Supporting online material

Thermodynamics of the Cu^{II} μ-thiolate and Cu^{I} disulfide equilibrium: a combined experimental and theoretical study

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S1. Crystallographic data

Table S1: Crystallographic and structure refinement data for complexes $[Cu^{II}_2(\mathbf{L^2S})_2](BF_4)_2{\cdot}C_3H_6O$ and $[Cu^{I}_2(\mathbf{L^4SSL^4})](BF_4)_2$

	$\mathbf{[Cu^{II}_2(L^2S)_2](BF_4)_2{\cdot}C_3H_6O}$	$\mathbf{[Cu^{I}_2(L^4SSL^4)](BF_4)_2}$
empirical formula	$[C_{30}H_{36}Cu_2N_6S_2](BF_4)_2{\cdot}C_3H_6O$	$[C_{30}H_{36}Cu_2N_6S_2](BF_4)_2$
formula weight	903.54	845.47
crystal system	orthorhombic	triclinic
space group	*Pna2₁*	*P*-1
a, Å	21.1268(2)	11.8258(3)
b, Å	10.28491(11)	12.2570(3)
c, Å	35.4103(4)	13.6442(3)
α, deg	90	110.331(2)
β, deg	90	97.1080(19)
γ, deg	90	108.254(2)
V, Å^3	7694.21(14)	1700.05(7)
Z	8	2
D_{calc}, g·cm^3	1.560	1.652
T, Kelvin	110(2)	110(2)
crystal size, mm	0.42 × 0.41 × 0.26	0.34 × 0.28 × 0.11
μ, mm^{-1}	3.045	1.451
no. of reflns measd	27801	31708
no. of unique reflns	13538	7816
no. of reflns obsd.	13151 [$I > 2\sigma(I)$]	6797 [$I > 2\sigma(I)$]
no. of parameters	1111	451
R_1 / wR_2 [$I > 2\sigma(I)$]	0.0497/0.1281	0.0279/0.0711
R_1 / wR_2 [all refl.]	0.0511/0.1291	0.0343/0.0734
goodness of fit	1.086	1.065
$\Delta\rho$, e·Å^{-3}	−0.56 /1.36	−0.53/0.75

Table S2: Crystallographic and structure refinement data for complexes $[Cu^{I}_{2}(\mathbf{L^{3}SSL^{3}})](BF_4)_2$

	$[Cu^{I}_{2}(L^{3}SSL^{3})](BF_4)_2$
empirical formula	$[C_{32}H_{40}Cu_2N_6S_2](BF_4)_2$
formula weight	873.52
crystal system	monoclinic
space group	$P2_1/n$
a, Å	11.3108(5)
b, Å	28.8420(11)
c, Å	11.9924(4)
α, deg	90
β, deg	104.604(4)
γ, deg	90
V, Å^3	3785.8(3)
Z	4
D_{calc}, g·cm^3	1.533
T, Kelvin	110(2)
crystal size, mm	0.21 × 0.17 × 0.13
μ, mm^{-1}	1.306
no. of reflns measd	23924
no. of unique reflns	7045
no. of reflns obsd.	5654
no. of parameters	473
R_1 / wR_2 [$I > 2\sigma(I)$]	0.0431/0.0995
R_1 / wR_2 [all refl.]	0.0595/0.1059
goodness of fit	1.041
$\Delta\rho$, e·Å^{-3}	−0.50/0.78

Structure determination

All reflection intensities for $[Cu^{I}_{2}(\mathbf{L^{3}SSL^{3}})](BF_4)_2$ were measured at 110(2) K using a KM4/Xcalibur (detector: Sapphire3) with enhanced graphite-monochromated Mo *K*α radiation (λ = 0.71073 Å) under the program CrysAlisPro (Version 1.171.35.11 Oxford Diffraction Ltd., 2011). The program CrysAlisPro was used to refine the cell dimensions and for data reduction. The structure was solved with the program SHELXS-97 (Sheldrick, 2008) and was refined on F^2 with SHELXL-97 (Sheldrick, 2008). Analytical

numeric absorption corrections based on a multifaceted crystal model were applied using CrysAlisPro. The temperature of the data collection was controlled using the system Cryojet (manufactured by Oxford Instruments). The H atoms were placed at calculated positions using the instructions AFIX 23, AFIX 43or AFIX 137 with isotropic displacement parameters having values 1.2 or 1.5 times *U*eq of the attached C atoms.

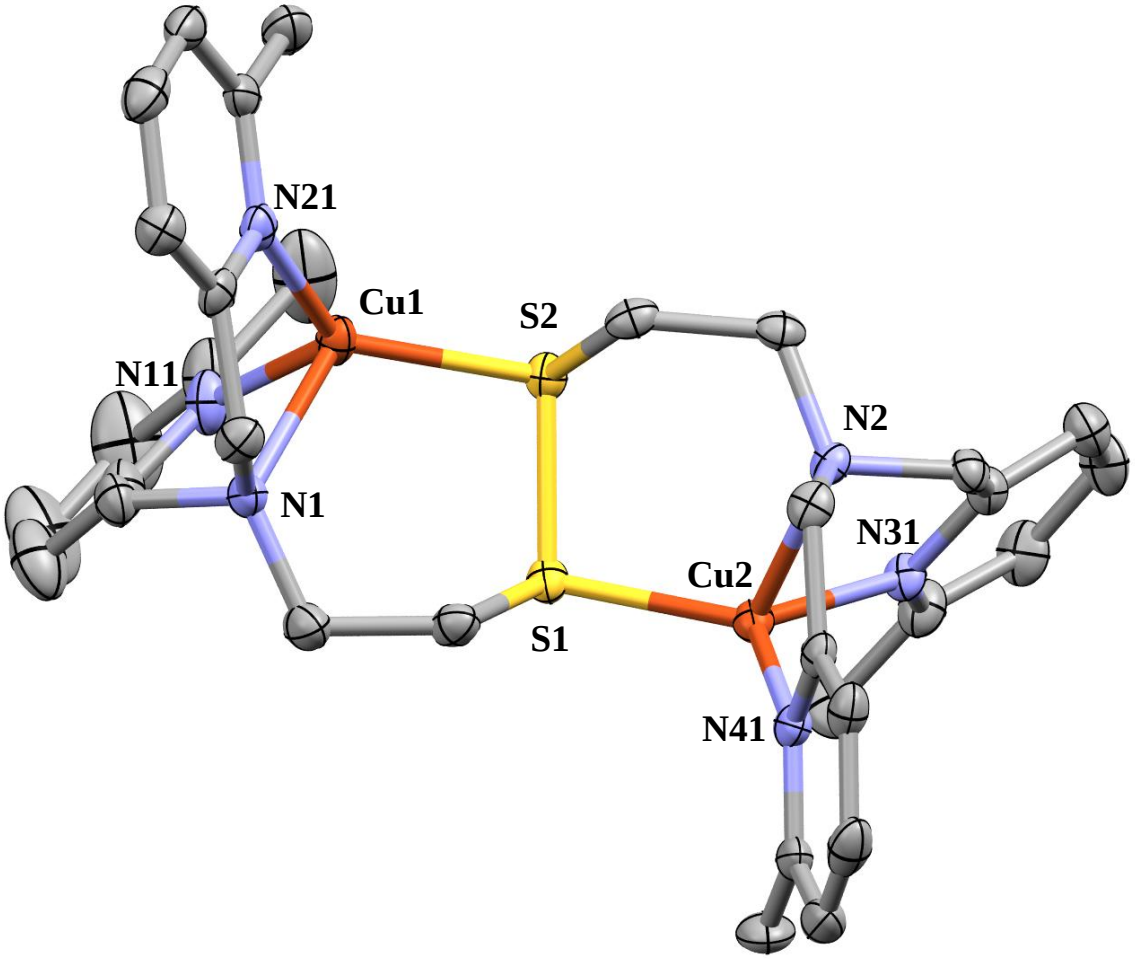
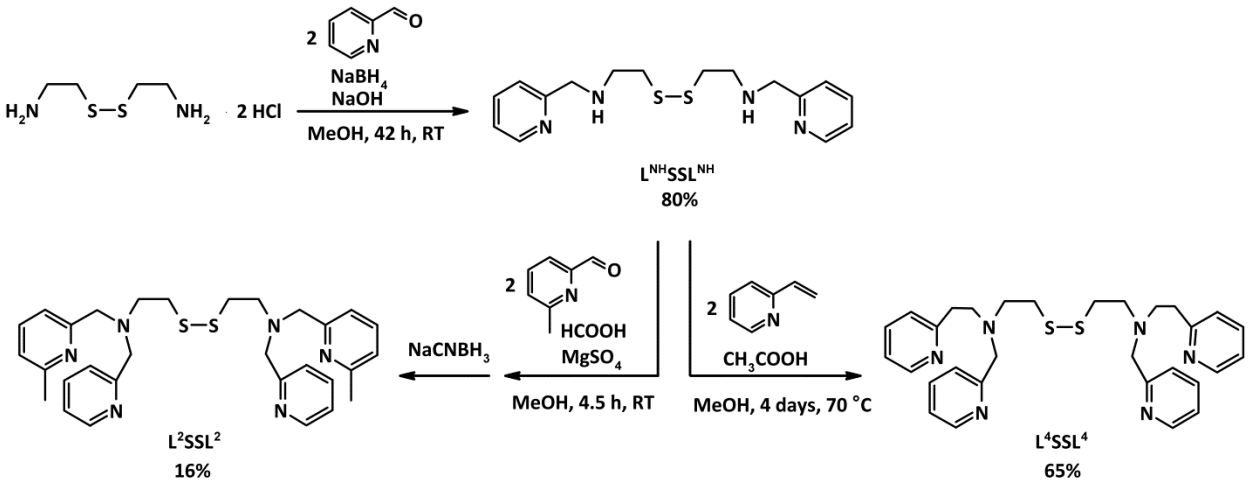


Figure S1: Projection of the cationic part of $[Cu^{I}_{2}(\mathbf{L^{3}SSL^{3}})](BF_4)_2$. Displacement ellipsoids are depicted at 50% probability level. All hydrogen atoms are omitted for clarity.

Table S3: Selected bond distances and angles for $[Cu^{I}_{2}(\mathbf{L^{3}SSL^{3}})](BF_4)_2$.

Bond distance (Å)		**Bond angle (°)**	
Cu1 - Cu2	5.1494(6)	Cu1 - S1 - Cu2	140.21(4)
S1 - S2	2.0872(12)	Cu1 - S2 - Cu2	137.12(4)
Cu1 - S1	3.2721(8)	S1 - Cu1 - S2	38.96(3)
Cu1 - S2	2.1925(8)	S2 - Cu1 - N1	110.53(7)
Cu1 - N1	2.186(3)	S2 - Cu1 - N11	119.79(8)
Cu1 - N11	2.035(3)	S2 - Cu1 - N21	124.72(8)
Cu1 - N21	2.005(3)	N1 - Cu1 - N11	83.48(11)
Cu2 - S1	2.1901(8)	N1 - Cu1 - N21	81.83(10)
Cu2 - S2	3.3219(8)	N11 - Cu1 - N21	114.99(11)
Cu2 - N2	2.167(3)	S1 - Cu2 - S2	37.94(3)
Cu2 - N31	2.024(3)	S1 - Cu2 - N2	108.51(7)
Cu2 - N41	2.012(3)	S1 - Cu2 - N31	125.10(8)
		S1 - Cu2 - N41	116.95(8)
		N2 - Cu2 - N31	84.04(10)
Dihedral angle (°)		N2 - Cu2 - N41	81.88(10)
Cu1 - S2 - S1 - Cu2	–161.75(4)	N31 - Cu2 - N41	117.70(10)

S2. Ligand synthesis scheme



Scheme S1: Schematic representation of the synthesis of $\mathbf{L^2SSL^2}$ and $\mathbf{L^4SSL^4}$ via $\mathbf{L^{NH}SSL^{NH}}$ (Y. Ueno et.al., *J. Am. Chem. Soc.* **2002,** *124*, 12428).

S3. NMR spectra

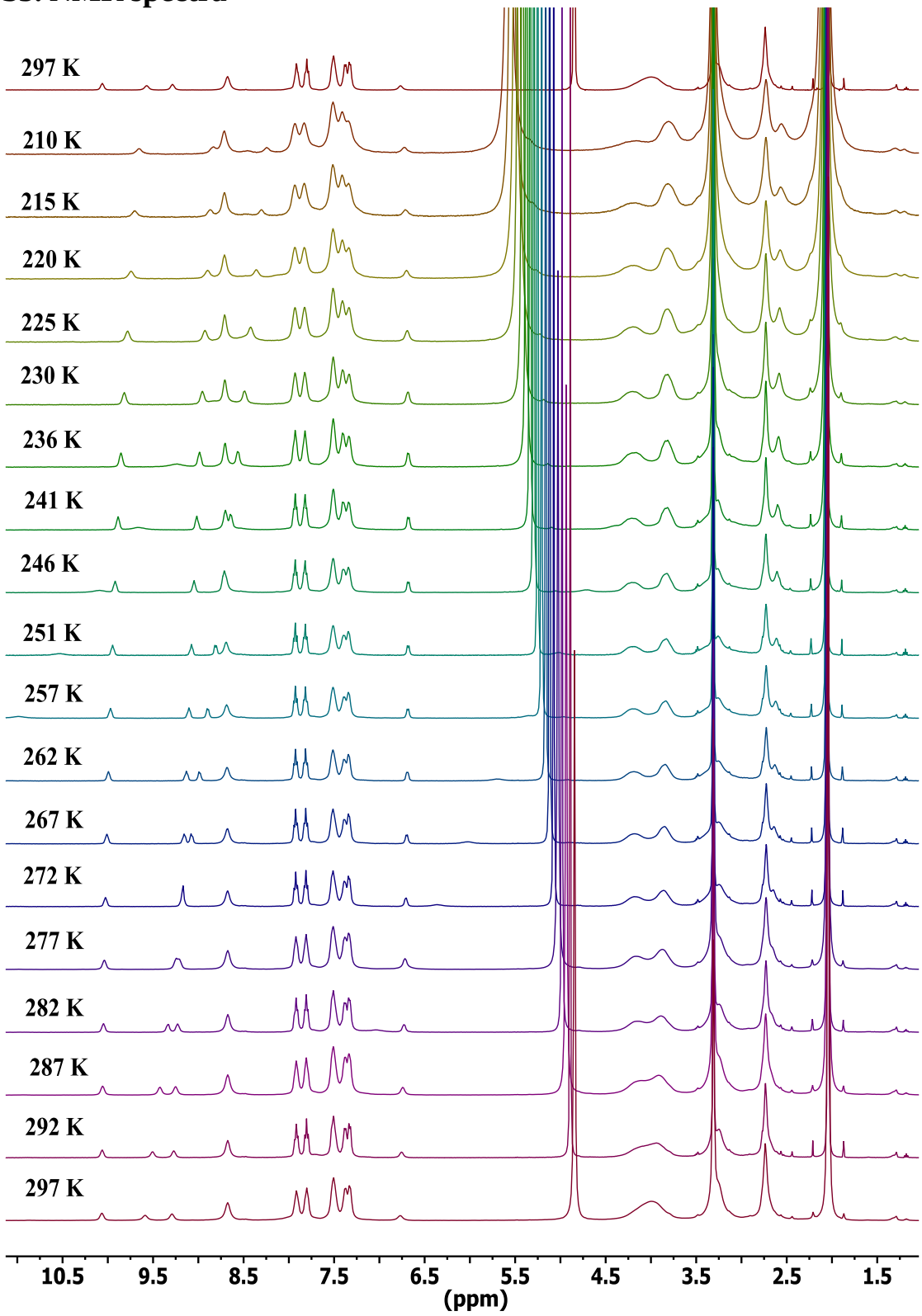


Figure S2: ^{1}H NMR spectra of $\mathbf{L^{2}SSL^{2}}$ and $[Cu(CH_3CN)_4](BF_4)$ in CD_3OD measured first at 297 K, then cooled down and measured from 210 K to 297 K in steps of 5 K.

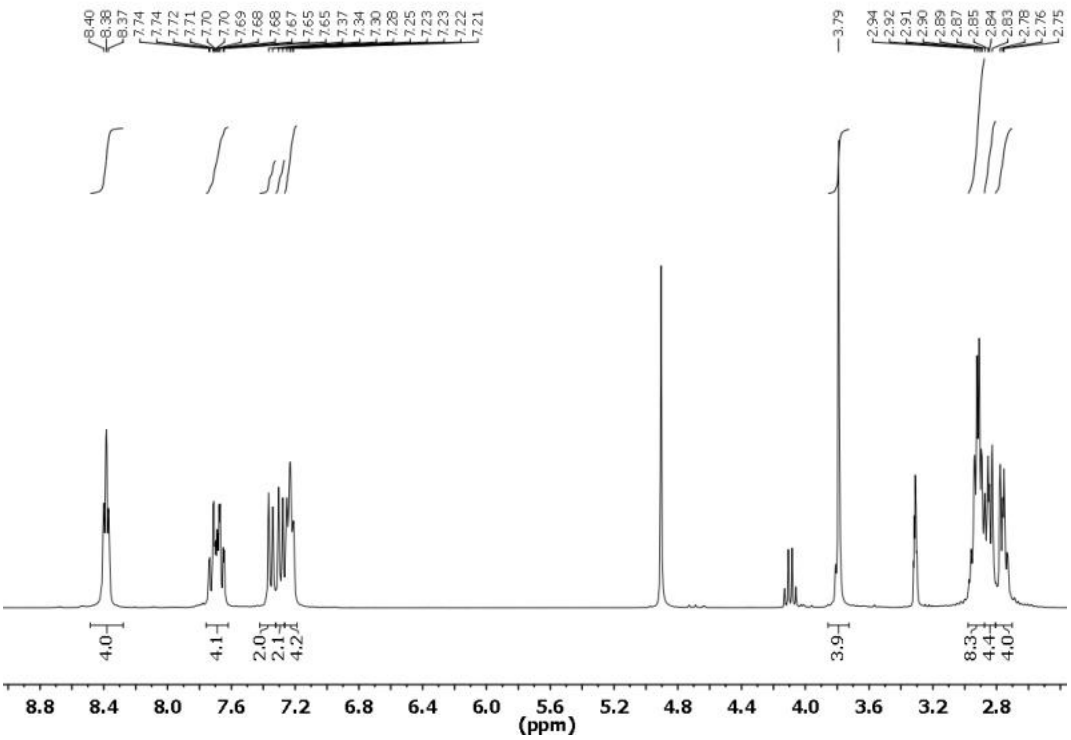


Figure S3: ^{1}H NMR spectrum of $\mathbf{L^4SSL^4}$ in CD_3OD at RT.

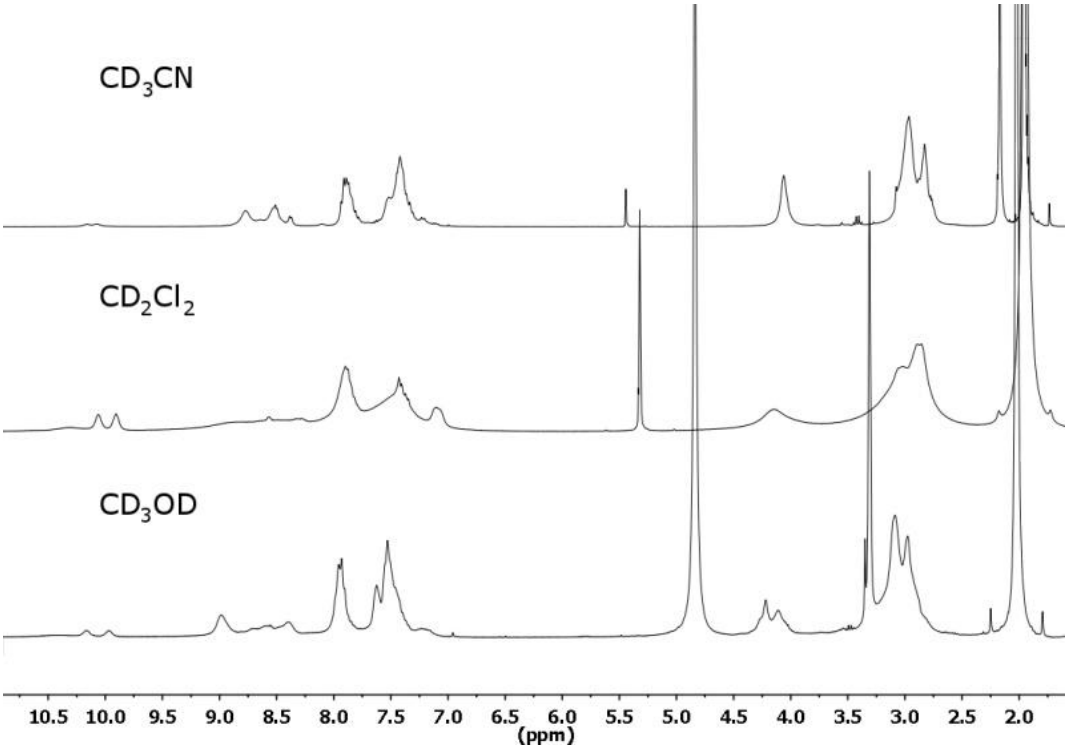


Figure S4: ^{1}H NMR spectra of $[Cu^{II}_2(\mathbf{L^4S})_2](BF_4)_2$ in CD_3CN, CD_2Cl_2 and CD_3OD at RT under argon.

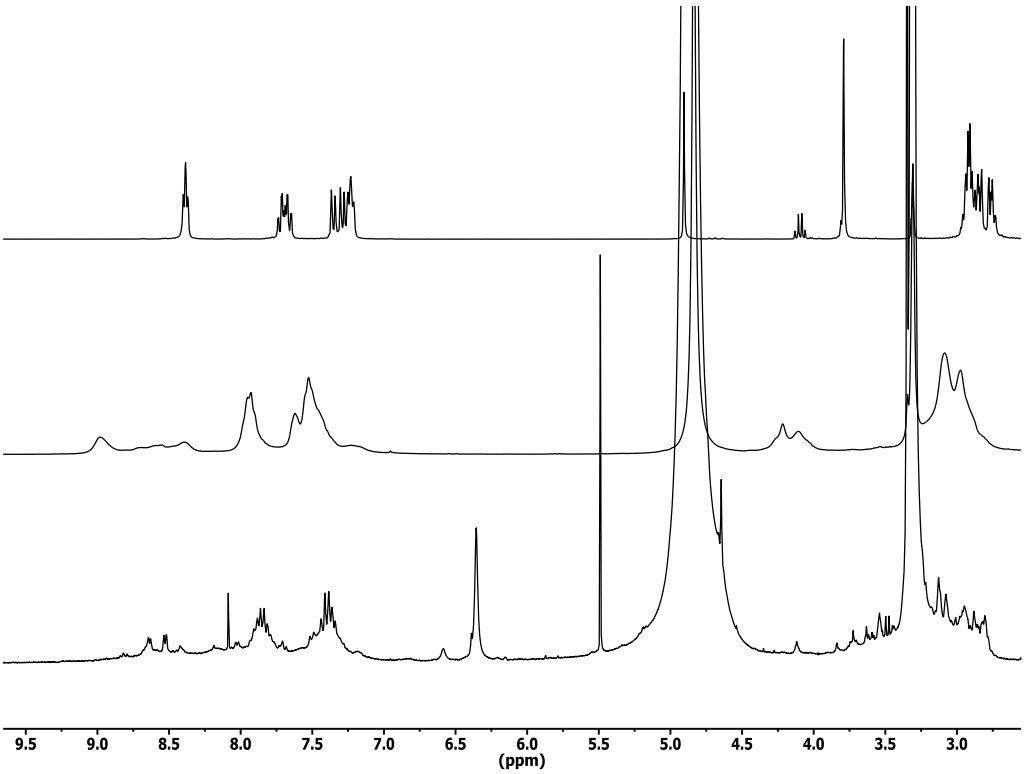


Figure S5: ^{1}H NMR spectra of $\mathbf{L^4SSL^4}$ (a), $[Cu^{II}_2(\mathbf{L^4S})_2](BF_4)_2$ (b) and $[Cu^{I}_2(\mathbf{L^4SSL^4})](BF_4)_2$ (c) in CD_3OD at RT.

S4. UV-Vis spectra

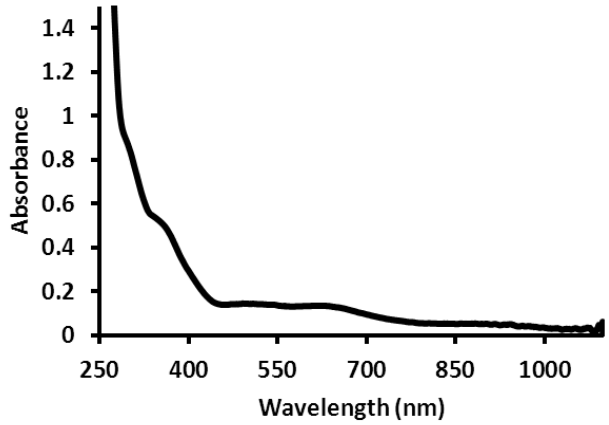


Figure S6: UV-Vis absorption spectrum of $[Cu^{II}_2(\mathbf{L^2S})_2](BF_4)_2$ in dichloromethane at 1 mM [Cu] concentration recorded with a transmission dip probe at a path length of 1.2 mm.

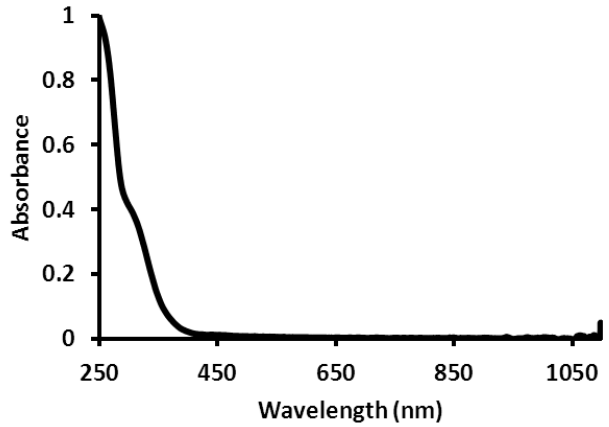


Figure S7: UV-Vis absorption spectrum of $[Cu^{I}_2(\mathbf{L^2SSL^2})](BF_4)_2$ in CH_3CN at 1 mM [Cu] concentration recorded with a transmission dip probe at a path length of 1.2 mm.

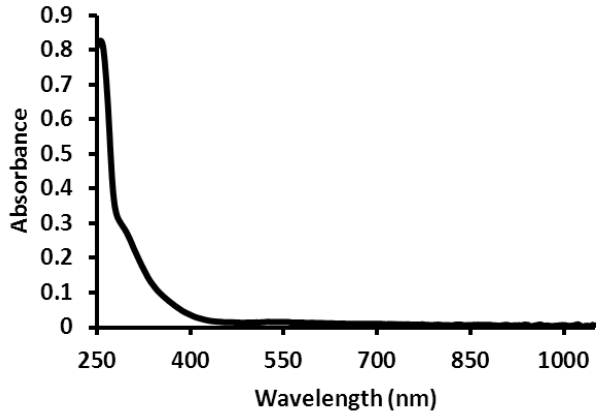


Figure S8: UV-Vis absorption spectrum of $[Cu^{I}_2(\mathbf{L^4SSL^4})](BF_4)_2$ in MeOH at 1 mM [Cu] concentration recorded with a transmission dip probe at a path length of 1.2 mm.

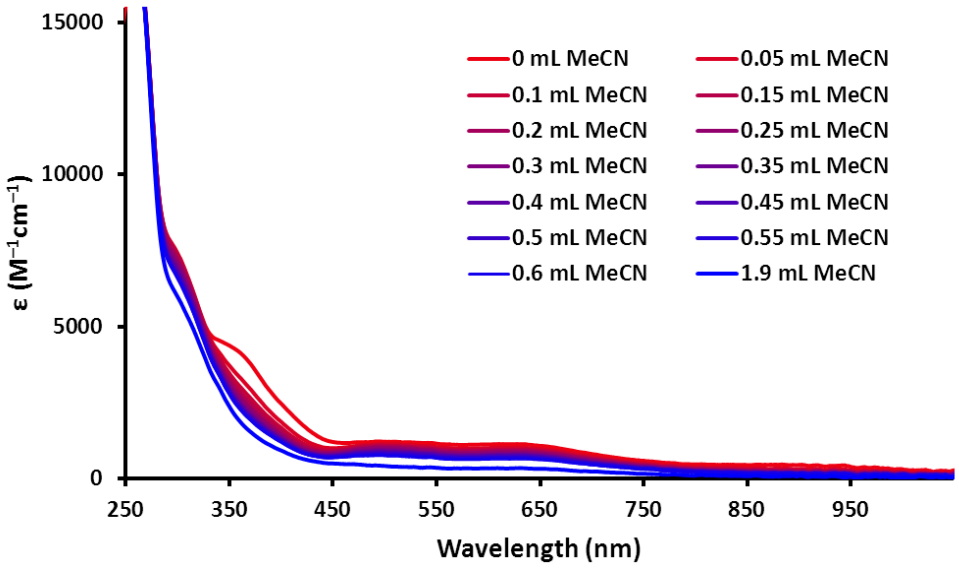


Figure S9: UV-Vis absorption spectra of a solution containing $\mathbf{L^2SSL^2}$ and 2 equivalents of $[Cu(CH_3CN)_4](BF_4)$ in 10 mL dichloromethane with variable amounts of added acetonitrile at 1 mM [Cu] concentration recorded with a transmission dip probe at a path length of 1.2 mm.

S5. Cyclic voltammetry

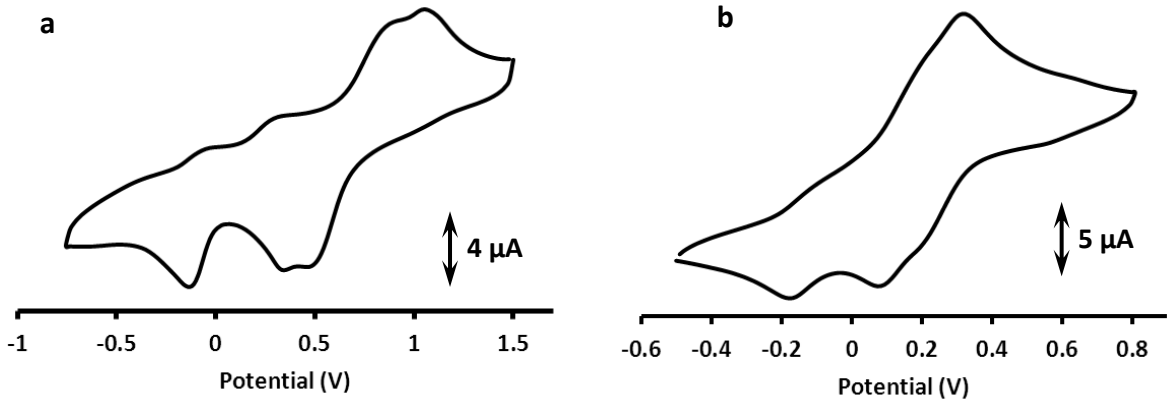


Figure S10: Cyclic voltammograms of (a) $[Cu^{II}_2(\mathbf{L^2S})_2](BF_4)_2$ in DCM and (b) $[Cu^{II}_2(\mathbf{L^4S})_2](BF_4)_2$ in MeOH at 1 mM [Cu] concentration at RT. The scanrate is 100 mV/s; potentials are given vs. Ag/AgCl.

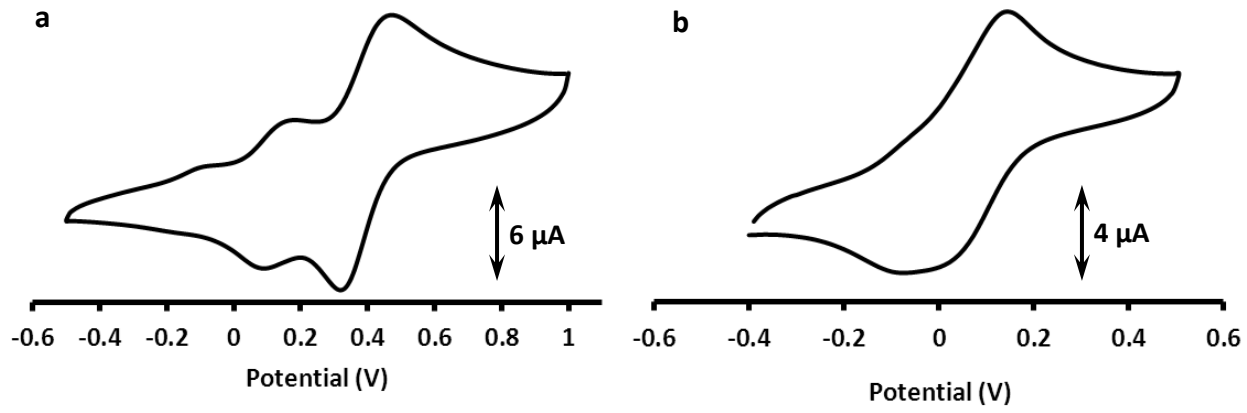


Figure S11: Cyclic voltammograms of (a) $[Cu^{I}_2(\mathbf{L^2SSL^2})](BF_4)_2$ in MeCN and (b) $[Cu^{I}_2(\mathbf{L^4SSL^4})](BF_4)_2$ in MeOH at 1 mM [Cu] concentration at RT. The scanrate is 100 mV/s; potentials are given vs. Ag/AgCl.

S6. DFT calculations

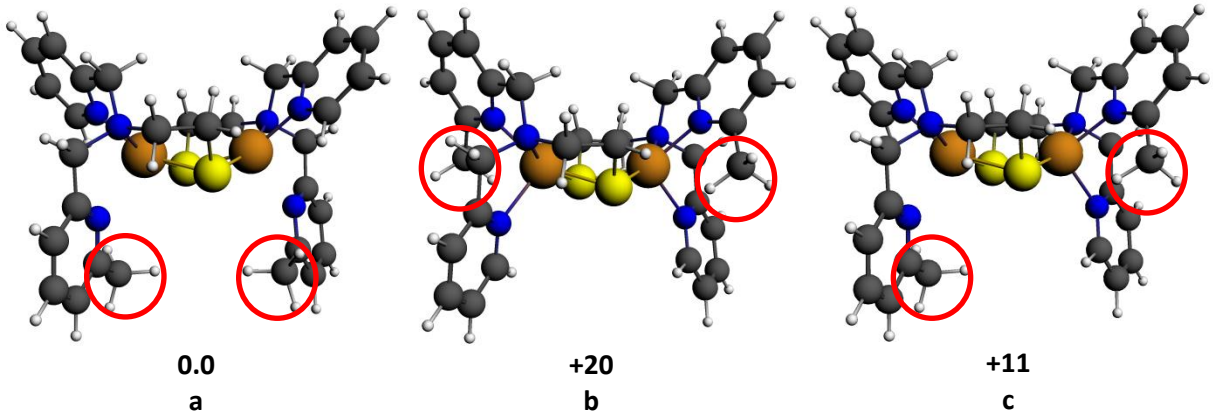


Figure S12: A projection of $[Cu^{II}_2(\mathbf{L}^2\mathbf{S})_2]^{2+}$ with three different ways of coordination (a,b and c) of the two 6-methylpyridyl groups and the relative energies in kJ/mol, computed at OPBE/TZ2P with COSMO for simulating solvation in MeCN. The methyl groups are highlighted with a red circle.

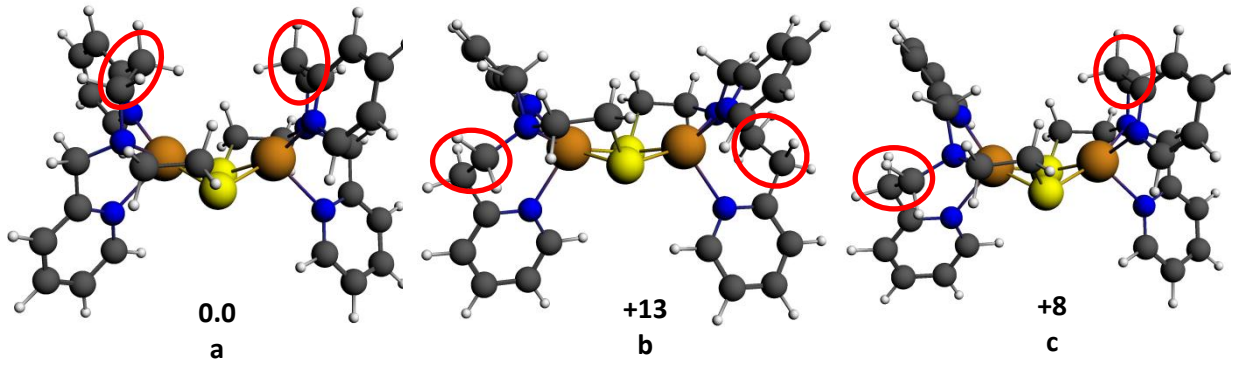


Figure S13: A projection of $[Cu^{II}_2(\mathbf{L}^4\mathbf{S})_2]^{2+}$ with three different ways of coordination (a,b and c) of the two pyridyl groups with ethylene bridges and the relative energies in kJ/mol, computed at OPBE/TZ2P with COSMO for simulating solvation in MeCN. The ethylene bridges are highlighted with a red circle.

Table S4: ADF total energies (kJ mol^{-1}) of all Cu^{II} μ-thiolate complexes computed at ZORA-OPBE/TZ2P.

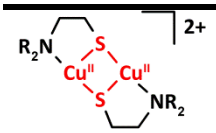
 A		MeCN			gas phase		
		E_{SF}	E_1	E_0	E_{SF}	E_1	E_0
L^{1}SSL^1		–40988.3	–40986.8	–40989.9	–40493.5	–40494.2	–40492.9
L^{2}SSL^2	**a**	–44188.9	–44187.7	–44190.0	–43699.6	–43700.7	–43698.5
	b	–44171.2	–44172.7	–44169.7			
	c	–44179.7	–44180.5	–44178.9			
L^{3}SSL^3		–47375.1	–47377.2	–47373.0	–46901.0	–46904.7	–46897.2
L^{4}SSL^4	**a**	–44135.9	–44137.4	–44134.3	–43655.1	–43658.8	–43651.7
	b	–44122.0	–44122.9	–44121.0			
	c	–44128.2	–44130.1	–44126.3			
L^{5}SSL^5		–47253.1	–47257.3	–47248.9	–46785.3	–46791.1	–46779.6

Table S5: ADF total energies (kJ mol^{-1}) of all Cu^{I} disulfide complexes computed at ZORA-OPBE/TZ2P.

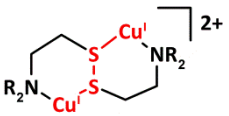
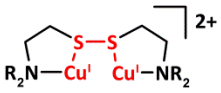
		 B		 C	
		MeCN	gas phase	MeCN	gas phase
L^{1}SSL^1		–40993.5	–40509.2	–40982.9	–40507.9
L^{2}SSL^2	**a**	–44203.1	–43725.4	–44199.3	–43729.9
	b	–44205.7		–44197.2	
	c	–44204.9		–44198.9	
L^{3}SSL^3		–47412.1	–46942.7	–47406.9	–46944.2
L^{4}SSL^4	**a**	–44150.0	–43676.0	–44182.2	–43705.4
	b	–44145.7			
	c	–44148.1			
L^{5}SSL^5		–47296.2	–46835.0	–47359.1	–46898.8

Table S6: Energies of formation (kJ mol^{-1}) of Cu^{II} μ-thiolate (**A**) and Cu^{I} disulfide (**B** or **C**) complexes for different **LSSL** ligands with and without coordinated acetonitrile and with or without coordinated pyridyl or sulfur groups.[a]

	L^1SSL^1	**L^2SSL^2**	**L^3SSL^3**	**L^4SSL^4**	**L^5SSL^5**
A $[Cu^{II}_2(LS)_2]^{2+}$ + 2 CH_3CN	–80	–73	–63	–44	27
A $[Cu^{II}_2(LS)_2(CH_3CN)_2]^{2+}$ - N-pyridyl uncoordinated	x[b]	+33	+42	+87[d]	+108[d]
B $[Cu^{I}_2(LSSL)]^{2+}$ + 2 CH_3CN	–83	–86	–102	–60	–20
B $[Cu^{I}_2(LSSL)(CH_3CN)_2]^{2+}$ - N-pyridyl uncoordinated	–2	+10	–5	+70[d]	+26
C $[Cu^{I}_2(LSSL)]^{2+}$ + 2 CH_3CN	–73	–83	–97	–93	–83
C $[Cu^{I}_2(LSSL)(CH_3CN)_2]^{2+}$ - N-pyridyl uncoordinated	–6	x[c]	x[c]	–3	–19
$[Cu^{I}_2(LSSL)(CH_3CN)_2]^{2+}$ - S uncoordinated	–73	–79	–91[d]	–38	–20

[a] Computed at ZORA-OPBE/TZ2P in CH_3CN (COSMO).

[b] Acetonitrile dissociates from the complex

[c] Sulfur dissociates and pyridyl group re-coordinates

[d] Imaginary frequency (in the range of –23 to –134 cm^{-1}) which shows rotation of the methyl group of CH_3CN

Table S7: Cartesian coordinates (Å) and ADF total energies of MeCN, $[Cu(CH_3CN)_4]^+$, **L^{1}SSL^1**, **L^{2}SSL^2**, **L^{3}SSL^3**, **L^{4}SSL^4** and **L^{5}SSL^5**, computed at ZORA-OPBE/TZ2P in the gas phase and/or solvated in MeCN (COSMO).

MeCN in MeCN (–857.39 kcal mol^{-1}) Symmetry C_{3v}				$[Cu(CH_3CN)_4]^+$ in MeCN (–3401.99 kcal mol^{-1}) No symmetry			
1.C	0.000000	0.000000	0.989163	1.Cu	10.858794	1.592929	9.009942
2.C	0.000000	0.000000	-0.453903	2.N	10.844608	3.568010	8.998085
3.N	0.000000	0.000000	2.151443	3.N	9.905155	0.920032	7.418454
4.H	-0.514958	-0.891933	-0.822864	4.N	12.723473	0.953817	8.994916
5.H	1.029915	0.000000	-0.822864	5.N	9.939618	0.943954	10.632230
6.H	-0.514958	0.891933	-0.822864	6.C	10.831789	4.728063	8.992720
				7.C	10.815032	6.167964	8.986576
				8.H	11.582401	6.548726	9.667553
				9.H	9.832422	6.524999	9.310541
				10.H	11.016083	6.533694	7.974891
				11.C	9.336828	0.523776	6.487943
				12.C	8.632693	0.031271	5.332560
				13.H	9.348770	-0.227453	4.546652
				14.H	7.950584	0.802034	4.960534
				15.H	8.057197	-0.859168	5.603856
				16.C	13.825805	0.592178	8.992548
				17.C	15.194564	0.144972	8.989067
				18.H	15.241311	-0.899206	9.313269
				19.H	15.785842	0.762544	9.672133
				20.H	15.605935	0.227844	7.978310
				21.C	9.379808	0.562229	11.573907
				22.C	8.682434	0.090080	12.742023
				23.H	9.399539	-0.324828	13.457013
				24.H	7.967499	-0.687110	12.455054
				25.H	8.145847	0.921188	13.210339
L^{1}SSL^1 in MeCN (–9833.05 kcal mol^{-1}) No symmetry				**L^{1}SSL^1** in the gas phase (–9810.23 kcal mol^{-1}) No symmetry			
1.C	-3.935905	2.998338	-1.209240	1.C	-3.987611	3.013536	-1.162041
2.C	-4.889536	2.084961	-1.663445	2.C	-4.980335	2.139763	-1.611375
3.C	-4.936464	1.762035	-3.014887	3.C	-5.061023	1.843075	-2.966422
4.C	-4.026927	2.361872	-3.876152	4.C	-4.146897	2.428242	-3.831259
5.C	-3.120513	3.269510	-3.336380	5.C	-3.201622	3.294977	-3.289001
6.N	-3.067560	3.593799	-2.041948	6.N	-3.115174	3.593985	-1.995267
7.H	-5.588128	1.630018	-0.964049	7.H	-5.680514	1.694248	-0.906450
8.H	-5.671802	1.050796	-3.386690	8.H	-5.825240	1.162135	-3.338284
9.H	-4.020715	2.142610	-4.941573	9.H	-4.165538	2.226837	-4.900765
10.H	-2.400907	3.772204	-3.984415	10.H	-2.472035	3.783772	-3.938117
11.H	1.365354	-3.155645	-4.303846	11.H	1.508220	-3.178829	-4.345339
12.C	-3.887869	3.410111	0.245282	12.C	-3.896097	3.405159	0.298099
13.N	-2.665809	3.062842	0.962839	13.N	-2.680091	3.013795	0.989387
14.C	-2.530431	3.887106	2.160951	14.C	-2.457817	3.839195	2.164942
15.H	-1.683133	2.904720	4.577001	15.H	-1.553260	2.897897	4.583326
16.C	-1.136294	3.904776	2.744020	16.C	-1.039959	3.811584	2.693729
17.N	-0.178673	4.500055	2.015304	17.N	-0.094862	4.336669	1.903629
18.C	1.055098	4.543746	2.524304	18.C	1.153617	4.353193	2.363484
19.C	1.405965	4.020689	3.765425	19.C	1.536757	3.869470	3.611915
20.C	0.409045	3.422620	4.524255	20.C	0.551766	3.338040	4.432079
21.C	-0.879581	3.365073	4.005387	21.C	-0.756538	3.308701	3.965119
22.H	1.293512	-1.370316	-6.076600	22.H	1.373305	-1.390599	-6.110030
23.H	1.808893	5.035339	1.907254	23.H	1.899071	4.788337	1.694004

24.H	2.430695	4.090598	4.123684	24.H	2.577164	3.916091	3.928948
25.H	0.627939	3.004589	5.505128	25.H	0.795188	2.948215	5.419287
26.C	-2.536988	1.635911	1.254201	26.C	-2.565476	1.584558	1.258408
27.C	-1.787125	0.857476	0.176628	27.C	-1.856616	0.807150	0.152076
28.S	-1.672816	-0.924436	0.517220	28.S	-1.728106	-0.973424	0.487634
29.S	-0.263787	-1.190225	1.952265	29.S	-0.293720	-1.221373	1.896128
30.C	1.266954	-1.654673	1.095992	30.C	1.231196	-1.643081	1.004583
31.C	1.983517	-0.533946	0.354356	31.C	1.947085	-0.493202	0.305457
32.N	3.240050	-0.980977	-0.235250	32.N	3.230409	-0.905567	-0.251591
33.C	4.325572	-1.060982	0.735609	33.C	4.292105	-0.962193	0.738361
34.H	2.277036	0.854995	-5.547471	34.H	2.269236	0.871411	-5.565887
35.C	5.419711	-2.028715	0.343511	35.C	5.387251	-1.952864	0.405622
36.C	6.699769	-1.576054	0.018157	36.C	6.691648	-1.531078	0.142088
37.C	7.685077	-2.499010	-0.317853	37.C	7.670030	-2.479039	-0.134048
38.C	7.361427	-3.849365	-0.316967	38.C	7.314369	-3.820156	-0.135798
39.C	6.062112	-4.207752	0.031889	39.C	5.989351	-4.142128	0.146286
40.N	5.106521	-3.334006	0.358242	40.N	5.041435	-3.246979	0.413687
41.H	6.924186	-0.511192	0.031734	41.H	6.939125	-0.470637	0.154643
42.H	8.688286	-2.165397	-0.576574	42.H	8.693126	-2.172107	-0.346088
43.H	8.094258	-4.611669	-0.572091	43.H	8.041670	-4.602060	-0.346025
44.H	5.775862	-5.260386	0.057554	44.H	5.673672	-5.187503	0.164054
45.C	3.610696	-0.215301	-1.409976	45.C	3.613273	-0.156891	-1.432946
46.H	2.424020	-2.607457	-2.099936	46.H	2.540352	-2.597888	-2.134253
47.C	2.887834	-0.591346	-2.684943	47.C	2.917011	-0.560973	-2.714820
48.N	2.848763	0.362906	-3.627698	48.N	2.847050	0.394248	-3.649539
49.C	2.287990	0.057847	-4.803144	49.C	2.307722	0.070289	-4.825029
50.C	1.739197	-1.183422	-5.102132	50.C	1.808394	-1.189874	-5.132634
51.C	1.779928	-2.165938	-4.118618	51.C	1.883256	-2.174038	-4.153873
52.C	2.363096	-1.867941	-2.893877	52.C	2.448707	-1.859385	-2.926416
53.H	-4.787551	3.015148	0.751662	53.H	-4.804530	3.038225	0.818255
54.H	-3.972984	4.502083	0.262779	54.H	-3.940810	4.499635	0.319370
55.H	-3.245206	3.599246	2.952668	55.H	-3.152730	3.596080	2.994046
56.H	-2.775203	4.916010	1.877291	56.H	-2.662285	4.876002	1.876241
57.H	-3.521185	1.165811	1.431790	57.H	-3.550980	1.123644	1.460674
58.H	-1.970697	1.525362	2.184003	58.H	-1.974074	1.453601	2.170123
59.H	-0.787962	1.269991	0.016076	59.H	-0.869606	1.231207	-0.048006
60.H	-2.313222	0.874794	-0.784803	60.H	-2.418873	0.825800	-0.788760
61.H	1.059414	-2.496413	0.428345	61.H	1.017271	-2.452646	0.300277
62.H	1.867788	-2.040873	1.929597	62.H	1.847340	-2.074705	1.804800
63.H	2.120689	0.334252	1.025273	63.H	2.046480	0.364134	0.996412
64.H	1.336828	-0.201749	-0.463851	64.H	1.319441	-0.155215	-0.524632
65.H	3.908232	-1.416234	1.681755	65.H	3.854442	-1.286279	1.687282
66.H	4.771798	-0.071752	0.940208	66.H	4.741593	0.032066	0.926418
67.H	4.677489	-0.386736	-1.602244	67.H	4.685122	-0.323834	-1.602885
68.H	3.511208	0.875566	-1.264953	68.H	3.495004	0.935480	-1.315263
L²SSL² in MeCN (–10599.44 kcal mol^{-1}) Symmetry C_2				**L²SSL²** in the gas phase (–10573.81 kcal mol^{-1}) Symmetry C_2			
1.N	4.518046	-2.553716	-1.406251	1.N	4.487940	-2.518726	-1.342841
2.N	4.798641	2.101280	-0.620997	2.N	4.775227	2.100482	-0.619800
3.S	-0.972907	-0.274912	0.377255	3.S	-0.955367	-0.321597	0.383537
4.S	0.972907	0.274912	0.377255	4.S	0.955367	0.321597	0.383537
5.C	-3.166812	0.266083	1.983332	5.C	-3.178257	0.195979	1.983459
6.H	-3.130664	-0.812873	2.163516	6.H	-3.131927	-0.889859	2.119336
7.H	-3.469615	0.726035	2.945450	7.H	-3.470129	0.615927	2.971311
8.C	-1.751658	0.740669	1.682732	8.C	-1.769713	0.690605	1.671954
9.H	-1.154447	0.630370	2.593024	9.H	-1.172882	0.616595	2.587485

10.H	-1.715673	1.790018	1.375462	10.H	-1.755878	1.735162	1.345802
11.C	3.166812	-0.266083	1.983332	11.C	3.178257	-0.195979	1.983459
12.H	3.130664	0.812873	2.163516	12.H	3.131927	0.889859	2.119336
13.H	3.469615	-0.726035	2.945450	13.H	3.470129	-0.615927	2.971311
14.C	1.751658	-0.740669	1.682732	14.C	1.769713	-0.690605	1.671954
15.H	1.154447	-0.630370	2.593024	15.H	1.172882	-0.616595	2.587485
16.H	1.715673	-1.790018	1.375462	16.H	1.755878	-1.735162	1.345802
17.C	-4.995340	-1.826581	0.674571	17.C	-5.029409	-1.862366	0.669004
18.C	-4.987554	-2.817038	1.658981	18.C	-5.082116	-2.879810	1.623281
19.H	-5.173489	-2.562996	2.700696	19.H	-5.308250	-2.653248	2.664032
20.C	-4.746537	-4.132451	1.282102	20.C	-4.847083	-4.186361	1.216147
21.H	-4.735193	-4.927858	2.025066	21.H	-4.881758	-5.004566	1.933872
22.C	-4.521128	-4.415300	-0.057653	22.C	-4.565564	-4.432237	-0.118825
23.H	-4.329446	-5.435110	-0.385498	23.H	-4.374504	-5.445349	-0.468219
24.C	-4.558920	-3.368161	-0.985105	24.C	-4.538377	-3.355729	-1.011710
25.C	-4.340571	-3.615256	-2.449204	25.C	-4.244624	-3.549574	-2.470669
26.H	-5.202937	-3.268840	-3.029884	26.H	-5.064163	-3.149887	-3.077901
27.H	-4.177771	-4.673894	-2.664844	27.H	-4.096429	-4.602258	-2.725849
28.H	-3.472157	-3.048971	-2.804446	28.H	-3.344445	-2.989557	-2.747676
29.C	-5.291227	-0.386308	1.028360	29.C	-5.322098	-0.425874	1.043192
30.H	-6.041428	-0.033528	0.314853	30.H	-6.066128	-0.063648	0.327045
31.H	-5.759256	-0.350867	2.030804	31.H	-5.799829	-0.403957	2.045544
32.C	-5.280497	2.360908	-0.318977	32.C	-5.277986	2.342822	-0.277271
33.C	-6.654957	2.610728	-0.324475	33.C	-6.645250	2.626612	-0.306404
34.H	-7.241334	2.463000	0.580439	34.H	-7.254508	2.488469	0.585767
35.C	-7.265285	3.054657	-1.492322	35.C	-7.217803	3.090980	-1.484468
36.H	-8.335089	3.254485	-1.514445	36.H	-8.282059	3.317727	-1.530253
37.C	-6.482055	3.236765	-2.624765	37.C	-6.405556	3.256368	-2.597321
38.H	-6.908819	3.582634	-3.563706	38.H	-6.804220	3.615514	-3.544425
39.C	-5.118701	2.975674	-2.522033	39.C	-5.051833	2.957520	-2.465211
40.H	5.229986	-2.128175	1.808727	40.H	5.267426	-2.078608	1.854522
41.N	4.145800	-0.515829	0.933543	41.N	4.180644	-0.474819	0.969226
42.C	4.578936	-1.910462	0.940747	42.C	4.603932	-1.866726	0.990032
43.H	3.689129	-2.536342	1.051315	43.H	3.712218	-2.486200	1.118868
44.C	-4.578936	1.910462	0.940747	44.C	-4.603932	1.866726	0.990032
45.H	-3.689129	2.536342	1.051315	45.H	-3.712218	2.486200	1.118868
46.H	-5.229986	2.128175	1.808727	46.H	-5.267426	2.078608	1.854522
47.C	4.995340	1.826581	0.674571	47.C	5.029409	1.862366	0.669004
48.C	4.987554	2.817038	1.658981	48.C	5.082116	2.879810	1.623281
49.H	5.173489	2.562996	2.700696	49.H	5.308250	2.653248	2.664032
50.C	4.746537	4.132451	1.282102	50.C	4.847083	4.186361	1.216147
51.H	4.735193	4.927858	2.025066	51.H	4.881758	5.004566	1.933872
52.C	4.521128	4.415300	-0.057653	52.C	4.565564	4.432237	-0.118825
53.H	4.329446	5.435110	-0.385498	53.H	4.374504	5.445349	-0.468219
54.C	4.558920	3.368161	-0.985105	54.C	4.538377	3.355729	-1.011710
55.C	4.340571	3.615256	-2.449204	55.C	4.244624	3.549574	-2.470669
56.H	5.202937	3.268840	-3.029884	56.H	5.064163	3.149887	-3.077901
57.H	4.177771	4.673894	-2.664844	57.H	4.096429	4.602258	-2.725849
58.H	3.472157	3.048971	-2.804446	58.H	3.344445	2.989557	-2.747676
59.C	5.291227	0.386308	1.028360	59.C	5.322098	0.425874	1.043192
60.H	6.041428	0.033528	0.314853	60.H	6.066128	0.063648	0.327045
61.H	5.759256	0.350867	2.030804	61.H	5.799829	0.403957	2.045544
62.C	5.280497	-2.360908	-0.318977	62.C	5.277986	-2.342822	-0.277271
63.C	6.654957	-2.610728	-0.324475	63.C	6.645250	-2.626612	-0.306404
64.H	7.241334	-2.463000	0.580439	64.H	7.254508	-2.488469	0.585767
65.C	7.265285	-3.054657	-1.492322	65.C	7.217803	-3.090980	-1.484468

66.H	8.335089	-3.254485	-1.514445	66.H	8.282059	-3.317727	-1.530253
67.C	6.482055	-3.236765	-2.624765	67.C	6.405556	-3.256368	-2.597321
68.H	6.908819	-3.582634	-3.563706	68.H	6.804220	-3.615514	-3.544425
69.C	5.118701	-2.975674	-2.522033	69.C	5.051833	-2.957520	-2.465211
70.N	-4.518046	2.553716	-1.406251	70.N	-4.487940	2.518726	-1.342841
71.N	-4.798641	-2.101280	-0.620997	71.N	-4.775227	-2.100482	-0.619800
72.N	-4.145800	0.515829	0.933543	72.N	-4.180644	0.474819	0.969226
73.H	-4.469547	3.125069	-3.386368	73.H	-4.377834	3.087202	-3.314571
74.H	4.469547	-3.125069	-3.386368	74.H	4.377834	-3.087202	-3.314571
L^3**SSL**^{3} in MeCN (–11362.72 kcal mol^{-1}) Symmetry C_2				**L**^{3}**SSL**^{3} in the gas phase (–11343.28 kcal mol^{-1}) Symmetry C_2			
1.N	-2.378300	-4.443704	-0.824096	1.N	-2.105745	-4.629905	-1.129703
2.N	2.510167	-4.635158	-0.421872	2.N	2.468046	-4.602699	-0.247341
3.S	-0.414039	0.921050	0.853735	3.S	-0.379487	0.934257	0.698446
4.S	0.414039	-0.921050	0.853735	4.S	0.379487	-0.934257	0.698446
5.C	-0.133351	3.224722	2.385304	5.C	0.010430	3.189423	2.290393
6.H	-1.210711	3.085997	2.519826	6.H	-1.065742	3.073853	2.458215
7.H	0.248666	3.589266	3.360443	7.H	0.438519	3.518972	3.263098
8.C	0.492668	1.857050	2.137608	8.C	0.586307	1.811904	1.980798
9.H	0.446663	1.285546	3.069863	9.H	0.551240	1.215632	2.899061
10.H	1.539968	1.931636	1.830282	10.H	1.628973	1.858808	1.651525
11.C	0.133351	-3.224722	2.385304	11.C	-0.010430	-3.189423	2.290393
12.H	1.210711	-3.085997	2.519826	12.H	1.065742	-3.073853	2.458215
13.H	-0.248666	-3.589266	3.360443	13.H	-0.438519	-3.518972	3.263098
14.C	-0.492668	-1.857050	2.137608	14.C	-0.586307	-1.811904	1.980798
15.H	-0.446663	-1.285546	3.069863	15.H	-0.551240	-1.215632	2.899061
16.H	-1.539968	-1.931636	1.830282	16.H	-1.628973	-1.858808	1.651525
17.C	-2.327138	4.803745	0.893421	17.C	-2.201969	4.890082	1.029262
18.C	-3.359501	4.634189	1.818919	18.C	-3.187782	4.893958	2.017748
19.H	-3.186572	4.807554	2.879252	19.H	-2.939837	5.148850	3.046908
20.C	-4.613604	4.252177	1.358697	20.C	-4.490833	4.574276	1.660405
21.H	-5.439581	4.113736	2.054020	21.H	-5.284464	4.569667	2.406028
22.C	-4.796857	4.051187	-0.002298	22.C	-4.764616	4.259571	0.338377
23.H	-5.767049	3.751264	-0.393631	23.H	-5.775687	4.002968	0.026966
24.C	-3.716133	4.258046	-0.866397	24.C	-3.719539	4.284674	-0.591155
25.C	-3.856018	4.075120	-2.349415	25.C	-3.945032	3.953825	-2.037720
26.H	-3.584866	4.995814	-2.878102	26.H	-3.558984	4.756957	-2.674123
27.H	-4.873903	3.797446	-2.633197	27.H	-5.002685	3.796343	-2.265639
28.H	-3.170072	3.295712	-2.699775	28.H	-3.390934	3.046051	-2.303314
29.C	-0.950578	5.250195	1.334577	29.C	-0.775181	5.277633	1.350675
30.H	-0.629692	6.017798	0.625740	30.H	-0.484453	6.034325	0.615404
31.H	-1.029434	5.737880	2.325894	31.H	-0.751212	5.768534	2.346698
32.C	1.899499	5.334254	0.053943	32.C	1.942025	5.406594	-0.056496
33.C	1.886087	6.705911	-0.206279	33.C	2.157069	6.785332	-0.088262
34.H	1.521959	7.409282	0.539884	34.H	2.029440	7.387773	0.809606
35.C	2.354934	7.158518	-1.433773	35.C	2.539558	7.371327	-1.287497
36.H	2.354680	8.221414	-1.668548	36.H	2.715247	8.444339	-1.348248
37.C	2.824223	6.233384	-2.355352	37.C	2.690159	6.568507	-2.407741
38.H	3.195355	6.555582	-3.326401	38.H	2.985673	6.998743	-3.363096
39.C	2.827986	4.877516	-2.009047	39.C	2.463487	5.193365	-2.287530
40.C	3.363307	3.835241	-2.947030	40.C	2.616020	4.266081	-3.457676
41.H	2.683320	2.978991	-2.991937	41.H	1.672367	3.742003	-3.644806
42.H	4.329189	3.457636	-2.588696	42.H	3.364451	3.496916	-3.237033
43.H	3.509853	4.230928	-3.955088	43.H	2.913170	4.795330	-4.367067
44.C	1.410136	4.780089	1.373706	44.C	1.555947	4.705744	1.227796
45.H	2.105161	3.986995	1.658737	45.H	2.234505	3.855152	1.334790

46.H	1.485432	5.564906	2.150233	46.H	1.756190	5.383672	2.083762
47.C	2.327138	-4.803745	0.893421	47.C	2.201969	-4.890082	1.029262
48.C	3.359501	-4.634189	1.818919	48.C	3.187782	-4.893958	2.017748
49.H	3.186572	-4.807554	2.879252	49.H	2.939837	-5.148850	3.046908
50.C	4.613604	-4.252177	1.358697	50.C	4.490833	-4.574276	1.660405
51.H	5.439581	-4.113736	2.054020	51.H	5.284464	-4.569667	2.406028
52.C	4.796857	-4.051187	-0.002298	52.C	4.764616	-4.259571	0.338377
53.H	5.767049	-3.751264	-0.393631	53.H	5.775687	-4.002968	0.026966
54.C	3.716133	-4.258046	-0.866397	54.C	3.719539	-4.284674	-0.591155
55.C	3.856018	-4.075120	-2.349415	55.C	3.945032	-3.953825	-2.037720
56.H	3.584866	-4.995814	-2.878102	56.H	3.558984	-4.756957	-2.674123
57.H	4.873903	-3.797446	-2.633197	57.H	5.002685	-3.796343	-2.265639
58.H	3.170072	-3.295712	-2.699775	58.H	3.390934	-3.046051	-2.303314
59.C	0.950578	-5.250195	1.334577	59.C	0.775181	-5.277633	1.350675
60.H	0.629692	-6.017798	0.625740	60.H	0.484453	-6.034325	0.615404
61.H	1.029434	-5.737880	2.325894	61.H	0.751212	-5.768534	2.346698
62.C	-1.899499	-5.334254	0.053943	62.C	-1.942025	-5.406594	-0.056496
63.C	-1.886087	-6.705911	-0.206279	63.C	-2.157069	-6.785332	-0.088262
64.H	-1.521959	-7.409282	0.539884	64.H	-2.029440	-7.387773	0.809606
65.C	-2.354934	-7.158518	-1.433773	65.C	-2.539558	-7.371327	-1.287497
66.H	-2.354680	-8.221414	-1.668548	66.H	-2.715247	-8.444339	-1.348248
67.C	-2.824223	-6.233384	-2.355352	67.C	-2.690159	-6.568507	-2.407741
68.H	-3.195355	-6.555582	-3.326401	68.H	-2.985673	-6.998743	-3.363096
69.C	-2.827986	-4.877516	-2.009047	69.C	-2.463487	-5.193365	-2.287530
70.C	-3.363307	-3.835241	-2.947030	70.C	-2.616020	-4.266081	-3.457676
71.H	-2.683320	-2.978991	-2.991937	71.H	-1.672367	-3.742003	-3.644806
72.H	-4.329189	-3.457636	-2.588696	72.H	-3.364451	-3.496916	-3.237033
73.H	-3.509853	-4.230928	-3.955088	73.H	-2.913170	-4.795330	-4.367067
74.C	-1.410136	-4.780089	1.373706	74.C	-1.555947	-4.705744	1.227796
75.H	-2.105161	-3.986995	1.658737	75.H	-2.234505	-3.855152	1.334790
76.H	-1.485432	-5.564906	2.150233	76.H	-1.756190	-5.383672	2.083762
77.N	0.067716	4.203713	1.326849	77.N	0.193736	4.195149	1.258487
78.N	-0.067716	-4.203713	1.326849	78.N	-0.193736	-4.195149	1.258487
79.N	-2.510167	4.635158	-0.421872	79.N	-2.468046	4.602699	-0.247341
80.N	2.378300	4.443704	-0.824096	80.N	2.105745	4.629905	-1.129703
L^{4}SSL^4 in MeCN (–10593.12 kcal mol^{-1})				**L^{4}SSL^4** in the gas phase (–10574.39 kcal mol^{-1})			
No symmetry				No symmetry			
1.S	1.935973	0.421146	-0.618525	1.S	1.588775	0.405528	-0.678925
2.S	1.614336	2.096820	0.469248	2.S	1.482040	1.993162	0.568485
3.N	2.315010	-4.761864	-3.641155	3.N	2.586998	-4.601587	-4.082644
4.N	-1.915564	0.502759	-5.348952	4.N	-1.895203	0.198779	-5.210039
5.N	1.862669	-1.082579	-3.583283	5.N	1.964020	-1.022956	-3.550042
6.N	-0.631678	-0.922619	5.312564	6.N	-1.555933	-0.652422	5.303346
7.N	-1.341670	5.861943	4.213210	7.N	-0.858234	5.887418	4.182012
8.N	-0.909335	1.670498	2.684674	8.N	-1.174648	1.810821	2.621287
9.C	1.932540	-5.858905	-2.979065	9.C	2.255835	-5.799121	-3.597476
10.C	1.173994	-5.837653	-1.813932	10.C	1.589897	-5.994699	-2.393244
11.C	0.795181	-4.598781	-1.308701	11.C	1.253341	-4.870443	-1.647694
12.C	1.184676	-3.448556	-1.984247	12.C	1.593335	-3.615871	-2.133680
13.C	1.943016	-3.569555	-3.147735	13.C	2.259277	-3.525768	-3.356946
14.C	2.444453	-2.368608	-3.927838	14.C	2.730320	-2.200278	-3.926118
15.H	-0.497095	2.369669	-0.646158	15.H	-0.489595	2.718263	-0.607225
16.C	-2.746639	1.007835	-6.266807	16.C	-2.820736	0.653391	-6.053862
17.C	-3.098639	0.355760	-7.443401	17.C	-3.273864	-0.044289	-7.168312
18.C	-2.549851	-0.899395	-7.679729	18.C	-2.723031	-1.294695	-7.417450
19.C	-1.682427	-1.437866	-6.737399	19.C	-1.755980	-1.782962	-6.549256

20.C	-1.387104	-0.711324	-5.579484
21.C	-0.450451	-1.255917	-4.536767
22.C	0.928205	-0.589255	-4.586111
23.C	2.848033	-0.082515	-3.194215
24.C	2.327369	1.033399	-2.296487
25.C	0.261587	-1.449885	6.156860
26.C	1.615776	-1.135435	6.149191
27.C	2.064833	-0.221189	5.202117
28.C	1.150302	0.334354	4.315578
29.C	-0.190539	-0.038184	4.403862
30.C	-1.250980	0.487239	3.453613
31.H	-2.108288	1.676781	0.920558
32.C	-1.956281	6.970562	4.640444
33.C	-2.773759	7.024592	5.763659
34.C	-2.963928	5.852172	6.486174
35.C	-2.334746	4.691359	6.054102
36.C	-1.527287	4.729037	4.912811
37.C	-0.836398	3.492142	4.409525
38.C	-1.539199	2.883348	3.189739
39.C	-1.062917	1.507819	1.247370
40.C	-0.176923	2.411339	0.400085
41.H	2.249748	-6.810234	-3.408144
42.H	0.891397	-6.765546	-1.321732
43.H	0.202133	-4.529235	-0.397847
44.H	0.909920	-2.459377	-1.630465
45.H	2.316026	-2.593379	-4.997685
46.H	3.532428	-2.336195	-3.783075
47.H	-0.828669	0.469747	0.990255
48.H	-0.251898	3.462034	0.707052
49.H	-3.159778	1.992785	-6.044453
50.H	-3.785204	0.819673	-8.147980
51.H	-2.794691	-1.454272	-8.583733
52.H	-1.241573	-2.420771	-6.892813
53.H	-0.883978	-1.085372	-3.545453
54.H	-0.354567	-2.336750	-4.673903
55.H	0.782581	0.482784	-4.425721
56.H	1.350960	-0.697161	-5.604062
57.H	3.662163	-0.593612	-2.669973
58.H	3.309597	0.408786	-4.072480
59.H	3.112511	1.789569	-2.195906
60.H	1.438943	1.516668	-2.713097
61.H	-0.130784	-2.162798	6.883167
62.H	2.293655	-1.594583	6.865276
63.H	3.116884	0.056274	5.153393
64.H	1.452773	1.052068	3.558571
65.H	-2.170369	0.639712	4.039943
66.H	-1.494977	-0.338325	2.771678
67.H	-2.602585	2.699054	3.436051
68.H	-1.535771	3.634808	2.394481
69.H	-1.778567	7.870911	4.050846
70.H	-3.241327	7.960221	6.061941
71.H	-3.590732	5.840578	7.376165
72.H	-2.460628	3.759944	6.602829
73.H	-0.787544	2.759561	5.219951
74.H	0.192665	3.744459	4.131363

20.C	-1.365968	-1.009646	-5.451768
21.C	-0.325585	-1.497696	-4.480505
22.C	0.952968	-0.658135	-4.536365
23.C	2.795933	0.104815	-3.160256
24.C	2.110818	1.134498	-2.272586
25.C	-0.849573	-1.295775	6.234456
26.C	0.538944	-1.339165	6.266066
27.C	1.231961	-0.674638	5.260030
28.C	0.515303	-0.003024	4.280201
29.C	-0.879681	-0.014999	4.340431
30.C	-1.736319	0.641576	3.272551
31.H	-2.281828	2.196310	0.836680
32.C	-1.158148	7.102612	4.638828
33.C	-1.712364	7.354101	5.889424
34.C	-1.976933	6.265789	6.710896
35.C	-1.673671	4.992182	6.249402
36.C	-1.107665	4.838514	4.980102
37.C	-0.737875	3.481000	4.448453
38.C	-1.576476	3.070897	3.233613
39.C	-1.296843	1.812341	1.176489
40.C	-0.224766	2.617009	0.450854
41.H	2.537286	-6.655063	-4.214195
42.H	1.342694	-6.998662	-2.053104
43.H	0.732763	-4.968854	-0.695688
44.H	1.347738	-2.711178	-1.585315
45.H	2.801803	-2.320795	-5.019342
46.H	3.766050	-2.073017	-3.583980
47.H	-1.235724	0.778561	0.820551
48.H	-0.142958	3.634423	0.854912
49.H	-3.230538	1.638840	-5.822604
50.H	-4.036718	0.381982	-7.816958
51.H	-3.042440	-1.884406	-8.275665
52.H	-1.306704	-2.760655	-6.715249
53.H	-0.735642	-1.432152	-3.466374
54.H	-0.108268	-2.550307	-4.679666
55.H	0.658515	0.381073	-4.367308
56.H	1.374598	-0.700098	-5.560179
57.H	3.655707	-0.290032	-2.608508
58.H	3.207852	0.649425	-4.035718
59.H	2.825879	1.931692	-2.043842
60.H	1.243894	1.588439	-2.763472
61.H	-1.432497	-1.803765	7.005431
62.H	1.058998	-1.877152	7.056606
63.H	2.321248	-0.680946	5.237390
64.H	1.014223	0.532943	3.477310
65.H	-2.719066	0.847631	3.727801
66.H	-1.926110	-0.129124	2.513581
67.H	-2.645460	3.042387	3.520225
68.H	-1.481835	3.870041	2.492486
69.H	-0.936840	7.931220	3.962879
70.H	-1.927486	8.372843	6.206109
71.H	-2.411809	6.405401	7.699757
72.H	-1.865168	4.118791	6.870511
73.H	-0.831213	2.740425	5.246968
74.H	0.315379	3.501768	4.145269

L^{5}SSL^5 in MeCN (–11354.53 kcal mol^{-1}) No symmetry			
1.S	10.806050	3.136248	1.658329
2.S	10.566243	4.543643	3.095204
3.N	11.225854	-1.777747	-1.382046
4.N	7.224396	3.482700	-2.794221
5.N	11.302650	2.164110	-1.395277
6.N	8.422797	2.246794	8.323579
7.N	8.107275	8.749827	6.650601
8.N	7.802018	4.552744	5.087954
9.C	10.379053	-2.680022	-0.875319
10.C	10.052263	-2.769821	0.473123
11.C	10.645038	-1.864017	1.345599
12.C	11.521909	-0.916958	0.833140
13.C	11.790107	-0.896747	-0.538538
14.C	12.747603	0.096755	-1.139446
15.C	12.111643	1.145337	-2.057910
16.C	6.308840	3.989720	-3.627225
17.C	6.058816	3.500461	-4.904351
18.C	6.808925	2.414420	-5.341741
19.C	7.765175	1.876611	-4.489834
20.C	7.949596	2.433576	-3.219566
21.C	8.984705	1.890119	-2.275460
22.C	10.286570	2.702314	-2.292618
23.C	12.130439	3.199457	-0.794378
24.C	11.437398	4.086906	0.228841
25.C	9.300680	2.297686	9.331130
26.C	10.679839	2.340304	9.160733
27.C	11.172758	2.331975	7.860723
28.C	10.273017	2.285816	6.803508
29.C	8.900799	2.243884	7.066935
30.C	7.882243	2.180434	5.960946
31.C	7.079728	3.470355	5.747581
32.C	7.719580	9.947787	7.102449
33.C	6.924328	10.136849	8.226909
34.C	6.503482	9.008819	8.922209
35.C	6.894185	7.757095	8.463661
36.C	7.700795	7.659371	7.324978
37.C	8.149470	6.324244	6.801713
38.C	7.374275	5.863983	5.560177
39.C	7.768508	4.431659	3.639259
40.C	8.869857	5.184951	2.906329
41.H	9.941542	-3.378618	-1.590285
42.H	9.359374	-3.531155	0.824788
43.H	10.428152	-1.895111	2.412233
44.H	11.999699	-0.196215	1.492435
45.H	13.467145	-0.457771	-1.754992
46.H	13.326988	0.575530	-0.345015
47.H	11.474130	0.613830	-2.770792
48.H	12.919376	1.609115	-2.656943
49.H	5.736400	4.836886	-3.246271
50.H	5.295143	3.955777	-5.530949
51.H	6.649789	1.988487	-6.330877
52.H	8.362863	1.022581	-4.803365
53.H	8.586931	1.909544	-1.256248
54.H	9.193122	0.846508	-2.529180

L^{5}SSL^5 in the gas phase (–11336.38 kcal mol^{-1}) No symmetry			
1.S	10.952902	3.353596	1.641572
2.S	10.788096	4.814851	3.030244
3.N	10.954959	-1.538023	-1.037301
4.N	7.487884	3.684714	-2.813499
5.N	11.369633	2.222411	-1.343486
6.N	8.424664	2.130446	7.857964
7.N	7.894738	8.577258	6.709465
8.N	7.892763	4.601405	4.859297
9.C	10.077466	-2.370601	-0.478048
10.C	9.884334	-2.496878	0.893217
11.C	10.654036	-1.699538	1.730663
12.C	11.570437	-0.824561	1.164035
13.C	11.696168	-0.770545	-0.226593
14.C	12.708578	0.127548	-0.891422
15.C	12.136459	1.118605	-1.906944
16.C	6.543492	4.180859	-3.611643
17.C	6.033543	3.522317	-4.725515
18.C	6.546538	2.266985	-5.025730
19.C	7.532983	1.736008	-4.205839
20.C	7.980331	2.470737	-3.103206
21.C	9.039530	1.932736	-2.181865
22.C	10.355568	2.711404	-2.270549
23.C	12.224682	3.277342	-0.828754
24.C	11.561186	4.229164	0.156693
25.C	9.226555	2.100193	8.922025
26.C	10.615461	2.089418	8.853782
27.C	11.200372	2.119052	7.593985
28.C	10.380189	2.152830	6.474504
29.C	8.992844	2.153452	6.643214
30.C	8.050077	2.158888	5.467754
31.C	7.189368	3.420638	5.342890
32.C	7.501882	9.752634	7.198527
33.C	6.737591	9.906205	8.350394
34.C	6.355384	8.757356	9.031210
35.C	6.753163	7.523966	8.533390
36.C	7.527801	7.468609	7.370215
37.C	7.998504	6.158159	6.803489
38.C	7.378427	5.834540	5.440857
39.C	7.961918	4.648655	3.410198
40.C	9.104214	5.485188	2.846784
41.H	9.492630	-2.979831	-1.170669
42.H	9.152695	-3.199042	1.288386
43.H	10.540754	-1.754373	2.812616
44.H	12.181884	-0.182952	1.795223
45.H	13.409256	-0.515815	-1.441530
46.H	13.301190	0.641510	-0.128267
47.H	11.481400	0.549715	-2.572579
48.H	12.968387	1.491885	-2.538437
49.H	6.165198	5.168956	-3.341102
50.H	5.256798	3.981460	-5.334043
51.H	6.182267	1.706302	-5.885624
52.H	7.952394	0.752531	-4.412179
53.H	8.678924	2.002107	-1.149928
54.H	9.207831	0.873198	-2.393869

55.H	10.044409	3.723432	-1.984847	55.H	10.131434	3.755917	-2.038975
56.H	10.666675	2.779423	-3.328553	56.H	10.728904	2.705247	-3.312569
57.H	12.977647	2.711929	-0.301358	57.H	13.074125	2.807573	-0.321044
58.H	12.569394	3.875711	-1.557825	58.H	12.660018	3.896845	-1.643457
59.H	12.169577	4.804111	0.612891	59.H	12.301259	4.963496	0.491781
60.H	10.609196	4.652689	-0.208418	60.H	10.729048	4.773597	-0.301286
61.H	8.874637	2.297011	10.335735	61.H	8.726809	2.079860	9.893118
62.H	11.342848	2.374531	10.022513	62.H	11.215919	2.060633	9.761207
63.H	12.244650	2.361978	7.671208	63.H	12.284033	2.120505	7.482628
64.H	10.630102	2.285740	5.776654	64.H	10.809333	2.190071	5.476054
65.H	7.159744	1.394457	6.213130	65.H	7.361943	1.312601	5.593876
66.H	8.366051	1.876264	5.028091	66.H	8.606438	1.980399	4.542515
67.H	6.749598	3.821223	6.730209	67.H	6.784623	3.635258	6.336398
68.H	6.157612	3.214040	5.193240	68.H	6.315553	3.187649	4.703054
69.H	8.072395	10.808472	6.532590	69.H	7.822897	10.631561	6.635355
70.H	6.649624	11.139456	8.546788	70.H	6.454897	10.897112	8.700747
71.H	5.882641	9.100944	9.811688	71.H	5.757217	8.819443	9.939488
72.H	6.584476	6.856996	8.991554	72.H	6.473411	6.604995	9.046125
73.H	8.053085	5.577020	7.594580	73.H	7.793165	5.355356	7.517042
74.H	9.210811	6.382260	6.537608	74.H	9.085902	6.201683	6.674691
75.H	7.539115	6.600771	4.768272	75.H	7.609058	6.668430	4.771736
76.H	6.288209	5.882718	5.767962	76.H	6.274508	5.812461	5.525196
77.H	6.798925	4.777785	3.223297	77.H	7.017423	5.033777	2.968047
78.H	7.843935	3.370777	3.377554	78.H	8.071362	3.628007	3.027336
79.H	8.944537	6.223779	3.249275	79.H	9.171199	6.460863	3.344778
80.H	8.645871	5.226995	1.836071	80.H	8.928520	5.684533	1.784317

Table S8: Cartesian coordinates (Å) of complexes with ligand $\mathbf{L^1SSL^1}$ in **A**, **B** or **C** conformation computed at ZORA-OPBE/TZ2P in the gas phase and solvated in MeCN (COSMO).

$[Cu^{II}_2(\mathbf{L^1S})_2]^{2+}$ in MeCN Conformation **A**, symmetry C_2				$[Cu^{II}_2(\mathbf{L^1S})_2]^{2+}$ in the gas phase Conformation **A**, symmetry C_2			
1.Cu	-0.174891	-1.617972	-0.227314	1.Cu	-0.203182	-1.665828	-0.160990
2.Cu	0.174891	1.617972	-0.227314	2.Cu	0.203182	1.665828	-0.160990
3.S	1.475170	-0.164278	-0.858466	3.S	1.460799	-0.188372	-0.690988
4.S	-1.475170	0.164278	-0.858466	4.S	-1.460799	0.188372	-0.690988
5.N	-0.100427	-3.101375	-1.898218	5.N	-0.070712	-3.047392	-1.880081
6.N	-1.220371	-2.601550	1.213465	6.N	-1.273137	-2.739006	1.207728
7.N	1.354340	-2.906054	0.480449	7.N	1.333750	-2.995223	0.534970
8.N	0.100427	3.101375	-1.898218	8.N	0.070712	3.047392	-1.880081
9.N	1.220371	2.601550	1.213465	9.N	1.273137	2.739006	1.207728
10.N	-1.354340	2.906054	0.480449	10.N	-1.333750	2.995223	0.534970
11.C	-0.587971	-2.999637	-3.139347	11.C	-0.550795	-2.884229	-3.117635
12.C	-0.242793	-3.873924	-4.160939	12.C	-0.209298	-3.712864	-4.176712
13.C	0.663203	-4.890825	-3.880839	13.C	0.685526	-4.749236	-3.942634
14.C	1.178917	-4.999098	-2.594980	14.C	1.194491	-4.921148	-2.661482
15.C	0.765198	-4.087247	-1.627184	15.C	0.784283	-4.052906	-1.654856
16.C	1.205081	-4.209178	-0.191807	16.C	1.210162	-4.254807	-0.221911
17.C	-2.549252	-2.735246	1.323751	17.C	-2.602670	-2.894393	1.269178
18.C	-3.144396	-3.431287	2.364065	18.C	-3.222457	-3.670831	2.235678
19.C	-2.327272	-4.016940	3.324767	19.C	-2.430698	-4.318753	3.176032
20.C	-0.948429	-3.902874	3.199433	20.C	-1.050245	-4.182042	3.101140
21.C	-0.425711	-3.188340	2.127169	21.C	-0.502928	-3.386310	2.101162
22.C	1.050364	-3.011512	1.914671	22.C	0.980670	-3.185362	1.947233

23.C	2.689270	-2.322834	0.223607	23.C	2.662465	-2.375836	0.349777
24.C	2.692282	-0.813650	0.324952	24.C	2.638550	-0.868241	0.515220
25.C	0.587971	2.999637	-3.139347	25.C	0.550795	2.884229	-3.117635
26.C	0.242793	3.873924	-4.160939	26.C	0.209298	3.712864	-4.176712
27.C	-0.663203	4.890825	-3.880839	27.C	-0.685526	4.749236	-3.942634
28.C	-1.178917	4.999098	-2.594980	28.C	-1.194491	4.921148	-2.661482
29.C	-0.765198	4.087247	-1.627184	29.C	-0.784283	4.052906	-1.654856
30.C	-1.205081	4.209178	-0.191807	30.C	-1.210162	4.254807	-0.221911
31.C	2.549252	2.735246	1.323751	31.C	2.602670	2.894393	1.269178
32.C	3.144396	3.431287	2.364065	32.C	3.222457	3.670831	2.235678
33.C	2.327272	4.016940	3.324767	33.C	2.430698	4.318753	3.176032
34.C	0.948429	3.902874	3.199433	34.C	1.050245	4.182042	3.101140
35.C	0.425711	3.188340	2.127169	35.C	0.502928	3.386310	2.101162
36.C	-1.050364	3.011512	1.914671	36.C	-0.980670	3.185362	1.947233
37.C	-2.689270	2.322834	0.223607	37.C	-2.662465	2.375836	0.349777
38.C	-2.692282	0.813650	0.324952	38.C	-2.638550	0.868241	0.515220
39.H	-1.283805	-2.182266	-3.317593	39.H	-1.238856	-2.053171	-3.260411
40.H	-0.670030	-3.751268	-5.152963	40.H	-0.633113	-3.542874	-5.163448
41.H	0.969947	-5.590367	-4.655513	41.H	0.987407	-5.416100	-4.747775
42.H	1.890045	-5.782397	-2.343591	42.H	1.895437	-5.725304	-2.447289
43.H	2.130734	-4.791673	-0.115499	43.H	2.143478	-4.831348	-0.170970
44.H	0.433508	-4.778067	0.339276	44.H	0.439837	-4.864920	0.265108
45.H	-3.147206	-2.269497	0.546248	45.H	-3.181861	-2.380934	0.506558
46.H	-4.226883	-3.511742	2.411764	46.H	-4.305210	-3.768976	2.241892
47.H	-2.757754	-4.570777	4.155767	47.H	-2.880441	-4.938130	3.949354
48.H	-0.280422	-4.368920	3.918977	48.H	-0.402119	-4.696606	3.807201
49.H	1.611467	-3.827336	2.386903	49.H	1.531357	-4.025275	2.394273
50.H	1.368831	-2.084329	2.402868	50.H	1.276036	-2.285593	2.499519
51.H	3.430948	-2.755518	0.909966	51.H	3.396422	-2.826901	1.036318
52.H	2.975800	-2.608578	-0.792355	52.H	2.985538	-2.606635	-0.670004
53.H	3.684014	-0.438507	0.053010	53.H	3.637407	-0.473030	0.297481
54.H	2.465886	-0.462055	1.335504	54.H	2.373751	-0.558425	1.531366
55.H	1.283805	2.182266	-3.317593	55.H	1.238856	2.053171	-3.260411
56.H	0.670030	3.751268	-5.152963	56.H	0.633113	3.542874	-5.163448
57.H	-0.969947	5.590367	-4.655513	57.H	-0.987407	5.416100	-4.747775
58.H	-1.890045	5.782397	-2.343591	58.H	-1.895437	5.725304	-2.447289
59.H	-2.130734	4.791673	-0.115499	59.H	-2.143478	4.831348	-0.170970
60.H	-0.433508	4.778067	0.339276	60.H	-0.439837	4.864920	0.265108
61.H	3.147206	2.269497	0.546248	61.H	3.181861	2.380934	0.506558
62.H	4.226883	3.511742	2.411764	62.H	4.305210	3.768976	2.241892
63.H	2.757754	4.570777	4.155767	63.H	2.880441	4.938130	3.949354
64.H	0.280422	4.368920	3.918977	64.H	0.402119	4.696606	3.807201
65.H	-1.611467	3.827336	2.386903	65.H	-1.531357	4.025275	2.394273
66.H	-1.368831	2.084329	2.402868	66.H	-1.276036	2.285593	2.499519
67.H	-3.430948	2.755518	0.909966	67.H	-3.396422	2.826901	1.036318
68.H	-2.975800	2.608578	-0.792355	68.H	-2.985538	2.606635	-0.670004
69.H	-3.684014	0.438507	0.053010	69.H	-3.637407	0.473030	0.297481
70.H	-2.465886	0.462055	1.335504	70.H	-2.373751	0.558425	1.531366
$[Cu^{I}_2(\mathbf{L^1SSL^1})]^{2+}$ in MeCN Conformation **B**, symmetry C_2				$[Cu^{I}_2(\mathbf{L^1SSL^1})]^{2+}$ in the gas phase Conformation **B**, symmetry C_2			
1.Cu	0.491345	2.482446	-0.314980	1.Cu	0.520804	2.496614	-0.223651
2.Cu	-0.491345	-2.482446	-0.314980	2.Cu	-0.520804	-2.496614	-0.223651
3.S	-0.950092	-0.434396	-0.754603	3.S	-0.950726	-0.431722	-0.607591
4.S	0.950092	0.434396	-0.754603	4.S	0.950726	0.431722	-0.607591
5.C	-2.447998	1.796010	0.222929	5.C	-2.443779	1.843666	0.283002
6.H	-2.766151	1.820710	-0.823710	6.H	-2.747366	1.823470	-0.768838

7.H	-3.351775	1.959328	0.831166	7.H	-3.359836	2.031058	0.870108
8.C	-1.922292	0.405288	0.545286	8.C	-1.921392	0.461736	0.664866
9.H	-2.784420	-0.267531	0.631646	9.H	-2.785236	-0.205482	0.785144
10.H	-1.380051	0.345896	1.492976	10.H	-1.377677	0.442315	1.613972
11.C	2.447998	-1.796010	0.222929	11.C	2.443779	-1.843666	0.283002
12.H	2.766151	-1.820710	-0.823710	12.H	2.747366	-1.823470	-0.768838
13.H	3.351775	-1.959328	0.831166	13.H	3.359836	-2.031058	0.870108
14.C	1.922292	-0.405288	0.545286	14.C	1.921392	-0.461736	0.664866
15.H	2.784420	0.267531	0.631646	15.H	2.785236	0.205482	0.785144
16.H	1.380051	-0.345896	1.492976	16.H	1.377677	-0.442315	1.613972
17.C	-1.361893	4.069775	-1.763001	17.C	-1.293345	4.031428	-1.792192
18.C	-2.054099	4.687859	-2.799319	18.C	-1.936661	4.638428	-2.864892
19.H	-3.025491	5.138781	-2.611544	19.H	-2.904102	5.115924	-2.724875
20.C	-1.486176	4.722943	-4.067463	20.C	-1.321709	4.639484	-4.110722
21.H	-2.011306	5.200371	-4.891826	21.H	-1.804990	5.113749	-4.962436
22.C	-0.241440	4.135129	-4.263218	22.C	-0.083033	4.025801	-4.247846
23.H	0.241903	4.136711	-5.236704	23.H	0.437447	4.004194	-5.202027
24.C	0.380699	3.528119	-3.182406	24.C	0.485388	3.428604	-3.133655
25.H	1.350687	3.049640	-3.293523	25.H	1.449932	2.930382	-3.201276
26.N	-1.048270	-3.586329	1.243944	26.N	-1.031270	-3.705876	1.278481
27.N	1.048270	3.586329	1.243944	27.N	1.031270	3.705876	1.278481
28.N	0.161364	-3.493391	-1.955486	28.N	0.099413	-3.428850	-1.926857
29.C	-1.876029	4.088040	-0.345379	29.C	-1.852147	4.107251	-0.391530
30.H	-1.424157	4.959905	0.143603	30.H	-1.417280	5.001217	0.073766
31.H	-2.961501	4.253602	-0.331860	31.H	-2.939194	4.271029	-0.418987
32.C	0.049418	3.864141	2.104693	32.C	0.009902	4.042125	2.090182
33.C	0.249924	4.666353	3.224301	33.C	0.169765	4.944139	3.136384
34.H	-0.580505	4.880410	3.892698	34.H	-0.677650	5.204232	3.767170
35.C	1.514885	5.182954	3.473807	35.C	1.418524	5.507654	3.364887
36.H	1.691067	5.808968	4.345608	36.H	1.563377	6.214202	4.179432
37.C	2.546141	4.892261	2.586392	37.C	2.472482	5.160900	2.528261
38.H	3.551367	5.277472	2.735507	38.H	3.465663	5.582648	2.660908
39.C	2.267892	4.097883	1.486146	39.C	2.233092	4.265411	1.499111
40.H	3.042351	3.856176	0.762642	40.H	3.028521	3.981579	0.813797
41.N	1.493804	-2.897987	0.425281	41.N	1.495934	-2.954942	0.449443
42.N	-0.161364	3.493391	-1.955486	42.N	-0.099413	3.428850	-1.926857
43.N	-1.493804	2.897987	0.425281	43.N	-1.495934	2.954942	0.449443
44.C	-1.289016	3.219627	1.838018	44.C	-1.312714	3.351613	1.846648
45.H	-1.321150	2.286023	2.410192	45.H	-1.333587	2.446347	2.464949
46.H	-2.096129	3.848693	2.238189	46.H	-2.137907	3.984699	2.206865
47.C	1.361893	-4.069775	-1.763001	47.C	1.293345	-4.031428	-1.792192
48.C	2.054099	-4.687859	-2.799319	48.C	1.936661	-4.638428	-2.864892
49.H	3.025491	-5.138781	-2.611544	49.H	2.904102	-5.115924	-2.724875
50.C	1.486176	-4.722943	-4.067463	50.C	1.321709	-4.639484	-4.110722
51.H	2.011306	-5.200371	-4.891826	51.H	1.804990	-5.113749	-4.962436
52.C	0.241440	-4.135129	-4.263218	52.C	0.083033	-4.025801	-4.247846
53.H	-0.241903	-4.136711	-5.236704	53.H	-0.437447	-4.004194	-5.202027
54.C	-0.380699	-3.528119	-3.182406	54.C	-0.485388	-3.428604	-3.133655
55.H	-1.350687	-3.049640	-3.293523	55.H	-1.449932	-2.930382	-3.201276
56.H	2.096129	-3.848693	2.238189	56.H	2.137907	-3.984699	2.206865
57.C	1.289016	-3.219627	1.838018	57.C	1.312714	-3.351613	1.846648
58.H	1.321150	-2.286023	2.410192	58.H	1.333587	-2.446347	2.464949
59.C	1.876029	-4.088040	-0.345379	59.C	1.852147	-4.107251	-0.391530
60.H	1.424157	-4.959905	0.143603	60.H	1.417280	-5.001217	0.073766
61.H	2.961501	-4.253602	-0.331860	61.H	2.939194	-4.271029	-0.418987
62.C	-0.049418	-3.864141	2.104693	62.C	-0.009902	-4.042125	2.090182

63.C	-0.249924	-4.666353	3.224301	63.C	-0.169765	-4.944139	3.136384
64.H	0.580505	-4.880410	3.892698	64.H	0.677650	-5.204232	3.767170
65.C	-1.514885	-5.182954	3.473807	65.C	-1.418524	-5.507654	3.364887
66.H	-1.691067	-5.808968	4.345608	66.H	-1.563377	-6.214202	4.179432
67.C	-2.546141	-4.892261	2.586392	67.C	-2.472482	-5.160900	2.528261
68.H	-3.551367	-5.277472	2.735507	68.H	-3.465663	-5.582648	2.660908
69.C	-2.267892	-4.097883	1.486146	69.C	-2.233092	-4.265411	1.499111
70.H	-3.042351	-3.856176	0.762642	70.H	-3.028521	-3.981579	0.813797
$[Cu^{I}_2(\mathbf{L^1SSL^1})]^{2+}$ in MeCN Conformation **C**, symmetry C_2				$[Cu^{I}_2(\mathbf{L^1SSL^1})]^{2+}$ in the gas phase Conformation **C**, symmetry C_2			
1.Cu	2.535709	0.011545	-0.328127	1.Cu	2.606799	0.020852	-0.353294
2.Cu	-2.535709	-0.011545	-0.328127	2.Cu	-2.606799	-0.020852	-0.353294
3.S	0.930994	0.546574	1.022353	3.S	0.961265	0.519736	0.971614
4.S	-0.930994	-0.546574	1.022353	4.S	-0.961265	-0.519736	0.971614
5.N	3.122220	-1.274235	-1.708100	5.N	3.249767	-1.229951	-1.751862
6.N	4.022102	1.280667	0.131473	6.N	4.074754	1.270669	0.197757
7.N	3.539192	-1.337861	1.066422	7.N	3.570068	-1.383098	1.034158
8.N	-3.122220	1.274235	-1.708100	8.N	-3.249767	1.229951	-1.751862
9.N	-4.022102	-1.280667	0.131473	9.N	-4.074754	-1.270669	0.197757
10.N	-3.539192	1.337861	1.066422	10.N	-3.570068	1.383098	1.034158
11.C	3.092994	-1.099972	-3.041327	11.C	3.282456	-1.014491	-3.077857
12.C	3.723282	-1.958435	-3.927079	12.C	3.935975	-1.854239	-3.964205
13.C	4.426395	-3.043084	-3.413213	13.C	4.600253	-2.964944	-3.458371
14.C	4.460658	-3.228765	-2.037206	14.C	4.574809	-3.192633	-2.088857
15.C	3.792093	-2.332534	-1.208450	15.C	3.885005	-2.312620	-1.262172
16.H	-3.063823	1.784104	3.094553	16.H	-3.059642	1.851575	3.049995
17.C	3.727092	-2.559527	0.286312	17.C	3.749616	-2.585658	0.221776
18.C	4.158836	2.550404	-0.289416	18.C	4.226644	2.552765	-0.175809
19.C	5.193378	3.370462	0.125103	19.C	5.265349	3.348556	0.272449
20.C	6.125343	2.856335	1.022508	20.C	6.184977	2.797425	1.158335
21.C	5.985486	1.548041	1.461098	21.C	6.029307	1.476434	1.550746
22.C	4.920466	0.779080	0.993122	22.C	4.963709	0.733807	1.046661
23.H	-2.868069	3.214823	0.468227	23.H	-2.860774	3.214871	0.348998
24.C	4.790211	-0.668488	1.424847	24.C	4.826839	-0.733822	1.412942
25.C	2.574195	-1.460358	2.162564	25.C	2.587764	-1.513866	2.111471
26.C	1.821474	-0.172799	2.450578	26.C	1.824376	-0.229510	2.402561
27.C	-3.092994	1.099972	-3.041327	27.C	-3.282456	1.014491	-3.077857
28.C	-3.723282	1.958435	-3.927079	28.C	-3.935975	1.854239	-3.964205
29.C	-4.426395	3.043084	-3.413213	29.C	-4.600253	2.964944	-3.458371
30.C	-4.460658	3.228765	-2.037206	30.C	-4.574809	3.192633	-2.088857
31.C	-3.792093	2.332534	-1.208450	31.C	-3.885005	2.312620	-1.262172
32.H	-3.403485	-2.910010	-0.983452	32.H	-3.479527	-2.944740	-0.861979
33.C	-3.727092	2.559527	0.286312	33.C	-3.749616	2.585658	0.221776
34.C	-4.158836	-2.550404	-0.289416	34.C	-4.226644	-2.552765	-0.175809
35.C	-5.193378	-3.370462	0.125103	35.C	-5.265349	-3.348556	0.272449
36.C	-6.125343	-2.856335	1.022508	36.C	-6.184977	-2.797425	1.158335
37.C	-5.985486	-1.548041	1.461098	37.C	-6.029307	-1.476434	1.550746
38.C	-4.920466	-0.779080	0.993122	38.C	-4.963709	-0.733807	1.046661
39.H	-5.260560	-4.389648	-0.245786	39.H	-5.346851	-4.378762	-0.064622
40.C	-4.790211	0.668488	1.424847	40.C	-4.826839	0.733822	1.412942
41.C	-2.574195	1.460358	2.162564	41.C	-2.587764	1.513866	2.111471
42.C	-1.821474	0.172799	2.450578	42.C	-1.824376	0.229510	2.402561
43.H	2.542437	-0.234448	-3.401034	43.H	2.761762	-0.128431	-3.433803
44.H	3.667446	-1.769903	-4.995856	44.H	3.929696	-1.631786	-5.028272
45.H	4.945302	-3.733394	-4.074526	45.H	5.135888	-3.642748	-4.119775
46.H	5.002286	-4.065440	-1.602669	46.H	5.087188	-4.052276	-1.662182

47.H	-4.962652	0.728771	2.507654	47.H	-5.011837	0.848176	2.490835
48.H	-5.625410	1.210128	0.966009	48.H	-5.652720	1.257652	0.915769
49.H	4.609661	-3.124391	0.611112	49.H	4.599400	-3.192877	0.563595
50.H	2.868069	-3.214823	0.468227	50.H	2.860774	-3.214871	0.348998
51.H	3.403485	2.910010	-0.983452	51.H	3.479527	2.944740	-0.861979
52.H	5.260560	4.389648	-0.245786	52.H	5.346851	4.378762	-0.064622
53.H	6.950226	3.469609	1.378410	53.H	7.013632	3.390560	1.539651
54.H	6.697460	1.118167	2.161805	54.H	6.735748	1.019273	2.240729
55.H	-1.852816	2.235725	1.892584	55.H	-1.868559	2.285054	1.821977
56.H	-1.116831	0.322669	3.274015	56.H	-1.104660	0.402125	3.209872
57.H	4.962652	-0.728771	2.507654	57.H	5.011837	-0.848176	2.490835
58.H	5.625410	-1.210128	0.966009	58.H	5.652720	-1.257652	0.915769
59.H	1.852816	-2.235725	1.892584	59.H	1.868559	-2.285054	1.821977
60.H	3.063823	-1.784104	3.094553	60.H	3.059642	-1.851575	3.049995
61.H	1.116831	-0.322669	3.274015	61.H	1.104660	-0.402125	3.209872
62.H	-4.609661	3.124391	0.611112	62.H	-4.599400	3.192877	0.563595
63.H	-2.542437	0.234448	-3.401034	63.H	-2.761762	0.128431	-3.433803
64.H	-3.667446	1.769903	-4.995856	64.H	-3.929696	1.631786	-5.028272
65.H	-4.945302	3.733394	-4.074526	65.H	-5.135888	3.642748	-4.119775
66.H	-5.002286	4.065440	-1.602669	66.H	-5.087188	4.052276	-1.662182
67.H	-6.950226	-3.469609	1.378410	67.H	-7.013632	-3.390560	1.539651
68.H	-6.697460	-1.118167	2.161805	68.H	-6.735748	-1.019273	2.240729
69.H	2.492478	0.639518	2.755491	69.H	2.489015	0.575102	2.741169
70.H	-2.492478	-0.639518	2.755491	70.H	-2.489015	-0.575102	2.741169

Table S9: Cartesian coordinates (Å) of complexes with ligand $\mathbf{L^2SSL^2}$ in **A**, **B** or **C** conformation and with the methyl groups arranged in three different ways (**a**, **b** & **c**, Figure S11), computed at ZORA-OPBE/TZ2P in the gas phase and/or solvated in MeCN (COSMO).

$[Cu^{II}_2(\mathbf{L^2S})_2]^{2+}$ in MeCN Conformation **A** (**a**), symmetry C_2				$[Cu^{II}_2(\mathbf{L^2S})_2]^{2+}$ in the gas phase Conformation **A** (**a**), symmetry C_2			
1.Cu	-0.248792	1.626658	-0.076430	1.Cu	-0.275152	1.683687	-0.085745
2.Cu	0.248792	-1.626658	-0.076430	2.Cu	0.275152	-1.683687	-0.085745
3.S	1.484181	0.242735	0.449227	3.S	1.468456	0.258381	0.303090
4.S	-1.484181	-0.242735	0.449227	4.S	-1.468456	-0.258381	0.303090
5.C	2.526186	2.372916	-0.851904	5.C	2.484719	2.403570	-0.995873
6.H	2.948375	2.694701	0.104169	6.H	2.960835	2.674574	-0.048479
7.H	3.161209	2.785607	-1.648174	7.H	3.101450	2.825453	-1.805060
8.C	2.531464	0.861333	-0.901986	8.C	2.441446	0.891089	-1.095695
9.H	3.553982	0.502901	-0.748215	9.H	3.462360	0.499552	-1.023637
10.H	2.181032	0.472955	-1.862655	10.H	2.023001	0.544196	-2.046275
11.C	-2.526186	-2.372916	-0.851904	11.C	-2.484719	-2.403570	-0.995873
12.H	-2.948375	-2.694701	0.104169	12.H	-2.960835	-2.674574	-0.048479
13.H	-3.161209	-2.785607	-1.648174	13.H	-3.101450	-2.825453	-1.805060
14.C	-2.531464	-0.861333	-0.901986	14.C	-2.441446	-0.891089	-1.095695
15.H	-3.553982	-0.502901	-0.748215	15.H	-3.462360	-0.499552	-1.023637
16.H	-2.181032	-0.472955	-1.862655	16.H	-2.023001	-0.544196	-2.046275
17.C	0.928142	4.154193	1.227247	17.C	0.953770	4.114210	1.239167
18.C	1.590551	5.049082	2.060993	18.C	1.594890	4.980236	2.115757
19.H	2.292547	5.770290	1.650072	19.H	2.293351	5.727649	1.746508
20.C	1.323934	5.002762	3.422684	20.C	1.310069	4.877952	3.469855
21.H	1.821457	5.686107	4.107353	21.H	1.790580	5.538258	4.188598
22.C	0.409890	4.073249	3.894543	22.C	0.396600	3.924933	3.888260
23.H	0.170659	4.019512	4.953949	23.H	0.141196	3.831562	4.940996

24.C	-0.207946	3.195558	2.998534
25.C	1.090003	4.248324	-0.266659
26.H	0.213473	4.777799	-0.656130
27.H	1.965087	4.857643	-0.522056
28.C	-1.195081	2.182942	3.484855
29.H	-0.771966	1.174299	3.436530
30.H	-2.096648	2.185362	2.866301
31.H	-1.477980	2.377754	4.520977
32.C	-0.814800	3.224018	-2.337541
33.C	-1.477446	3.940661	-3.327547
34.H	-0.913637	4.404638	-4.132498
35.C	-2.860115	4.059948	-3.260738
36.H	-3.399059	4.616693	-4.023678
37.C	-3.539870	3.474817	-2.198028
38.H	-4.618395	3.558783	-2.096904
39.C	-2.810532	2.774952	-1.249915
40.H	-3.296600	2.304761	-0.400018
41.C	0.676119	3.039552	-2.323052
42.H	0.926621	2.109774	-2.845080
43.H	1.172874	3.852390	-2.866757
44.C	-0.928142	-4.154193	1.227247
45.C	-1.590551	-5.049082	2.060993
46.H	-2.292547	-5.770290	1.650072
47.C	-1.323934	-5.002762	3.422684
48.H	-1.821457	-5.686107	4.107353
49.C	-0.409890	-4.073249	3.894543
50.H	-0.170659	-4.019512	4.953949
51.C	0.207946	-3.195558	2.998534
52.C	-1.090003	-4.248324	-0.266659
53.H	-0.213473	-4.777799	-0.656130
54.H	-1.965087	-4.857643	-0.522056
55.C	1.195081	-2.182942	3.484855
56.H	0.771966	-1.174299	3.436530
57.H	2.096648	-2.185362	2.866301
58.H	1.477980	-2.377754	4.520977
59.C	0.814800	-3.224018	-2.337541
60.C	1.477446	-3.940661	-3.327547
61.H	0.913637	-4.404638	-4.132498
62.C	2.860115	-4.059948	-3.260738
63.H	3.399059	-4.616693	-4.023678
64.C	3.539870	-3.474817	-2.198028
65.H	4.618395	-3.558783	-2.096904
66.C	2.810532	-2.774952	-1.249915
67.H	3.296600	-2.304761	-0.400018
68.C	-0.676119	-3.039552	-2.323052
69.H	-0.926621	-2.109774	-2.845080
70.H	-1.172874	-3.852390	-2.866757
71.N	1.162560	2.939650	-0.938382
72.N	-1.162560	-2.939650	-0.938382
73.N	0.060361	3.238765	1.680615
74.N	-1.479578	2.640838	-1.323704
75.N	-0.060361	-3.238765	1.680615
76.N	1.479578	-2.640838	-1.323704

24.C	-0.200785	3.077087	2.952638
25.C	1.123333	4.284302	-0.248837
26.H	0.269185	4.871487	-0.606607
27.H	2.022816	4.874647	-0.469079
28.C	-1.199368	2.051878	3.385175
29.H	-0.847264	1.039545	3.168698
30.H	-2.148792	2.185650	2.857226
31.H	-1.394918	2.120411	4.456723
32.C	-0.906096	3.399215	-2.274925
33.C	-1.596772	4.187000	-3.188893
34.H	-1.062412	4.691464	-3.990990
35.C	-2.972186	4.329722	-3.053576
36.H	-3.532226	4.944274	-3.755471
37.C	-3.615165	3.692975	-1.998812
38.H	-4.686422	3.794442	-1.843289
39.C	-2.858442	2.922498	-1.129982
40.H	-3.316993	2.410958	-0.287419
41.C	0.583797	3.190384	-2.342403
42.H	0.791362	2.283406	-2.922467
43.H	1.063923	4.023023	-2.876206
44.C	-0.953770	-4.114210	1.239167
45.C	-1.594890	-4.980236	2.115757
46.H	-2.293351	-5.727649	1.746508
47.C	-1.310069	-4.877952	3.469855
48.H	-1.790580	-5.538258	4.188598
49.C	-0.396600	-3.924933	3.888260
50.H	-0.141196	-3.831562	4.940996
51.C	0.200785	-3.077087	2.952638
52.C	-1.123333	-4.284302	-0.248837
53.H	-0.269185	-4.871487	-0.606607
54.H	-2.022816	-4.874647	-0.469079
55.C	1.199368	-2.051878	3.385175
56.H	0.847264	-1.039545	3.168698
57.H	2.148792	-2.185650	2.857226
58.H	1.394918	-2.120411	4.456723
59.C	0.906096	-3.399215	-2.274925
60.C	1.596772	-4.187000	-3.188893
61.H	1.062412	-4.691464	-3.990990
62.C	2.972186	-4.329722	-3.053576
63.H	3.532226	-4.944274	-3.755471
64.C	3.615165	-3.692975	-1.998812
65.H	4.686422	-3.794442	-1.843289
66.C	2.858442	-2.922498	-1.129982
67.H	3.316993	-2.410958	-0.287419
68.C	-0.583797	-3.190384	-2.342403
69.H	-0.791362	-2.283406	-2.922467
70.H	-1.063923	-4.023023	-2.876206
71.N	1.140617	3.015357	-0.995617
72.N	-1.140617	-3.015357	-0.995617
73.N	0.090457	3.171066	1.641012
74.N	-1.535203	2.766672	-1.268369
75.N	-0.090457	-3.171066	1.641012
76.N	1.535203	-2.766672	-1.268369

$[Cu^{II}_2(\mathbf{L}^2\mathbf{S})_2]^{2+}$ in MeCN Conformation **A** (**b**), symmetry C_2			
1.Cu	-0.162029	-1.671730	-0.269156
2.Cu	0.162029	1.671730	-0.269156
3.S	1.455848	-0.136618	-0.822367
4.S	-1.455848	0.136618	-0.822367
5.N	0.164319	-3.164844	-1.894869
6.N	-1.267184	-2.813120	1.077016
7.N	1.381852	-2.831720	0.584465
8.N	-0.164319	3.164844	-1.894869
9.N	1.267184	2.813120	1.077016
10.N	-1.381852	2.831720	0.584465
11.C	-0.201006	-3.116574	-3.180474
12.C	0.267470	-4.010156	-4.133867
13.C	1.165848	-4.992472	-3.731671
14.C	1.554940	-5.044820	-2.398802
15.C	1.026521	-4.114273	-1.507259
16.C	1.344332	-4.167195	-0.034525
17.C	-2.576291	-3.138708	1.081336
18.C	-3.150751	-3.740538	2.204023
19.C	-2.366714	-4.048996	3.303316
20.C	-1.004365	-3.784442	3.253452
21.C	-0.492329	-3.166501	2.122279
22.C	0.974841	-2.866456	1.994284
23.C	2.703902	-2.199892	0.393027
24.C	2.639586	-0.690739	0.438583
25.C	0.201006	3.116574	-3.180474
26.C	-0.267470	4.010156	-4.133867
27.C	-1.165848	4.992472	-3.731671
28.C	-1.554940	5.044820	-2.398802
29.C	-1.026521	4.114273	-1.507259
30.C	-1.344332	4.167195	-0.034525
31.C	2.576291	3.138708	1.081336
32.C	3.150751	3.740538	2.204023
33.C	2.366714	4.048996	3.303316
34.C	1.004365	3.784442	3.253452
35.C	0.492329	3.166501	2.122279
36.C	-0.974841	2.866456	1.994284
37.C	-2.703902	2.199892	0.393027
38.C	-2.639586	0.690739	0.438583
39.H	-0.898012	-2.326748	-3.454286
40.H	-0.061485	-3.929789	-5.166821
41.H	1.565499	-5.706816	-4.448304
42.H	2.259147	-5.797826	-2.052905
43.H	2.285113	-4.702547	0.139974
44.H	0.555810	-4.749585	0.454446
45.C	-3.389399	-2.917678	-0.150189
46.H	-4.211751	-3.977755	2.195935
47.H	-2.805882	-4.518118	4.180454
48.H	-0.345024	-4.056304	4.073150
49.H	1.560979	-3.598154	2.565471
50.H	1.184679	-1.885686	2.434169
51.H	3.416764	-2.576163	1.140686
52.H	3.068276	-2.507278	-0.591384
53.H	3.626981	-0.284293	0.199520
54.H	2.350504	-0.309824	1.422175

$[Cu^{II}_2(\mathbf{L}^2\mathbf{S})_2]^{2+}$ in MeCN Conformation **A** (**c**), no symmetry			
1.Cu	0.072332	1.584450	-0.660705
2.Cu	-0.108716	-1.394097	0.860417
3.S	1.331550	-0.309954	-0.561648
4.S	-0.639448	0.786607	1.369322
5.N	1.882922	3.141504	-0.630615
6.N	-1.463949	2.747691	-1.286027
7.N	0.565952	1.712979	-2.713621
8.N	0.683342	-2.029141	2.839194
9.N	-0.442155	-3.255110	-0.014515
10.N	-1.909892	-1.936655	1.829099
11.C	2.697591	3.540218	0.363567
12.C	3.925389	4.152012	0.093336
13.C	4.319697	4.346345	-1.221481
14.C	3.473313	3.936798	-2.243155
15.C	2.261741	3.346170	-1.899984
16.C	1.262372	2.985469	-2.967011
17.C	-2.234957	3.566497	-0.557848
18.C	-3.281298	4.287855	-1.110721
19.C	-3.535234	4.153806	-2.471382
20.C	-2.724620	3.320567	-3.232372
21.C	-1.691419	2.631812	-2.607027
22.C	-0.761721	1.710971	-3.345798
23.C	1.395585	0.558517	-3.122173
24.C	1.087696	-0.688623	-2.323662
25.C	1.873268	-1.779408	3.396620
26.C	2.154937	-2.046532	4.729166
27.C	1.147409	-2.588551	5.519866
28.C	-0.093193	-2.844830	4.949125
29.C	-0.285362	-2.555681	3.600059
30.C	-1.579008	-2.889931	2.901113
31.C	0.418246	-4.114208	-0.599764
32.C	-0.059873	-5.222108	-1.304061
33.C	-1.421333	-5.469805	-1.366568
34.C	-2.290756	-4.623110	-0.692088
35.C	-1.762522	-3.526238	-0.027234
36.C	-2.645634	-2.575872	0.731564
37.C	-2.614845	-0.754212	2.367120
38.C	-2.422746	0.475340	1.508023
39.C	2.254817	3.310804	1.773246
40.H	4.562809	4.468792	0.915423
41.H	5.275918	4.812316	-1.448994
42.H	3.743055	4.077484	-3.286856
43.H	1.740464	2.970941	-3.953739
44.H	0.509565	3.781043	-2.994346
45.H	-1.996600	3.641430	0.499292
46.H	-3.878844	4.942029	-0.481865
47.H	-4.347981	4.703681	-2.940046
48.H	-2.882167	3.210197	-4.302021
49.H	-0.704402	1.986785	-4.405934
50.H	-1.161297	0.691833	-3.304729
51.H	1.275982	0.364328	-4.197270
52.H	2.439976	0.835352	-2.953036
53.H	1.782797	-1.481442	-2.616135
54.H	0.070818	-1.054753	-2.493459

55.H	0.898012	2.326748	-3.454286	55.H	2.630739	-1.348329	2.744672
56.H	0.061485	3.929789	-5.166821	56.H	3.139505	-1.827491	5.134275
57.H	-1.565499	5.706816	-4.448304	57.H	1.322517	-2.804456	6.571635
58.H	-2.259147	5.797826	-2.052905	58.H	-0.902975	-3.264829	5.541058
59.H	-2.285113	4.702547	0.139974	59.H	-2.400747	-2.965447	3.623113
60.H	-0.555810	4.749585	0.454446	60.H	-1.464483	-3.882910	2.452594
61.C	3.389399	2.917678	-0.150189	61.C	1.886032	-3.908623	-0.428227
62.H	4.211751	3.977755	2.195935	62.H	0.647980	-5.891885	-1.785990
63.H	2.805882	4.518118	4.180454	63.H	-1.801390	-6.330179	-1.912095
64.H	0.345024	4.056304	4.073150	64.H	-3.361179	-4.808750	-0.675093
65.H	-1.560979	3.598154	2.565471	65.H	-3.539277	-3.099804	1.095224
66.H	-1.184679	1.885686	2.434169	66.H	-2.997730	-1.790261	0.054482
67.H	-3.416764	2.576163	1.140686	67.H	-3.685136	-0.972810	2.490674
68.H	-3.068276	2.507278	-0.591384	68.H	-2.203114	-0.556622	3.360863
69.H	-3.626981	0.284293	0.199520	69.H	-2.894301	1.332556	1.998740
70.H	-2.350504	0.309824	1.422175	70.H	-2.870667	0.369741	0.515749
71.H	2.940832	2.177726	-0.812727	71.H	2.136014	-2.865080	-0.235210
72.H	4.408762	2.613862	0.099117	72.H	2.437468	-4.259341	-1.303392
73.H	3.462303	3.859961	-0.707268	73.H	2.235074	-4.494953	0.430921
74.H	-2.940832	-2.177726	-0.812727	74.H	2.887610	3.855951	2.476025
75.H	-4.408762	-2.613862	0.099117	75.H	2.311215	2.246429	2.026986
76.H	-3.462303	-3.859961	-0.707268	76.H	1.217281	3.624733	1.915333
$[Cu^1_2(\mathbf{L}^2\mathbf{SSL}^2)]^{2+}$ in MeCN Conformation **B** (**a**), symmetry C_2				$[Cu^1_2(\mathbf{L}^2\mathbf{SSL}^2)]^{2+}$ in the gas phase Conformation **B** (**a**), symmetry C_2			
1.Cu	0.436042	2.508063	-0.086464	1.Cu	0.461712	2.528343	-0.032744
2.Cu	-0.436042	-2.508063	-0.086464	2.Cu	-0.461712	-2.528343	-0.032744
3.S	-0.936240	-0.455386	-0.480532	3.S	-0.933983	-0.458997	-0.382687
4.S	0.936240	0.455386	-0.480532	4.S	0.933983	0.458997	-0.382687
5.C	-2.471470	1.728271	0.527246	5.C	-2.470625	1.765936	0.550508
6.H	-2.809152	1.748741	-0.513450	6.H	-2.786531	1.755933	-0.497993
7.H	-3.366903	1.874114	1.152535	7.H	-3.382331	1.930551	1.151653
8.C	-1.914720	0.347228	0.836301	8.C	-1.922138	0.387976	0.906337
9.H	-2.761949	-0.343620	0.925664	9.H	-2.773597	-0.297153	1.013150
10.H	-1.364328	0.292602	1.779290	10.H	-1.380422	0.359929	1.856245
11.C	2.471470	-1.728271	0.527246	11.C	2.470625	-1.765936	0.550508
12.H	2.809152	-1.748741	-0.513450	12.H	2.786531	-1.755933	-0.497993
13.H	3.366903	-1.874114	1.152535	13.H	3.382331	-1.930551	1.151653
14.C	1.914720	-0.347228	0.836301	14.C	1.922138	-0.387976	0.906337
15.H	2.761949	0.343620	0.925664	15.H	2.773597	0.297153	1.013150
16.H	1.364328	-0.292602	1.779290	16.H	1.380422	-0.359929	1.856245
17.C	-1.489274	4.051200	-1.468775	17.C	-1.436589	4.033949	-1.501643
18.C	-2.249706	4.644807	-2.467694	18.C	-2.167234	4.614061	-2.528222
19.H	-3.242008	5.028342	-2.244999	19.H	-3.163623	5.007576	-2.341736
20.C	-1.710234	4.746874	-3.743758	20.C	-1.590376	4.701310	-3.788404
21.H	-2.279238	5.206120	-4.548911	21.H	-2.133376	5.154616	-4.614842
22.C	-0.432375	4.259882	-3.973999	22.C	-0.307397	4.213328	-3.972635
23.H	0.021714	4.336878	-4.958684	23.H	0.176233	4.284827	-4.943714
24.C	0.278740	3.661120	-2.932451	24.C	0.372299	3.625547	-2.904825
25.C	1.654255	3.119676	-3.147749	25.C	1.754681	3.083891	-3.077387
26.H	2.320689	3.404701	-2.328118	26.H	2.387881	3.344077	-2.224100
27.H	2.075508	3.482669	-4.087181	27.H	2.220299	3.475356	-3.984149
28.H	1.637077	2.024549	-3.188729	28.H	1.736743	1.990822	-3.158695
29.C	-1.965549	4.034070	-0.037941	29.C	-1.948661	4.054521	-0.081813
30.H	-1.523927	4.912236	0.449151	30.H	-1.518294	4.945848	0.392484
31.H	-3.054032	4.171350	0.005532	31.H	-3.039337	4.193274	-0.069340
32.C	0.016725	3.852296	2.363015	32.C	-0.027265	3.983498	2.351806

33.C	0.217842	4.652364	3.484303	33.C	0.130817	4.860248	3.419912
34.H	-0.603064	4.835932	4.173195	34.H	-0.708975	5.078119	4.076417
35.C	1.471937	5.205648	3.709178	35.C	1.367978	5.452916	3.637056
36.H	1.648914	5.830509	4.581657	36.H	1.511422	6.140472	4.467939
37.C	2.491139	4.952836	2.796617	37.C	2.412134	5.159590	2.768255
38.H	3.487542	5.366996	2.926290	38.H	3.396166	5.605064	2.891564
39.C	2.211419	4.158969	1.696302	39.C	2.173434	4.287668	1.718878
40.H	2.976978	3.946529	0.954312	40.H	2.961368	4.046265	1.008987
41.N	1.534938	-2.848252	0.712635	41.N	1.540563	-2.891447	0.719427
42.N	-0.259137	3.554448	-1.699449	42.N	-0.201785	3.531689	-1.687752
43.N	-1.534938	2.848252	0.712635	43.N	-1.540563	2.891447	0.719427
44.C	-1.305856	3.166029	2.122884	44.C	-1.334394	3.260022	2.120946
45.H	-1.293805	2.228018	2.688504	45.H	-1.313950	2.340708	2.717950
46.H	-2.123106	3.765871	2.546910	46.H	-2.168868	3.859781	2.515361
47.C	1.489274	-4.051200	-1.468775	47.C	1.436589	-4.033949	-1.501643
48.C	2.249706	-4.644807	-2.467694	48.C	2.167234	-4.614061	-2.528222
49.H	3.242008	-5.028342	-2.244999	49.H	3.163623	-5.007576	-2.341736
50.C	1.710234	-4.746874	-3.743758	50.C	1.590376	-4.701310	-3.788404
51.H	2.279238	-5.206120	-4.548911	51.H	2.133376	-5.154616	-4.614842
52.C	0.432375	-4.259882	-3.973999	52.C	0.307397	-4.213328	-3.972635
53.H	-0.021714	-4.336878	-4.958684	53.H	-0.176233	-4.284827	-4.943714
54.C	-0.278740	-3.661120	-2.932451	54.C	-0.372299	-3.625547	-2.904825
55.C	-1.654255	-3.119676	-3.147749	55.C	-1.754681	-3.083891	-3.077387
56.H	-2.320689	-3.404701	-2.328118	56.H	-2.387881	-3.344077	-2.224100
57.H	-2.075508	-3.482669	-4.087181	57.H	-2.220299	-3.475356	-3.984149
58.H	-1.637077	-2.024549	-3.188729	58.H	-1.736743	-1.990822	-3.158695
59.C	1.965549	-4.034070	-0.037941	59.C	1.948661	-4.054521	-0.081813
60.H	1.523927	-4.912236	0.449151	60.H	1.518294	-4.945848	0.392484
61.H	3.054032	-4.171350	0.005532	61.H	3.039337	-4.193274	-0.069340
62.C	-0.016725	-3.852296	2.363015	62.C	0.027265	-3.983498	2.351806
63.C	-0.217842	-4.652364	3.484303	63.C	-0.130817	-4.860248	3.419912
64.H	0.603064	-4.835932	4.173195	64.H	0.708975	-5.078119	4.076417
65.C	-1.471937	-5.205648	3.709178	65.C	-1.367978	-5.452916	3.637056
66.H	-1.648914	-5.830509	4.581657	66.H	-1.511422	-6.140472	4.467939
67.C	-2.491139	-4.952836	2.796617	67.C	-2.412134	-5.159590	2.768255
68.H	-3.487542	-5.366996	2.926290	68.H	-3.396166	-5.605064	2.891564
69.C	-2.211419	-4.158969	1.696302	69.C	-2.173434	-4.287668	1.718878
70.H	-2.976978	-3.946529	0.954312	70.H	-2.961368	-4.046265	1.008987
71.N	1.003005	3.612451	1.477362	71.N	0.983429	3.700697	1.507806
72.N	-1.003005	-3.612451	1.477362	72.N	-0.983429	-3.700697	1.507806
73.N	0.259137	-3.554448	-1.699449	73.N	0.201785	-3.531689	-1.687752
74.C	1.305856	-3.166029	2.122884	74.C	1.334394	-3.260022	2.120946
75.H	1.293805	-2.228018	2.688504	75.H	1.313950	-2.340708	2.717950
76.H	2.123106	-3.765871	2.546910	76.H	2.168868	-3.859781	2.515361
$[Cu^{1}_{2}(\mathbf{L}^{2}\mathbf{SSL}^{2})]^{2+}$ in MeCN Conformation **B** (**b**), no symmetry				$[Cu^{1}_{2}(\mathbf{L}^{2}\mathbf{SSL}^{2})]^{2+}$ in MeCN Conformation **B** (**c**), no symmetry			
1.Cu	0.880679	-0.133442	-2.393900	1.Cu	0.272343	2.486396	-0.116334
2.Cu	-0.817538	-0.393806	2.382938	2.Cu	-0.352415	-2.559388	-0.213805
3.S	-0.917461	-0.773858	0.276171	3.S	-0.940954	-0.523204	-0.560635
4.S	1.075769	-0.527177	-0.295863	4.S	0.888345	0.477597	-0.548060
5.C	-2.170417	0.085602	-2.141292	5.C	-2.602375	1.553597	0.461255
6.H	-2.390694	-0.984218	-2.205490	6.H	-2.957235	1.539574	-0.573729
7.H	-3.090233	0.614931	-2.437101	7.H	-3.495978	1.645605	1.099116
8.C	-1.883139	0.440501	-0.690460	8.C	-1.948239	0.216086	0.772634
9.H	-2.838017	0.439706	-0.151747	9.H	-2.744265	-0.529882	0.885827
10.H	-1.447667	1.434231	-0.554905	10.H	-1.374911	0.208834	1.703540

11.C	2.095256	0.551108	2.144732	11.C	2.522924	-1.667447	0.391710
12.H	2.564925	-0.436196	2.187667	12.H	2.851319	-1.647372	-0.651967
13.H	2.862018	1.278719	2.455046	13.H	3.429440	-1.789333	1.005725
14.C	1.730196	0.858584	0.700608	14.C	1.909513	-0.320222	0.740304
15.H	2.657699	1.093955	0.165347	15.H	2.727811	0.401902	0.845836
16.H	1.072896	1.724553	0.584530	16.H	1.361919	-0.313757	1.686569
17.C	-0.577307	-1.794924	-4.185971	17.C	-1.736695	3.854742	-1.595182
18.C	-1.061493	-2.899352	-4.880069	18.C	-2.491652	4.382604	-2.637958
19.H	-1.963664	-2.811934	-5.480716	19.H	-3.494037	4.758551	-2.447862
20.C	-0.374989	-4.105127	-4.797484	20.C	-1.945501	4.426085	-3.915508
21.H	-0.736304	-4.980690	-5.332436	21.H	-2.518703	4.834897	-4.744729
22.C	0.774160	-4.173409	-4.017623	22.C	-0.660087	3.934522	-4.114357
23.H	1.342815	-5.094605	-3.921361	23.H	-0.191907	3.945609	-5.095184
24.C	1.186632	-3.031138	-3.347655	24.C	0.024118	3.414339	-3.025758
25.H	2.075994	-3.042940	-2.721982	25.N	1.638890	-2.832274	0.557013
26.N	0.531228	-1.863605	-3.427432	26.N	-1.739537	2.735058	0.621594
27.N	-1.088740	0.376121	-3.095806	27.H	1.383920	-2.274900	2.549639
28.N	0.976817	0.555359	3.101087	28.H	2.287338	-3.765897	2.363085
29.C	-1.216195	-0.434630	-4.312836	29.C	-2.230664	3.870050	-0.170030
30.H	-0.689311	0.090739	-5.119013	30.H	-1.845241	4.788372	0.289967
31.H	-2.261451	-0.528753	-4.636204	31.H	-3.325861	3.945795	-0.143207
32.C	0.395294	2.184802	-3.909941	32.C	-0.281942	3.904136	2.250090
33.C	0.566739	3.298727	-4.722457	33.C	-0.174008	4.762511	3.337281
34.H	-0.295651	3.873982	-5.049098	34.H	-1.018725	4.904057	4.006418
35.C	1.853424	3.657934	-5.099953	35.C	1.027310	5.425347	3.548546
36.H	2.020618	4.528894	-5.729378	36.H	1.144390	6.098735	4.394414
37.C	2.923036	2.884306	-4.670973	37.C	2.073741	5.224411	2.658825
38.H	3.940593	3.135810	-4.958466	38.H	3.022936	5.736614	2.793102
39.C	2.690331	1.765995	-3.872052	39.C	1.903164	4.365200	1.574681
40.C	3.805068	0.882612	-3.417821	40.C	2.986989	4.144142	0.571687
41.H	3.774217	0.737400	-2.333261	41.H	3.185243	3.075694	0.438583
42.H	4.776504	1.302073	-3.685600	42.H	3.913222	4.635408	0.874930
43.H	3.721715	-0.108507	-3.878974	43.H	2.692754	4.542516	-0.406387
44.C	-0.975964	1.800817	-3.409006	44.C	-1.541169	3.102961	2.023841
45.H	-1.160935	2.367047	-2.489634	45.H	-1.453898	2.180413	2.608433
46.H	-1.740840	2.126600	-4.127735	46.H	-2.405910	3.643081	2.434062
47.C	0.996053	-1.696209	4.148150	47.C	1.629703	-3.973216	-1.656122
48.C	1.730578	-2.667614	4.821076	48.C	2.411073	-4.493082	-2.679541
49.H	2.589214	-2.380318	5.423239	49.H	3.423688	-4.831871	-2.476741
50.C	1.348473	-3.999891	4.716333	50.C	1.866413	-4.580189	-3.954622
51.H	1.909387	-4.774745	5.234275	51.H	2.451537	-4.981539	-4.778883
52.C	0.243765	-4.323280	3.936212	52.C	0.562787	-4.153800	-4.159176
53.H	-0.092160	-5.350713	3.823004	53.H	0.104596	-4.222155	-5.142580
54.C	-0.429749	-3.298626	3.287836	54.C	-0.169391	-3.627755	-3.093181
55.H	-1.293768	-3.508915	2.661944	55.C	-1.573815	-3.153750	-3.279021
56.N	-1.726200	0.976442	3.513728	56.H	-2.215934	-3.502776	-2.464747
57.N	-0.068271	-2.010798	3.388184	57.H	-1.984050	-3.506192	-4.227355
58.N	1.435465	1.436716	-3.492572	58.H	-1.615970	-2.058611	-3.281877
59.C	1.297098	-0.226327	4.301744	59.C	2.115237	-3.977357	-0.228387
60.H	0.665268	0.143673	5.118566	60.H	1.714288	-4.886765	0.235860
61.H	2.336627	-0.077874	4.622594	61.H	3.208911	-4.068898	-0.195043
62.C	-0.892664	1.941207	3.949941	62.C	0.152456	-3.953741	2.190540
63.C	-1.321059	2.962157	4.789417	63.C	0.003146	-4.803365	3.282995
64.H	-0.619399	3.718978	5.130354	64.H	0.840333	-4.973122	3.955663
65.C	-2.654186	2.994208	5.175288	65.C	-1.220187	-5.424634	3.499929
66.H	-3.020874	3.784253	5.826429	66.H	-1.355818	-6.089967	4.349582

67.C	-3.510316	1.997873	4.726798	67.C	-2.261945	-5.187046	2.609201
68.H	-4.556801	1.991678	5.020419	68.H	-3.235745	-5.653216	2.733836
69.C	-3.021333	0.987398	3.900475	69.C	-2.034029	-4.340054	1.536813
70.C	-3.893803	-0.127864	3.426326	70.N	-0.855570	-3.729275	1.325341
71.H	-3.826374	-0.245459	2.340118	71.N	-0.495744	3.373761	-1.789978
72.H	-4.937759	0.044459	3.694186	72.N	0.735751	3.709548	1.388618
73.H	-3.579040	-1.077886	3.874027	73.N	0.373866	-3.532405	-1.861567
74.C	0.528558	1.905887	3.442582	74.C	1.437974	-3.196878	1.960510
75.H	0.569709	2.518131	2.534989	75.H	1.028634	3.013707	-3.139536
76.H	1.196949	2.390664	4.167903	76.H	-2.817910	-4.137118	0.811459
$[Cu^{I}_{2}(\mathbf{L}^{2}\mathbf{SSL}^{2})]^{2+}$ in MeCN Conformation **C** (**a**), symmetry C_2				$[Cu^{I}_{2}(\mathbf{L}^{2}\mathbf{SSL}^{2})]^{2+}$ in the gas phase Conformation **C** (**a**), symmetry C_2			
1.Cu	0.018216	2.552802	0.053224	1.Cu	0.038838	2.675630	0.104249
2.Cu	-0.018216	-2.552802	0.053224	2.Cu	-0.038838	-2.675630	0.104249
3.S	0.516553	0.947400	-1.317333	3.S	0.444789	1.000754	-1.225269
4.S	-0.516553	-0.947400	-1.317333	4.S	-0.444789	-1.000754	-1.225269
5.N	-1.198898	3.135208	1.499216	5.N	-1.055699	3.370228	1.608950
6.N	1.265330	4.023052	-0.525359	6.N	1.216690	4.099647	-0.695296
7.N	-1.404045	3.514313	-1.277613	7.N	-1.510459	3.543995	-1.162190
8.N	1.198898	-3.135208	1.499216	8.N	1.055699	-3.370228	1.608950
9.N	-1.265330	-4.023052	-0.525359	9.N	-1.216690	-4.099647	-0.695296
10.N	1.404045	-3.514313	-1.277613	10.N	1.510459	-3.543995	-1.162190
11.C	-0.943867	3.113810	2.825978	11.C	-0.681043	3.472838	2.901871
12.C	-1.804510	3.736258	3.728380	12.C	-1.456908	4.183827	3.816021
13.C	-2.927775	4.401746	3.257593	13.C	-2.619631	4.807658	3.392536
14.C	-3.178158	4.420871	1.892055	14.C	-2.996598	4.695932	2.060958
15.C	-2.297905	3.766901	1.039157	15.C	-2.196485	3.960499	1.198711
16.H	1.916724	-3.053513	-3.293337	16.H	2.167990	-2.982525	-3.110378
17.C	-2.593556	3.667692	-0.442141	17.C	-2.626380	3.713755	-0.232503
18.C	2.568658	4.152375	-0.223087	18.C	2.541955	4.249249	-0.534152
19.C	3.362501	5.161372	-0.740358	19.C	3.270313	5.240212	-1.168331
20.C	2.783893	6.073044	-1.618770	20.C	2.599418	6.110725	-2.020220
21.C	1.439826	5.940391	-1.936386	21.C	1.232115	5.955872	-2.195801
22.C	0.701635	4.903314	-1.367914	22.C	0.565546	4.941204	-1.512926
23.H	3.220276	-2.779630	-0.579456	23.H	3.207445	-2.784077	-0.235317
24.C	-0.782922	4.786562	-1.648031	24.C	-0.941832	4.810523	-1.626224
25.C	-1.553845	2.558547	-2.378751	25.C	-1.726249	2.536984	-2.202834
26.C	-0.268748	1.822418	-2.719403	26.C	-0.458473	1.795696	-2.604824
27.C	0.943867	-3.113810	2.825978	27.C	0.681043	-3.472838	2.901871
28.C	1.804510	-3.736258	3.728380	28.C	1.456908	-4.183827	3.816021
29.C	2.927775	-4.401746	3.257593	29.C	2.619631	-4.807658	3.392536
30.C	3.178158	-4.420871	1.892055	30.C	2.996598	-4.695932	2.060958
31.C	2.297905	-3.766901	1.039157	31.C	2.196485	-3.960499	1.198711
32.H	-0.275441	-2.217623	4.349991	32.H	-0.655507	-2.687781	4.390140
33.C	2.593556	-3.667692	-0.442141	33.C	2.626380	-3.713755	-0.232503
34.C	-2.568658	-4.152375	-0.223087	34.C	-2.541955	-4.249249	-0.534152
35.C	-3.362501	-5.161372	-0.740358	35.C	-3.270313	-5.240212	-1.168331
36.C	-2.783893	-6.073044	-1.618770	36.C	-2.599418	-6.110725	-2.020220
37.C	-1.439826	-5.940391	-1.936386	37.C	-1.232115	-5.955872	-2.195801
38.C	-0.701635	-4.903314	-1.367914	38.C	-0.565546	-4.941204	-1.512926
39.H	-4.411363	-5.223365	-0.462966	39.H	-4.341127	-5.321950	-0.999663
40.C	0.782922	-4.786562	-1.648031	40.C	0.941832	-4.810523	-1.626224
41.C	1.553845	-2.558547	-2.378751	41.C	1.726249	-2.536984	-2.202834
42.C	0.268748	-1.822418	-2.719403	42.C	0.458473	-1.795696	-2.604824
43.C	0.299503	2.419718	3.277216	43.C	0.599278	2.816452	3.307020
44.H	-1.582979	3.703462	4.792012	44.H	-1.138989	4.253183	4.853368

45.H	-3.601007	4.903608	3.948731	45.H	-3.226838	5.377648	4.092276
46.H	-4.049044	4.931249	1.489017	46.H	-3.905384	5.169567	1.697303
47.H	0.965636	-5.018094	-2.705743	47.H	1.244705	-5.022610	-2.662003
48.H	1.270352	-5.589036	-1.082129	48.H	1.368480	-5.619094	-1.019460
49.H	-3.208510	4.521612	-0.752022	49.H	-3.318081	4.505706	-0.552279
50.H	-3.220276	2.779630	-0.579456	50.H	-3.207445	2.784077	-0.235317
51.H	-0.438042	-1.476065	2.739792	51.H	-0.705655	-1.835709	2.831531
52.H	4.411363	5.223365	-0.462966	52.H	4.341127	5.321950	-0.999663
53.H	3.374487	6.876141	-2.054096	53.H	3.135562	6.899697	-2.543636
54.H	0.959216	6.636540	-2.619830	54.H	0.681183	6.623332	-2.855385
55.H	2.311324	-1.826005	-2.088901	55.H	2.447944	-1.808688	-1.822394
56.H	0.444441	-1.110210	-3.531262	56.H	0.695616	-1.037311	-3.358685
57.H	-0.965636	5.018094	-2.705743	57.H	-1.244705	5.022610	-2.662003
58.H	-1.270352	5.589036	-1.082129	58.H	-1.368480	5.619094	-1.019460
59.H	-2.311324	1.826005	-2.088901	59.H	-2.447944	1.808688	-1.822394
60.H	-1.916724	3.053513	-3.293337	60.H	-2.167990	2.982525	-3.110378
61.H	-0.444441	1.110210	-3.531262	61.H	-0.695616	1.037311	-3.358685
62.H	3.208510	-4.521612	-0.752022	62.H	3.318081	-4.505706	-0.552279
63.C	-0.299503	-2.419718	3.277216	63.C	-0.599278	-2.816452	3.307020
64.H	1.582979	-3.703462	4.792012	64.H	1.138989	-4.253183	4.853368
65.H	3.601007	-4.903608	3.948731	65.H	3.226838	-5.377648	4.092276
66.H	4.049044	-4.931249	1.489017	66.H	3.905384	-5.169567	1.697303
67.H	-3.374487	-6.876141	-2.054096	67.H	-3.135562	-6.899697	-2.543636
68.H	-0.959216	-6.636540	-2.619830	68.H	-0.681183	-6.623332	-2.855385
69.H	0.519745	2.503544	-3.061511	69.H	0.284148	2.468031	-3.051096
70.H	-0.519745	-2.503544	-3.061511	70.H	-0.284148	-2.468031	-3.051096
71.H	0.275441	2.217623	4.349991	71.H	0.655507	2.687781	4.390140
72.H	0.438042	1.476065	2.739792	72.H	0.705655	1.835709	2.831531
73.H	-1.180266	-3.041563	3.075507	73.H	-1.457172	-3.429805	3.004564
74.H	1.180266	3.041563	3.075507	74.H	1.457172	3.429805	3.004564
75.H	2.980039	3.412200	0.458529	75.H	3.028248	3.539843	0.131366
76.H	-2.980039	-3.412200	0.458529	76.H	-3.028248	-3.539843	0.131366
$[Cu^{I}_{2}(\mathbf{L}^{2}\mathbf{SSL}^{2})]^{2+}$ in MeCN Conformation **C** (**b**), symmetry C_2				$[Cu^{I}_{2}(\mathbf{L}^{2}\mathbf{SSL}^{2})]^{2+}$ in MeCN Conformation **C** (**c**), no symmetry			
1.Cu	2.497565	-0.022754	-0.189722	1.Cu	2.330824	-6.789788	0.142561
2.Cu	-2.497565	0.022754	-0.189722	2.Cu	2.441651	-1.781007	0.132036
3.S	0.924457	0.546865	1.193784	3.S	2.903467	-5.242342	1.547603
4.S	-0.924457	-0.546865	1.193784	4.S	1.886429	-3.351211	1.525268
5.N	2.969302	-1.355422	-1.572764	5.N	1.067809	-7.238203	-1.307465
6.N	4.023226	1.216700	0.235300	6.N	3.499656	-8.341285	0.667528
7.N	3.472052	-1.401438	1.184684	7.N	0.864337	-7.718073	1.456187
8.N	-2.969302	1.355422	-1.572764	8.N	3.739462	-1.297013	-1.276009
9.N	-4.023226	-1.216700	0.235300	9.N	1.196252	-0.277310	0.618391
10.N	-3.472052	1.401438	1.184684	10.N	3.844999	-0.820649	1.481769
11.C	2.895031	-1.203011	-2.906959	11.C	1.307694	-7.161923	-2.635297
12.C	3.445344	-2.105899	-3.801647	12.C	0.410949	-7.702308	-3.554823
13.C	4.115434	-3.215435	-3.296566	13.C	-0.736435	-8.338760	-3.101596
14.C	4.194484	-3.380515	-1.919740	14.C	-0.974664	-8.408150	-1.735653
15.C	3.604500	-2.438579	-1.081616	15.C	-0.055503	-7.837276	-0.863906
16.H	-3.070584	1.790413	3.239994	16.H	4.288733	-1.234060	3.524156
17.C	3.586384	-2.640637	0.418285	17.C	-0.334367	-7.794674	0.623936
18.C	4.172251	2.494462	-0.180809	18.C	4.793693	-8.528096	0.354818
19.C	5.229423	3.274315	0.280355	19.C	5.542523	-9.581117	0.851002
20.C	6.135240	2.734271	1.184316	20.C	4.927974	-10.477687	1.720451
21.C	5.971436	1.422643	1.602472	21.C	3.593609	-10.286524	2.048965
22.C	4.902505	0.686213	1.100226	22.C	2.901289	-9.207860	1.500805

23.H	-2.711147	3.260802	0.641396	23.H	5.695921	-1.571664	0.895275
24.C	4.761239	-0.775217	1.480575	24.C	1.425966	-9.026306	1.793696
25.C	2.550313	-1.476480	2.321523	25.C	0.766508	-6.782780	2.580147
26.C	1.836149	-0.167139	2.608632	26.C	2.086596	-6.117056	2.930802
27.C	-2.895031	1.203011	-2.906959	27.C	3.556193	-1.357936	-2.607033
28.C	-3.445344	2.105899	-3.801647	28.C	4.439390	-0.800818	-3.516718
29.C	-4.115434	3.215435	-3.296566	29.C	5.562052	-0.138644	-3.030572
30.C	-4.194484	3.380515	-1.919740	30.C	5.758573	-0.072744	-1.657416
31.C	-3.604500	2.438579	-1.081616	31.C	4.834492	-0.667963	-0.803246
32.C	-3.170054	-3.025389	-1.152732	32.C	-0.648711	-1.129544	-0.720383
33.C	-3.586384	2.640637	0.418285	33.C	5.068853	-0.696765	0.691745
34.C	-4.172251	-2.494462	-0.180809	34.C	-0.100192	-0.144940	0.259639
35.C	-5.229423	-3.274315	0.280355	35.C	-0.883601	0.878138	0.787511
36.C	-6.135240	-2.734271	1.184316	36.C	-0.326739	1.766850	1.698051
37.C	-5.971436	-1.422643	1.602472	37.C	1.005321	1.621936	2.055113
38.C	-4.902505	-0.686213	1.100226	38.C	1.743169	0.586956	1.488582
39.H	-5.333745	-4.298986	-0.066624	39.H	-1.924190	0.968787	0.487250
40.C	-4.761239	0.775217	1.480575	40.C	3.222550	0.466146	1.797207
41.C	-2.550313	1.476480	2.321523	41.C	3.947516	-1.748503	2.612023
42.C	-1.836149	0.167139	2.608632	42.C	2.643636	-2.459578	2.930842
43.H	3.366597	4.071994	-1.391466	43.C	2.569734	-6.490142	-3.068118
44.H	3.355206	-1.931944	-4.870629	44.H	0.622375	-7.628640	-4.618418
45.H	4.573598	-3.940863	-3.965078	45.H	-1.438462	-8.777695	-3.806776
46.H	4.711228	-4.236047	-1.491527	46.H	-1.864911	-8.895084	-1.345990
47.H	-5.015518	0.890943	2.542348	47.H	3.391645	0.735810	2.848042
48.H	-5.542344	1.312632	0.930286	48.H	3.723063	1.243702	1.208603
49.H	4.457883	-3.234760	0.720028	49.H	-0.974359	-8.641387	0.900461
50.H	2.711147	-3.260802	0.641396	50.H	-0.932935	-6.895285	0.806474
51.C	3.170054	3.025389	-1.152732	51.H	2.571498	-6.302955	-4.143551
52.H	5.333745	4.298986	-0.066624	52.H	6.585528	-9.687677	0.565135
53.H	6.961332	3.333477	1.560449	53.H	5.483093	-11.313601	2.140377
54.H	6.664297	0.968551	2.306434	54.H	3.085001	-10.969048	2.725833
55.H	-1.801908	2.241829	2.101056	55.H	4.703414	-2.498046	2.364974
56.H	-1.152214	0.284721	3.454717	56.H	2.784435	-3.156851	3.762231
57.H	5.015518	-0.890943	2.542348	57.H	1.238883	-9.272208	2.847330
58.H	5.542344	-1.312632	0.930286	58.H	0.897311	-9.791506	1.213749
59.H	1.801908	-2.241829	2.101056	59.H	0.044430	-6.007183	2.312445
60.H	3.070584	-1.790413	3.239994	60.H	0.384795	-7.280760	3.485320
61.H	1.152214	-0.284721	3.454717	61.H	1.951169	-5.419724	3.763051
62.H	-4.457883	3.234760	0.720028	62.H	5.664967	0.175306	0.987699
63.H	3.194771	2.450986	-2.085554	63.H	2.702937	-5.538236	-2.542741
64.H	-3.355206	1.931944	-4.870629	64.H	4.240713	-0.878828	-4.582315
65.H	-4.573598	3.940863	-3.965078	65.H	6.273254	0.323878	-3.711213
66.H	-4.711228	4.236047	-1.491527	66.H	6.624678	0.438329	-1.244050
67.H	-6.961332	-3.333477	1.560449	67.H	-0.928319	2.565343	2.126380
68.H	-6.664297	-0.968551	2.306434	68.H	1.472924	2.302317	2.762337
69.H	2.535036	0.634795	2.876227	69.H	2.845521	-6.843126	3.246354
70.H	-2.535036	-0.634795	2.876227	70.H	1.854399	-1.761326	3.234804
71.H	-2.155339	-2.947424	-0.747562	71.H	-0.576331	-2.149849	-0.327927
72.H	-3.194771	-2.450986	-2.085554	72.H	-0.082045	-1.098552	-1.657462
73.H	-3.366597	-4.071994	-1.391466	73.H	-1.696087	-0.922120	-0.945971
74.H	2.155339	2.947424	-0.747562	74.H	3.439937	-7.115070	-2.834510
75.H	2.373834	-0.317601	-3.262092	75.H	5.235963	-7.797745	-0.317960
76.H	-2.373834	0.317601	-3.262092	76.H	2.660656	-1.872559	-2.946643

Table S10: Cartesian coordinates (Å) of complexes with ligand $\mathbf{L^3SSL^3}$ in **A**, **B** or **C** conformation computed at ZORA-OPBE/TZ2P in the gas phase and solvated in MeCN (COSMO).

$[Cu^{II}_2(\mathbf{L^3S})_2]^{2+}$ in MeCN Conformation **A**, symmetry C_2				$[Cu^{II}_2(\mathbf{L^3S})_2]^{2+}$ in the gas phase Conformation **A**, symmetry C_2			
1.Cu	-0.174217	-1.691142	0.029886	1.Cu	-0.211109	-1.736475	0.066835
2.Cu	0.174217	1.691142	0.029886	2.Cu	0.211109	1.736475	0.066835
3.S	1.465010	-0.159049	-0.430526	3.S	1.453477	-0.186931	-0.249179
4.S	-1.465010	0.159049	-0.430526	4.S	-1.453477	0.186931	-0.249179
5.N	0.413557	-3.264266	-1.641063	5.N	0.438973	-3.178959	-1.591136
6.N	-1.387761	-2.864231	1.237378	6.N	-1.468583	-2.972495	1.179896
7.N	1.299498	-2.833862	1.005529	7.N	1.244570	-2.916108	1.100345
8.N	-0.413557	3.264266	-1.641063	8.N	-0.438973	3.178959	-1.591136
9.N	1.387761	2.864231	1.237378	9.N	1.468583	2.972495	1.179896
10.N	-1.299498	2.833862	1.005529	10.N	-1.244570	2.916108	1.100345
11.C	0.236555	-3.264285	-2.975794	11.C	0.282839	-3.102019	-2.925075
12.C	0.911186	-4.171807	-3.796682	12.C	0.991266	-3.944603	-3.786797
13.C	1.789294	-5.084943	-3.232254	13.C	1.873829	-4.874673	-3.267110
14.C	1.971327	-5.077500	-1.856544	14.C	2.028685	-4.951621	-1.889384
15.C	1.256782	-4.153775	-1.099716	15.C	1.287649	-4.090909	-1.091476
16.C	1.349141	-4.174811	0.403737	16.C	1.344679	-4.210920	0.410382
17.C	-2.686830	-3.208170	1.112657	17.C	-2.757072	-3.316924	0.970300
18.C	-3.350176	-3.851382	2.160120	18.C	-3.459007	-4.048369	1.931858
19.C	-2.664860	-4.176334	3.319573	19.C	-2.826558	-4.456896	3.093414
20.C	-1.311466	-3.880134	3.406987	20.C	-1.483691	-4.151184	3.268196
21.C	-0.708497	-3.222509	2.344966	21.C	-0.840590	-3.407937	2.289986
22.C	0.754200	-2.877471	2.368106	22.C	0.617312	-3.050873	2.417572
23.C	2.621799	-2.177031	0.943921	23.C	2.547354	-2.225383	1.147638
24.C	2.521363	-0.668826	0.955946	24.C	2.408750	-0.717131	1.200213
25.C	-0.236555	3.264285	-2.975794	25.C	-0.282839	3.102019	-2.925075
26.C	-0.911186	4.171807	-3.796682	26.C	-0.991266	3.944603	-3.786797
27.C	-1.789294	5.084943	-3.232254	27.C	-1.873829	4.874673	-3.267110
28.C	-1.971327	5.077500	-1.856544	28.C	-2.028685	4.951621	-1.889384
29.C	-1.256782	4.153775	-1.099716	29.C	-1.287649	4.090909	-1.091476
30.C	-1.349141	4.174811	0.403737	30.C	-1.344679	4.210920	0.410382
31.C	2.686830	3.208170	1.112657	31.C	2.757072	3.316924	0.970300
32.C	3.350176	3.851382	2.160120	32.C	3.459007	4.048369	1.931858
33.C	2.664860	4.176334	3.319573	33.C	2.826558	4.456896	3.093414
34.C	1.311466	3.880134	3.406987	34.C	1.483691	4.151184	3.268196
35.C	0.708497	3.222509	2.344966	35.C	0.840590	3.407937	2.289986
36.C	-0.754200	2.877471	2.368106	36.C	-0.617312	3.050873	2.417572
37.C	-2.621799	2.177031	0.943921	37.C	-2.547354	2.225383	1.147638
38.C	-2.521363	0.668826	0.955946	38.C	-2.408750	0.717131	1.200213
39.C	-0.708221	-2.264772	-3.561613	39.C	-0.697061	-2.117940	-3.479520
40.H	0.747858	-4.151441	-4.871458	40.H	0.846684	-3.861583	-4.861670
41.H	2.330075	-5.791520	-3.858001	41.H	2.438582	-5.531351	-3.925380
42.H	2.652044	-5.775419	-1.375515	42.H	2.710821	-5.671837	-1.443458
43.H	2.251849	-4.708363	0.724851	43.H	2.252549	-4.747597	0.717560
44.H	0.494682	-4.747485	0.780251	44.H	0.494720	-4.827095	0.725650
45.C	-3.384047	-2.952119	-0.180308	45.C	-3.402640	-2.960803	-0.326878
46.H	-4.401187	-4.105138	2.047864	46.H	-4.499687	-4.306201	1.750338
47.H	-3.173589	-4.678801	4.138664	47.H	-3.365568	-5.030038	3.844640
48.H	-0.727605	-4.156693	4.280453	48.H	-0.940684	-4.490904	4.146874
49.H	1.300850	-3.590434	2.998652	49.H	1.131642	-3.799141	3.038624
50.H	0.887832	-1.890124	2.822856	50.H	0.712317	-2.092429	2.941121
51.H	3.259112	-2.524410	1.769516	51.H	3.146079	-2.585609	1.999380

52.H	3.094721	-2.491369	0.009209	52.H	3.087055	-2.492769	0.233895
53.H	3.519244	-0.242089	0.815334	53.H	3.403671	-0.260400	1.154420
54.H	2.123630	-0.281853	1.898583	54.H	1.932677	-0.370324	2.123211
55.C	0.708221	2.264772	-3.561613	55.C	0.697061	2.117940	-3.479520
56.H	-0.747858	4.151441	-4.871458	56.H	-0.846684	3.861583	-4.861670
57.H	-2.330075	5.791520	-3.858001	57.H	-2.438582	5.531351	-3.925380
58.H	-2.652044	5.775419	-1.375515	58.H	-2.710821	5.671837	-1.443458
59.H	-2.251849	4.708363	0.724851	59.H	-2.252549	4.747597	0.717560
60.H	-0.494682	4.747485	0.780251	60.H	-0.494720	4.827095	0.725650
61.C	3.384047	2.952119	-0.180308	61.C	3.402640	2.960803	-0.326878
62.H	4.401187	4.105138	2.047864	62.H	4.499687	4.306201	1.750338
63.H	3.173589	4.678801	4.138664	63.H	3.365568	5.030038	3.844640
64.H	0.727605	4.156693	4.280453	64.H	0.940684	4.490904	4.146874
65.H	-1.300850	3.590434	2.998652	65.H	-1.131642	3.799141	3.038624
66.H	-0.887832	1.890124	2.822856	66.H	-0.712317	2.092429	2.941121
67.H	-3.259112	2.524410	1.769516	67.H	-3.146079	2.585609	1.999380
68.H	-3.094721	2.491369	0.009209	68.H	-3.087055	2.492769	0.233895
69.H	-3.519244	0.242089	0.815334	69.H	-3.403671	0.260400	1.154420
70.H	-2.123630	0.281853	1.898583	70.H	-1.932677	0.370324	2.123211
71.H	3.015985	2.049805	-0.670511	71.H	3.048301	2.003353	-0.712851
72.H	4.462999	2.870414	-0.035455	72.H	4.489876	2.928983	-0.230116
73.H	3.206087	3.792540	-0.862665	73.H	3.163214	3.725891	-1.075950
74.H	-0.773144	-2.373955	-4.645449	74.H	-0.358212	-1.726248	-4.442094
75.H	-0.380047	-1.245783	-3.338784	75.H	-0.865195	-1.284884	-2.797949
76.H	-1.712165	-2.380272	-3.142705	76.H	-1.664189	-2.605173	-3.656331
77.H	-3.206087	-3.792540	-0.862665	77.H	-3.163214	-3.725891	-1.075950
78.H	-3.015985	-2.049805	-0.670511	78.H	-3.048301	-2.003353	-0.712851
79.H	-4.462999	-2.870414	-0.035455	79.H	-4.489876	-2.928983	-0.230116
80.H	0.773144	2.373955	-4.645449	80.H	0.358212	1.726248	-4.442094
81.H	0.380047	1.245783	-3.338784	81.H	0.865195	1.284884	-2.797949
82.H	1.712165	2.380272	-3.142705	82.H	1.664189	2.605173	-3.656331
$[Cu^{I}_2(\mathbf{L^3SSL^3})]^{2+}$ in MeCN Conformation **B**, symmetry C_2				$[Cu^{I}_2(\mathbf{L^3SSL^3})]^{2+}$ in the gas phase Conformation **B**, symmetry C_2			
1.Cu	0.320393	2.534835	-0.078536	1.Cu	0.347731	2.556025	-0.038595
2.Cu	-0.320393	-2.534835	-0.078536	2.Cu	-0.347731	-2.556025	-0.038595
3.S	-0.914225	-0.496339	-0.431062	3.S	-0.911111	-0.501395	-0.358200
4.S	0.914225	0.496339	-0.431062	4.S	0.911111	0.501395	-0.358200
5.C	-2.537354	1.617085	0.583296	5.C	-2.538978	1.648891	0.588048
6.H	-2.896321	1.611485	-0.450386	6.H	-2.875341	1.618515	-0.453685
7.H	-3.425810	1.729945	1.225420	7.H	-3.444630	1.778040	1.207079
8.C	-1.914917	0.265092	0.893735	8.C	-1.925021	0.298473	0.939870
9.H	-2.729593	-0.460757	1.000634	9.H	-2.743274	-0.423445	1.058605
10.H	-1.351190	0.241795	1.829938	10.H	-1.372794	0.297018	1.884001
11.C	2.537354	-1.617085	0.583296	11.C	2.538978	-1.648891	0.588048
12.H	2.896321	-1.611485	-0.450386	12.H	2.875341	-1.618515	-0.453685
13.H	3.425810	-1.729945	1.225420	13.H	3.444630	-1.778040	1.207079
14.C	1.914917	-0.265092	0.893735	14.C	1.925021	-0.298473	0.939870
15.H	2.729593	0.460757	1.000634	15.H	2.743274	0.423445	1.058605
16.H	1.351190	-0.241795	1.829938	16.H	1.372794	-0.297018	1.884001
17.C	-1.734058	3.917418	-1.467926	17.C	-1.679308	3.908275	-1.506242
18.C	-2.566194	4.437071	-2.450956	18.C	-2.480620	4.420927	-2.516000
19.H	-3.560005	4.793850	-2.193424	19.H	-3.481127	4.784456	-2.293936
20.C	-2.096639	4.498421	-3.756719	20.C	-1.970525	4.478601	-3.806019
21.H	-2.721636	4.900315	-4.550949	21.H	-2.569044	4.880324	-4.620737
22.C	-0.817074	4.040215	-4.030799	22.C	-0.683052	4.023400	-4.035408
23.H	-0.417745	4.081363	-5.041034	23.H	-0.251651	4.067658	-5.032435

24.C	-0.031428	3.517020	-3.001746	24.C	0.069748	3.503259	-2.981131
25.C	1.344858	3.005153	-3.275757	25.C	1.454921	2.992187	-3.212978
26.H	2.058004	3.370470	-2.531965	26.H	2.129140	3.299214	-2.409624
27.H	1.684623	3.310751	-4.267100	27.H	1.855433	3.359877	-4.159911
28.H	1.366070	1.910255	-3.236093	28.H	1.462979	1.896731	-3.252694
29.C	-2.145168	3.934008	-0.017694	29.C	-2.130206	3.951257	-0.067477
30.H	-1.704951	4.834798	0.427519	30.H	-1.702490	4.861248	0.372590
31.H	-3.234267	4.043583	0.070835	31.H	-3.223016	4.061500	-0.010905
32.C	-0.135298	3.907397	2.344520	32.C	-0.186662	4.019009	2.325722
33.C	0.012087	4.729279	3.455030	33.C	-0.092131	4.912735	3.382630
34.H	-0.812524	4.857950	4.151303	34.H	-0.941130	5.075217	4.042469
35.C	1.227274	5.369379	3.656155	35.C	1.104559	5.587408	3.582794
36.H	1.376328	6.012879	4.520068	36.H	1.212159	6.290773	4.405468
37.C	2.246871	5.180534	2.734239	37.C	2.156903	5.354597	2.712785
38.H	3.208246	5.671684	2.861392	38.H	3.104691	5.871808	2.841156
39.C	2.035160	4.360991	1.626263	39.C	1.997701	4.460158	1.654464
40.C	3.092987	4.171338	0.589960	40.C	3.099642	4.231603	0.671785
41.H	3.166677	3.123347	0.285613	41.H	3.104889	3.198029	0.314666
42.H	4.067502	4.501005	0.955133	42.H	4.074962	4.458701	1.108182
43.H	2.856320	4.757246	-0.306268	43.H	2.972003	4.884003	-0.200985
44.C	-1.408034	3.122963	2.139345	44.C	-1.440757	3.200105	2.126450
45.H	-1.314631	2.191961	2.709015	45.H	-1.338423	2.285372	2.721926
46.H	-2.255875	3.665815	2.579910	46.H	-2.306441	3.738800	2.541471
47.C	1.734058	-3.917418	-1.467926	47.C	1.679308	-3.908275	-1.506242
48.C	2.566194	-4.437071	-2.450956	48.C	2.480620	-4.420927	-2.516000
49.H	3.560005	-4.793850	-2.193424	49.H	3.481127	-4.784456	-2.293936
50.C	2.096639	-4.498421	-3.756719	50.C	1.970525	-4.478601	-3.806019
51.H	2.721636	-4.900315	-4.550949	51.H	2.569044	-4.880324	-4.620737
52.C	0.817074	-4.040215	-4.030799	52.C	0.683052	-4.023400	-4.035408
53.H	0.417745	-4.081363	-5.041034	53.H	0.251651	-4.067658	-5.032435
54.C	0.031428	-3.517020	-3.001746	54.C	-0.069748	-3.503259	-2.981131
55.C	-1.344858	-3.005153	-3.275757	55.C	-1.454921	-2.992187	-3.212978
56.H	-2.058004	-3.370470	-2.531965	56.H	-2.129140	-3.299214	-2.409624
57.H	-1.684623	-3.310751	-4.267100	57.H	-1.855433	-3.359877	-4.159911
58.H	-1.366070	-1.910255	-3.236093	58.H	-1.462979	-1.896731	-3.252694
59.C	2.145168	-3.934008	-0.017694	59.C	2.130206	-3.951257	-0.067477
60.H	1.704951	-4.834798	0.427519	60.H	1.702490	-4.861248	0.372590
61.H	3.234267	-4.043583	0.070835	61.H	3.223016	-4.061500	-0.010905
62.C	0.135298	-3.907397	2.344520	62.C	0.186662	-4.019009	2.325722
63.C	-0.012087	-4.729279	3.455030	63.C	0.092131	-4.912735	3.382630
64.H	0.812524	-4.857950	4.151303	64.H	0.941130	-5.075217	4.042469
65.C	-1.227274	-5.369379	3.656155	65.C	-1.104559	-5.587408	3.582794
66.H	-1.376328	-6.012879	4.520068	66.H	-1.212159	-6.290773	4.405468
67.C	-2.246871	-5.180534	2.734239	67.C	-2.156903	-5.354597	2.712785
68.H	-3.208246	-5.671684	2.861392	68.H	-3.104691	-5.871808	2.841156
69.C	-2.035160	-4.360991	1.626263	69.C	-1.997701	-4.460158	1.654464
70.C	-3.092987	-4.171338	0.589960	70.C	-3.099642	-4.231603	0.671785
71.H	-3.166677	-3.123347	0.285613	71.H	-3.104889	-3.198029	0.314666
72.H	-4.067502	-4.501005	0.955133	72.H	-4.074962	-4.458701	1.108182
73.H	-2.856320	-4.757246	-0.306268	73.H	-2.972003	-4.884003	-0.200985
74.C	1.408034	-3.122963	2.139345	74.C	1.440757	-3.200105	2.126450
75.H	1.314631	-2.191961	2.709015	75.H	1.338423	-2.285372	2.721926
76.H	2.255875	-3.665815	2.579910	76.H	2.306441	-3.738800	2.541471
77.N	-1.648484	2.778952	0.738444	77.N	-1.655754	2.814102	0.732213
78.N	1.648484	-2.778952	0.738444	78.N	1.655754	-2.814102	0.732213
79.N	-0.497493	3.456270	-1.736320	79.N	-0.435279	3.445111	-1.731239

80.N	0.854103	3.728346	1.446965	80.N	0.834666	3.797354	1.473825
81.N	0.497493	-3.456270	-1.736320	81.N	0.435279	-3.445111	-1.731239
82.N	-0.854103	-3.728346	1.446965	82.N	-0.834666	-3.797354	1.473825
$[Cu^{I}_2(\mathbf{L^3SSL^3})]^{2+}$ in MeCN Conformation **C**, symmetry C_2				$[Cu^{I}_2(\mathbf{L^3SSL^3})]^{2+}$ in the gas phase Conformation **C**, symmetry C_2			
1.Cu	-0.042477	-2.532271	-0.007770	1.Cu	-0.038115	-2.672641	-0.077680
2.Cu	0.042477	2.532271	-0.007770	2.Cu	0.038115	2.672641	-0.077680
3.S	0.495422	-0.950635	1.397818	3.S	0.417499	-1.006038	1.271605
4.S	-0.495422	0.950635	1.397818	4.S	-0.417499	1.006038	1.271605
5.N	-1.316398	-2.982143	-1.467206	5.N	-1.203340	-3.249665	-1.596886
6.N	1.171696	-4.034623	0.611990	6.N	1.104901	-4.125704	0.757376
7.N	-1.515453	-3.423929	1.298410	7.N	-1.628387	-3.455334	1.172642
8.N	1.316398	2.982143	-1.467206	8.N	1.203340	3.249665	-1.596886
9.N	-1.171696	4.034623	0.611990	9.N	-1.104901	4.125704	0.757376
10.N	1.515453	3.423929	1.298410	10.N	1.628387	3.455334	1.172642
11.C	-1.094962	-2.917785	-2.798505	11.C	-0.871573	-3.326187	-2.903707
12.C	-2.006051	-3.461313	-3.704166	12.C	-1.707521	-3.963525	-3.820121
13.C	-3.149535	-4.090101	-3.235300	13.C	-2.891302	-4.538994	-3.388293
14.C	-3.374079	-4.142453	-1.865812	14.C	-3.230720	-4.445642	-2.045376
15.C	-2.444485	-3.566392	-1.010119	15.C	-2.370771	-3.783269	-1.181542
16.H	1.978875	3.034447	3.340676	16.H	2.226526	2.944134	3.153439
17.C	-2.720374	-3.491999	0.475415	17.C	-2.766191	-3.547637	0.260597
18.C	2.497824	-4.178479	0.392215	18.C	2.440622	-4.299085	0.664019
19.C	3.218551	-5.194178	1.017731	19.C	3.084210	-5.296747	1.395355
20.C	2.570403	-6.064363	1.883000	20.C	2.349491	-6.115963	2.236475
21.C	1.210661	-5.903950	2.104862	21.C	0.978445	-5.924693	2.329853
22.C	0.540118	-4.878575	1.446940	22.C	0.388573	-4.923169	1.570493
23.H	3.296239	2.575024	0.642110	23.H	3.298652	2.589854	0.291466
24.C	-0.959589	-4.742390	1.605177	24.C	-1.118821	-4.765828	1.579862
25.C	-1.617228	-2.511916	2.441415	25.C	-1.791060	-2.479908	2.252390
26.C	-0.307040	-1.825087	2.787686	26.C	-0.493804	-1.789707	2.649837
27.C	1.094962	2.917785	-2.798505	27.C	0.871573	3.326187	-2.903707
28.C	2.006051	3.461313	-3.704166	28.C	1.707521	3.963525	-3.820121
29.C	3.149535	4.090101	-3.235300	29.C	2.891302	4.538994	-3.388293
30.C	3.374079	4.142453	-1.865812	30.C	3.230720	4.445642	-2.045376
31.C	2.444485	3.566392	-1.010119	31.C	2.370771	3.783269	-1.181542
32.C	-3.158371	3.227128	-0.549951	32.C	-3.210998	3.415525	-0.262965
33.C	2.720374	3.491999	0.475415	33.C	2.766191	3.547637	0.260597
34.C	-2.497824	4.178479	0.392215	34.C	-2.440622	4.299085	0.664019
35.C	-3.218551	5.194178	1.017731	35.C	-3.084210	5.296747	1.395355
36.C	-2.570403	6.064363	1.883000	36.C	-2.349491	6.115963	2.236475
37.C	-1.210661	5.903950	2.104862	37.C	-0.978445	5.924693	2.329853
38.C	-0.540118	4.878575	1.446940	38.C	-0.388573	4.923169	1.570493
39.H	-4.284459	5.290540	0.828043	39.H	-4.160645	5.420722	1.303895
40.C	0.959589	4.742390	1.605177	40.C	1.118821	4.765828	1.579862
41.C	1.617228	2.511916	2.441415	41.C	1.791060	2.479908	2.252390
42.C	0.307040	1.825087	2.787686	42.C	0.493804	1.789707	2.649837
43.C	0.162937	-2.264671	-3.269048	43.C	0.425318	-2.720811	-3.333180
44.H	-1.806834	-3.394547	-4.770915	44.H	-1.419076	-4.012711	-4.867347
45.H	-3.860780	-4.532219	-3.929120	45.H	-3.544762	-5.053138	-4.089685
46.H	-4.264164	-4.617501	-1.461489	46.H	-4.157426	-4.876116	-1.673312
47.H	1.248564	5.071201	2.612480	47.H	1.508317	5.055922	2.566777
48.H	1.407086	5.466070	0.913570	48.H	1.507752	5.507516	0.870703
49.H	-3.378653	-4.318467	0.770503	49.H	-3.492657	-4.310265	0.574855
50.H	-3.296239	-2.575024	0.642110	50.H	-3.298652	-2.589854	0.291466
51.C	3.158371	-3.227128	-0.549951	51.C	3.210998	-3.415525	-0.262965

52.H	4.284459	-5.290540	0.828043	52.H	4.160645	-5.420722	1.303895
53.H	3.122139	-6.855696	2.385253	53.H	2.840038	-6.893115	2.818488
54.H	0.670846	-6.564237	2.778821	54.H	0.371785	-6.549408	2.981421
55.H	2.358674	1.747005	2.197430	55.H	2.498954	1.717888	1.914301
56.H	0.453530	1.123263	3.614161	56.H	0.694042	1.036200	3.418999
57.H	-1.248564	-5.071201	2.612480	57.H	-1.508317	-5.055922	2.566777
58.H	-1.407086	-5.466070	0.913570	58.H	-1.507752	-5.507516	0.870703
59.H	-2.358674	-1.747005	2.197430	59.H	-2.498954	-1.717888	1.914301
60.H	-1.978875	-3.034447	3.340676	60.H	-2.226526	-2.944134	3.153439
61.H	-0.453530	-1.123263	3.614161	61.H	-0.694042	-1.036200	3.418999
62.H	3.378653	4.318467	0.770503	62.H	3.492657	4.310265	0.574855
63.C	-0.162937	2.264671	-3.269048	63.C	-0.425318	2.720811	-3.333180
64.H	1.806834	3.394547	-4.770915	64.H	1.419076	4.012711	-4.867347
65.H	3.860780	4.532219	-3.929120	65.H	3.544762	5.053138	-4.089685
66.H	4.264164	4.617501	-1.461489	66.H	4.157426	4.876116	-1.673312
67.H	-3.122139	6.855696	2.385253	67.H	-2.840038	6.893115	2.818488
68.H	-0.670846	6.564237	2.778821	68.H	-0.371785	6.549408	2.981421
69.H	0.461875	-2.537187	3.110184	69.H	0.231285	-2.494554	3.073809
70.H	-0.461875	2.537187	3.110184	70.H	-0.231285	2.494554	3.073809
71.H	-2.882500	2.192732	-0.324205	71.H	-2.722539	2.446569	-0.389724
72.H	-2.849064	3.432181	-1.580713	72.H	-3.296765	3.884009	-1.251089
73.H	-4.245028	3.317099	-0.502025	73.H	-4.227327	3.251576	0.103716
74.H	0.973756	-2.999501	-3.336856	74.H	1.255274	-3.408705	-3.133040
75.H	0.482027	-1.479652	-2.578040	75.H	0.624129	-1.789747	-2.793109
76.H	0.034154	-1.833199	-4.264654	76.H	0.427683	-2.511527	-4.405322
77.H	2.882500	-2.192732	-0.324205	77.H	2.722539	-2.446569	-0.389724
78.H	2.849064	-3.432181	-1.580713	78.H	3.296765	-3.884009	-1.251089
79.H	4.245028	-3.317099	-0.502025	79.H	4.227327	-3.251576	0.103716
80.H	-0.034154	1.833199	-4.264654	80.H	-0.427683	2.511527	-4.405322
81.H	-0.973756	2.999501	-3.336856	81.H	-1.255274	3.408705	-3.133040
82.H	-0.482027	1.479652	-2.578040	82.H	-0.624129	1.789747	-2.793109

Table S11: Cartesian coordinates (Å) of complexes with ligand **L^{4}SSL^4** in **A**, **B** or **C** conformation and with the ethylene groups arranged in three different ways (**a**, **b** & **c**, Figure S12), computed at ZORA-OPBE/TZ2P in the gas phase and/or solvated in MeCN (COSMO).

$[Cu^{II}_2(\mathbf{L^4S})_2]^{2+}$ in MeCN Conformation **A** (**a**), symmetry C_2				$[Cu^{II}_2(\mathbf{L^4S})_2]^{2+}$ in the gas phase Conformation **A** (**a**), symmetry C_2			
1.Cu	-0.045600	1.625360	0.306325	1.Cu	-0.071008	1.667516	0.269783
2.Cu	0.045600	-1.625360	0.306325	2.Cu	0.071008	-1.667516	0.269783
3.S	1.444446	0.072955	1.029555	3.S	1.434569	0.096279	0.913066
4.S	-1.444446	-0.072955	1.029555	4.S	-1.434569	-0.096279	0.913066
5.N	0.168074	3.176729	1.921727	5.N	0.191514	3.145546	1.916375
6.N	-1.272288	2.669413	-0.920523	6.N	-1.301270	2.766805	-0.914469
7.N	1.676766	2.780170	-0.420741	7.N	1.671377	2.859110	-0.458219
8.N	-0.168074	-3.176729	1.921727	8.N	-0.191514	-3.145546	1.916375
9.N	1.272288	-2.669413	-0.920523	9.N	1.301270	-2.766805	-0.914469
10.N	-1.676766	-2.780170	-0.420741	10.N	-1.671377	-2.859110	-0.458219
11.C	-0.325809	3.173341	3.164408	11.C	-0.287936	3.088242	3.163639
12.C	0.024636	4.116798	4.120401	12.C	0.060869	3.997579	4.151633
13.C	0.942757	5.100590	3.769616	13.C	0.963049	5.004658	3.832165
14.C	1.468009	5.103780	2.483399	14.C	1.477063	5.061894	2.543106
15.C	1.049796	4.125923	1.582912	15.C	1.061167	4.116317	1.609902
16.H	0.382525	1.197375	-2.346381	16.H	0.339487	1.341016	-2.402544

17.C	-2.423727	3.213439	-0.499267	17.C	-2.442855	3.308361	-0.463911
18.C	-3.206178	4.023485	-1.305326	18.C	-3.227247	4.152983	-1.231658
19.C	-2.772750	4.284828	-2.600545	19.C	-2.808183	4.455007	-2.521658
20.C	-1.579956	3.724026	-3.037665	20.C	-1.624815	3.899570	-2.990044
21.C	-0.843750	2.912637	-2.175229	21.C	-0.886006	3.053612	-2.164751
22.C	-1.694331	-2.835074	-1.904919	22.C	-1.660086	-2.967945	-1.936549
23.C	2.902688	2.140466	0.109513	23.C	2.893151	2.187114	0.035951
24.C	2.849659	0.631567	0.024404	24.C	2.826559	0.679149	-0.097038
25.C	0.325809	-3.173341	3.164408	25.C	0.287936	-3.088242	3.163639
26.C	-0.024636	-4.116798	4.120401	26.C	-0.060869	-3.997579	4.151633
27.C	-0.942757	-5.100590	3.769616	27.C	-0.963049	-5.004658	3.832165
28.C	-1.468009	-5.103780	2.483399	28.C	-1.477063	-5.061894	2.543106
29.C	-1.049796	-4.125923	1.582912	29.C	-1.061167	-4.116317	1.609902
30.H	-3.002702	-2.430716	1.160012	30.H	-3.003688	-2.438313	1.095944
31.C	2.423727	-3.213439	-0.499267	31.C	2.442855	-3.308361	-0.463911
32.C	3.206178	-4.023485	-1.305326	32.C	3.227247	-4.152983	-1.231658
33.C	2.772750	-4.284828	-2.600545	33.C	2.808183	-4.455007	-2.521658
34.C	1.579956	-3.724026	-3.037665	34.C	1.624815	-3.899570	-2.990044
35.C	0.843750	-2.912637	-2.175229	35.C	0.886006	-3.053612	-2.164751
36.H	-0.769952	-4.660933	-0.444145	36.H	-0.762316	-4.737207	-0.392655
37.C	-2.902688	-2.140466	0.109513	37.C	-2.893151	-2.187114	0.035951
38.C	-2.849659	-0.631567	0.024404	38.C	-2.826559	-0.679149	-0.097038
39.H	-1.032384	2.379821	3.399572	39.H	-0.980867	2.275748	3.375131
40.H	-0.408423	4.073229	5.116582	40.H	-0.361928	3.911403	5.149713
41.H	1.252753	5.853861	4.490826	41.H	1.269805	5.734151	4.579082
42.H	2.192802	5.855402	2.179508	42.H	2.190454	5.835104	2.265313
43.H	-0.583479	-2.354211	-3.657344	43.H	-0.516628	-2.534128	-3.686013
44.H	-3.785973	-2.523265	-0.423136	44.H	-3.780903	-2.578875	-0.487025
45.H	-2.721237	2.983877	0.519760	45.H	-2.729198	3.048880	0.551751
46.H	-4.133456	4.436816	-0.918383	46.H	-4.146012	4.563822	-0.820579
47.H	-3.358038	4.916714	-3.264858	47.H	-3.395638	5.114828	-3.157133
48.H	-1.216381	3.905081	-4.045967	48.H	-1.273370	4.115521	-3.996577
49.H	1.858764	3.868292	-2.227816	49.H	1.812944	4.013368	-2.229845
50.H	2.452669	4.698484	0.061216	50.H	2.451116	4.757885	0.102253
51.H	3.785973	2.523265	-0.423136	51.H	3.780903	2.578875	-0.487025
52.H	3.002702	2.430716	1.160012	52.H	3.003688	2.438313	1.095944
53.H	3.767550	0.209246	0.446278	53.H	3.749238	0.238867	0.298229
54.H	2.753519	0.271835	-1.004380	54.H	2.719187	0.349571	-1.135548
55.H	1.032384	-2.379821	3.399572	55.H	0.980867	-2.275748	3.375131
56.H	0.408423	-4.073229	5.116582	56.H	0.361928	-3.911403	5.149713
57.H	-1.252753	-5.853861	4.490826	57.H	-1.269805	-5.734151	4.579082
58.H	-2.192802	-5.855402	2.179508	58.H	-2.190454	-5.835104	2.265313
59.H	-3.767550	-0.209246	0.446278	59.H	-3.749238	-0.238867	0.298229
60.H	-2.753519	-0.271835	-1.004380	60.H	-2.719187	-0.349571	-1.135548
61.H	2.721237	-2.983877	0.519760	61.H	2.729198	-3.048880	0.551751
62.H	4.133456	-4.436816	-0.918383	62.H	4.146012	-4.563822	-0.820579
63.H	3.358038	-4.916714	-3.264858	63.H	3.395638	-5.114828	-3.157133
64.H	1.216381	-3.905081	-4.045967	64.H	1.273370	-4.115521	-3.996577
65.H	0.769952	4.660933	-0.444145	65.H	0.762316	4.737207	-0.392655
66.H	-2.452669	-4.698484	0.061216	66.H	-2.451116	-4.757885	0.102253
67.C	1.519060	4.128358	0.151746	67.C	1.517710	4.181059	0.174231
68.C	-1.519060	-4.128358	0.151746	68.C	-1.517710	-4.181059	0.174231
69.H	-0.382525	-1.197375	-2.346381	69.H	-0.339487	-1.341016	-2.402544
70.H	0.583479	2.354211	-3.657344	70.H	0.516628	2.534128	-3.686013
71.H	2.548702	2.257191	-2.265104	71.H	2.512954	2.411711	-2.337383
72.C	1.694331	2.835074	-1.904919	72.C	1.660086	2.967945	-1.936549

73.C	-0.445235	-2.268020	-2.576029	73.C	-0.398046	-2.418199	-2.603667
74.C	0.445235	2.268020	-2.576029	74.C	0.398046	2.418199	-2.603667
75.H	-2.548702	-2.257191	-2.265104	75.H	-2.512954	-2.411711	-2.337383
76.H	-1.858764	-3.868292	-2.227816	76.H	-1.812944	-4.013368	-2.229845
$[Cu^{II}_2(\mathbf{L^4S})_2]^{2+}$ in MeCN Conformation **A** (**b**), symmetry C_2				$[Cu^{II}_2(\mathbf{L^4S})_2]^{2+}$ in MeCN Conformation **A** (**c**), no symmetry			
1.Cu	0.015000	1.723157	0.032934	1.Cu	0.127756	1.743415	0.314265
2.Cu	-0.015000	-1.723157	0.032934	2.Cu	-0.028743	-1.582250	0.089885
3.S	1.493345	0.021989	0.366686	3.S	1.581448	0.010855	0.594719
4.S	-1.493345	-0.021989	0.366686	4.S	-1.322000	0.045948	0.970244
5.N	-0.065722	2.946315	1.911081	5.N	0.108749	3.070893	2.154813
6.N	-1.066492	2.964640	-1.162140	6.N	-0.971720	2.897404	-0.946538
7.N	1.666487	2.822856	-0.804439	7.N	1.762380	2.822053	-0.576144
8.N	0.065722	-2.946315	1.911081	8.N	-0.258156	-3.160763	1.658302
9.N	1.066492	-2.964640	-1.162140	9.N	1.010496	-2.701989	-1.245878
10.N	-1.666487	-2.822856	-0.804439	10.N	-1.887516	-2.568815	-0.549095
11.C	-0.587821	2.429032	3.032111	11.C	-0.344352	2.597428	3.323682
12.C	-0.691240	3.125063	4.226355	12.C	-0.434668	3.358275	4.479170
13.C	-0.221712	4.432702	4.263708	13.C	-0.031425	4.686989	4.421779
14.C	0.327362	4.976249	3.111124	14.C	0.449238	5.185283	3.218901
15.C	0.394098	4.211091	1.943450	15.C	0.511287	4.353447	2.097621
16.C	-0.979238	-4.804359	0.692172	16.H	-0.582485	-1.012390	-2.489090
17.C	-2.373135	3.249942	-1.075135	17.C	-2.281897	3.173423	-0.882906
18.C	-2.995868	4.154395	-1.920431	18.C	-2.914538	4.003135	-1.794837
19.C	-2.231146	4.791170	-2.892162	19.C	-2.156094	4.575109	-2.810601
20.C	-0.872811	4.513371	-2.970811	20.C	-0.793920	4.310683	-2.865449
21.C	-0.319617	3.594787	-2.083994	21.C	-0.231207	3.467608	-1.912246
22.C	1.131312	3.215660	-2.122195	22.C	-2.009461	-2.551228	-2.028810
23.C	2.833296	1.922286	-0.988314	23.C	2.955654	1.944645	-0.689936
24.C	2.431131	0.471052	-1.122896	24.C	2.599173	0.483833	-0.832235
25.C	0.587821	-2.429032	3.032111	25.C	0.325837	-3.244485	2.858757
26.C	0.691240	-3.125063	4.226355	26.C	-0.007073	-4.212172	3.796300
27.C	0.221712	-4.432702	4.263708	27.C	-1.002368	-5.128139	3.472513
28.C	-0.327362	-4.976249	3.111124	28.C	-1.621410	-5.039594	2.232013
29.C	-0.394098	-4.211091	1.943450	29.C	-1.217434	-4.041753	1.346813
30.H	-3.474804	-2.023139	-0.110805	30.H	-3.054935	-2.180125	1.142323
31.C	2.373135	-3.249942	-1.075135	31.C	2.118475	-3.384088	-0.920265
32.C	2.995868	-4.154395	-1.920431	32.C	2.751757	-4.244288	-1.801888
33.C	2.231146	-4.791170	-2.892162	33.C	2.211907	-4.404658	-3.073438
34.C	0.872811	-4.513371	-2.970811	34.C	1.065607	-3.697950	-3.412714
35.C	0.319617	-3.594787	-2.083994	35.C	0.479620	-2.846948	-2.476217
36.C	-1.131312	-3.215660	-2.122195	36.H	-1.146815	-4.514429	-0.714291
37.C	-2.833296	-1.922286	-0.988314	37.C	-3.011869	-1.856937	0.097738
38.C	-2.431131	-0.471052	-1.122896	38.C	-2.840761	-0.354866	0.058468
39.H	-0.948903	1.405522	2.964666	39.H	-0.656322	1.555837	3.327953
40.H	-1.128594	2.649131	5.100383	40.H	-0.812607	2.914539	5.396890
41.H	-0.278649	5.020606	5.177603	41.H	-0.084108	5.325330	5.301513
42.H	0.708486	5.994698	3.109310	42.H	0.781093	6.217936	3.141760
43.C	0.979238	4.804359	0.692172	43.C	1.038923	4.883587	0.794424
44.H	-3.424912	-2.237070	-1.858269	44.H	-3.962198	-2.144864	-0.375644
45.H	-2.928425	2.735213	-0.296510	45.H	-2.832347	2.716005	-0.066903
46.H	-4.058347	4.353978	-1.811316	46.H	-3.979733	4.196362	-1.702083
47.H	-2.684394	5.507590	-3.573311	47.H	-2.617047	5.232041	-3.544433
48.H	-0.242109	5.008008	-3.704920	48.H	-0.167674	4.757787	-3.633024
49.H	1.730266	4.022378	-2.564557	49.H	0.208916	5.054541	0.100891
50.H	1.227564	2.352523	-2.791675	50.H	2.847432	3.759761	0.934332

51.H	3.424912	2.237070	-1.858269	51.H	3.586455	2.268014	-1.529483
52.H	3.474804	2.023139	-0.110805	52.H	3.542628	2.069483	0.222275
53.H	3.332057	-0.146716	-1.185708	53.H	3.517304	-0.112320	-0.828138
54.H	1.829318	0.281203	-2.017536	54.H	2.065708	0.267057	-1.762603
55.H	0.948903	-1.405522	2.964666	55.H	1.093888	-2.504001	3.073875
56.H	1.128594	-2.649131	5.100383	56.H	0.499908	-4.240219	4.757495
57.H	0.278649	-5.020606	5.177603	57.H	-1.299713	-5.898972	4.180288
58.H	-0.708486	-5.994698	3.109310	58.H	-2.408562	-5.735480	1.951314
59.H	-3.332057	0.146716	-1.185708	59.H	-3.687451	0.123256	0.561244
60.H	-1.829318	-0.281203	-2.017536	60.H	-2.791066	0.030685	-0.964032
61.H	2.928425	-2.735213	-0.296510	61.H	2.505195	-3.227333	0.082447
62.H	4.058347	-4.353978	-1.811316	62.H	3.648600	-4.772689	-1.490676
63.H	2.684394	-5.507590	-3.573311	63.H	2.679936	-5.070904	-3.794812
64.H	0.242109	-5.008008	-3.704920	64.H	0.621553	-3.797033	-4.399861
65.H	-1.730266	-4.022378	-2.564557	65.H	2.705575	4.705652	-0.542919
66.H	-1.227564	-2.352523	-2.791675	66.H	-2.780226	-4.437425	-0.071277
67.C	2.076422	3.993479	0.011914	67.C	2.147777	4.059609	0.150085
68.C	-2.076422	-3.993479	0.011914	68.C	-1.798221	-3.947322	-0.040301
69.H	-1.432968	-5.763428	0.958445	69.H	-2.284935	-3.550371	-2.382806
70.H	-0.173762	-5.054897	-0.006499	70.H	-2.832935	-1.887944	-2.303860
71.H	1.432968	5.763428	0.958445	71.H	1.464541	5.873716	0.981409
72.H	0.173762	5.054897	-0.006499	72.H	-0.975593	-2.079999	-3.832550
73.H	2.750930	3.618198	0.785582	73.C	-0.760914	-2.060917	-2.760612
74.H	2.664860	4.670776	-0.623900	74.C	1.225179	3.108399	-1.920513
75.H	-2.750930	-3.618198	0.785582	75.H	1.812682	3.890129	-2.418996
76.H	-2.664860	-4.670776	-0.623900	76.H	1.338464	2.201296	-2.525702
$[Cu^{I}_2(\mathbf{L^4SSL^4})]^{2+}$ in MeCN Conformation **B** (**a**), symmetry C_2				$[Cu^{I}_2(\mathbf{L^4SSL^4})]^{2+}$ in the gas phase Conformation **B** (**a**), symmetry C_2			
1.Cu	0.150926	-2.580859	0.289153	1.Cu	0.150833	-2.600128	0.238659
2.Cu	-0.150926	2.580859	0.289153	2.Cu	-0.150833	2.600128	0.238659
3.S	-0.861498	0.581719	0.727586	3.S	-0.853715	0.594832	0.645670
4.S	0.861498	-0.581719	0.727586	4.S	0.853715	-0.594832	0.645670
5.C	-2.668960	-1.390362	-0.230670	5.C	-2.689037	-1.404043	-0.209334
6.H	-2.996401	-1.321874	0.809788	6.H	-2.981095	-1.294225	0.838920
7.H	-3.582646	-1.421592	-0.844271	7.H	-3.627694	-1.448659	-0.787298
8.C	-1.919875	-0.116552	-0.585595	8.C	-1.938889	-0.145683	-0.629486
9.H	-2.658721	0.681280	-0.727553	9.H	-2.675429	0.651277	-0.795415
10.H	-1.341192	-0.179746	-1.511467	10.H	-1.375459	-0.253166	-1.561246
11.C	2.668960	1.390362	-0.230670	11.C	2.689037	1.404043	-0.209334
12.H	2.996401	1.321874	0.809788	12.H	2.981095	1.294225	0.838920
13.H	3.582646	1.421592	-0.844271	13.H	3.627694	1.448659	-0.787298
14.C	1.919875	0.116552	-0.585595	14.C	1.938889	0.145683	-0.629486
15.H	2.658721	-0.681280	-0.727553	15.H	2.675429	-0.651277	-0.795415
16.H	1.341192	0.179746	-1.511467	16.H	1.375459	0.253166	-1.561246
17.C	-0.877277	-4.753271	1.947854	17.C	-0.777533	-4.796804	1.945044
18.C	-1.013724	-5.572540	3.070033	18.C	-0.789639	-5.673684	3.029609
19.H	-1.778610	-6.345201	3.077465	19.H	-1.537669	-6.461816	3.076004
20.C	-0.172995	-5.402118	4.161381	20.C	0.152951	-5.543575	4.039172
21.H	-0.270192	-6.040013	5.037421	21.H	0.153542	-6.227903	4.885266
22.C	0.792463	-4.402423	4.110171	22.C	1.090423	-4.522590	3.946948
23.H	1.477641	-4.226067	4.935202	23.H	1.849259	-4.373936	4.711038
24.C	0.867370	-3.619480	2.970370	24.C	1.040037	-3.683702	2.847611
25.H	1.606160	-2.825788	2.894115	25.H	1.754390	-2.870333	2.743584
26.N	-0.545183	3.549353	-1.416412	26.N	-0.446793	3.645858	-1.452303
27.N	0.545183	-3.549353	-1.416412	27.N	0.446793	-3.645858	-1.452303
28.N	-0.060063	3.780252	1.906401	28.N	-0.137949	3.808029	1.858324

29.C	-1.792037	-2.989856	-1.814595	29.C	-1.905321	-3.088761	-1.755852
30.H	-3.479949	-4.070571	-0.212736	30.H	-3.548994	-4.023745	0.027377
31.C	1.792037	2.989856	-1.814595	31.C	1.905321	3.088761	-1.755852
32.C	-0.532411	-3.720061	-2.202529	32.C	-0.670842	-3.852393	-2.169984
33.C	-0.475136	-4.478505	-3.369108	33.C	-0.684353	-4.679991	-3.288894
34.H	-1.366687	-4.605891	-3.978379	34.H	-1.607221	-4.834802	-3.844034
35.C	0.728603	-5.062984	-3.740186	35.C	0.490230	-5.305210	-3.685034
36.H	0.792837	-5.658605	-4.648044	36.H	0.499992	-5.957189	-4.556004
37.C	1.844531	-4.879057	-2.929886	37.C	1.646639	-5.091248	-2.943929
38.H	2.806791	-5.319367	-3.177285	38.H	2.587644	-5.566134	-3.210006
39.C	1.705921	-4.122093	-1.777933	39.C	1.576923	-4.262706	-1.836472
40.H	2.548330	-3.965223	-1.108939	40.H	2.454741	-4.085785	-1.219055
41.N	1.915224	2.653551	-0.385068	41.N	1.953444	2.678263	-0.341169
42.N	0.060063	-3.780252	1.906401	42.N	0.137949	-3.808029	1.858324
43.N	-1.915224	-2.653551	-0.385068	43.N	-1.953444	-2.678263	-0.341169
44.C	-1.705921	4.122093	-1.777933	44.C	-1.576923	4.262706	-1.836472
45.H	-2.806791	5.319367	-3.177285	45.H	-2.587644	5.566134	-3.210006
46.H	-2.548330	3.965223	-1.108939	46.H	-2.454741	4.085785	-1.219055
47.C	0.877277	4.753271	1.947854	47.C	0.777533	4.796804	1.945044
48.C	1.013724	5.572540	3.070033	48.C	0.789639	5.673684	3.029609
49.H	1.778610	6.345201	3.077465	49.H	1.537669	6.461816	3.076004
50.C	0.172995	5.402118	4.161381	50.C	-0.152951	5.543575	4.039172
51.H	0.270192	6.040013	5.037421	51.H	-0.153542	6.227903	4.885266
52.C	-0.792463	4.402423	4.110171	52.C	-1.090423	4.522590	3.946948
53.H	-1.477641	4.226067	4.935202	53.H	-1.849259	4.373936	4.711038
54.C	-0.867370	3.619480	2.970370	54.C	-1.040037	3.683702	2.847611
55.H	-1.606160	2.825788	2.894115	55.H	-1.754390	2.870333	2.743584
56.C	2.612888	3.721210	0.367514	56.C	2.610043	3.702160	0.506649
57.H	-2.461592	-5.752329	0.968760	57.H	-2.491391	-5.726031	1.126128
58.C	1.766999	4.935602	0.752934	58.C	1.782210	4.944491	0.835562
59.C	-0.728603	5.062984	-3.740186	59.C	-0.490230	5.305210	-3.685034
60.H	-0.792837	5.658605	-4.648044	60.H	-0.499992	5.957189	-4.556004
61.C	-1.844531	4.879057	-2.929886	61.C	-1.646639	5.091248	-2.943929
62.C	0.532411	3.720061	-2.202529	62.C	0.670842	3.852393	-2.169984
63.C	0.475136	4.478505	-3.369108	63.C	0.684353	4.679991	-3.288894
64.H	1.366687	4.605891	-3.978379	64.H	1.607221	4.834802	-3.844034
65.C	-1.766999	-4.935602	0.752934	65.C	-1.782210	-4.944491	0.835562
66.C	-2.612888	-3.721210	0.367514	66.C	-2.610043	-3.702160	0.506649
67.H	-2.670766	-3.549389	-2.164978	67.H	-2.805669	-3.659378	-2.029894
68.H	-1.789269	-2.053689	-2.384773	68.H	-1.930158	-2.181595	-2.372177
69.H	-1.165452	-5.274226	-0.098486	69.H	-1.280531	-5.329064	-0.060528
70.H	-3.008590	-3.272047	1.282744	70.H	-2.887883	-3.215240	1.446547
71.H	2.670766	3.549389	-2.164978	71.H	2.805669	3.659378	-2.029894
72.H	1.789269	2.053689	-2.384773	72.H	1.930158	2.181595	-2.372177
73.H	3.008590	3.272047	1.282744	73.H	2.887883	3.215240	1.446547
74.H	3.479949	4.070571	-0.212736	74.H	3.548994	4.023745	0.027377
75.H	1.165452	5.274226	-0.098486	75.H	1.280531	5.329064	-0.060528
76.H	2.461592	5.752329	0.968760	76.H	2.491391	5.726031	1.126128
$[Cu^{I}_2(\mathbf{L^4SSL^4})]^{2+}$ in MeCN Conformation **B** (**b**), symmetry C_2				$[Cu^{I}_2(\mathbf{L^4SSL^4})]^{2+}$ in MeCN Conformation **B** (**c**), no symmetry			
1.Cu	0.295256	2.516575	-0.396483	1.Cu	0.366341	2.550699	-0.226597
2.Cu	-0.295256	-2.516575	-0.396483	2.Cu	-0.303084	-2.524918	-0.386671
3.S	-0.900511	-0.538064	-1.007917	3.S	-0.811965	-0.478034	-0.867960
4.S	0.900511	0.538064	-1.007917	4.S	0.997257	0.556508	-0.756420
5.C	-2.655199	1.556831	-0.219172	5.C	-2.598343	1.571594	-0.049441
6.H	-3.192060	1.316555	-1.141194	6.H	-3.184572	1.328076	-0.940526

7.H	-3.432008	1.766290	0.527797	7.H	-3.334096	1.795610	0.733036
8.C	-1.911914	0.316096	0.248970	8.C	-1.846388	0.330177	0.400301
9.H	-2.661317	-0.437924	0.517496	9.H	-2.586450	-0.437262	0.657180
10.H	-1.285595	0.488291	1.128591	10.H	-1.224838	0.497542	1.284443
11.C	2.655199	-1.556831	-0.219172	11.C	2.582078	-1.601859	0.207841
12.H	3.192060	-1.316555	-1.141194	12.H	2.929290	-1.550611	-0.827300
13.H	3.432008	-1.766290	0.527797	13.H	3.481048	-1.720634	0.832870
14.C	1.911914	-0.316096	0.248970	14.C	1.939472	-0.272479	0.569856
15.H	2.661317	0.437924	0.517496	15.H	2.742727	0.450976	0.755165
16.H	1.285595	-0.488291	1.128591	16.H	1.325605	-0.304492	1.474496
17.C	-0.989028	4.244377	-2.257612	17.C	-0.915917	4.161752	-2.200524
18.C	-1.241875	5.288367	-3.143102	18.C	-1.167659	5.153412	-3.144525
19.H	-2.263418	5.519376	-3.435197	19.H	-2.186997	5.352621	-3.466328
20.C	-0.174654	6.022052	-3.646314	20.C	-0.102465	5.876146	-3.667208
21.H	-0.349660	6.840931	-4.340630	21.H	-0.276612	6.654410	-4.406924
22.C	1.115945	5.695270	-3.244099	22.C	1.185071	5.590783	-3.225550
23.H	1.981460	6.241075	-3.610519	23.H	2.049301	6.129733	-3.604979
24.C	1.283887	4.650563	-2.348055	24.C	1.351601	4.597678	-2.272471
25.H	2.275597	4.368335	-2.003150	25.H	2.341108	4.349309	-1.896470
26.N	-0.802570	-3.345306	1.363664	26.N	-0.835270	-3.449965	1.306815
27.N	0.802570	3.345306	1.363664	27.N	0.843242	3.479640	1.482275
28.N	-0.257844	-3.935436	-1.861763	28.N	-0.300033	-3.740444	-1.995606
29.C	-1.580883	3.466582	1.997608	29.C	-1.547306	3.606160	2.073826
30.C	2.093000	-3.800144	0.600766	30.H	-2.060695	2.404480	-2.344483
31.C	1.580883	-3.466582	1.997608	31.C	1.536813	-3.132155	1.760692
32.C	-0.121723	3.698764	2.282612	32.C	-0.100182	3.913778	2.346230
33.C	0.259617	4.262864	3.502214	33.C	0.253218	4.625690	3.494405
34.H	-0.505044	4.537364	4.224693	34.H	-0.526932	4.966320	4.170555
35.C	1.601291	4.474270	3.785407	35.C	1.587090	4.896444	3.765899
36.H	1.902398	4.912751	4.734373	36.H	1.866707	5.451274	4.658934
37.C	2.546910	4.123887	2.828009	37.C	2.552624	4.449452	2.870923
38.H	3.610716	4.274798	2.990567	38.H	3.611574	4.634780	3.030051
39.C	2.101244	3.569070	1.641016	39.C	2.134251	3.752461	1.750629
40.H	2.811327	3.285040	0.868427	40.H	2.860538	3.390072	1.027399
41.N	1.837293	-2.774948	-0.433746	41.N	1.719282	-2.795868	0.337399
42.N	0.257844	3.935436	-1.861763	42.N	0.327503	3.893616	-1.766316
43.N	-1.837293	2.774948	-0.433746	43.N	-1.781542	2.781587	-0.314554
44.C	-2.101244	-3.569070	1.641016	44.C	-2.054855	-3.908337	1.636615
45.H	-3.610716	-4.274798	2.990567	45.H	-3.300860	-4.999850	2.999976
46.H	-2.811327	-3.285040	0.868427	46.H	-2.861580	-3.666779	0.949143
47.C	0.989028	-4.244377	-2.257612	47.C	0.534687	-4.803116	-2.013290
48.C	1.241875	-5.288367	-3.143102	48.C	0.595772	-5.651085	-3.120701
49.H	2.263418	-5.519376	-3.435197	49.H	1.278390	-6.497249	-3.108862
50.C	0.174654	-6.022052	-3.646314	50.C	-0.215250	-5.414525	-4.222263
51.H	0.349660	-6.840931	-4.340630	51.H	-0.177084	-6.073791	-5.086900
52.C	-1.115945	-5.695270	-3.244099	52.C	-1.073383	-4.320311	-4.196631
53.H	-1.981460	-6.241075	-3.610519	53.H	-1.729711	-4.088423	-5.031291
54.C	-1.283887	-4.650563	-2.348055	54.C	-1.077533	-3.515444	-3.069798
55.H	-2.275597	-4.368335	-2.003150	55.H	-1.732112	-2.649454	-3.013169
56.C	2.092655	-3.345989	-1.764813	56.C	2.332749	-3.913913	-0.414545
57.C	-2.093000	3.800144	0.600766	57.C	-2.064663	3.857023	0.660229
58.H	-3.054399	3.876035	-1.801361	58.C	1.392479	-5.054071	-0.807299
59.C	-1.601291	-4.474270	3.785407	59.C	-1.222427	-4.949955	3.615116
60.H	-1.902398	-4.912751	4.734373	60.H	-1.366969	-5.540461	4.517032
61.C	-2.546910	-4.123887	2.828009	61.C	-2.294540	-4.654038	2.779185
62.C	0.121723	-3.698764	2.282612	62.C	0.200476	-3.730324	2.117058

63.C	-0.259617	-4.262864	3.502214	63.C	0.041059	-4.483331	3.277662
64.H	0.505044	-4.537364	4.224693	64.H	0.900882	-4.699710	3.907088
65.H	-2.163413	2.514297	-2.475514	65.H	-2.984472	3.787494	-1.765891
66.C	-2.092655	3.345989	-1.764813	66.C	-2.016023	3.275114	-1.679854
67.H	-2.151380	4.081237	2.699911	67.H	-2.146160	4.222627	2.750039
68.H	-1.837603	2.433305	2.263193	68.H	-1.754578	2.572151	2.377743
69.H	1.629297	-4.732283	0.260062	69.H	2.017846	-5.927459	-1.012471
70.H	3.176741	-3.986574	0.665263	70.H	0.754631	-5.338217	0.037783
71.H	2.151380	-4.081237	2.699911	71.H	2.345565	-3.784809	2.118314
72.H	1.837603	-2.433305	2.263193	72.H	1.622271	-2.207332	2.342717
73.H	2.163413	-2.514297	-2.475514	73.H	2.769429	-3.495579	-1.325735
74.H	3.054399	-3.876035	-1.801361	74.H	3.165228	-4.334287	0.169487
75.H	-1.629297	4.732283	0.260062	75.H	-1.619556	4.779140	0.271283
76.H	-3.176741	3.986574	0.665263	76.H	-3.152104	4.024242	0.711864
$[Cu^{I}_{2}(\mathbf{L^{4}SSL^{4}})]^{2+}$ in MeCN Conformation **C** (**a**), no symmetry				$[Cu^{I}_{2}(\mathbf{L^{4}SSL^{4}})]^{2+}$ in the gas phase Conformation **C** (**a**), no symmetry			
1.Cu	5.213218	8.438129	4.991487	1.Cu	5.208823	8.428198	5.189108
2.Cu	5.439095	8.791730	0.208072	2.Cu	5.478185	8.867347	0.028537
3.S	3.697451	8.708589	3.350244	3.S	3.820785	8.697309	3.434347
4.S	4.090295	7.713992	1.518939	4.S	4.130927	7.922350	1.443311
5.C	3.091346	6.460972	4.930036	5.C	3.227254	6.333713	4.852261
6.H	2.277193	5.865772	5.374444	6.H	2.417725	5.663383	5.190461
7.H	3.618782	5.808438	4.226864	7.H	3.854857	5.759192	4.162842
8.C	2.483434	7.617203	4.162298	8.C	2.612970	7.496010	4.094066
9.H	1.924138	8.302507	4.809542	9.H	1.948007	8.100319	4.722036
10.H	1.776636	7.249744	3.412893	10.H	2.003972	7.117842	3.266923
11.C	2.620628	9.406604	-0.189007	11.C	2.721558	9.804647	-0.126790
12.H	1.706272	9.490469	-0.797843	12.H	1.764999	10.011918	-0.637648
13.H	2.579080	10.206350	0.555121	13.H	2.854102	10.591255	0.621840
14.C	2.602070	8.068895	0.523548	14.C	2.611108	8.467745	0.584601
15.H	2.576235	7.224886	-0.176402	15.H	2.404315	7.646013	-0.111946
16.H	1.714709	7.981396	1.156724	16.H	1.782527	8.491725	1.299291
17.C	6.229949	5.847927	5.345806	17.C	6.392713	5.901657	5.613270
18.C	6.966189	4.689254	5.117353	18.C	7.270818	4.827780	5.504790
19.H	6.633758	3.745274	5.542350	19.H	6.974954	3.844057	5.863236
20.C	8.122232	4.755838	4.350177	20.C	8.527910	5.029081	4.952469
21.H	8.708921	3.859904	4.160121	21.H	9.230978	4.203010	4.868157
22.C	8.513595	5.986435	3.832445	22.C	8.871209	6.304633	4.518594
23.H	9.415026	6.090374	3.234113	23.H	9.850079	6.514652	4.094636
24.C	7.724121	7.094374	4.092882	24.C	7.937482	7.319442	4.642801
25.H	7.994909	8.075260	3.710592	25.H	8.166423	8.331262	4.315421
26.C	5.028585	5.843431	6.257225	26.C	5.069222	5.746372	6.325786
27.H	4.564678	4.848207	6.270104	27.H	4.678695	4.728999	6.182031
28.H	5.403884	6.011776	7.273181	28.H	5.279322	5.829571	7.398897
29.C	4.427751	9.803634	7.401613	29.C	4.165376	9.619368	7.599286
30.C	4.006738	10.895177	8.163650	30.C	3.676712	10.642280	8.411796
31.H	3.559434	10.722026	9.139250	31.H	3.195092	10.394035	9.354693
32.C	4.169947	12.188000	7.684546	32.C	3.818683	11.968190	8.028592
33.H	3.848754	13.041219	8.278152	33.H	3.447139	12.769367	8.664249
34.C	4.757317	12.367436	6.436423	34.C	4.451683	12.247485	6.823848
35.H	4.919392	13.356687	6.016600	35.H	4.601200	13.268213	6.481110
36.C	5.140014	11.244907	5.724164	36.C	4.898734	11.187808	6.055651
37.H	5.600630	11.342546	4.743944	37.H	5.394989	11.366005	5.104517
38.C	4.308180	8.406918	7.941377	38.C	4.074684	8.186223	8.048372
39.H	3.909449	8.469748	8.957438	39.H	3.592631	8.170116	9.030513
40.H	5.317487	7.986305	8.041848	40.H	5.094044	7.812943	8.216310

41.C	3.420930	7.429272	7.164808	41.C	3.307257	7.211903	7.149174
42.H	3.135401	6.608317	7.838467	42.H	2.992062	6.346567	7.753006
43.H	2.493976	7.931883	6.875707	43.H	2.389062	7.693099	6.800477
44.C	5.052033	8.026574	-2.522056	44.C	4.734243	8.126549	-2.642603
45.C	5.301821	7.528009	-3.799259	45.C	4.802470	7.585719	-3.923901
46.H	4.622573	7.763751	-4.615177	46.H	4.096898	7.904230	-4.688630
47.C	6.415555	6.727943	-4.012560	47.C	5.770266	6.634551	-4.211196
48.H	6.625267	6.329795	-5.002975	48.H	5.837874	6.200348	-5.206515
49.C	7.255660	6.445238	-2.940005	49.C	6.647586	6.247325	-3.204713
50.H	8.137488	5.820547	-3.055214	50.H	7.418681	5.501160	-3.378870
51.C	6.948403	6.988363	-1.703822	51.C	6.524888	6.841436	-1.960792
52.H	7.582118	6.795353	-0.841878	52.H	7.194244	6.567168	-1.148620
53.C	3.791914	8.813989	-2.243239	53.C	3.619083	9.084871	-2.280420
54.H	3.555586	9.446173	-3.107479	54.H	3.411329	9.742728	-3.134106
55.H	2.972905	8.087687	-2.185210	55.H	2.709251	8.484112	-2.157255
56.C	6.199382	11.573726	0.165907	56.C	6.559743	11.542657	-0.198180
57.C	7.066038	12.667810	0.147198	57.C	7.541356	12.516652	-0.378713
58.H	6.669847	13.658993	-0.059033	58.H	7.247890	13.544513	-0.579166
59.C	8.420304	12.489493	0.395807	59.C	8.884229	12.175635	-0.300782
60.H	9.099276	13.339408	0.386007	60.H	9.654866	12.930847	-0.441540
61.C	8.887684	11.206073	0.657391	61.C	9.220507	10.853210	-0.039178
62.H	9.936698	11.008587	0.861239	62.H	10.256607	10.532345	0.034670
63.C	7.976927	10.163859	0.651976	63.C	8.197390	9.935549	0.121612
64.H	8.306411	9.145948	0.846073	64.H	8.422267	8.890500	0.323912
65.C	4.727137	11.759076	-0.063022	65.C	5.101595	11.905601	-0.248074
66.H	4.537445	12.826105	-0.207905	66.H	5.023621	12.988536	-0.384833
67.H	4.193010	11.483951	0.855996	67.H	4.653517	11.696366	0.732335
68.C	4.117724	11.019092	-1.257036	68.C	4.271673	11.245424	-1.353534
69.H	3.201104	11.544508	-1.564469	69.H	3.390248	11.874056	-1.558478
70.H	4.809852	11.070005	-2.102659	70.H	4.863353	11.222960	-2.273857
71.N	4.054844	6.893891	5.949266	71.N	4.071488	6.761012	5.973386
72.N	3.824457	9.596807	-1.005368	72.N	3.850379	9.863110	-1.059693
73.N	6.599065	7.036602	4.827230	73.N	6.717324	7.132385	5.174865
74.N	4.983823	9.986153	6.179513	74.N	4.767077	9.898089	6.419155
75.N	5.874089	7.766918	-1.491459	75.N	5.594291	7.767388	-1.676613
76.N	6.662318	10.327335	0.415685	76.N	6.893090	10.255452	0.046160

Table S12: Cartesian coordinates (Å) of complexes with ligand $\mathbf{L^5SSL^5}$ in **A**, **B** or **C** conformation computed at ZORA-OPBE/TZ2P in the gas phase and solvated in MeCN (COSMO).

$[Cu^{II}_2(\mathbf{L^5S})_2]^{2+}$ in MeCN Conformation **A**, symmetry C_2				$[Cu^{II}_2(\mathbf{L^5S})_2]^{2+}$ in the gas phase Conformation **A**, symmetry C_2			
1.Cu	0.171866	1.690955	0.344489	1.Cu	0.128749	1.738904	0.269870
2.Cu	-0.171866	-1.690955	0.344489	2.Cu	-0.128749	-1.738904	0.269870
3.S	1.425995	-0.070059	0.976224	3.S	1.427317	-0.028109	0.784113
4.S	-1.425995	0.070059	0.976224	4.S	-1.427317	0.028109	0.784113
5.N	-0.087966	3.264858	1.984320	5.N	-0.045762	3.171007	1.987738
6.N	-0.927995	2.651407	-1.079238	6.N	-1.006209	2.780321	-1.075547
7.N	2.104142	2.651976	-0.295725	7.N	2.082434	2.748737	-0.407450
8.N	0.087966	-3.264858	1.984320	8.N	0.045762	-3.171007	1.987738
9.N	0.927995	-2.651407	-1.079238	9.N	1.006209	-2.780321	-1.075547
10.N	-2.104142	-2.651976	-0.295725	10.N	-2.082434	-2.748737	-0.407450
11.C	-0.765570	2.968058	3.101487	11.C	-0.662607	2.782449	3.112944
12.C	-1.062536	3.894199	4.090242	12.C	-0.867747	3.610945	4.204603
13.C	-0.635030	5.204183	3.910131	13.C	-0.408884	4.919252	4.130604

14.C	0.078535	5.520617	2.762190	14.C	0.242086	5.330162	2.976194
15.C	0.343376	4.528740	1.814490	15.C	0.414589	4.434980	1.919626
16.C	-1.151127	-4.846503	0.588473	16.C	-1.154655	-4.859265	0.680877
17.C	-2.122126	3.212499	-0.835519	17.C	-2.189431	3.328559	-0.758615
18.C	-2.862283	3.855046	-1.813535	18.C	-2.955259	4.041140	-1.665843
19.C	-2.343362	3.916746	-3.102112	19.C	-2.475006	4.194473	-2.960925
20.C	-1.105474	3.341620	-3.356099	20.C	-1.247749	3.635443	-3.290519
21.C	-0.413116	2.712481	-2.321879	21.C	-0.528476	2.931663	-2.325459
22.C	-2.046265	-2.865221	-1.768530	22.C	-1.957507	-3.052958	-1.857277
23.C	3.199523	1.718211	0.067123	23.C	3.175705	1.781836	-0.148544
24.C	2.848430	0.259260	-0.096848	24.C	2.791899	0.332692	-0.352434
25.C	0.765570	-2.968058	3.101487	25.C	0.662607	-2.782449	3.112944
26.C	1.062536	-3.894199	4.090242	26.C	0.867747	-3.610945	4.204603
27.C	0.635030	-5.204183	3.910131	27.C	0.408884	-4.919252	4.130604
28.C	-0.078535	-5.520617	2.762190	28.C	-0.242086	-5.330162	2.976194
29.C	-0.343376	-4.528740	1.814490	29.C	-0.414589	-4.434980	1.919626
30.H	-3.440130	-1.887631	1.119432	30.H	-3.476621	-1.897676	0.896043
31.C	2.122126	-3.212499	-0.835519	31.C	2.189431	-3.328559	-0.758615
32.C	2.862283	-3.855046	-1.813535	32.C	2.955259	-4.041140	-1.665843
33.C	2.343362	-3.916746	-3.102112	33.C	2.475006	-4.194473	-2.960925
34.C	1.105474	-3.341620	-3.356099	34.C	1.247749	-3.635443	-3.290519
35.C	0.413116	-2.712481	-2.321879	35.C	0.528476	-2.931663	-2.325459
36.H	-3.135017	-4.489240	-0.163546	36.H	-3.103314	-4.591049	-0.202696
37.C	-3.199523	-1.718211	0.067123	37.C	-3.175705	-1.781836	-0.148544
38.C	-2.848430	-0.259260	-0.096848	38.C	-2.791899	-0.332692	-0.352434
39.H	-1.091059	1.935402	3.202565	39.H	-1.015758	1.753994	3.132330
40.H	-1.616508	3.590181	4.974930	40.H	-1.376997	3.234755	5.088619
41.H	-0.846310	5.968196	4.655703	41.H	-0.548601	5.609064	4.960744
42.H	0.438217	6.533574	2.597412	42.H	0.622501	6.345832	2.892579
43.C	1.151127	4.846503	0.588473	43.C	1.154655	4.859265	0.680877
44.H	-4.102866	-1.955466	-0.514270	44.H	-4.055722	-2.027759	-0.764607
45.H	-2.489391	3.136793	0.183387	45.H	-2.523118	3.187478	0.265702
46.H	-3.824828	4.292437	-1.563004	46.H	-3.906593	4.467341	-1.357132
47.H	-2.894572	4.409157	-3.900088	47.H	-3.046246	4.746544	-3.704726
48.H	-0.669595	3.376140	-4.351290	48.H	-0.842534	3.744705	-4.294032
49.H	0.509524	4.833680	-0.299765	49.H	0.468878	4.907580	-0.172543
50.H	2.786731	3.713706	1.373572	50.H	2.847074	3.705858	1.292250
51.H	4.102866	1.955466	-0.514270	51.H	4.055722	2.027759	-0.764607
52.H	3.440130	1.887631	1.119432	52.H	3.476621	1.897676	0.896043
53.H	3.691393	-0.350819	0.244048	53.H	3.645563	-0.300682	-0.085029
54.H	2.629982	-0.018030	-1.131118	54.H	2.517501	0.098533	-1.384814
55.H	1.091059	-1.935402	3.202565	55.H	1.015758	-1.753994	3.132330
56.H	1.616508	-3.590181	4.974930	56.H	1.376997	-3.234755	5.088619
57.H	0.846310	-5.968196	4.655703	57.H	0.548601	-5.609064	4.960744
58.H	-0.438217	-6.533574	2.597412	58.H	-0.622501	-6.345832	2.892579
59.H	-3.691393	0.350819	0.244048	59.H	-3.645563	0.300682	-0.085029
60.H	-2.629982	0.018030	-1.131118	60.H	-2.517501	-0.098533	-1.384814
61.H	2.489391	-3.136793	0.183387	61.H	2.523118	-3.187478	0.265702
62.H	3.824828	-4.292437	-1.563004	62.H	3.906593	-4.467341	-1.357132
63.H	2.894572	-4.409157	-3.900088	63.H	3.046246	-4.746544	-3.704726
64.H	0.669595	-3.376140	-4.351290	64.H	0.842534	-3.744705	-4.294032
65.H	3.135017	4.489240	-0.163546	65.H	3.103314	4.591049	-0.202696
66.H	-2.786731	-3.713706	1.373572	66.H	-2.847074	-3.705858	1.292250
67.C	2.362090	3.941840	0.393212	67.C	2.366620	3.992320	0.353433
68.C	-2.362090	-3.941840	0.393212	68.C	-2.366620	-3.992320	0.353433
69.H	-1.515745	-5.873555	0.674157	69.H	-1.513063	-5.882189	0.829304

70.H	-0.509524	-4.833680	-0.299765	70.H	-0.468878	-4.907580	-0.172543
71.H	1.515745	5.873555	0.674157	71.H	1.513063	5.882189	0.829304
72.C	2.046265	2.865221	-1.768530	72.C	1.957507	3.052958	-1.857277
73.C	-0.943771	-2.114128	-2.515965	73.C	-0.821965	-2.346803	-2.604354
74.C	0.943771	2.114128	-2.515965	74.C	0.821965	2.346803	-2.604354
75.H	-3.012913	-2.583037	-2.203216	75.H	-2.906086	-2.808505	-2.355006
76.H	-1.922450	-3.934962	-1.958499	76.H	-1.821832	-4.132563	-1.974397
77.H	3.012913	2.583037	-2.203216	77.H	2.906086	2.808505	-2.355006
78.H	1.922450	3.934962	-1.958499	78.H	1.821832	4.132563	-1.974397
79.H	-1.197618	-2.127793	-3.579296	79.H	-1.033493	-2.423205	-3.675680
80.H	-0.926073	-1.062746	-2.208048	80.H	-0.814004	-1.278647	-2.359947
81.H	1.197618	2.127793	-3.579296	81.H	1.033493	2.423205	-3.675680
82.H	0.926073	1.062746	-2.208048	82.H	0.814004	1.278647	-2.359947
$[Cu^{I}_2(\mathbf{L^5SSL^5})]^{2+}$ in MeCN Conformation **B**, symmetry C_2				$[Cu^{I}_2(\mathbf{L^5SSL^5})]^{2+}$ in the gas phase Conformation **B**, symmetry C_2			
1.Cu	-0.009178	2.615866	-0.409179	1.Cu	0.038385	2.648641	-0.346614
2.Cu	0.009178	-2.615866	-0.409179	2.Cu	-0.038385	-2.648641	-0.346614
3.S	-0.782678	-0.686299	-1.008956	3.S	-0.792376	-0.673186	-0.835101
4.S	0.782678	0.686299	-1.008956	4.S	0.792376	0.673186	-0.835101
5.C	-2.729769	1.225761	-0.223929	5.C	-2.722279	1.267145	-0.075582
6.H	-2.865628	1.207719	-1.309415	6.H	-2.876807	1.199541	-1.157074
7.H	-3.737986	1.186830	0.220214	7.H	-3.725656	1.246856	0.384807
8.C	-2.013361	-0.055237	0.177052	8.C	-1.996594	-0.000786	0.361562
9.H	-2.752952	-0.865822	0.149631	9.H	-2.737399	-0.811332	0.390233
10.H	-1.598653	-0.049745	1.185648	10.H	-1.554567	0.047799	1.358260
11.C	2.729769	-1.225761	-0.223929	11.C	2.722279	-1.267145	-0.075582
12.H	2.865628	-1.207719	-1.309415	12.H	2.876807	-1.199541	-1.157074
13.H	3.737986	-1.186830	0.220214	13.H	3.725656	-1.246856	0.384807
14.C	2.013361	0.055237	0.177052	14.C	1.996594	0.000786	0.361562
15.H	2.752952	0.865822	0.149631	15.H	2.737399	0.811332	0.390233
16.H	1.598653	0.049745	1.185648	16.H	1.554567	-0.047799	1.358260
17.C	-1.063478	4.905008	-1.930065	17.C	-1.046224	4.828435	-2.004866
18.C	-1.137283	5.875226	-2.931053	18.C	-1.133387	5.729623	-3.065529
19.H	-1.921073	6.627721	-2.890724	19.H	-1.911606	6.489444	-3.064901
20.C	-0.210867	5.874711	-3.965263	20.C	-0.227417	5.655209	-4.113957
21.H	-0.257228	6.629896	-4.747252	21.H	-0.284861	6.356928	-4.943753
22.C	0.771022	4.890004	-3.981996	22.C	0.747551	4.665882	-4.082820
23.H	1.518945	4.841860	-4.769179	23.H	1.478439	4.560634	-4.880711
24.C	0.780211	3.954386	-2.960444	24.C	0.771980	3.802559	-3.000911
25.H	1.530357	3.167703	-2.940270	25.H	1.517939	3.013008	-2.943625
26.N	-0.759801	-3.543082	1.204287	26.N	-0.779083	-3.688884	1.210323
27.N	0.759801	3.543082	1.204287	27.N	0.779083	3.688884	1.210323
28.N	0.105790	-3.953456	-1.949597	28.N	0.092644	-3.873584	-1.974367
29.C	-1.021436	2.462961	2.462498	29.C	-0.990021	2.662680	2.530086
30.C	2.225236	-2.807351	1.581185	30.C	2.205260	-2.943937	1.639019
31.C	1.021436	-2.462961	2.462498	31.C	0.990021	-2.662680	2.530086
32.C	0.133421	3.415113	2.393321	32.C	0.151474	3.628861	2.403828
33.C	0.556175	4.131185	3.513457	33.C	0.554438	4.425033	3.474630
34.H	0.029940	4.011368	4.457208	34.H	0.028013	4.360675	4.424330
35.C	1.648630	4.983056	3.416268	35.C	1.627982	5.292606	3.324595
36.H	1.990031	5.542743	4.284389	36.H	1.953224	5.916801	4.154479
37.C	2.295713	5.103165	2.191298	37.C	2.275143	5.346366	2.096396
38.H	3.157701	5.752256	2.061746	38.H	3.121018	6.007775	1.926473
39.C	1.815549	4.370884	1.118077	39.C	1.814872	4.535081	1.073152
40.H	2.291208	4.442277	0.143180	40.H	2.288299	4.558052	0.094398
41.N	2.099791	-2.519958	0.126513	41.N	2.088906	-2.575838	0.202638

42.N	-0.105790	3.953456	-1.949597	42.N	-0.092644	3.873584	-1.974367
43.N	-2.099791	2.519958	0.126513	43.N	-2.088906	2.575838	0.202638
44.C	-1.815549	-4.370884	1.118077	44.C	-1.814872	-4.535081	1.073152
45.H	-3.157701	-5.752256	2.061746	45.H	-3.121018	-6.007775	1.926473
46.H	-2.291208	-4.442277	0.143180	46.H	-2.288299	-4.558052	0.094398
47.C	1.063478	-4.905008	-1.930065	47.C	1.046224	-4.828435	-2.004866
48.C	1.137283	-5.875226	-2.931053	48.C	1.133387	-5.729623	-3.065529
49.H	1.921073	-6.627721	-2.890724	49.H	1.911606	-6.489444	-3.064901
50.C	0.210867	-5.874711	-3.965263	50.C	0.227417	-5.655209	-4.113957
51.H	0.257228	-6.629896	-4.747252	51.H	0.284861	-6.356928	-4.943753
52.C	-0.771022	-4.890004	-3.981996	52.C	-0.747551	-4.665882	-4.082820
53.H	-1.518945	-4.841860	-4.769179	53.H	-1.478439	-4.560634	-4.880711
54.C	-0.780211	-3.954386	-2.960444	54.C	-0.771980	-3.802559	-3.000911
55.H	-1.530357	-3.167703	-2.940270	55.H	-1.517939	-3.013008	-2.943625
56.C	2.814212	-3.571908	-0.639807	56.C	2.796634	-3.590875	-0.620399
57.C	-2.225236	2.807351	1.581185	57.C	-2.205260	2.943937	1.639019
58.C	2.050151	-4.884902	-0.799711	58.C	2.019975	-4.884985	-0.861546
59.C	-1.648630	-4.983056	3.416268	59.C	-1.627982	-5.292606	3.324595
60.H	-1.990031	-5.542743	4.284389	60.H	-1.953224	-5.916801	4.154479
61.C	-2.295713	-5.103165	2.191298	61.C	-2.275143	-5.346366	2.096396
62.C	-0.133421	-3.415113	2.393321	62.C	-0.151474	-3.628861	2.403828
63.C	-0.556175	-4.131185	3.513457	63.C	-0.554438	-4.425033	3.474630
64.H	-0.029940	-4.011368	4.457208	64.H	-0.028013	-4.360675	4.424330
65.C	-2.050151	4.884902	-0.799711	65.C	-2.019975	4.884985	-0.861546
66.C	-2.814212	3.571908	-0.639807	66.C	-2.796634	3.590875	-0.620399
67.H	-1.381709	2.423792	3.494490	67.H	-1.342821	2.673535	3.566648
68.H	-0.650730	1.459542	2.229773	68.H	-0.608465	1.652523	2.346730
69.H	2.435599	-3.874041	1.700023	69.H	2.423526	-4.014469	1.699402
70.H	3.103866	-2.277351	1.974766	70.H	3.079962	-2.433730	2.070259
71.H	1.381709	-2.423792	3.494490	71.H	1.342821	-2.673535	3.566648
72.H	0.650730	-1.459542	2.229773	72.H	0.608465	-1.652523	2.346730
73.H	3.032740	-3.170483	-1.632912	73.H	3.022702	-3.137300	-1.589481
74.H	3.784299	-3.776225	-0.164298	74.H	3.765563	-3.829557	-0.155608
75.H	-2.435599	3.874041	1.700023	75.H	-2.423526	4.014469	1.699402
76.H	-3.103866	2.277351	1.974766	76.H	-3.079962	2.433730	2.070259
77.H	2.781310	-5.680674	-0.965151	77.H	2.746981	-5.676748	-1.065632
78.H	1.534251	-5.141779	0.134176	78.H	1.492516	-5.193300	0.050228
79.H	-2.781310	5.680674	-0.965151	79.H	-2.746981	5.676748	-1.065632
80.H	-1.534251	5.141779	0.134176	80.H	-1.492516	5.193300	0.050228
81.H	-3.032740	3.170483	-1.632912	81.H	-3.022702	3.137300	-1.589481
82.H	-3.784299	3.776225	-0.164298	82.H	-3.765563	3.829557	-0.155608
$[Cu^{I}_2(\mathbf{L^5SSL^5})]^{2+}$ in MeCN Conformation **C**, no symmetry				$[Cu^{I}_2(\mathbf{L^5SSL^5})]^{2+}$ in the gas phase Conformation **C**, no symmetry			
1.Cu	9.844060	2.439773	0.285422	1.Cu	9.906982	2.339565	0.128808
2.Cu	8.463444	4.096711	4.533371	2.Cu	8.442408	4.138047	4.732003
3.S	8.227648	3.800313	0.900692	3.S	8.391053	3.738883	0.903860
4.S	8.693085	5.036845	2.557420	4.S	8.669300	4.927291	2.687625
5.N	11.532902	1.880618	1.151052	5.N	11.573887	1.532601	0.852304
6.N	8.941698	1.058699	-0.873804	6.N	8.905802	1.189523	-1.187823
7.N	10.571300	3.838333	-1.216509	7.N	10.746589	3.855512	-1.218128
8.N	8.215617	2.223370	5.117914	8.N	8.305740	2.323722	5.534869
9.N	9.510645	5.285581	5.781003	9.N	9.325604	5.520319	5.901611
10.N	6.455506	4.897379	4.780023	10.N	6.351644	4.788170	4.847639
11.C	11.648483	0.675003	1.737850	11.C	11.614512	0.246422	1.244291
12.C	12.838034	0.187332	2.251055	12.C	12.776184	-0.394499	1.638149
13.C	13.976342	0.979690	2.146045	13.C	13.965541	0.323582	1.618140

14.C	13.867765	2.223272	1.538195	14.C	13.934721	1.650474	1.212303
15.C	12.634320	2.659033	1.050820	15.C	12.726766	2.238026	0.837628
16.C	12.491567	4.009320	0.413670	16.C	12.667917	3.676450	0.409428
17.C	12.026331	4.011663	-1.043696	17.C	12.209339	3.917355	-1.030800
18.C	7.918728	0.316908	-0.412848	18.C	7.834441	0.464564	-0.820288
19.C	7.161266	-0.522292	-1.211891	19.C	7.073682	-0.279130	-1.705047
20.C	7.468171	-0.594524	-2.566434	20.C	7.428105	-0.268323	-3.048348
21.C	8.522932	0.166807	-3.051840	21.C	8.528582	0.480860	-3.438866
22.C	9.253008	0.984612	-2.187343	22.C	9.258745	1.199960	-2.492309
23.C	10.410271	1.796046	-2.691858	23.C	10.468011	1.993416	-2.900406
24.C	10.265711	3.314620	-2.561827	24.C	10.412792	3.495738	-2.610699
25.C	9.866511	5.102449	-0.959842	25.C	10.118420	5.122251	-0.821397
26.C	8.427890	4.905278	-0.532703	26.C	8.665940	4.965323	-0.416720
27.C	9.231308	1.515320	5.645403	27.C	9.338747	1.771789	6.196539
28.C	9.080142	0.245926	6.176903	28.C	9.254652	0.567921	6.874099
29.C	7.811230	-0.323816	6.175514	29.C	8.037346	-0.101900	6.881221
30.C	6.756475	0.401236	5.637415	30.C	6.964457	0.460869	6.204041
31.C	6.980293	1.673013	5.107427	31.C	7.121084	1.673037	5.532619
32.C	5.859013	2.461948	4.499599	32.C	5.978003	2.292618	4.780723
33.C	5.549489	3.800884	5.171704	33.C	5.514092	3.657762	5.294162
34.C	10.815693	5.540319	5.579054	34.C	10.615753	5.863010	5.738900
35.C	11.537943	6.461784	6.317992	35.C	11.241823	6.856331	6.470998
36.C	10.876267	7.167374	7.317220	36.C	10.495049	7.545757	7.418226
37.C	9.528618	6.912069	7.532763	37.C	9.161452	7.203901	7.589864
38.C	8.862983	5.961964	6.755700	38.C	8.595143	6.183935	6.824870
39.C	7.411519	5.659654	6.987927	39.C	7.158926	5.787524	7.021663
40.C	6.474336	5.951328	5.812758	40.C	6.253070	5.917138	5.794255
41.C	6.074167	5.436963	3.466861	41.C	5.991513	5.192961	3.482660
42.C	7.224372	6.097824	2.738233	42.C	7.121741	5.889027	2.750507
43.H	10.739489	0.081253	1.794408	43.H	10.666274	-0.285819	1.236806
44.H	12.864238	-0.793303	2.718899	44.H	12.743614	-1.436405	1.946506
45.H	14.933690	0.635872	2.531750	45.H	14.904298	-0.142005	1.911702
46.H	14.738263	2.867390	1.440300	46.H	14.849766	2.237818	1.184652
47.H	13.460486	4.514738	0.453961	47.H	13.665600	4.112634	0.519168
48.H	11.807495	4.616192	1.021491	48.H	12.016410	4.225990	1.102099
49.H	12.532254	3.205831	-1.582957	49.H	12.669620	3.167159	-1.680642
50.H	12.346744	4.951859	-1.517618	50.H	12.588130	4.893586	-1.372939
51.H	7.706064	0.405553	0.650095	51.H	7.585237	0.486136	0.238337
52.H	6.350876	-1.101095	-0.776697	52.H	6.223336	-0.852384	-1.344318
53.H	6.897358	-1.235892	-3.234591	53.H	6.858024	-0.835508	-3.781456
54.H	8.791392	0.129407	-4.104798	54.H	8.831771	0.506060	-4.483010
55.H	11.325036	1.465880	-2.183797	55.H	11.356376	1.554372	-2.428196
56.H	10.553456	1.564976	-3.750906	56.H	10.611341	1.867767	-3.977746
57.H	9.241342	3.599418	-2.818081	57.H	9.406615	3.864128	-2.832310
58.H	10.918295	3.796705	-3.304800	58.H	11.091109	4.018688	-3.302761
59.H	10.395674	5.638202	-0.166863	59.H	10.671922	5.530684	0.029616
60.H	9.888495	5.754091	-1.847917	60.H	10.187915	5.869646	-1.630061
61.H	7.951403	5.866763	-0.320595	61.H	8.253173	5.931426	-0.109355
62.H	7.821933	4.415449	-1.304552	62.H	8.039231	4.601975	-1.240211
63.H	10.206139	1.996583	5.635437	63.H	10.271828	2.329876	6.177357
64.H	9.942045	-0.276980	6.583166	64.H	10.126719	0.172465	7.388753
65.H	7.644935	-1.317387	6.586237	65.H	7.922992	-1.047442	7.407624
66.H	5.752191	-0.015011	5.620264	66.H	5.998594	-0.039129	6.192899
67.H	4.950825	1.853758	4.532942	67.H	5.122837	1.611186	4.825148
68.H	6.077885	2.624471	3.435885	68.H	6.252223	2.369647	3.719989
69.H	5.609030	3.679647	6.257068	69.H	5.512337	3.644365	6.388136

70.H	4.509186	4.081182	4.947029	70.H	4.469146	3.824173	4.987605
71.H	11.296198	4.970605	4.786912	71.H	11.165213	5.304624	4.984181
72.H	12.593250	6.617618	6.110020	72.H	12.291538	7.080728	6.298999
73.H	11.401671	7.904153	7.921198	73.H	10.943577	8.336718	8.016006
74.H	8.983218	7.444412	8.308214	74.H	8.552783	7.724090	8.325888
75.H	7.071371	6.253168	7.840850	75.H	6.737203	6.414025	7.813286
76.H	7.310553	4.609649	7.290306	76.H	7.124140	4.759511	7.404939
77.H	6.772853	6.891932	5.341029	77.H	6.505290	6.839138	5.261874
78.H	5.457271	6.107815	6.201781	78.H	5.210484	6.031007	6.129807
79.H	5.249632	6.161307	3.562330	79.H	5.105317	5.850243	3.484790
80.H	5.697663	4.614890	2.851870	80.H	5.714519	4.297012	2.918845
81.H	7.618334	6.969076	3.275194	81.H	7.419713	6.826333	3.235790
82.H	6.906902	6.451581	1.753173	82.H	6.810443	6.146091	1.733078

Table S13: Cartesian coordinates (Å) and ADF total energies of $[Cu^{II}_2(\mathbf{L^xS})_2(CH_3CN)_2]^{2+}$ (**A**) and $[Cu^{I}_2(\mathbf{L^XSSL^X})(CH_3CN)_2]^{2+}$ (**B** or **C**) with X = 1, 2, 3, 4 or 5 with an uncoordinated pyridyl group unless mentioned otherwise. All structures are computed at ZORA-OPBE/TZP in MeCN (COSMO).

$[Cu^{I}_2(\mathbf{L^1SSL^1})_2(CH_3CN)_2]^{2+}$ (–11492.91 kcal mol^{-1}) Conformation **B**, symmetry C_2				$[Cu^{I}_2(\mathbf{L^1SSL^1})_2(CH_3CN)_2]^{2+}$ (–11493.88 kcal mol^{-1}) Conformation **C**, symmetry C_2			
1.Cu	2.228436	-1.455199	-0.997284	1.Cu	0.073227	2.492386	0.428878
2.Cu	-2.228436	1.455199	-0.997284	2.Cu	-0.073227	-2.492386	0.428878
3.S	-0.057500	1.028668	-1.212220	3.S	0.662089	0.813704	-1.002210
4.S	0.057500	-1.028668	-1.212220	4.S	-0.662089	-0.813704	-1.002210
5.C	2.474554	1.632639	-0.043339	5.N	-3.831943	5.940635	-0.544164
6.H	2.680686	2.051085	-1.032010	6.N	1.455750	3.846573	-0.062843
7.H	2.872514	2.352237	0.687747	7.N	-1.074188	3.612421	-1.293724
8.C	0.971595	1.601390	0.174601	8.N	3.831943	-5.940635	-0.544164
9.H	0.638084	2.641745	0.275690	9.N	-1.455750	-3.846573	-0.062843
10.H	0.659048	1.090496	1.088786	10.N	1.074188	-3.612421	-1.293724
11.C	-2.474554	-1.632639	-0.043339	11.C	-4.214606	6.927977	0.270847
12.H	-2.680686	-2.051085	-1.032010	12.C	-3.558630	7.256056	1.451897
13.H	-2.872514	-2.352237	0.687747	13.C	-2.448247	6.501442	1.807392
14.C	-0.971595	-1.601390	0.174601	14.C	-2.048086	5.459564	0.979036
15.H	-0.638084	-2.641745	0.275690	15.C	-2.761391	5.209526	-0.192545
16.H	-0.659048	-1.090496	1.088786	16.H	1.338635	-2.999017	-3.310915
17.C	5.519028	1.464119	0.054402	17.C	-2.468525	4.079694	-1.150931
18.C	6.441436	1.090417	1.035125	18.C	2.682514	3.861475	0.493675
19.H	6.482212	0.063827	1.391813	19.C	3.700585	4.687360	0.053094
20.C	7.329571	2.036380	1.533669	20.C	3.446680	5.536244	-1.020878
21.H	8.057470	1.761407	2.294551	21.C	2.186449	5.525879	-1.598077
22.C	7.275526	3.330681	1.032973	22.C	1.206089	4.671181	-1.094360
23.H	7.951096	4.106138	1.386645	23.H	3.064703	-3.213952	-0.837779
24.C	6.337469	3.609786	0.044403	24.C	-0.185261	4.717322	-1.674846
25.H	6.278378	4.609915	-0.386236	25.C	-1.102829	2.561707	-2.326407
26.N	-3.040673	2.404612	0.555851	26.C	0.174477	1.770887	-2.467868
27.N	3.040673	-2.404612	0.555851	27.C	4.214606	-6.927977	0.270847
28.N	-5.478658	-2.710909	-0.445510	28.C	3.558630	-7.256056	1.451897
29.C	4.552891	0.459172	-0.541390	29.C	2.448247	-6.501442	1.807392
30.H	4.416550	0.708406	-1.596460	30.C	2.048086	-5.459564	0.979036
31.H	5.003011	-0.535928	-0.492827	31.C	2.761391	-5.209526	-0.192545
32.C	3.522840	-1.617610	1.535733	32.H	-2.840441	-3.178664	1.324343
33.C	4.202986	-2.145900	2.629086	33.C	2.468525	-4.079694	-1.150931
34.H	4.583938	-1.483137	3.402061	34.C	-2.682514	-3.861475	0.493675

35.C	4.382459	-3.520338	2.719896	35.C	-3.700585	-4.687360	0.053094
36.H	4.911211	-3.950564	3.567427	36.C	-3.446680	-5.536244	-1.020878
37.C	3.880960	-4.331596	1.707741	37.C	-2.186449	-5.525879	-1.598077
38.H	3.999162	-5.411561	1.732271	38.C	-1.206089	-4.671181	-1.094360
39.C	3.222584	-3.732912	0.645703	39.H	-4.671105	-4.658742	0.540813
40.H	2.821513	-4.329911	-0.169370	40.C	0.185261	-4.717322	-1.674846
41.N	-3.193352	-0.349262	0.051771	41.C	1.102829	-2.561707	-2.326407
42.N	5.478658	2.710909	-0.445510	42.C	-0.174477	-1.770887	-2.467868
43.N	3.193352	0.349262	0.051771	43.H	-5.091430	7.493239	-0.045812
44.C	3.225819	-0.145769	1.432052	44.H	-3.909065	8.080132	2.068761
45.H	2.231412	0.007002	1.866511	45.H	-1.897065	6.715869	2.720966
46.H	3.918255	0.422803	2.066750	46.H	-1.187986	4.852548	1.243483
47.C	-5.519028	-1.464119	0.054402	47.H	0.117182	-4.818267	-2.767437
48.C	-6.441436	-1.090417	1.035125	48.H	0.630361	-5.655238	-1.324076
49.H	-6.482212	-0.063827	1.391813	49.H	-2.868299	4.389043	-2.127165
50.C	-7.329571	-2.036380	1.533669	50.H	-3.064703	3.213952	-0.837779
51.H	-8.057470	-1.761407	2.294551	51.H	2.840441	3.178664	1.324343
52.C	-7.275526	-3.330681	1.032973	52.H	4.671105	4.658742	0.540813
53.H	-7.951096	-4.106138	1.386645	53.H	4.221320	6.196709	-1.403987
54.C	-6.337469	-3.609786	0.044403	54.H	1.953336	6.176927	-2.437226
55.H	-6.278378	-4.609915	-0.386236	55.H	1.921272	-1.876970	-2.082959
56.H	-3.918255	-0.422803	2.066750	56.H	-0.104491	-1.100047	-3.327878
57.C	-3.225819	0.145769	1.432052	57.H	-0.117182	4.818267	-2.767437
58.H	-2.231412	-0.007002	1.866511	58.H	-0.630361	5.655238	-1.324076
59.C	-4.552891	-0.459172	-0.541390	59.H	-1.921272	1.876970	-2.082959
60.H	-4.416550	-0.708406	-1.596460	60.H	-1.338635	2.999017	-3.310915
61.H	-5.003011	0.535928	-0.492827	61.H	0.104491	1.100047	-3.327878
62.C	-3.522840	1.617610	1.535733	62.H	2.868299	-4.389043	-2.127165
63.C	-4.202986	2.145900	2.629086	63.H	5.091430	-7.493239	-0.045812
64.H	-4.583938	1.483137	3.402061	64.H	3.909065	-8.080132	2.068761
65.C	-4.382459	3.520338	2.719896	65.H	1.897065	-6.715869	2.720966
66.H	-4.911211	3.950564	3.567427	66.H	1.187986	-4.852548	1.243483
67.C	-3.880960	4.331596	1.707741	67.H	-4.221320	-6.196709	-1.403987
68.H	-3.999162	5.411561	1.732271	68.H	-1.953336	-6.176927	-2.437226
69.C	-3.222584	3.732912	0.645703	69.H	1.053333	2.401968	-2.647013
70.H	-2.821513	4.329911	-0.169370	70.H	-1.053333	-2.401968	-2.647013
71.N	-2.940684	1.809410	-2.737015	71.N	0.756763	-2.146646	2.062352
72.N	2.940684	-1.809410	-2.737015	72.N	-0.756763	2.146646	2.062352
73.C	-3.354565	2.061768	-3.791650	73.C	-1.275405	1.888274	3.068230
74.C	-3.872194	2.373646	-5.098359	74.C	-1.918487	1.567121	4.315274
75.C	3.354565	-2.061768	-3.791650	75.C	1.275405	-1.888274	3.068230
76.C	3.872194	-2.373646	-5.098359	76.C	1.918487	-1.567121	4.315274
77.H	3.525576	-1.628263	-5.820969	77.H	2.700680	-2.303183	4.527693
78.H	3.522199	-3.363900	-5.406447	78.H	1.185137	-1.584256	5.127884
79.H	-4.966515	2.370877	-5.073118	79.H	-2.700680	2.303183	4.527693
80.H	-3.525576	1.628263	-5.820969	80.H	-1.185137	1.584256	5.127884
81.H	-3.522199	3.363900	-5.406447	81.H	-2.374871	0.573693	4.256482
82.H	4.966515	-2.370877	-5.073118	82.H	2.374871	-0.573693	4.256482
$[Cu^{I}_2(\mathbf{L^1SSL^1})_2(CH_3CN)_2]^{2+}$ (–11510.02 kcal mol^{-1}) S uncoordinated, no symmetry				$[Cu^{II}_2(\mathbf{L^2S})_2(CH_3CN)_2]^{2+}$ E^T = –12250.96 kcal mol^{-1} E^{BS} = –12250.83 kcal mol^{-1} E^S = –12250.70 kcal mol^{-1} Conformation **A**, no symmetry			
1.Cu	-5.951858	0.512697	0.450159	1.Cu	-0.676061	1.591139	-0.485390
2.Cu	5.933586	-0.531660	0.454181	2.Cu	0.673465	-1.588939	-0.482857

3.S	-0.346930	-0.925948	-0.224822	3.S	1.363437	0.659319	-0.384254
4.S	0.358285	0.970570	-0.258298	4.S	-1.367177	-0.657208	-0.381500
5.N	-6.701453	-1.298915	0.000948	5.C	1.675687	2.789910	-2.019468
6.N	-5.199389	1.565320	-1.093225	6.H	2.364415	3.179242	-1.268922
7.N	-3.988186	-0.672711	0.094961	7.H	1.976514	3.204523	-2.993181
8.N	6.734862	1.256673	-0.003053	8.C	1.809318	1.281402	-2.028826
9.N	5.156008	-1.572778	-1.084686	9.H	2.851443	1.015807	-2.235007
10.N	4.007496	0.705189	0.087027	10.H	1.192128	0.807086	-2.798728
11.C	-7.990439	-1.546355	-0.292239	11.C	-1.676469	-2.792643	-2.010621
12.C	-8.466080	-2.808922	-0.606800	12.H	-2.362116	-3.182167	-1.257274
13.C	-7.565800	-3.869226	-0.634250	13.H	-1.978892	-3.210397	-2.982305
14.C	-6.231073	-3.619350	-0.344533	14.C	-1.814501	-1.284679	-2.023565
15.C	-5.830938	-2.325466	-0.021225	15.H	-2.857858	-1.023181	-2.229189
16.H	3.312353	0.215862	1.970314	16.H	-1.199368	-0.810923	-2.795262
17.C	-4.403388	-2.039917	0.376627	17.C	1.082622	5.001548	0.077364
18.C	-5.595641	2.790931	-1.473876	18.C	2.440747	5.319707	0.066090
19.C	-4.980399	3.500970	-2.493502	19.H	3.010255	5.320132	-0.860306
20.C	-3.900260	2.919374	-3.148072	20.C	3.053407	5.667781	1.265239
21.C	-3.483672	1.652561	-2.757728	21.H	4.112463	5.916176	1.290730
22.C	-4.157290	0.998193	-1.730628	22.C	2.291176	5.709387	2.420612
23.H	4.381043	2.222849	1.446229	23.H	2.741549	5.985792	3.372466
24.C	-3.809361	-0.414595	-1.335266	24.C	0.922106	5.422632	2.342231
25.C	-2.903711	-0.194432	0.961024	25.C	0.337356	4.671288	-1.193678
26.C	-1.608369	-0.999234	1.088815	26.H	-0.702976	4.966675	-1.043094
27.C	8.031074	1.467408	-0.293386	27.H	0.741639	5.283996	-2.013388
28.C	8.542982	2.715648	-0.607984	28.C	0.049016	5.526090	3.557495
29.C	7.673574	3.801315	-0.637955	29.H	0.420461	4.885951	4.365615
30.C	6.331557	3.589355	-0.351821	30.H	-0.976026	5.238216	3.318612
31.C	5.893898	2.307582	-0.028975	31.H	0.043548	6.551256	3.946211
32.H	6.345056	-3.256180	-0.909859	32.C	-2.028125	3.188745	-2.369758
33.C	4.457120	2.062623	0.363012	33.C	-3.028138	3.869673	-3.053992
34.C	5.514923	-2.813005	-1.454803	34.H	-2.782487	4.451379	-3.938451
35.C	4.880726	-3.511547	-2.470761	35.C	-4.333855	3.800063	-2.582567
36.C	3.821127	-2.901691	-3.133109	36.H	-5.131583	4.327603	-3.100319
37.C	3.442883	-1.619752	-2.753435	37.C	-4.602318	3.057609	-1.438089
38.C	4.133032	-0.979016	-1.728832	38.H	-5.606940	2.982578	-1.030942
39.H	5.212878	-4.513616	-2.729209	39.C	-3.553078	2.404539	-0.809781
40.C	3.826671	0.445750	-1.342743	40.H	-3.711726	1.810885	0.085728
41.C	2.907654	0.260669	0.951481	41.C	-0.592886	3.173575	-2.809403
42.C	1.622764	1.086685	1.049631	42.H	-0.404312	2.230543	-3.334179
43.H	-8.660808	-0.690471	-0.269432	43.H	-0.398763	3.979630	-3.528112
44.H	-9.520131	-2.950740	-0.830718	44.C	-1.077862	-5.003863	0.082095
45.H	-7.896494	-4.875004	-0.883881	45.C	-2.434115	-5.329861	0.065555
46.H	-5.497486	-4.421857	-0.366209	46.H	-3.001031	-5.331354	-0.862479
47.H	2.832207	0.727713	-1.707233	47.C	-3.048754	-5.684480	1.261762
48.H	4.543664	1.077403	-1.883591	48.H	-4.106289	-5.939624	1.282822
49.H	-3.753053	-2.795320	-0.086678	49.C	-2.290122	-5.724019	2.419588
50.H	-4.330280	-2.191107	1.461451	50.H	-2.741463	-6.005862	3.369361
51.H	-6.440734	3.212147	-0.934586	51.C	-0.922657	-5.427968	2.346452
52.H	-5.342814	4.490197	-2.760671	52.C	-0.329739	-4.669015	-1.186060
53.H	-3.385229	3.445787	-3.948700	53.H	0.711658	-4.958214	-1.031064
54.H	-2.644617	1.167382	-3.250603	54.H	-0.727252	-5.284480	-2.006977
55.H	2.659243	-0.770404	0.677792	55.C	-0.053424	-5.526875	3.564843
56.H	1.136532	0.844679	2.000451	56.H	-0.429614	-4.886034	4.370263
57.H	-2.805387	-0.667955	-1.694354	57.H	0.971530	-5.236458	3.328761
58.H	-4.504502	-1.070249	-1.876080	58.H	-0.047124	-6.551022	3.956089

59.H	-2.668423	0.834689	0.669320	59.C	2.027621	-3.182019	-2.369128
60.H	-3.317625	-0.135876	1.975677	60.C	3.028372	-3.858851	-3.056264
61.H	-1.124052	-0.712491	2.028190	61.H	2.783131	-4.439196	-3.941766
62.H	3.829548	2.831800	-0.108706	62.C	4.334699	-3.786444	-2.586743
63.H	8.677128	0.593118	-0.268184	63.H	5.133112	-4.310702	-3.106799
64.H	9.601128	2.827277	-0.829724	64.C	4.602958	-3.045704	-1.441139
65.H	8.033390	4.797153	-0.887127	65.H	5.608025	-2.968785	-1.035439
66.H	5.621089	4.412327	-0.375873	66.C	3.552903	-2.396798	-0.809783
67.H	3.292174	-3.417872	-3.931280	67.H	3.711374	-1.804901	0.086844
68.H	2.620396	-1.112765	-3.252233	68.C	0.591367	-3.169973	-2.805488
69.H	-1.800293	-2.076028	1.166532	69.H	0.399341	-2.227470	-3.329829
70.H	1.826381	2.163718	1.082125	70.H	0.397371	-3.976478	-3.523995
71.N	-6.428873	1.366849	2.026873	71.N	0.321516	3.251532	-1.654354
72.N	6.386791	-1.386228	2.037363	72.N	-0.320036	-3.249607	-1.647978
73.C	6.716015	-1.923043	3.015461	73.N	0.336571	5.074495	1.189634
74.C	7.124143	-2.584586	4.228071	74.N	-2.296426	2.466075	-1.268217
75.C	-6.770942	1.898960	3.003151	75.N	-0.335054	-5.073974	1.196689
76.C	-7.194274	2.553696	4.214256	76.N	2.295876	-2.460687	-1.266614
77.H	6.460713	-2.293046	5.048874	77.N	-1.183277	1.847412	1.746577
78.H	8.150296	-2.297986	4.480462	78.N	1.179823	-1.843210	1.748000
79.H	7.075575	-3.670400	4.097236	79.C	-1.391710	1.719415	2.878841
80.H	-7.299917	3.629489	4.040931	80.C	-1.645895	1.566666	4.291203
81.H	-6.451409	2.389592	5.001669	81.C	1.388744	-1.718129	2.880479
82.H	-8.156386	2.145542	4.540619	82.C	1.643964	-1.568520	4.292989
				83.H	-0.719803	1.711705	4.856316
				84.H	-2.039891	0.565993	4.493861
				85.H	-2.382119	2.306650	4.619568
				86.H	2.032778	-0.566357	4.497983
				87.H	2.384359	-2.305608	4.618327
				88.H	0.719469	-1.719138	4.859237
$[Cu^{I}_2(\mathbf{L^2SSL^2})_2(CH_3CN)_2]^{2+}$ (–12256.56 kcal mol^{-1}) Conformation **B**, symmetry C_2				$[Cu^{I}_2(\mathbf{L^2SSL^2})_2(CH_3CN)_2]^{2+}$ (–12277.72 kcal mol^{-1}) S uncoordinated, no symmetry			
1.Cu	1.049651	2.534740	0.151099	1.Cu	-5.829722	0.237501	0.546373
2.Cu	-1.049651	-2.534740	0.151099	2.Cu	5.752840	-0.281461	0.536798
3.S	-0.985938	-0.290862	0.061712	3.S	-0.226721	-0.854683	-0.474725
4.S	0.985938	0.290862	0.061712	4.S	0.277675	1.096616	-0.643081
5.C	-2.174444	2.002082	1.252612	5.N	-6.531776	-1.598042	0.108826
6.H	-2.700297	2.068407	0.297243	6.N	-5.272237	1.352205	-1.049884
7.H	-2.915996	2.231996	2.038663	7.N	-3.855368	-0.804907	0.040076
8.C	-1.769500	0.555805	1.466619	8.N	6.697310	1.435432	0.080208
9.H	-2.694888	-0.021933	1.585604	9.N	5.088031	-1.353716	-1.053262
10.H	-1.182236	0.376154	2.370083	10.N	3.949469	0.995380	-0.038530
11.C	2.174444	-2.002082	1.252612	11.C	-7.828551	-1.903382	-0.125025
12.H	2.700297	-2.068407	0.297243	12.C	-8.213144	-3.205018	-0.442306
13.H	2.915996	-2.231996	2.038663	13.C	-7.252739	-4.202968	-0.535415
14.C	1.769500	-0.555805	1.466619	14.C	-5.922864	-3.876931	-0.309675
15.H	2.694888	0.021933	1.585604	15.C	-5.599665	-2.565310	0.017926
16.H	1.182236	-0.376154	2.370083	16.H	3.091705	0.637942	1.803049
17.C	-2.478357	4.432639	-0.396094	17.C	-4.173370	-2.193514	0.343207
18.C	-3.875265	4.430966	-0.378770	18.C	-5.771058	2.550330	-1.393916
19.H	-4.418191	4.328133	0.558013	19.C	-5.275865	3.300565	-2.449600
20.C	-4.557491	4.575096	-1.579143	20.C	-4.207649	2.791585	-3.180164
21.H	-5.645470	4.582107	-1.599676	21.C	-3.684326	1.553601	-2.827439
22.C	-3.827354	4.716970	-2.750138	22.C	-4.242660	0.855109	-1.760597
23.H	-4.331630	4.837452	-3.706740	23.H	4.286461	2.529862	1.310462
24.C	-2.430153	4.722397	-2.683115	24.C	-3.777320	-0.532612	-1.396567

25.C	-1.598411	4.885837	-3.919983	25.C	-2.754768	-0.261744	0.843793
26.H	-0.834158	5.655286	-3.772284	26.C	-1.412551	-0.990865	0.901934
27.H	-2.209469	5.155731	-4.784249	27.C	8.027856	1.559977	-0.128273
28.H	-1.074946	3.950903	-4.151861	28.C	8.589456	2.790609	-0.463903
29.C	-1.707729	4.342609	0.899373	29.C	7.773216	3.904811	-0.602126
30.H	-0.886192	5.063362	0.858490	30.C	6.407016	3.763652	-0.403112
31.H	-2.380219	4.654108	1.714279	31.C	5.904554	2.515325	-0.055408
32.C	0.742352	3.935499	2.633367	32.H	9.923914	0.555150	-0.133493
33.C	1.004999	4.847453	3.650672	33.C	4.434025	2.340999	0.239455
34.H	0.244381	5.055564	4.398853	34.C	5.424791	-2.617064	-1.358255
35.C	2.242263	5.477610	3.697954	35.C	4.848512	-3.321315	-2.404607
36.H	2.465561	6.192737	4.486522	36.C	3.872645	-2.691323	-3.169186
37.C	3.183544	5.181308	2.718449	37.C	3.517451	-1.384750	-2.857475
38.H	4.165593	5.646632	2.712725	38.C	4.146778	-0.741392	-1.795838
39.C	2.843811	4.275209	1.726576	39.H	5.159331	-4.342882	-2.607597
40.H	3.547489	4.025481	0.936635	40.C	3.866946	0.704099	-1.471067
41.N	1.113595	-3.022715	1.245307	41.C	2.775678	0.614385	0.753511
42.N	-1.772137	4.588465	-1.521704	42.C	1.493406	1.445730	0.671032
43.N	-1.113595	3.022715	1.245307	43.C	-8.826349	-0.795798	-0.032266
44.C	-0.533280	3.145781	2.589049	44.H	-9.262365	-3.426214	-0.620441
45.H	-0.288400	2.140484	2.948711	45.H	-7.536940	-5.221772	-0.788685
46.H	-1.254612	3.567761	3.304770	46.H	-5.140171	-4.627549	-0.385069
47.C	2.478357	-4.432639	-0.396094	47.H	2.914551	1.012499	-1.917754
48.C	3.875265	-4.430966	-0.378770	48.H	4.646930	1.294158	-1.969903
49.H	4.418191	-4.328133	0.558013	49.H	-3.503565	-2.909693	-0.152980
50.C	4.557491	-4.575096	-1.579143	50.H	-4.035057	-2.334308	1.423019
51.H	5.645470	-4.582107	-1.599676	51.H	8.737603	-0.113467	1.005918
52.C	3.827354	-4.716970	-2.750138	52.H	-5.718713	4.264836	-2.684995
53.H	4.331630	-4.837452	-3.706740	53.H	-3.784048	3.351772	-4.010914
54.C	2.430153	-4.722397	-2.683115	54.H	-2.851018	1.125065	-3.379226
55.C	1.598411	-4.885837	-3.919983	55.H	2.541516	-0.432429	0.529410
56.H	0.834158	-5.655286	-3.772284	56.H	0.969752	1.365676	1.629172
57.H	2.209469	-5.155731	-4.784249	57.H	-2.780600	-0.716564	-1.813362
58.H	1.074946	-3.950903	-4.151861	58.H	-4.456499	-1.232782	-1.900432
59.C	1.707729	-4.342609	0.899373	59.H	-2.593373	0.776797	0.535281
60.H	0.886192	-5.063362	0.858490	60.H	-3.113528	-0.220014	1.879801
61.H	2.380219	-4.654108	1.714279	61.H	-0.896767	-0.671809	1.813903
62.C	-0.742352	-3.935499	2.633367	62.H	3.874986	3.122492	-0.294136
63.C	-1.004999	-4.847453	3.650672	63.C	8.865658	0.331547	0.013165
64.H	-0.244381	-5.055564	4.398853	64.H	9.662367	2.865613	-0.621072
65.C	-2.242263	-5.477610	3.697954	65.H	8.196209	4.870266	-0.870134
66.H	-2.465561	-6.192737	4.486522	66.H	5.733410	4.609593	-0.514655
67.C	-3.183544	-5.181308	2.718449	67.H	3.390594	-3.210762	-3.994529
68.H	-4.165593	-5.646632	2.712725	68.H	2.759707	-0.861620	-3.435784
69.C	-2.843811	-4.275209	1.726576	69.H	-1.536554	-2.076822	0.991247
70.H	-3.547489	-4.025481	0.936635	70.H	1.694553	2.513486	0.524091
71.N	1.650114	3.660065	1.677473	71.H	-9.842063	-1.164448	-0.186441
72.N	-1.650114	-3.660065	1.677473	72.H	-8.776732	-0.309466	0.948002
73.N	1.772137	-4.588465	-1.521704	73.H	8.569030	-0.425111	-0.722102
74.C	0.533280	-3.145781	2.589049	74.H	-8.621835	-0.027129	-0.786290
75.H	0.288400	-2.140484	2.948711	75.H	-6.601290	2.916392	-0.794310
76.H	1.254612	-3.567761	3.304770	76.H	6.188205	-3.075962	-0.734219
77.N	1.615388	3.099334	-1.583103	77.N	5.902681	-1.148686	2.170581
78.N	-1.615388	-3.099334	-1.583103	78.N	-6.125234	1.096848	2.164916
79.C	2.081518	3.374261	-2.609277	79.C	-6.303947	1.638521	3.178737
80.C	2.646369	3.716787	-3.889163	80.C	-6.529482	2.305581	4.435543

81.C	-2.081518	-3.374261	-2.609277	81.C	5.989692	-1.695417	3.193669
82.C	-2.646369	-3.716787	-3.889163	82.C	6.099660	-2.370343	4.461716
83.H	-2.478369	-2.901496	-4.600217	83.H	-5.582128	2.689399	4.827978
84.H	-3.723039	-3.884105	-3.786421	84.H	-6.959739	1.604472	5.158007
85.H	3.723039	3.884105	-3.786421	85.H	-7.219806	3.143458	4.293034
86.H	2.179138	4.630914	-4.268914	86.H	6.446168	-1.669768	5.228474
87.H	2.478369	2.901496	-4.600217	87.H	6.813722	-3.196562	4.381855
88.H	-2.179138	-4.630914	-4.268914	88.H	5.124097	-2.770961	4.756044
$[Cu^{II}_2(\mathbf{L^3S})_2(CH_3CN)_2]^{2+}$ (–xxxxx.xx kcal mol^{-1}) E^T = –13012.16 kcal mol^{-1} E^{BS} = –13012.83 kcal mol^{-1} E^S = –13013.50 kcal mol^{-1} Conformation **A**, no symmetry				$[Cu^{I}_2(\mathbf{L^3SSL^3})_2(CH_3CN)_2]^{2+}$ (–13023.39 kcal mol^{-1}) Conformation **B**, symmetry C_2			
1.Cu	-1.658615	0.596832	0.409150	1.Cu	0.829294	-2.626945	-0.078168
2.Cu	1.658988	-0.599058	0.409512	2.Cu	-0.829294	2.626945	-0.078168
3.S	-0.550277	-1.377107	0.244493	3.S	-0.974546	0.307501	-0.112087
4.S	0.550472	1.374700	0.244053	4.S	0.974546	-0.307501	-0.112087
5.N	-5.345260	-0.270010	-1.030657	5.C	-2.149029	-2.027052	-1.260287
6.N	-2.612493	2.150026	1.353232	6.H	-2.636923	-2.106960	-0.286730
7.N	-3.178181	-0.556933	1.583007	7.H	-2.910132	-2.268214	-2.022915
8.N	5.345941	0.274067	-1.033778	8.C	-1.780067	-0.570479	-1.484146
9.N	2.612728	-2.151882	1.354721	9.H	-2.725290	-0.019420	-1.574452
10.N	3.178400	0.555911	1.582360	10.H	-1.234370	-0.380891	-2.411541
11.C	-5.805601	-0.709402	-2.209504	11.C	2.149029	2.027052	-1.260287
12.C	-6.005877	-2.070770	-2.465063	12.H	2.636923	2.106960	-0.286730
13.C	-5.759412	-2.986637	-1.454439	13.H	2.910132	2.268214	-2.022915
14.C	-5.298347	-2.527476	-0.226184	14.C	1.780067	0.570479	-1.484146
15.C	-5.074907	-1.159030	-0.064646	15.H	2.725290	0.019420	-1.574452
16.C	-4.634706	-0.569655	1.254741	16.H	1.234370	0.380891	-2.411541
17.C	-2.701547	3.456332	1.021709	17.C	-2.181840	-4.717463	0.318394
18.C	-3.312434	4.364806	1.889646	18.C	-3.465504	-4.376057	0.748470
19.C	-3.850080	3.927991	3.089462	19.H	-4.150677	-3.837030	0.099049
20.C	-3.783295	2.577263	3.402107	20.C	-3.865906	-4.761945	2.021466
21.C	-3.154078	1.721366	2.510111	21.H	-4.858156	-4.505847	2.387484
22.C	-3.010424	0.256554	2.800111	22.C	-2.988534	-5.488601	2.812414
23.C	-2.678755	-1.927997	1.804344	23.H	-3.277522	-5.807204	3.811976
24.C	-1.169209	-2.022731	1.816910	24.C	-1.734882	-5.829321	2.294749
25.C	5.805371	0.716077	-2.212021	25.C	-0.774739	-6.678915	3.072819
26.C	6.001727	2.078227	-2.466321	26.H	-0.842196	-7.723994	2.744004
27.C	5.752859	2.992341	-1.454653	27.H	-0.988296	-6.656066	4.144401
28.C	5.293285	2.530569	-0.226832	28.H	0.254785	-6.353944	2.901026
29.C	5.073244	1.161326	-0.066839	29.C	-1.687087	-4.386921	-1.069501
30.C	4.634572	0.569432	1.251901	30.H	-0.918513	-5.123956	-1.310267
31.C	2.700395	-3.458637	1.024651	31.H	-2.512906	-4.520234	-1.786898
32.C	3.310931	-4.366822	1.893240	32.C	0.856229	-3.827295	-2.642296
33.C	3.849957	-3.929244	3.092085	33.C	1.240244	-4.578234	-3.745793
34.C	3.784976	-2.578000	3.403036	34.H	0.561918	-4.698849	-4.586270
35.C	3.155759	-1.722516	2.510701	35.C	2.501724	-5.157828	-3.751351
36.C	3.013754	-0.257318	2.799996	36.H	2.834148	-5.748885	-4.601551
37.C	2.677764	1.926416	1.804947	37.C	3.330192	-4.974969	-2.653556
38.C	1.168095	2.019438	1.817395	38.H	4.323442	-5.415624	-2.629111
39.C	-6.143831	0.328320	-3.238119	39.C	2.885193	-4.223672	-1.566078
40.H	-6.372511	-2.401310	-3.435095	40.C	3.740768	-4.019118	-0.359929
41.H	-5.935333	-4.048471	-1.614136	41.H	3.836921	-2.954158	-0.123895
42.H	-5.139749	-3.225024	0.592532	42.H	4.738722	-4.434304	-0.510764

43.H	-5.154280	-1.093641	2.071476
44.H	-4.970112	0.468805	1.263513
45.C	-2.166092	3.912090	-0.292937
46.H	-3.363913	5.413324	1.608038
47.H	-4.328760	4.629643	3.768392
48.H	-4.211544	2.187669	4.321339
49.H	-3.715853	-0.047339	3.584506
50.H	-2.005663	0.077987	3.196987
51.H	-3.090177	-2.340166	2.738431
52.H	-3.045898	-2.542256	0.981140
53.H	-0.880423	-3.075490	1.903833
54.H	-0.715584	-1.490908	2.658678
55.C	6.146925	-0.319619	-3.241613
56.H	6.367342	2.410822	-3.436036
57.H	5.925719	4.054827	-1.613360
58.H	5.133243	3.226401	0.593009
59.H	5.155088	1.091543	2.069134
60.H	4.969591	-0.469177	1.257609
61.C	2.163992	-3.915550	-0.289166
62.H	3.360917	-5.415750	1.612791
63.H	4.328630	-4.630488	3.771443
64.H	4.214911	-2.187669	4.321164
65.H	3.722082	0.046672	3.581676
66.H	2.010343	-0.077537	3.199944
67.H	3.089100	2.338449	2.739120
68.H	3.043973	2.541831	0.982248
69.H	0.878061	3.071763	1.904533
70.H	0.714294	1.486459	2.658360
71.H	1.183695	-3.480671	-0.496520
72.H	2.087304	-5.003547	-0.316722
73.H	2.833014	-3.601295	-1.097860
74.H	-7.205485	0.598778	-3.168016
75.H	-5.972226	-0.038217	-4.254156
76.H	-5.561698	1.237667	-3.074351
77.H	-2.834130	3.594371	-1.101085
78.H	-1.184621	3.479303	-0.499196
79.H	-2.092183	5.000212	-0.322695
80.H	7.208641	-0.589233	-3.169335
81.H	5.977455	0.048322	-4.257481
82.H	5.565351	-1.229823	-3.080820
83.N	-2.054720	0.810178	-1.791003
84.N	2.055879	-0.814897	-1.788707
85.C	-2.030590	0.796610	-2.948702
86.C	-2.009917	0.779576	-4.391398
87.C	2.032954	-0.801454	-2.946435
88.C	2.014713	-0.784600	-4.389073
89.H	-2.880023	1.313927	-4.784629
90.H	-2.034422	-0.253651	-4.751860
91.H	-1.103536	1.270531	-4.758394
92.H	2.038568	0.248464	-4.749991
93.H	1.109671	-1.276845	-4.757586
94.H	2.886100	-1.318364	-4.780098

43.H	3.294376	-4.504780	0.514970
44.C	-0.451653	-3.085305	-2.625928
45.H	-0.234037	-2.058023	-2.935395
46.H	-1.129171	-3.502336	-3.384553
47.C	2.181840	4.717463	0.318394
48.C	3.465504	4.376057	0.748470
49.H	4.150677	3.837030	0.099049
50.C	3.865906	4.761945	2.021466
51.H	4.858156	4.505847	2.387484
52.C	2.988534	5.488601	2.812414
53.H	3.277522	5.807204	3.811976
54.C	1.734882	5.829321	2.294749
55.C	0.774739	6.678915	3.072819
56.H	0.842196	7.723994	2.744004
57.H	0.988296	6.656066	4.144401
58.H	-0.254785	6.353944	2.901026
59.C	1.687087	4.386921	-1.069501
60.H	0.918513	5.123956	-1.310267
61.H	2.512906	4.520234	-1.786898
62.C	-0.856229	3.827295	-2.642296
63.C	-1.240244	4.578234	-3.745793
64.H	-0.561918	4.698849	-4.586270
65.C	-2.501724	5.157828	-3.751351
66.H	-2.834148	5.748885	-4.601551
67.C	-3.330192	4.974969	-2.653556
68.H	-4.323442	5.415624	-2.629111
69.C	-2.885193	4.223672	-1.566078
70.C	-3.740768	4.019118	-0.359929
71.H	-3.836921	2.954158	-0.123895
72.H	-4.738722	4.434304	-0.510764
73.H	-3.294376	4.504780	0.514970
74.C	0.451653	3.085305	-2.625928
75.H	0.234037	2.058023	-2.935395
76.H	1.129171	3.502336	-3.384553
77.N	-1.079731	-3.043296	-1.298337
78.N	1.079731	3.043296	-1.298337
79.N	-1.346533	-5.446557	1.070510
80.N	1.656564	-3.659944	-1.571931
81.N	1.346533	5.446557	1.070510
82.N	-1.656564	3.659944	-1.571931
83.N	-0.912977	2.832044	1.793610
84.N	0.912977	-2.832044	1.793610
85.C	-0.957896	2.818437	2.953098
86.C	-1.005336	2.802232	4.393256
87.C	0.957896	-2.818437	2.953098
88.C	1.005336	-2.802232	4.393256
89.H	1.409574	-3.747938	4.768095
90.H	-0.001714	-2.658761	4.798869
91.H	0.001714	2.658761	4.798869
92.H	-1.648659	1.985068	4.735070
93.H	-1.409574	3.747938	4.768095
94.H	1.648659	-1.985068	4.735070

$[Cu^{I}_2(\mathbf{L^3SSL^3})_2(CH_3CN)_2]^{2+}$ (–13044.03 kcal mol^{-1}) S uncoordinated, no symmetry				$[Cu^{II}_2(\mathbf{L^4S})_2(CH_3CN)_2]^{2+}$ E^T = –12231.86 kcal mol^{-1} E^{BS} = –12232.96 kcal mol^{-1} E^S = –12234.06 kcal mol^{-1} Conformation **A**, no symmetry			
1.Cu	5.703133	-0.347604	0.561112	1.Cu	-0.258963	1.627707	1.106876
2.Cu	-5.760449	0.285860	0.561209	2.Cu	0.256886	-1.626884	1.104712
3.S	0.297804	1.161919	-0.764777	3.S	1.367510	0.274386	1.893211
4.S	-0.220568	-0.791296	-0.682024	4.S	-1.367835	-0.274370	1.895409
5.N	6.698731	1.338710	0.001852	5.N	-0.134505	3.363004	2.468615
6.N	5.057377	-1.525044	-0.965518	6.N	-0.312965	5.499829	-2.502857
7.N	3.948075	0.914206	-0.106700	7.N	1.453520	2.895006	0.217767
8.N	-6.512194	-1.521235	0.005766	8.N	0.134725	-3.362075	2.466395
9.N	-5.267216	1.548627	-0.958781	9.N	0.327328	-5.483255	-2.500418
10.N	-3.837519	-0.717411	-0.079926	10.N	-1.459466	-2.894778	0.218523
11.C	8.030880	1.447834	-0.200232	11.C	-0.689041	3.457223	3.682800
12.C	8.602275	2.658474	-0.590121	12.C	-0.558100	4.579724	4.486622
13.C	7.793525	3.768227	-0.790372	13.C	0.193783	5.647810	4.008860
14.C	6.425297	3.643616	-0.594723	14.C	0.780639	5.550422	2.754456
15.C	5.914559	2.416005	-0.189441	15.C	0.589540	4.389551	2.006809
16.H	-3.044332	-0.267192	1.776149	16.H	-0.305176	3.109769	-1.922351
17.C	4.441760	2.267723	0.106353	17.C	-0.269465	6.790923	-2.850992
18.C	5.382946	-2.816812	-1.195964	18.C	0.873056	7.434470	-3.309431
19.C	4.794680	-3.531441	-2.239837	19.C	2.038225	6.683347	-3.426060
20.C	3.857612	-2.914308	-3.055605	20.C	2.009852	5.341146	-3.072639
21.C	3.527059	-1.588815	-2.810364	21.C	0.816086	4.782070	-2.602687
22.C	4.149981	-0.924787	-1.760693	22.C	-1.741096	-2.760629	-1.236078
23.H	-3.984522	-2.356593	1.175388	23.C	2.655011	2.441617	0.956935
24.C	3.894648	0.542036	-1.520413	24.C	2.800139	0.937959	1.008447
25.C	2.756070	0.587625	0.682127	25.C	0.691119	-3.455548	3.679791
26.C	1.499727	1.453666	0.575766	26.C	0.559162	-4.576584	4.485530
27.C	-7.814797	-1.815268	-0.204134	27.C	-0.195732	-5.643836	4.010698
28.C	-8.206544	-3.084397	-0.629129	28.C	-0.784408	-5.547241	2.757061
29.C	-7.246900	-4.060399	-0.857149	29.C	-0.592070	-4.387923	2.007307
30.C	-5.911079	-3.747607	-0.647566	30.H	-2.580968	-2.816431	1.985888
31.C	-5.582280	-2.471472	-0.205636	31.C	0.298037	-6.776255	-2.842482
32.C	-6.896520	3.255834	-0.338701	32.C	-0.838525	-7.435970	-3.292815
33.C	-4.148626	-2.126721	0.114800	33.C	-2.013286	-6.699678	-3.407780
34.C	-5.766574	2.782694	-1.193081	34.C	-1.999724	-5.355643	-3.060442
35.C	-5.242727	3.590936	-2.202823	35.C	-0.810937	-4.779941	-2.598177
36.C	-4.190052	3.129182	-2.979105	36.H	-0.382874	-4.655476	-0.076174
37.C	-3.684896	1.859556	-2.733957	37.C	-2.658304	-2.440879	0.961428
38.C	-4.252535	1.095602	-1.721577	38.C	-2.802821	-0.937095	1.013825
39.H	-5.662950	4.579487	-2.369525	39.H	-1.261596	2.595727	4.019927
40.C	-3.807980	-0.326638	-1.489814	40.H	-1.030695	4.609515	5.464974
41.C	-2.710649	-0.242863	0.731330	41.H	0.328164	6.545167	4.608946
42.C	-1.378056	-0.989794	0.710073	42.H	1.381858	6.364434	2.356326
43.C	8.864823	0.224749	-0.003396	43.H	-0.899220	-2.743989	-3.158865
44.H	9.677199	2.720958	-0.739755	44.H	-3.563190	-2.885068	0.517882
45.H	8.223799	4.717266	-1.101980	45.H	-1.207116	7.340165	-2.756400
46.H	5.756926	4.486592	-0.751206	46.H	0.846730	8.489284	-3.573594
47.H	-2.833057	-0.495771	-1.961113	47.H	2.958025	7.135209	-3.793029
48.H	-4.523824	-0.968413	-2.020244	48.H	2.907570	4.733663	-3.169630
49.H	3.891502	3.024671	-0.469711	49.H	2.717872	3.196027	-1.442997
50.H	4.289505	2.511198	1.165541	50.H	2.018445	4.926865	0.508095

51.C	6.389327	-3.456033	-0.296436	51.H	3.558075	2.886196	0.510369
52.H	5.074318	-4.569153	-2.403027	52.H	2.581055	2.817303	1.981634
53.H	3.386881	-3.460935	-3.869607	53.H	3.695046	0.678554	1.583414
54.H	2.799098	-1.069302	-3.428094	54.H	2.890273	0.478646	0.021341
55.H	-2.543494	0.812060	0.489020	55.H	1.266328	-2.594841	4.014388
56.H	-0.836715	-0.731688	1.626620	56.H	1.033299	-4.605919	5.463177
57.H	2.960257	0.843485	-2.008258	57.H	-0.331181	-6.539832	4.612581
58.H	4.698634	1.088163	-2.031109	58.H	-1.388385	-6.360435	2.361344
59.H	2.493464	-0.456591	0.478794	59.H	-3.696521	-0.678043	1.590874
60.H	3.061816	0.626450	1.734452	60.H	-2.895332	-0.477301	0.027141
61.H	0.954686	1.375601	1.522393	61.H	1.242825	-7.313478	-2.749576
62.H	-3.491257	-2.797798	-0.455467	62.H	-0.800403	-8.491572	-3.552332
63.C	-8.817207	-0.732224	0.024839	63.H	-2.928966	-7.164399	-3.768958
64.H	-9.261461	-3.296189	-0.784268	64.H	-2.905062	-4.759491	-3.155965
65.H	-7.536248	-5.051988	-1.197643	65.H	0.378251	4.656682	-0.076561
66.H	-5.128590	-4.482142	-0.820549	66.H	-2.022063	-4.927399	0.510626
67.H	-3.766836	3.751465	-3.764402	67.C	1.140569	4.273060	0.608634
68.H	-2.864953	1.458401	-3.324061	68.C	-1.144819	-4.272432	0.609764
69.H	1.733305	2.517244	0.448911	69.H	0.293199	-3.090731	-1.931556
70.H	-1.514056	-2.077552	0.740950	70.H	0.875058	2.742801	-3.155442
71.H	-6.593798	3.302457	0.712524	71.H	1.824763	1.687514	-1.430503
72.H	-7.747366	2.569832	-0.399457	72.C	1.729829	2.758629	-1.237713
73.H	-7.231677	4.248106	-0.645778	73.C	-0.729513	-3.314565	-2.236277
74.H	8.653982	-0.510825	-0.788062	74.C	0.718403	3.319372	-2.234282
75.H	8.644942	-0.249593	0.958125	75.H	-1.842484	-1.689960	-1.428729
76.H	9.929520	0.462211	-0.041835	76.H	-2.727915	-3.202597	-1.438532
77.H	6.029397	-3.468413	0.737690	77.N	1.788100	-2.359429	0.098392
78.H	7.331841	-2.899516	-0.303371	78.N	-1.794617	2.360916	0.106164
79.H	6.593813	-4.483309	-0.603225	79.C	2.752592	-2.857468	-0.304164
80.H	-9.835855	-1.122258	-0.015633	80.C	3.939206	-3.488459	-0.815109
81.H	-8.722417	0.044555	-0.742536	81.C	-2.764330	2.856438	-0.287055
82.H	-8.661874	-0.253132	0.996527	82.C	-3.958475	3.484068	-0.784267
83.N	5.815322	-0.915225	2.329621	83.H	-4.498413	3.952582	0.044730
84.N	-5.946048	0.853708	2.325353	84.H	-4.601211	2.736826	-1.259510
85.C	-6.037010	1.155984	3.444820	85.H	4.662591	-2.727497	-1.123375
86.C	-6.152539	1.531678	4.830978	86.H	3.678714	-4.110119	-1.677670
87.C	5.871159	-1.211997	3.452935	87.H	4.384776	-4.115573	-0.036331
88.C	5.942154	-1.581160	4.843907	88.H	-3.688468	4.249484	-1.518885
89.H	-7.081596	1.130692	5.249244				
90.H	-6.158009	2.622588	4.924408				
91.H	-5.305294	1.129286	5.395869				
92.H	5.024142	-1.274513	5.356004				
93.H	6.796771	-1.087730	5.318401				
94.H	6.056420	-2.666076	4.938046				

$[Cu^{I}_2(\mathbf{L^4SSL^4})_2(CH_3CN)_2]^{2+}$ (–12235.92 kcal mol^{-1}) Conformation **B**, no symmetry				$[Cu^{I}_2(\mathbf{L^4SSL^4})_2(CH_3CN)_2]^{2+}$ (–12253.41 kcal mol^{-1}) Conformation **C**, no symmetry			
1.Cu	0.786785	2.576146	-0.428772	1.Cu	-0.013360	-0.179125	2.301368
2.Cu	-0.785440	-2.577860	-0.438546	2.Cu	0.070167	0.027585	-2.336543
3.S	-0.911394	-0.490027	-1.297491	3.S	-1.644442	0.267296	0.854205
4.S	0.922925	0.490517	-1.285775	4.S	-1.363047	-0.904421	-0.867814
5.C	-2.156940	1.967320	-0.930512	5.C	-2.626543	-1.838103	2.447693
6.H	-1.869596	1.891914	-1.982556	6.H	-3.524830	-2.208454	2.970756
7.H	-3.239407	2.166264	-0.916508	7.H	-2.387438	-2.565617	1.668327
8.C	-1.893760	0.622699	-0.252186	8.C	-2.989814	-0.534200	1.774559
9.H	-2.830765	0.074987	-0.104338	9.H	-3.286326	0.252663	2.478591
10.H	-1.401552	0.712632	0.719273	10.H	-3.842878	-0.683170	1.106219

11.C	2.160954	-1.969977	-0.920837	11.C	-2.844634	0.815679	-2.485311
12.H	1.877687	-1.889142	-1.973597	12.H	-3.801466	0.970749	-3.007198
13.H	3.243551	-2.169244	-0.903977	13.H	-2.815232	1.551183	-1.677238
14.C	1.893382	-0.629011	-0.236409	14.C	-2.836005	-0.563570	-1.872349
15.H	2.828987	-0.082907	-0.073851	15.H	-2.808892	-1.362549	-2.623423
16.H	1.390364	-0.725276	0.728874	16.H	-3.732818	-0.730465	-1.268927
17.C	0.706534	5.010053	-2.127286	17.C	-0.587685	-4.063000	2.647368
18.C	1.116723	5.908060	-3.113652	18.C	-1.482783	-4.955027	2.047881
19.H	0.566663	6.835122	-3.254614	19.H	-2.530414	-4.966745	2.341331
20.C	2.220792	5.613079	-3.901759	20.C	-1.017966	-5.843398	1.086288
21.H	2.550395	6.307976	-4.671384	21.H	-1.699218	-6.546484	0.610868
22.C	2.892833	4.414771	-3.687771	22.C	0.330999	-5.820723	0.755880
23.H	3.763209	4.134460	-4.275081	23.H	0.745540	-6.499815	0.013889
24.C	2.425945	3.568039	-2.695921	24.C	1.150440	-4.917051	1.423850
25.H	2.926616	2.623323	-2.501379	25.H	2.220567	-4.892809	1.212282
26.N	0.757897	-4.684182	2.557776	26.C	-1.041193	-3.128574	3.741717
27.N	-0.776813	4.677573	2.564355	27.H	-1.867804	-3.612397	4.286614
28.N	-1.354669	-3.846679	-1.936894	28.H	-0.212263	-3.021006	4.444184
29.C	-2.102836	3.427854	0.948926	29.C	-0.364318	0.961552	5.027128
30.H	-2.557457	4.737986	-1.166854	30.C	-0.394404	1.961171	6.000230
31.C	2.097902	-3.437577	0.952031	31.H	-0.625767	1.698445	7.029529
32.C	-1.779905	4.711500	1.675673	32.C	-0.132790	3.278566	5.648755
33.C	-2.578870	5.846043	1.500524	33.H	-0.155181	4.064837	6.400395
34.H	-3.416084	5.831192	0.806684	34.C	0.153478	3.570962	4.319731
35.C	-2.304759	6.991861	2.235971	35.H	0.364415	4.584542	3.989309
36.H	-2.916852	7.883386	2.114083	36.C	0.164147	2.529986	3.406708
37.C	-1.245492	6.970326	3.134365	37.H	0.384787	2.717789	2.358612
38.H	-0.992866	7.839991	3.736787	38.C	-0.660090	-0.466809	5.370340
39.C	-0.524086	5.787999	3.262010	39.H	-0.865704	-0.530928	6.441501
40.H	0.296747	5.726017	3.977666	40.H	0.239311	-1.070077	5.197812
41.N	1.433363	-3.130529	-0.356279	41.C	-1.845609	-1.059777	4.602506
42.N	1.360678	3.847432	-1.925143	42.H	-2.392211	-1.751085	5.261977
43.N	-1.431994	3.125634	-0.357396	43.H	-2.543558	-0.256163	4.355634
44.C	0.496214	-5.794532	3.252075	44.C	-1.083894	0.608565	-5.842088
45.H	0.953992	-7.849171	3.726453	45.C	-0.972884	1.689461	-6.721688
46.H	-0.329096	-5.730310	3.962375	46.H	-1.623943	2.554970	-6.618603
47.C	-0.697824	-5.007237	-2.142557	47.C	-0.034750	1.639237	-7.745853
48.C	-1.101070	-5.899330	-3.137093	48.H	0.065261	2.469621	-8.442100
49.H	-0.548898	-6.824688	-3.280897	49.C	0.760607	0.506634	-7.866414
50.C	-2.200951	-5.600804	-3.929705	50.H	1.506832	0.416671	-8.652665
51.H	-2.524882	-6.291179	-4.705786	51.C	0.560553	-0.529986	-6.960548
52.C	-2.876376	-4.405195	-3.711413	52.H	1.148057	-1.445528	-7.041421
53.H	-3.744111	-4.122557	-4.301502	53.C	-2.126426	0.592093	-4.752087
54.C	-2.416538	-3.564244	-2.711464	54.H	-2.988107	1.192673	-5.081395
55.H	-2.920018	-2.621800	-2.513275	55.H	-2.467882	-0.439669	-4.646201
56.C	1.588868	-4.254860	-1.313143	56.C	0.768539	2.888076	-2.175780
57.H	-0.894850	6.267643	-1.555724	57.C	1.614419	3.998371	-2.143399
58.C	0.478337	-5.306273	-1.264029	58.H	1.185133	4.997232	-2.141640
59.C	2.279405	-7.003639	2.236191	59.C	2.990523	3.821674	-2.110258
60.H	2.889003	-7.897315	2.117396	60.H	3.656530	4.681280	-2.079994
61.C	1.213954	-6.979444	3.127250	61.C	3.496606	2.526214	-2.118804
62.C	1.766518	-4.720875	1.675478	62.H	4.565189	2.329546	-2.095843
63.C	2.562645	-5.857935	1.503950	63.C	2.600533	1.471833	-2.161117
64.H	3.404544	-5.844813	0.815692	64.H	2.956976	0.445311	-2.180610
65.C	-0.473916	5.305263	-1.253256	65.C	-0.719285	3.056557	-2.195701
66.C	-1.583292	4.253232	-1.311237	66.H	-0.947989	4.123602	-2.129644

67.H	-3.188527	3.421001	0.768384	67.H	-1.136921	2.602432	-1.288513
68.H	-1.877032	2.604999	1.630503	68.C	-1.423495	2.509067	-3.437835
69.H	-0.124570	5.431002	-0.222489	69.H	-2.360158	3.068684	-3.587785
70.H	-1.606144	3.829216	-2.319075	70.H	-0.795612	2.703090	-4.310486
71.H	3.184141	-3.435275	0.775081	71.N	-1.474910	-1.758335	3.353998
72.H	1.872895	-2.614719	1.633861	72.N	-1.711707	1.061052	-3.399339
73.H	1.617007	-3.828036	-2.319779	73.N	0.719541	-4.059947	2.352571
74.H	2.562064	-4.740836	-1.165505	74.N	-0.084694	1.251475	3.739228
75.H	0.124192	-5.435195	-0.235314	75.N	-0.339285	-0.497846	-5.974784
76.H	0.900131	-6.267812	-1.568010	76.N	1.265612	1.632553	-2.183579
77.N	-1.814422	-2.752677	1.155155	77.N	1.005399	-1.531165	-2.970254
78.N	1.811633	2.762021	1.166512	78.N	1.740952	-0.701207	1.845759
79.C	2.475101	2.924297	2.103762	79.C	2.833022	-0.961835	1.556015
80.C	3.285346	3.144240	3.273804	80.C	4.185025	-1.300229	1.192539
81.C	-2.470414	-2.913279	2.097940	81.C	1.548716	-2.536214	-3.171470
82.C	-3.271163	-3.126663	3.275710	82.C	2.218762	-3.787396	-3.420855
83.H	-3.858721	-4.043247	3.161652	83.H	1.919069	-4.182439	-4.396779
84.H	-3.951911	-2.282669	3.424149	84.H	1.948809	-4.514941	-2.648474
85.H	3.967604	3.982320	3.098422	85.H	4.620352	-0.502263	0.582733
86.H	3.870873	2.247264	3.499000	86.H	4.198336	-2.236186	0.624276
87.H	2.642558	3.374010	4.129934	87.H	4.791658	-1.423859	2.095084
88.H	-2.621687	-3.219646	4.152295	88.H	3.303268	-3.639965	-3.413752
$[Cu^{I}_2(\mathbf{L}^{4}\mathbf{SSL}^{4})_2(CH_3CN)_2]^{2+}$ (–12261.70 kcal mol^{-1}) S uncoordinated, no symmetry				$[Cu^{II}_2(\mathbf{L}^{5}\mathbf{S})_2(CH_3CN)_2]^{2+}$ E^{T} = –12988.18 kcal mol^{-1} E^{BS} = –12989.20 kcal mol^{-1} E^{S} = –12990.22 kcal mol^{-1} Conformation **A**, no symmetry			
1.Cu	0.193167	4.210591	0.842059	1.Cu	0.294901	-1.674861	1.435455
2.Cu	-0.118980	-4.202541	0.849050	2.Cu	-0.295217	1.668469	1.430404
3.S	-0.453212	0.799052	-3.293654	3.S	-1.370597	-0.354924	2.121430
4.S	0.781673	-0.789150	-3.153034	4.S	1.372571	0.351850	2.118481
5.C	-0.635621	3.288643	-2.255248	5.N	1.061305	-3.096741	3.007972
6.H	-0.653860	3.529700	-3.330943	6.N	-0.060413	-3.445764	-3.408299
7.H	-1.675317	3.142869	-1.950257	7.N	-1.360150	-3.104138	0.764296
8.C	0.123869	1.987242	-2.031854	8.N	-1.060831	3.095628	3.003768
9.H	-0.065260	1.590058	-1.031274	9.N	0.058309	3.445096	-3.416214
10.H	1.200757	2.106247	-2.172856	10.N	1.360529	3.098733	0.756069
11.C	0.585627	-3.337656	-2.282697	11.C	1.727694	-2.637095	4.075597
12.H	0.543902	-3.580593	-3.356685	12.C	2.366771	-3.458113	4.992519
13.H	1.644501	-3.269964	-2.016230	13.C	2.318909	-4.832092	4.788847
14.C	-0.057396	-1.977552	-2.046198	14.C	1.620562	-5.319255	3.692468
15.H	0.059111	-1.664981	-1.005089	15.C	0.995155	-4.427155	2.819287
16.H	-1.116419	-1.960532	-2.314359	16.C	-0.195706	4.923905	1.644181
17.C	2.897890	4.540203	-0.244974	17.C	0.117981	-3.908385	-4.648383
18.C	4.253964	4.252165	-0.415301	18.C	-0.856722	-3.873586	-5.640326
19.H	4.800798	4.719145	-1.230962	19.C	-2.092825	-3.326353	-5.318751
20.C	4.897207	3.390318	0.461655	20.C	-2.294740	-2.840491	-4.032231
21.H	5.955550	3.168821	0.341047	21.C	-1.253263	-2.914815	-3.104146
22.C	4.163517	2.825786	1.500126	22.C	1.306760	3.493224	-0.675465
23.H	4.621749	2.156421	2.223664	23.C	-2.671709	-2.491617	1.106777
24.C	2.818813	3.139141	1.599802	24.C	-2.688737	-0.979651	1.055501
25.H	2.209366	2.716416	2.395314	25.C	-1.728345	2.638458	4.071764
26.N	0.482291	-6.109358	0.776436	26.C	-2.367650	3.461662	4.986629
27.N	-0.502353	6.083312	0.799423	27.C	-2.319314	4.835192	4.780158
28.N	-2.108763	-3.929851	0.922906	28.C	-1.620113	5.319812	3.683200

29.C	-1.122455	5.489617	-1.473991	29.C	-0.994183	4.425623	2.812598
30.H	0.930895	5.662368	-2.872874	30.H	2.930528	2.787870	2.112699
31.C	0.929572	-5.579616	-1.553476	31.C	-0.119447	3.915355	-4.653441
32.C	-0.961254	6.519576	-0.389044	32.C	0.858884	3.895054	-5.642315
33.C	-1.353637	7.840461	-0.584474	33.C	2.097980	3.354128	-5.320834
34.H	-1.709035	8.160781	-1.560899	34.C	2.299426	2.860688	-4.037120
35.C	-1.289964	8.734711	0.477292	35.C	1.254359	2.921110	-3.112041
36.H	-1.593975	9.770517	0.343676	36.H	1.894655	5.097916	1.163014
37.C	-0.826453	8.280790	1.707484	37.C	2.672384	2.484949	1.095506
38.H	-0.756966	8.940525	2.568428	38.C	2.686311	0.973005	1.045216
39.C	-0.438929	6.954786	1.820720	39.H	1.752217	-1.556848	4.196050
40.H	-0.059920	6.564869	2.762287	40.H	2.889830	-3.024020	5.840911
41.N	0.004735	-4.438697	-1.486237	41.H	2.809675	-5.516081	5.478380
42.N	2.185291	3.971772	0.754029	42.H	1.550888	-6.389219	3.511540
43.N	-0.100805	4.433616	-1.490289	43.C	0.198142	-4.928273	1.651067
44.C	0.457136	-6.965742	1.812044	44.H	3.457170	2.886575	0.439261
45.H	0.710950	-8.962233	2.556111	45.H	1.099965	-4.332474	-4.862931
46.H	0.195065	-6.542849	2.778854	46.H	-0.649278	-4.265687	-6.633416
47.C	-2.916781	-4.467859	-0.018496	47.H	-2.891055	-3.277011	-6.056993
48.C	-4.281853	-4.173462	-0.048293	48.H	-3.252475	-2.406482	-3.751712
49.H	-4.906525	-4.616542	-0.820116	49.H	0.753133	-4.748477	0.724379
50.C	-4.834204	-3.334841	0.909351	50.H	-1.553307	-4.119376	2.581570
51.H	-5.898174	-3.108071	0.897154	51.H	-3.458263	-2.895509	0.453964
52.C	-4.000896	-2.799468	1.886040	52.H	-2.925162	-2.793946	2.125227
53.H	-4.383881	-2.148207	2.667576	53.H	-3.646479	-0.615747	1.442937
54.C	-2.654433	-3.118761	1.847456	54.H	-2.557417	-0.581320	0.049309
55.H	-1.969480	-2.719002	2.591788	55.H	-1.753378	1.558469	4.194584
56.C	-1.329102	-4.796241	-2.014684	56.H	-2.891232	3.029490	5.835692
57.H	2.948790	5.994993	-1.778752	57.H	-2.810168	5.520778	5.468006
58.C	-2.314880	-5.409053	-1.017675	58.H	-1.549993	6.389315	3.499937
59.C	1.056093	-8.810802	0.421370	59.H	3.644942	0.606831	1.427985
60.H	1.275315	-9.866136	0.275116	60.H	2.548378	0.574683	0.039839
61.C	0.742742	-8.315944	1.682825	61.H	-1.104166	4.333162	-4.868483
62.C	0.797784	-6.585723	-0.442489	62.H	0.651585	4.292813	-6.633195
63.C	1.080505	-7.931943	-0.654539	63.H	2.898884	3.315614	-6.056859
64.H	1.319934	-8.284001	-1.655098	64.H	3.259445	2.431459	-3.756596
65.C	2.197633	5.506624	-1.150765	65.H	-1.890286	-5.105553	1.162918
66.C	1.158895	4.909127	-2.103213	66.H	1.551183	4.107450	2.576727
67.H	-1.203769	5.991227	-2.449693	67.C	-1.209732	-4.344252	1.569330
68.H	-2.090072	5.004603	-1.293933	68.C	1.210949	4.336580	1.564334
69.H	1.744778	6.295758	-0.541573	69.H	-0.106829	6.010189	1.722712
70.H	1.622900	4.070560	-2.629184	70.H	-0.751003	4.743482	0.717807
71.H	0.869379	-6.092112	-2.524813	71.H	0.111018	-6.014530	1.731334
72.H	1.948456	-5.179396	-1.479186	72.C	-1.307237	-3.495683	-0.668126
73.H	-1.784564	-3.894190	-2.430254	73.C	1.429013	2.383687	-1.711860
74.H	-1.213847	-5.497985	-2.855462	74.C	-1.428391	-2.383501	-1.701666
75.H	-1.848311	-6.242840	-0.482564	75.H	2.107245	4.231370	-0.847266
76.H	-3.126155	-5.842944	-1.609834	76.H	0.359578	4.008809	-0.844347
77.N	0.963880	-2.901237	1.646970	77.H	-2.108680	-4.232384	-0.840329
78.N	-0.787535	2.883771	1.729998	78.H	-0.360541	-4.011925	-0.837590
79.C	-1.424421	2.107423	2.316584	79.H	2.406774	1.900310	-1.654750
80.C	-2.221679	1.150395	3.040942	80.H	0.663267	1.620285	-1.533708
81.C	1.680224	-2.132521	2.145624	81.H	-2.405971	-1.900038	-1.643594
82.C	2.579882	-1.186778	2.756399	82.H	-0.662784	-1.620592	-1.520404
83.H	-1.592005	0.336054	3.413957	83.N	1.672614	-2.183905	0.083618
84.H	-2.996430	0.742950	2.383431	84.N	-1.672269	2.176161	0.078713

85.H	-2.703946	1.640199	3.892856	85.C	-2.514805	2.480051	-0.654798
86.H	3.189127	-1.690650	3.513572	86.C	-3.551436	2.865711	-1.573986
87.H	2.016216	-0.380892	3.237940	87.C	2.513090	-2.491193	-0.650835
88.H	3.243592	-0.765294	1.994161	88.C	3.545976	-2.880974	-1.572480
				89.H	-4.216531	2.017815	-1.764931
				90.H	-3.097484	3.193197	-2.514110
				91.H	-4.135384	3.686429	-1.145543
				92.H	3.093427	-3.144300	-2.533179
				93.H	4.084778	-3.746852	-1.175026
				94.H	4.252556	-2.057254	-1.713686
$[Cu^{I}_2(\mathbf{L^5SSL^5})_2(CH_3CN)_2]^{2+}$ (–13007.77 kcal mol^{-1}) Conformation **B**, no symmetry				$[Cu^{I}_2(\mathbf{L^5SSL^5})_2(CH_3CN)_2]^{2+}$ (–13018.48 kcal mol^{-1}) Conformation **C**, no symmetry			
1.Cu	0.953868	-2.531097	0.341513	1 Cu	2.298484	0.361056	-0.601738
2.Cu	-0.949509	2.530488	0.341245	2 Cu	-2.303351	-0.365087	-0.603590
3.S	-0.972390	0.327911	0.713401	3 S	0.649647	0.816592	0.863862
4.S	0.979444	-0.327976	0.710433	4 S	-0.656637	-0.823054	0.864134
5.C	-2.077521	-2.146556	-0.133571	5 N	4.920599	-4.636801	-0.241159
6.H	-2.218917	-2.211998	0.949681	6 N	3.326719	2.080483	-0.893478
7.H	-3.033263	-2.445720	-0.593925	7 N	3.560470	-0.508468	1.128407
8.C	-1.852410	-0.690034	-0.510169	8 N	-4.901016	4.652141	-0.243903
9.H	-2.832618	-0.196845	-0.518365	9 N	-3.337175	-2.081227	-0.894472
10.H	-1.424893	-0.549584	-1.504591	10 N	-3.564022	0.510524	1.124257
11.C	2.081644	2.146546	-0.137737	11 C	5.540395	-5.812105	-0.084440
12.H	2.225590	2.210639	0.945327	12 C	5.260600	-6.708875	0.940196
13.H	3.035947	2.446674	-0.600336	13 C	4.274458	-6.363300	1.856850
14.C	1.853574	0.690910	-0.516605	14 C	3.622094	-5.145871	1.708784
15.H	2.832845	0.196215	-0.534718	15 C	3.970655	-4.305526	0.647477
16.H	1.418062	0.553652	-1.507885	16 C	3.304799	-2.965567	0.471035
17.C	-1.166771	-6.848249	0.569149	17 C	4.196665	-1.841219	0.995118
18.C	-0.677900	-7.314249	1.792200	18 C	2.711690	3.153587	-1.419947
19.H	0.139256	-6.795959	2.288692	19 C	3.348194	4.361023	-1.650972
20.C	-1.233426	-8.453860	2.360495	20 C	4.693862	4.469243	-1.317019
21.H	-0.860206	-8.833593	3.309894	21 C	5.336137	3.367507	-0.768741
22.C	-2.268189	-9.097581	1.692641	22 C	4.632141	2.179762	-0.565672
23.H	-2.734911	-9.993864	2.094573	23 C	5.294098	0.977945	0.038172
24.C	-2.691338	-8.564215	0.480522	24 C	4.641821	0.482947	1.330970
25.H	-3.496363	-9.044272	-0.076941	25 C	2.671533	-0.518485	2.300302
26.N	-2.088189	3.337769	-1.096057	26 C	1.687655	0.626736	2.341008
27.N	2.089874	-3.340094	-1.096118	27 C	-5.516168	5.829142	-0.081149
28.N	2.164963	7.469250	-0.079794	28 C	-5.238448	6.715934	0.952692
29.C	0.324922	-2.642810	-2.618556	29 C	-4.259093	6.358328	1.872066
30.C	0.943514	3.235375	-1.997838	30 C	-3.611338	5.139285	1.717559
31.C	-0.323349	2.645051	-2.620343	31 C	-3.957842	4.309186	0.647527
32.C	1.601786	-3.379928	-2.354964	32 C	-3.298606	2.966707	0.465394
33.C	2.275230	-4.063116	-3.367870	33 C	-4.194974	1.845591	0.989080
34.H	1.857989	-4.081515	-4.371628	34 C	-2.725307	-3.157159	-1.418816
35.C	3.475821	-4.702256	-3.088774	35 C	-3.365405	-4.363082	-1.647780
36.H	4.012934	-5.232185	-3.872577	36 C	-4.711351	-4.466733	-1.313737
37.C	3.979398	-4.646102	-1.793395	37 C	-5.350476	-3.361981	-0.767830
38.H	4.918545	-5.122518	-1.524648	38 C	-4.643031	-2.175932	-0.567031
39.C	3.253123	-3.961230	-0.833444	39 C	-5.301963	-0.970992	0.034090
40.H	3.609451	-3.898598	0.191661	40 C	-4.649609	-0.476177	1.326837
41.N	1.043577	3.137165	-0.515764	41 C	-2.676310	0.518361	2.297018
42.N	-2.164130	-7.470391	-0.080348	42 C	-1.696350	-0.630197	2.339820
43.N	-1.040955	-3.137017	-0.514873	43 H	6.304772	-6.049539	-0.825144
44.C	-3.252092	3.957021	-0.831882	44 H	5.799969	-7.650524	1.012055

45.H	-4.919103	5.117783	-1.520262	45 H	4.014395	-7.031275	2.675994
46.H	-3.607921	3.892106	0.193199	46 H	2.845178	-4.850013	2.411354
47.C	1.167550	6.847554	0.569915	47 H	2.344787	-2.983304	0.993395
48.C	0.679243	7.313595	1.793120	48 H	3.097349	-2.805782	-0.589749
49.H	-0.137603	6.795349	2.290216	49 H	5.049365	-1.737553	0.318808
50.C	1.234916	8.453337	2.360933	50 H	4.612497	-2.126338	1.975837
51.H	0.861988	8.833266	3.310366	51 H	1.659876	3.028482	-1.666573
52.C	2.269375	9.097054	1.692584	52 H	2.796556	5.192476	-2.081423
53.H	2.736092	9.993569	2.094015	53 H	5.235128	5.399040	-1.478328
54.C	2.692390	8.563126	0.480651	54 H	6.386506	3.420548	-0.493527
55.H	3.497752	9.042610	-0.076878	55 H	5.319851	0.170463	-0.704138
56.C	1.522873	4.422181	0.060762	56 H	6.337274	1.226519	0.248655
57.C	-0.942258	-3.233448	-1.996985	57 H	4.231768	1.339483	1.872428
58.C	0.588928	5.619169	-0.083828	58 H	5.415170	0.048060	1.981432
59.C	-3.476340	4.702374	-3.085572	59 H	2.110262	-1.455673	2.301216
60.H	-4.013982	5.233662	-3.868028	60 H	3.254424	-0.501531	3.235647
61.C	-3.979436	4.643047	-1.790172	61 H	1.050604	0.553161	3.226735
62.C	-1.600734	3.380500	-2.355032	62 H	2.175039	1.608409	2.392794
63.C	-2.275139	4.065106	-3.366291	63 H	-6.275086	6.076355	-0.824222
64.H	-1.858222	4.086017	-4.370105	64 H	-5.774226	7.659244	1.029572
65.C	-0.588066	-5.619939	-0.084913	65 H	-4.000895	7.018234	2.698327
66.C	-1.520782	-4.422153	0.061092	66 H	-2.839722	4.834053	2.421933
67.H	0.160282	-2.595988	-3.699147	67 H	-2.337190	2.978186	0.985377
68.H	0.455888	-1.611220	-2.275133	68 H	-3.094791	2.808693	-0.596314
69.H	1.019671	4.284575	-2.292703	69 H	-5.047016	1.744344	0.311562
70.H	1.806332	2.735214	-2.454467	70 H	-4.610945	2.132759	1.969148
71.H	-0.158629	2.599894	-3.701100	71 H	-1.672976	-3.035695	-1.665257
72.H	-0.453172	1.612781	-2.278633	72 H	-2.816239	-5.196960	-2.076744
73.H	1.695430	4.240664	1.126324	73 H	-5.255244	-5.395299	-1.473123
74.H	2.499230	4.674079	-0.382100	74 H	-6.400932	-3.411552	-0.492212
75.H	-1.018983	-4.282193	-2.293160	75 H	-6.345878	-1.216382	0.244563
76.H	-1.805610	-2.733210	-2.453023	76 H	-5.324937	-0.164214	-0.709130
77.H	0.418199	5.856450	-1.138469	77 H	-4.244105	-1.333301	1.870725
78.H	-0.380367	5.392854	0.365681	78 H	-5.422192	-0.037045	1.975321
79.H	-0.418605	-5.856773	-1.139855	79 H	-3.260366	0.504821	3.231781
80.H	0.382024	-5.394880	0.363437	80 H	-2.111358	1.453351	2.297337
81.H	-1.692614	-4.240914	1.126922	81 H	-2.187022	-1.610305	2.391187
82.H	-2.497690	-4.673005	-0.381353	82 H	-1.060216	-0.558487	3.226459
83.N	-1.211815	3.241233	2.128440	83 N	-2.039525	0.662328	-2.167974
84.N	1.206945	-3.240055	2.130645	84 N	2.039958	-0.669389	-2.165013
85.C	-1.423481	3.526912	3.233533	85 C	1.837355	-1.224427	-3.164317
86.C	-1.681090	3.881772	4.605663	86 C	1.576483	-1.919561	-4.398260
87.C	1.416990	-3.525806	3.235994	87 C	-1.832252	1.212839	-3.168841
88.C	1.670790	-3.880626	4.608834	88 C	-1.565024	1.902703	-4.404249
89.H	1.709828	-4.969689	4.713263	89 H	-0.544969	2.301302	-4.400319
90.H	0.873164	-3.486888	5.247150	90 H	-1.680133	1.213953	-5.247156
91.H	-0.853825	3.541687	5.237230	91 H	1.692069	-1.233432	-5.243283
92.H	-2.607989	3.405952	4.941575	92 H	0.557802	-2.321502	-4.395831
93.H	-1.782881	4.967896	4.699184	93 H	2.284013	-2.746876	-4.514265
94.H	2.628448	-3.457838	4.928767	94 H	-2.269456	2.731911	-4.525422

$[Cu^{I}_2(\mathbf{L^5SSL^5})_2(CH_3CN)_2]^{2+}$ (–13018.74 kcal mol^{-1})
S uncoordinated, symmetry C_2

1.Cu	6.136294	-0.217270	0.183736
2.Cu	-6.136294	0.217270	0.183736
3.S	0.355713	0.947724	0.056883
4.S	-0.355713	-0.947724	0.056883

5.N	7.330050	1.305927	0.657492
6.N	5.986673	-0.773096	-1.733168
7.N	4.041415	1.094574	0.179630
8.N	-7.330050	-1.305927	0.657492
9.N	-5.986673	0.773096	-1.733168
10.N	-4.041415	-1.094574	0.179630
11.C	8.600622	1.329266	0.212439
12.C	9.491891	2.348448	0.502756
13.C	9.050960	3.408609	1.288215
14.C	7.740651	3.396105	1.747499
15.C	6.896569	2.332748	1.422641
16.C	5.473141	2.302060	1.887210
17.C	4.443448	2.388139	0.751301
18.C	6.482280	-1.963795	-2.121027
19.C	6.367362	-2.457945	-3.408918
20.C	5.693770	-1.689213	-4.353126
21.C	5.175754	-0.462099	-3.963190
22.C	5.339282	-0.016916	-2.649060
23.C	4.797654	1.310061	-2.215682
24.C	3.628845	1.242738	-1.222680
25.C	3.051628	0.381689	1.002277
26.C	1.684821	1.014437	1.305800
27.C	-8.600622	-1.329266	0.212439
28.C	-9.491891	-2.348448	0.502756
29.C	-9.050960	-3.408609	1.288215
30.C	-7.740651	-3.396105	1.747499
31.C	-6.896569	-2.332748	1.422641
32.C	-5.473141	-2.302060	1.887210
33.C	-4.443448	-2.388139	0.751301
34.C	-6.482280	1.963795	-2.121027
35.C	-6.367362	2.457945	-3.408918
36.C	-5.693770	1.689213	-4.353126
37.C	-5.175754	0.462099	-3.963190
38.C	-5.339282	0.016916	-2.649060
39.C	-4.797654	-1.310061	-2.215682
40.C	-3.628845	-1.242738	-1.222680
41.C	-3.051628	-0.381689	1.002277
42.C	-1.684821	-1.014437	1.305800
43.H	8.908532	0.485868	-0.401093
44.H	10.507206	2.306113	0.117173
45.H	9.716066	4.232375	1.539147
46.H	7.362263	4.209463	2.362026
47.H	5.311745	3.144244	2.565318
48.H	5.304306	1.393756	2.478289
49.H	4.862038	2.996405	-0.055852
50.H	3.570141	2.948204	1.114818
51.H	6.997014	-2.538742	-1.354949
52.H	6.798027	-3.424002	-3.659242
53.H	5.575889	-2.038210	-5.376908
54.H	4.646765	0.165316	-4.676617
55.H	5.612784	1.905318	-1.786274
56.H	4.455615	1.848558	-3.103899
57.H	2.988479	0.394942	-1.481241
58.H	3.015096	2.145669	-1.358348
59.H	2.901472	-0.608304	0.558069
60.H	3.517844	0.204275	1.978597

61.H	1.290567	0.562048	2.221544
62.H	1.761353	2.088765	1.512634
63.H	-8.908532	-0.485868	-0.401093
64.H	-10.507206	-2.306113	0.117173
65.H	-9.716066	-4.232375	1.539147
66.H	-7.362263	-4.209463	2.362026
67.H	-5.311745	-3.144244	2.565318
68.H	-5.304306	-1.393756	2.478289
69.H	-4.862038	-2.996405	-0.055852
70.H	-3.570141	-2.948204	1.114818
71.H	-6.997014	2.538742	-1.354949
72.H	-6.798027	3.424002	-3.659242
73.H	-5.575889	2.038210	-5.376908
74.H	-4.646765	-0.165316	-4.676617
75.H	-4.455615	-1.848558	-3.103899
76.H	-5.612784	-1.905318	-1.786274
77.H	-2.988479	-0.394942	-1.481241
78.H	-3.015096	-2.145669	-1.358348
79.H	-3.517844	-0.204275	1.978597
80.H	-2.901472	0.608304	0.558069
81.H	-1.761353	-2.088765	1.512634
82.H	-1.290567	-0.562048	2.221544
83.N	-6.034677	1.627238	1.441193
84.C	-6.080272	2.481894	2.227842
85.C	-6.138350	3.533844	3.210496
86.N	6.034677	-1.627238	1.441193
87.C	6.080272	-2.481894	2.227842
88.C	6.138350	-3.533844	3.210496
89.H	-5.328537	3.406806	3.936346
90.H	-7.097764	3.496078	3.736556
91.H	-6.031830	4.508338	2.723345
92.H	7.097764	-3.496078	3.736556
93.H	6.031830	-4.508338	2.723345
94.H	5.328537	-3.406806	3.936346