Supplementary information

Extended isomerism in heteronuclear metal-organic frameworks: synthetic strategies and crystal structures of lanthanide-cobalt-oxydiacetate systems

Fernando Igoa[a], Agustín López[a], Javier González-Platas[b], Leopoldo Suescun[c], Carlos Kremer[a], Julia Torres[a*]

[a] Área Química Inorgánica, Departamento Estrella Campos (DEC), Facultad de Química, Universidad de la República, Montevideo, Uruguay

[b] Departamento de Física, Instituto Universitario de Estudios Avanzados en Física Atómica, Molecular y Fotónica (IUDEA), MALTA-Cosolider Team, Universidad de La Laguna, Tenerife, Spain

[c] Cryssmat-Lab, DETEMA, Facultad de Química, Universidad de la República, Montevideo, Uruguay

[*]Corresponding author. **jtorres@fq.edu.uy**

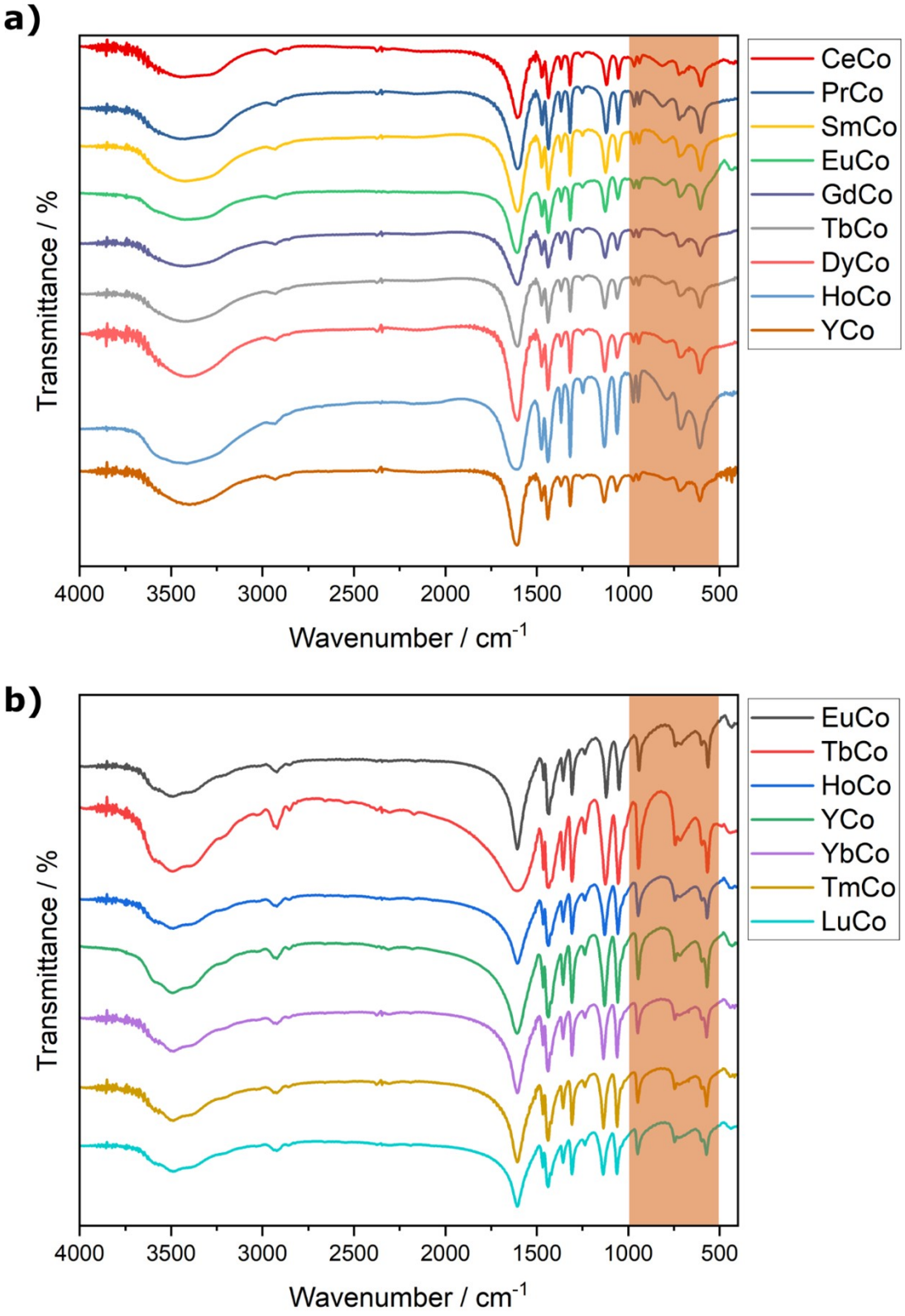

Figure S1 – a) Infrared spectra of the new LnCo compounds showing hexagonal or b) cubic structures. The zone where spectra of both types of compounds show most marked differences is highlighted.

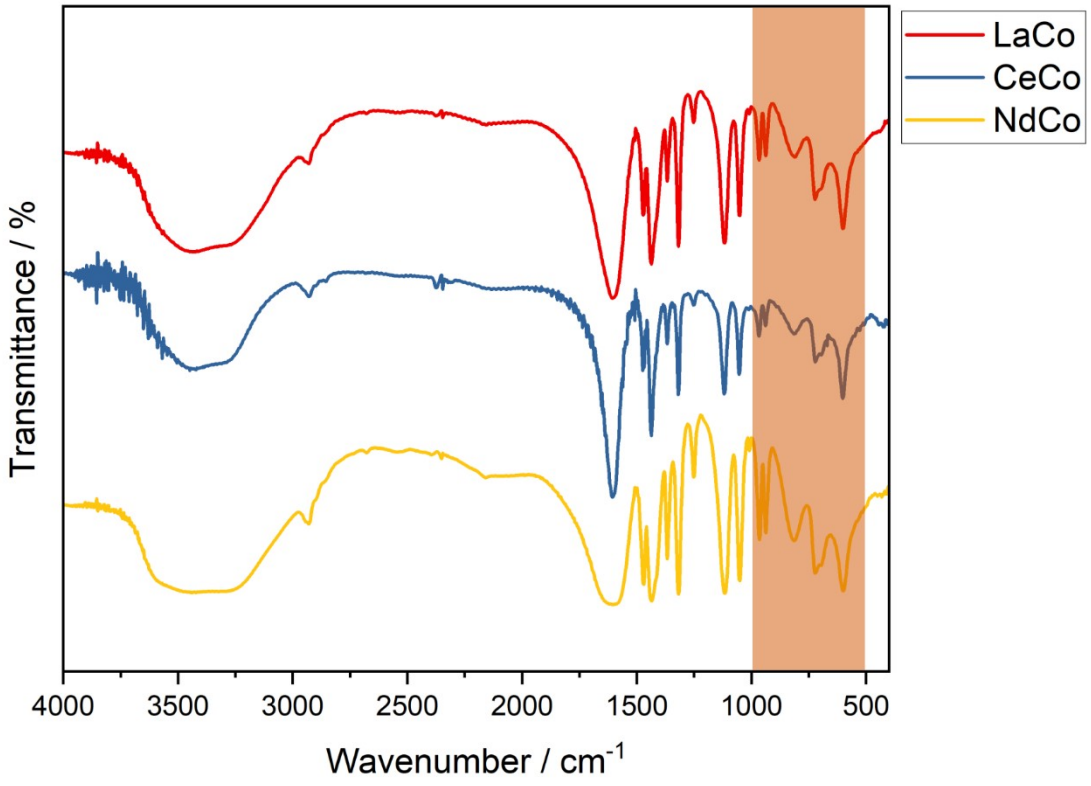

Figure S2 – Infrared spectra of **LaCo^{H}**, **CeCo^{H}** and **NdCo^{H}** prepared following the hydrothermal synthesis (at 180 °C for 3 days).

Table S1 – Numbering scheme for the compounds prepared in this work.

Number	Nomenclature in this work	Comment
1	$LaCo^{H}$	Hexagonal, single crystal structure previously reported in[1]
2	$CeCo^{H}$	Hexagonal, single crystal structure reported in this work
3	$PrCo^{H}$	Hexagonal, single crystal structure reported in this work
4	$NdCo^{H}$	Hexagonal, single crystal structure previously reported in[2]
5	$SmCo^{H}$	Hexagonal, single crystal structure reported in this work
6	$EuCo^{H}$	Hexagonal, single crystal structure reported in this work
7	$GdCo^{H}$	Hexagonal, single crystal structure reported in this work
8	$TbCo^{H}$	Hexagonal, single crystal structure reported in this work
9	$DyCo^{H}$	Hexagonal, single crystal structure reported in this work
10	$HoCo^{H}$	Hexagonal, single crystal structure reported in this work
11	YCo^{H}	Hexagonal, single crystal structure reported in this work
12	$EuCo^{C}$	Cubic, single crystal structure reported in this work
13	$TbCo^{C}$	Cubic, single crystal structure reported in this work
14	$HoCo^{C}$	Cubic, single crystal structure reported in this work
15	YCo^{C}	Cubic, single crystal structure reported in this work
16	$TmCo^{C}$	Cubic, single crystal structure reported in this work
17	$YbCo^{C}$	Cubic, single crystal structure reported in this work
18	$LuCo^{C}$	Cubic, single crystal structure reported in this work

Table S2 – Channel dimensions and water content variation among hexagonal compounds obtained in this work.

Ln	Shannon's radii (Å)[a]	Channel volume (Å^3)[b]	Channel diameter (Å)[c]	Crystallization water content	Coordination water content
La[d]	1.216	1034	9.31	14	6
Ce	1.196	1041	9.33	14	6
Pr	1.179	1041	9.32	14	6
Nd[d]	1.163	1021	9.18	14	6
Sm	1.132	973	8.92	13	6
Eu	1.120	957	8.82	13	6
Gd	1.107	941	8.74	13	6
Tb	1.095	936	8.70	13	6
Dy	1.083	912	8.54	12	6
Y	1.075	905[e]	8.54	12	6
Ho	1.072	913	8.55	12	6

[a]Shannon's ionic radii for coordination number 9.[3] [b]Channel volume calculated from single-crystal data in PLATON software.[4] [c]Channel diameter calculated from modeling the empty volume as a cylinder of base radii equal to the calculated diameter and height *c* (crystallographic edge). [d]Although these compounds were previously reported, they were prepared *de novo* under the same conditions of this work in order to determine the water content from a pure hexagonal sample. [e]Only the major occupied part of the disordered oda ligand was considered for calculating the channel volume in this structure.

References

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