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Apêndice

Dados cristalográficos suplementares para $[Cu_2(\mu\text{-}L1)_2(HL1)(ClO_4)_2(OH_2)]\cdot 2H_2O$

Tabela A. Comprimentos de ligação selecionados [Å] para $[Cu_2(\mu\text{-}L1)_2(HL1)(ClO_4)_2(OH_2)]\cdot 2H_2O$

Cu(1)-N(3)	1.925(3)
Cu(1)-O(8)	1.965(2)
Cu(1)-N(27)	1.993(3)
Cu(1)-N(23)	2.011(3)
Cu(1)-O(1W)	2.212(3)
Cu(2)-O(28)	1.924(3)
Cu(2)-O(8)	1.941(3)
Cu(2)-N(43)	2.002(3)
Cu(2)-N(47)	2.051(3)
Cu(2)-O(1P)	2.447(3)
Cu(2)-O(5P)	2.705(5)
Cu(1)-N(3)	1.925(3)
Cu(1)-O(8)	1.965(2)
Cu(1)-N(27)	1.993(3)
Cu(1)-N(23)	2.011(3)
Cu(1)-O(1W)	2.212(3)
Cu(2)-O(28)	1.924(3)
Cu(2)-O(8)	1.941(3)
Cu(2)-N(43)	2.002(3)
Cu(2)-N(47)	2.051(3)
Cu(2)-O(1P)	2.447(3)
Cu(2)-O(5P)	2.705(5)
O(1W)-H(1WA)	0.7435
O(1W)-H(1WB)	0.7819
N(1)-N(2)	1.347(4)
N(1)-C(5)	1.354(4)
N(1)-C(11)	1.437(5)
N(2)-N(3)	1.307(4)
N(3)-C(4)	1.367(4)
C(4)-C(5)	1.373(5)
C(4)-C(6)	1.446(5)
C(5)-H(5)	0.9500

Tabela A. Comprimentos de ligação selecionados [Å] para [Cu_2(*μ-L1*)$_2$(H*L1*)(ClO_4)$_2$(OH_2)]·2H_2O (continuação 1)

C(6)-N(7)	1.285(5)
C(6)-H(6)	0.9500
N(7)-O(8)	1.384(4)
C(11)-C(16)	1.380(5)
C(11)-C(12)	1.390(5)
C(12)-C(13)	1.385(6)
C(12)-H(12)	0.9500
C(13)-C(14)	1.384(6)
C(13)-H(13)	0.9500
C(14)-C(15)	1.382(6)
C(14)-H(14)	0.9500
C(15)-C(16)	1.379(6)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500
N(21)-N(22)	1.347(4)
N(21)-C(25)	1.351(5)
N(21)-C(31)	1.447(5)
N(22)-N(23)	1.304(4)
N(23)-C(24)	1.361(5)
C(24)-C(25)	1.362(5)
C(24)-C(26)	1.445(5)
C(25)-H(25)	0.9500
C(26)-N(27)	1.287(4)
C(26)-H(26)	0.9500
N(27)-O(28)	1.322(4)
C(31)-C(36)	1.381(6)
C(31)-C(32)	1.390(5)
C(32)-C(33)	1.392(6)
C(32)-H(32)	0.9500
C(33)-C(34)	1.369(7)
C(33)-H(33)	0.9500
C(34)-C(35)	1.379(6)
C(34)-H(34)	0.9500
C(35)-C(36)	1.386(6)
C(35)-H(35)	0.9500
C(36)-H(36)	0.9500
N(41)-N(42)	1.342(4)

Tabela A. Comprimentos de ligação selecionados [Å] para [Cu_2(μ-*L1*)$_2$(H*L1*)(ClO_4)$_2$(OH_2)]·2H_2O (continuação 2)

N(41)-C(45)	1.362(5)
N(41)-C(51)	1.438(5)
N(42)-N(43)	1.306(4)
N(43)-C(44)	1.366(5)
C(44)-C(45)	1.355(5)
C(44)-C(46)	1.459(5)
C(45)-H(45)	0.9500
C(46)-N(47)	1.274(5)
C(46)-H(46)	0.9500
N(47)-O(48)	1.374(4)
O(48)-H(48)	0.8475
C(51)-C(56)	1.379(6)
C(51)-C(52)	1.386(6)
C(52)-C(53)	1.379(6)
C(52)-H(52)	0.9500
C(53)-C(54)	1.384(8)
C(53)-H(53)	0.9500
C(54)-C(55)	1.386(8)
C(54)-H(54)	0.9500
C(55)-C(56)	1.400(6)
C(55)-H(55)	0.9500
C(56)-H(56)	0.9500
Cl(1)-O(3P)	1.429(3)
Cl(1)-O(2P)	1.433(3)
Cl(1)-O(4P)	1.438(3)
Cl(1)-O(1P)	1.451(3)
Cl(2)-O(7P)	1.406(4)
Cl(2)-O(5P)	1.417(4)
Cl(2)-O(8P)	1.417(4)
Cl(2)-O(6P)	1.450(4)
O(2W)-H(2WA)	0.9119
O(2W)-H(2WB)	0.8956
O(3W)-H(3WA)	0.9106
O(3W)-H(3WB)	0.8805

Tabela B. Ângulos de ligação selecionados [°] para $[Cu_2(\mu\text{-}L1)_2(HL1)(ClO_4)_2(OH_2)]\cdot 2H_2O$

N(3)-Cu(1)-O(8)	91.58(11)
N(3)-Cu(1)-N(27)	171.59(14)
O(8)-Cu(1)-N(27)	86.55(11)
N(3)-Cu(1)-N(23)	99.00(13)
O(8)-Cu(1)-N(23)	161.55(13)
N(27)-Cu(1)-N(23)	80.78(13)
N(3)-Cu(1)-O(1W)	96.03(13)
O(8)-Cu(1)-O(1W)	97.59(11)
N(27)-Cu(1)-O(1W)	92.34(12)
N(23)-Cu(1)-O(1W)	96.29(12)
O(28)-Cu(2)-O(8)	92.28(11)
O(28)-Cu(2)-N(43)	88.91(12)
O(8)-Cu(2)-N(43)	177.15(13)
O(28)-Cu(2)-N(47)	166.77(13)
O(8)-Cu(2)-N(47)	100.05(12)
N(43)-Cu(2)-N(47)	78.99(12)
O(28)-Cu(2)-O(1P)	92.86(12)
O(8)-Cu(2)-O(1P)	88.45(12)
N(43)-Cu(2)-O(1P)	88.90(12)
N(47)-Cu(2)-O(1P)	92.25(12)
O(28)-Cu(2)-O(5P)	96.85(14)
O(8)-Cu(2)-O(5P)	92.69(15)
N(43)-Cu(2)-O(5P)	89.74(16)
N(47)-Cu(2)-O(5P)	77.93(14)
O(1P)-Cu(2)-O(5P)	170.17(12)
Cu(2)-O(8)-Cu(1)	117.89(12)
N(3)-Cu(1)-O(8)	91.58(11)
N(3)-Cu(1)-N(27)	171.59(14)
O(8)-Cu(1)-N(27)	86.55(11)
N(3)-Cu(1)-N(23)	99.00(13)
O(8)-Cu(1)-N(23)	161.55(13)
N(27)-Cu(1)-N(23)	80.78(13)
N(3)-Cu(1)-O(1W)	96.03(13)
O(8)-Cu(1)-O(1W)	97.59(11)
N(27)-Cu(1)-O(1W)	92.34(12)
N(23)-Cu(1)-O(1W)	96.29(12)
O(28)-Cu(2)-O(8)	92.28(11)

Tabela B. Ângulos de ligação selecionados [°] para $[Cu_2(\mu\text{-}L1)_2(HL1)(ClO_4)_2(OH_2)]\cdot 2H_2O$ (continuação 1)

O(28)-Cu(2)-N(43)	88.91(12)
O(8)-Cu(2)-N(43)	177.15(13)
O(28)-Cu(2)-N(47)	166.77(13)
O(8)-Cu(2)-N(47)	100.05(12)
N(43)-Cu(2)-N(47)	78.99(12)
O(28)-Cu(2)-O(1P)	92.86(12)
O(8)-Cu(2)-O(1P)	88.45(12)
N(43)-Cu(2)-O(1P)	88.90(12)
N(47)-Cu(2)-O(1P)	92.25(12)
O(28)-Cu(2)-O(5P)	96.85(14)
O(8)-Cu(2)-O(5P)	92.69(15)
N(43)-Cu(2)-O(5P)	89.74(16)
N(47)-Cu(2)-O(5P)	77.93(14)
O(1P)-Cu(2)-O(5P)	170.17(12)
Cu(1)-O(1W)-H(1WA)	124.4
Cu(1)-O(1W)-H(1WB)	118.1
H(1WA)-O(1W)-H(1WB)	109.5
N(2)-N(1)-C(5)	111.4(3)
N(2)-N(1)-C(11)	118.7(3)
C(5)-N(1)-C(11)	129.8(3)
N(3)-N(2)-N(1)	106.1(3)
N(2)-N(3)-C(4)	110.7(3)
N(2)-N(3)-Cu(1)	124.6(2)
C(4)-N(3)-Cu(1)	124.7(2)
N(3)-C(4)-C(5)	107.0(3)
N(3)-C(4)-C(6)	123.0(3)
C(5)-C(4)-C(6)	129.7(3)
N(1)-C(5)-C(4)	104.9(3)
N(1)-C(5)-H(5)	127.5
C(4)-C(5)-H(5)	127.5
N(7)-C(6)-C(4)	129.9(3)
N(7)-C(6)-H(6)	115.1
C(4)-C(6)-H(6)	115.1
C(6)-N(7)-O(8)	120.1(3)
N(7)-O(8)-Cu(2)	111.5(2)
N(7)-O(8)-Cu(1)	127.9(2)
Cu(2)-O(8)-Cu(1)	117.89(12)

Tabela B. Ângulos de ligação selecionados [°] para $[Cu_2(\mu\text{-}L1)_2(HL1)(ClO_4)_2(OH_2)]\cdot 2H_2O$ (continuação 2)

C(16)-C(11)-C(12)	121.8(4)
C(16)-C(11)-N(1)	120.3(3)
C(12)-C(11)-N(1)	117.8(3)
C(13)-C(12)-C(11)	118.3(4)
C(13)-C(12)-H(12)	120.8
C(11)-C(12)-H(12)	120.8
C(14)-C(13)-C(12)	120.7(4)
C(14)-C(13)-H(13)	119.7
C(12)-C(13)-H(13)	119.7
C(15)-C(14)-C(13)	119.6(4)
C(15)-C(14)-H(14)	120.2
C(13)-C(14)-H(14)	120.2
C(16)-C(15)-C(14)	121.0(4)
C(16)-C(15)-H(15)	119.5
C(14)-C(15)-H(15)	119.5
C(15)-C(16)-C(11)	118.6(3)
C(15)-C(16)-H(16)	120.7
C(11)-C(16)-H(16)	120.7
N(22)-N(21)-C(25)	111.8(3)
N(22)-N(21)-C(31)	119.8(3)
C(25)-N(21)-C(31)	128.3(3)
N(23)-N(22)-N(21)	105.2(3)
N(22)-N(23)-C(24)	111.1(3)
N(22)-N(23)-Cu(1)	138.1(2)
C(24)-N(23)-Cu(1)	110.8(2)
N(23)-C(24)-C(25)	107.2(3)
N(23)-C(24)-C(26)	117.6(3)
C(25)-C(24)-C(26)	135.1(3)
N(21)-C(25)-C(24)	104.7(3)
C(16)-C(11)-N(1)	120.3(3)
C(12)-C(11)-N(1)	117.8(3)
N(21)-C(25)-H(25)	127.7
C(24)-C(25)-H(25)	127.7
N(27)-C(26)-C(24)	113.7(3)
N(27)-C(26)-H(26)	123.1
C(24)-C(26)-H(26)	123.1
C(26)-N(27)-O(28)	118.6(3)

Tabela B. Ângulos de ligação selecionados [°] para $[Cu_2(\mu\text{-}L1)_2(HL1)(ClO_4)_2(OH_2)]\cdot 2H_2O$ (continuação 3)

C(26)-N(27)-Cu(1)	116.4(3)
O(28)-N(27)-Cu(1)	124.7(2)
N(27)-O(28)-Cu(2)	117.1(2)
C(36)-C(31)-C(32)	121.9(4)
C(36)-C(31)-N(21)	119.4(3)
C(32)-C(31)-N(21)	118.7(4)
C(31)-C(32)-C(33)	118.1(4)
C(31)-C(32)-H(32)	121.0
C(33)-C(32)-H(32)	121.0
C(34)-C(33)-C(32)	120.9(4)
C(34)-C(33)-H(33)	119.6
C(32)-C(33)-H(33)	119.6
C(33)-C(34)-C(35)	119.8(4)
C(33)-C(34)-H(34)	120.1
C(35)-C(34)-H(34)	120.1
C(34)-C(35)-C(36)	121.1(5)
C(34)-C(35)-H(35)	119.4
C(31)-C(36)-C(35)	118.1(4)
C(31)-C(36)-H(36)	120.9
C(35)-C(36)-H(36)	120.9
N(42)-N(41)-C(45)	111.3(3)
N(42)-N(41)-C(51)	119.9(3)
C(45)-N(41)-C(51)	128.7(3)
N(43)-N(42)-N(41)	106.1(3)
N(42)-N(43)-C(44)	110.0(3)
N(42)-N(43)-Cu(2)	136.0(2)
C(44)-N(43)-Cu(2)	114.0(2)
C(45)-C(44)-N(43)	108.0(3)
C(45)-C(44)-N(46)	136.1(4)
C(31)-C(36)-C(35)	118.1(4)
N(43)-C(44)-C(46)	115.9(3)
C(44)-C(45)-N(41)	104.4(3)
C(44)-C(45)-H(45)	127.8
N(41)-C(45)-H(45)	127.8
N(47)-C(46)-C(44)	114.2(3)
N(47)-C(46)-H(46)	122.9

Tabela B. Ângulos de ligação selecionados [°] para $[Cu_2(\mu\text{-}L1)_2(HL1)(ClO_4)_2(OH_2)]\cdot 2H_2O$ (continuação 4)

C(44)-C(46)-H(46)	122.9
C(46)-N(47)-O(48)	115.3(3)
C(46)-N(47)-Cu(2)	117.0(3)
O(48)-N(47)-Cu(2)	127.7(2)
N(47)-O(48)-H(48)	103.2
C(56)-C(51)-C(52)	121.8(4)
C(56)-C(51)-N(41)	118.7(4)
C(52)-C(51)-N(41)	119.5(4)
C(53)-C(52)-C(51)	119.5(5)
C(53)-C(52)-H(52)	120.3
C(51)-C(52)-H(52)	120.3
C(52)-C(53)-C(54)	120.1(5)
C(52)-C(53)-H(53)	119.9
C(54)-C(53)-H(53)	119.9
C(53)-C(54)-C(55)	120.0(4)
C(53)-C(54)-H(54)	120.0
C(55)-C(54)-H(54)	120.0
C(54)-C(55)-C(56)	120.6(5)
C(54)-C(55)-H(55)	119.7
C(56)-C(55)-H(55)	119.7
C(51)-C(56)-C(55)	118.1(5)
C(51)-C(56)-H(56)	120.9
C(55)-C(56)-H(56)	120.9
O(3P)-Cl(1)-O(2P)	110.54(19)
O(3P)-Cl(1)-O(4P)	109.6(2)
O(2P)-Cl(1)-O(4P)	110.7(2)
O(3P)-Cl(1)-O(1P)	108.94(18)
O(2P)-Cl(1)-O(1P)	108.7(2)
O(4P)-Cl(1)-O(1P)	108.36(19)
Cl(1)-O(1P)-Cu(2)	131.27(17)
O(7P)-Cl(2)-O(5P)	110.4(3)
O(7P)-Cl(2)-O(8P)	111.5(3)
O(5P)-Cl(2)-O(8P)	107.2(3)
O(7P)-Cl(2)-O(6P)	109.0(3)
O(5P)-Cl(2)-O(6P)	108.8(3)
O(8P)-Cl(2)-O(6P)	109.9(3)
Cl(2)-O(5P)-Cu(2)	133.0(3)

Tabela B. Ângulos de ligação selecionados [°] para $[Cu_2(\mu\text{-}L1)_2(HL1)(ClO_4)_2(OH_2)]\cdot 2H_2O$ (continuação 5)

H(2WA)-O(2W)-H(2WB)	106.3
H(3WA)-O(3W)-H(3WB)	107.8