ЖУРНАЛ СТРУКТУРНОЙ ХИМИИ

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SUPPLEMENTARY MATERIALS TO:

DFT ANALYSIS OF COPPER(II) COMPLEXES of *cis*-1,2-DIAMINOCYCLOHEXANE (Dach), $[Cu(Dach)_2(N_3)]Cl\cdot 3H_2O$ AND $[Cu(Dach)_2—Ag(CN)_2—Cu(Dach)_2][Ag(CN)_2]_3$

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NBO charges of all atoms in complexes **1** and **2** along with illustrative Figures.

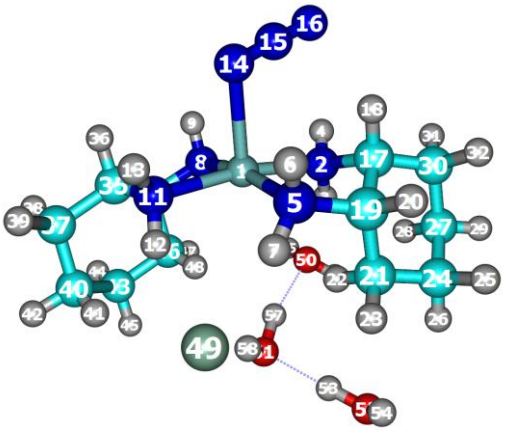


Fig. S1. NBO charges of all atoms in complex **1.**

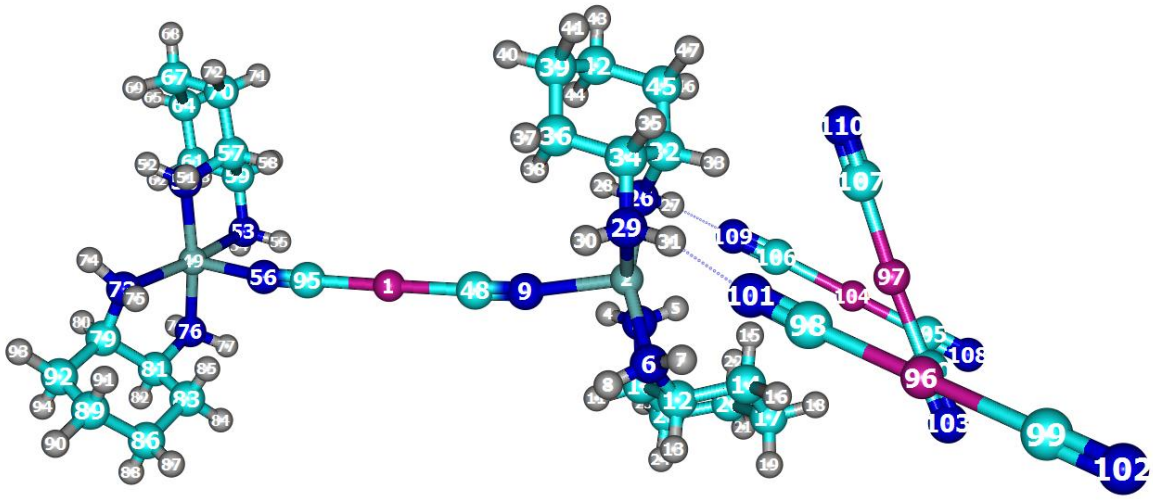


Fig. S2. NBO charges of all atoms in complex **2.**

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Table S1

NBO charges of atoms in complex **1**

Atom	Number	Charge
1	2	3
Cu	1	0.88548
N	2	–0.92747
H	3	0.43637
H	4	0.43280
N	5	–0.91837
H	6	0.43330
H	7	0.43514
N	8	–0.91262
H	9	0.43606
H	10	0.43142
N	11	–0.92972
H	12	0.42845
H	13	0.43611
N	14	–0.54866
N	15	0.18451
N	16	–0.46800
C	17	–0.00549
H	18	0.23098
C	19	0.00662
H	20	0.22293
C	21	–0.43702
H	22	0.20535
H	23	0.22642
C	24	–0.40634
H	25	0.20407
H	26	0.22537
C	27	–0.40715
H	28	0.19254
H	29	0.22449
C	30	–0.42653
H	31	0.22409
H	32	0.22130
C	33	0.00696
H	34	0.22387
C	35	–0.00287
H	36	0.22973
C	37	–0.42693
H	38	0.22060
H	39	0.22472
C	40	–0.41418
H	41	0.20834
H	42	0.22197
C	43	–0.40387
H	44	0.20484

Continued Table S1

1	2	3
H	45	0.22245
C	46	–0.42972
H	47	0.22380
H	48	0.20202
Cl	49	–0.82565
O	50	–1.00059
O	51	–1.03637
O	52	–1.03617
H	53	0.50602
H	54	0.48603
H	55	0.52819
H	56	0.52704
H	57	0.50878
H	58	0.49456
Total		0.00000

Table S2

NBO charges of atoms in complex **2**

Atom	Number	Charge
1	2	3
Ag	1	0.48148
Cu	2	0.89331
N	3	–0.92067
H	4	0.43743
H	5	0.42974
N	6	–0.91916
H	7	0.43795
H	8	0.43297
N	9	–0.60338
C	10	–0.00172
H	11	0.23034
C	12	0.00783
H	13	0.22352
C	14	–0.42754
H	15	0.20603
H	16	0.23004
C	17	–0.39992
H	18	0.22584
H	19	0.20544
C	20	–0.40668
H	21	0.22390
H	22	0.19761
C	23	–0.42611
H	24	0.22166
H	25	0.22418
N	26	–0.93096

Continued Table S2

1	2	3
H	27	0.44979
H	28	0.41842
N	29	–0.91612
H	30	0.42764
H	31	0.44939
C	32	–0.00249
H	33	0.23684
C	34	0.00459
H	35	0.22178
C	36	–0.42994
H	37	0.22336
H	38	0.20828
C	39	–0.40300
H	40	0.22118
H	41	0.20518
C	42	–0.40988
H	43	0.22524
H	44	0.19518
C	45	–0.42745
H	46	0.22455
H	47	0.22147
C	48	0.02121
Cu	49	0.91050
N	50	–0.91648
H	51	0.44495
H	52	0.42785
N	53	–0.91037
H	54	0.43690
H	55	0.44172
N	56	–0.62574
C	57	–0.00281
H	58	0.23676
C	59	0.00536
H	60	0.22982
C	61	–0.43245
H	62	0.20528
H	63	0.23021
C	64	–0.40311
H	65	0.22565
H	66	0.20884
C	67	–0.41179
H	68	0.23026
H	69	0.19672
C	70	–0.42869
H	71	0.22643
H	72	0.22867
N	73	–0.91704

Continued Table S2

1	2	3
H	74	0.44220
H	75	0.42960
N	76	–0.91036
H	77	0.43969
H	78	0.44051
C	79	–0.00235
H	80	0.23445
C	81	0.00501
H	82	0.22997
C	83	–0.43367
H	84	0.22876
H	85	0.21224
C	86	–0.40321
H	87	0.22519
H	88	0.20751
C	89	–0.41178
H	90	0.22965
H	91	0.19738
C	92	–0.42910
H	93	0.22824
H	94	0.22627
C	95	0.03443
Ag	96	0.42725
Ag	97	0.31405
C	98	–0.00460
C	99	–0.09965
C	100	–0.10923
N	101	–0.64627
N	102	–0.58490
N	103	–0.57964
Ag	104	0.41720
C	105	–0.09920
C	106	–0.01671
C	107	–0.10181
N	108	–0.58049
N	109	–0.64305
N	110	–0.58928
Total		0.00000