Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting information

"Interactions of Coinage Metal Clusters with Histidine and their Effects on Histidine Acidity; Theoretical Investigation"

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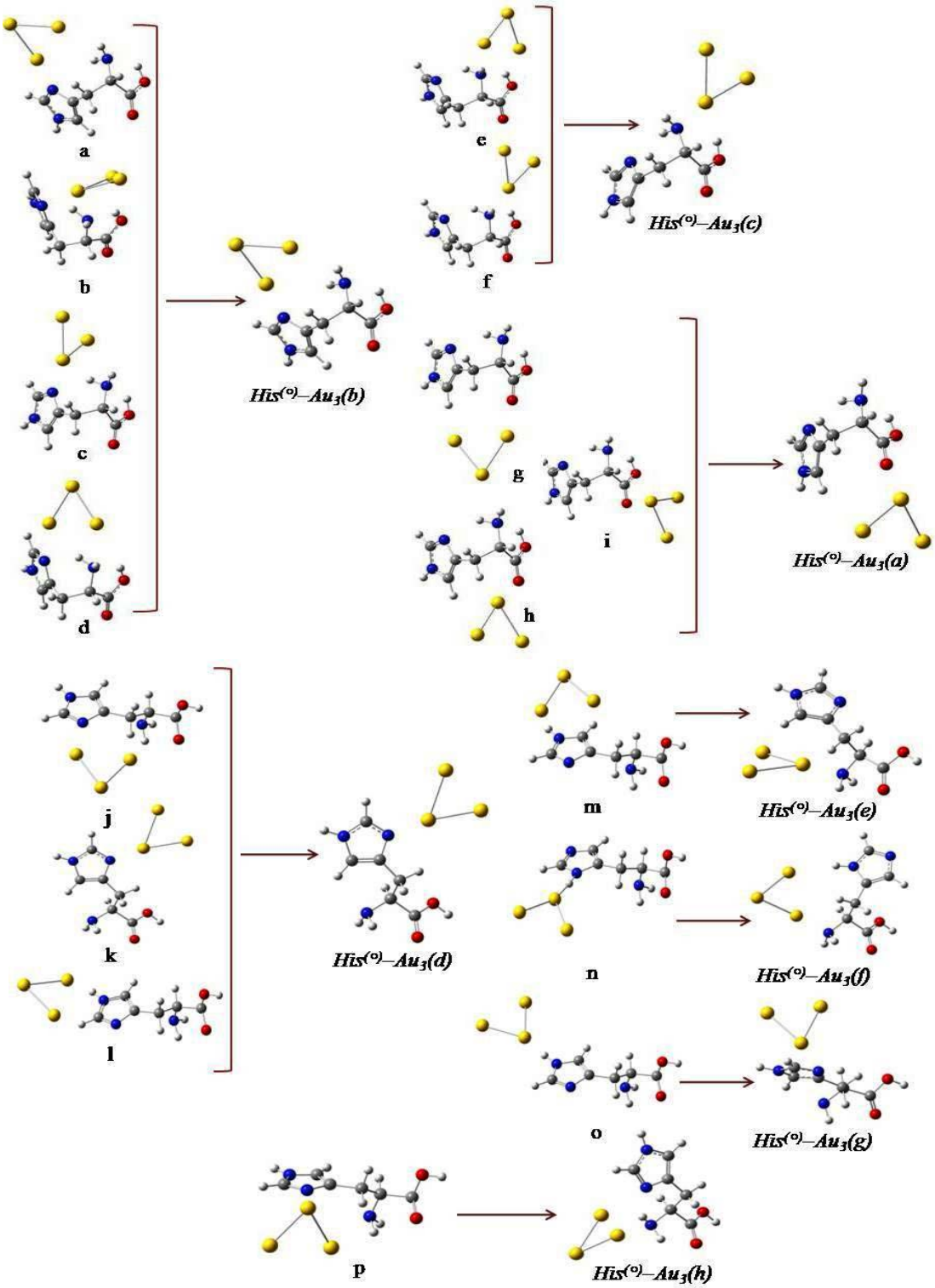
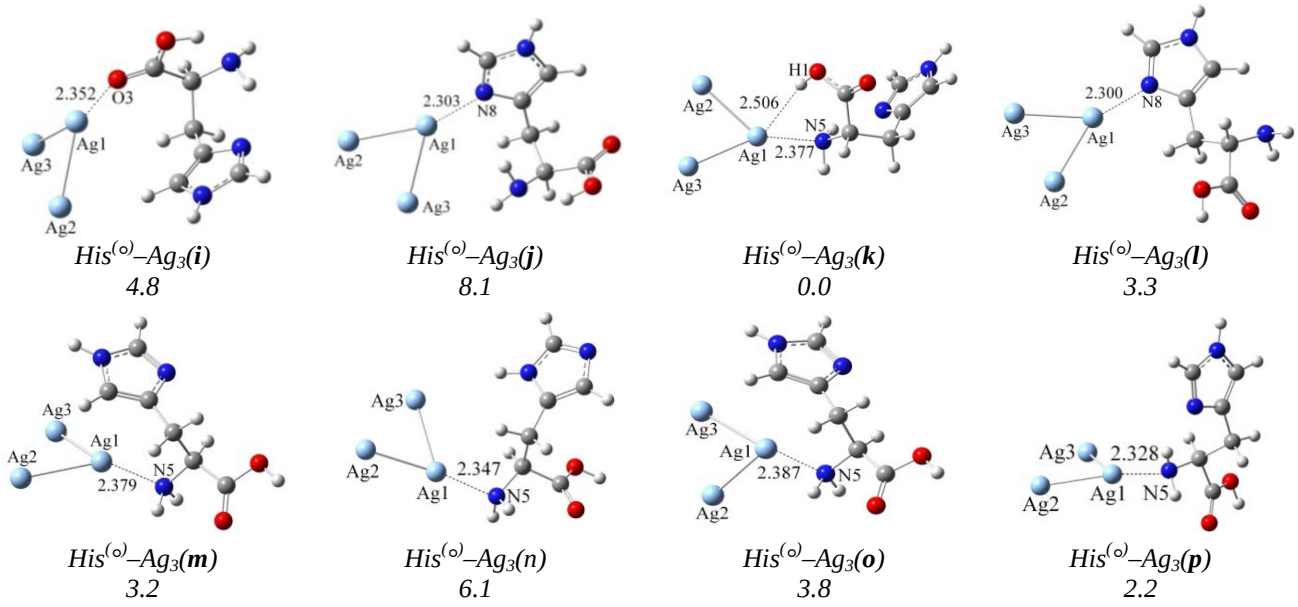


Fig **S1.** The initial structures (**a**, **b**, **c**, **d, e, f, g, h, i, j**, **k**, **l**, **m, n, o** and **p**) for optimization are shown in the left and the optimized structures (*His*$^{(o)}$*–Au*$_3$***(a)***, *His*$^{(o)}$*–Au*$_3$***(b)***, *His*$^{(o)}$*–Au*$_3$***(c)***, *His*$^{(o)}$*–Au*$_3$***(d)***, *His*$^{(o)}$*–Au*$_3$***(e)***, *His*$^{(o)}$*–Au*$_3$***(f)***, *His*$^{(o)}$*–Au*$_3$***(g)*** and *His*$^{(o)}$*–Au*$_3$***(h)***) of *His*$^{(o)}$*-Au*$_3$ complexes calculated at B3LYP/6-31+G** ∪ LANL2DZ are depicted in the right.



His$^{(\circ)}$*–Ag*$_3$***(i)*** *4.8*

His$^{(\circ)}$*–Ag*$_3$***(j)*** *8.1*

His$^{(\circ)}$*–Ag*$_3$***(k)*** *0.0*

His$^{(\circ)}$*–Ag*$_3$***(l)*** *3.3*

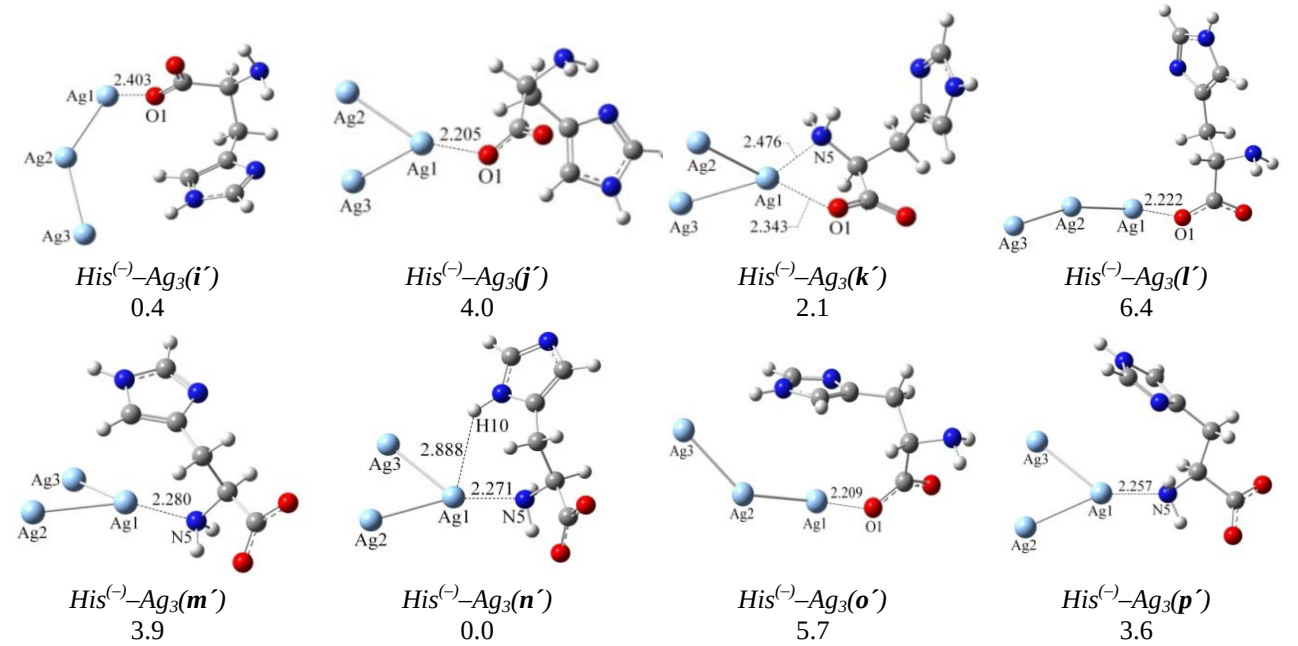
His$^{(\circ)}$*–Ag*$_3$***(m)*** *3.2*

His$^{(\circ)}$*–Ag*$_3$*(n)* *6.1*

His$^{(\circ)}$*–Ag*$_3$***(o)*** *3.8*

His$^{(\circ)}$*–Ag*$_3$***(p)*** *2.2*

Fig **S2.** Optimized geometries (B3LYP/6-31+G** ∪ LANL2DZ) of neutral histidine with Ag_3 cluster. Relative potential energies including the ZPE values, in kcal/mol. Distances in Å.



His$^{(-)}$*–Ag*$_3$***(i´)*** 0.4

His$^{(-)}$*–Ag*$_3$***(j´)*** 4.0

His$^{(-)}$*–Ag*$_3$***(k´)*** 2.1

His$^{(-)}$*–Ag*$_3$***(l´)*** 6.4

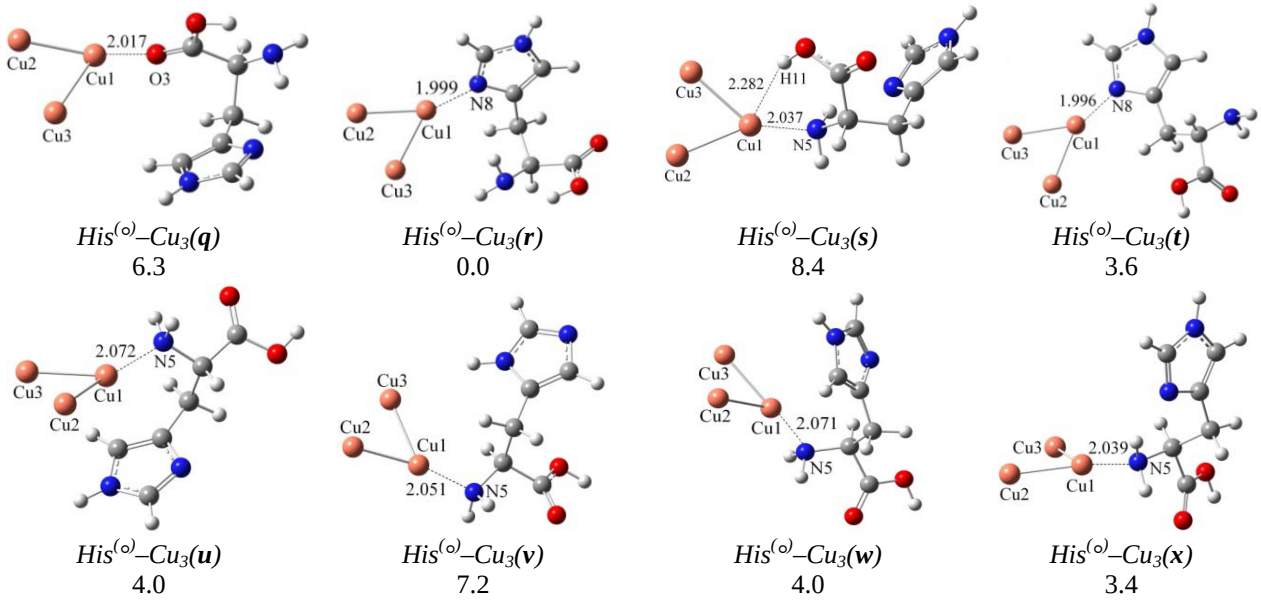
His$^{(-)}$*–Ag*$_3$***(m´)*** 3.9

His$^{(-)}$*–Ag*$_3$***(n´)*** 0.0

His$^{(-)}$*–Ag*$_3$***(o´)*** 5.7

His$^{(-)}$*–Ag*$_3$***(p´)*** 3.6

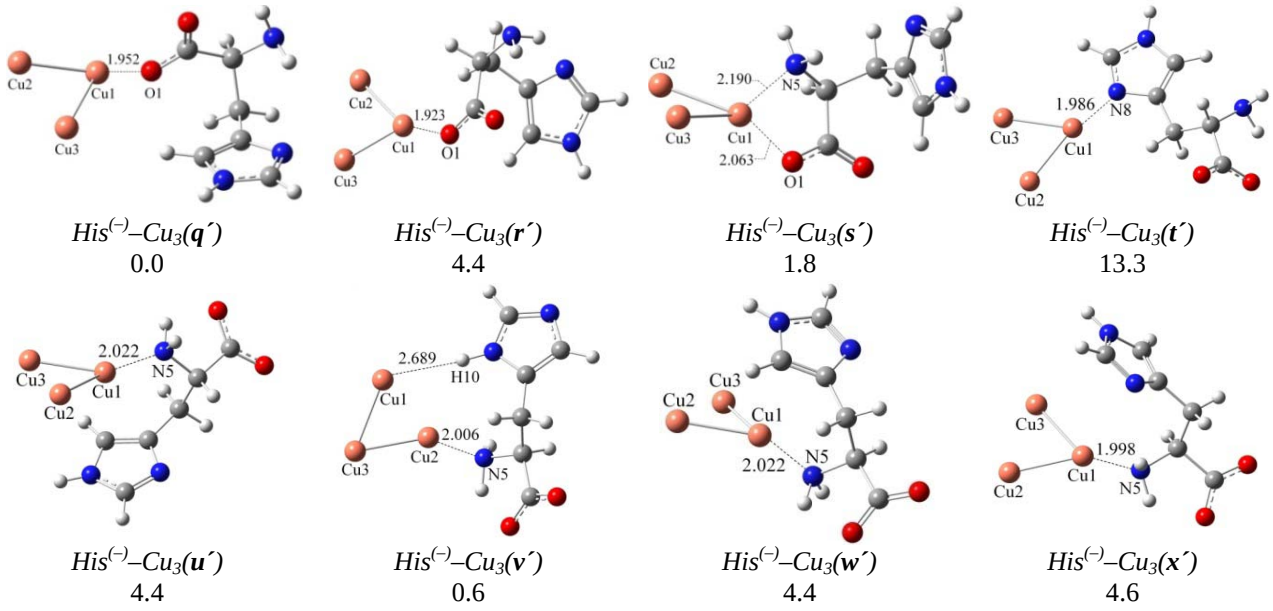
Fig **S3.** Optimized geometries (B3LYP/6-31+G** ∪ LANL2DZ) of anionic histidine with Ag_3 cluster. Relative potential energies including the ZPE values, in kcal/mol. Distances in Å.



His$^{(\circ)}$–*Cu*$_3$(***q***) 6.3 | *His*$^{(\circ)}$–*Cu*$_3$(***r***) 0.0 | *His*$^{(\circ)}$–*Cu*$_3$(***s***) 8.4 | *His*$^{(\circ)}$–*Cu*$_3$(***t***) 3.6

His$^{(\circ)}$–*Cu*$_3$(***u***) 4.0 | *His*$^{(\circ)}$–*Cu*$_3$(***v***) 7.2 | *His*$^{(\circ)}$–*Cu*$_3$(***w***) 4.0 | *His*$^{(\circ)}$–*Cu*$_3$(***x***) 3.4

Fig **S4.** Optimized geometries (B3LYP/6-31+G** ∪ LANL2DZ) of neutral histidine with Cu_3 cluster. Relative potential energies including the ZPE values, in kcal/mol. Distances in Å.



His$^{(-)}$–*Cu*$_3$(***q´***) 0.0 | *His*$^{(-)}$–*Cu*$_3$(***r´***) 4.4 | *His*$^{(-)}$–*Cu*$_3$(***s´***) 1.8 | *His*$^{(-)}$–*Cu*$_3$(***t´***) 13.3

His$^{(-)}$–*Cu*$_3$(***u´***) 4.4 | *His*$^{(-)}$–*Cu*$_3$(***v´***) 0.6 | *His*$^{(-)}$–*Cu*$_3$(***w´***) 4.4 | *His*$^{(-)}$–*Cu*$_3$(***x´***) 4.6

Fig **S5.** Optimized geometries (B3LYP/6-31+G** ∪ LANL2DZ) of anionic histidine with Cu_3 cluster. Relative potential energies including the ZPE values, in kcal/mol. Distances in Å.

Table **S**1. Geometric Features of Anionic and Neutral Histidine with Ag_3 Cluster [a]

Complex	Anchor bond	$r_{M\text{-}X}$ [a]	E_b [b]	Complex	Anchor bond	$r_{M\text{-}X}$	E_b
His$^{(\circ)}$–*Ag*$_3$(***i***)	Ag_1-O_3	2.352	-2.45	*His*$^{(-)}$–*Ag*$_3$(***i´***)	Ag_1-O_1	2.403	-25.49
His$^{(\circ)}$–*Ag*$_3$(***j***)	Ag_1-N_8	2.303	1.02	*His*$^{(-)}$–*Ag*$_3$(***j´***)	Ag_1-O_1	2.205	-22.00
His$^{(\circ)}$–*Ag*$_3$(***k***)	Ag_1-N_5 Ag_1-H_1	2.377 2.506	-7.00	*His*$^{(-)}$–*Ag*$_3$(***k´***)	Ag_1-O_1 Ag_1-N_5	2.343 2.476	-23.78
His$^{(\circ)}$–*Ag*$_3$(***l***)	Ag_1-N_8	2.300	-3.85	*His*$^{(-)}$–*Ag*$_3$(***l´***)	Ag_1-O_1	2.222	-19.69
His$^{(\circ)}$–*Ag*$_3$(***m***)	Ag_1-N_5	2.379	-3.70	*His*$^{(-)}$–*Ag*$_3$(***m´***)	Ag_1-N_5	2.280	-22.52
His$^{(\circ)}$–*Ag*$_3$(***n***)	Ag_1-N_5	2.347	-0.84	*His*$^{(-)}$–*Ag*$_3$(***n´***)	Ag_1-H_{10} Ag_1-N_5	2.888 2.271	-25.95
His$^{(\circ)}$–*Ag*$_3$(***o***)	Ag_1-N_5	2.387	-3.74	*His*$^{(-)}$–*Ag*$_3$(***o´***)	Ag_1-O_1	2.209	-20.34
His$^{(\circ)}$–*Ag*$_3$(***p***)	Ag_1-N_5	2.328	-4.54	*His*$^{(-)}$–*Ag*$_3$(***p´***)	Ag_1-N_5	2.257	-22.09

[a] r(M-X) is the length of the anchoring bond or nonconventional H-bonds, (X = O, N, and H). [b] The binding energy, E_b, includes zero-point vibrational energy in kcal/mol.

Table **S**2. Geometric Features of Anionic and Neutral Histidine with Cu_3 Cluster [a]

Complex	Anchor bond	$r_{M\text{-}X}$ [a]	E_b [b]	Complex	Anchor bond	$r_{M\text{-}X}$	E_b
His$^{(\circ)}$–*Cu*$_3$(***q***)	Cu_1-O_3	2.017	-14.58	*His*$^{(-)}$–*Cu*$_3$(***q´***)	Cu_1-O_1	1.952	-39.48
His$^{(\circ)}$–*Cu*$_3$(***r***)	Cu_1-N_8	1.999	-20.69	*His*$^{(-)}$–*Cu*$_3$(***r´***)	Cu_1-O_1	1.923	-35.25
His$^{(\circ)}$–*Cu*$_3$(***s***)	Cu_1-N_5 Cu_1-H_{11}	2.037 2.282	-12.51	*His*$^{(-)}$–*Cu*$_3$(***s´***)	Cu_1-N_5 Cu_1-O_1	2.190 2.063	-37.62
His$^{(\circ)}$–*Cu*$_3$(***t***)	Cu_1-N_8	1.996	-16.28	*His*$^{(-)}$–*Cu*$_3$(***t´***)	Cu_1-N_8	1.986	-25.44
His$^{(\circ)}$–*Cu*$_3$(***u***)	Cu_1-N_5	2.072	-15.69	*His*$^{(-)}$–*Cu*$_3$(***u´***)	Cu_1-N_5	2.022	-34.12
His$^{(\circ)}$–*Cu*$_3$(***v***)	Cu_1-N_5	2.051	-12.54	*His*$^{(-)}$–*Cu*$_3$(***v´***)	Cu_1-H10 Cu_2-N_5	2.689 2.006	-38.21
His$^{(\circ)}$–*Cu*$_3$(***w***)	Cu_1-N_5	2.071	-15.69	*His*$^{(-)}$–*Cu*$_3$(***w´***)	Cu_1-N_5	2.022	-34.12
His$^{(\circ)}$–*Cu*$_3$(***x***)	Cu_1-N_5	2.039	-16.11	*His*$^{(-)}$–*Cu*$_3$(***x´***)	Cu_1-N_5	1.998	-33.88

[a] r(M-X) is the length of the anchoring bond or nonconventional H-bonds, (X = O, N, and H). [b] The binding energy, E_b, includes zero-point vibrational energy in kcal/mol.

Table **S**3. Geometric Features of Neutral Histidine with M_3 Clusters (M = Au, Ag and Cu) [a]

Complex	Anchor bond	$\upsilon_{M\text{-}X}$	$\Delta\upsilon_{A\text{-}X}$	$\Delta r_{A\text{-}X}$	$-\Delta H_f$
His$^{(\circ)}$–*Au*$_3$(***a***)	Au_1-O_3	177.73	C_2-O_3(146.96)	C_2-O_3(0.020)	-10.05
His$^{(\circ)}$–*Au*$_3$(***b***)	Au_1-N_8 Au_1-H_5	199.81 59.83	N_8-C_9(4.44) N_5-H_5(-84.16)	N_8-C_9(0.009) N_5-H_5(0.010)	-18.48
His$^{(\circ)}$–*Au*$_3$(***c***)	Au_1-H_1 Au_1-N_5	104.31 165.27	O_1-H_1(-159.62) C_4-N_5(-123.62)	O_3-H_3(0.009) C_4-N_5(0.019)	-9.93
His$^{(\circ)}$–*Au*$_3$(***d***)	Au_1-N_8	209.55	N_8-C_9(4.86)	N_8-C_9(0.007)	-14.90
His$^{(\circ)}$–*Au*$_3$(***e***)	Au_1-N_5	158.14	C_4-N_5(-30.22)	C_4-N_5(0.008)	-13.00
His$^{(\circ)}$–*Au*$_3$(***f***)	Au_1-H_{10} Au_2-N_5	81.61 169.02	N_{10}-H_{10}(-173.65) C_4-N_5(-34.53)	N_{10}-H_{10}(0.740) C_4-N_5(0.012)	-11.30
His$^{(\circ)}$–*Au*$_3$(***g***)	Au_1-C_{11}	135.58	C_7-C_{11}(-103.51)	C_7-C_{11}(0.043)	-4.90
His$^{(\circ)}$–*Au*$_3$(***h***)	Cu_1-N_5	146.12	C_4-N_5(-23.08)	C_4-N_5(0.009)	-15.40
His$^{(\circ)}$–*Ag*$_3$(***i***)	Ag_1-O_3	181.40	C_2-O_3(-49.81)	C_2-O_3(0.012)	-1.56
His$^{(\circ)}$–*Ag*$_3$(***j***)	Ag_1-N_8	187.90	N_8-C_9(2.05)	N_8-C_9(0.006)	1.91
His$^{(\circ)}$–*Ag*$_3$(***k***)	Ag_1-N_5	167.56	C_4-N_5(-29.70)	C_4-N_5(0.010)	-6.12
His$^{(\circ)}$–*Ag*$_3$(***l***)	Ag_1-N_8	181.67	N_8-C_9(2.01)	N_8-C_9(0.004)	-2.97
His$^{(\circ)}$–*Ag*$_3$(***m***)	Ag_1-N_5	167.09	C_4-N_5(-45.59)	C_4-N_5(-0.002)	-2.81
His$^{(\circ)}$–*Ag*$_3$(***o***)	Ag_1-N_5	163.99	C_4-N_5(-47.45)	C_4-N_5(-0.002)	0.05
His$^{(\circ)}$–*Ag*$_3$(***n***)	Ag_1-N_5	177.55	C_4-N_5(-45.95)	C_4-N_5(0.005)	-2.86
His$^{(\circ)}$–*Ag*$_3$(***p***)	Ag_1-N_5	177.55	C_4-N_5(-18.06)	C_4-N_5(0.001)	-3.65
His$^{(\circ)}$–*Cu*$_3$(***q***)	Cu_1-O_3	166.07	C_2-O_3(-63.27)	C_2-O_3(0.018)	-13.69
His$^{(\circ)}$–*Cu*$_3$(***r***)	Cu_1-N_8	170.16	N_8-C_9(4.17)	N_8-C_9(-0.008)	-19.80
His$^{(\circ)}$–*Cu*$_3$(***s***)	Cu_1-N_5 Cu_2-H_1	159.81 107.49	C_4-N_5(-27.65) O_1-H_1(92.00)	C_4-N_5(0.014) O_1-H_1(-0.009)	-11.63
His$^{(\circ)}$–*Cu*$_3$(***t***)	Cu_1-N_8	169.94	N_8-C_9(4.37)	N_8-C_9(0.007)	-16.28
His$^{(\circ)}$–*Cu*$_3$(***u***)	Cu_1-N_5	144.59	C_4-N_5(-32.71)	C_4-N_5(0.001)	-15.69
His$^{(\circ)}$–*Cu*$_3$(***v***)	Cu_1-N_5	147.36	C_4-N_5(-35.96)	C_4-N_5(0.009)	-12.54
His$^{(\circ)}$–*Cu*$_3$(***w***)	Cu_1-N_5	144.83	C_4-N_5(-32.73)	C_4-N_5(0.001)	-15.69
His$^{(\circ)}$–*Cu*$_3$(***x***)	Cu_1-N_5	129.06	C_4-N_5(-19.22)	C_4-N_5(0.006)	-16.11

[a]Δr(A-X) is the difference, in angstroms, between the bond lengths of N-C, O-C, N-H, and O-H in the complexed and isolated fragments. $\Delta\upsilon$(A-X), in cm^{-1}, is the difference between the frequency of N-C, O-C, N-H, and O-H bonds in the complexed and isolated fragments. [b]The ΔH_f, includes thermal Enthalpies in kcal/mol. The notations "(◦)" and "(–)" indicate neutral and anionic histidine, respectively.

Table **S4**. Geometric Features of Anionic Histidine with M_3 Clusters (M = Au, Ag and Cu) [a]

Complex	Anchor bond	$\upsilon_{M\text{-}X}$	$\Delta\upsilon_{A\text{-}X}$	$\Delta r_{A\text{-}X}$	$-\Delta H_f$
*His$^{(-)}$–Au$_3$(**a´**)*	Au_1-O_1	169.61	C_2-O_1(34.69)	C_2-O_1(0.039)	-38.38
*His$^{(-)}$–Au$_3$(**b´**)*	Au_1-O_1	136.06	C_2-O_1(19.69)	C_2-O_1(0.042)	-33.36
*His$^{(-)}$–Au$_3$(**c´**)*	Au_1-O_1 Au_1-N_5	140.61 172.51	C_2-O_1(14.20) C_4-N_5(47.95)	C_2-O_1(0.010) C_4-N_5 (-0.007)	-31.94
*His$^{(-)}$–Au$_3$(**d´**)*	Au_1-N_8	215.32	N_8-C_9(83.69)	N_8-C_9(0.004)	-26.58
*His$^{(-)}$–Au$_3$(**e´**)*	Au_1-N_5	218.86	C_4-N_5(46.96)	C_4-N_5 (0.017)	-36.41
*His$^{(-)}$–Au$_3$(**f´**)*	Au_1-H_{10} Au_2-N_5	62.21 144.74	N_{10}-H_{10}(-148.38) C_4-N_5(77.28)	N_{10}-H_{10}(0.009) C_4-N_5(0.018)	-42.00
*His$^{(-)}$–Au$_3$(**g´**)*	Au_1-C_{11}	137.16	C_7-C_{11}(-103.66)	C_7-C_{11}(0.048)	-16.87
*His$^{(-)}$–Au$_3$(**h´**)*	Au_1-N_5	146.12	C_4-N_5(57.74)	C_4-N_5(0.017)	-37.35
*His$^{(-)}$–Ag$_3$(**i´**)*	Ag_1-O_1	143.83	C_2-O_1(-55.90)	C_2-O_1(0.009)	-24.60
*His$^{(-)}$–Ag$_3$(**j´**)*	Ag_1-O_1	144.12	C_2-O_1(4.76)	C_2-O_1(0.030)	-21.11
*His$^{(-)}$–Ag$_3$(**k´**)*	Ag_1-O_1 Ag_1-N_5	179.19 141.58	C_2-O_1(15.70) C_4-N_5(52.79)	C_2-O_1(0.009) C_4-N_5(-0.007)	-22.89
*His$^{(-)}$–Ag$_3$(**l´**)*	Ag_1-O_1	152.58	C_2-O_1(5.27)	C_2-O_1(0.024)	-18.80
*His$^{(-)}$–Ag$_3$(**m´**)*	Ag_1-N_5	174.44	C_4-N_5(43.83)	C_4-N_5(0.001)	-21.63
*His$^{(-)}$–Ag$_3$(**n´**)*	Ag_1-H_{10} Ag_1-N_5	92.63 150.21	N_{10}-H_{10}(-151.62) C_4-N_5(74.43)	N_{10}-H_{10}(0.008) C_4-N_5(0.007)	-25.06
*His$^{(-)}$–Ag$_3$(**o´**)*	Ag_1-O_1	147.71	C_2-O_1(5.25)	C_2-O_1(0.026)	-19.45
*His$^{(-)}$–Ag$_3$(**p´**)*	Ag_1-N_5	150.42	C_4-N_5(76.36)	C_4-N_5(0.011)	-21.20
*His$^{(-)}$–Cu$_3$(**q´**)*	Cu_1-O_1	138.56	Cu_1-O_1(8.01)	Cu_1-O_1(0.031)	-38.59
*His$^{(-)}$–Cu$_3$(**r´**)*	Cu_1-O_1	130.85	Cu_1-O_1(11.55)	Cu_1-O_1(0.033)	-34.36
*His$^{(-)}$–Cu$_3$(**s´**)*	Cu_1-N_5 Cu_1-O_1	165.52 181.69	C_4-N_5(64.97) C_2-O_1(23.17)	C_4-N_5(-0.006) C_2-O_1(0.013)	-36.74
*His$^{(-)}$–Cu$_3$(**t´**)*	Cu_1-N_8	178.95	N_8-C_9(331.41)	N_8-C_9(0.010)	-25.44
*His$^{(-)}$–Cu$_3$(**u´**)*	Cu_1-N_5	198.62	C_4-N_5(44.61)	C_4-N_5(0.012)	-34.12
*His$^{(-)}$–Cu$_3$(**v´**)*	Cu_1-H_{10} Cu_2-N_5	102.75 203.22	N_{10}-H_{10}(-233.37) C_4-N_5(77.01)	N_{10}-H_{10}(0.012) C_4-N_5(0.014)	-38.21
*His$^{(-)}$–Cu$_3$(**w´**)*	Cu_1-N_5	198.64	C_4-N_5(44.47)	C_4-N_5(0.011)	-34.12
*His$^{(-)}$–Cu$_3$(**x´**)*	Cu_1-N_5	129.06	C_4-N_5(-19.22)	C_4-N_5(0.006)	-33.88

[a] Δr(A-X) is the difference, in angstroms, between the bond lengths of N-C, O-C, N-H, and O-H in the complexed and isolated fragments. $\Delta\upsilon$(A-X), in cm^{-1}, is the difference between the frequency of N-C, O-C, N-H, and O-H bonds in the complexed and isolated fragments. [b]The ΔH_f, includes thermal Enthalpies in kcal/mol. The notations "(◦)" and "(–)" indicate neutral and anionic histidine, respectively.

Table **S5**. The values of total energy (in a.u.), Gibbs free energy (a.u.), and entropy (cal mol^{-1} K^{-1}) are given at 298 K for His, His-OMe, His-M_3, His-OMe-M_3, and their anion.

Name	E	G	S	Name	E	G	S
His$^{(\circ)}$	-548.8175657	-548.692697	99.595	*His*$^{(\circ)}$*-OMe*	-588.1014817	-587.952364	109.667
His$^{(-)}$	-548.2621749	-548.151745	100.160	*His*$^{(-)}$*-OMe*	-587.5489193	-587.411643	105.683
His$^{(\circ)}$*–Au*$_3$***(b)***	-955.2723904	-955.162658	150.789	*His*$^{(\circ)}$*-OMe–Au*$_3$	-994.5249524	-994.3932160	158.178
His$^{(-)}$*–Au*$_3$***(f´)***	-954.7538392	-954.654945	142.425	*His*$^{(-)}$*-OMe–Au*$_3$	-994.0556734	-993.9369600	165.218
His$^{(\circ)}$*–Ag*$_3$***(k)***	-986.1895962	-986.079899	150.377	*His*$^{(\circ)}$*-OMe–Ag*$_3$	-1025.466183	-1025.339076	172.403
His$^{(-)}$*–Ag*$_3$***(n´)***	-985.6647644	-985.570033	152.841	*His*$^{(-)}$*-OMe–Ag*$_3$	-1024.964246	-1024.844339	162.127
His$^{(\circ)}$*–Cu*$_3$***(h)***	-1137.315130	-1137.202109	143.771	*His*$^{(\circ)}$*-OMe–Cu*$_3$	-1176.570174	-1176.440283	168.472
His$^{(-)}$*–Cu*$_3$***(g´)***	-1136.790228	-1136.691687	145.573	*His*$^{(-)}$*-OMe–Cu*$_3$	-1176.088611	-1175.965764	156.350

Table **S6.** Bond critical point data (in a.u.) from quantum theory of atoms in molecules.

Name	BCP	ρ(r)	$\nabla^2\rho(r)$	H(r)
*His$^{(-)}$–Au$_3$(**f´**)*	Au_1-N_5	0.099	0.296	-0.030
His$^{(-)}$-OMe–Au$_3$	Au_1-N_{10}	0.113	0.334	-0.039
*His$^{(-)}$–Ag$_3$(**n´**)*	A_{g1}-N_5	0.065	0.251	-0.009
His$^{(-)}$-OMe–Ag$_3$	Ag_1-N_{10}	0.074	0.302	-0.011
*His$^{(-)}$–Cu$_3$(**q´**)*	Cu_1-O_1	0.085	0.454	-0.018
His$^{(-)}$-OMe–Cu$_3$	Cu_1-N_{10}	0.097	0.398	-0.032

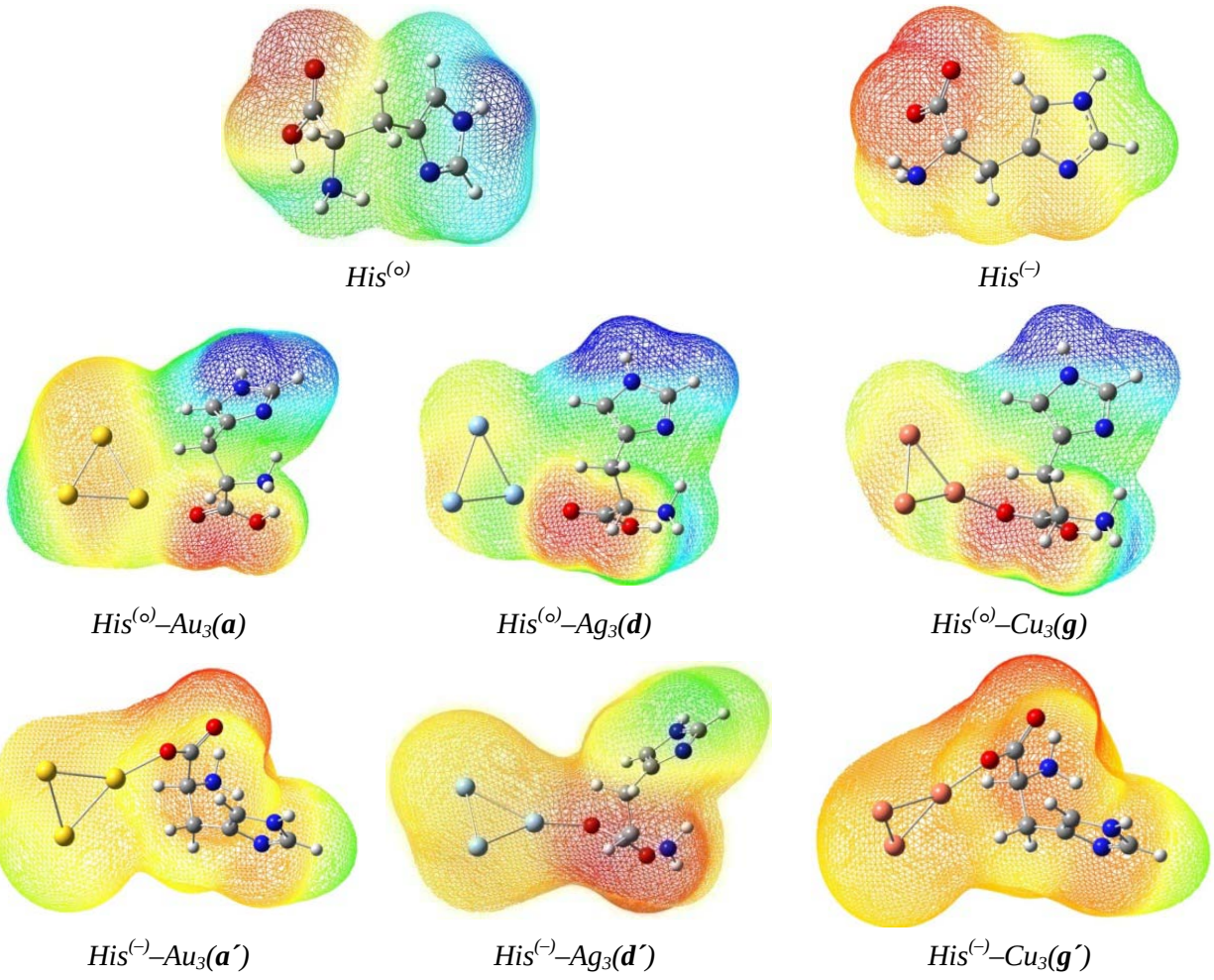


Fig **S**6**.** Illustration of electron density plots (ESP) [a] for histidine and the complexes in both neutral and anionic forms.

[a]In ESP plots, the intensity of electron density can be classified in the order of red > yellow > green> blue. The red color shows the highest electron density and blue color shows the lowest one.

List of energies and Cartesian coordinates

*$His^{(o)}$–Au_3**(a)***

E_{total} = -955.2560639 a.u.

Electronic and zero-point Energy = -955.093010

Thermal Energies = -955.076171

Enthalpy = -955.075227

Free Energy = -955.148444

0 2

N	-5.08629700	-1.63363400	0.95709800
C	-4.30329900	-1.66014900	-0.28950800
C	-2.81957900	-1.77800000	0.10649300
O	-1.91694800	-1.71267500	-0.73104500
H	-5.89131400	-2.24910800	0.92402200
H	-5.39733900	-0.68215800	1.16757800
H	-4.54592600	-2.56672000	-0.85663800
C	-4.50509100	-0.42551000	-1.20613200
C	-4.11808600	0.85113600	-0.52192700
H	-5.55954100	-0.39687000	-1.50338800
H	-3.90479700	-0.56246900	-2.10916400
C	-3.00535600	1.63450600	-0.72536000
N	-4.86005400	1.35117700	0.53735400
H	-2.17550900	1.55744600	-1.41088200
H	-2.37893200	3.34255900	0.37721500
C	-4.20586300	2.41719400	0.96033200
N	-3.08053200	2.63152900	0.22205500
H	-4.50180300	3.05886100	1.77818000
O	-2.60217300	-1.93664100	1.39081000
H	-3.52701300	-1.93470400	1.78497200
Au	2.72527500	-0.53843600	0.21710100
Au	0.92095000	1.67513100	-0.06659200
Au	0.18880000	-1.04873100	-0.24404000

His$^{(\circ)}$*–Au*$_3$***(b)***

E $_{total}$ = -955.2584434 a.u.

Electronic and zero-point Energy = -955.094837

Thermal Energies = -955.078111

Enthalpy = -955.077167

Free Energy = -955.150351

0 2

N	2.53003000	-1.62425100	0.99332400
C	3.36321700	-1.49483800	-0.20744000
C	4.84562900	-1.42520600	0.22414900
O	5.73145000	-0.99646700	-0.48666800
H	1.64114400	-2.07958800	0.78634700
H	2.29555900	-0.71322900	1.38345300
H	3.27201900	-2.43778900	-0.76253500
C	3.00992600	-0.35513700	-1.19364000
C	3.07815300	1.02110100	-0.60407300
H	1.99796000	-0.52841100	-1.57266200
H	3.70285300	-0.41761200	-2.03696000
C	4.17019400	1.83793300	-0.43554100
N	1.96065600	1.69220700	-0.11488300
H	5.21085500	1.67547400	-0.66823100
H	4.25706700	3.80183400	0.40143800
C	2.36565000	2.87569700	0.32812400
N	3.70120500	2.99696200	0.14949500
H	1.73707400	3.63740700	0.76267100
O	5.06921300	-1.90967100	1.45142000
H	4.17316600	-2.13030600	1.80864200
Au	-0.05522400	0.96736300	-0.03015700
Au	-2.65914500	0.57591500	0.15447400
Au	-1.04554100	-1.71758700	-0.17096500

His$^{(\circ)}$*–Au*$_3$***(c)***

E $_{total}$ = -955.2723904 a.u.

Electronic and zero-point Energy = -955.108702

Thermal Energies = -955.091957

Enthalpy = -955.091013

Free Energy = -955.162658

0 2

N	2.00416700	-1.22209500	-0.52864500
C	2.87563800	-1.47360100	0.65803000
C	2.78919000	-0.43401400	1.80175500
O	3.56495600	-0.53653500	2.72821000
H	2.08401400	-2.03967900	-1.13462400
H	2.41525200	-0.44997200	-1.07621300
H	2.55082300	-2.41671500	1.10494000
C	4.35861900	-1.61250500	0.22141200
C	4.91906100	-0.34874300	-0.36366300
H	4.42226800	-2.42905600	-0.50967100
H	4.94133300	-1.90736500	1.09667700
C	6.04427000	0.35135700	-0.00167900
N	4.27659200	0.30778200	-1.40335500
H	6.78108200	0.18456900	0.76816100
H	6.78525800	2.17308300	-0.83902800
C	5.00002900	1.37919800	-1.66324300
N	6.08665400	1.44432800	-0.84461600
H	4.78430100	2.12346200	-2.41635700
O	1.89555400	0.55967500	1.77240100
H	1.22547900	0.50416200	1.05758400
Au	-2.75630400	-0.61391200	-0.05285200
Au	-1.15287700	1.72537500	0.12968000
Au	-0.16887600	-0.94447400	-0.31145700

His$^{(\circ)}$*–Au*$_3$***(d)***

E $_{total}$ = -955.2666109 a.u.

Electronic and zero-point Energy = -955.103728

Thermal Energies = -955.086334

Enthalpy = -955.08539

Free Energy = -955.161436

0 2

N	6.03736100	0.45242400	-0.12464700
C	4.90901800	-0.32813700	0.37175800
H	6.83429300	0.35940300	0.50042900
H	4.73811700	-0.06976900	1.42252800
C	3.62096100	-0.00123500	-0.42237600
C	3.12654900	1.40197800	-0.22880800
H	2.81988500	-0.68397400	-0.12173000
H	3.81253400	-0.19112100	-1.48749700
C	3.81306000	2.59100800	-0.17728900
N	1.77266600	1.67935000	-0.08317600
H	4.86952100	2.78882300	-0.24946400
H	3.04055200	4.56792500	0.08476300
C	1.64349100	2.99178000	0.05244600
N	2.86157800	3.57772600	0.00121100
H	0.71310200	3.52188600	0.18717900
Au	-1.58989000	-1.70178600	-0.13078900
Au	0.09699700	0.33854500	-0.07838700
Au	-2.66425600	0.90088200	0.15902900
H	6.34023700	0.07823700	-1.02278100
C	5.15437000	-1.84096600	0.30278700
O	5.97872500	-2.37680800	-0.40834100
O	4.32635900	-2.52602700	1.12138600
H	4.49999100	-3.47545200	0.99904300

His$^{(\circ)}$*–Au*$_3$***(e)***

E $_{total}$ = -955.2639946 a.u.

Electronic and zero-point Energy = -955.100360

Thermal Energies = -955.083171

Enthalpy = -955.082227

Free Energy = -955.157395

0 2

N	2.48619400	-0.89272600	-0.95697600
C	3.62820100	-0.16907400	-0.35027100
H	2.59982500	-0.90586700	-1.96964300
H	3.74654700	0.79013800	-0.86280300
C	3.41003000	0.13011700	1.15715300
C	2.49301000	1.29363700	1.38234200
H	4.38955300	0.35494800	1.59285300
H	3.02578600	-0.76708100	1.65556200
C	1.30641900	1.34799300	2.07932600
N	2.79681000	2.53633900	0.86121800
H	0.73122900	0.59454200	2.59484700
H	0.01303600	3.02460700	2.32663900
C	1.81174700	3.32792600	1.23216600
N	0.88811700	2.65755200	1.98195000
H	1.71874200	4.37821200	0.99390900
Au	-2.00687100	0.88659800	-0.86599000
Au	-1.69371700	-1.21812400	1.00016800
Au	0.39232900	-0.23565100	-0.62333400
H	2.53755800	-1.87241900	-0.67252400
C	4.89552400	-0.99763300	-0.54870100
O	4.90509900	-2.17573600	-0.84633000
O	6.01321000	-0.27748200	-0.33849900
H	6.77632700	-0.87029700	-0.45229300

His$^{(\circ)}$*–Au*$_3$***(f)***

E $_{total}$ = -955.2611106 a.u.

Electronic and zero-point Energy = -955.097402

Thermal Energies = -955.080444

Enthalpy = - -955.0795

Free Energy = -955.152338

0 2

N	1.62472000	-2.20170900	-0.15168200
C	2.74693000	-1.23701300	-0.28840200
H	1.58528000	-2.80454400	-0.97298600
H	2.50717600	-0.56070900	-1.11163200
C	2.90507400	-0.41787400	1.03015200
C	3.58416000	0.90177200	0.87328800
H	3.44685300	-1.02065300	1.76755700
H	1.89083800	-0.26842300	1.42195100
C	4.84667500	1.35046100	1.19498100
H	5.64905700	0.79035300	1.65660300
C	3.84587900	3.03340600	0.32852000
N	5.00142100	2.67439700	0.85224300
H	3.59958700	4.01669000	-0.04755400
Au	-0.34789300	-1.22432100	0.04687100
Au	-0.69690300	1.57092900	-0.50605000
Au	-2.75566300	-0.21675500	0.31071900
H	1.81115000	-2.82890000	0.63182000
C	4.03217500	-1.99238900	-0.61095300
O	4.23620200	-3.14618900	-0.28732200
O	4.91561300	-1.23064200	-1.27379300
H	5.73140900	-1.74693300	-1.39904600
N	2.95297800	1.99986600	0.31297100
H	1.98110800	2.04134600	0.01035600

His$^{(\circ)}$*–Au*$_3$***(g)***

E $_{total}$ = -955.2485977 a.u.

Electronic and zero-point Energy = -955.086849

Thermal Energies = -955.07028

Enthalpy = -955.069335

Free Energy = -955.140458

0 2

N	3.40495200	0.12516500	2.00507400
C	3.41629600	-0.57836500	0.72773200
H	2.98771600	-0.45948800	2.72487400
H	2.41922700	-1.00665900	0.55765300
C	3.72401900	0.38119400	-0.43955700
C	2.75786200	1.51341400	-0.64793600
H	3.78992100	-0.17923000	-1.37641100
H	4.71645000	0.82863600	-0.27858800
C	1.84632500	2.12406900	0.25243000
N	2.80883200	2.21804900	-1.82313400
H	1.88755600	2.09525200	1.33395000
H	0.72263900	3.92580000	-0.11855200
C	2.00777700	3.25844600	-1.65693000
N	1.43418300	3.28144100	-0.43468700
H	1.79978700	4.00537200	-2.41184800
Au	0.24877300	0.54396200	-0.07185900
Au	-1.20116400	-1.65663800	-0.59931700
Au	-2.41862200	0.61136400	0.62776000
H	4.36084600	0.30476700	2.30780100
C	4.41790000	-1.74016600	0.69716100
O	5.28375100	-1.93116000	1.52557700
O	4.23660200	-2.54235900	-0.37574500
H	4.90619000	-3.24684100	-0.33580700

His$^{(\circ)}$*–Au*$_3$***(h)***

E $_{total}$ = -955.2681575 a.u.

Electronic and zero-point Energy = -955.103929

Thermal Energies = -955.0871

Enthalpy = -955.086156

Free Energy = -955.160216

0 2

N	2.14281900	-0.28940300	-1.21495400
C	2.86935100	0.87103700	-0.64559900
H	2.22710400	-0.25642300	-2.23251900
H	2.46275500	1.09234600	0.34386000
C	4.39880500	0.61448700	-0.52083400
C	4.71722300	-0.50777200	0.42175400
H	4.87897900	1.53427800	-0.17280900
H	4.79776900	0.39359200	-1.51975700
C	5.48102900	-0.49526600	1.56566900
N	4.20952800	-1.77900800	0.21324600
H	6.03386000	0.28876400	2.06010300
H	5.88943100	-2.12527000	2.88889200
C	4.65399700	-2.51872100	1.20925200
N	5.43436900	-1.78685800	2.05359600
H	4.44410700	-3.56763300	1.36355300
Au	0.00801400	-0.38604900	-0.71684700
Au	-2.58401400	-0.80387800	-0.42183500
Au	-1.32824400	0.99803900	1.37405500
H	2.58904200	-1.15188000	-0.88159300
C	2.63390800	2.06888200	-1.55412300
O	2.37743700	1.98752800	-2.73700600
O	2.80018500	3.23578600	-0.90326400
H	2.65843900	3.95593900	-1.54194600

His$^{(-)}$*–Au*$_3$***(a´)***

E $_{total}$ = -954.7491579 a.u.

Electronic and zero-point Energy = -954.599466

Thermal Energies = -954.582456

Enthalpy = -954.581512

Free Energy = -954.655426

-1 2

N	-5.18722500	-2.00249700	0.88947800
C	-4.23380100	-1.83222100	-0.21082300
C	-2.75832100	-1.69498100	0.27151400
O	-1.94333200	-1.37039500	-0.68656000
H	-5.50818600	-1.08580300	1.19760800
H	-4.67268800	-2.39478900	1.67728900
H	-4.24958100	-2.74481700	-0.82625600
C	-4.64943500	-0.66305700	-1.13536300
C	-4.51153500	0.69406000	-0.50436000
H	-5.69553200	-0.81022800	-1.42699300
H	-4.03028200	-0.71244900	-2.03434300
C	-3.37281600	1.46252400	-0.39116100
N	-5.57180700	1.33520500	0.12029300
H	-2.35444800	1.28908400	-0.70357800
H	-3.13503200	3.33433200	0.59688600
C	-5.08086800	2.46192600	0.59945800
N	-3.75112600	2.58780900	0.31141500
H	-5.63348300	3.21264100	1.14791800
O	-2.46802300	-1.92296300	1.44925500
Au	2.72653900	-0.68577300	0.13870000
Au	1.23722300	1.71190100	0.00186900
Au	0.08410900	-0.89643400	-0.22606300

His$^{(-)}$*–Au*$_3$(***b´***)

E $_{total}$ = -954.7399646 a.u.

Electronic and zero-point Energy = -954.590810

Thermal Energies = -954.574466

Enthalpy = -954.573521

Free Energy = -954.644446

-1 2

N	4.27057200	0.14033700	2.46058900
C	3.11847000	0.02709800	1.55962800
C	2.91666900	-1.41380600	1.00762400
O	1.87926000	-1.64217400	0.25274400
H	5.09868200	0.37331100	1.91459400
H	4.45585500	-0.78808000	2.83727200
H	2.20525500	0.27236700	2.12161000
C	3.22596700	1.06923600	0.41650300
C	4.29620000	0.76696600	-0.59195200
H	3.43204100	2.04494500	0.86971700
H	2.25632500	1.13668100	-0.08512100
C	4.22218400	-0.09526900	-1.66369900
N	5.56731300	1.31794900	-0.52378900
H	3.42443000	-0.73514100	-2.00849500
H	5.76125700	-0.60735800	-3.05397300
C	6.24278600	0.79782800	-1.52883100
N	5.47010100	-0.06549200	-2.25486000
H	7.27323400	1.00977300	-1.78003400
O	3.74416400	-2.28942000	1.28281000
Au	0.03823200	-0.58411200	0.13186600
Au	-1.55355100	1.63556000	0.15939900
Au	-2.66422500	-0.89848000	-0.36809100

His$^{(-)}$*–Au*$_3$***(c´)***

E $_{total}$ = -954.7390123 a.u.

Electronic and zero-point Energy = -954.588933

Thermal Energies = -954.572196

Enthalpy = -954.571252

Free Energy = -954.643915

-1 2

N	2.08308200	0.73221300	-0.62441100
C	2.96876200	-0.17433500	-1.38118000
C	2.86327000	-1.64554600	-0.83990400
O	3.83784300	-2.39048700	-1.07773600
H	1.91982800	1.60647500	-1.11610900
H	2.49540400	0.96582000	0.27710000
H	2.57311800	-0.20900400	-2.40478700
C	4.43130600	0.32199300	-1.45296500
C	5.09656600	0.46550800	-0.11261100
H	4.46367700	1.29930800	-1.94928000
H	4.98225900	-0.39500600	-2.06801600
C	5.46430500	-0.53079400	0.76647500
N	5.41000800	1.70535100	0.42612200
H	5.35135600	-1.60216300	0.69816900
H	6.36212800	-0.31966400	2.69285400
C	5.95631900	1.46233800	1.60117400
N	6.01451600	0.11959400	1.85399100
H	6.32150500	2.20429200	2.29821200
O	1.79103700	-1.96203800	-0.23537800
Au	-2.45580400	-1.16388100	0.38418000
Au	0.04733100	-0.33254000	-0.15608300
Au	-1.82870100	1.67332100	-0.11416100

His$^{(-)}$*–Au*$_3$***(d´)***

E $_{total}$ = -954.7301427 a.u.

Electronic and zero-point Energy = -954.580704

Thermal Energies = -954.563658

Enthalpy = -954.562714

Free Energy = -954.636506

-1 2

N	6.13446000	0.67362700	-0.25088900
C	5.16125300	-0.25743500	0.36932400
H	6.91580600	0.76378600	0.39754500
H	5.07306100	-0.02151800	1.43654400
C	3.76516000	-0.10131400	-0.27189000
C	3.15320500	1.26101300	-0.13175700
H	3.09719700	-0.84277100	0.17848100
H	3.84303800	-0.35451800	-1.33909900
C	3.76798800	2.49074200	-0.11003200
N	1.78163700	1.47906500	-0.00658200
H	4.81782000	2.71909500	-0.19738100
H	2.89133600	4.43286700	0.09094100
C	1.57837700	2.78817700	0.09177200
N	2.76463000	3.43411500	0.03325100
H	0.61916200	3.26943900	0.20419700
Au	-1.80415800	-1.66707800	-0.06684000
Au	0.13362800	0.13638700	-0.02243100
Au	-2.61393200	1.03459900	0.06272400
H	6.53474900	0.11971100	-1.01703900
C	5.59626200	-1.76787200	0.23494800
O	6.44236900	-1.99956900	-0.67378300
O	5.03035100	-2.56072400	1.02607900

*$His^{(-)}$–Au_3(**e´**)*

E_{total} = -954.7462652 a.u.

Electronic and zero-point Energy = -954.596034

Thermal Energies = -954.579317

Enthalpy = -954.578373

Free Energy = -954.652125

-1 2

N	2.54645400	-0.75281400	-0.99549200
C	3.72917000	-0.05118600	-0.39583100
H	2.56035700	-0.57463000	-1.99812700
H	3.95433700	0.83408700	-0.99603900
C	3.51681700	0.39446900	1.06397600
C	2.52559100	1.50260700	1.24906600
H	4.50364800	0.71218800	1.41707000
H	3.21678500	-0.47100400	1.66732100
C	1.32872400	1.47274600	1.93327300
N	2.70591200	2.75455600	0.68325700
H	0.83069100	0.68907900	2.48270600
H	-0.15629000	2.99951500	2.05367600
C	1.64100200	3.45540800	1.01120600
N	0.77939500	2.73221000	1.78715800
H	1.44350500	4.47958500	0.72479300
Au	-1.85875300	0.99584100	-0.87177200
Au	-1.82867200	-1.18910500	0.87040700
Au	0.48488000	-0.46178600	-0.42254500
H	2.84343200	-1.74693100	-0.91053100
C	4.94502400	-1.06071700	-0.46413200
O	4.61736100	-2.25596700	-0.72790400
O	6.06567200	-0.56785800	-0.22981800

His$^{(-)}$*–Au*$_3$***(f´)***

E $_{total}$ = -954.7538392 a.u.

Electronic and zero-point Energy = -954.603695

Thermal Energies = -954.588219

Enthalpy = -954.587275

Free Energy = -954.654945

-1 2

N	2.27106800	-0.93171600	-1.19709000
C	3.50530300	-0.74427200	-0.36265000
H	2.30862800	-0.35666900	-2.03518400
H	4.24119400	-0.20795700	-0.97536900
C	3.31394900	0.03920600	0.94496200
C	3.20982200	1.52910900	0.81035600
H	4.19235500	-0.19455200	1.55339300
H	2.44166900	-0.36528400	1.47623000
C	4.14707700	2.52842400	0.98292600
H	5.18097000	2.41012700	1.27880400
C	2.34947800	3.54011500	0.40973600
N	3.60741200	3.77430400	0.73159200
H	1.60846900	4.28516000	0.15455300
Au	0.27933700	-0.73787400	-0.40641400
Au	-1.57106400	1.45580900	-0.45380500
Au	-2.14906100	-1.04804100	0.67601300
H	2.40236500	-1.93886200	-1.46653200
C	4.10653600	-2.19346600	-0.13296800
O	3.57787700	-3.08340700	-0.86442500
O	5.03849800	-2.27550100	0.68809500
N	2.05998600	2.20526200	0.43955600
H	1.15338500	1.78805600	0.24444600

*$His^{(-)}$–Au_3(**g´**)*

E $_{total}$ = -954.7134533 a.u.

Electronic and zero-point Energy = -954.565330

Thermal Energies = -954.548174

Enthalpy = -954.54723

Free Energy = -954.621864

-1 2

N	3.79715500	-0.00277900	1.79416800
C	3.87309200	-0.55946900	0.42397000
H	3.33745000	-0.69578800	2.38246700
H	2.98524200	-1.17842100	0.23389500
C	3.91504200	0.55375300	-0.63516800
C	2.80656100	1.55291100	-0.63382500
H	3.99203300	0.09300900	-1.62602300
H	4.84521100	1.13060300	-0.50599600
C	1.83500000	1.78565100	0.38341500
N	2.68458900	2.48707000	-1.62935800
H	2.04508600	1.58921700	1.43238200
H	0.37492400	3.37864200	0.38094200
C	1.72313200	3.31209500	-1.23431500
N	1.21460400	2.99360100	-0.02960600
H	1.35132400	4.14519300	-1.81791200
Au	0.34499500	0.17511100	0.01477500
Au	-1.51822800	-1.71326900	-0.30286800
Au	-2.40713600	0.90786100	0.33281700
H	4.77212900	-0.02755200	2.11500000
C	5.15064200	-1.46527800	0.20083100
O	6.01699300	-1.40341900	1.11555600
O	5.16431600	-2.10467300	-0.87853900

His$^{(-)}$*–Au*$_3$***(h´)***

E $_{total}$ = -954.7478802 a.u.

Electronic and zero-point Energy = -954.597405

Thermal Energies = -954.580814

Enthalpy = -954.57987

Free Energy = -954.652731

-1 2

N	2.42794800	-1.03573300	0.63026800
C	3.40066700	-0.71432000	-0.46702300
H	2.66726000	-2.02933400	0.82648500
H	2.84268000	-0.59086600	-1.39916000
C	4.18308800	0.58125200	-0.17435200
C	3.29393700	1.74619400	0.14655700
H	4.81345400	0.77457200	-1.04588100
H	4.85424600	0.41296700	0.67649100
C	2.58235800	2.56195300	-0.70473900
N	2.97800100	2.06028500	1.46012600
H	2.52167000	2.60603500	-1.78126400
H	1.08669500	3.99983900	-0.20044400
C	2.09079000	3.03356000	1.39792200
N	1.82757700	3.38714700	0.10737700
H	1.61219600	3.51154300	2.24120500
Au	0.32794000	-0.74061200	0.29202500
Au	-2.32600900	-1.13802500	0.04656300
Au	-1.39542400	1.46416000	-0.36707200
H	2.66101700	-0.49492100	1.46450000
C	4.36517700	-1.94787500	-0.64659200
O	4.11787900	-2.92467600	0.11933400
O	5.24411200	-1.81190500	-1.52267000

His$^{(\circ)}$*–Ag*$_3$***(i)***

E $_{total}$ = -986.181893 a.u.

Electronic and zero-point Energy = -986.019074

Thermal Energies = -986.002131

Enthalpy = -986.001187

Free Energy = -986.073576

0 2

N	4.87831800	1.10075400	-0.89262600
C	4.38397800	0.45255500	0.33446900
C	3.50237300	-0.74099700	-0.08803300
O	2.82859800	-1.38803200	0.70573500
H	5.85835300	1.35295100	-0.82797700
H	4.33045800	1.93992600	-1.09832900
H	5.23366300	0.02066300	0.87757400
C	3.60631500	1.38534900	1.29682200
C	2.37834000	1.96698600	0.66314200
H	4.28885000	2.18234700	1.61513900
H	3.32631100	0.81141500	2.18404400
C	1.05733800	1.70964300	0.95111400
N	2.46288600	2.83235900	-0.41644200
H	0.58500600	1.08024500	1.68870900
H	-0.67856000	2.39758100	-0.06770300
C	1.21510000	3.08718500	-0.76884000
N	0.33004600	2.43719400	0.03613600
H	0.90579500	3.72747700	-1.58277700
O	3.53007200	-1.00363700	-1.38493500
H	4.13474300	-0.29721000	-1.75655800
Ag	-3.42609200	1.23403500	0.01093800
Ag	-1.99373800	-1.06299800	-0.14191700
Ag	0.53869500	-1.99738800	0.10927600

*His$^{(\circ)}$–Ag$_3$**(j)***

E $_{total}$ = -986.1766233 a.u.

Electronic and zero-point Energy = -986.013619

Thermal Energies = -985.996602

Enthalpy = -985.995658

Free Energy = -986.069585

0 2

N	1.58259700	-1.06344400	-0.24860800
C	2.51925200	-1.20082600	0.89467900
C	2.58905100	0.03282300	1.81729300
O	3.37772400	0.06061300	2.73564600
H	1.44245500	-1.99308200	-0.64275600
H	2.05550900	-0.53316200	-0.99090500
H	2.14051800	-2.00833800	1.53154700
C	3.95612200	-1.57315400	0.43909500
C	4.60238300	-0.50669200	-0.39585000
H	3.89690500	-2.51235400	-0.12642200
H	4.56079800	-1.76105800	1.32916500
C	5.77572000	0.17436300	-0.17178500
N	4.01070800	-0.04431600	-1.56234900
H	6.49824700	0.12254900	0.62789500
H	6.64913700	1.71821800	-1.36494900
C	4.81074000	0.89342300	-2.03069600
N	5.89772400	1.05864200	-1.22527800
H	4.65344000	1.47069700	-2.93082000
O	1.76746900	1.06919400	1.58669000
H	1.13624700	0.88788300	0.86496300
Ag	-2.31451100	1.71631000	0.07049600
Ag	-0.71629600	-0.46807200	-0.14222900
Ag	-3.35539700	-1.05686900	-0.24612200

*His$^{(\circ)}$–Ag$_3$(**k**)*

E $_{total}$ = -986.1895962 a.u.

Electronic and zero-point Energy = -986.026324

Thermal Energies = -986.009394

Enthalpy = -986.00845

Free Energy = -986.079899

0 2

N	-2.22468100	-1.66574200	-0.83784100
C	-3.04149400	-1.43204900	0.35958200
C	-4.52650600	-1.34364400	-0.06065600
O	-5.39261500	-0.86156700	0.63960900
H	-1.36260300	-2.16234500	-0.61760500
H	-1.94835600	-0.78830700	-1.27457600
H	-2.97421900	-2.33790300	0.97644800
C	-2.64102300	-0.23588900	1.25627600
C	-2.64830600	1.09087200	0.55674800
H	-1.63739800	-0.42373800	1.65135100
H	-3.33463700	-0.20564000	2.10086500
C	-3.70597800	1.93909600	0.32523700
N	-1.50052900	1.65166400	0.00828900
H	-4.75132400	1.85206800	0.57747500
H	-3.70281100	3.82398400	-0.68132800
C	-1.85648400	2.80684300	-0.53235600
N	-3.18578300	3.01716700	-0.36234600
H	-1.19976000	3.50087300	-1.03572300
O	-4.77690200	-1.87759400	-1.26252100
H	-3.89141900	-2.14182100	-1.61605100
Ag	3.31470900	0.64561700	-0.07961500
Ag	0.62708900	0.77059600	0.03536800
Ag	1.69765600	-1.78167900	0.08290100

His$^{(\circ)}$*–Ag*$_3$***(l)***

E $_{total}$ = -986.1843858 a.u.

Electronic and zero-point Energy = -986.021917

Thermal Energies = -986.004373

Enthalpy = -986.003428

Free Energy = -986.078703

0 2

N	5.38010100	0.15534600	-0.22947300
C	4.18870000	-0.49836800	0.30191100
H	6.18952900	-0.06171700	0.34693000
H	4.09422600	-0.24589100	1.36376200
C	2.91700300	-0.00400700	-0.42827600
C	2.58651200	1.43929800	-0.17896400
H	2.05830600	-0.60583500	-0.11299200
H	3.04605600	-0.18427400	-1.50476600
C	3.40605300	2.54073800	-0.10081300
N	1.27164900	1.84820300	-0.00528500
H	4.47672300	2.62609400	-0.18580800
H	2.85686300	4.57976800	0.23770800
C	1.29468200	3.15875500	0.17323300
N	2.57000100	3.61845300	0.12437200
H	0.43399700	3.78973400	0.33927100
H	5.58680200	-0.21712900	-1.15508800
C	4.24753700	-2.02733600	0.19407800
O	4.96133800	-2.64173000	-0.57142800
O	3.38799000	-2.62757900	1.04636900
H	3.43131100	-3.58712800	0.89197300
Ag	-3.36511900	0.63937300	0.06677900
Ag	-0.64005300	0.56849600	-0.01991400
Ag	-1.85362900	-1.86632900	-0.11101100

His$^{(\circ)}$*–Ag*$_3$***(m)***

E $_{total}$ = -986.1844895 a.u.

Electronic and zero-point Energy = -986.004122

Thermal Energies = -986.004122

Enthalpy = -986.003178

Free Energy = -986.077698

0 2

N	2.11521300	-1.18052800	-0.68556400
C	3.28116700	-0.32637600	-0.40554300
H	2.10828000	-1.43669800	-1.67110200
H	3.33583900	0.45906800	-1.16551100
C	3.16174900	0.37374500	0.97459600
C	2.12833800	1.45913700	0.97452800
H	4.13775300	0.80720000	1.21829500
H	2.93244400	-0.37405100	1.74279200
C	1.00183500	1.59363300	1.75917200
N	2.23942600	2.53640600	0.11702000
H	0.58317100	0.97993500	2.54183200
H	-0.45472300	3.15324900	1.69528900
C	1.20462800	3.30841600	0.37720100
N	0.43138400	2.79027500	1.37498500
H	0.96758200	4.23827700	-0.12037300
H	2.22444000	-2.06029700	-0.17990500
C	4.56935700	-1.14566700	-0.45816000
O	4.62000400	-2.35733400	-0.38878600
O	5.66568400	-0.36714300	-0.56889800
H	6.44491100	-0.94967400	-0.56550800
Ag	-2.39754200	0.73282800	-1.17582300
Ag	-0.10205600	-0.42789400	-0.26480600
Ag	-2.39720700	-1.23305300	0.99785900

*His$^{(\circ)}$–Ag$_3$(**n**)*

E $_{total}$ = -986.179892 a.u.

Electronic and zero-point Energy = -986.016691

Thermal Energies = -985.999569

Enthalpy = -985.998624

Free Energy = -986.070869

0 2

N	-1.09548300	-2.20769000	0.09380400
C	-2.19651600	-1.24156100	0.30063200
H	-1.02186300	-2.82759000	0.89926600
H	-1.94455600	-0.62225500	1.16512300
C	-2.33540900	-0.34120000	-0.95974900
C	-3.19288900	0.86813800	-0.78072400
H	-2.73278300	-0.94616300	-1.78268500
H	-1.31746100	-0.04037500	-1.24049900
C	-4.47597700	1.17259700	-1.18069000
H	-5.15450700	0.55121800	-1.75011300
C	-3.78624300	2.89905000	-0.11753500
N	-4.83686000	2.43442400	-0.76324800
H	-3.70642700	3.87349900	0.34410200
H	-1.32452100	-2.81280200	-0.69538900
C	-3.51187400	-1.96959000	0.56860200
O	-3.83988300	-2.99837900	0.01143000
O	-4.27140000	-1.33873200	1.48121300
H	-5.11694700	-1.81568500	1.55450900
N	-2.76441000	1.99165500	-0.09384600
H	-1.83599800	2.13308500	0.29331000
Ag	1.25482200	1.54710700	0.64007800
Ag	0.98609000	-1.14306800	-0.11399500
Ag	3.43815300	-0.11998300	-0.36372000

*His$^{(o)}$–Ag$_3$(**o**)*

E $_{total}$ = -986.183589 a.u.

Electronic and zero-point Energy = -986.020588

Thermal Energies = -986.004197

Enthalpy = -986.003252

Free Energy = -986.072901

0 2

N	1.99681500	-1.33298800	-0.14188500
C	3.26843600	-0.60103500	-0.25950200
H	1.88024300	-1.95120600	-0.94285500
H	3.35749600	-0.20505300	-1.27553300
C	3.32681000	0.60625800	0.71355000
C	2.39208700	1.70356400	0.30714500
H	4.35403600	0.98690900	0.71806600
H	3.09749600	0.26544300	1.73004800
C	1.35890400	2.27704500	1.01758700
N	2.50679100	2.30639100	-0.93063600
H	0.96877200	2.09579900	2.00707800
H	0.00626300	3.78845400	0.36302300
C	1.56514500	3.22760800	-0.96653900
N	0.85473900	3.26467300	0.19688800
H	1.35740700	3.88745500	-1.79718800
H	2.04902200	-1.95421400	0.66661300
C	4.44968500	-1.53135300	0.00778300
O	4.37195000	-2.59619400	0.58699400
O	5.61300300	-1.02538900	-0.45201200
H	6.32115300	-1.65051500	-0.21888600
Ag	-2.44939700	1.17890300	0.09945200
Ag	-0.14978800	-0.29533900	-0.00873000
Ag	-2.48478000	-1.73568000	-0.11457100

*His$^{(o)}$–Ag$_3$**(p)***

E $_{total}$ = -954.7478802 a.u.

Electronic and zero-point Energy = -986.022497

Thermal Energies = -986.005466

Enthalpy = -986.004522

Free Energy = -986.078143

0 2

N	1.64884400	0.17564100	-1.20594200
C	2.41054700	1.04201000	-0.28635100
H	1.68641100	0.57924600	-2.14224000
H	2.05625500	0.87788200	0.73585700
C	3.94708500	0.78809500	-0.32145000
C	4.31267600	-0.58886100	0.14688600
H	4.44212800	1.53077500	0.31225000
H	4.30050500	0.94265000	-1.34937000
C	5.10936200	-0.95965200	1.20581300
N	3.82959700	-1.71871200	-0.49170900
H	5.65793400	-0.38469700	1.93615800
H	5.59887800	-2.93946200	1.85139600
C	4.32201900	-2.74877500	0.16616500
N	5.10866900	-2.34120600	1.20263300
H	4.14512300	-3.79048800	-0.06161600
H	2.09645400	-0.74402100	-1.23957800
C	2.13738400	2.49232700	-0.65570000
O	1.78356900	2.86781600	-1.75394400
O	2.38277000	3.33122400	0.37176400
H	2.21083600	4.23672400	0.06072900
Ag	-2.05689900	0.55604000	1.59874300
Ag	-3.16370500	-0.92048100	-0.68517400
Ag	-0.58938300	-0.12198200	-0.63938100

*$His^{(-)}$–Ag_3(**i'**)*

E_{total} = -985.664168 a.u.

Electronic and zero-point Energy = -985.514711

Thermal Energies = -985.497631

Enthalpy = -985.496687

Free Energy = -985.568954

-1 2

N	4.82990200	0.58465100	-1.09645500
C	4.31238700	0.20983800	0.22587000
C	3.15417900	-0.82363600	0.19547800
O	2.63100900	-1.14397600	1.30063900
H	4.30005800	1.38413900	-1.44173400
H	4.60935000	-0.17684400	-1.73616300
H	5.12427200	-0.25819400	0.80220700
C	3.86164300	1.46758400	1.01705800
C	2.59582100	2.08404400	0.49190300
H	4.67080100	2.20617900	0.97461400
H	3.71669700	1.17171500	2.05894800
C	1.29918900	1.75038600	0.82118600
N	2.58860000	3.04251200	-0.51032200
H	0.90206200	1.02200100	1.51009400
H	-0.51549400	2.43675400	-0.05536900
C	1.31499800	3.26986800	-0.77929100
N	0.49359500	2.51683500	0.00767800
H	0.93794900	3.96230800	-1.51940300
O	2.77396500	-1.25994400	-0.93475500
Ag	-3.33797100	1.26418700	0.03938000
Ag	-2.00430700	-1.12132000	-0.05260200
Ag	0.62739600	-1.91463700	-0.07528400

*$His^{(-)}$–Ag_3(**j'**)*

E_{total} = -985.6583933 a.u.

Electronic and zero-point Energy = -985.509275

Thermal Energies = -985.49207

Enthalpy = -985.491125

Free Energy = -985.564868

-1 2

N	-3.77765700	-2.52515300	-0.28710500
C	-2.61861300	-1.62811100	-0.18296400
C	-2.37861300	-1.11004300	1.27137500
O	-1.41550500	-0.26711700	1.43450600
H	-4.58785400	-1.99334300	-0.60032900
H	-3.99788700	-2.82140800	0.66425000
H	-1.71279900	-2.19533100	-0.44967100
C	-2.72458300	-0.46626200	-1.20042200
C	-3.80534800	0.53009900	-0.88611500
H	-2.92257200	-0.88860100	-2.19196100
H	-1.75661500	0.04167200	-1.24523300
C	-3.81547100	1.47527300	0.11681900
N	-4.99967200	0.58338700	-1.58969400
H	-3.09144200	1.69913600	0.88550900
H	-5.37593400	2.84192500	0.62484900
C	-5.71319000	1.53593400	-1.02263100
N	-5.03749700	2.11114600	0.01784400
H	-6.70450900	1.85073600	-1.31948600
O	-3.12051100	-1.52644200	2.17616500
Ag	2.74023800	1.58139300	0.09939800
Ag	0.60511800	-0.12194400	0.56418400
Ag	2.81371700	-1.19122100	-0.68096500

His$^{(-)}$*–Ag*$_3$***(k')***

E $_{total}$ = -985.6613444 a.u.

Electronic and zero-point Energy = -985.511719

Thermal Energies = -985.494908

Enthalpy = -985.493964

Free Energy = -985.566249

-1 2

N	1.53639400	-0.27400100	-1.08764500
C	2.40508700	-1.35949200	-0.59241400
C	2.29819500	-1.52874800	0.96930300
O	3.26521700	-2.09907400	1.52164300
H	1.44969800	-0.31153400	-2.10020700
H	1.94902900	0.63009200	-0.86398500
H	2.00221500	-2.29253500	-1.01076400
C	3.87531800	-1.23469600	-1.06294700
C	4.56161700	0.01798900	-0.59459200
H	3.91033000	-1.24471600	-2.15940200
H	4.41129200	-2.11299300	-0.69241700
C	4.91845000	0.35968700	0.69251200
N	4.90765200	1.04343400	-1.46394300
H	4.78201300	-0.17379600	1.62100900
H	5.83900500	2.16492100	1.36824000
C	5.46110400	1.97985400	-0.71871200
N	5.49424400	1.61229000	0.59815000
H	5.84905100	2.92623500	-1.07053200
O	1.23961000	-1.10833000	1.53076200
Ag	-3.15437200	-0.97892200	-0.46098000
Ag	-0.54800400	-0.30210600	0.24845100
Ag	-2.48736700	1.70643000	0.25516700

His$^{(-)}$*–Ag*$_3$***(I′)***

E $_{total}$ = -985.6546256 a.u.

Electronic and zero-point Energy = -985.505726

Thermal Energies = -985.488391

Enthalpy = -985.487447

Free Energy = -985.562986

-1 2

N	4.38002100	-0.93069100	1.77769700
C	3.50748900	-0.86221400	0.58868900
H	3.82716000	-1.29152700	2.55417100
H	2.59487400	-0.32079700	0.86684100
C	4.20873400	-0.08967700	-0.54857300
C	4.48405100	1.36306300	-0.27516000
H	3.59265600	-0.14695400	-1.45181000
H	5.14636200	-0.61445100	-0.78219900
C	4.79736500	1.98780400	0.91207500
N	4.45832300	2.29839700	-1.30010700
H	4.91739100	1.58464900	1.90430900
H	5.16892400	4.06900500	1.24934000
C	4.74243500	3.45751600	-0.74444900
N	4.95914100	3.32722300	0.59946500
H	4.79903200	4.40974100	-1.25455000
H	5.05269200	-1.67535600	1.58040700
C	3.12263000	-2.27701200	0.05538900
O	3.97730400	-3.17460400	0.17686200
O	1.97445000	-2.41248000	-0.50539700
Ag	-2.24861200	0.12826800	-0.12058500
Ag	-4.88955200	0.69264000	0.26333700
Ag	0.14940300	-1.15407900	-0.34499500

His$^{(-)}$*–Ag*$_3$***(m´)***

E $_{total}$ = -985.658558 a.u.

Electronic and zero-point Energy = -985.508779

Thermal Energies = -985.492899

Enthalpy = -985.491955

Free Energy = -985.559885

-1 2

N	2.13637800	-0.97510400	-0.91375400
C	3.36209300	-0.23950000	-0.48118600
H	2.10211600	-0.94965600	-1.93084400
H	3.62084200	0.50361900	-1.24094700
C	3.17708000	0.49650400	0.86131900
C	2.15950300	1.59566700	0.84117000
H	4.16126900	0.89920400	1.12254600
H	2.90717300	-0.23212800	1.63628300
C	0.98129000	1.68156200	1.55647800
N	2.29096200	2.71394400	0.03279800
H	0.53687900	1.03357100	2.29618700
H	-0.52603800	3.19284900	1.43763200
C	1.22249100	3.44995500	0.25469000
N	0.39989900	2.88184000	1.18518200
H	0.99278000	4.39275400	-0.22338900
H	2.39574800	-1.95363900	-0.69363000
C	4.55273600	-1.26928400	-0.34434400
O	4.20722000	-2.48589300	-0.39590800
O	5.68348200	-0.76326700	-0.17899700
Ag	-2.30562400	-1.09465600	1.13421200
Ag	0.00060800	-0.48513400	-0.28221300
Ag	-2.41494600	0.56856700	-1.19376400

His$^{(\circ)}$*–Ag*$_3$***(n′)***

E $_{total}$ = -985.6647644 a.u.

Electronic and zero-point Energy = -985.514959

Thermal Energies = -985.498358

Enthalpy = -985.497414

Free Energy = -985.570033

-1 2

N	-1.73600200	-1.10197100	1.22967700
C	-2.93309100	-1.18097300	0.34437600
H	-1.90677100	-0.49847100	2.03010000
H	-3.82595500	-0.93304100	0.93641800
C	-2.89138400	-0.22762800	-0.85982900
C	-3.08779800	1.22419300	-0.53974600
H	-3.68796300	-0.55775600	-1.53223100
H	-1.94473300	-0.37812800	-1.39891500
C	-4.21323800	2.02447200	-0.54838200
H	-5.21706500	1.73667700	-0.83091600
C	-2.62718300	3.30174500	0.11450300
N	-3.92129800	3.31137000	-0.13978000
H	-2.03775000	4.14417300	0.44973900
H	-1.66174600	-2.08562500	1.55006300
C	-3.11300600	-2.69770000	-0.07522100
O	-2.47651500	-3.51006700	0.65663400
O	-3.88621600	-2.91217600	-1.03145700
N	-2.07930700	2.06863200	-0.10601900
H	-1.09651500	1.82898200	-0.00785500
Ag	1.86190400	1.66654100	0.15457200
Ag	2.90690200	-0.94216400	-0.46341400
Ag	0.32972200	-0.64969100	0.40034800

His$^{(\circ)}$*–Ag*$_3$***(o′)***

E $_{total}$ = -985.6556695 a.u.

Electronic and zero-point Energy = -985.506555

Thermal Energies = -985.489427

Enthalpy = -985.488483

Free Energy = -985.560911

-1 2

N	4.96239900	0.15395700	1.86268500
C	3.78071100	0.23318000	0.98118700
H	5.05254300	-0.80669200	2.19050000
H	2.92806000	-0.18120300	1.53293400
C	3.50859900	1.72878800	0.67989300
C	2.15676900	2.04334600	0.10315300
H	4.27004300	2.09534800	-0.01683800
H	3.64975600	2.26594700	1.62686800
C	0.91116800	1.70524500	0.59826000
N	2.00554000	2.77513700	-1.06027900
H	0.59984100	1.17201200	1.48274400
H	-1.00314600	2.06203900	-0.26809100
C	0.70417600	2.86461600	-1.26587100
N	-0.00608200	2.24548500	-0.28166200
H	0.22924400	3.35726900	-2.10325700
H	5.77286200	0.29244900	1.25544600
C	3.99014800	-0.58392900	-0.33308600
O	5.12552200	-0.53650200	-0.84028300
O	3.00196700	-1.26286700	-0.80036200
Ag	-3.79499600	0.74595500	0.19684600
Ag	-1.85639900	-1.17808200	0.07599900
Ag	0.85221400	-1.27067500	-0.28990000

His$^{(\circ)}$*–Ag*$_3$***(p′)***

E $_{total}$ = -985.6589518 a.u.

Electronic and zero-point Energy = -985.508992

Thermal Energies = -985.492217

Enthalpy = -985.491272

Free Energy = -985.563932

-1 2

N	1.96872200	-1.13017800	0.68374700
C	2.98916700	-0.80260700	-0.35840400
H	2.15931900	-2.13200100	0.85912500
H	2.47396800	-0.62829800	-1.31010000
C	3.78759800	0.46565300	-0.00126500
C	2.92069500	1.66459700	0.24982500
H	4.48906600	0.63982400	-0.82125800
H	4.38408500	0.27403600	0.89932500
C	2.32701200	2.51101000	-0.66116300
N	2.52139200	2.01372300	1.53157800
H	2.36226600	2.55051200	-1.73906900
H	0.90296500	4.06010000	-0.28687600
C	1.70181000	3.03707400	1.39271300
N	1.55986200	3.38878500	0.08230300
H	1.19231800	3.55605400	2.19284800
H	2.19667400	-0.63582600	1.54640100
C	3.94173700	-2.04002100	-0.57545700
O	3.66000900	-3.05665800	0.12131100
O	4.84868400	-1.87023000	-1.42062200
Ag	-1.93761800	1.32518400	-0.65587400
Ag	-2.89337900	-1.21765800	0.24178200
Ag	-0.20279400	-0.68603300	0.25862800

His$^{(\circ)}$*–Cu*$_3$***(q)***

E $_{total}$ = -1137.305095 a.u.

Electronic and zero-point Energy = -1137.141358

Thermal Energies = -1137.125003

Enthalpy = -1137.124059

Free Energy = -1137.192266

0 2

N	3.76540800	-1.81701200	-0.75740700
C	2.87958400	-1.74102800	0.41682400
C	1.43089800	-1.69785600	-0.09948300
O	0.47279700	-1.51853300	0.65248100
H	4.49245200	-2.51549100	-0.64995800
H	4.19766400	-0.90888000	-0.94275800
H	2.96983400	-2.66440300	1.00188500
C	3.14382000	-0.53220600	1.35064300
C	2.98046800	0.77759700	0.63967700
H	4.16177000	-0.62746200	1.74546000
H	2.45015600	-0.58831200	2.19345000
C	1.96362200	1.69806100	0.74968200
N	3.87346000	1.17594100	-0.34379400
H	1.07314500	1.72947100	1.35862800
H	1.67656000	3.48113800	-0.37828400
C	3.40407400	2.31685900	-0.81269300
N	2.25282200	2.67582000	-0.17699900
H	3.85355600	2.91429000	-1.59327300
O	1.30219900	-1.85762900	-1.39944300
H	2.24820600	-1.96387600	-1.71643900
Cu	-2.09837800	1.52248900	-0.05744000
Cu	-1.33879700	-0.75665400	0.19880000
Cu	-3.64489200	-0.45614500	-0.12630900

His$^{(\circ)}$*–Cu*$_3$***(r)***

E $_{total}$ = -1137.31513 a.u.

Electronic and zero-point Energy = -1137.151210

Thermal Energies = -1137.134743

Enthalpy = -1137.133799

Free Energy = -1137.202109

0 2

N	-1.56489200	-1.73080900	-0.79106800
C	-2.40722500	-1.41743900	0.36962700
C	-3.85919600	-1.20064600	-0.11353200
O	-4.70698900	-0.63571000	0.54595400
H	-0.75005300	-2.28252100	-0.52666500
H	-1.20207100	-0.88397100	-1.22531000
H	-2.44663400	-2.32226300	0.99052400
C	-1.94185000	-0.25781200	1.28330300
C	-1.79746900	1.06064600	0.58452200
H	-0.97844700	-0.53321400	1.72431400
H	-2.66936900	-0.15983100	2.09343600
C	-2.75058400	2.01946900	0.33838400
N	-0.58627300	1.49424300	0.05145500
H	-3.80277400	2.04740200	0.57463100
H	-2.52607800	3.89360400	-0.66453300
C	-0.80603500	2.68337300	-0.49339900
N	-2.10562900	3.03444000	-0.34056500
H	-0.06801900	3.29913800	-0.98525900
O	-4.10612500	-1.72264500	-1.32151100
H	-3.23428100	-2.06941000	-1.63530900
Cu	1.16721100	0.53403400	0.05895800
Cu	3.51795400	0.44320300	-0.20630600
Cu	2.18912300	-1.63353900	0.20274200

His$^{(\circ)}$*–Cu*$_3$***(s)***

E $_{total}$ = -1137.301671 a.u.

Electronic and zero-point Energy = -955.094837

Thermal Energies = -1137.12171

Enthalpy = -1137.120766

Free Energy = -1137.189142

0 2

N	-0.63686900	-0.39634900	-0.95232200
C	-1.50537900	0.79129100	-1.17788700
C	-1.57171000	1.79351900	-0.00408200
O	-2.38873000	2.68839300	-0.03504400
H	-0.56586300	-0.88581200	-1.84559000
H	-1.14976200	-1.05051000	-0.34596200
H	-1.06503700	1.35790700	-2.00674500
C	-2.94538900	0.37859000	-1.57897000
C	-3.66794500	-0.36529900	-0.49408500
H	-2.87772000	-0.24195200	-2.48267300
H	-3.50209700	1.28087300	-1.83986100
C	-4.86625300	-0.06541900	0.10933100
N	-3.13578200	-1.51447200	0.07242800
H	-5.55886800	0.75013700	-0.02943200
H	-5.85062900	-1.12941100	1.68056300
C	-3.99534300	-1.89831600	0.99588800
N	-5.06423500	-1.05483600	1.05194500
H	-3.89398300	-2.76217700	1.63747900
O	-0.72653400	1.68125300	1.02848300
H	-0.03756400	0.98699200	0.92140000
Cu	2.70044200	0.16148500	1.46947900
Cu	1.32247400	-0.27291400	-0.40864800
Cu	3.65273800	-0.45097800	-0.78297600

His$^{(o)}$*–Cu*$_3$***(t)***

E $_{total}$ = -1137.309395 a.u.

Electronic and zero-point Energy = -1137.146053

Thermal Energies = -1137.12913

Enthalpy = -1137.128185

Free Energy = -1137.198773

0 2

N	4.51666500	0.47202800	-0.27774000
C	3.42432800	-0.32629500	0.26954200
H	5.36447200	0.33214400	0.26663500
H	3.33190400	-0.10687600	1.33890300
C	2.08396900	0.02777700	-0.41604400
C	1.60088700	1.42164600	-0.13910200
H	1.30629300	-0.67008100	-0.08671300
H	2.19842300	-0.12420100	-1.49862300
C	2.29120600	2.60506000	-0.03392700
N	0.24612200	1.68149600	0.03373100
H	3.34581600	2.81018300	-0.11368800
H	1.51813900	4.56414300	0.34014300
C	0.12291800	2.98490500	0.23816400
N	1.33988600	3.57946800	0.20704400
H	-0.80430600	3.51118100	0.40878500
H	4.73216900	0.15130700	-1.22057000
C	3.65683800	-1.83540500	0.12551800
O	4.40239600	-2.34783400	-0.68362900
O	2.91332100	-2.54720400	1.00035400
H	3.05931600	-3.49203900	0.82039400
Cu	-3.64720000	0.15394200	-0.03203200
Cu	-1.27781600	0.39299300	-0.01198800
Cu	-2.12248600	-1.83012500	-0.05236700

His$^{(\circ)}$*–Cu*$_3$***(u)***

E $_{total}$ = -1137.30882 a.u.

Electronic and zero-point Energy = -1137.144919

Thermal Energies = -1137.128178

Enthalpy = -1137.127234

Free Energy = -1137.196329

0 2

N	-1.43416200	-1.27445000	0.25950700
C	-2.55071700	-0.31096700	0.30488800
H	-1.43129600	-1.83000700	1.11437600
H	-2.52000400	0.21620900	1.26342400
C	-2.41894700	0.75175800	-0.81802800
C	-1.25729000	1.66803200	-0.58598600
H	-3.34357500	1.33729500	-0.84161200
H	-2.32134900	0.24484000	-1.78531000
C	-0.08986900	1.79871300	-1.31082000
N	-1.25539700	2.54682200	0.47996000
H	0.26642700	1.31847400	-2.20904500
H	1.56537500	3.07764000	-0.89567400
C	-0.11373900	3.19822000	0.40152600
N	0.62087200	2.79643200	-0.67619400
H	0.22844000	3.95943000	1.08842600
H	-1.61288400	-1.94508300	-0.48998000
C	-3.88616200	-1.03988100	0.18711300
O	-4.01602300	-2.17804700	-0.21696900
O	-4.92423800	-0.26604600	0.56369900
H	-5.74040300	-0.77978400	0.43509600
Cu	2.51695000	-0.10507200	1.28762900
Cu	0.51240000	-0.58762800	0.08025300
Cu	2.58487500	-1.06327100	-1.02197100

His$^{(\circ)}$*–Cu*$_3$***(v)***

E $_{total}$ = -1137.303635 a.u.

Electronic and zero-point Energy = -1137.139773

Thermal Energies = -1137.123158

Enthalpy = -1137.122214

Free Energy = -1137.191338

0 2

N	0.19714300	2.04344800	-0.03939600
C	1.40968200	1.23096400	0.22557900
H	0.08014200	2.73519500	0.70146300
H	1.23894500	0.66443900	1.14434000
C	1.63478500	0.24132300	-0.95678700
C	2.49385300	-0.93655800	-0.63840800
H	2.06272200	0.78574900	-1.80612400
H	0.63615600	-0.09975000	-1.26240200
C	3.78794500	-1.27282700	-0.97094000
H	4.48428500	-0.70411100	-1.57289400
C	3.06597200	-2.89635400	0.22476800
N	4.13571800	-2.49030800	-0.42954000
H	2.97272000	-3.82435300	0.77171000
H	0.34518100	2.59178900	-0.88844800
C	2.62654800	2.13178000	0.40782600
O	2.76534100	3.20260700	-0.15025800
O	3.53480300	1.60007400	1.24330000
H	4.30764400	2.19143900	1.26882700
N	2.04424600	-1.99341500	0.13510800
H	1.10202400	-2.09889400	0.50322600
Cu	-1.82916200	-1.39257600	0.64439000
Cu	-1.50153100	0.89568200	-0.10384100
Cu	-3.64804700	-0.00555300	-0.36880600

*His$^{(\circ)}$–Cu$_3$(**w**)*

E $_{total}$ = -1137.30882 a.u.

Electronic and zero-point Energy = -1137.144918

Thermal Energies = -1137.128178

Enthalpy = -1137.127234

Free Energy = -1137.196333

0 2

N	-1.43418200	-1.27436400	0.25870600
C	-2.55077700	-0.31095000	0.30473100
H	-1.43102600	-1.83023300	1.11336800
H	-2.51987200	0.21581800	1.26349100
C	-2.41915100	0.75231100	-0.81773000
C	-1.25727200	1.66823600	-0.58544500
H	-3.34372600	1.33793700	-0.84084100
H	-2.32175900	0.24582500	-1.78525700
C	-0.09006900	1.79895200	-1.31067700
N	-1.25471900	2.54635500	0.48098800
H	0.26576200	1.31910100	-2.20929500
H	1.56547600	3.07765300	-0.89567500
C	-0.11292100	3.19753900	0.40245200
N	0.62124500	2.79600100	-0.67561800
H	0.22976600	3.95816600	1.08974200
H	-1.61303300	-1.94473800	-0.49097300
C	-3.88623100	-1.03984500	0.18699000
O	-4.01614100	-2.17805400	-0.21694100
O	-4.92431100	-0.26595200	0.56350600
H	-5.74047500	-0.77974200	0.43508900
Cu	2.58528900	-1.06241400	-1.02166000
Cu	0.51225200	-0.58726500	0.07932700
Cu	2.51641100	-0.10622200	1.28776000

*His$^{(o)}$–Cu$_3$(**x**)*

E $_{total}$ = -1137.309753 a.u.

Electronic and zero-point Energy = -1137.145271

Thermal Energies = -1137.12885

Enthalpy = -1137.127905

Free Energy = - -1137.196842

0 2

N	0.75284700	0.25229300	-1.09086300
C	1.47990300	1.09601500	-0.11620500
H	0.71880600	0.74777700	-1.98374200
H	1.20162200	0.78608100	0.89508800
C	3.02697000	1.01126100	-0.25809800
C	3.55344100	-0.36157600	0.03637100
H	3.48391100	1.73163400	0.42773900
H	3.29981500	1.30934400	-1.27898800
C	4.44475900	-0.75909400	1.00618300
N	3.14042300	-1.46107200	-0.69711200
H	4.97983300	-0.21176500	1.76710400
H	5.15689900	-2.73657800	1.40427000
C	3.76656100	-2.49994400	-0.18221000
N	4.57349800	-2.12595000	0.85118800
H	3.67426400	-3.52460500	-0.51364000
H	1.28641000	-0.61096000	-1.23620300
C	1.03612700	2.53777800	-0.31268000
O	0.61138500	2.98826800	-1.35623600
O	1.22240700	3.27980500	0.79720300
H	0.93791500	4.18816500	0.59648300
Cu	-2.52243800	0.17456400	1.41514200
Cu	-1.15214000	-0.20285600	-0.52267800
Cu	-3.30900000	-1.16575000	-0.55068800

*$His^{(-)}$–Cu_3(**q´**)*

E_{total} = -1136.790228 a.u.

Electronic and zero-point Energy = -1136.640069

Thermal Energies = -1136.623465

Enthalpy = -1136.622521

Free Energy = -1136.691687

-1 2

N	-3.70953600	-2.07598900	0.85608400
C	-2.77249400	-1.87664800	-0.25691400
C	-1.30490000	-1.65522200	0.20810000
O	-0.48795400	-1.33341600	-0.73986700
H	-4.11067000	-1.17671100	1.11819200
H	-3.15332200	-2.37206100	1.65825500
H	-2.75111400	-2.79681200	-0.86158200
C	-3.24937600	-0.74205000	-1.19623200
C	-3.16040200	0.62963800	-0.58881800
H	-4.29155600	-0.93763000	-1.47423100
H	-2.63778600	-0.78093000	-2.10106700
C	-2.04931100	1.43937000	-0.49278700
N	-4.23800800	1.24021300	0.03714900
H	-1.02625900	1.29649900	-0.80456700
H	-1.86379900	3.32214300	0.48174200
C	-3.78263000	2.38814500	0.50200900
N	-2.46062200	2.55755200	0.20169400
H	-4.35666900	3.12450900	1.04800200
O	-1.01213600	-1.81576700	1.40399000
Cu	2.23173200	1.55843600	0.14429800
Cu	3.64022800	-0.46560200	0.01524100
Cu	1.26472000	-0.66653700	-0.19727600

*His$^{(-)}$–Cu$_3$(**r´**)*

E $_{total}$ = -1136.783256 a.u.

Electronic and zero-point Energy = -1136.633103

Thermal Energies = -1136.616725

Enthalpy = -1136.61578

Free Energy = -1136.686071

-1 2

N	-2.96702100	2.24481000	1.11236900
C	-1.75569000	1.50283300	0.73481000
C	-1.43117100	1.60802500	-0.78736900
O	-0.39951100	0.95234900	-1.21137500
H	-3.75643900	1.60269700	1.15284600
H	-3.17132700	2.88005700	0.34069800
H	-0.89343200	1.95244800	1.25150900
C	-1.83542400	0.03569100	1.22110200
C	-2.83700200	-0.80884500	0.48627000
H	-2.10424400	0.04102000	2.28346700
H	-0.83910700	-0.40946600	1.14214000
C	-2.73610600	-1.32163100	-0.78913400
N	-4.06250800	-1.15961100	1.03358700
H	-1.96069500	-1.22549100	-1.53362300
H	-4.18364600	-2.45888000	-1.87204300
C	-4.68712000	-1.86092700	0.10850400
N	-3.92274500	-1.99069600	-1.01779300
H	-5.67305900	-2.29675100	0.19767500
O	-2.15991800	2.30725000	-1.50597600
Cu	2.61730000	-0.23253300	1.46112700
Cu	1.23595800	0.30965300	-0.43023100
Cu	3.43703100	-0.58590700	-0.85731300

*His$^{(-)}$–Cu$_3$(**s´**)*

E $_{total}$ = -1136.787336 a.u.

Electronic and zero-point Energy = -1136.636707

Thermal Energies = -1136.620504

Enthalpy = -1136.619559

Free Energy = -1136.687681

-1 2

N	0.60854900	-0.18410700	-1.03516200
C	1.43882000	-1.31293900	-0.56706700
C	1.30164100	-1.50101300	0.98784400
O	2.24270300	-2.08117900	1.56787200
H	0.40515100	-0.25918800	-2.02815500
H	1.10206200	0.69678100	-0.89835200
H	0.99655400	-2.21990900	-1.00161100
C	2.91264100	-1.23908000	-1.02694600
C	3.63721100	-0.01033300	-0.55266200
H	2.95708000	-1.25180600	-2.12264500
H	3.41441700	-2.13525300	-0.65059800
C	3.99166300	0.32198200	0.73754700
N	4.02454000	1.00186600	-1.41995600
H	3.82872600	-0.20447900	1.66575700
H	4.96268400	2.09794900	1.41984000
C	4.60043800	1.92119600	-0.67049700
N	4.60842700	1.55508400	0.64708400
H	5.02226600	2.85384200	-1.01991300
O	0.21969400	-1.08128400	1.51297800
Cu	-3.24965200	-0.49202700	-0.94865100
Cu	-1.15272800	-0.17650000	0.26717000
Cu	-2.98979900	1.35931900	0.65375000

His$^{(-)}$*–Cu*$_3$***(t´)***

E $_{total}$ = -1136.769003 a.u.

Electronic and zero-point Energy = -1136.619135

Thermal Energies = -1136.602503

Enthalpy = -1136.601559

Free Energy = -1136.670847

-1 2

N	4.64362900	0.70588100	-0.28341900
C	3.70000900	-0.23877000	0.36203900
H	5.43273900	0.82020300	0.35172100
H	3.61580500	0.01508400	1.42551000
C	2.29635200	-0.12606900	-0.26988000
C	1.64336400	1.21861500	-0.13470400
H	1.65355100	-0.88359800	0.19052200
H	2.37555900	-0.38688800	-1.33534200
C	2.21511800	2.46911500	-0.13710200
N	0.26478900	1.37490700	0.00740700
H	3.25285400	2.74090300	-0.24132300
H	1.26303700	4.37741300	0.05645600
C	0.01804600	2.67631400	0.09325600
N	1.17613200	3.37395800	0.00968600
H	-0.95634900	3.12567000	0.21591600
H	5.04377600	0.15303400	-1.05014000
C	4.17155400	-1.73903700	0.25203800
O	5.00286300	-1.97130500	-0.67049700
O	3.64541300	-2.52884500	1.07401700
Cu	-1.22239000	0.05909000	-0.01210400
Cu	-3.62339900	0.44388600	0.20039900
Cu	-2.66199300	-1.80314300	-0.25626400

*His$^{(-)}$–Cu$_3$(**u´**)*

E $_{total}$ = -1136.783263 a.u.

Electronic and zero-point Energy = -1136.632612

Thermal Energies = -1136.616341

Enthalpy = -1136.615396

Free Energy = -1136.682668

-1 2

N	1.49589900	-1.15188500	-0.50878700
C	2.65800800	-0.21360800	-0.43274300
H	1.46237900	-1.51279200	-1.46163800
H	2.75196500	0.31343500	-1.38634600
C	2.47710200	0.83292300	0.68701700
C	1.27943100	1.71547500	0.52159200
H	3.39140900	1.43406100	0.70044300
H	2.41257500	0.31183400	1.65067000
C	0.10577900	1.69968200	1.25210500
N	1.19355300	2.67792400	-0.47159600
H	-0.19312300	1.13939800	2.12466400
H	-1.66802400	2.83676500	0.91174100
C	0.00386800	3.22643100	-0.34068100
N	-0.69068300	2.69234400	0.70646300
H	-0.40421200	4.00722800	-0.96816900
H	1.84360300	-1.95946000	0.03751700
C	3.97200300	-1.03928200	-0.15300700
O	3.77229000	-2.22279600	0.24886300
O	5.04392300	-0.42055900	-0.32884600
Cu	-2.50149300	-1.06938200	1.04576900
Cu	-0.40662900	-0.60353200	-0.09659000
Cu	-2.50893900	-0.12991500	-1.23391300

*His$^{(-)}$–Cu$_3$(**v´**)*

E $_{total}$ = -1136.789282 a.u.

Electronic and zero-point Energy = -1136.638919

Thermal Energies = -1136.622848

Enthalpy = -1136.621903

Free Energy = -1136.69183

-1 2

N	0.78234800	1.23029100	1.10112500
C	2.05594900	1.34337600	0.32191700
H	0.95945700	0.81044000	2.01144300
H	2.89926600	1.23465200	1.01750700
C	2.22261200	0.29243600	-0.78663300
C	2.53267800	-1.09813100	-0.31778100
H	3.04420200	0.65081100	-1.41337100
H	1.32293900	0.29230600	-1.41753800
C	3.72916300	-1.75868300	-0.11696300
H	4.72559200	-1.37639500	-0.29439000
C	2.21266100	-3.16197600	0.44709000
N	3.52370900	-3.03878000	0.35992900
H	1.67769000	-4.04270500	0.77537200
H	0.56615100	2.24001200	1.24319700
C	2.14605300	2.82866400	-0.22169900
O	1.34222400	3.62904000	0.33922400
O	3.01708600	3.04012500	-1.08989700
N	1.57165400	-2.02051800	0.05603000
H	0.56244500	-1.88384800	-0.00241200
Cu	-2.07409600	-1.53853400	-0.40261600
Cu	-3.27355000	0.58765900	-0.04004600
Cu	-0.89962500	0.42847200	0.35681400

*$His^{(-)}$–Cu_3(**w´**)*

E_{total} = -1136.783263a.u.

Electronic and zero-point Energy = -1136.632612

Thermal Energies = -1136.61634

Enthalpy = -1136.615396

Free Energy = -1136.682669

-1 2

N	1.49579300	-1.15219000	-0.50810100
C	2.65795100	-0.21386000	-0.43258400
H	1.46258600	-1.51380400	-1.46068300
H	2.75140800	0.31299600	-1.38633500
C	2.47710800	0.83286100	0.68701900
C	1.27945900	1.71545300	0.52155500
H	3.39141800	1.43400200	0.70032600
H	2.41260300	0.31192800	1.65075900
C	0.10579300	1.69979600	1.25206900
N	1.19367500	2.67789900	-0.47163700
H	-0.19331900	1.13930300	2.12441400
H	-1.66775500	2.83746700	0.91205600
C	0.00403200	3.22651900	-0.34075200
N	-0.69061200	2.69240900	0.70631700
H	-0.40399200	4.00734700	-0.96823900
H	1.84306800	-1.95931000	0.03893600
C	3.97209300	-1.03932100	-0.15303600
O	3.77259900	-2.22243700	0.25002400
O	5.04391500	-0.42071600	-0.33024700
Cu	-2.50126500	-1.06909000	1.04591000
Cu	-0.40674400	-0.60331500	-0.09688300
Cu	-2.50918900	-0.13036200	-1.23389400

*$His^{(-)}$–Cu_3(**x´**)*

E $_{total}$ = -1136.782884 a.u.

Electronic and zero-point Energy = -1136.632248

Thermal Energies = -1136.615959

Enthalpy = -1136.615014

Free Energy = -1136.683526

-1 2

N	-1.29280700	-1.04834200	-0.70176600
C	-2.34270800	-0.61838600	0.27704700
H	-1.55408100	-2.03758100	-0.86358700
H	-1.87640900	-0.54124500	1.26623600
C	-2.93631800	0.75434200	-0.08762100
C	-1.90364300	1.83389100	-0.22994300
H	-3.67007800	0.99598300	0.68557300
H	-3.48371700	0.67106200	-1.03484700
C	-1.26497500	2.55725600	0.75354300
N	-1.37975400	2.17548700	-1.46789700
H	-1.36017000	2.55398100	1.82839200
H	0.37191300	3.91218400	0.53940800
C	-0.44404300	3.07374200	-1.23271400
N	-0.34396000	3.35372300	0.09913100
H	0.17930800	3.55084400	-1.97637100
H	-1.45929500	-0.57260700	-1.59004700
C	-3.45501600	-1.72923200	0.38374600
O	-3.22211200	-2.77768600	-0.28357600
O	-4.41905300	-1.44838300	1.13043600
Cu	2.24654700	0.57711300	1.02683600
Cu	2.96170800	-1.25221300	-0.46616700
Cu	0.62546000	-0.74972100	-0.22688500