Synthesis of Two Novel Copper (II) Complexes as Potential Inhibitors of HIV-1 Protease Enzyme: Experimental and Theoretical Investigations

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(a)

(b)

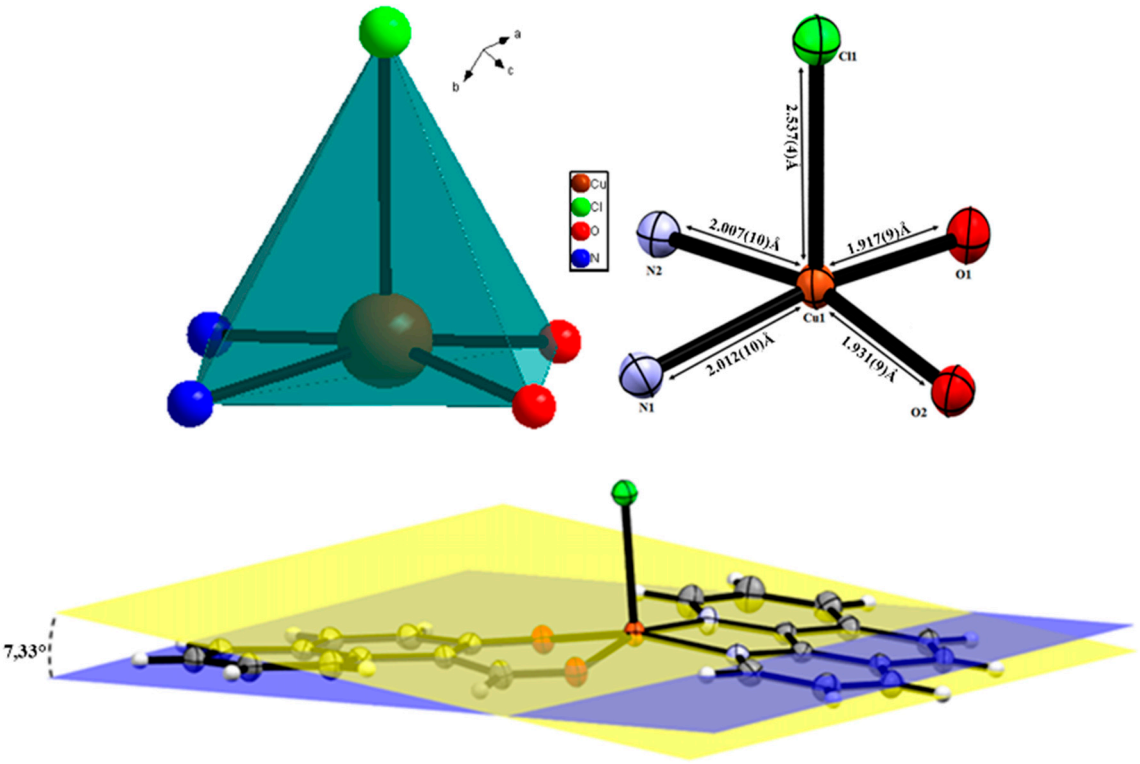

Figure S1. The copper square-pyramidal environment (a), and the dihedral angle between the two ligands (b) of C-2.

Table S1. Selected experimental and calculated bond lengths (Å) and angles (°) for C-1.

Bond lengths (Å)	Experimental	Calculated
Cu1- O1	1.908 (17)	1.946
Cu1- O2	1.943 (18)	1.976
Cu1- N2	2.001 (2)	2.040
Cu1- N1	2.005 (19)	2.039
Cu1- N3	2.188 (2)	2.138
Angles (°)		
O1- Cu1- O2	91.79 (8)	89.62
O1- Cu1- N2	162.97 (8)	162.00
O2- Cu1- N2	92.24 (8)	92.73
O1- Cu1- N1	91.19 (8)	92.70
O2- Cu1- N1	164.11 (8)	162.03
N2- Cu1- N1	80.63 (8)	79.76
O1- Cu1- N3	99.23 (9)	105.30
O2- Cu1- N3	93.77 (9)	103.14
N2- Cu1- N3	97.01 (9)	91.54
N1- Cu1- N3	101.15 (9)	93.43

Table S2. Selected experimental and calculated bond lengths (Å) and angles (°) for C-2.

Bond lengths (Å)	Experimental	Calculated
Cu1- O1	1.917 (9)	1.945
Cu1- O2	1.931 (9)	1.985
Cu1- N2	2.007 (10)	2.056
Cu1-N1	2.012 (10)	2.047
Cu1- Cl1	2.537 (4)	2.451
Angles (°)		
O1- Cu1- O2	92.46 (4)	89.30
O1- Cu1- N2	91.78 (4)	91.76
O2- Cu1- N2	164.59 (4)	159.44
O1- Cu1- N1	163.34 (4)	161.05
O2- Cu1- N1	89.87 (4)	91.62
N2- Cu1- N1	81.95 (4)	80.89
O1- Cu1- Cl1	98.46 (3)	105.79
O2- Cu1- Cl1	96.92 (3)	104.01
N2- Cu1- Cl1	97.09 (3)	95.45
N1- Cu1- Cl1	97.63 (3)	92.35