

⁵ **Figure S1** ORTEP of **3b** with ellipsoids at 50% level and hydrogen atoms omitted for clarity.

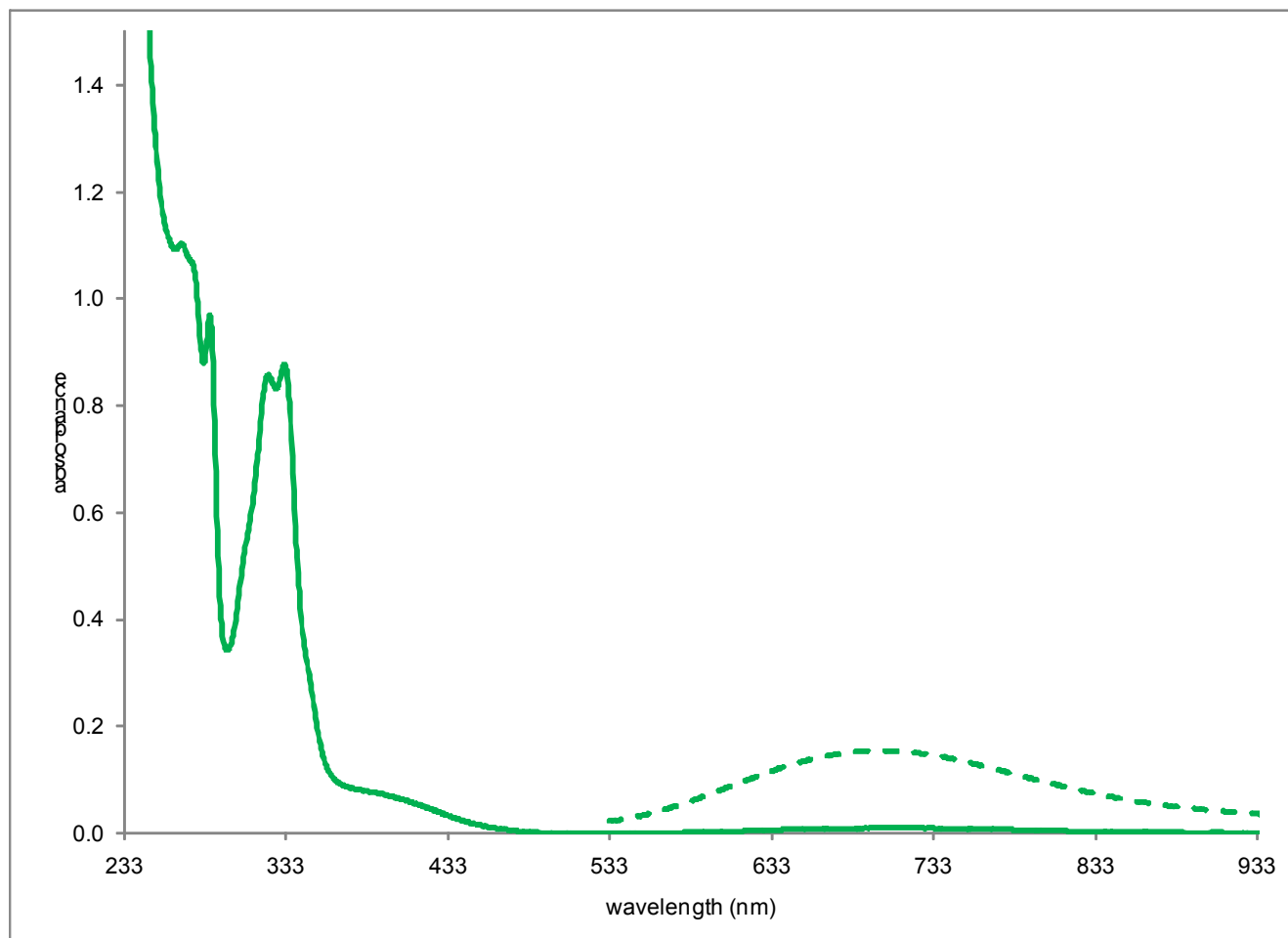


Figure S2 UV-vis absorption spectrum for **2** (18.5 mg) dissolved in CH_2Cl_2 (5 ml) and serially diluted 1 ml solution to 10 ml twice (solid line) and **2** (18.5 mg) dissolved in CH_2Cl_2 (5 ml) (dashed line, insert). See text for discussion of species present.

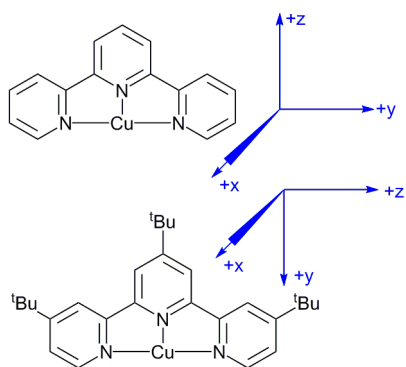


Figure S3 Cartesian coordinate systems used in DFT calculations with Cu at {0,0,0}.

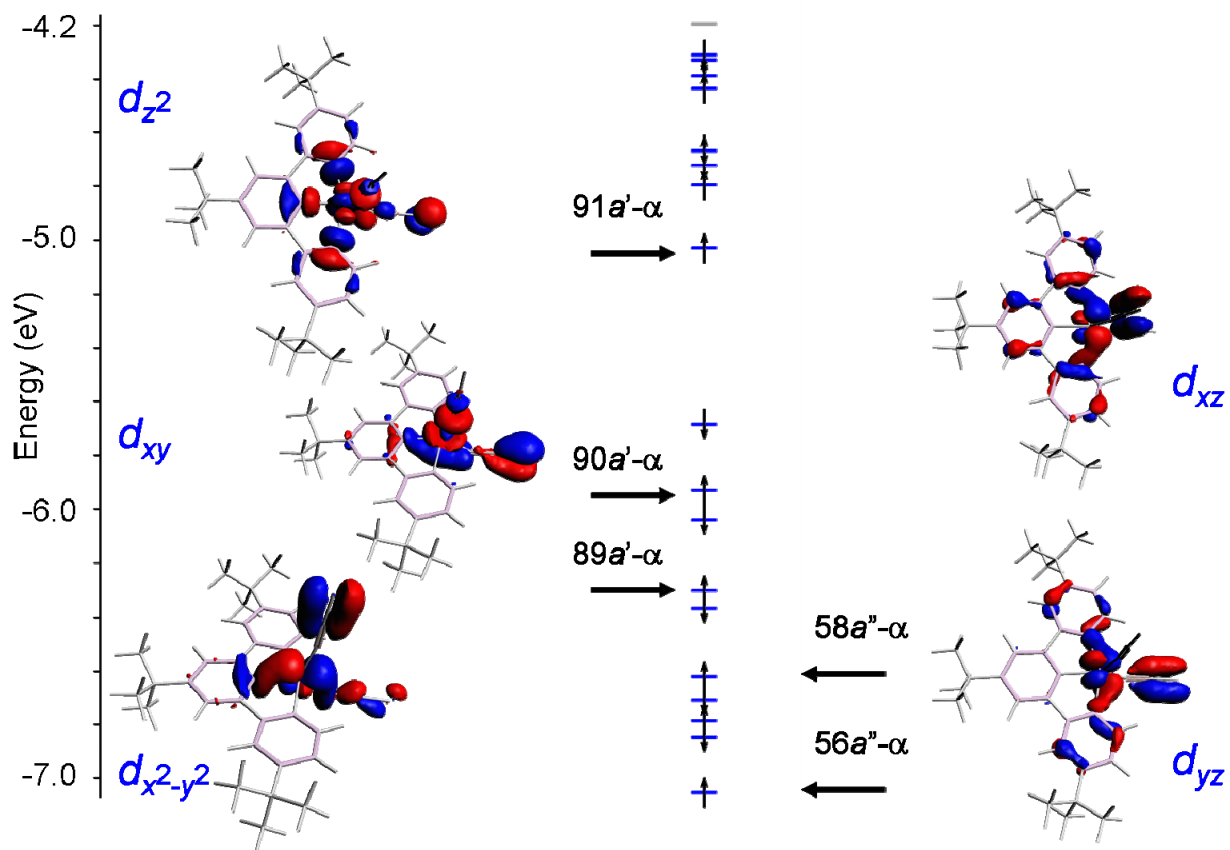


Figure S3 Energy level diagram for $[\text{Cu}(\text{L}_3')(\text{NCS})_2]$ in C_s symmetry based on **3b** showing α -spin orbitals only.

Table S1. Orbital compositions for frontier orbitals in DFT calculations.

[Cu(terpy)(NCS)₂] in C₂ Symmetry

5 List of all MOs, ordered by energy, with the most significant SFO gross populations

Each percentage contribution in the table below corresponds to the indicated SFO.
In general, a SFO may be a linear combination of several Fragment Orbitals on the same,
10 or on symmetry-related Fragments. Only the first 'member' of such a combination is
specified here. A full definition of all SFOs is given in an earlier part of the output.
The numbering of the SFOs in this table does NOT include the Core Orbitals, and starts
from one for each symmetry representation, as in the SFO definition list earlier.

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*** SPIN 1 ***

E(eV)	Occ	MO	%	SFO (first member)	E(eV)	Occ	Fragment
-7.446	1.00	50 A	60.76%	1 D:xy	-5.630	2.00	1 Cu
		8.50%	1 P:x	-5.430 0.67			11 C
		7.48%	1 P:x	-5.430 0.67			8 C
		3.68%	1 P:x	-5.430 0.67			9 C
		2.83%	1 P:x	-5.430 0.67			13 C
		2.27%	2 P:y	-7.128 1.33			24 S
		2.09%	1 P:z	-5.430 0.67			15 C
		1.78%	1 P:x	-5.430 0.67			14 C
		1.49%	2 P:z	-7.128 1.33			24 S
		1.15%	1 P:x	-5.430 0.67			10 C
		1.14%	1 P:x	-7.265 1.00			2 N
		1.13%	1 P:y	-5.430 0.67			15 C
-7.295	1.00	47 B	53.24%	1 D:yz	-5.630	2.00	1 Cu
		8.44%	1 P:y	-7.265 1.00			2 N
		3.96%	2 P:y	-7.128 1.33			24 S
		3.71%	1 P:x	-5.430 0.67			15 C
		3.07%	1 P:z	-5.430 0.67			15 C
		2.84%	2 P:x	-7.128 1.33			24 S
		2.65%	1 P:y	-5.430 0.67			15 C
		2.36%	1 P:y	-7.265 1.00			4 N
		1.65%	1 P:x	-5.430 0.67			10 C
		1.56%	2 S	-18.424 2.00			2 N
		1.52%	2 P:z	-7.128 1.33			24 S
		1.28%	1 P:x	-5.430 0.67			8 C
		1.27%	3 P:y	-0.074 0.00			1 Cu
		1.19%	1 P:y	-5.430 0.67			11 C
		1.08%	1 P:x	-5.430 0.67			7 C
-7.053	1.00	51 A	23.35%	1 P:x	-5.430	0.67	13 C
		16.96%	1 P:x	-5.430 0.67			10 C
		11.66%	1 D:xy	-5.630 2.00			1 Cu
		10.95%	1 P:x	-5.430 0.67			7 C
		10.25%	1 P:x	-5.430 0.67			8 C
		8.76%	1 P:x	-5.430 0.67			14 C
		5.93%	1 P:x	-5.430 0.67			11 C
		2.35%	1 P:x	-7.265 1.00			2 N
-6.715	1.00	52 A	31.55%	1 D:z2	-5.630	2.00	1 Cu
		26.79%	1 D:x2-y2	-5.630 2.00			1 Cu

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7.72% 2 P:z -7.128 1.33 24 S
 6.22% 1 P:z -7.265 1.00 3 N
 4.01% 2 P:x -7.128 1.33 24 S
 3.68% 3 P:z -0.074 0.00 1 Cu
 5 3.55% 1 P:x -5.430 0.67 15 C
 2.92% 1 P:z -5.430 0.67 15 C
 2.24% 1 P:y -7.265 1.00 4 N
 2.03% 2 S -18.424 2.00 4 N
 1.21% 2 S -18.424 2.00 3 N
 10 1.15% 1 P:y -5.430 0.67 15 C
 -6.498 1.00 48 B 49.60% 1 D:xz -5.630 2.00 1 Cu
 7.31% 2 P:x -7.128 1.33 24 S
 6.86% 2 S -18.424 2.00 4 N
 6.41% 1 P:y -7.265 1.00 4 N
 15 4.98% 3 P:x -0.074 0.00 1 Cu
 3.13% 1 P:z -7.265 1.00 4 N
 2.29% 1 P:x -5.430 0.67 15 C
 2.19% 1 P:x -5.430 0.67 14 C
 2.15% 1 P:x -5.430 0.67 8 C
 20 1.68% 1 P:x -5.430 0.67 12 C
 1.64% 1 P:x -5.430 0.67 11 C
 1.41% 1 P:y -5.430 0.67 15 C
 1.34% 2 D:xz 11.536 0.00 1 Cu
 1.14% 1 D:yz -5.630 2.00 1 Cu
 25 -5.619 1.00 53 A 24.26% 2 P:x -7.128 1.33 24 S
 12.93% 1 D:x2-y2 -5.630 2.00 1 Cu
 11.14% 1 P:y -7.265 1.00 4 N
 8.77% 1 P:y -7.265 1.00 2 N
 8.10% 1 D:z2 -5.630 2.00 1 Cu
 30 5.04% 2 P:y -7.128 1.33 24 S
 5.02% 1 P:z -7.265 1.00 3 N
 3.98% 1 P:x -7.265 1.00 4 N
 3.50% 2 S -18.424 2.00 4 N
 2.45% 2 P:z -7.128 1.33 24 S
 35 1.90% 2 S -18.424 2.00 2 N
 1.48% 2 D:x2-y2 11.536 0.00 1 Cu
 -5.174 1.00 49 B 32.02% 2 P:z -7.128 1.33 24 S
 22.01% 2 P:y -7.128 1.33 24 S
 12.29% 1 P:y -7.265 1.00 4 N
 40 9.73% 1 P:z -7.265 1.00 4 N
 7.41% 2 P:x -7.128 1.33 24 S
 2.10% 1 P:x -7.265 1.00 4 N
 1.80% 1 D:yz -5.630 2.00 1 Cu
 1.25% 3 P:x -0.074 0.00 1 Cu
 45 1.21% 1 D:xz -5.630 2.00 1 Cu
 1.06% 1 P:x -5.430 0.67 9 C
 -4.943 1.00 54 A 36.34% 2 P:x -7.128 1.33 24 S
 14.82% 1 D:z2 -5.630 2.00 1 Cu
 13.34% 1 P:x -7.265 1.00 4 N
 50 7.30% 1 P:y -7.265 1.00 2 N
 5.08% 1 P:z -7.265 1.00 3 N
 4.74% 2 P:z -7.128 1.33 24 S
 3.37% 1 D:x2-y2 -5.630 2.00 1 Cu
 2.03% 2 S -18.424 2.00 2 N
 55 1.75% 2 D:z2 11.536 0.00 1 Cu
 1.73% 1 P:z -7.265 1.00 4 N
 1.00% 2 P:y -7.128 1.33 24 S
 -4.876 1.00 50 B 47.36% 2 P:x -7.128 1.33 24 S

20.96% 1 P:x -7.265 1.00 4 N
 17.15% 2 P:z -7.128 1.33 24 S
 6.19% 1 P:z -7.265 1.00 4 N
 3.21% 1 D:xz -5.630 2.00 1 Cu
 5 -4.861 1.00 55 A 38.52% 2 P:z -7.128 1.33 24 S
 17.44% 1 P:z -7.265 1.00 4 N
 17.30% 2 P:y -7.128 1.33 24 S
 8.81% 1 D:x2-y2 -5.630 2.00 1 Cu
 5.11% 1 P:y -7.265 1.00 4 N
 10 3.83% 1 P:y -7.265 1.00 2 N
 1.60% 1 D:xy -5.630 2.00 1 Cu
 1.13% 2 S -18.424 2.00 2 N
 -3.782 0.00 51 B 19.05% 1 P:x -7.265 1.00 3 N
 14.04% 1 P:x -5.430 0.67 14 C
 15 13.76% 1 P:x -5.430 0.67 12 C
 10.40% 1 P:x -5.430 0.67 10 C
 10.36% 1 P:x -7.265 1.00 2 N
 8.36% 1 P:x -5.430 0.67 7 C
 6.90% 1 P:x -5.430 0.67 9 C
 20 3.99% 1 D:xz -5.630 2.00 1 Cu
 3.57% 1 P:x -5.430 0.67 13 C
 2.34% 1 P:x -5.430 0.67 8 C
 -2.13% 2 P:x 7.646 0.00 3 N
 1.53% 2 P:y -7.128 1.33 24 S
 25 1.30% 1 P:x -5.430 0.67 11 C
 -1.21% 2 P:x 4.600 0.00 12 C
 1.20% 2 P:x -7.128 1.33 24 S
 -1.07% 2 P:x 7.646 0.00 2 N
 -3.741 0.00 56 A 37.55% 1 P:x -5.430 0.67 13 C
 30 17.26% 1 P:x -5.430 0.67 14 C
 14.07% 1 P:x -5.430 0.67 10 C
 10.63% 1 P:x -5.430 0.67 7 C
 8.55% 1 P:x -5.430 0.67 8 C
 8.53% 1 P:x -7.265 1.00 2 N
 35 -2.23% 2 P:x 4.600 0.00 13 C
 -2.12% 2 P:x 4.600 0.00 14 C
 1.82% 1 P:x -5.430 0.67 9 C
 1.51% 1 P:x 10.964 0.00 31 H
 -2.751 0.00 57 A 31.09% 1 P:x -5.430 0.67 9 C
 40 27.32% 1 P:x -5.430 0.67 11 C
 22.08% 1 P:x -5.430 0.67 8 C
 17.10% 1 P:x -7.265 1.00 2 N
 -3.45% 2 P:x 4.600 0.00 9 C
 -2.48% 2 P:x 7.646 0.00 2 N
 45 -1.95% 2 P:x 4.600 0.00 8 C
 -1.36% 2 P:x 4.600 0.00 11 C
 1.19% 1 P:x 10.964 0.00 27 H
 1.11% 1 P:x -5.430 0.67 14 C

50 *** SPIN 2 ***

E(eV) Occ MO % SFO (first member) E(eV) Occ Fragment

55 -----
 -7.247 1.00 50 A 34.40% 1 D:xy -5.630 2.00 1 Cu
 13.17% 1 P:x -5.430 0.67 11 C

13.12% 1 P:x -5.430 0.67 8 C
 12.50% 1 P:x -5.430 0.67 13 C
 7.93% 1 P:x -5.430 0.67 10 C
 6.04% 1 P:x -5.430 0.67 14 C
 5 3.25% 1 P:x -5.430 0.67 7 C
 1.39% 1 P:x -5.430 0.67 9 C
 1.14% 2 P:y -7.128 1.33 24 S
 -7.029 1.00 47 B 60.98% 1 D:yz -5.630 2.00 1 Cu
 7.50% 1 P:y -7.265 1.00 2 N
 10 3.82% 2 P:y -7.128 1.33 24 S
 3.34% 2 P:x -7.128 1.33 24 S
 3.33% 1 P:x -5.430 0.67 15 C
 2.37% 1 P:z -5.430 0.67 15 C
 2.25% 1 P:y -5.430 0.67 15 C
 15 1.64% 2 P:z -7.128 1.33 24 S
 1.42% 2 S -18.424 2.00 2 N
 1.42% 3 P:y -0.074 0.00 1 Cu
 -6.949 1.00 51 A 42.26% 1 D:xy -5.630 2.00 1 Cu
 13.84% 1 P:x -5.430 0.67 13 C
 20 10.11% 1 P:x -5.430 0.67 10 C
 8.22% 1 P:x -5.430 0.67 7 C
 4.52% 1 P:x -5.430 0.67 14 C
 3.76% 1 P:x -5.430 0.67 8 C
 2.67% 1 P:x -7.265 1.00 2 N
 25 2.30% 1 P:x -5.430 0.67 9 C
 1.70% 1 P:z -5.430 0.67 15 C
 1.58% 2 P:y -7.128 1.33 24 S
 1.08% 1 P:y -5.430 0.67 15 C
 1.02% 2 P:z -7.128 1.33 24 S
 30 -6.464 1.00 52 A 31.97% 1 D:z2 -5.630 2.00 1 Cu
 27.47% 1 D:x2-y2 -5.630 2.00 1 Cu
 8.73% 2 P:z -7.128 1.33 24 S
 5.54% 1 P:z -7.265 1.00 3 N
 4.91% 2 P:x -7.128 1.33 24 S
 35 3.69% 3 P:z -0.074 0.00 1 Cu
 3.06% 1 P:x -5.430 0.67 15 C
 2.60% 1 P:z -5.430 0.67 15 C
 2.19% 1 P:y -7.265 1.00 4 N
 1.70% 2 S -18.424 2.00 4 N
 40 1.10% 2 S -18.424 2.00 3 N
 -6.256 1.00 48 B 51.17% 1 D:xz -5.630 2.00 1 Cu
 8.35% 2 P:x -7.128 1.33 24 S
 6.17% 1 P:y -7.265 1.00 4 N
 6.13% 2 S -18.424 2.00 4 N
 45 4.82% 3 P:x -0.074 0.00 1 Cu
 2.96% 1 P:z -7.265 1.00 4 N
 2.46% 1 P:x -5.430 0.67 14 C
 2.12% 1 P:x -5.430 0.67 15 C
 1.78% 1 P:x -5.430 0.67 8 C
 50 1.78% 1 P:x -5.430 0.67 12 C
 1.69% 1 D:yz -5.630 2.00 1 Cu
 1.36% 1 P:x -5.430 0.67 11 C
 1.19% 1 P:y -5.430 0.67 15 C
 -5.356 1.00 53 A 40.49% 2 P:x -7.128 1.33 24 S
 55 12.95% 1 P:y -7.265 1.00 4 N
 9.09% 1 P:x -7.265 1.00 4 N
 8.93% 2 P:y -7.128 1.33 24 S
 7.63% 1 D:x2-y2 -5.630 2.00 1 Cu

2.72% 2 S -18.424 2.00 4 N
 2.70% 2 P:z -7.128 1.33 24 S
 2.60% 1 D:z2 -5.630 2.00 1 Cu
 2.44% 1 P:y -7.265 1.00 2 N
 5 1.68% 1 D:xy -5.630 2.00 1 Cu
 1.53% 1 P:z -7.265 1.00 3 N
 -5.091 1.00 49 B 36.93% 2 P:z -7.128 1.33 24 S
 21.09% 2 P:y -7.128 1.33 24 S
 12.15% 1 P:y -7.265 1.00 4 N
 10 11.50% 1 P:z -7.265 1.00 4 N
 3.30% 2 P:x -7.128 1.33 24 S
 2.20% 1 D:yz -5.630 2.00 1 Cu
 1.22% 3 P:x -0.074 0.00 1 Cu
 1.03% 1 P:x -5.430 0.67 9 C
 15 -4.809 1.00 50 B 49.49% 2 P:x -7.128 1.33 24 S
 21.79% 1 P:x -7.265 1.00 4 N
 11.99% 2 P:z -7.128 1.33 24 S
 4.58% 1 D:xz -5.630 2.00 1 Cu
 4.31% 1 P:z -7.265 1.00 4 N
 20 -4.807 1.00 54 A 39.77% 2 P:z -7.128 1.33 24 S
 17.08% 1 P:z -7.265 1.00 4 N
 11.45% 2 P:x -7.128 1.33 24 S
 8.88% 2 P:y -7.128 1.33 24 S
 7.97% 1 D:z2 -5.630 2.00 1 Cu
 25 4.26% 1 P:x -7.265 1.00 4 N
 2.82% 1 P:y -7.265 1.00 4 N
 2.06% 1 D:x2-y2 -5.630 2.00 1 Cu
 1.33% 1 P:z -7.265 1.00 3 N
 -4.387 0.00 55 A 21.27% 1 D:x2-y2 -5.630 2.00 1 Cu
 30 17.53% 1 D:z2 -5.630 2.00 1 Cu
 14.98% 1 P:y -7.265 1.00 2 N
 7.81% 2 P:x -7.128 1.33 24 S
 6.17% 1 P:z -7.265 1.00 3 N
 5.29% 2 P:y -7.128 1.33 24 S
 35 4.23% 2 S -18.424 2.00 2 N
 3.54% 1 P:x -7.265 1.00 4 N
 1.80% 1 P:z -7.265 1.00 4 N
 1.56% 2 P:z -7.128 1.33 24 S
 1.49% 2 D:x2-y2 11.536 0.00 1 Cu
 40 1.32% 1 D:xy -5.630 2.00 1 Cu
 1.11% 1 P:z -7.265 1.00 2 N
 1.08% 2 S -18.424 2.00 3 N
 1.06% 2 D:z2 11.536 0.00 1 Cu

[Cu(L₃')(NCS)₂] in C_s Symmetry

List of all MOs, ordered by energy, with the most significant SFO gross populations

Each percentage contribution in the table below corresponds to the indicated SFO.
 In general, a SFO may be a linear combination of several Fragment Orbitals on the same,
 or on symmetry-related Fragments. Only the first 'member' of such a combination is
 specified here. A full definition of all SFOs is given in an earlier part of the output.
 The numbering of the SFOs in this table does NOT include the Core Orbitals, and starts
 from one for each symmetry representation, as in the SFO definition list earlier.

*** SPIN 1 ***

E(eV)	Occ	MO	%	SFO (first member)	E(eV)	Occ	Fragment
-7.050	1.00	56 AAA	38.15%	1 D:xz	-5.630	2.00	1 Cu
		25.87%	1 D:yz	-5.630	2.00	1 Cu	
		6.92%	1 P:z	-5.430	0.67	9 C	
		5.85%	2 P:z	-7.128	1.33	3 S	
		4.21%	1 P:x	-5.430	0.67	14 C	
		3.13%	1 P:x	-5.430	0.67	11 C	
		2.64%	1 P:z	-7.265	1.00	6 N	
		2.11%	1 P:x	-5.430	0.67	13 C	
		1.17%	1 P:x	-5.430	0.67	17 C	
-6.783	1.00	57 AAA	21.19%	1 P:x	-5.430	0.67	17 C
		13.95%	1 P:x	-5.430	0.67	12 C	
		11.94%	1 P:x	-5.430	0.67	14 C	
		11.53%	1 D:yz	-5.630	2.00	1 Cu	
		9.20%	1 P:x	-5.430	0.67	16 C	
		8.62%	1 P:x	-5.430	0.67	11 C	
		7.36%	1 P:x	-5.430	0.67	15 C	
		1.71%	1 P:z	-7.265	1.00	6 N	
-6.622	1.00	58 AAA	33.19%	1 D:xz	-5.630	2.00	1 Cu
		25.61%	1 D:yz	-5.630	2.00	1 Cu	
		5.61%	1 P:z	-5.430	0.67	10 C	
		4.79%	1 P:x	-5.430	0.67	17 C	
		4.78%	2 P:z	-7.128	1.33	2 S	
		4.47%	1 P:z	-7.265	1.00	6 N	
		3.04%	1 P:x	-5.430	0.67	12 C	
		2.99%	1 P:x	-7.265	1.00	6 N	
		2.67%	1 P:x	-5.430	0.67	15 C	
		1.72%	1 P:x	-5.430	0.67	13 C	
		1.60%	1 P:x	-5.430	0.67	16 C	
		1.06%	3 P:z	-0.074	0.00	1 Cu	
		1.05%	2 S	-18.424	2.00	6 N	
-6.302	1.00	89 AA	43.16%	1 D:x ² -y ²	-5.630	2.00	1 Cu
		17.57%	1 D:xy	-5.630	2.00	1 Cu	
		6.82%	2 P:y	-7.128	1.33	2 S	
		5.11%	1 P:y	-5.430	0.67	10 C	
		3.97%	1 P:y	-7.265	1.00	7 N	
		2.94%	3 P:y	-0.074	0.00	1 Cu	
		2.36%	1 P:y	-7.265	1.00	4 N	
		1.97%	2 S	-18.424	2.00	4 N	

			1.69%	2 P:x	-7.128	1.33	3 S	
			1.56%	1 P:x	-5.430	0.67	9 C	
			1.38%	2 P:y	-7.128	1.33	3 S	
	-5.929	1.00	90 AA	36.82%	1 D:xy	-5.630	2.00	1 Cu
5			13.18%	2 P:x	-7.128	1.33	3 S	
			9.48%	1 D:x2-y2	-5.630	2.00	1 Cu	
			5.94%	3 P:x	-0.074	0.00	1 Cu	
			3.97%	1 P:x	-7.265	1.00	5 N	
			3.40%	2 S	-18.424	2.00	5 N	
10			2.96%	1 P:y	-7.265	1.00	4 N	
			2.67%	1 P:x	-5.430	0.67	9 C	
			2.46%	1 P:y	-7.265	1.00	7 N	
			1.67%	2 S	-18.424	2.00	4 N	
			1.47%	1 P:x	-5.430	0.67	16 C	
15			1.20%	2 P:y	-7.128	1.33	3 S	
			1.17%	1 P:x	-5.430	0.67	18 C	
			1.13%	1 D:z2	-5.630	2.00	1 Cu	
			1.05%	2 D:xy	11.536	0.00	1 Cu	
			1.03%	1 P:x	-5.430	0.67	14 C	
20	-5.027	1.00	91 AA	38.26%	1 D:z2	-5.630	2.00	1 Cu
			15.90%	1 P:z	-7.265	1.00	6 N	
			7.49%	2 P:x	-7.128	1.33	3 S	
			4.89%	1 P:y	-7.265	1.00	7 N	
			4.37%	2 S	-18.424	2.00	6 N	
25			3.18%	2 D:z2	11.536	0.00	1 Cu	
			3.03%	1 P:y	-7.265	1.00	4 N	
			1.91%	1 P:x	-7.265	1.00	5 N	
			1.82%	1 P:x	-7.265	1.00	4 N	
			1.79%	2 S	-18.424	2.00	5 N	
30			1.43%	2 S	-18.424	2.00	4 N	
			1.34%	1 P:y	-7.265	1.00	6 N	
			1.23%	1 S	-6.357	1.00	38 H	
	-4.795	1.00	59 AAA	66.98%	2 P:z	-7.128	1.33	3 S
			25.54%	1 P:z	-7.265	1.00	4 N	
35			2.48%	1 D:yz	-5.630	2.00	1 Cu	
			1.55%	1 D:yz	33.631	0.00	9 C	
			1.12%	1 D:xz	-5.630	2.00	1 Cu	
	-4.669	1.00	92 AA	40.75%	2 P:x	-7.128	1.33	3 S
			17.70%	1 P:x	-7.265	1.00	4 N	
40			7.84%	1 D:x2-y2	-5.630	2.00	1 Cu	
			7.34%	2 P:y	-7.128	1.33	3 S	
			4.96%	1 D:z2	-5.630	2.00	1 Cu	
			4.37%	1 D:xy	-5.630	2.00	1 Cu	
			3.22%	1 P:y	-7.265	1.00	7 N	
45			2.96%	1 P:z	-7.265	1.00	6 N	
			1.18%	1 P:y	-7.265	1.00	4 N	
	-4.435	1.00	93 AA	60.01%	2 P:y	-7.128	1.33	2 S
			22.88%	1 P:y	-7.265	1.00	5 N	
			5.78%	2 P:x	-7.128	1.33	2 S	
50			3.90%	1 D:x2-y2	-5.630	2.00	1 Cu	
			2.04%	1 P:x	-7.265	1.00	5 N	
			1.17%	1 D:xy	33.631	0.00	10 C	
	-4.387	1.00	60 AAA	68.44%	2 P:z	-7.128	1.33	2 S
			25.50%	1 P:z	-7.265	1.00	5 N	
55			1.98%	1 D:xz	-5.630	2.00	1 Cu	
			1.60%	1 D:xz	33.631	0.00	10 C	
	-3.404	0.00	61 AAA	36.20%	1 P:x	-5.430	0.67	17 C
			16.88%	1 P:x	-5.430	0.67	16 C	

13.12%	1 P:x	-5.430	0.67	12 C
10.27%	1 P:x	-5.430	0.67	15 C
8.74%	1 P:x	-5.430	0.67	14 C
7.23%	1 P:x	-7.265	1.00	6 N
-2.17%	2 P:x	4.600	0.00	17 C
-2.13%	2 P:x	4.600	0.00	16 C
1.55%	1 P:x	-5.430	0.67	13 C
1.55%	1 P:x	10.964	0.00	41 H

*** SPIN 2 ***

E(eV)	Occ	MO	%	SFO (first member)	E(eV)	Occ	Fragment
-6.848	1.00	56 AAA	22.04%	1 D:xz	-5.630	2.00	1 Cu
		14.00%	1 P:x	-5.430	0.67	17 C	
		11.87%	1 P:x	-5.430	0.67	14 C	
		10.20%	1 D:yz	-5.630	2.00	1 Cu	
		9.29%	1 P:x	-5.430	0.67	11 C	
		7.50%	1 P:x	-5.430	0.67	12 C	
		6.57%	1 P:x	-5.430	0.67	16 C	
		4.03%	1 P:x	-5.430	0.67	15 C	
		2.60%	2 P:z	-7.128	1.33	3 S	
		2.58%	1 P:z	-5.430	0.67	9 C	
-6.705	1.00	57 AAA	25.06%	1 D:yz	-5.630	2.00	1 Cu
		17.07%	1 D:xz	-5.630	2.00	1 Cu	
		12.00%	1 P:x	-5.430	0.67	17 C	
		8.85%	1 P:x	-5.430	0.67	12 C	
		5.18%	1 P:x	-5.430	0.67	15 C	
		4.69%	1 P:x	-5.430	0.67	16 C	
		4.63%	2 P:z	-7.128	1.33	3 S	
		4.01%	1 P:z	-5.430	0.67	9 C	
		3.51%	1 P:x	-5.430	0.67	14 C	
		2.16%	1 P:z	-7.265	1.00	6 N	
		1.96%	1 P:x	-5.430	0.67	11 C	
		1.90%	1 P:x	-7.265	1.00	6 N	
-6.366	1.00	58 AAA	36.94%	1 D:xz	-5.630	2.00	1 Cu
		32.55%	1 D:yz	-5.630	2.00	1 Cu	
		5.68%	2 P:z	-7.128	1.33	2 S	
		5.30%	1 P:z	-5.430	0.67	10 C	
		4.47%	1 P:z	-7.265	1.00	6 N	
		1.74%	1 P:x	-7.265	1.00	6 N	
		1.54%	1 P:x	-5.430	0.67	13 C	
		1.29%	1 P:x	-5.430	0.67	17 C	
		1.27%	3 P:z	-0.074	0.00	1 Cu	
		1.16%	1 P:x	-5.430	0.67	15 C	
		1.04%	2 S	-18.424	2.00	6 N	
-6.039	1.00	89 AA	46.65%	1 D:x2-y2	-5.630	2.00	1 Cu
		14.96%	1 D:xy	-5.630	2.00	1 Cu	
		7.51%	2 P:y	-7.128	1.33	2 S	
		4.62%	1 P:y	-5.430	0.67	10 C	
		4.24%	1 P:y	-7.265	1.00	7 N	
		3.09%	3 P:y	-0.074	0.00	1 Cu	
		2.50%	2 P:x	-7.128	1.33	3 S	
		1.63%	1 P:x	-5.430	0.67	9 C	
		1.56%	1 P:y	-7.265	1.00	4 N	

			1.47%	2 S	-18.424	2.00	4 N	
			1.45%	2 P:y	-7.128	1.33	3 S	
	-5.683	1.00	90 AA	39.85%	1 D:xy	-5.630	2.00	1 Cu
			14.79%	2 P:x	-7.128	1.33	3 S	
5			6.53%	1 D:x2-y2	-5.630	2.00	1 Cu	
			6.01%	3 P:x	-0.074	0.00	1 Cu	
			3.29%	1 P:x	-7.265	1.00	5 N	
			3.11%	1 P:y	-7.265	1.00	4 N	
			2.95%	2 S	-18.424	2.00	5 N	
10			2.43%	1 P:x	-5.430	0.67	9 C	
			1.79%	1 P:x	-5.430	0.67	16 C	
			1.78%	1 D:z2	-5.630	2.00	1 Cu	
			1.62%	1 P:x	-7.265	1.00	4 N	
			1.53%	2 S	-18.424	2.00	4 N	
15			1.47%	2 P:y	-7.128	1.33	3 S	
			1.35%	1 P:x	-5.430	0.67	18 C	
			1.22%	1 P:y	-7.265	1.00	7 N	
			1.04%	1 P:x	-5.430	0.67	13 C	
	-4.724	1.00	59 AAA	65.93%	2 P:z	-7.128	1.33	3 S
20			25.35%	1 P:z	-7.265	1.00	4 N	
			3.31%	1 D:yz	-5.630	2.00	1 Cu	
			1.54%	1 D:yz	33.631	0.00	9 C	
			1.46%	1 D:xz	-5.630	2.00	1 Cu	
	-4.665	1.00	91 AA	33.54%	2 P:x	-7.128	1.33	3 S
25			16.19%	1 D:z2	-5.630	2.00	1 Cu	
			12.31%	1 P:x	-7.265	1.00	4 N	
			4.49%	2 P:y	-7.128	1.33	3 S	
			4.40%	1 P:z	-7.265	1.00	6 N	
			3.89%	1 D:x2-y2	-5.630	2.00	1 Cu	
30			3.77%	1 P:y	-7.265	1.00	4 N	
			3.17%	1 D:xy	-5.630	2.00	1 Cu	
			2.43%	2 P:y	-7.128	1.33	2 S	
			2.43%	1 P:x	-7.265	1.00	5 N	
			2.05%	2 S	-18.424	2.00	5 N	
35			1.32%	2 S	-18.424	2.00	6 N	
	-4.333	1.00	60 AAA	67.70%	2 P:z	-7.128	1.33	2 S
			25.30%	1 P:z	-7.265	1.00	5 N	
			2.63%	1 D:xz	-5.630	2.00	1 Cu	
			1.59%	1 D:xz	33.631	0.00	10 C	
40			1.01%	1 D:yz	-5.630	2.00	1 Cu	
	-4.311	1.00	92 AA	49.27%	2 P:y	-7.128	1.33	2 S
			18.87%	1 P:y	-7.265	1.00	5 N	
			9.70%	1 D:x2-y2	-5.630	2.00	1 Cu	
			4.83%	2 P:x	-7.128	1.33	2 S	
45			3.86%	2 P:x	-7.128	1.33	3 S	
			2.34%	1 P:y	-7.265	1.00	7 N	
			2.11%	1 D:z2	-5.630	2.00	1 Cu	
			1.51%	1 P:x	-7.265	1.00	5 N	
			1.27%	1 P:x	-7.265	1.00	4 N	
50	-4.197	0.00	93 AA	32.44%	1 D:z2	-5.630	2.00	1 Cu
			11.28%	1 P:z	-7.265	1.00	6 N	
			8.42%	2 P:y	-7.128	1.33	2 S	
			8.27%	2 P:x	-7.128	1.33	3 S	
			4.90%	1 D:xy	-5.630	2.00	1 Cu	
55			4.85%	1 P:x	-7.265	1.00	4 N	
			4.56%	1 P:y	-7.265	1.00	7 N	
			3.38%	1 P:y	-7.265	1.00	5 N	
			3.27%	2 S	-18.424	2.00	6 N	

2.42%	2 P:y	-7.128	1.33	3 S
1.94%	2 D:z2	11.536	0.00	1 Cu
1.25%	2 S	-18.424	2.00	4 N
1.21%	1 D:x2-y2	-5.630	2.00	1 Cu

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