	630 and 723	Intense wide band with a shoulder (symmetry loss)

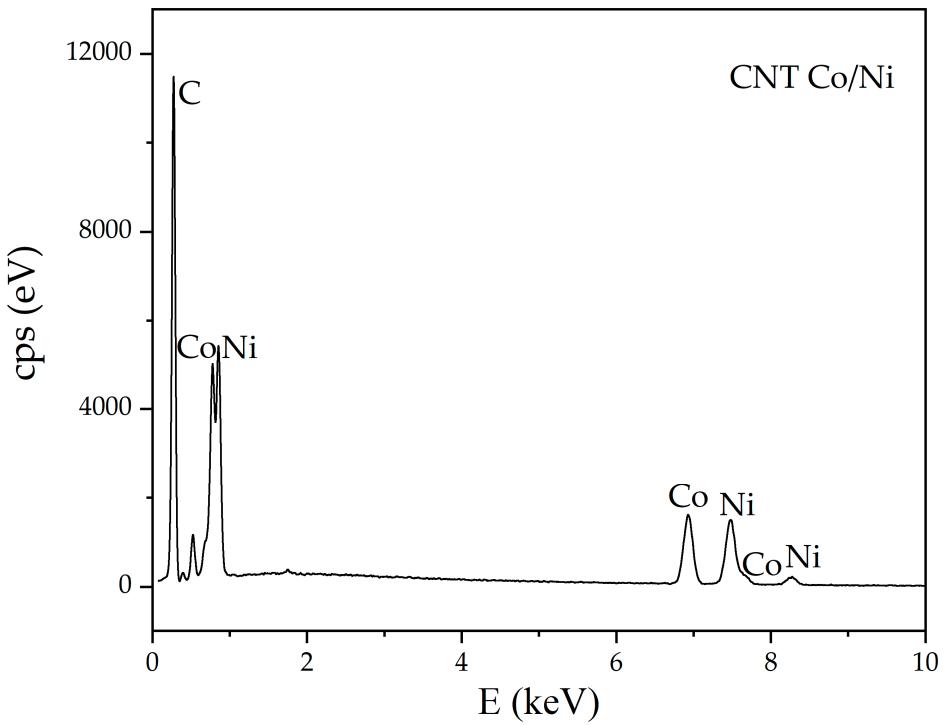


Figure S7. EDS spectrum of the CNTs obtained with the calcination of [TPrA][Co_{0.5}Ni_{0.5}(dca)₃].