Supplementary Material

Polynuclear 2D Copper(II) Complex of Pyrazine Containing Perchlorate as a Counter-Ion: Crystal Structure and DFT Calculations

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Table S1: Cartesian coordinates of the optimized geometry of $[CuCl(pyz)_4]^+$ as obtained in the gas phase with M06-2X/6-31G(d) (T = 298 K)

N	-2.58775000	4.05217200	-0.47352400
C	-2.66235500	3.05321900	-1.35217500
C	-1.79258800	3.86842900	0.57765600
H	-3.31241000	3.19189500	-2.21079700
C	-1.94444800	1.87308000	-1.18728100
C	-1.05868600	2.69684700	0.76005400
H	-1.73466200	4.67278600	1.30451600
N	-1.13651100	1.70238500	-0.13288100
H	-2.02066700	1.05573100	-1.89874300
H	-0.42530600	2.53183200	1.62734800
Cu	0.00001500	0.00000700	0.23006300
N	-1.70243700	-1.13652900	-0.13225200
N	1.13648800	-1.70238000	-0.13301700
N	1.70240300	1.13650500	-0.13269100
Cl	0.00027300	0.00008700	2.57887100
C	-2.69663400	-1.05893000	0.76099400
C	-1.87347800	-1.94412000	-1.18686500
H	-2.53132700	-0.42582600	1.62843300
C	-3.86830600	-1.79271800	0.57869600
C	-3.05369700	-2.66191800	-1.35164400
H	-1.05633400	-2.02015800	-1.89858200
N	-4.05239500	-2.58753900	-0.47268100
H	-4.67245400	-1.73497300	1.30580200
C	1.05896500	-2.69675900	0.76003700
C	1.94409100	-1.87315800	-1.18765900
C	2.69681000	1.05893400	0.76032300
C	1.87320400	1.94404800	-1.18738000
H	-3.19265500	-3.31169600	-2.21043000
H	0.42585200	-2.53167500	1.62751300
C	1.79283300	-3.86834300	0.57751400
C	2.66196800	-3.05329800	-1.35267200
H	2.02007100	-1.05587100	-1.89921800
H	2.53170000	0.42587100	1.62782900
C	3.86844600	1.79270300	0.57771800
C	3.05339300	2.66182600	-1.35246800
H	1.05589300	2.02006400	-1.89890700
H	1.73515300	-4.67263400	1.30446700
H	3.31174800	-3.19204500	-2.21149100
H	4.67276300	1.73498400	1.30463900
H	3.19215500	3.31156400	-2.21131700
N	2.58766200	-4.05217100	-0.47390300
N	4.05229500	2.58747600	-0.47373700

Table S2: Cartesian coordinates of the optimized geometry of $[CuCl(pyz)_4]^+$ as obtained in the gas phase with M06-2X/6-31+G(d) (T = 298 K)

N	3.38503400	-3.46193400	-0.44154700
C	3.26759200	-2.47383700	-1.32846800
C	2.55341600	-3.43845700	0.59777500
H	3.94523300	-2.48232100	-2.17696000
C	2.32054200	-1.46364400	-1.18369900
C	1.59249900	-2.43906800	0.76071700
H	2.64986600	-4.23372900	1.33063700
N	1.48024700	-1.45513500	-0.14035900
H	2.23986500	-0.65250100	-1.90234400
H	0.92510600	-2.40043200	1.61777100
Cu	-0.00001700	-0.00001300	0.18143300
N	1.45515600	1.48023100	-0.14012500
N	-1.48020800	1.45514100	-0.14053700
N	-1.45512300	-1.48022200	-0.14060000
Cl	-0.00027400	-0.00014100	2.54473700
C	2.43893500	1.59253800	0.76111200
C	1.46385400	2.32044800	-1.18352600
H	2.40014200	0.92521000	1.61820800
C	3.43836100	2.55343500	0.59827100
C	2.47408100	3.26747800	-1.32819200
H	0.65283300	2.23972600	-1.90230400
N	3.46202600	3.38497600	-0.44110900
H	4.23350800	2.64993100	1.33126100
C	-1.59268100	2.43896100	0.76063500
C	-2.32024700	1.46378000	-1.18408200
C	-2.43909100	-1.59261000	0.76041900
C	-1.46361800	-2.32032700	-1.18409400
H	2.48271700	3.94505700	-2.17673100
H	-0.92549800	2.40021900	1.61784700
C	-2.55356000	3.43837000	0.59758300
C	-3.26726100	2.47399100	-1.32895800
H	-2.23939200	0.65272700	-1.90280900
H	-2.40046900	-0.92537300	1.61759500
C	-3.43850100	-2.55347100	0.59726700
C	-2.47383200	-3.26732300	-1.32907200
H	-0.65244700	-2.23954000	-1.90269500
H	-2.65018900	4.23355000	1.33051900
H	-3.94469400	2.48258100	-2.17761500
H	-4.23380300	-2.65003100	1.33008100
H	-2.48230300	-3.94481000	-2.17768700
N	-3.38492200	3.46197700	-0.44194100
N	-3.46196400	-3.38489900	-0.44220700

Table S3: Cartesian coordinates of the optimized geometry of $[CuCl(pyz)_4]^+\cdots ClO_4^-$ as obtained with M06-2X/6-31+G(d) in the gas phase (T = 298 K)

N	2.43373400	3.52703700	0.04563000
C	2.18608300	2.72057400	1.07452700
C	1.78628900	3.26302200	-1.08736500
H	2.74618500	2.88434700	1.98894700
C	1.25688500	1.68375900	0.99273700
C	0.84800700	2.24011600	-1.19292300
H	2.00809500	3.89149700	-1.94459300
N	0.57060500	1.46832000	-0.13451400
H	1.08915500	1.01068100	1.82748100
H	0.30684000	2.02821000	-2.11124200
Cu	-0.87262600	0.01696600	-0.30113300
N	0.53962100	-1.47608600	-0.16890800
N	-2.33642300	-1.43752500	0.26077700
N	-2.33838100	1.49695700	0.17012600
Cl	-1.36258900	-0.06777500	-2.63655200
C	1.45384800	-1.56965100	-1.13615500
C	0.63019500	-2.33429500	0.85682500
H	1.39137900	-0.86188400	-1.95558000
C	2.44025700	-2.56012800	-1.08532700
C	1.61029400	-3.31522100	0.88009800
H	-0.09772100	-2.24093700	1.65811200
N	2.50512300	-3.44708400	-0.09965500
H	3.19023300	-2.62144800	-1.86705600
C	-2.50872500	-2.47714100	-0.56231100
C	-3.05793300	-1.40707100	1.38635900
C	-3.47000400	1.49427400	-0.54415900
C	-2.19395800	2.44670000	1.10077400
H	1.67196700	-4.01424400	1.70876100
H	-1.93023600	-2.47376500	-1.48254000
C	-3.41345700	-3.48988600	-0.24043500
C	-3.95148900	-2.43039600	1.69092500
H	-2.92146400	-0.55437500	2.04628100
H	-3.55406800	0.74238900	-1.32437400
C	-4.46097400	2.44562700	-0.30410800
C	-3.19902600	3.38447300	1.32736200
H	-1.26328600	2.46462200	1.66034900
H	-3.55694100	-4.33193400	-0.91057500
H	-4.53237600	-2.40535400	2.60811300
H	-5.37607100	2.44524500	-0.88843300
H	-3.07845000	4.15107100	2.08693400
N	-4.13258400	-3.47332500	0.88055100
N	-4.33507800	3.38634400	0.63089800
O	3.34517800	0.56727000	-0.77826200
Cl	4.02343400	-0.00725700	0.41757100
O	2.97318700	-0.60712300	1.29333000
O	4.96202800	-1.05267500	-0.00662600
O	4.70641600	1.06608000	1.15651900

Table S4: Cartesian coordinates of the optimized geometry of $\{CuCl(\mu\text{-}pyz)_4(ZnCl_2(H_2O)_3)_4\}^+$ as obtained with M06-2X/6-31G(d) in the gas phase (T = 298 K)

N	-3.26860500	-3.46547600	0.05720000
C	-2.28882200	-3.29716900	-0.83212100
Zn	-4.84015600	-4.95558800	-0.25151300
C	-3.29373100	-2.68932400	1.13933100
H	-2.29041500	-3.96126000	-1.69329300
C	-1.31810500	-2.32264100	-0.63526900
O	-6.06750500	-6.73254300	-0.07070400
O	-3.67229400	-6.10541300	1.15348700
C	-2.31996800	-1.71306700	1.34037800
H	-4.11154300	-2.84746200	1.83760000
N	-1.34305600	-1.53033100	0.44424600
H	-0.51030300	-2.17877200	-1.34661300
H	-2.30308100	-1.08280400	2.22505600
Cu	0.01259700	0.00548700	0.80578700
N	1.54432000	-1.34503200	0.40430400
N	1.35821300	1.54240100	0.43130900
N	-1.53522700	1.34534000	0.43846200
Cl	0.03399500	-0.00694800	3.14618100
C	1.71451100	-2.35147500	1.27006000
C	2.36999500	-1.27129900	-0.64689700
H	1.05718000	-2.37671200	2.13463300
C	2.71572000	-3.29924200	1.06989500
C	3.36798200	-2.21796400	-0.84536100
H	2.23669800	-0.44223700	-1.33527800
N	3.52905200	-3.22388000	0.01652000
H	2.87445400	-4.13078100	1.75293600
C	2.36146200	1.71223200	1.30076400
C	1.29681000	2.35752300	-0.62924400
C	-1.75400800	2.30991800	1.33970500
C	-2.33255800	1.29143400	-0.63637100
H	4.05176600	-2.18293700	-1.69037900
Zn	5.14695100	-4.67310100	-0.28995300
H	2.37535400	1.06361600	2.17217900
C	3.32202500	2.69999200	1.09230500
C	2.25913300	3.33775600	-0.83864200
H	0.46829700	2.22617500	-1.31862600
H	-1.11758900	2.31736400	2.22018000
C	-2.77807000	3.23703000	1.15203000
C	-3.35338500	2.21498100	-0.82042200
H	-2.15894400	0.49429700	-1.35295200
O	3.78627500	-5.86746300	-1.42056900
O	6.11441400	-3.50155800	1.25592700
H	4.14656300	2.86572400	1.78224300
H	2.24576700	3.99901500	-1.70176900
H	-2.97398400	4.04001100	1.85875500
H	-4.02512900	2.18642500	-1.67482000
N	3.26445100	3.49542800	0.02463100
Zn	4.77653500	5.03672800	-0.36036400
O	6.05629200	3.47012500	-1.05506100
O	5.78724500	6.95911400	-0.44342700

N	-3.56175900	3.18063900	0.07652900
Zn	-5.18153800	4.61087000	-0.27431300
O	-3.69387000	5.56179100	-1.53899200
O	-6.31124800	6.28115000	-1.07926600
O	-6.23007000	3.70626500	1.34226200
O	3.43367200	6.27281200	0.79956700
O	7.08012500	-5.65454900	-0.15707600
O	-5.49534900	-3.73667800	-1.88905000
H	-3.41495000	6.23502900	-0.88977200
H	-4.23552100	6.04494100	-2.18465000
H	-7.13056800	5.98402800	-1.50765200
H	-6.52462000	6.96569600	-0.42500200
H	-7.07379700	3.29149600	1.10256800
H	-6.37468500	4.32750100	2.07450000
H	3.61893700	7.17047700	0.47786800
H	3.90509100	6.20748700	1.65127800
H	6.61260300	6.99454000	0.06614100
H	5.96661800	7.22840900	-1.35903800
H	6.84633200	3.40486700	-0.49360200
H	6.33040800	3.57918600	-1.97953400
H	5.95944500	-4.12154400	1.99326400
H	7.06075900	-3.58245100	1.05317900
H	7.51523400	-5.70373000	-1.02385300
H	7.04918000	-6.54230700	0.23405800
H	4.07519700	-6.04063600	-2.33041600
H	3.62748700	-6.71310600	-0.96924000
H	-3.21375900	-6.67049800	0.50395500
H	-4.31640200	-6.68761000	1.58869400
H	-6.09412100	-7.29015400	-0.86448400
H	-6.97546300	-6.50628800	0.18976700
H	-5.50062900	-4.22620900	-2.72727900
H	-6.38218200	-3.37576300	-1.72650100
Cl	-4.45802700	6.17369200	1.39288400
Cl	-6.36956800	3.29704800	-1.77137300
Cl	-6.43627100	-3.91284900	1.06711000
Cl	-3.66346200	-6.17202400	-1.94869800
Cl	4.52604100	-6.12835700	1.51488000
Cl	5.94081900	-3.78494500	-2.28470800
Cl	4.18267200	5.45090700	-2.56606500
Cl	5.96486500	4.73644300	1.69933900