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Magneto-structural maps and bridged-ligand effect for dichloro-bridged dinuclear Copper(II) complexes: A theoretical perspective

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Table S1. Structural and magnetic coupling constant for some di-μ-chloro-bridged binuclear Cu(II) complexes[25,26].

Complex	α(Cu-μ-Cl-Cu)[°]	R_{Cu-Cl}[Å]	R_0(Cu•••Cu)[Å]	α/R_{Cu-Cl}[°/Å]	J[cm^{-1}]
$[Cu(TMSO)_2Cl_2]_2$	88.50	2.28	3.02	38.82	-16.00
$[Cu_2(dpt)_2Cl_2]$ $(Cl)_2$	91.40	2.55	3.55	35.91	85.90
$[Cu(2\text{-methylpyridine})_2Cl_2]_2$	100.63	2.29	3.36	44.00	-7.40
$[Cu(HL)Cl]_2\cdot H_2O$	84.66	2.67	3.34	31.73	43.20
$[Cu(apyhist)Cl]_2(ClO_4)_2$	87.46	2.27	2.74	38.51	-3.09
$[Cu(pmpe)Cl]_2$	89.31	2.30	2.77	38.86	-4.54
$[Cu(pdon)Cl_2]_2\cdot 2DMF$	87.66	2.27	2.69	38.70	-1.16
$[Cu(dmg)Cl_2]_2$	88.00	2.24	2.70	39.32	0.62
$[Cu(dbea)Cl_2]_2$	87.10	2.30	2.74	37.90	5.00
$[Cu(pzPh)(opo)Cl]_2$	93.60	2.29	2.83	40.89	8.72
$[Cu(iydio)Cl]_2(ClO_4)_2$	88.81	2.32	2.66	38.20	1.16
$[Cu(dien)Cl]_2(ClO_4)_2$	92.00	2.31	2.77	39.78	0.40
	92.10	2.23	2.74	41.37	0.40
$[Cu(Hfsaaep)Cl]_2$	95.27	2.31	2.85	41.28	0.30
$[Cu(bpdio)Cl_2]_2$	96.68	2.27	2.84	42.53	4.87
$[Cu(pmdio)Cl]_2(ClO_4)_2$	88.20	2.29	2.58	38.50	2.28
$[Cu(2,2\text{-dimethylaziridine})_2Cl_2]_2$	93.14	2.35	2.68	39.68	-3.70
$[Cu(aamo)Cl]_2$	82.90	2.33	2.81	35.59	12.00
$[Cu(L1)Cl]_2\cdot H_2O$ (2)	88.47	2.30	2.71	38.42	-1.40
	84.79	2.29	2.66	37.03	-1.40
$[Cu(pbpe)Cl]_2(ClO_4)_2$	88.09	2.29	2.73	38.53	6.00
$[Cu_2(L3)_2Cl_2]n\cdot 3nH_2O$ (6)	85.61	2.29	2.65	37.47	4.95
$[Cu(Hbpmdio)Cl_2]_2(ClO_4)_2$	94.70	2.29	2.92	41.32	10.70
$[Cu_2(pmdip)_2Cl_2](ClO_4)_2$	86.44	2.28	2.64	37.91	-1.95
$[\{Cu(terpy)Cl\}_2](PF_6)_2$	89.90	2.22	2.72	40.53	-5.90
$[Cu(HL2)Cl_2]_2\cdot 2DMF$ (3)	86.76	2.28	2.63	38.10	-4.00
$[Cu(mebta)_2Cl_2]_2$	88.10	2.30	2.63	38.27	6.70

$[CuCl_2(PyTn)]_2$	88.60	2.91	3.61	30.49	13.73
$[Cu(bpdio)Cl_2]_2$	96.68	2.84	3.84	33.99	4.87
$[Cu(dmgH)Cl_2]_2$	88.00	2.70	3.45	32.62	0.62
$[Cu(Hfsaaep)Cl]_2$	95.27	2.85	3.45	33.48	0.30
$[Cu(ppmma)Cl_2]_2$	89.73	2.70	3.51	33.28	0.00
$C_{22}H_{32}Cl_4Cu_2N_4O_2$	92.65	2.83	3.71	32.77	-0.47
$[Cu(4\text{-}Metz)(DMF)Cl_2]_2$	95.30	2.72	3.39	34.99	-3.60
$[Cu(guaH)Cl_3]_2$	95.34	2.45	3.57	38.96	-38.80
	85.12	2.36	3.57	36.05	-2.99
$[Cu(DMEN)C1_2]_2$	86.13	2.73	3.46	31.50	-2.10
$[Cu(TMSO)C1_2]_2$	88.50	3.02	3.74	29.30	-17.00
$[Cu(TMEN)C1_2]_2$	96.80	3.15	4.09	30.76	-5.60
$[Cu(GuaH)Cl_3]_2$	97.90	2.45	3.58	40.01	-82.60

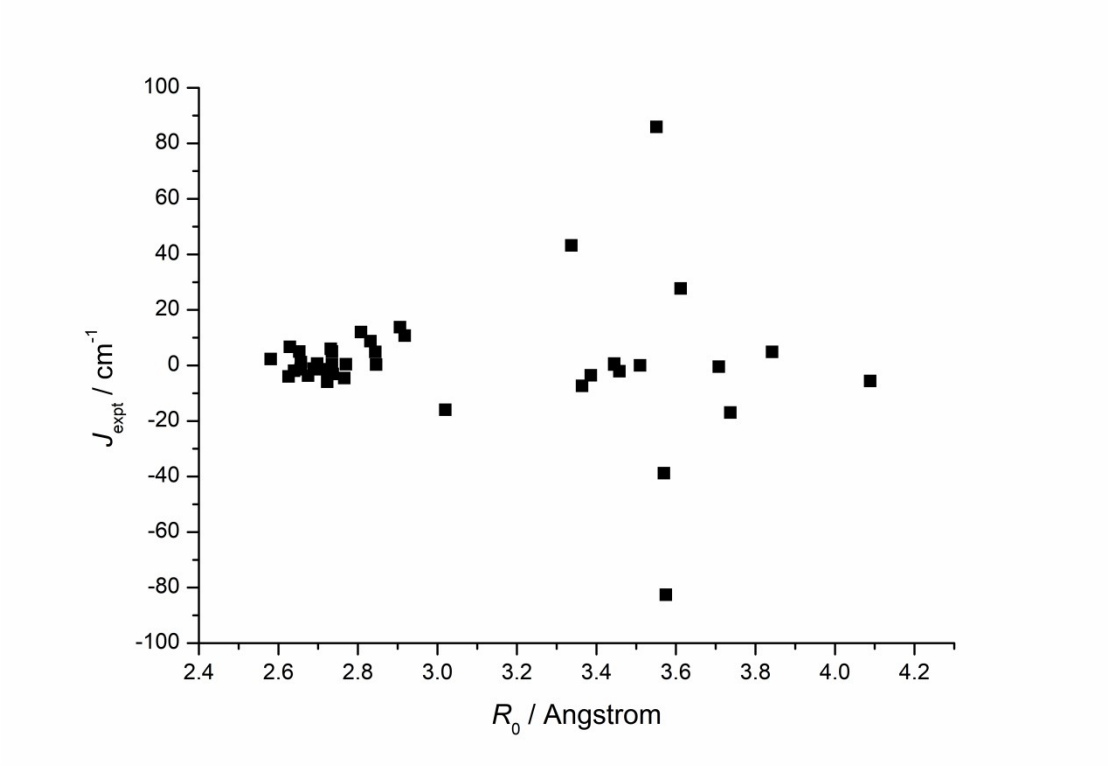

Figure S1. The magneto-structural correlation of J_{expt} and R_0 were obtained by ref. 19,20.

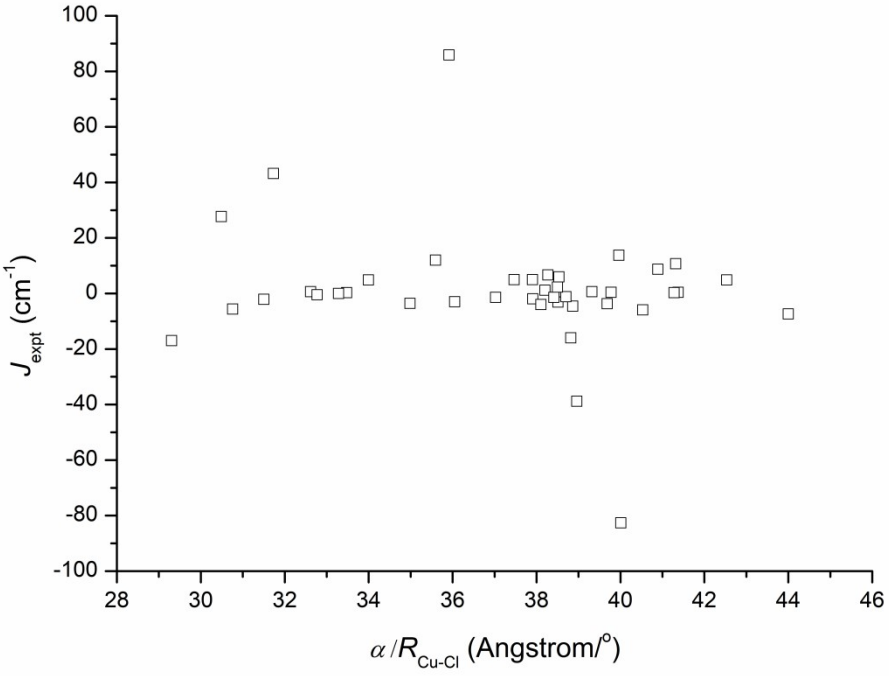

Figure S2. The magneto-structural correlation of J_{expt} and $\alpha/R_{Cu\text{-}Cl}$ were obtained by ref. 19,20.

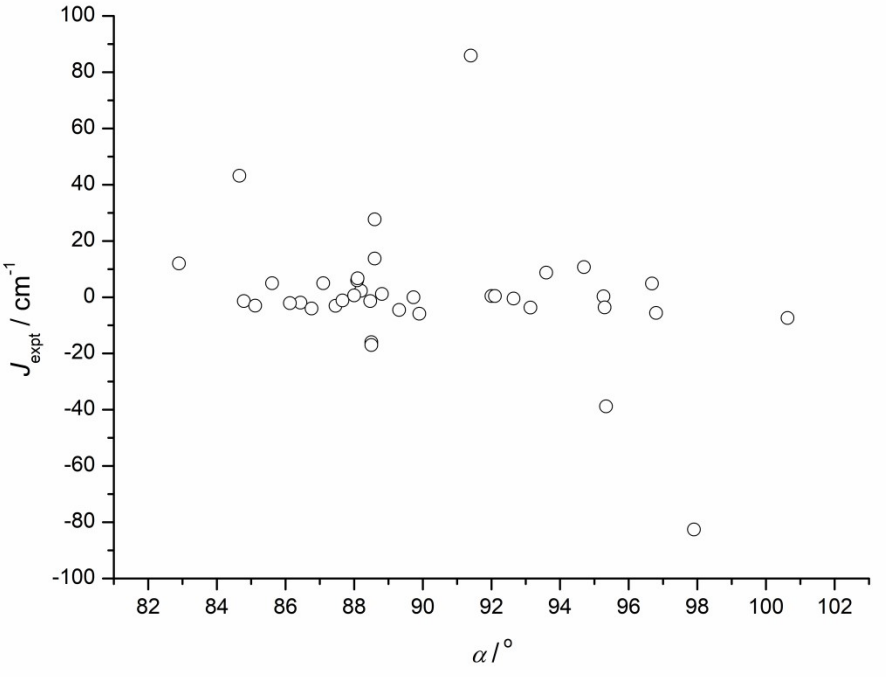

Figure S3. The magneto-structural correlation of J_{expt} and α were obtained by ref. 19,20.

Table S2. Some selected bond lengths [Å] and angles [°] for complex A.

Cu1-Cl3	2.319	Cu2-N10	2.117
Cu1-Cl4	2.670	Cu1-Cl3-Cu2	85.26
Cu1-Cl5	2.277	Cu1-Cl4-Cu2	85.26
Cu1-N6	2.096	Cl3-Cu1-Cl5	100.72
Cu1-N7	2.117	Cl3-Cu2-Cl8	107.01
Cu2-Cl3	2.670	Cl4-Cu1-Cl5	107.01
Cu2-Cl4	2.319	Cl4-Cu2-Cl8	100.73
Cu2-Cl8	2.277	N6-Cu1-N7	76.21
Cu2-N9	2.096	N9-Cu2-N10	76.21

Table S3. Calculated energies (E_{HS} and E_{BS}), S^2_{HS}, S^2_{BS} and J_{calc} with different functions under the ZORA-def2-TZVPP basis set (J_{expt} = 13.73 cm^{-1}).

Functional	E_{HS}/eV	E_{BS}/eV	S^2_{HS}	S^2_{BS}	$^{J}_{cacl}$/cm^{-1}
OLYP	-184265.56662	-184265.56469	2.00419	1.00402	15.57
PBE	-184179.38588	-184179.38427	2.00301	1.00296	12.98
BP86	-184271.08909	-184271.08751	2.00308	1.00303	12.73
PW91	-184248.14705	-184248.14549	2.00293	1.00288	12.61
BLYP	-184245.32417	-184245.32268	2.00285	1.00280	11.97
XLYP	-184300.17483	-184300.17338	2.00287	1.00281	11.63
O3LYP	-184168.67089	-184168.67000	2.00523	1.00521	7.14
B3P86	-184242.98046	-184242.98000	2.00597	1.00598	3.65
B3PW91	-184232.70437	-184232.70393	2.00585	1.00587	3.61
B3LYP	-184222.38426	-184222.38383	2.00571	1.00573	3.49
B3LYP*	-184252.04824	-184252.04781	2.00566	1.00568	3.48
X3LYP	-184209.47090	-184209.47052	2.00595	1.00597	3.10
B1P86	-184263.03709	-184263.03677	2.00672	1.00673	2.60
PBE0	-184185.21537	-184185.21505	2.00654	1.00656	2.55
B1LYP	-184236.91656	-184236.91625	2.00638	1.00641	2.45

Table S4. Calculated energies (E_{HS} and E_{BS}), S^2_{HS} , S^2_{BS} and J_{calc} with different basis sets at the PBE function (J_{expt} = 13.73 cm^{-1}).

Basis set	E_{HS}/eV	E_{BS}/eV	S^2_{HS}	S^2_{BS}	J_{calc}/cm^{-1}
ZORA-def2-QZVPP	-184187.09530	-184187.09374	2.00306	1.00303	12.54
ZORA-def2-TZVPP	-184179.38588	-184179.38427	2.00301	1.00296	12.98
ZORA-def2-TZVP(-f)	-184178.36917	-184178.36751	2.00287	1.00282	13.40
ZORA-def2-TZVP	-184179.10722	-184179.10556	2.00299	1.00294	13.40
ZORA-def2-SVP	-184114.04534	-184114.04366	2.00259	1.00246	13.57

Table S5. The Mulliken spin population of HS and BS states for complex A.

Atoms	HS state	BS state
Cu(1)	0.49322	-0.49341
Cu(2)	0.49323	0.49342
Cl(3)	0.16772	-0.16786
Cl(4)	0.16778	0.16792
Cl(5)	0.18374	-0.18370
N(6)	0.06822	-0.06792
N(7)	0.06770	-0.06776
Cl(8)	0.18367	0.18363
N(9)	0.06769	0.06793
N(10)	0.06822	0.06776

Table S6. Distribution of spin electrons in atomic orbitals of BS state complex A.

Atoms	Atomic orbitals		
	s	*p*	*d*
Cu(1)	0.00989	0.00566	-0.50894
Cu(2)	-0.00990	-0.00566	0.50896
Cl(3)	-0.00150	-0.16585	-0.00045
Cl(4)	0.00149	0.16591	0.00045
Cl(5)	-0.00160	-0.18206	0.00004
N(6)	-0.01415	-0.05304	-0.00073
N(7)	-0.01509	-0.05185	-0.00081
Cl(8)	0.00160	0.18200	-0.00004
N(9)	0.01415	0.05304	0.00073
N(10)	0.01509	0.05184	0.00081

Table S7. Calculated energies (E_{HS} and E_{BS}), S_{HS}^2, S_{BS}^2 and magnetic coupling constants with different bond distance at the PBE/ZORA-def2-TZVP level.

R_0/Å	E_{HS}/eV	E_{BS}/eV	S_{HS}^2	S_{BS}^2	J_{cacl}/cm^{-1}	$R_{Cu\text{-}Cl\text{-}1}$/Å	$R_{Cu\text{-}Cl\text{-}2}$/Å	α/°	$\alpha/R_{Cu\text{-}Cl\text{-}1}$ [°/Å]	$\alpha/R_{Cu\text{-}Cl\text{-}2}$ [°/Å]
3.0	-184179.00812	-184179.00623	2.00295	1.00268	15.25	2.300	2.655	74.1	32.22	27.91
3.1	-184179.05284	-184179.05100	2.00295	1.00282	14.78	2.300	2.660	77.0	33.48	28.95
3.2	-184179.08566	-184179.08396	2.00295	1.00290	13.72	2.303	2.661	79.9	34.69	30.03
3.3	-184179.10170	-184179.10017	2.00296	1.00294	12.38	2.303	2.659	82.9	36.00	31.18
3.4	-184179.09684	-184179.09544	2.00295	1.00295	11.24	2.317	2.673	85.6	36.94	32.02
3.5	-184179.10061	-184179.09922	2.00298	1.00288	11.22	2.325	2.698	88.0	37.85	32.62
3.6	-184179.08769	-184179.08647	2.00298	1.00273	9.86	2.325	2.728	90.5	38.92	33.17
3.7	-184179.06030	-184179.05928	2.00298	1.00264	8.24	2.324	2.775	92.6	39.85	33.37
3.8	-184179.03617	-184179.03543	2.00296	1.00260	5.98	2.317	2.858	93.9	40.53	32.86
3.9	-184179.02717	-184179.02660	2.00297	1.00258	4.57	2.312	2.939	95.2	41.18	32.39

Table S8. Calculated energies (E_{HS} and E_{BS}), S_{HS}^2, S_{BS}^2 and magnetic coupling constants with different bond angle at the PBE/ZORA-def2-TZVP level.

α/°	E_{HS}/eV	E_{BS}/eV	S_{HS}^2	S_{BS}^2	J_{cacl}/cm^{-1}	$R_{Cu\text{-}Cl}$/Å	$R_{Cu\text{-}Cl}$/Å	R_0/Å	$\alpha/R_{Cu\text{-}Cl\text{-}1}$ [°/Å]	$\alpha/R_{Cu\text{-}Cl\text{-}2}$ [°/Å]
80.0	-184179.09314	-184179.09185	2.00295	1.00280	10.40	2.307	2.709	3.239	34.68	29.53
83.0	-184179.10255	-184179.10111	2.00296	1.00292	11.62	2.312	2.669	3.311	35.90	31.10
86.0	-184179.09745	-184179.09592	2.00296	1.00294	12.31	2.314	2.646	3.392	37.17	32.50
89.0	-184179.08926	-184179.08761	2.00299	1.00263	13.35	2.319	2.646	3.488	38.38	33.64
92.0	-184179.05873	-184179.05714	2.00300	1.00233	12.80	2.320	2.646	3.580	39.66	34.77
95.0	-184179.01204	-184179.01043	2.00300	1.00207	12.92	2.324	2.653	3.676	40.88	35.81
98.0	-184178.95090	-184178.94926	2.00299	1.00168	13.22	2.327	2.675	3.782	42.11	36.64
101.0	-184178.89198	-184178.89057	2.00299	1.00096	11.30	2.323	2.734	3.911	43.48	36.94
104.0	-184178.83725	-184178.83604	2.00298	1.00072	9.76	2.308	2.850	4.078	45.06	36.49

Table S9. Calculated energies (E_{HS} and E_{BS}), S^2_{HS}, S^2_{BS} and magnetic coupling constants with different Cu-Cl-Cu-Cl dihedral angle (τ) at the PBE/ZORA-def2-TZVP level.

τ/°	E_{HS}/eV	E_{BS}/eV	S^2_{HS}	S^2_{BS}	J_{cacl}/cm^{-1}	$R_{Cu\text{-}Cl}$/Å	$R_{Cu\text{-}Cl}$/Å	R_0/Å	α/°	$\alpha/R_{Cu\text{-}Cl\text{-}1}$ [°/Å]	$\alpha/R_{Cu\text{-}Cl\text{-}2}$ [°/Å]
0	-184179.10128	-184179.09981	2.002955	1.002938	11.82	2.311	2.658	3.338	84.1	36.39	31.64
3	-184179.09104	-184179.08970	2.002938	1.002927	10.85	2.306	2.677	3.350	83.9	36.38	31.34
6	-184179.08558	-184179.08424	2.002955	1.002954	10.85	2.306	2.657	3.356	83.9	36.38	31.58
9	-184179.06323	-184179.06197	2.002946	1.002946	10.16	2.310	2.675	3.366	84.05	36.39	31.42
12	-184179.04558	-184179.04452	2.002936	1.002941	8.49	2.310	2.695	3.391	84.2	36.45	31.24
15	-184178.97379	-184178.97285	2.002884	1.002904	7.60	2.298	2.735	3.355	82.3	35.81	30.09
18	-184178.96165	-184178.96083	2.002890	1.002900	6.63	2.290	2.740	3.364	81.8	35.72	29.85
21	-184178.96699	-184178.96623	2.002911	1.002890	6.09	2.284	2.759	3.348	80.45	35.22	29.16

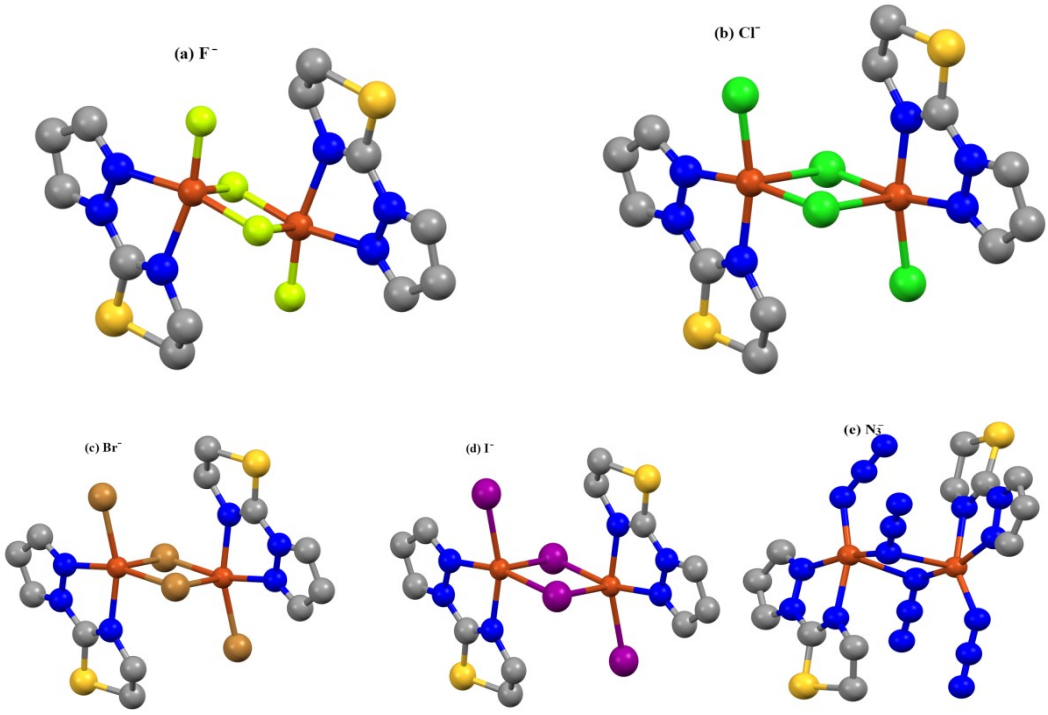

Figure S4. Molecular structure optimized (**I**) for different ligands.

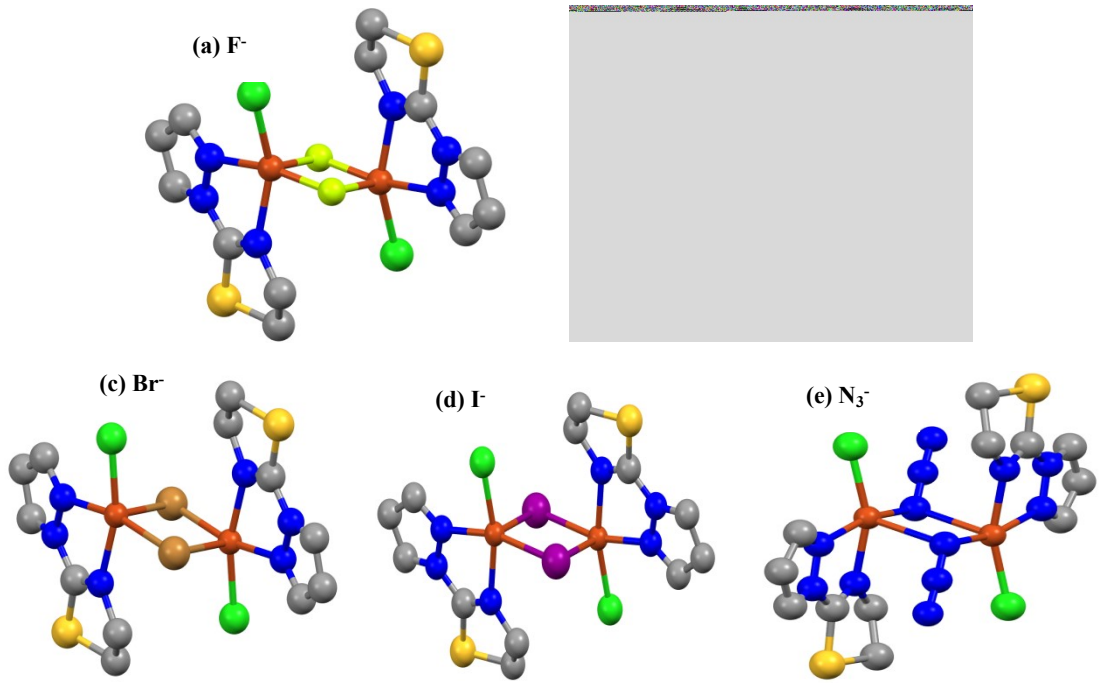

Figure S5. Molecular structure optimized (**II**) for different ligands.

Table S9. Calculated energies (E_{HS} and E_{BS}), S_{HS}^2, S_{BS}^2 and magnetic coupling constants with different ligands at the PBE/ZORA-def2-TZVP level.

Ligands	E_{HS}/eV	E_{BS}/eV	S_{HS}^2	S_{BS}^2	J_{cacl}/cm^{-1}
F^-	-144736.69512	-144736.69287	2.00320	1.00317	18.17
Cl^-	-184179.10722	-184179.10556	2.00299	1.00294	13.40
Br^-	-419474.28663	-419474.28518	2.00299	1.00299	11.68
I^-	-920122.93826	-920122.93738	2.00299	1.00234	7.12
N_3^-	-151736.02343	-151736.02300	2.00495	1.00334	3.42

Table S10. Calculated energies (E_{HS} and E_{BS}), S_{HS}^2, S_{BS}^2 and magnetic coupling constants with different ligands at the PBE/ZORA-def2-TZVP level.

Ligands	E_{HS}/eV	E_{BS}/eV	S_{HS}^2	S_{BS}^2	J_{cacl}/cm^{-1}
F^-	-164457.98007	-164457.97835	2.00304	1.00044	13.80
Cl^-	-184179.10722	-184179.10556	2.00299	1.00294	13.40
Br^-	-301826.66903	-301826.66849	2.00298	1.00229	4.38
I^-	-552151.00188	-552151.00045	2.00307	1.00307	11.60

N_3^-	-167957.76973	-167957.76854	2.00404	1.00356	9.61

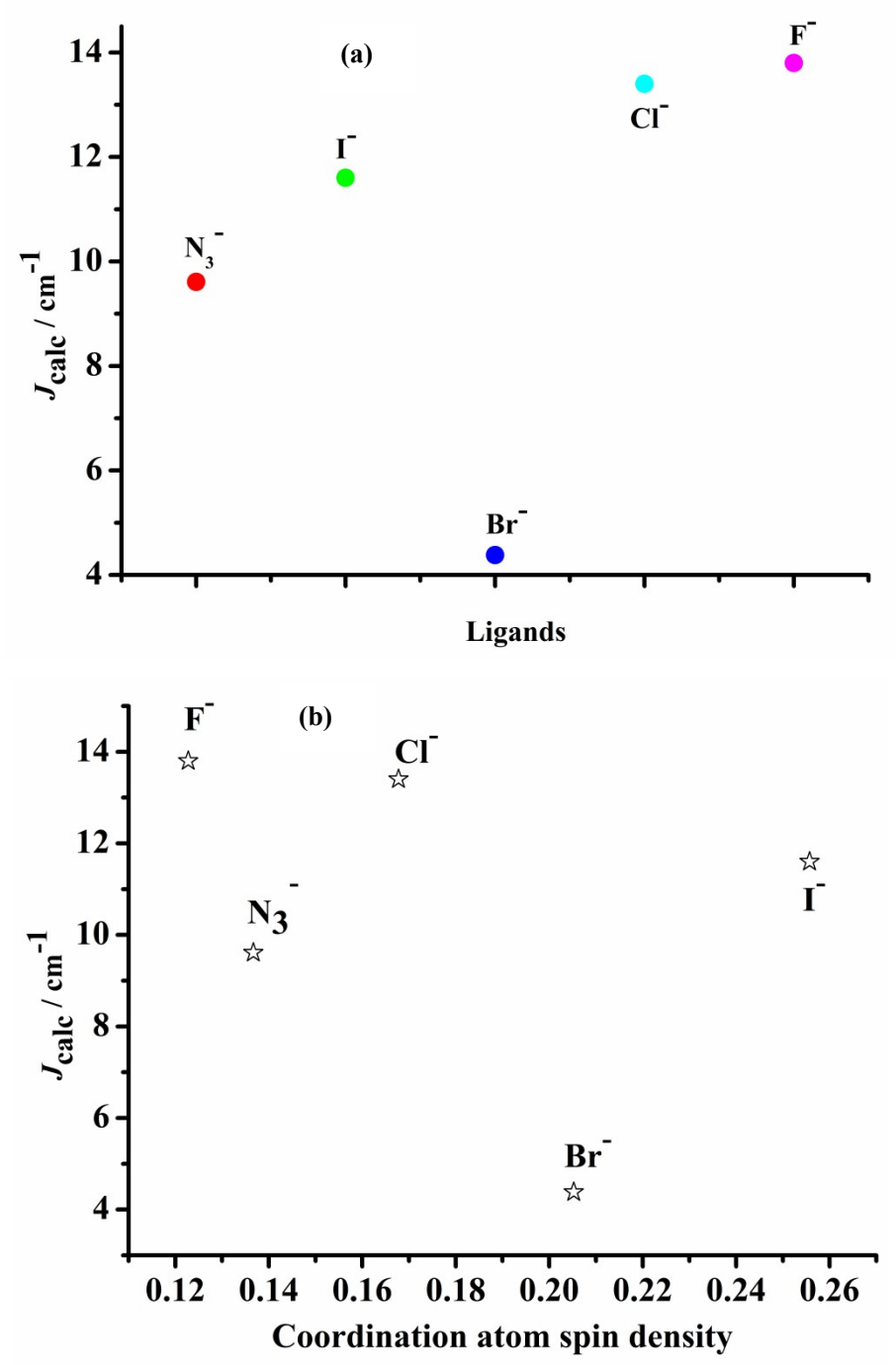

Figure S6. Magneto-structural correlation of J_{calc} and ligands were obtained by BS-DFT (Model **II**). (a) The magneto-structural correlation of J_{calc}-ligand; (b) spin density variation of Cu(II) and bridging coordination atoms in the triplet state (S=1).

Table S11. DFT-optimized Cartesian coordinates of dichloro-bridged dinuclear copper(II) complexes (M06-2X/def2-TZVPP).

Cu•••Cu distance (R_0 = 3.0 Å)			
E = -182658.29388 eV			
Cu	0.311801	-0.111298	-0.073383
Cu	3.299929	0.111294	0.073398
Cl	1.954176	1.973847	-0.018215
Cl	1.657545	-1.973856	0.018251
Cl	-0.372965	-0.255878	-2.240044
Cl	3.984742	0.255871	2.240046
C	-0.289802	1.072560	2.468986
C	0.856232	-0.772988	3.111666
H	1.784537	-1.219649	2.765644
H	0.146183	-1.563532	3.366060
C	-1.727402	2.342460	-0.364718
H	-1.903217	2.188039	-1.416959
C	-2.049135	3.434925	0.473599
H	-2.565194	4.338820	0.206492
C	-1.552672	3.100331	1.703631
H	-1.540849	3.621657	2.645490
C	1.114380	0.168370	4.288830
H	2.083001	0.652059	4.186145
H	1.025410	-0.322703	5.253164
S	-0.178580	1.458071	4.161869
N	-1.097444	1.414348	0.314036
N	0.269678	0.021161	2.035101
N	-0.991291	1.871547	1.575265
C	3.901487	-1.072559	-2.468982
C	2.755538	0.773047	-3.111649
H	1.827245	1.219739	-2.765636
H	3.465626	1.563568	-3.366012
C	5.339035	-2.342540	0.364711
H	5.514860	-2.188131	1.416952
C	5.660708	-3.435019	-0.473611
H	6.176721	-4.338941	-0.206509
C	5.164255	-3.100396	-1.703638
H	5.152397	-3.621719	-2.645498
C	2.497377	-0.168276	-4.288838
H	1.528733	-0.651926	-4.186182
H	2.586390	0.322813	-5.253160
S	3.790278	-1.458035	-4.161874
N	4.709125	-1.414391	-0.314037
N	3.342040	-0.021146	-2.035087
N	4.602943	-1.871581	-1.575267

Cu•••Cu distance (R_0 = 3.1 Å)			
E = -182658.34753 eV			
Cu	0.261171	-0.098910	-0.081628
Cu	3.350542	0.098934	0.081614
Cl	1.970178	1.937290	0.000717
Cl	1.641522	-1.937275	-0.000745
Cl	-0.403359	-0.222432	-2.254325
Cl	4.015068	0.222479	2.254309
C	-0.313601	1.084492	2.466531
C	0.840452	-0.760394	3.098114
H	1.765869	-1.202002	2.737531
H	0.140153	-1.555044	3.365828
C	-1.756443	2.370133	-0.358725
H	-1.931159	2.222788	-1.412161
C	-2.085394	3.453245	0.488654
H	-2.607378	4.355876	0.229061
C	-1.586927	3.111523	1.715999
H	-1.579296	3.624674	2.662400
C	1.114758	0.184003	4.269971
H	2.084202	0.663621	4.156138
H	1.035221	-0.304793	5.236275
S	-0.174889	1.478315	4.155412
N	-1.120843	1.440501	0.312833
N	0.232334	0.027904	2.029173
N	-1.017462	1.887820	1.577745
C	3.925294	-1.084503	-2.466526
C	2.771316	0.760421	-3.098138
H	1.845914	1.202069	-2.737566
H	3.471649	1.555041	-3.365852
C	5.368082	-2.370159	0.358750
H	5.542803	-2.222807	1.412184
C	5.696999	-3.453293	-0.488615
H	6.218951	-4.355939	-0.229011
C	5.198535	-3.111574	-1.715963
H	5.190877	-3.624741	-2.662355
C	2.496987	-0.183974	-4.269991
H	1.527522	-0.663551	-4.156166
H	2.576559	0.304812	-5.236298
S	3.786577	-1.478340	-4.155403
N	4.732523	-1.440510	-0.312823
N	3.379394	-0.027890	-2.029184
N	4.629124	-1.887844	-1.577728

Cu•••Cu distance (R_0 = 3.2 Å)

E = -182658.38292 eV

Cu	0.210702	-0.079245	-0.095680
Cu	3.401040	0.079271	0.095672
Cl	1.988922	1.896900	0.021967
Cl	1.622807	-1.896881	-0.021961
Cl	-0.451911	-0.188796	-2.267575
Cl	4.063690	0.188834	2.267556
C	-0.338284	1.098997	2.462395
C	0.826110	-0.744041	3.079489
H	1.748533	-1.181460	2.706262
H	0.136032	-1.543493	3.359169
C	-1.789357	2.403545	-0.351804
H	-1.964119	2.264831	-1.406267
C	-2.128483	3.473762	0.507311
H	-2.659493	4.373844	0.257672
C	-1.626213	3.123602	1.731061
H	-1.624167	3.625778	2.683179
C	1.114521	0.201621	4.247809
H	2.083802	0.679408	4.123622
H	1.046133	-0.286766	5.215144
S	-0.174769	1.497345	4.148364
N	-1.144414	1.472969	0.310102
N	0.196444	0.039521	2.019914
N	-1.044323	1.907708	1.579081
C	3.949979	-1.098998	-2.462394
C	2.785644	0.744075	-3.079494
H	1.863234	1.181520	-2.706265
H	3.475744	1.543506	-3.359179
C	5.401011	-2.403582	0.351809
H	5.575785	-2.264865	1.406269
C	5.740080	-3.473825	-0.507297
H	6.271046	-4.373931	-0.257651
C	5.237811	-3.123659	-1.731045
H	5.235728	-3.625846	-2.683157
C	2.497203	-0.201584	-4.247811
H	1.527907	-0.679339	-4.123624
H	2.565609	0.286798	-5.215147
S	3.786449	-1.497351	-4.148359
N	4.756114	-1.472979	-0.310104
N	3.415289	-0.039501	-2.019918
N	4.655990	-1.907730	-1.579077

Cu•••Cu distance (R_0 = 3.3 Å)

E = -182658.40136 eV

Cu	0.160299	-0.058286	-0.105652
Cu	3.451462	0.058303	0.105663
Cl	2.001166	1.854393	0.047715
Cl	1.610587	-1.854379	-0.047667
Cl	-0.494541	-0.137659	-2.281626
Cl	4.106348	0.137670	2.281626
C	-0.365488	1.113464	2.460407
C	0.804128	-0.730007	3.065602
H	1.718524	-1.170699	2.676040
H	0.119684	-1.527741	3.363609
C	-1.828054	2.433209	-0.341637
H	-2.002708	2.302583	-1.397354
C	-2.174721	3.492791	0.527406
H	-2.713059	4.390958	0.286242
C	-1.667536	3.136011	1.747171
H	-1.668773	3.630018	2.703837
C	1.117267	0.220724	4.223738
H	2.087017	0.693097	4.082726
H	1.063211	-0.263708	5.194062
S	-0.168305	1.521430	4.140323
N	-1.174170	1.502307	0.311141
N	0.153369	0.047854	2.014216
N	-1.075265	1.926884	1.583858
C	3.977178	-1.113459	-2.460404
C	2.807637	0.730059	-3.065597
H	1.893255	1.170784	-2.676038
H	3.492114	1.527768	-3.363596
C	5.439710	-2.433267	0.341627
H	5.614388	-2.302644	1.397339
C	5.786284	-3.492885	-0.527411
H	6.324560	-4.391090	-0.286246
C	5.279101	-3.136083	-1.747170
H	5.280278	-3.630103	-2.703828
C	2.494469	-0.220653	-4.223741
H	1.524700	-0.692990	-4.082739
H	2.548551	0.263784	-5.194061
S	3.779989	-1.521410	-4.140323
N	4.785885	-1.502323	-0.311150
N	3.458359	-0.047831	-2.014210
N	4.686927	-1.926908	-1.583861

Cu•••Cu distance (R_0 = 3.4 Å)

E = -182658.40223 eV

Cu•••Cu distance (R_0 = 3.5 Å)

E = -182658.38324 eV

Cu	0.110636	-0.029151	-0.124156
Cu	3.501056	0.029175	0.124142
Cl	2.029533	1.818971	0.094181
Cl	1.582164	-1.818940	-0.094198
Cl	-0.512449	-0.028458	-2.311109
Cl	4.124122	0.028474	2.311101
C	-0.396206	1.128074	2.453136
C	0.784063	-0.712772	3.040975
H	1.686767	-1.160737	2.633034
H	0.105172	-1.504762	3.365588
C	-1.877476	2.465444	-0.331524
H	-2.053970	2.344226	-1.387891
C	-2.231567	3.511863	0.549800
H	-2.779338	4.407122	0.319689
C	-1.716556	3.147352	1.764266
H	-1.719157	3.631042	2.726080
C	1.131080	0.247594	4.180899
H	2.095242	0.720303	4.006516
H	1.109384	-0.228898	5.156364
S	-0.160048	1.544358	4.125862
N	-1.212513	1.533766	0.309803
N	0.107905	0.058304	2.000064
N	-1.113144	1.946229	1.586098
C	4.007899	-1.128084	-2.453135
C	2.827641	0.712762	-3.040999
H	1.924943	1.160743	-2.633062
H	3.506539	1.504737	-3.365630
C	5.489164	-2.465423	0.331542
H	5.665657	-2.344193	1.387908
C	5.843252	-3.511855	-0.549768
H	6.391018	-4.407113	-0.319645
C	5.328240	-3.147359	-1.764238
H	5.330840	-3.631062	-2.726046
C	2.480613	-0.247622	-4.180905
H	1.516449	-0.720322	-4.006509
H	2.502303	0.228855	-5.156379
S	3.771733	-1.544393	-4.125854
N	4.824205	-1.533751	-0.309796
N	3.503794	-0.058304	-2.000079
N	4.724833	-1.946230	-1.586086

Cu•••Cu distance (R_0 = 3.6 Å)

E = -182658.35703 eV

Cu	0.017342	0.127438	-0.158858
Cu	3.594223	-0.127479	0.158856
Cu	0.063579	0.086257	-0.139903
Cu	3.548113	-0.086212	0.139872
Cl	2.148867	1.770548	0.167670
Cl	1.462810	-1.770516	-0.167716
Cl	-0.530332	0.207312	-2.328485
Cl	4.142012	-0.207233	2.328459
C	-0.461227	1.186668	2.462716
C	0.765063	-0.636780	3.003870
H	1.664464	-1.070812	2.574727
H	0.103188	-1.438132	3.339989
C	-1.954706	2.565240	-0.295705
H	-2.108984	2.474708	-1.358378
C	-2.381009	3.553519	0.619672
H	-2.974446	4.425166	0.414126
C	-1.866318	3.169260	1.828475
H	-1.915830	3.610352	2.809089
C	1.126039	0.323899	4.136848
H	2.066343	0.830280	3.928723
H	1.161448	-0.157600	5.109262
S	-0.207117	1.579704	4.139742
N	-1.248094	1.646922	0.321075
N	0.055014	0.134005	1.985085
N	-1.192864	2.012494	1.613918
C	4.072922	-1.186683	-2.462716
C	2.846634	0.636753	-3.003912
H	1.947249	1.070815	-2.574767
H	3.508515	1.438080	-3.340082
C	5.566402	-2.565196	0.295734
H	5.720679	-2.474644	1.358405
C	5.992720	-3.553486	-0.619626
H	6.586168	-4.425121	-0.414064
C	5.478024	-3.169255	-1.828436
H	5.527545	-3.610363	-2.809042
C	2.485624	-0.323969	-4.136842
H	1.545326	-0.830344	-3.928670
H	2.450186	0.157491	-5.109273
S	3.818782	-1.579772	-4.139724
N	4.859781	-1.646897	-0.321064
N	3.556695	-0.133999	-1.985111
N	4.804557	-2.012492	-1.613900

Cu•••Cu distance (R_0 = 3.7 Å)

E = -182658.32006 eV

Cu	-0.029925	0.138907	-0.181979
Cu	3.641633	-0.138917	0.181991

Cl	2.194137	1.727049	0.222388
Cl	1.417442	-1.727081	-0.222463
Cl	-0.555868	0.295817	-2.348023
Cl	4.167306	-0.295867	2.348051
C	-0.495092	1.202607	2.456353
C	0.753772	-0.613391	2.967903
H	1.642049	-1.048449	2.517120
H	0.101271	-1.414274	3.323472
C	-2.002329	2.603875	-0.283467
H	-2.154465	2.527514	-1.347803
C	-2.439983	3.574768	0.644752
H	-3.041962	4.443272	0.450405
C	-1.922425	3.179082	1.848771
H	-1.977773	3.607485	2.834931
C	1.140953	0.352892	4.085710
H	2.066112	0.871826	3.842808
H	1.218254	-0.124782	5.057553
S	-0.209717	1.590136	4.130150
N	-1.286887	1.684342	0.321499
N	0.016465	0.153828	1.965523
N	-1.237122	2.032453	1.619810
C	4.106786	-1.202640	-2.456333
C	2.858091	0.613449	-2.967968
H	1.969809	1.048575	-2.517268
H	3.510694	1.414282	-3.323463
C	5.613861	-2.603931	0.283558
H	5.765947	-2.527570	1.347901
C	6.051542	-3.574834	-0.644639
H	6.653498	-4.443347	-0.450264
C	5.534046	-3.179141	-1.848682
H	5.589435	-3.607545	-2.834839
C	2.470946	-0.352785	-4.085829
H	1.545724	-0.871651	-3.843028
H	2.393777	0.124915	-5.057670
S	3.821522	-1.590132	-4.130159
N	4.898456	-1.684392	-0.321440
N	3.595242	-0.153844	-1.965528
N	4.848746	-2.032505	-1.619752

Cu•••Cu distance (R_0 = 3.8 Å)

E = -182658.28124 eV

Cu	-0.077449	0.134090	-0.212306
Cu	3.689221	-0.134058	0.212302
Cl	2.257185	1.682190	0.352091
Cl	1.354621	-1.682128	-0.352080

Cl	2.218428	1.695576	0.287396
Cl	1.393305	-1.695566	-0.287375
Cl	-0.580222	0.353905	-2.371842
Cl	4.191893	-0.353943	2.371862
C	-0.518041	1.199853	2.440973
C	0.748951	-0.609555	2.926826
H	1.622486	-1.049895	2.452984
H	0.107815	-1.407100	3.309838
C	-2.038023	2.621493	-0.281912
H	-2.192599	2.554251	-1.346542
C	-2.467281	3.588054	0.654051
H	-3.064541	4.461539	0.467360
C	-1.947441	3.181753	1.853798
H	-1.995928	3.604721	2.842671
C	1.169571	0.366802	4.022872
H	2.081019	0.891111	3.742710
H	1.285350	-0.103062	4.994728
S	-0.188783	1.595079	4.104568
N	-1.325914	1.693537	0.314972
N	-0.018769	0.149245	1.941001
N	-1.269964	2.032766	1.615281
C	4.129744	-1.199849	-2.440967
C	2.862854	0.609627	-2.926831
H	1.989327	1.050001	-2.453009
H	3.504041	1.407148	-3.309809
C	5.649613	-2.621583	0.281929
H	5.804177	-2.554356	1.346562
C	6.078827	-3.588166	-0.654032
H	6.676031	-4.461688	-0.467337
C	5.559022	-3.181831	-1.853783
H	5.607492	-3.604802	-2.842655
C	2.442222	-0.366691	-4.022909
H	1.530738	-0.890958	-3.742790
H	2.326502	0.103198	-4.994761
S	3.800517	-1.595035	-4.104579
N	4.937574	-1.693579	-0.314961
N	3.630505	-0.149227	-1.940993
N	4.881618	-2.032800	-1.615271

Cu•••Cu distance (R_0 = 3.9 Å)

E = -182658.24374 eV

Cu	-0.126796	0.121496	-0.229046
Cu	3.738576	-0.121485	0.229059
Cl	2.291577	1.675408	0.383753
Cl	1.320260	-1.675348	-0.383716

Cl	-0.602767	0.404968	-2.399831
Cl	4.214532	-0.404957	2.399827
C	-0.524539	1.192892	2.415687
C	0.749285	-0.615769	2.879304
H	1.604741	-1.068882	2.385139
H	0.115057	-1.404782	3.290754
C	-2.070198	2.626490	-0.286928
H	-2.233982	2.564213	-1.350360
C	-2.484139	3.592848	0.655353
H	-3.077646	4.470459	0.476643
C	-1.954507	3.180422	1.849105
H	-1.989684	3.600952	2.839407
C	1.207533	0.370406	3.950898
H	2.107850	0.892850	3.634226
H	1.356116	-0.090544	4.922608
S	-0.149332	1.598402	4.066117
N	-1.358353	1.691929	0.301096
N	-0.043269	0.137021	1.908466
N	-1.287517	2.027736	1.601161
C	4.136244	-1.192886	-2.415692
C	2.862491	0.615827	-2.879307
H	2.007060	1.068976	-2.385131
H	3.496745	1.404814	-3.290768
C	5.681835	-2.626555	0.286926
H	5.845628	-2.564280	1.350356
C	6.095693	-3.592957	-0.655346
H	6.689134	-4.470611	-0.476630
C	5.566083	-3.180505	-1.849100
H	5.601218	-3.601051	-2.839396
C	2.404191	-0.370336	-3.950890
H	1.503858	-0.892743	-3.634202
H	2.255613	0.090613	-4.922601
S	3.761006	-1.598389	-4.066117
N	4.970058	-1.691947	-0.301104
N	3.655026	-0.136989	-1.908473
N	4.899185	-2.027764	-1.601166

Cu-(μ-Cl)-Cu bond angle (α = 80°)

E = -182658.38879 eV

Cu	0.191621	-0.086835	-0.102005
Cu	3.419865	0.086804	0.101988
Cl	2.012557	1.914284	0.039598
Cl	1.598927	-1.914312	-0.039759
Cl	-0.454614	-0.161566	-2.280283
Cl	4.065921	0.161540	2.280320

Cl	-0.639269	0.420487	-2.413106
Cl	4.251034	-0.420523	2.413117
C	-0.526657	1.192495	2.399628
C	0.753573	-0.616716	2.845919
H	1.602725	-1.066780	2.338426
H	0.127565	-1.408915	3.263552
C	-2.099371	2.628846	-0.286106
H	-2.274801	2.567156	-1.347772
C	-2.497131	3.598492	0.659396
H	-3.087067	4.479617	0.486131
C	-1.956376	3.184517	1.847692
H	-1.976986	3.607122	2.837577
C	1.224561	0.367700	3.914140
H	2.123778	0.887655	3.590917
H	1.379846	-0.094837	4.884026
S	-0.126832	1.600784	4.043189
N	-1.386463	1.690626	0.295148
N	-0.054290	0.135149	1.886815
N	-1.299012	2.027738	1.594053
C	4.138370	-1.192472	-2.399633
C	2.858222	0.616801	-2.845900
H	2.009096	1.066898	-2.338390
H	3.484257	1.408978	-3.263534
C	5.710985	-2.628958	0.286087
H	5.886418	-2.567292	1.347754
C	6.108656	-3.598635	-0.659420
H	6.698510	-4.479816	-0.486160
C	5.567934	-3.184607	-1.847712
H	5.588497	-3.607214	-2.837597
C	2.387178	-0.367586	-3.914123
H	1.487942	-0.887503	-3.590894
H	2.231904	0.094964	-4.884004
S	3.738516	-1.600728	-4.043195
N	4.998160	-1.690671	-0.295160
N	3.666062	-0.135106	-1.886809
N	4.910676	-2.027770	-1.594066

Cu-(μ-Cl)-Cu bond angle (α = 83°)

E = -182658.40245 eV

Cu	0.154978	-0.061127	-0.107269
Cu	3.456760	0.061127	0.107283
Cl	2.002710	1.857724	0.051904
Cl	1.609024	-1.857725	-0.051860
Cl	-0.501628	-0.137557	-2.281942
Cl	4.113389	0.137531	2.281949

C	-0.332812	1.101987	2.453622
C	0.825073	-0.745605	3.070385
H	1.743434	-1.187797	2.692642
H	0.133423	-1.541006	3.356703
C	-1.792846	2.407074	-0.355721
H	-1.969322	2.268254	-1.409741
C	-2.135883	3.473515	0.506358
H	-2.673218	4.370537	0.259831
C	-1.627779	3.124477	1.728009
H	-1.625770	3.624467	2.681169
C	1.125180	0.202595	4.233925
H	2.096661	0.673978	4.103965
H	1.057834	-0.281864	5.203226
S	-0.156266	1.506692	4.136112
N	-1.140036	1.479579	0.303000
N	0.191878	0.037007	2.011580
N	-1.038341	1.912885	1.572081
C	3.944484	-1.102064	-2.453580
C	2.786941	0.745696	-3.070510
H	1.868551	1.187986	-2.692959
H	3.478760	1.541022	-3.356629
C	5.404231	-2.407157	0.355902
H	5.580629	-2.268319	1.409932
C	5.747210	-3.473676	-0.506105
H	6.284429	-4.370746	-0.259501
C	5.239287	-3.124605	-1.727821
H	5.237339	-3.624610	-2.680975
C	2.486998	-0.202379	-4.234189
H	1.515396	-0.673588	-4.104531
H	2.554704	0.282128	-5.203441
S	3.768163	-1.506732	-4.136104
N	4.751507	-1.479652	-0.302890
N	3.419826	-0.037040	-2.011601
N	4.649884	-1.912988	-1.571964

Cu-(μ-Cl)-Cu bond angle (α = 86°)

E = -182658.40011 eV

Cu	0.114431	-0.029708	-0.120869
Cu	3.497294	0.029753	0.120846
Cl	2.011863	1.804156	0.079720
Cl	1.599861	-1.804111	-0.079743
Cl	-0.532378	-0.065811	-2.298341
Cl	4.144092	0.065872	2.298320
C	-0.397909	1.126053	2.455992
C	0.784073	-0.714565	3.042879

C	-0.364363	1.112796	2.457469
C	0.805285	-0.731356	3.061174
H	1.718611	-1.172361	2.669638
H	0.121760	-1.529115	3.361053
C	-1.827913	2.434370	-0.342982
H	-2.003493	2.304275	-1.398538
C	-2.172976	3.494044	0.526595
H	-2.710610	4.392730	0.286023
C	-1.665235	3.136518	1.745904
H	-1.665349	3.630302	2.702614
C	1.121196	0.219599	4.218480
H	2.091367	0.690667	4.076242
H	1.067756	-0.264395	5.189020
S	-0.162642	1.522014	4.136525
N	-1.174342	1.502740	0.309085
N	0.151859	0.045962	2.010958
N	-1.074195	1.926912	1.581818
C	3.976052	-1.112790	-2.457467
C	2.806443	0.731391	-3.061157
H	1.893125	1.172412	-2.669621
H	3.489987	1.529138	-3.361026
C	5.439589	-2.434414	0.342966
H	5.615183	-2.304327	1.398520
C	5.784600	-3.494103	-0.526614
H	6.322199	-4.392810	-0.286048
C	5.276853	-3.136559	-1.745916
H	5.276929	-3.630346	-2.702624
C	2.490516	-0.219546	-4.218474
H	1.520334	-0.690595	-4.076243
H	2.543967	0.264458	-5.189009
S	3.774326	-1.521988	-4.136527
N	4.786053	-1.502755	-0.309094
N	3.459850	-0.045950	-2.010946
N	4.685870	-1.926926	-1.581825

Cu-(μ-Cl)-Cu bond angle (α = 89°)

E = -182658.37924 eV

Cu	0.072633	0.131024	-0.143527
Cu	3.538986	-0.131089	0.143552
Cl	2.155477	1.730132	0.181811
Cl	1.456146	-1.730198	-0.181793
Cl	-0.526278	0.260771	-2.333380
Cl	4.137852	-0.260868	2.333413
C	-0.481336	1.197535	2.472833
C	0.752562	-0.621659	3.006227

H	1.688300	-1.158513	2.634121
H	0.107305	-1.510081	3.362779
C	-1.873985	2.467010	-0.329349
H	-2.048555	2.345823	-1.385973
C	-2.224766	3.515208	0.551401
H	-2.767972	4.412873	0.320516
C	-1.713271	3.148446	1.766485
H	-1.714980	3.631303	2.728579
C	1.126840	0.243125	4.186225
H	2.091864	0.715786	4.017222
H	1.099656	-0.234933	5.160635
S	-0.163306	1.541080	4.129555
N	-1.213411	1.532720	0.312495
N	0.106794	0.056738	2.002621
N	-1.114356	1.944753	1.589248
C	4.009606	-1.126062	-2.455992
C	2.827655	0.714563	-3.042915
H	1.923446	1.158547	-2.634156
H	3.504440	1.510052	-3.362850
C	5.485672	-2.466990	0.329368
H	5.660254	-2.345781	1.385987
C	5.836401	-3.515228	-0.551356
H	6.379573	-4.412908	-0.320452
C	5.324923	-3.148472	-1.766448
H	5.326607	-3.631354	-2.728530
C	2.484850	-0.243155	-4.186226
H	1.519819	-0.715792	-4.017190
H	2.512025	0.234874	-5.160651
S	3.774975	-1.541129	-4.129540
N	4.825120	-1.532696	-0.312494
N	3.504929	-0.056725	-2.002643
N	4.726044	-1.944756	-1.589236

Cu-(μ-Cl)-Cu bond angle (α = 92°)

E = -182658.34745 eV

Cu	0.031722	0.171613	-0.162505
Cu	3.580044	-0.171650	0.162552
Cl	2.174060	1.672746	0.235716
Cl	1.437703	-1.672793	-0.235590
Cl	-0.546666	0.341218	-2.352790
Cl	4.158490	-0.341296	2.352818
C	-0.516603	1.205701	2.468732
C	0.737664	-0.605234	2.975999
H	1.619828	-1.048827	2.521424
H	0.085143	-1.399742	3.345687
H	1.646911	-1.060703	2.571970
H	0.089876	-1.418732	3.351270
C	-1.972686	2.588220	-0.281219
H	-2.120457	2.506927	-1.345710
C	-2.416275	3.562035	0.641441
H	-3.019315	4.428405	0.441299
C	-1.903581	3.171719	1.849187
H	-1.964956	3.602839	2.833715
C	1.124210	0.342841	4.131207
H	2.056772	0.856408	3.905782
H	1.180509	-0.135631	5.104083
S	-0.220082	1.586904	4.150605
N	-1.258264	1.672333	0.330180
N	0.036518	0.148097	1.990505
N	-1.215008	2.025448	1.627274
C	4.093028	-1.197536	-2.472821
C	2.859182	0.621695	-3.006209
H	1.964808	1.060727	-2.571994
H	3.521899	1.418778	-3.351167
C	5.584301	-2.588282	0.281239
H	5.732045	-2.507011	1.345735
C	6.027912	-3.562079	-0.641430
H	6.630943	-4.428455	-0.441291
C	5.515252	-3.171734	-1.849181
H	5.576653	-3.602833	-2.833716
C	2.487601	-0.342742	-4.131267
H	1.555010	-0.856299	-3.905942
H	2.431390	0.135782	-5.104121
S	3.831866	-1.586834	-4.150623
N	4.869898	-1.672380	-0.330159
N	3.575149	-0.148117	-1.990478
N	4.826674	-2.025469	-1.627260

Cu-(μ-Cl)-Cu bond angle (α = 95°)

E = -182658.29784 eV

Cu	-0.013195	0.191838	-0.178479
Cu	3.624842	-0.191884	0.178504
Cl	2.173511	1.619503	0.286784
Cl	1.438142	-1.619549	-0.286773
Cl	-0.568816	0.395841	-2.370168
Cl	4.180432	-0.395897	2.370200
C	-0.545403	1.204664	2.460812
C	0.726412	-0.599999	2.943747
H	1.595209	-1.044904	2.465223
H	0.088460	-1.394056	3.338908

C	-2.018661	2.621186	-0.268320
H	-2.164483	2.551838	-1.333813
C	-2.465861	3.581782	0.665720
H	-3.072065	4.448186	0.475982
C	-1.951387	3.179099	1.869072
H	-2.013286	3.597998	2.858619
C	1.138363	0.367812	4.082791
H	2.056693	0.890557	3.822930
H	1.232828	-0.104351	5.055788
S	-0.219315	1.597547	4.139895
N	-1.301311	1.700145	0.332950
N	-0.006768	0.157518	1.975558
N	-1.259377	2.037888	1.633723
C	4.128294	-1.205666	-2.468733
C	2.874000	0.605275	-2.975920
H	1.991834	1.048833	-2.521313
H	3.526500	1.399809	-3.345591
C	5.630371	-2.621265	0.268252
H	5.776213	-2.551952	1.333744
C	6.077537	-3.581838	-0.665827
H	6.683726	-4.448261	-0.476128
C	5.563038	-3.179116	-1.869154
H	5.624901	-3.597991	-2.858714
C	2.473297	-0.367736	-4.082742
H	1.554975	-0.890501	-3.822891
H	2.378816	0.104459	-5.055721
S	3.830985	-1.597457	-4.139905
N	4.913044	-1.700180	-0.332979
N	3.618463	-0.157500	-1.975517
N	4.871073	-2.037887	-1.633762

Cu-(μ-Cl)-Cu bond angle (α = 98°)

E = -182658.22996 eV

Cu	-0.063496	0.206286	-0.195066
Cu	3.675251	-0.206263	0.195066
Cl	2.177167	1.568318	0.334033
Cl	1.434591	-1.568296	-0.334031
Cl	-0.594589	0.453547	-2.386765
Cl	4.206362	-0.453517	2.386762
C	-0.571894	1.203513	2.449896
C	0.714712	-0.596971	2.906612
H	1.567952	-1.044652	2.403281
H	0.090963	-1.389361	3.327335
C	-2.099129	2.658712	-0.253768
H	-2.249911	2.607691	-1.319817
C	-2.057174	2.641105	-0.260958
H	-2.203897	2.580912	-1.326867
C	-2.496304	3.597654	0.680422
H	-3.096981	4.469394	0.497944
C	-1.980918	3.183875	1.879859
H	-2.036911	3.596969	2.872108
C	1.157911	0.381706	4.030901
H	2.065537	0.906402	3.739656
H	1.283234	-0.083678	5.003656
S	-0.203406	1.606678	4.121046
N	-1.344469	1.711117	0.332729
N	-0.050440	0.152683	1.960489
N	-1.297578	2.039633	1.635729
C	4.157098	-1.204663	-2.460798
C	2.885346	0.600045	-2.943738
H	2.016535	1.044955	-2.465248
H	3.523340	1.394098	-3.338839
C	5.668769	-2.641187	0.260981
H	5.815461	-2.581022	1.326895
C	6.107962	-3.597688	-0.680419
H	6.708658	-4.469417	-0.497954
C	5.592542	-3.183922	-1.879844
H	5.648536	-3.597005	-2.872098
C	2.453883	-0.381612	-4.030952
H	1.546227	-0.906294	-3.739780
H	2.328629	0.083809	-5.003698
S	3.815170	-1.606619	-4.121061
N	4.956106	-1.711167	-0.332706
N	3.662128	-0.152690	-1.960465
N	4.909236	-2.039659	-1.635712

Cu-(μ-Cl)-Cu bond angle (α = 101°)

E = -182658.14462 eV

Cu	-0.124050	0.229713	-0.213995
Cu	3.735814	-0.229738	0.214025
Cl	2.213939	1.517276	0.377986
Cl	1.397819	-1.517312	-0.377906
Cl	-0.623778	0.531488	-2.403703
Cl	4.235593	-0.531547	2.403716
C	-0.594258	1.216924	2.435778
C	0.713254	-0.579049	2.855479
H	1.558992	-1.010873	2.326745
H	0.109738	-1.383529	3.282115
C	-2.156201	2.685484	-0.240993
H	-2.315708	2.642884	-1.306161

C	-2.527107	3.612640	0.694933	C	-2.577809	3.630991	0.718504
H	-3.122108	4.490083	0.520213	H	-3.176394	4.508275	0.555901
C	-2.008631	3.188526	1.889575	C	-2.046809	3.199584	1.905195
H	-2.056829	3.597499	2.884197	H	-2.086210	3.601412	2.903100
C	1.179387	0.392465	3.972830	C	1.193802	0.405442	3.919811
H	2.077145	0.915871	3.650168	H	2.086876	0.930334	3.587512
H	1.335087	-0.066944	4.944138	H	1.363860	-0.059350	4.886035
S	-0.180381	1.617398	4.096135	S	-0.163566	1.630864	4.071998
N	-1.389731	1.720421	0.331264	N	-1.438995	1.744481	0.330552
N	-0.093169	0.147399	1.942162	N	-0.124726	0.162918	1.915581
N	-1.334652	2.041145	1.636219	N	-1.372556	2.055958	1.637607
C	4.183590	-1.203512	-2.449897	C	4.205941	-1.216903	-2.435780
C	2.897040	0.597013	-2.906611	C	2.898431	0.579087	-2.855414
H	2.043821	1.044725	-2.403271	H	2.052710	1.010904	-2.326643
H	3.520808	1.389379	-3.327349	H	3.501936	1.383573	-3.282054
C	5.710787	-2.658759	0.253763	C	5.767913	-2.685545	0.240929
H	5.861581	-2.607738	1.319810	H	5.927445	-2.642969	1.306095
C	6.138702	-3.612721	-0.694933	C	6.189480	-3.631043	-0.718595
H	6.733654	-4.490195	-0.520211	H	6.788049	-4.508343	-0.556021
C	5.620244	-3.188583	-1.889576	C	5.658464	-3.199602	-1.905266
H	5.668416	-3.597564	-2.884195	H	5.697837	-3.601412	-2.903179
C	2.432318	-0.392415	-3.972817	C	2.417846	-0.405382	-3.919749
H	1.534548	-0.915790	-3.650137	H	1.524778	-0.930274	-3.587434
H	2.276617	0.066991	-4.944126	H	2.247763	0.059430	-4.885959
S	3.792045	-1.617393	-4.096130	S	3.775201	-1.630810	-4.071996
N	5.001431	-1.720437	-0.331269	N	5.050719	-1.744513	-0.330582
N	3.704909	-0.147376	-1.942166	N	3.736438	-0.162899	-1.915555
N	4.946324	-2.041168	-1.636221	N	4.984245	-2.055965	-1.637643

Cu-(μ-Cl)-Cu bond angle (α = 104°)

E = -182658.04930 eV

Cu	-0.205586	0.221342	-0.249157
Cu	3.817257	-0.221343	0.249157
Cl	2.261736	1.473099	0.433772
Cl	1.349940	-1.473097	-0.433783
Cl	-0.688756	0.566735	-2.428255
Cl	4.300425	-0.566721	2.428258
C	-0.601665	1.219938	2.404469
C	0.710856	-0.580950	2.788758
H	1.540481	-1.013437	2.235787
H	0.117513	-1.385834	3.228591
C	-2.214874	2.700952	-0.235144
H	-2.395582	2.662919	-1.297109
C	-2.611184	3.646184	0.734878
H	-3.207641	4.527522	0.587221

C	-2.057418	3.209140	1.909356
H	-2.071922	3.608686	2.908814
C	1.220747	0.399112	3.843707
H	2.109386	0.919238	3.493474
H	1.407796	-0.068294	4.805440
S	-0.123679	1.635203	4.026097
N	-1.491616	1.753934	0.319299
N	-0.151406	0.163316	1.872093
N	-1.396182	2.062228	1.625217
C	4.213360	-1.219943	-2.404466
C	2.900838	0.580943	-2.788766
H	2.071201	1.013419	-2.235805
H	3.494183	1.385835	-3.228583
C	5.826550	-2.700951	0.235164
H	6.007251	-2.662914	1.297130
C	6.222862	-3.646189	-0.734851
H	6.819315	-4.527528	-0.587186
C	5.669119	-3.209139	-1.909339
H	5.683639	-3.608683	-2.908797
C	2.390970	-0.399114	-3.843731
H	1.502323	-0.919243	-3.493520
H	2.203940	0.068298	-4.805466
S	3.735400	-1.635202	-4.026103
N	5.103289	-1.753938	-0.319286
N	3.763090	-0.163324	-1.872093
N	5.007870	-2.062232	-1.625205

Cu-Cl-Cu-Cl dihedral angle (τ = 0°)

E = -182658.40217 eV

Cu	0.141627	-0.061806	-0.107874
Cu	3.470104	0.061822	0.107876
Cl	1.993083	1.838599	0.055896
Cl	1.618644	-1.838587	-0.055895
Cl	-0.516971	-0.138268	-2.281960
Cl	4.128696	0.138270	2.281961
C	-0.374438	1.109695	2.459477
C	0.800673	-0.732115	3.059470
H	1.712975	-1.171105	2.663135
H	0.121520	-1.531706	3.364295
C	-1.838324	2.435460	-0.339018
H	-2.015360	2.306053	-1.394406
C	-2.175830	3.497751	0.530277
H	-2.707811	4.399831	0.289859
C	-1.668971	3.137733	1.749252
H	-1.664259	3.632271	2.705550

Cu-Cl-Cu-Cl dihedral angle (τ = 3°)

E = -182658.39169 eV

Cu	-0.136120	0.211240	-0.129524
Cu	3.171533	0.280198	-0.655394
Cl	1.649644	1.950458	-1.146737
Cl	1.408577	-1.395284	0.462164
Cl	-1.188331	-0.813915	-1.857574
Cl	4.251785	1.282354	1.072432
C	-0.166148	2.455256	1.652900
C	1.177919	1.033741	2.792436
H	2.000894	0.398861	2.473348
H	0.608993	0.519951	3.570836
C	-2.176192	2.446139	-1.120681
H	-2.562092	1.858169	-1.937562
C	-2.310234	3.823152	-0.833485
H	-2.858757	4.560927	-1.389494
C	-1.571632	4.025350	0.300577
H	-1.354528	4.908087	0.877051

C	1.121207	0.220804	4.214127
H	2.090484	0.692368	4.067195
H	1.072672	-0.262124	5.185447
S	-0.164118	1.522046	4.136779
N	-1.189960	1.499984	0.312898
N	0.139133	0.042044	2.012161
N	-1.085986	1.924191	1.585357
C	3.986137	-1.109691	-2.459477
C	2.811056	0.732134	-3.059477
H	1.898760	1.171141	-2.663143
H	3.490222	1.531713	-3.364305
C	5.449999	-2.435478	0.339020
H	5.627046	-2.306069	1.394406
C	5.787457	-3.497791	-0.530266
H	6.319401	-4.399891	-0.289843
C	5.280593	-3.137770	-1.749238
H	5.275845	-3.632322	-2.705528
C	2.490506	-0.220784	-4.214130
H	1.521223	-0.692333	-4.067196
H	2.539048	0.262141	-5.185452
S	3.775812	-1.522044	-4.136777
N	4.801676	-1.499977	-0.312902
N	3.472583	-0.042030	-2.012164
N	4.697673	-1.924196	-1.585355

Cu-Cl-Cu-Cl dihedral angle (τ = 6°)

E = -182658.37507 eV

Cu	-0.200315	0.207916	-0.128067
Cu	3.120516	0.229034	-0.609639
Cl	1.653575	1.939204	-1.137910
Cl	1.344781	-1.349981	0.580152
Cl	-1.224215	-0.844055	-1.853403
Cl	4.199863	1.232361	1.122322
C	-0.227982	2.532859	1.553967
C	1.048188	1.129614	2.791333
H	1.857501	0.457327	2.517160
H	0.452853	0.668181	3.582628
C	-2.150759	2.445999	-1.278293
H	-2.522635	1.830492	-2.081307
C	-2.263113	3.836505	-1.055555
H	-2.777719	4.559794	-1.660874
C	-1.556141	4.072705	0.092014
H	-1.338211	4.975080	0.636756
C	1.603353	2.493216	3.205005
H	2.511043	2.721316	2.650211
C	1.701330	2.392453	3.260063
H	2.586040	2.675909	2.693964
H	1.899695	2.426302	4.327089
S	0.369243	3.583574	2.865011
N	-1.426149	1.860083	-0.217034
N	0.283700	1.272031	1.662402
N	-1.062090	2.819682	0.653968
C	3.199636	-1.915035	-2.494994
C	1.844206	-0.465216	-3.584039
H	1.004903	0.140343	-3.250788
H	2.419857	0.092976	-4.326148
C	5.248602	-1.968943	0.249366
H	5.639702	-1.402447	1.078776
C	5.413226	-3.329964	-0.095262
H	5.993564	-4.073631	0.419338
C	4.657578	-3.508117	-1.221840
H	4.454709	-4.373615	-1.828983
C	1.354817	-1.809520	-4.125687
H	0.469992	-2.139399	-3.586190
H	1.171189	-1.794470	-5.195728
S	2.708075	-2.990345	-3.772810
N	4.463354	-1.369311	-0.614119
N	2.722273	-0.742321	-2.450638
N	4.105136	-2.304268	-1.514408

Cu-Cl-Cu-Cl dihedral angle (τ = 9°)

E = -182658.36035 eV

Cu	-0.169233	0.207579	-0.198273
Cu	3.168667	0.249601	-0.629699
Cl	1.692768	1.962371	-1.118310
Cl	1.377046	-1.316973	0.590919
Cl	-1.170805	-0.866097	-1.923802
Cl	4.245358	1.252136	1.105098
C	-0.291272	2.561440	1.455657
C	1.001870	1.210579	2.731078
H	1.818541	0.539444	2.475838
H	0.413250	0.766932	3.537327
C	-2.148532	2.392605	-1.416108
H	-2.485739	1.758900	-2.220157
C	-2.309595	3.780329	-1.208061
H	-2.835463	4.481106	-1.829945
C	-1.633954	4.048468	-0.048524
H	-1.457591	4.962042	0.492412
C	1.541492	2.592042	3.102342
H	2.441880	2.818826	2.534883

H	1.774651	2.574460	4.274008
S	0.322994	3.705482	2.714479
N	-1.443599	1.885013	-0.325590
N	0.179627	1.337003	1.635611
N	-1.085946	2.873309	0.514156
C	3.203223	-1.948322	-2.479400
C	1.819152	-0.510331	-3.547815
H	0.959504	0.067546	-3.218061
H	2.397040	0.079702	-4.263304
C	5.259418	-1.983528	0.260025
H	5.623183	-1.420642	1.104392
C	5.511641	-3.316344	-0.139526
H	6.151342	-4.035927	0.337739
C	4.758068	-3.502002	-1.266222
H	4.615629	-4.352424	-1.910899
C	1.377336	-1.852383	-4.133075
H	0.495823	-2.225776	-3.616626
H	1.207698	-1.812399	-5.204813
S	2.763532	-2.999989	-3.796171
N	4.425015	-1.407442	-0.571959
N	2.683335	-0.794960	-2.405624
N	4.118386	-2.329310	-1.504031

Cu-Cl-Cu-Cl dihedral angle (τ = 12°)

E = -182658.33620 eV

Cu	-0.148194	0.199667	-0.272487
Cu	3.221908	0.281374	-0.642224
Cl	1.762913	2.016367	-1.091056
Cl	1.401797	-1.286481	0.578380
Cl	-1.112663	-0.897506	-2.001685
Cl	4.293810	1.274913	1.098907
C	-0.347544	2.575920	1.344451
C	0.967319	1.276625	2.650532
H	1.796149	0.616110	2.406262
H	0.390751	0.838397	3.468254
C	-2.150839	2.324790	-1.556559
H	-2.452909	1.674980	-2.361524
C	-2.373654	3.704661	-1.354673
H	-2.923813	4.379640	-1.983964
C	-1.724585	4.004655	-0.187374
H	-1.598815	4.925985	0.354519
C	1.482952	2.675721	2.990029
H	2.379792	2.905349	2.417634
H	1.660794	2.816489	4.051805
S	0.161522	3.821521	2.449069

H	1.720565	2.705642	4.167133
S	0.240137	3.771586	2.588116
N	-1.442451	1.862478	-0.444683
N	0.129891	1.373274	1.570283
N	-1.134451	2.868279	0.393039
C	3.223454	-1.946613	-2.468252
C	1.885588	-0.489275	-3.570724
H	1.029026	0.102364	-3.257055
H	2.483256	0.090678	-4.278073
C	5.233447	-1.994751	0.303602
H	5.602048	-1.426271	1.142170
C	5.435793	-3.347029	-0.057253
H	6.031057	-4.081384	0.453603
C	4.697246	-3.529941	-1.194062
H	4.527322	-4.391518	-1.816626
C	1.433572	-1.826268	-4.160488
H	0.533108	-2.180590	-3.664057
H	1.290573	-1.788086	-5.236152
S	2.788483	-2.998528	-3.786066
N	4.442013	-1.405524	-0.560369
N	2.724812	-0.782409	-2.412794
N	4.115464	-2.336682	-1.476181

Cu-Cl-Cu-Cl dihedral angle (τ = 15°)

E = -182658.31028 eV

Cu	0.038578	0.161227	-0.294428
Cu	3.370436	0.349352	-0.644613
Cl	1.911153	2.092198	-1.076247
Cl	1.576836	-1.267125	0.639435
Cl	-0.616369	-1.046278	-2.095049
Cl	4.456613	1.325718	1.084399
C	-0.354602	2.555933	1.223334
C	1.154512	1.463206	2.505518
H	2.008471	0.838453	2.255297
H	0.668840	1.066134	3.399958
C	-2.266338	1.992309	-1.567476
H	-2.515794	1.292405	-2.348027
C	-2.692789	3.321323	-1.352167
H	-3.384377	3.895041	-1.941165
C	-2.020369	3.734849	-0.233247
H	-2.010045	4.668682	0.302754
C	1.593778	2.916251	2.684447
H	2.410992	3.155358	2.006057
H	1.861535	3.157342	3.708766
S	0.137410	3.915286	2.193247

N	-1.433409	1.828970	-0.574943
N	0.089159	1.396668	1.488923
N	-1.179261	2.848688	0.262909
C	3.242662	-1.935489	-2.446582
C	1.970474	-0.447938	-3.588432
H	1.119549	0.160867	-3.292031
H	2.594143	0.121661	-4.281167
C	5.200261	-2.010791	0.360975
H	5.576538	-1.441789	1.195857
C	5.348899	-3.378395	0.033035
H	5.899584	-4.127360	0.572091
C	4.624921	-3.553265	-1.114326
H	4.425559	-4.420675	-1.719734
C	1.503700	-1.774809	-4.191587
H	0.576052	-2.102794	-3.729099
H	1.403478	-1.736396	-5.271944
S	2.808137	-2.985315	-3.764350
N	4.453882	-1.405922	-0.531669
N	2.777159	-0.756422	-2.412578
N	4.104001	-2.341183	-1.434365

Cu-Cl-Cu-Cl dihedral angle (τ = 18°)

E = -182658.28172 eV

Cu	0.030016	0.152809	-0.345182
Cu	3.375509	0.355563	-0.638768
Cl	1.973073	2.133344	-1.096619
Cl	1.556560	-1.210200	0.682521
Cl	-0.579955	-1.088272	-2.133205
Cl	4.459117	1.325076	1.098181
C	-0.384541	2.589762	1.103056
C	1.109423	1.538005	2.434668
H	1.967621	0.906741	2.218721
H	0.608773	1.166894	3.332237
C	-2.261542	1.938989	-1.693339
H	-2.493789	1.217643	-2.459749
C	-2.715807	3.262718	-1.505511
H	-3.417148	3.810461	-2.107501
C	-2.056271	3.711434	-0.391909
H	-2.066298	4.655512	0.125991
C	1.544312	2.995316	2.577252
H	2.367505	3.216497	1.899911
H	1.800717	3.265010	3.597269
S	0.090347	3.976126	2.042919
N	-1.402575	1.611842	-0.754577
N	0.156405	1.468617	1.326529

N	-1.411172	1.628768	-0.638891
N	0.185296	1.426985	1.410827
N	-1.265036	2.688584	0.176895
C	3.217502	-1.860770	-2.424317
C	2.250027	-0.218720	-3.662511
H	1.406120	0.420238	-3.412857
H	2.967283	0.358986	-4.247999
C	4.972132	-2.145450	0.499369
H	5.415033	-1.617610	1.328043
C	4.812253	-3.531703	0.276628
H	5.129158	-4.341194	0.908275
C	4.140710	-3.627777	-0.911026
H	3.773769	-4.472681	-1.468235
C	1.777204	-1.474385	-4.415477
H	0.736895	-1.692541	-4.196477
H	1.939556	-1.401738	-5.486541
S	2.778947	-2.861854	-3.773357
N	4.449668	-1.456774	-0.487928
N	2.908432	-0.630931	-2.429176
N	3.947091	-2.359747	-1.352975

Cu-Cl-Cu-Cl dihedral angle (τ = 21°)

E = -182658.25764 eV

Cu	-0.057051	0.117386	-0.301508
Cu	3.273952	0.314445	-0.578520
Cl	1.940777	2.129744	-1.079211
Cl	1.437573	-1.185649	0.832887
Cl	-0.624152	-1.155252	-2.078983
Cl	4.364018	1.281731	1.158860
C	-0.437190	2.646177	1.000847
C	0.987423	1.635206	2.434273
H	1.825148	0.959303	2.282116
H	0.453591	1.345845	3.342386
C	-2.208748	1.908367	-1.841427
H	-2.431740	1.154972	-2.579202
C	-2.595028	3.263497	-1.763991
H	-3.224357	3.809348	-2.442360
C	-1.976935	3.747013	-0.641143
H	-1.956136	4.723673	-0.188736
C	1.474192	3.081244	2.484377
H	2.309301	3.228635	1.801346
H	1.731328	3.409931	3.486645
S	0.060492	4.071174	1.866565
N	-1.429908	1.595177	-0.830399
N	0.057179	1.523274	1.307755

N	-1.281169	2.689927	0.040691
C	3.219097	-1.868014	-2.402940
C	2.284037	-0.223502	-3.663211
H	1.436053	0.416721	-3.431346
H	3.014218	0.355114	-4.231360
C	4.950782	-2.148695	0.535120
H	5.390474	-1.619594	1.364708
C	4.794603	-3.535444	0.311991
H	5.111750	-4.344057	0.944661
C	4.128473	-3.633614	-0.878544
H	3.767851	-4.479654	-1.438284
C	1.827886	-1.477737	-4.430122
H	0.779488	-1.689290	-4.247461
H	2.027755	-1.407472	-5.495056
S	2.798479	-2.871192	-3.755493
N	4.431213	-1.461374	-0.454630
N	2.915322	-0.636816	-2.416768
N	3.933255	-2.365809	-1.320837

Model **I** for F^-.

E= -143434.32070 eV

Cu	0.335484	-0.101645	-0.247404
Cu	3.276314	0.101234	0.247649
F	1.900928	1.414604	0.100149
F	1.710994	-1.414855	-0.099595
F	-0.009955	-0.090526	-2.072411
F	3.621822	0.089791	2.072650
C	-0.233609	1.018366	2.297851
C	0.919147	-0.837406	2.892498
H	1.797667	-1.303742	2.454529
H	0.234532	-1.604958	3.262265
C	-1.709502	2.376284	-0.485019
H	-1.885163	2.271528	-1.542600
C	-2.081646	3.407085	0.406649
H	-2.641197	4.297605	0.187035
C	-1.565392	3.031495	1.617867
H	-1.581250	3.499379	2.587176
C	1.335792	0.144627	3.989381
H	2.297574	0.585900	3.738662
H	1.346964	-0.301672	4.979336
S	0.065246	1.465678	3.954785
N	-1.035776	1.443405	0.144382
N	0.221930	-0.076587	1.860720
N	-0.945357	1.842620	1.425183
C	3.845175	-1.018262	-2.297896

N	-1.295149	2.713441	-0.095413
C	3.205020	-1.894543	-2.383890
C	2.216167	-0.263169	-3.615236
H	1.351791	0.357847	-3.392875
H	2.946947	0.334941	-4.163088
C	4.977537	-2.157271	0.530919
H	5.382488	-1.626486	1.376968
C	4.975310	-3.538695	0.227012
H	5.406531	-4.339408	0.799214
C	4.293587	-3.644945	-0.953717
H	4.023308	-4.492575	-1.560122
C	1.802904	-1.518758	-4.399908
H	0.771308	-1.786159	-4.193531
H	1.969816	-1.415370	-5.467922
S	2.862462	-2.872574	-3.777094
N	4.353988	-1.481526	-0.403555
N	2.834810	-0.681776	-2.363255
N	3.935420	-2.385407	-1.310036

Model **I** for Cl^-.

E= -182658.40366 eV

Cu	2.163254	3.444815	0.082750
Cu	-1.108554	4.312179	-0.082775
Cl	0.005904	3.234728	1.642135
Cl	1.049025	4.523090	-1.641818
Cl	2.511432	1.397575	-0.852280
Cl	-1.457914	6.359373	0.851923
C	2.905981	5.129503	2.285582
C	1.983833	6.638307	0.874093
H	1.095447	6.620264	0.248303
H	2.780926	7.174087	0.353402
C	3.871635	1.841891	2.277604
H	3.901141	0.927496	1.707681
C	4.298917	2.124817	3.594860
H	4.761401	1.453013	4.294394
C	3.984350	3.441282	3.798616
H	4.105219	4.092483	4.647393
C	1.667789	7.256401	2.234823
H	0.658201	6.998112	2.548176
H	1.811433	8.332390	2.259713
S	2.845371	6.469825	3.396383
N	3.350523	2.912577	1.726061
N	2.445440	5.272065	1.114460
N	3.419385	3.888239	2.650054
C	-1.850466	2.626705	-2.285275

C	2.692030	0.837446	-2.891970
H	1.813624	1.303690	-2.453683
H	3.376454	1.605069	-3.261921
C	5.321856	-2.376378	0.484443
H	5.497654	-2.271804	1.542019
C	5.694132	-3.406894	-0.407499
H	6.253961	-4.297307	-0.188159
C	5.177582	-3.031191	-1.618555
H	5.193457	-3.498843	-2.587976
C	2.275041	-0.144599	-3.988730
H	1.313408	-0.586015	-3.737663
H	2.263375	0.301761	-4.978653
S	3.545814	-1.465443	-3.954776
N	4.647796	-1.443531	-0.144655
N	3.389648	0.076572	-1.860507
N	4.557271	-1.842517	-1.425522

Model **I** for Br^-.

E= -412757.69524 eV

Cu	0.064254	0.010599	-0.100277
Cu	3.547578	-0.010386	0.100166
Br	2.102331	1.991771	0.098282
Br	1.509472	-1.991580	-0.098493
Br	-0.685547	-0.012258	-2.417254
Br	4.297358	0.012580	2.417146
C	-0.438100	1.166307	2.483807
C	0.766617	-0.664037	3.057002
H	1.683767	-1.089981	2.657176
H	0.099901	-1.476207	3.355582
C	-1.928490	2.517717	-0.288411
H	-2.105720	2.408448	-1.346024
C	-2.300502	3.546297	0.605978
H	-2.862540	4.435079	0.385108
C	-1.783220	3.173973	1.816515
H	-1.797668	3.643560	2.785230
C	1.079138	0.281895	4.218531
H	2.038328	0.773659	4.069372
H	1.051106	-0.211386	5.185386
S	-0.230239	1.558797	4.165538
N	-1.248613	1.587737	0.341029
N	0.092218	0.113391	2.019284
N	-1.159618	1.984953	1.623661
C	4.049840	-1.166326	-2.483818
C	2.845151	0.663988	-3.057162
H	1.928060	1.090030	-2.657301
C	-0.926985	1.118777	-0.873691
H	-0.038435	1.137685	-0.248129
H	-1.723496	0.582408	-0.352719
C	-2.817057	5.914076	-2.278252
H	-2.846843	6.828625	-1.708593
C	-3.244128	5.630671	-3.595475
H	-3.706650	6.302179	-4.295267
C	-2.929275	4.314209	-3.798809
H	-3.049865	3.662752	-4.647429
C	-0.610707	0.500754	-2.234408
H	0.398615	0.759830	-2.547996
H	-0.753477	-0.575356	-2.259124
S	-1.789178	1.286208	-3.395823
N	-2.295810	4.843655	-1.726327
N	-1.389743	2.484614	-1.114162
N	-2.364341	3.867699	-2.650054

Model **I** for I^-.

E= -164952.75029 eV

Cu	-0.115493	0.116944	-0.114724
Cu	3.727205	-0.116883	0.114692
I	2.296989	2.113426	0.226828
I	1.314718	-2.113367	-0.226887
I	-1.001347	0.136050	-2.608198
I	4.613039	-0.135955	2.608172
C	-0.552887	1.239304	2.497156
C	0.730693	-0.557341	2.999100
H	1.653714	-0.937343	2.567076
H	0.112500	-1.406916	3.296658
C	-2.096056	2.651661	-0.217453
H	-2.281191	2.581388	-1.276845
C	-2.494549	3.630779	0.718580
H	-3.083660	4.510041	0.534276
C	-1.961262	3.225868	1.911170
H	-1.987617	3.654431	2.898260
C	1.040344	0.377112	4.169493
H	1.976947	0.906868	4.005443
H	1.062361	-0.136296	5.125738
S	-0.314325	1.606023	4.180667
N	-1.382632	1.717197	0.370217
N	-0.006845	0.210618	1.997868
N	-1.301930	2.065624	1.668827
C	4.164593	-1.239315	-2.497159
C	2.881037	0.557331	-2.999154
H	1.958028	0.937367	-2.567133

H	3.511874	1.476082	-3.355935
C	5.540182	-2.517589	0.288499
H	5.717437	-2.408236	1.346098
C	5.912084	-3.546288	-0.605800
H	6.474043	-4.435101	-0.384857
C	5.394816	-3.174029	-1.816363
H	5.409195	-3.643713	-2.785032
C	2.532473	-0.282104	-4.218512
H	1.573291	-0.773822	-4.069168
H	2.560405	0.211030	-5.185446
S	3.841823	-1.559032	-4.165476
N	4.860384	-1.587606	-0.341021
N	3.519623	-0.113314	-2.019392
N	4.771330	-1.984933	-1.623613

Model **I** for N_3^-.

E= -412757.69524 eV

Cu	0.180632	0.259433	-0.091656
Cu	3.324258	0.031923	-0.128809
C	-0.235156	1.160223	2.634875
C	0.802273	-0.837767	2.942646
H	1.816474	-1.108425	2.652476
H	0.173357	-1.720511	2.820112
C	-1.470776	3.022542	0.039317
H	-1.633956	3.072854	-1.024566
C	-1.783746	3.950135	1.058347
H	-2.248284	4.912816	0.950278
C	-1.350954	3.367763	2.217100
H	-1.352545	3.701042	3.240539
C	0.756049	-0.304031	4.391844
H	1.734335	0.012980	4.737152
H	0.327538	-1.024659	5.082411
S	-0.314775	1.174397	4.367861
N	-0.898951	1.956258	0.546918
N	0.314161	0.189687	2.033192
N	-0.824678	2.164790	1.874967
C	4.029692	-1.388064	-2.551056
C	2.582385	0.162293	-3.340224
H	1.606294	0.493858	-2.989908
H	3.119296	1.032741	-3.723503
C	5.512322	-2.251275	0.419582
H	5.603573	-2.020745	1.468441
C	6.103313	-3.276538	-0.350954
H	6.781610	-4.040605	-0.018501
C	5.619753	-3.094511	-1.619246

H	3.499245	1.406881	-3.296751
C	5.707720	-2.651632	0.217494
H	5.892849	-2.581336	1.276885
C	6.106197	-3.630784	-0.718511
H	6.695289	-4.510053	-0.534180
C	5.572920	-3.225896	-1.911114
H	5.599265	-3.654490	-2.898191
C	2.571357	-0.377162	-4.169505
H	1.634755	-0.906908	-4.005416
H	2.549323	0.136210	-5.125770
S	3.926018	-1.606083	-4.180657
N	4.994325	-1.717165	-0.370207
N	3.618569	-0.210605	-1.997900
N	4.913619	-2.065627	-1.668806

Model **II** for F^-.

E= -163046.55293 eV

Cu	0.002380	-0.050710	0.128319
Cu	2.984828	0.050310	-0.128104
F	1.623471	1.368646	-0.077008
F	1.363814	-1.369009	0.077098
C	-0.073181	1.282076	2.659606
C	1.036899	-0.613541	3.212259
H	1.862668	-1.120517	2.716316
H	0.359703	-1.359884	3.634452
C	-1.804247	2.574170	-0.003393
H	-2.147217	2.403117	-1.010872
C	-1.925503	3.710850	0.827593
H	-2.406756	4.644272	0.600270
C	-1.286442	3.372340	1.989283
H	-1.109693	3.914778	2.901983
C	1.555230	0.361199	4.277588
H	2.533638	0.746099	4.001663
H	1.574426	-0.074189	5.272169
S	0.376750	1.762773	4.273590
N	-1.152283	1.619908	0.615919
N	0.294921	0.154286	2.223240
N	-0.835224	2.103371	1.831095
C	3.062572	-1.281290	-2.660200
C	1.949426	0.612770	-3.211834
H	1.123313	1.118896	-2.715624
H	2.625724	1.359755	-3.634352
C	4.794503	-2.572404	0.002720
H	5.136554	-2.401464	1.010532
C	4.917926	-3.708375	-0.828903

H	5.772909	-3.634924	-2.537406
C	2.460141	-0.946538	-4.389819
H	1.610873	-1.593778	-4.188758
H	2.409255	-0.565780	-5.404967
S	3.977075	-1.952883	-4.194931
N	4.735634	-1.503859	-0.330456
N	3.341602	-0.377521	-2.214173
N	4.803264	-2.013792	-1.573651
N	-0.781766	0.317150	-1.812054
N	3.856980	0.216549	1.770602
N	-0.696408	-0.295991	-2.829116
N	3.332930	0.987911	2.517230
N	-0.646048	-0.835068	-3.831620
N	2.847456	1.693704	3.267052
N	2.062656	1.570308	-0.367102
N	1.391763	-1.360912	-0.157353
N	1.989206	2.639975	0.182783
N	1.450968	-2.202218	-1.011906
N	1.860586	3.655538	0.661024
N	1.566317	-3.005744	-1.802742
H	5.400487	-4.641194	-0.601884
C	4.279415	-3.369927	-1.990929
H	4.104415	-3.911891	-2.904250
C	1.431811	-0.362649	-4.276790
H	0.454615	-0.749732	-3.999572
H	1.410319	0.072919	-5.271238
S	2.613428	-1.761585	-4.274546
N	4.141078	-1.618901	-0.616218
N	2.692623	-0.154347	-2.223138
N	3.825667	-2.101945	-1.831986
Cl	-1.152041	-0.483520	-1.784031
Cl	4.138679	0.482530	1.784840

Model **II** for Br^-.

E= -297708.00355 eV

Cu	0.005640	-0.148703	-0.005665
Cu	3.483230	0.148451	0.005825
Br	1.965776	2.091921	0.004569
Br	1.523125	-2.092157	-0.004423
C	-0.302808	1.166523	2.514578
C	0.939776	-0.635802	3.100446
H	1.823161	-1.089750	2.658129
H	0.292195	-1.424913	3.489758
C	-1.929846	2.379029	-0.239770
H	-2.175956	2.200989	-1.273989
C	-2.166521	3.501691	0.585378
H	-2.674537	4.412279	0.326016
C	-1.598114	3.187365	1.789542
H	-1.509753	3.733847	2.712694
C	1.335748	0.373636	4.177855
H	2.275101	0.859021	3.921984
H	1.386097	-0.064108	5.170108
S	0.017124	1.642844	4.155631
N	-1.279355	1.452836	0.423289
N	0.196866	0.088192	2.070855
N	-1.080430	1.939549	1.662169
C	3.791741	-1.166716	-2.514439

Model **II** for I^-.

E= -173810.94654 eV

Cu	0.023338	0.007796	-0.062713
Cu	3.833254	-0.008653	0.063678
I	2.346641	2.177227	0.079348
I	1.511082	-2.177695	-0.076120
C	-0.316186	1.317818	2.467095
C	1.117282	-0.348586	3.009375
H	2.013457	-0.732341	2.528558
H	0.575384	-1.184571	3.456748
C	-2.129815	2.378667	-0.237960
H	-2.368874	2.194502	-1.272830
C	-2.534707	3.413723	0.634689
H	-3.193469	4.234420	0.417796
C	-1.896780	3.156582	1.817670
H	-1.885646	3.675026	2.761090
C	1.489112	0.721118	4.034926
H	2.364246	1.281073	3.709600
H	1.646935	0.316119	5.029807
S	0.060008	1.865428	4.074701
N	-1.317926	1.552857	0.380421
N	0.245020	0.274988	2.015169
N	-1.177502	2.021919	1.633188
C	4.172437	-1.317512	-2.467093

C	2.549279	0.635687	-3.100338	C	2.738405	0.348716	-3.008558
H	1.665860	1.089636	-2.658099	H	1.842007	0.731907	-2.527592
H	3.196929	1.424803	-3.489524	H	3.280204	1.185060	-3.455378
C	5.418647	-2.379311	0.239953	C	5.986869	-2.379176	0.237184
H	5.664725	-2.201290	1.274184	H	6.225960	-2.195497	1.272129
C	5.655303	-3.501974	-0.585195	C	6.392464	-3.413271	-0.636310
H	6.163271	-4.412586	-0.325827	H	7.051937	-4.233587	-0.420132
C	5.086951	-3.187612	-1.789375	C	5.753968	-3.155926	-1.818927
H	4.998600	-3.734081	-2.712536	H	5.742787	-3.673883	-2.762615
C	2.153401	-0.373665	-4.177864	C	2.367165	-0.720565	-4.034774
H	1.213983	-0.859006	-3.922157	H	1.492459	-1.281315	-3.709648
H	2.103219	0.064142	-5.170098	H	2.208954	-0.315095	-5.029400
S	3.471940	-1.642959	-4.155538	S	3.796992	-1.863972	-4.075285
N	4.768217	-1.453084	-0.423117	N	5.174291	-1.553537	-0.380505
N	3.292054	-0.088393	-2.070711	N	3.610707	-0.275215	-2.014610
N	4.569309	-1.939779	-1.662012	N	5.033848	-2.021925	-1.633522
Cl	-0.793914	-0.270490	-2.117705	Cl	-0.734300	-0.075165	-2.193026
Cl	4.282721	0.270202	2.117889	Cl	4.590398	0.072416	2.193956

Model **II** for N_3^-.

E= -166547.89912 eV

Cu	0.086516	-0.052197	0.242286
Cu	3.252208	0.175086	0.145376
C	-0.551686	2.740651	-0.059065
C	0.747418	2.760948	1.795971
H	1.698667	2.291923	2.035340
H	0.107297	2.750789	2.681862
C	-1.985880	0.445992	-2.162694
H	-2.111672	-0.600416	-2.388405
C	-2.455303	1.593667	-2.839311
H	-3.045155	1.631599	-3.736679
C	-1.986564	2.654373	-2.112697
H	-2.063023	3.718840	-2.252628
C	0.954883	4.175112	1.253756
H	1.865061	4.228775	0.659262
H	0.954665	4.933740	2.030382
S	-0.465607	4.468200	0.136642
N	-1.293795	0.789131	-1.100782
N	0.077263	1.994588	0.750674
N	-1.299843	2.136516	-1.065753
C	3.890251	-2.617552	0.443868
C	2.576558	-2.637637	-1.400720
H	1.624229	-2.167469	-1.633387
H	3.209618	-2.629601	-2.291693
C	5.341958	-0.321898	2.534796

H	5.470918	0.724665	2.758088
C	5.811230	-1.469122	3.212059
H	6.405077	-1.506411	4.106831
C	5.336541	-2.530379	2.489878
H	5.410576	-3.594721	2.632108
C	2.371106	-4.050621	-0.854905
H	1.466116	-4.102175	-0.252165
H	2.362294	-4.809983	-1.630716
S	3.800634	-4.345112	0.250235
N	4.644736	-0.665602	1.476367
N	3.256303	-1.871196	-0.361724
N	4.647062	-2.013230	1.444350
N	1.837601	0.479636	-1.260165
N	1.504012	-0.359343	1.643134
N	1.666842	1.554012	-1.773176
N	1.675045	-1.432364	2.158678
N	1.458018	2.553936	-2.260091
N	1.885355	-2.430981	2.647633
Cl	3.946885	2.308748	0.492533
Cl	-0.633197	-2.181511	-0.090918