
ANNEX 1

ANÀLISIS ELEMENTALS

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1. Compostos dinuclears $[\text{Ln}(\text{DMF})_4(\text{H}_2\text{O})_3(\mu\text{-CN})\text{M}(\text{CN})_5] \cdot n\text{H}_2\text{O}$

Els percentatges teòrics de C, H i N per als compostos següents han estat calculats a partir de la fórmula empírica $\text{LnMC}_{18}\text{H}_{36}\text{N}_{10}\text{O}_8$ on s'ha considerat una única molècula d'aigua de cristal·lització. En els casos en què ha estat possible resoldre l'estructura del compost per difracció de raigs X de monocristall i aquest no presenta la fórmula empírica anterior, la fórmula empírica emprada s'indica al cosat del compost pertinent.

[LaFe] (Calc.: C 30,22; H 5,07; N 19,58/ Exp.: C 29,97; H 4,99; N 19,56)

[CeFe] (Calc.: C 30,17; H 5,06; N 19,54/ Exp.: C 29,88; H 5,02; N 19,52)

[PrFe] (Calc.: C 30,14; H 5,06; N 19,53/ Exp.: C 30,61; H 5,16; N 19,68)

[NdFe] (Calc.: C 30,00; H 5,04; N 19,44/ Exp.: C 30,08; H 5,04; N 19,72)

[SmFe] (Calc.: C 29,75; H 4,99; N 19,27/ Exp.: C 29,24; H 4,99; N 18,97)

[EuFe] (Calc.: C 29,68; H 4,98; N 19,23/ Exp.: C 29,79; H 5,09; N 19,30)

[GdFe] (Calc.: C 29,47; H 4,95; N 19,09/ Exp.: C 29,66; H 5,06; N 19,26)

[TbFe] (Calc.: C 29,40; H 4,93; N 19,05/ Exp.: C 28,69; H 4,83; N 18,84)

[DyFe] (Calc.: C 29,26; H 4,91; N 18,96/ Exp.: C 29,36; H 4,83; N 18,83)

[HoFe] (Calc.: C 29,16; H 4,89; N 18,89/ Exp.: C 28,91; H 4,83; N 18,64)

[ErFe] (Calc.: C 29,07; H 4,88; N 18,84/ Exp.: C 28,49; H 4,84; N 18,57)

[TmFe] (Calc.: C 28,83; H 4,91; N 18,68/ Exp.: C 28,27; H 4,91; N 18,46)

Fórmula empírica: $\text{TmFeC}_{18}\text{H}_{36,5}\text{N}_{10}\text{O}_{8,25}$

[YbFe] (Calc.: C 28,85; H 4,84; N 18,69/ Exp.: C 28,27; H 4,55; N 18,03)

[CeCo] (Calc.: C 30,04; H 5,04; N 19,46/ Exp.: C 29,43; H 5,10; N 19,21)

[PrCo] (Calc.: C 30,01; H 5,04; N 19,44/ Exp.: C 29,39; H 5,11; N 19,22)

[NdCo] (Calc.: C 29,87; H 5,01; N 19,35/ Exp.: C 29,28; H 4,97; N 19,22)

[SmCo] (Calc.: C 28,91; H 5,12; N 18,73/ Exp.: C 29,11; H 5,09; N 18,92)

Fórmula empírica: SmCoC₁₈H₃₈N₁₀O₉

[EuCo] (Calc.: C 29,56; H 4,96; N 19,15/ Exp.: C 28,55; H 4,79; N 18,73)

[GdCo] (Calc.: C 29,35; H 4,93; N 19,01/ Exp.: C 28,83; H 4,82; N 19,15)

[TbCo] (Calc.: C 29,28; H 4,91; N 18,97/ Exp.: C 29,10; H 4,83; N 19,23)

[DyCo] (Calc.: C 29,14; H 4,89; N 18,88/ Exp.: C 28,63; H 4,78; N 19,12)

[HoCo] (Calc.: C 29,04; H 4,87; N 18,82/ Exp.: C 28,51; H 4,79; N 18,77)

[ErCo] (Calc.: C 28,95; H 4,86; N 18,76/ Exp.: C 28,26; H 4,74; N 18,84)

[TmCo] (Calc.: C 28,89; H 4,85; N 18,72/ Exp.: C 28,29; H 4,68; N 18,91)

[YbCo] (Calc.: C 28,39; H 4,90; N 18,39/ Exp.: C 28,25; H 4,79; N 18,70)

Fórmula empírica: YbCoC₁₈H₃₇N₁₀O_{8,5}

2. Compostos trinuclears *trans*-[Ln(H₂O)₄(bpy)₂]₂(μ-CN)₂M(CN)₄ [M(CN)₆]·8H₂O

Els percentatges teòrics de C, H i N per als compostos següents han estat calculats a partir de la fórmula empírica Ln₂M₂C₅₂H₆₄N₂₀O₁₆.

[La₂Febpy] (Calc.: C 38,68; H 4,00; N 17,35/ Exp.: C 38,5; H 3,9; N 17,3)

[Ce₂Febpy] (Calc.: C 38,62; H 3,99; N 17,32/ Exp.: C 33,7; H 3,8; N 17,2)

[Pr₂Febpy] (Calc.: C 38,58; H 3,98; N 17,31/ Exp.: C 38,7; H 3,7; N 17,8)

[Nd₂Febpy] (Calc.: C 38,42; H 3,97; N 17,24/ Exp.: C 38,2; H 4,1; N 17,1)

[Ce₂Cobpy] (Calc.: C 38,47; H 3,97; N 17,26/ Exp.: C 38,5; H 3,8; N 17,1)

[Pr₂Cobpy] (Calc.: C 38,44; H 3,97; N 17,24/ Exp.: C 38,3; H 4,1; N 17,3)

[Nd₂Cobpy] (Calc.: C 38,28; H 3,95; N 17,17/ Exp.: C 38,4; H 4,1; N 17,1)

[Sm₂Cobpy] (Calc.: C 38,00; H 3,92; N 17,04/ Exp.: C 38,2; H 4,1; N 17,0)

3. Compostos monodimensionals amb 2,2'-bipiridina *trans*- $[\text{Ln}(\text{H}_2\text{O})_4(\text{bpy})(\mu\text{-CN})_2\text{Fe}(\text{CN})_4]_n \cdot 4n\text{H}_2\text{O} \cdot 1,5n\text{bpy}$

Els percentatges teòrics de C, H i N per als compostos següents han estat calculats a partir de la fórmula empírica $\text{Ln}_2\text{M}_2\text{C}_{62}\text{H}_{72}\text{N}_{22}\text{O}_{16}$, excepte per al compost $[\text{SmFebpy}]_n$ que presenta una molècula d'aigua de cristal·lització més que la resta i la seva fórmula empírica és $\text{Sm}_2\text{Fe}_2\text{C}_{62}\text{H}_{76}\text{N}_{22}\text{O}_{18}$.

$[\text{SmFebpy}]_n$ (Calc.: C 40,70; H 4,19; N 16,84/ Exp.: C 40,9; H 4,0; N 17,0)

$[\text{EuFebpy}]_n$ (Calc.: C 41,44; H 4,04; N 17,15/ Exp.: C 41,5; H 4,0; N 17,2)

$[\text{GdFebpy}]_n$ (Calc.: C 41,20; H 4,01; N 17,05/ Exp.: C 41,1; H 3,9; N 17,2)

$[\text{TbFebpy}]_n$ (Calc.: C 41,12; H 4,00; N 17,02/ Exp.: C 41,0; H 3,9; N 17,2)

$[\text{DyFebpy}]_n$ (Calc.: C 40,96; H 3,99; N 16,95/ Exp.: C 41,1; H 3,9; N 17,0)

$[\text{HoFebpy}]_n$ (Calc.: C 40,85; H 3,98; N 16,90/ Exp.: C 40,9; H 4,1; N 17,1)

$[\text{ErFebpy}]_n$ (Calc.: C 40,74; H 3,97; N 16,86/ Exp.: C 40,8; H 3,9; N 17,2)

$[\text{TmFebpy}]_n$ (Calc.: C 40,67; H 3,96; N 16,83/ Exp.: C 40,6; H 3,9; N 16,8)

$[\text{YbFebpy}]_n$ (Calc.: C 40,49; H 3,95; N 16,75/ Exp.: C 40,6; H 3,9; N 16,9)

$[\text{LuFebpy}]_n$ (Calc.: C 40,40; H 3,94; N 16,72/ Exp.: C 40,2; H 3,8; N 16,6)

$[\text{EuCobpy}]_n$ (Calc.: C 41,30; H 4,02; N 17,09/ Exp.: C 41,2; H 4,2; N 17,0)

$[\text{GdCobpy}]_n$ (Calc.: C 41,06; H 4,00; N 16,99/ Exp.: C 41,3; H 4,0; N 17,1)

$[\text{TbCobpy}]_n$ (Calc.: C 40,98; H 3,99; N 16,95/ Exp.: C 41,0; H 3,9; N 17,0)

$[\text{DyCobpy}]_n$ (Calc.: C 40,82; H 3,98; N 16,90/ Exp.: C 40,9; H 4,1; N 17,0)

$[\text{HoCobpy}]_n$ (Calc.: C 40,71; H 3,96; N 16,85/ Exp.: C 40,8; H 4,1; N 16,9)

$[\text{ErCobpy}]_n$ (Calc.: C 40,60; H 3,96; N 16,80/ Exp.: C 40,7; H 4,0; N 16,7)

$[\text{TmCobpy}]_n$ (Calc.: C 40,53; H 3,95; N 16,77/ Exp.: C 40,6; H 3,9; N 16,7)

$[\text{YbCobpy}]_n$ (Calc.: C 40,35; H 3,93; N 16,70/ Exp.: C 40,2; H 3,8; N 16,8)

$[\text{GdCr bpy}]_n$ (Calc.: C 41,37; H 4,03; N 17,12/ Exp.: C 41,2; H 4,0; N 17,3)

**4. Compostos monodimensionals amb 2,2':6',2''-terpiridina *trans*-
[Ln(H₂O)₄(terpy)(μ-CN)₂M(CN)₄]_n**

Els percentatges teòrics de C, H i N per als compostos següents han estat calculats a partir de la fórmula empírica Ln₂M₂C₄₂H₃₈N₁₈O₈.

[SmFeterpy]_n (Calc.: C 40,70; H 4,19; N 16,84/ Exp.: C 40,9; H 4,0; N 17,0)

[SmCoterpy]_n (Calc.: C 41,44; H 4,04; N 17,15/ Exp.: C 41,5; H 4,0; N 17,2)

[LaFeterpy]_n (Calc.: C 41,20; H 4,01; N 17,05/ Exp.: C 41,1; H 3,9; N 17,2)

**5. Compost monodimensional amb 1,10-fenantrolina *trans*-
[Ce(H₂O)(phen)₃(μ-CN)₂Fe(CN)₄]_n·15nH₂O**

Els percentatges teòrics de C, H i N per als compostos següents han estat calculats a partir de la fórmula empírica Ce₂Fe₂C₈₄H₈₂N₂₄O₁₇.

[CeFephen]_n (Calc.: C 48,24; H 3,95; N 16,07/ Exp.: C 46,7; H 3,7; N 15,7)

**6. Compostos monodimensionals amb N,N'-dimetilformamida *cis*-
[Ln(DMF)₄(H₂O)₂(μ-CN)₂Cr(CN)₄]_n·nH₂O**

Els percentatges teòrics de C, H i N per als compostos següents han estat calculats a partir de la fórmula empírica LnMC₁₈H₃₄N₁₀O₇.

[CeCr]_n (Calc.: C 31,12; H 4,93; N 20,16/ Exp.: C 30,2; H 4,3; N 19,7)

[GdCr]_n (Calc.: C 30,37; H 4,81; N 19,68/ Exp.: C 29,1; H 5,0; N 19,5)

[YbCr]_n (Calc.: C 29,71; H 4,71; N 19,25/ Exp.: C 29,0; H 4,4; N 18,4)

7. Compost tipus *clúster* [CeMn₈(O)₈(OOCCH₃)₁₂(H₂O)₄]**·2H₂O**

Els percentatges teòrics de C i H per al compost següent han estat calculats a partir de la fórmula empírica CeMn₈C₂₄H₄₈O₃₈.

[CeMn₈] (Calc.: C 18,91; H 3,17/ Exp.: C 18,0; H 3,26)

8. Compostos triangulars de crom(III)

Els percentatges teòrics de C, H, N i S han estat calculats a partir de la fórmula empírica Cr₃C₄₆H₄₅N₂O₂₀ per al compost [Cr₃O] i Cr₃C₄₁H₃₆N₇O₇S₃ per al compost [Cr₃Obpy].

[Cr₃O] (Calc.: C 50,14; H 4,12; N 2,54/ Exp.: C 50,0; H 3,8; N 1,4)

[Cr₃Obpy] (Calc.: C 49,69; H 3,66; N 9,89; S 9,71/ Exp.: C 50,1; H 3,7; N 9,8; S 8,2)

ANNEX 2

DADES ESTRUCTURALS

Taula A2. 1. Distàncies i angles d'enllaç per al compost $[\text{Ce}^{\text{IV}}\text{Mn}^{\text{III}}_8(\text{O})_8(\text{OOCCH}_3)_{12}(\text{H}_2\text{O})_4]\cdot 2\text{H}_2\text{O}$

Ce-O(1) #1	2.322 (3)
Ce-O(1)	2.322 (3)
Ce-O(1) #2	2.322 (3)
Ce-O(1) #3	2.322 (3)
Ce-O(2) #2	2.393 (3)
Ce-O(2) #3	2.393 (3)
Ce-O(2) #1	2.393 (3)
Ce-O(2)	2.393 (3)
Ce-Mn(2) #3	3.3183 (11)
Ce-Mn(2) #2	3.3183 (11)
Ce-Mn(2)	3.3183 (11)
Ce-Mn(2) #1	3.3183 (11)
Mn(1)-O(1)	1.832 (3)
Mn(1)-O(2) #2	1.893 (3)
Mn(1)-O(3)	1.982 (4)
Mn(1)-O(8) #2	2.001 (4)
Mn(1)-O(9)	2.175 (4)
Mn(1)-O(5)	2.246 (4)
Mn(1)-Mn(2) #2	3.0241 (15)
Mn(1)-Mn(2)	3.238 (2)
Mn(2)-O(1)	1.844 (3)
Mn(2)-O(2)	1.873 (3)
Mn(2)-O(4)	1.931 (4)
Mn(2)-O(7)	1.958 (4)
Mn(2)-O(6)	2.160 (5)
Mn(2)-O(5) #1	2.305 (4)
Mn(2)-Mn(1) #1	3.0241 (15)
O(2)-Mn(1) #1	1.893 (3)
O(3)-C(1)	1.286 (8)
O(4)-C(1)	1.218 (8)
C(1)-C(2)	1.534 (8)
O(5)-C(3)	1.300 (7)
O(5)-Mn(2) #2	2.305 (4)
O(6)-C(3)	1.239 (7)
C(3)-C(4)	1.471 (8)
O(7)-C(5)	1.210 (8)
O(8)-C(5)	1.285 (8)
O(8)-Mn(1) #1	2.001 (4)
C(5)-C(6)	1.504 (8)
O(1) #1-Ce-O(1)	97.48 (6)
O(1) #1-Ce-O(1) #2	137.71 (16)
O(1)-Ce-O(1) #2	97.48 (5)
O(1) #1-Ce-O(1) #3	97.48 (6)
O(1)-Ce-O(1) #3	137.71 (16)
O(1) #2-Ce-O(1) #3	97.48 (6)
O(1) #1-Ce-O(2) #2	154.78 (11)
O(1)-Ce-O(2) #2	65.72 (11)
O(1) #2-Ce-O(2) #2	65.94 (11)
O(1) #3-Ce-O(2) #2	85.08 (11)
O(1) #1-Ce-O(2) #3	85.08 (11)
O(1)-Ce-O(2) #3	154.78 (11)
O(1) #2-Ce-O(2) #3	65.72 (11)
O(1) #3-Ce-O(2) #3	65.94 (11)
O(2) #2-Ce-O(2) #3	118.34 (9)
O(1) #1-Ce-O(2) #1	65.94 (11)
O(1)-Ce-O(2) #1	85.08 (11)

O(1)#2-Ce-O(2)#1	154.78(11)
O(1)#3-Ce-O(2)#1	65.72(11)
O(2)#2-Ce-O(2)#1	92.91(15)
O(2)#3-Ce-O(2)#1	118.34(9)
O(1)#1-Ce-O(2)	65.72(11)
O(1)-Ce-O(2)	65.94(11)
O(1)#2-Ce-O(2)	85.08(11)
O(1)#3-Ce-O(2)	154.78(11)
O(2)#2-Ce-O(2)	118.34(9)
O(2)#3-Ce-O(2)	92.91(15)
O(2)#1-Ce-O(2)	118.34(9)
O(1)#1-Ce-Mn(2)#3	89.70(8)
O(1)-Ce-Mn(2)#3	169.23(8)
O(1)#2-Ce-Mn(2)#3	82.33(8)
O(1)#3-Ce-Mn(2)#3	32.47(8)
O(2)#2-Ce-Mn(2)#3	104.76(8)
O(2)#3-Ce-Mn(2)#3	33.58(8)
O(2)#1-Ce-Mn(2)#3	90.57(7)
O(2)-Ce-Mn(2)#3	124.63(8)
O(1)#1-Ce-Mn(2)#2	169.23(8)
O(1)-Ce-Mn(2)#2	82.33(8)
O(1)#2-Ce-Mn(2)#2	32.47(8)
O(1)#3-Ce-Mn(2)#2	89.70(8)
O(2)#2-Ce-Mn(2)#2	33.58(8)
O(2)#3-Ce-Mn(2)#2	90.57(7)
O(2)#1-Ce-Mn(2)#2	124.63(8)
O(2)-Ce-Mn(2)#2	104.76(8)
Mn(2)#3-Ce-Mn(2)#2	92.117(6)
O(1)#1-Ce-Mn(2)	82.33(8)
O(1)-Ce-Mn(2)	32.47(8)
O(1)#2-Ce-Mn(2)	89.70(8)
O(1)#3-Ce-Mn(2)	169.23(8)
O(2)#2-Ce-Mn(2)	90.57(7)
O(2)#3-Ce-Mn(2)	124.63(8)
O(2)#1-Ce-Mn(2)	104.76(8)
O(2)-Ce-Mn(2)	33.58(8)
Mn(2)#3-Ce-Mn(2)	157.84(3)
Mn(2)#2-Ce-Mn(2)	92.117(7)
O(1)#1-Ce-Mn(2)#1	32.47(8)
O(1)-Ce-Mn(2)#1	89.70(8)
O(1)#2-Ce-Mn(2)#1	169.23(8)
O(1)#3-Ce-Mn(2)#1	82.33(8)
O(2)#2-Ce-Mn(2)#1	124.63(8)
O(2)#3-Ce-Mn(2)#1	104.76(8)
O(2)#1-Ce-Mn(2)#1	33.58(8)
O(2)-Ce-Mn(2)#1	90.57(7)
Mn(2)#3-Ce-Mn(2)#1	92.117(6)
Mn(2)#2-Ce-Mn(2)#1	157.84(3)
Mn(2)-Ce-Mn(2)#1	92.117(6)
O(1)-Mn(1)-O(2)#2	86.75(13)
O(1)-Mn(1)-O(3)	92.14(18)
O(2)#2-Mn(1)-O(3)	173.96(18)
O(1)-Mn(1)-O(8)#2	176.66(17)
O(2)#2-Mn(1)-O(8)#2	90.07(17)
O(3)-Mn(1)-O(8)#2	91.13(19)
O(1)-Mn(1)-O(9)	94.27(15)
O(2)#2-Mn(1)-O(9)	97.37(16)
O(3)-Mn(1)-O(9)	88.63(19)
O(8)#2-Mn(1)-O(9)	85.13(17)
O(1)-Mn(1)-O(5)	96.04(14)
O(2)#2-Mn(1)-O(5)	84.10(14)

O(3)-Mn(1)-O(5)	90.12(17)
O(8)#2-Mn(1)-O(5)	84.62(16)
O(9)-Mn(1)-O(5)	169.65(14)
O(1)-Mn(1)-Mn(2)#2	99.59(11)
O(2)#2-Mn(1)-Mn(2)#2	36.35(10)
O(3)-Mn(1)-Mn(2)#2	138.40(14)
O(8)#2-Mn(1)-Mn(2)#2	78.36(14)
O(9)-Mn(1)-Mn(2)#2	129.52(13)
O(5)-Mn(1)-Mn(2)#2	49.21(10)
O(1)-Mn(1)-Mn(2)	28.36(10)
O(2)#2-Mn(1)-Mn(2)	103.32(11)
O(3)-Mn(1)-Mn(2)	73.39(15)
O(8)#2-Mn(1)-Mn(2)	154.26(13)
O(9)-Mn(1)-Mn(2)	114.20(12)
O(5)-Mn(1)-Mn(2)	75.19(10)
Mn(2)#2-Mn(1)-Mn(2)	99.42(5)
O(1)-Mn(1)-Ce	42.16(11)
O(2)#2-Mn(1)-Ce	44.84(10)
O(3)-Mn(1)-Ce	133.24(15)
O(8)#2-Mn(1)-Ce	134.76(13)
O(9)-Mn(1)-Ce	101.66(12)
O(5)-Mn(1)-Ce	86.64(10)
Mn(2)#2-Mn(1)-Ce	62.77(3)
Mn(2)-Mn(1)-Ce	60.69(3)
O(1)-Mn(2)-O(2)	87.34(14)
O(1)-Mn(2)-O(4)	92.09(16)
O(2)-Mn(2)-O(4)	178.42(17)
O(1)-Mn(2)-O(7)	171.82(18)
O(2)-Mn(2)-O(7)	90.62(17)
O(4)-Mn(2)-O(7)	89.74(18)
O(1)-Mn(2)-O(6)	102.09(15)
O(2)-Mn(2)-O(6)	92.46(16)
O(4)-Mn(2)-O(6)	89.10(18)
O(7)-Mn(2)-O(6)	85.91(18)
O(1)-Mn(2)-O(5)#1	86.97(13)
O(2)-Mn(2)-O(5)#1	82.91(13)
O(4)-Mn(2)-O(5)#1	95.59(17)
O(7)-Mn(2)-O(5)#1	84.91(17)
O(6)-Mn(2)-O(5)#1	169.66(14)
O(1)-Mn(2)-Mn(1)#1	94.73(11)
O(2)-Mn(2)-Mn(1)#1	36.81(10)
O(4)-Mn(2)-Mn(1)#1	141.85(14)
O(7)-Mn(2)-Mn(1)#1	78.99(14)
O(6)-Mn(2)-Mn(1)#1	125.68(13)
O(5)#1-Mn(2)-Mn(1)#1	47.53(9)
O(1)-Mn(2)-Mn(1)	28.16(10)
O(2)-Mn(2)-Mn(1)	103.41(11)
O(4)-Mn(2)-Mn(1)	76.65(13)
O(7)-Mn(2)-Mn(1)	159.29(15)
O(6)-Mn(2)-Mn(1)	78.44(12)
O(5)#1-Mn(2)-Mn(1)	111.59(9)
Mn(1)#1-Mn(2)-Mn(1)	121.24(4)
O(1)-Mn(2)-Ce	42.53(10)
O(2)-Mn(2)-Ce	44.96(11)
O(4)-Mn(2)-Ce	134.56(13)
O(7)-Mn(2)-Ce	135.45(14)
O(6)-Mn(2)-Ce	97.32(12)
O(5)#1-Mn(2)-Ce	85.95(9)
Mn(1)#1-Mn(2)-Ce	63.10(3)
Mn(1)-Mn(2)-Ce	60.991(19)
Mn(1)-O(1)-Mn(2)	123.48(18)

Mn(1)-O(1)-Ce	105.86(16)
Mn(2)-O(1)-Ce	105.01(14)
Mn(2)-O(2)-Mn(1)#1	106.84(15)
Mn(2)-O(2)-Ce	101.46(14)
Mn(1)#1-O(2)-Ce	101.24(14)
C(1)-O(3)-Mn(1)	130.8(5)
C(1)-O(4)-Mn(2)	130.6(5)
O(4)-C(1)-O(3)	127.0(7)
O(4)-C(1)-C(2)	119.3(8)
O(3)-C(1)-C(2)	113.6(7)
C(3)-O(5)-Mn(1)	128.3(4)
C(3)-O(5)-Mn(2)#2	123.4(3)
Mn(1)-O(5)-Mn(2)#2	83.26(12)
C(3)-O(6)-Mn(2)	128.3(5)
O(6)-C(3)-O(5)	126.4(6)
O(6)-C(3)-C(4)	119.0(6)
O(5)-C(3)-C(4)	114.6(7)
C(5)-O(7)-Mn(2)	128.3(5)
C(5)-O(8)-Mn(1)#1	125.4(5)
O(7)-C(5)-O(8)	128.5(7)
O(7)-C(5)-C(6)	119.1(7)
O(8)-C(5)-C(6)	112.4(7)

Symmetry transformations used to generate equivalent atoms:
#1 $y, -x+2, -z$ #2 $-y+2, x, -z$ #3 $-x+2, -y+2, z$

Taula A2. 2. Distàncies i angles d'enllaç per al compost $[\text{Cr}_3(\mu_3\text{-O})(\mu_2\text{-PhCOO})_6(\text{H}_2\text{O})_3](\text{NO}_3)\cdot\text{CH}_3\text{CH}_2\text{OH}\cdot\text{CH}_3\text{CN}$.

Cr(1)-O(1)	1.8925(18)	C(9)-C(14)	1.367(7)
Cr(1)-O(3)	1.959(3)	C(9)-C(10)	1.378(7)
Cr(1)-O(2)	1.967(3)	C(10)-C(11)	1.395(8)
Cr(1)-O(6)	1.975(3)	C(10)-H(10A)	0.9500
Cr(1)-O(5)#1	1.977(3)	C(11)-C(12)	1.326(10)
Cr(1)-O(8)	2.047(3)	C(11)-H(11A)	0.9500
Cr(2)-O(1)	1.903(3)	C(12)-C(13)	1.399(10)
Cr(2)-O(9)	1.955(3)	C(12)-H(12A)	0.9500
Cr(2)-O(9)#1	1.955(3)	C(13)-C(14)	1.392(8)
Cr(2)-O(4)	1.977(3)	C(13)-H(13A)	0.9500
Cr(2)-O(4)#1	1.977(3)	C(14)-H(14A)	0.9500
Cr(2)-O(7)	2.025(4)	C(15)-C(16)	1.489(6)
O(1)-Cr(1)#1	1.8925(18)	C(16)-C(17)	1.342(8)
O(2)-C(1)	1.251(5)	C(16)-C(21)	1.379(9)
O(3)-C(8)	1.256(5)	C(17)-C(18)	1.401(8)
O(4)-C(8)	1.249(5)	C(17)-H(17A)	0.9500
O(5)-C(15)	1.239(6)	C(18)-C(19)	1.326(13)
O(5)-Cr(1)#1	1.977(3)	C(18)-H(18A)	0.9500
O(6)-C(15)	1.247(6)	C(19)-C(20)	1.379(14)
O(7)-H(7B)	1.11(4)	C(19)-H(19A)	0.9500
O(9)-C(1)	1.256(5)	C(20)-C(21)	1.391(9)
C(1)-C(2)	1.484(6)	C(20)-H(20A)	0.9500
C(2)-C(7)	1.381(7)	C(21)-H(21A)	0.9500
C(2)-C(3)	1.393(6)	O(1X)-C(3S)	1.46(2)
C(3)-C(4)	1.371(7)	O(1Y)-C(4Y)	1.21(4)
C(3)-H(3A)	0.9500	O(1Y)-O(4S)	1.23(8)
C(4)-C(5)	1.356(8)	O(1Y)-H(4C)	1.02(7)
C(4)-H(4A)	0.9500	O(1Y)-H(4D)	1.26(10)
C(5)-C(6)	1.383(9)	O(3X)-N(2S)	1.178(15)
C(5)-H(5B)	0.9500	O(3Y)-N(2S)	1.41(3)
C(6)-C(7)	1.384(8)	O(2S)-N(2S)	1.227(8)
C(6)-H(6A)	0.9500	O(4S)-C(4Y)	1.09(5)
C(7)-H(7A)	0.9500	O(4S)-H(4C)	0.96(5)
C(8)-C(9)	1.483(6)	O(4S)-H(4D)	1.11(7)

N(2S)-O(3X)#2	1.178(15)	O(4)-Cr(2)-O(4)#1	172.50(18)
N(2S)-O(3Y)#2	1.41(3)	O(1)-Cr(2)-O(7)	180.000(1)
C(3S)-C(4X)	1.64(2)	O(9)-Cr(2)-O(7)	84.15(8)
C(3S)-H(3SA)	0.9900	O(9)#1-Cr(2)-O(7)	84.15(8)
C(3S)-H(3SB)	0.9900	O(4)-Cr(2)-O(7)	86.25(9)
C(4Y)-H(4C)	1.50(5)	O(4)#1-Cr(2)-O(7)	86.25(9)
N(1S)-C(1S)	1.02(3)	Cr(1)#1-O(1)-Cr(1)	120.00(18)
N(1S)-C(2S)	1.96(2)	Cr(1)#1-O(1)-Cr(2)	120.00(9)
C(1S)-C(2S)	1.16(2)	Cr(1)-O(1)-Cr(2)	120.00(9)
C(2S)-H(2SB)	0.9800	C(1)-O(2)-Cr(1)	132.5(3)
C(2S)-H(2SC)	0.9800	C(8)-O(3)-Cr(1)	134.0(3)
C(2S)-H(2SD)	0.9800	C(8)-O(4)-Cr(2)	131.8(3)
		C(15)-O(5)-Cr(1)#1	132.1(3)
O(1)-Cr(1)-O(3)	94.01(10)	C(15)-O(6)-Cr(1)	133.0(3)
O(1)-Cr(1)-O(2)	94.61(10)	Cr(2)-O(7)-H(7B)	135(2)
O(3)-Cr(1)-O(2)	94.41(13)	C(1)-O(9)-Cr(2)	133.5(3)
O(1)-Cr(1)-O(6)	95.43(12)	O(2)-C(1)-O(9)	124.5(4)
O(3)-Cr(1)-O(6)	88.08(13)	O(2)-C(1)-C(2)	117.9(4)
O(2)-Cr(1)-O(6)	169.46(13)	O(9)-C(1)-C(2)	117.5(4)
O(1)-Cr(1)-O(5)#1	95.50(12)	C(7)-C(2)-C(3)	118.9(4)
O(3)-Cr(1)-O(5)#1	170.39(13)	C(7)-C(2)-C(1)	120.2(4)
O(2)-Cr(1)-O(5)#1	86.24(14)	C(3)-C(2)-C(1)	120.9(4)
O(6)-Cr(1)-O(5)#1	89.62(15)	C(4)-C(3)-C(2)	120.5(5)
O(1)-Cr(1)-O(8)	177.57(14)	C(4)-C(3)-H(3A)	119.8
O(3)-Cr(1)-O(8)	84.31(13)	C(2)-C(3)-H(3A)	119.8
O(2)-Cr(1)-O(8)	83.78(14)	C(5)-C(4)-C(3)	120.0(5)
O(6)-Cr(1)-O(8)	86.28(14)	C(5)-C(4)-H(4A)	120.0
O(5)#1-Cr(1)-O(8)	86.23(14)	C(3)-C(4)-H(4A)	120.0
O(1)-Cr(2)-O(9)	95.85(8)	C(4)-C(5)-C(6)	121.0(6)
O(1)-Cr(2)-O(9)#1	95.85(8)	C(4)-C(5)-H(5B)	119.5
O(9)-Cr(2)-O(9)#1	168.30(17)	C(6)-C(5)-H(5B)	119.5
O(1)-Cr(2)-O(4)	93.75(9)	C(5)-C(6)-C(7)	119.2(7)
O(9)-Cr(2)-O(4)	91.67(15)	C(5)-C(6)-H(6A)	120.4
O(9)#1-Cr(2)-O(4)	87.56(14)	C(7)-C(6)-H(6A)	120.4
O(1)-Cr(2)-O(4)#1	93.75(9)	C(2)-C(7)-C(6)	120.3(5)
O(9)-Cr(2)-O(4)#1	87.56(14)		
O(9)#1-Cr(2)-O(4)#1	91.67(15)		

C(2)-C(7)-H(7A)	119.8	C(17)-C(18)-H(18A)	119.9
C(6)-C(7)-H(7A)	119.8	C(18)-C(19)-C(20)	120.6(7)
O(4)-C(8)-O(3)	125.3(4)	C(18)-C(19)-H(19A)	119.7
O(4)-C(8)-C(9)	117.3(4)	C(20)-C(19)-H(19A)	119.7
O(3)-C(8)-C(9)	117.3(4)	C(19)-C(20)-C(21)	118.7(9)
C(14)-C(9)-C(10)	118.9(5)	C(19)-C(20)-H(20A)	120.6
C(14)-C(9)-C(8)	120.7(5)	C(21)-C(20)-H(20A)	120.6
C(10)-C(9)-C(8)	120.4(4)	C(16)-C(21)-C(20)	120.6(8)
C(9)-C(10)-C(11)	120.1(6)	C(16)-C(21)-H(21A)	119.7
C(9)-C(10)-H(10A)	120.0	C(20)-C(21)-H(21A)	119.7
C(11)-C(10)-H(10A)	120.0	C(4Y)-O(1Y)-O(4S)	53(2)
C(12)-C(11)-C(10)	121.7(6)	C(4Y)-O(1Y)-H(4C)	84(3)
C(12)-C(11)-H(11A)	119.1	O(4S)-O(1Y)-H(4C)	49(4)
C(10)-C(11)-H(11A)	119.1	C(4Y)-O(1Y)-H(4D)	90(5)
C(11)-C(12)-C(13)	118.7(6)	O(4S)-O(1Y)-H(4D)	53(5)
C(11)-C(12)-H(12A)	120.6	H(4C)-O(1Y)-H(4D)	83(7)
C(13)-C(12)-H(12A)	120.6	C(4Y)-O(4S)-O(1Y)	62(4)
C(14)-C(13)-C(12)	120.2(6)	C(4Y)-O(4S)-H(4C)	94(6)
C(14)-C(13)-H(13A)	119.9	O(1Y)-O(4S)-H(4C)	54(5)
C(12)-C(13)-H(13A)	119.9	C(4Y)-O(4S)-H(4D)	105(5)
C(9)-C(14)-C(13)	120.2(6)	O(1Y)-O(4S)-H(4D)	65(5)
C(9)-C(14)-H(14A)	119.9	H(4C)-O(4S)-H(4D)	94(5)
C(13)-C(14)-H(14A)	119.9	O(3X)-N(2S)-O(3X)#2	119.0(16)
O(5)-C(15)-O(6)	126.0(4)	O(3X)-N(2S)-O(2S)	120.5(8)
O(5)-C(15)-C(16)	117.8(5)	O(3X)#2-N(2S)-O(2S)	120.5(8)
O(6)-C(15)-C(16)	116.1(4)	O(3X)-N(2S)-O(3Y)	35.8(10)
C(17)-C(16)-C(21)	118.8(5)	O(3X)#2-N(2S)-O(3Y)	113.5(11)
C(17)-C(16)-C(15)	122.6(5)	O(2S)-N(2S)-O(3Y)	114.0(9)
C(21)-C(16)-C(15)	118.7(5)	O(3X)-N(2S)-O(3Y)#2	113.5(11)
C(16)-C(17)-C(18)	120.8(7)	O(3X)#2-N(2S)-O(3Y)#2	35.8(10)
C(16)-C(17)-H(17A)	119.6	O(2S)-N(2S)-O(3Y)#2	114.0(9)
C(18)-C(17)-H(17A)	119.6	O(3Y)-N(2S)-O(3Y)#2	132.0(18)
C(19)-C(18)-C(17)	120.3(7)	O(1X)-C(3S)-C(4X)	108.5(14)
C(19)-C(18)-H(18A)	119.9	O(1X)-C(3S)-H(3SA)	110.0

C(4X)-C(3S)-H(3SA)	110.0	C(1S)-C(2S)-N(1S)	24.6(15)
O(1X)-C(3S)-H(3SB)	110.0	C(1S)-C(2S)-H(2SB)	109.5
C(4X)-C(3S)-H(3SB)	110.0	N(1S)-C(2S)-H(2SB)	127.6
H(3SA)-C(3S)-H(3SB)	108.4	C(1S)-C(2S)-H(2SC)	109.5
O(4S)-C(4Y)-O(1Y)	65(5)	N(1S)-C(2S)-H(2SC)	111.2
O(4S)-C(4Y)-H(4C)	40(3)	H(2SB)-C(2S)-H(2SC)	109.5
O(1Y)-C(4Y)-H(4C)	43(3)	C(1S)-C(2S)-H(2SD)	109.5
C(1S)-N(1S)-C(2S)	28.2(16)	N(1S)-C(2S)-H(2SD)	86.5
N(1S)-C(1S)-C(2S)	127(3)	H(2SB)-C(2S)-H(2SD)	109.5
		H(2SC)-C(2S)-H(2SD)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 $-x+2, y, -z+1/2$ #2 $-x+1, y, -z+1/2$

Taula A2. 3. Distàncies i angles d'enllaç per al compost $[\text{Cr}_3(\mu_3\text{-O})(\mu_2\text{-PhCOO})_2(\mu_2\text{-OCH}_2\text{CH}_3)_2(\text{bpy})_2(\text{NCS})_3]$.

Cr (1) - Cr (2)	2.8832	C (9) - C (10)	1.3750
Cr (1) - Cr (3)	2.8660	C (11) - C (12)	1.5001
Cr (1) - O (1)	1.9220	C (12) - C (13)	1.3947
Cr (1) - O (2)	2.0145	C (12) - C (17)	1.3916
Cr (1) - O (5)	1.9926	C (13) - C (14)	1.3891
Cr (1) - O (6)	1.9643	C (14) - C (15)	1.3667
Cr (1) - O (7)	1.9680	C (15) - C (16)	1.3677
Cr (1) - N (1)	2.0132	C (16) - C (17)	1.3781
Cr (2) - O (1)	1.8953	C (18) - C (19)	1.4473
Cr (2) - O (6)	1.9368	C (211) - C (212)	1.3789
Cr (2) - N (2)	2.0186	C (212) - C (213)	1.3706
Cr (2) - N (21)	2.0647	C (213) - C (214)	1.3675
Cr (2) - N (22)	2.0767	C (214) - C (215)	1.3837
Cr (3) - O (1)	1.9017	C (215) - C (221)	1.4868
Cr (3) - O (4)	1.9881	C (221) - C (222)	1.3703
Cr (3) - O (7)	1.9575	C (222) - C (223)	1.3908
Cr (3) - N (3)	2.0147	C (223) - C (224)	1.3534
Cr (3) - N (31)	2.0634	C (224) - C (225)	1.3716
Cr (3) - N (32)	2.0496	C (311) - C (312)	1.3614
S (1) - C (1)	1.6178	C (312) - C (313)	1.3553
S (2) - C (2)	1.5983	C (313) - C (314)	1.3560
S (3) - C (3)	1.6079	C (314) - C (315)	1.3831
O (2) - C (4)	1.2529	C (315) - C (321)	1.4814
O (3) - C (4)	1.2646	C (321) - C (322)	1.3774
O (4) - C (11)	1.2723	C (322) - C (323)	1.3700
O (5) - C (11)	1.2576	C (323) - C (324)	1.3627
O (7) - C (18)	1.4509	C (324) - C (325)	1.3679
N (1) - C (1)	1.1407		
N (2) - C (2)	1.1659	O (1) - Cr (1) - O (2)	89.26 (15)
N (3) - C (3)	1.1579	O (1) - Cr (1) - O (5)	90.92 (15)
N (21) - C (211)	1.3454	O (1) - Cr (1) - O (6)	80.40 (15)
N (21) - C (215)	1.3438	O (1) - Cr (1) - O (7)	81.99 (15)
N (22) - C (221)	1.3590	O (1) - Cr (1) - N (1)	176.9 (2)
N (22) - C (225)	1.3334	O (2) - Cr (1) - O (5)	78.92 (16)
N (31) - C (311)	1.3380	O (2) - Cr (1) - O (6)	91.11 (16)
N (31) - C (315)	1.3546	O (2) - Cr (1) - O (7)	91.53 (15)
N (32) - C (321)	1.3474	O (2) - Cr (1) - N (1)	88.39 (18)
N (32) - C (325)	1.3384	O (5) - Cr (1) - O (6)	87.87 (16)
C (4) - C (5)	1.5126	O (5) - Cr (1) - O (7)	89.55 (15)
C (5) - C (6)	1.4059	O (5) - Cr (1) - N (1)	91.46 (18)
C (5) - C (10)	1.3712	O (6) - Cr (1) - O (7)	62.15 (15)
C (6) - C (7)	1.3873	O (6) - Cr (1) - N (1)	101.7 (2)
C (7) - C (8)	1.3554	O (7) - Cr (1) - N (1)	96.0 (2)
C (8) - C (9)	1.3805	O (1) - Cr (2) - O (3)	91.50 (16)

O(1)-Cr(2)-O(6)	81.78(15)	O(4)-Cr(3)-O(7)	93.61(15)
O(1)-Cr(2)-N(2)	176.16(19)	O(4)-Cr(3)-N(3)	90.11(17)
O(1)-Cr(2)-N(21)	91.98(17)	O(4)-Cr(3)-N(31)	93.94(17)
O(1)-Cr(2)-N(22)	95.21(17)	O(4)-Cr(3)-N(32)	172.78(17)
O(3)-Cr(2)-O(6)	91.82(18)	O(7)-Cr(3)-N(3)	94.98(17)
O(3)-Cr(2)-N(2)	90.6(2)	O(7)-Cr(3)-N(31)	171.67(18)
O(3)-Cr(2)-N(21)	168.9(2)	O(7)-Cr(3)-N(32)	93.60(17)
O(3)-Cr(2)-N(22)	91.05(19)	N(3)-Cr(3)-N(31)	88.51(19)
O(6)-Cr(2)-N(2)	94.97(19)	N(3)-Cr(3)-N(32)	89.69(19)
O(6)-Cr(2)-N(21)	99.14(18)	N(31)-Cr(3)-N(32)	78.83(19)
O(6)-Cr(2)-N(22)	175.90(18)	Cr(1)-O(1)-Cr(2)	98.10(16)
N(2)-Cr(2)-N(21)	86.5(2)	Cr(1)-O(1)-Cr(3)	97.10(16)
N(2)-Cr(2)-N(22)	87.9(2)	Cr(2)-O(1)-Cr(3)	164.5(2)
N(21)-Cr(2)-N(22)	78.11(19)	Cr(1)-O(2)-C(4)	126.4(4)
O(1)-Cr(3)-O(4)	90.39(15)	Cr(2)-O(3)-C(4)	125.5(4)
O(1)-Cr(3)-O(7)	82.78(15)	Cr(3)-O(4)-C(11)	124.5(4)
O(1)-Cr(3)-N(3)	177.73(18)	Cr(1)-O(5)-C(11)	126.8(4)
O(1)-Cr(3)-N(31)	93.66(17)	Cr(1)-O(6)-Cr(2)	95.30(15)
O(1)-Cr(3)-N(32)	90.09(17)	Cr(1)-O(6)-C(20)	128.2(6)

