

Electronic Supplementary Information

**Copper Complexation of Rosarin: Formation of a Bis-copper
Rosarin and a Mono-copper Linear Tridipyrin**

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1, Supporting figures and tables

Rosarin Cu 1 #13 RT: 0.19 AV: 1 NL: 3.13E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]

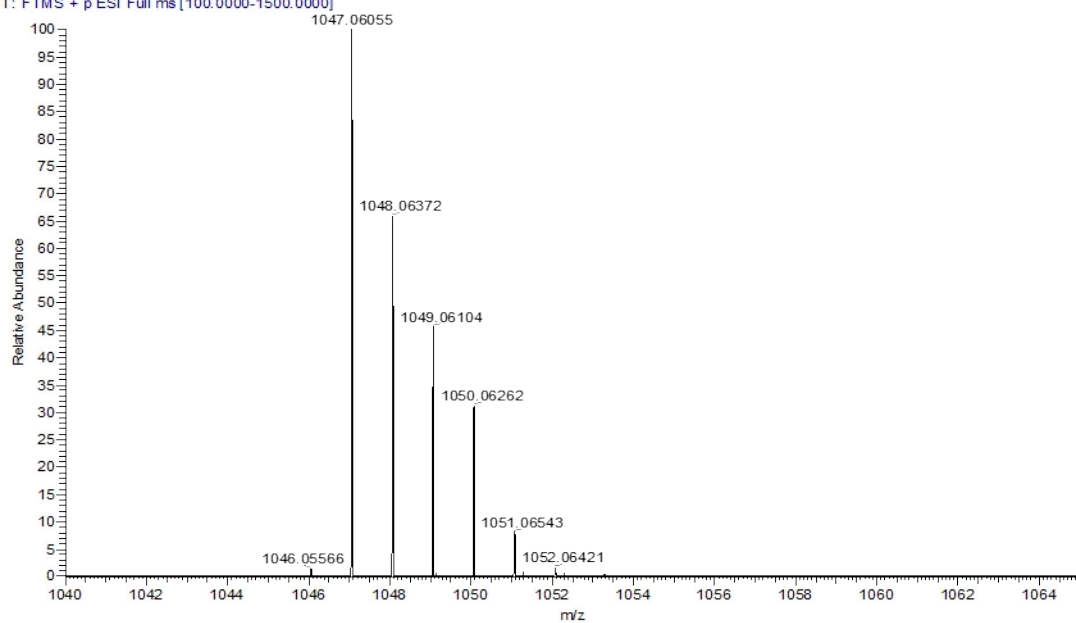


Figure S1. HR-APCI mass spectrum of Cu-1..

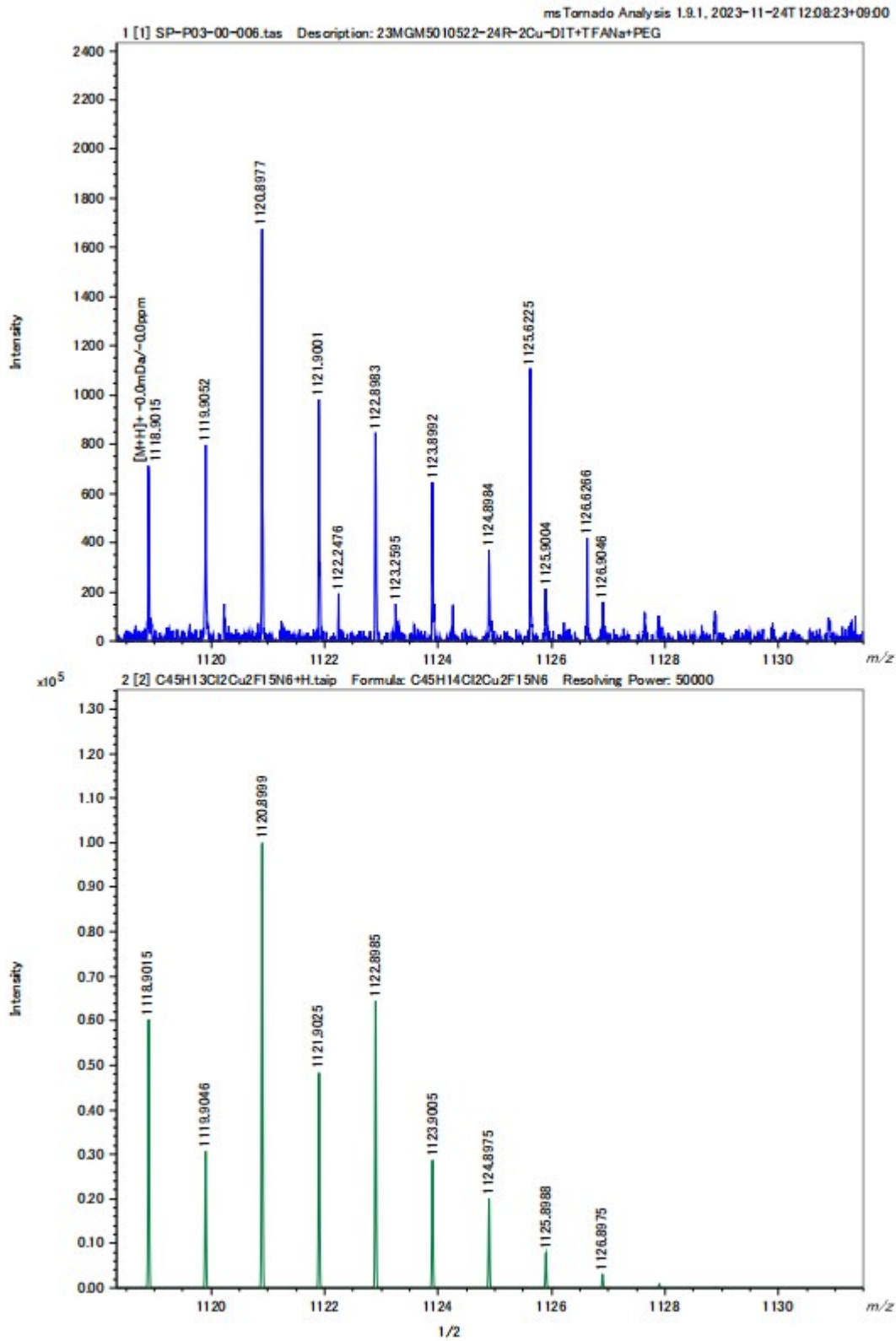


Figure S2. HR-MALDI mass spectrum of 2Cu-1.

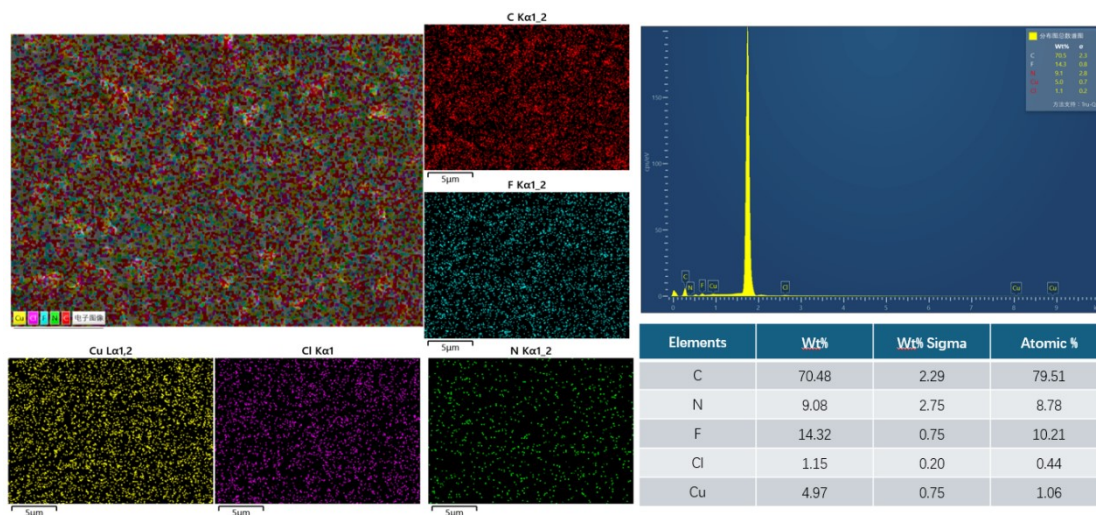


Figure S3. EDS elemental distribution of **2Cu-1**.

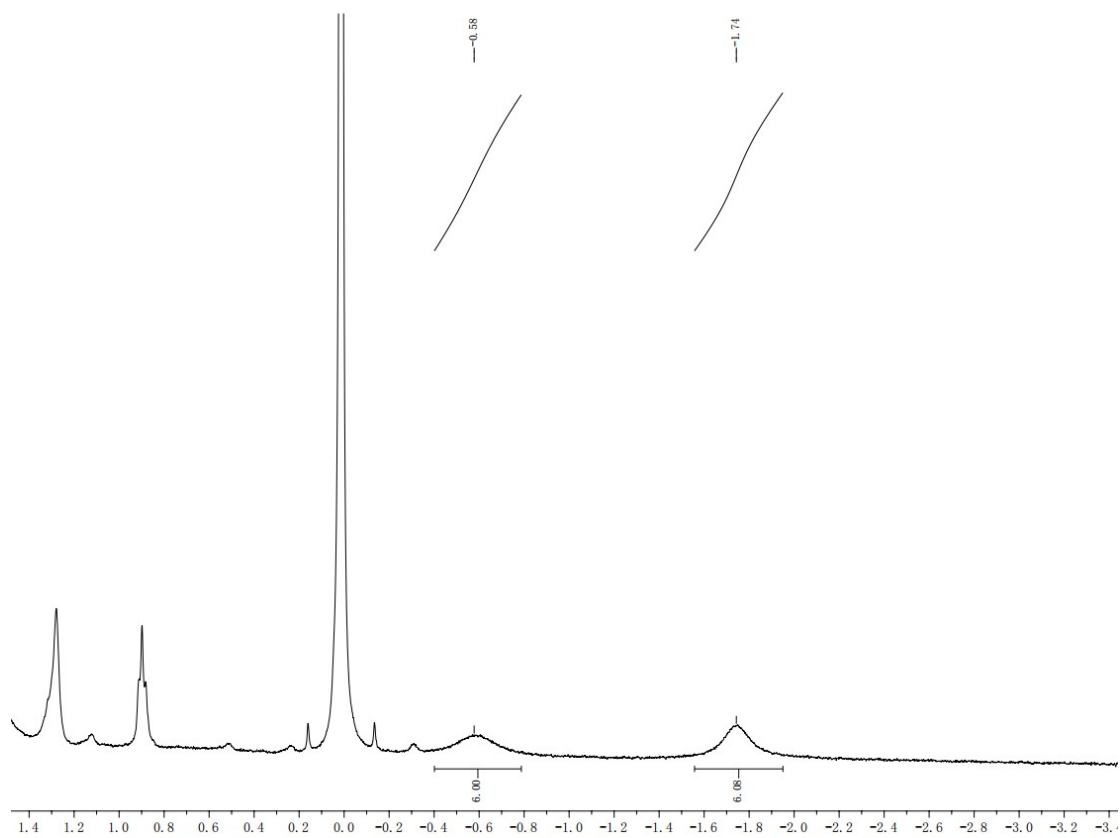


Figure S4. ^1H NMR spectrum of 2Cu-1 in CDCl_3 .

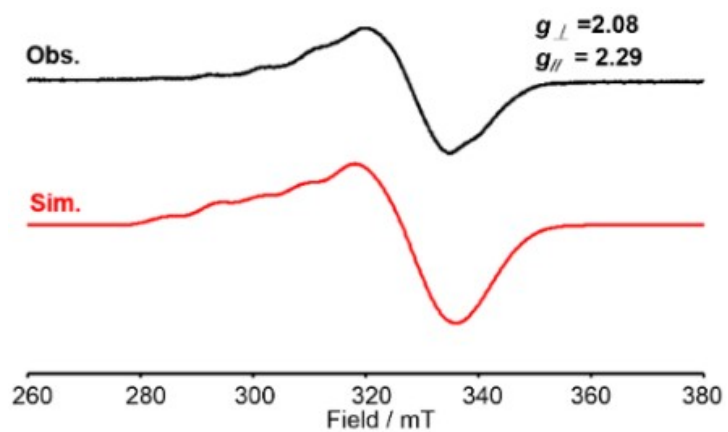


Figure S5. Observed and simulated EPR spectra of **2Cu-1** in frozen dichloromethane. The spectrum was obtained at 215 K 0.4 μ s after the laser excitation pulse with 14.5 mW of microwave power and an integration time of 0.2 μ s per point.

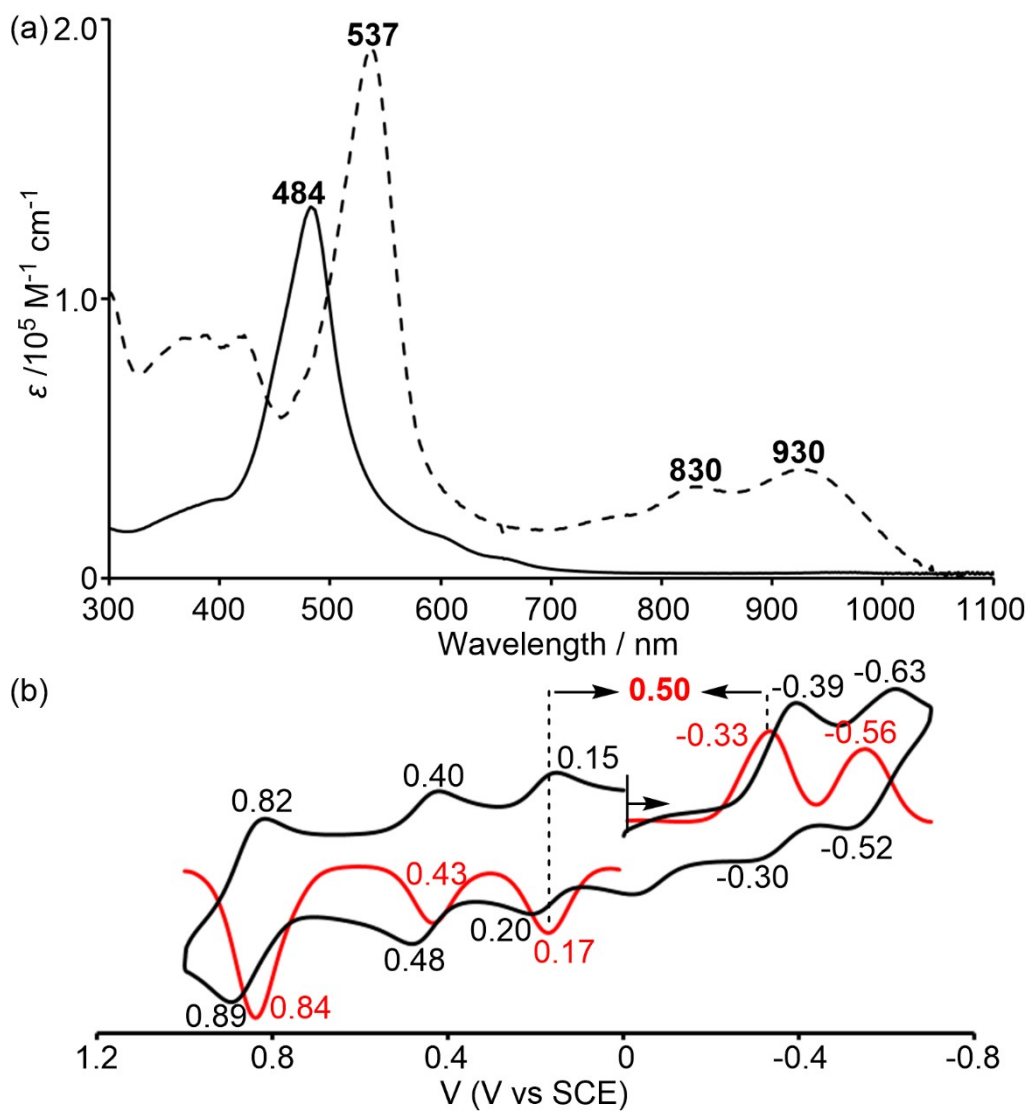


Figure S6. (a) UV-vis-NIR absorption spectra of **Cu-1** (black dotted line) and **2Cu-1** (black solid line) in CH_2Cl_2 . (b) CV (black line) and DPV (red line) line of **2Cu-1** in CH_2Cl_2 (0.1 M TBAP). The scan rate is 0.1 V s^{-1} . Forward scan: from negative potential to positive potential.

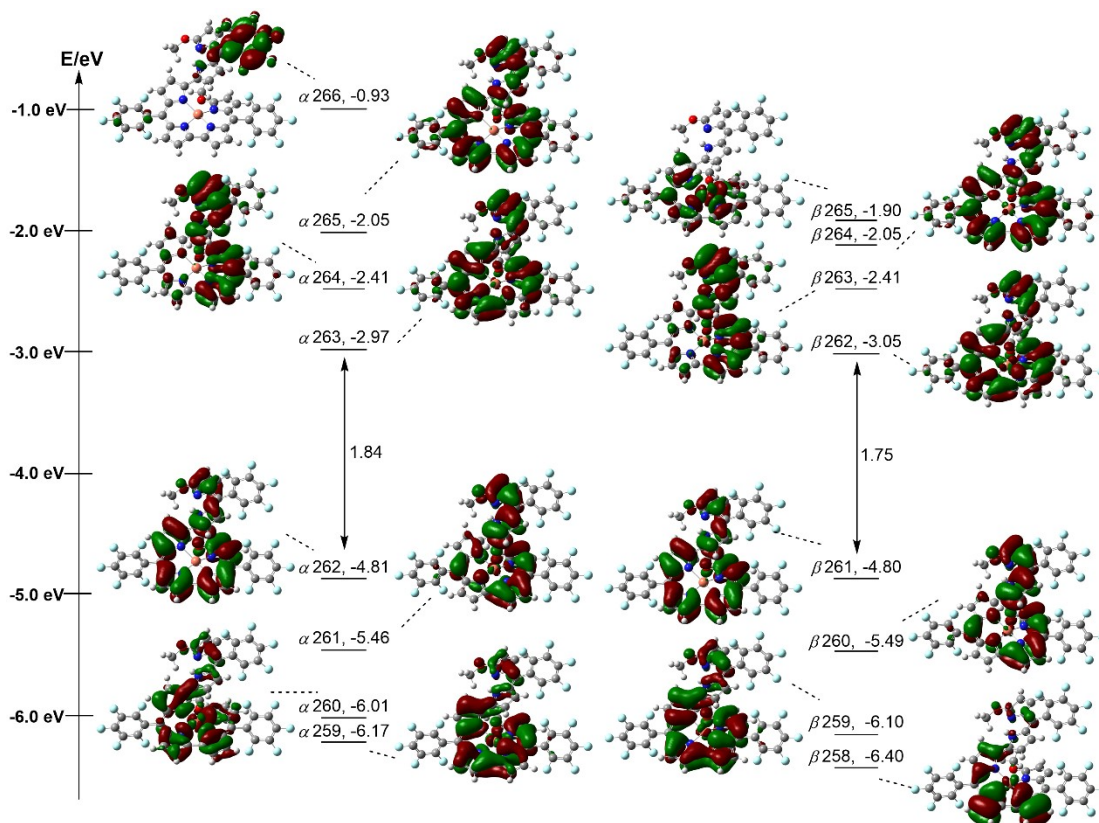


Figure S7. Frontier molecular orbitals and energy diagrams of **1Cu-1**, calculated at the UB3LYP/6-31G(d, p) level of theory.

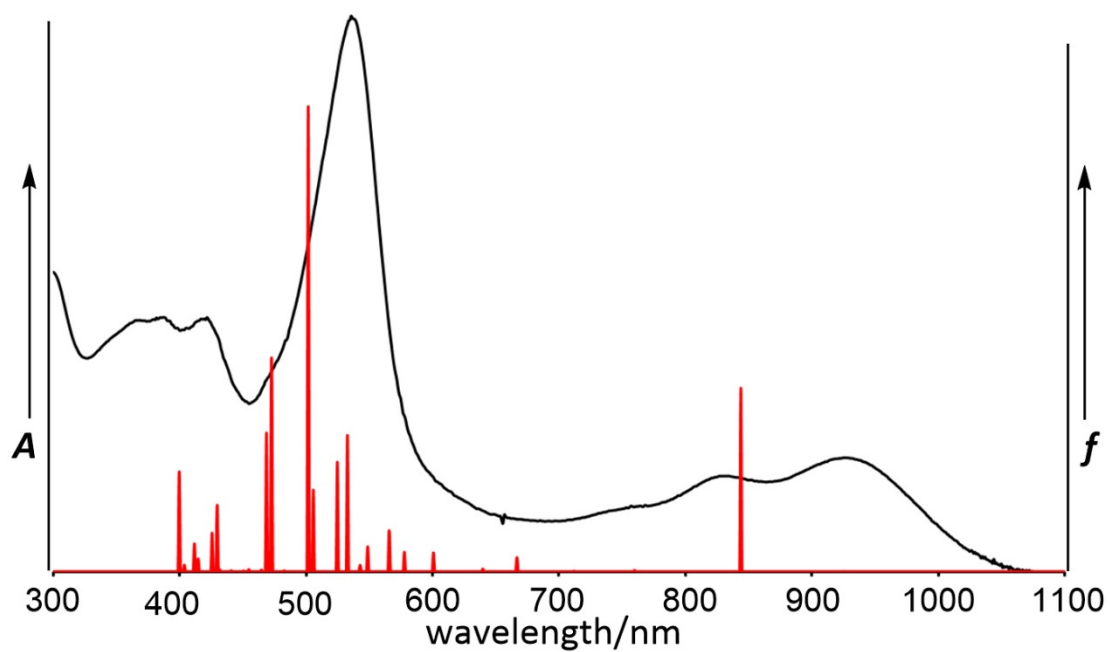


Figure S8. The UV-Vis absorption spectrum (black line, left axis) of **1Cu-1** and oscillator strengths (red bar, right axis) is calculated at the UB3LYP/6-31G(d, p) level of theory.

Table S1. Major composition, vertical excitation energies (E , eV/nm) and oscillator strengths (f) for the lowest optically allowed excited states of **1Cu-1**, calculated at the UB3LYP/6-31G(d,p) level of theory.

State	Major Composition	Exci. (eV/nm)	f
1	260B -> 262B (0.47676)		
	261B -> 263B (0.47682)	1.3339/926.00	0.0001
2	261A -> 263A (-0.46125)		
	262A -> 263A (0.73356)		
	261B -> 262B (0.65432)	1.4699/843.51	0.1395
3	259A -> 263A (0.41738)		
	262A -> 265A (-0.41022)	2.4713/501.70	0.3538
	261B -> 264B (-0.38757)		
4	261A -> 264A (0.41712)		
	259A -> 263A (0.38576)	2.6207/473.10	0.1626
	260B -> 263B (0.40575)		

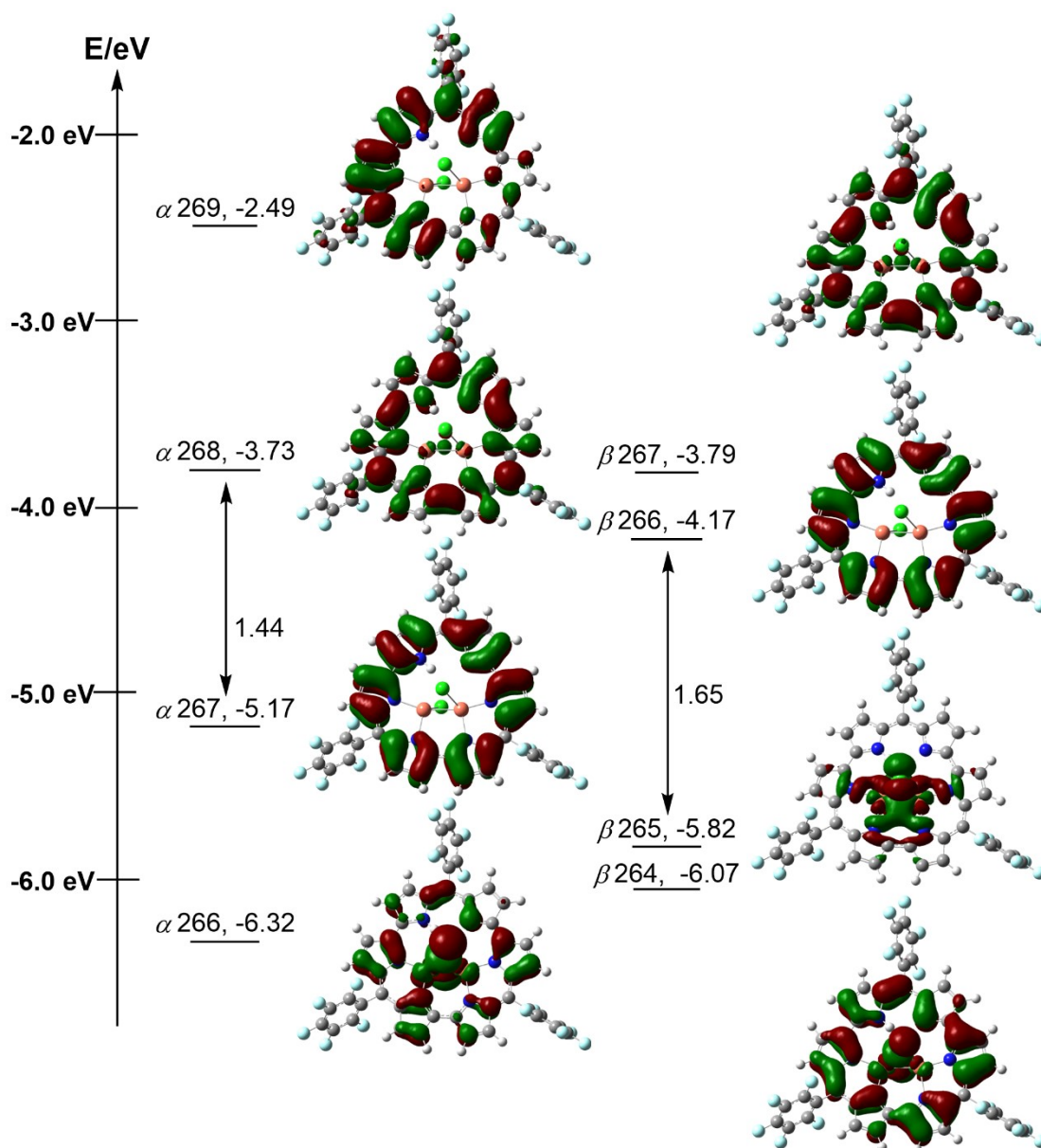


Figure S9. Frontier molecular orbitals and energy diagrams of **2Cu-1**, calculated at the UB3LYP/6-31G(d, p) level of theory.

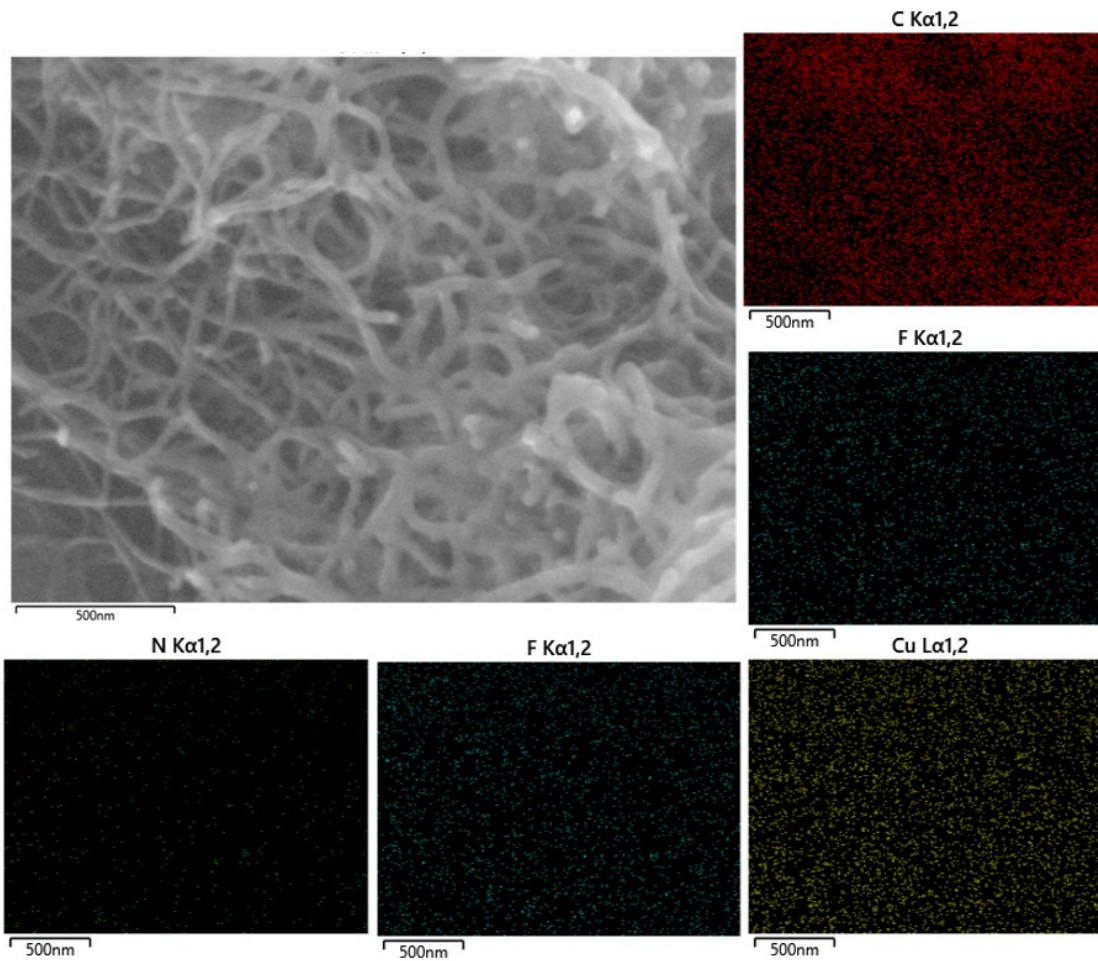


Figure S10. SEM and mapping images of 2Cu-1@CNT.

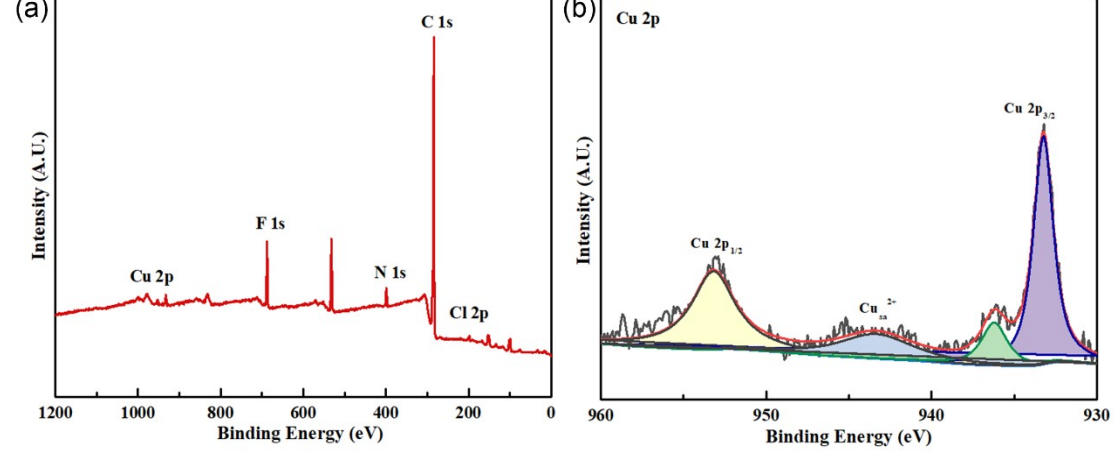


Figure S11. XPS scan spectrum of **2Cu-1@CNT** and the corresponding Cu 2p binding energy region.

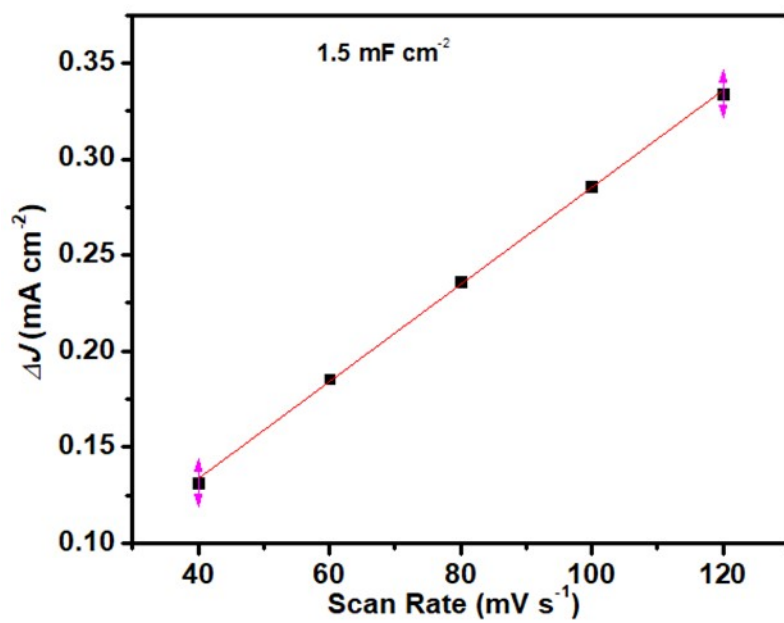


Figure S12. Linear fitting of the current densities vs scan rates for 2Cu-1@CNT.

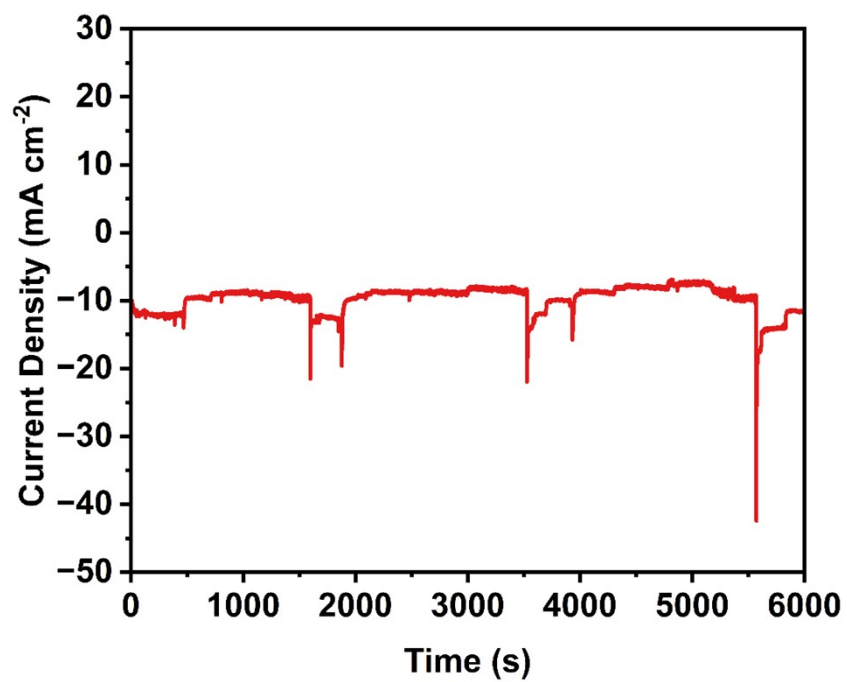


Figure S13. Stability test of **2Cu-1@CNT** during electrolysis at -0.6 V (vs RHE).

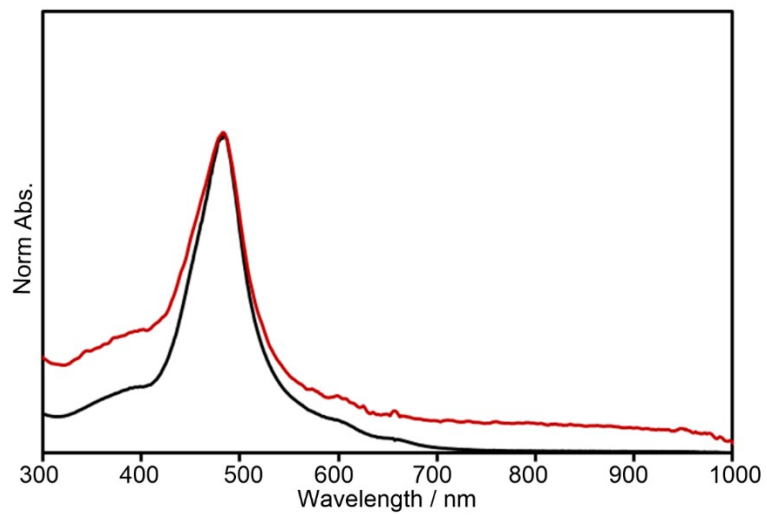
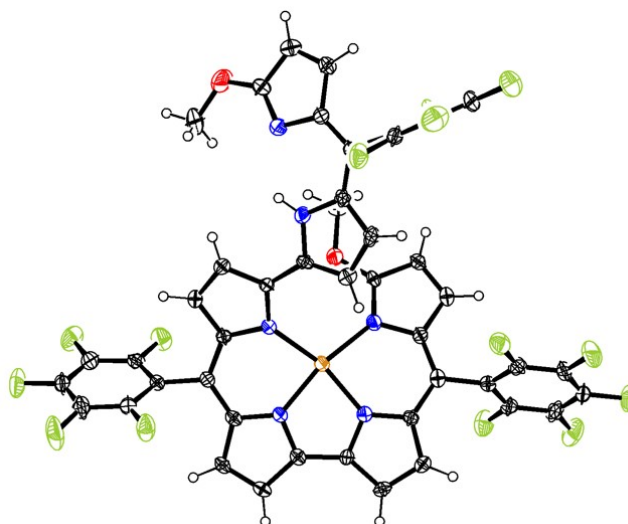


Figure S14. UV-Vis absorption spectra of **2Cu-1** before (black line) and after (red line) HER electrolysis.

Table S2. Crystal data of **Cu-1**.

Empirical formula	C ₄₇ H ₁₉ CuF ₁₅ N ₆ O ₂
Formula weight	1048.22
Temperature/K	193.00
Crystal system	triclinic
Space group	<i>P</i> -1
<i>a</i> /Å	10.5020(5)
<i>b</i> /Å	13.5350(7)
<i>c</i> /Å	15.0523(8)
α /°	91.912(2)
β /°	103.429(2)
γ /°	99.557(2)
Volume/Å ³	2046.44(18)
<i>Z</i>	2
ρ_{calc} /g/cm ³	1.701
μ /mm ⁻¹	0.654
<i>F</i> (000)	1046.0
Crystal size/mm ³	0.13 × 0.12 × 0.1
Radiation	MoK α (λ = 0.71073)
2 θ range for data collection/°	3.984 to 55.004
Index ranges	-13 ≤ <i>h</i> ≤ 12, -17 ≤ <i>k</i> ≤ 17, -17 ≤ <i>l</i> ≤ 19
Reflections collected	19324
Independent reflections	9345 [<i>R</i> _{int} = 0.0589, <i>R</i> _{sigma} = 0.1015]
Data/restraints/parameters	9345/411/742
Goodness-of-fit on <i>F</i> ²	1.097
Final <i>R</i> indexes [<i>I</i> ≥ 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0695, <i>wR</i> ₂ = 0.0942
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.1287, <i>wR</i> ₂ = 0.1156
Largest diff. peak/hole / e Å ⁻³	0.37/-0.43

**Figure S15.** Crystal structure of **Cu-1**. The thermal ellipsoids represent for 40% probability.**Table S3.** Crystal data of **2Cu-1**.

Empirical formula	C ₄₆ H ₁₄ Cl ₄ Cu ₂ F ₁₅ N ₆
Formula weight	1204.51
Temperature/K	193.15

Crystal system	monoclinic
Space group	P21/c
a/Å	8.8187(4)
b/Å	33.2549(14)
c/Å	16.0729(6)
$\alpha/^\circ$	90
$\beta/^\circ$	95.606(2)
$\gamma/^\circ$	90
Volume/Å ³	4691.1(3)
Z	4
$\rho_{\text{calc}}/\text{g}/\text{cm}^3$	1.705
μ/mm^{-1}	6.861
$F(000)$	2372.0
Radiation	GaK α ($\lambda = 1.34139$)
2 θ range for data collection/ $^\circ$	4.624 to 108.082
Index ranges	$-10 \leq h \leq 10, -40 \leq k \leq 39, -19 \leq l \leq 19$
Reflections collected	33962
Independent reflections	8601 [$R_{\text{int}} = 0.0757, R_{\text{sigma}} = 0.0766$]
Data/restraints/parameters	8601/0/667
Goodness-of-fit on F^2	1.071
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0612, wR_2 = 0.1504$
Final R indexes [all data]	$R_1 = 0.1025, wR_2 = 0.1687$
Largest diff. peak/hole / e Å ⁻³	0.76/ -0.63

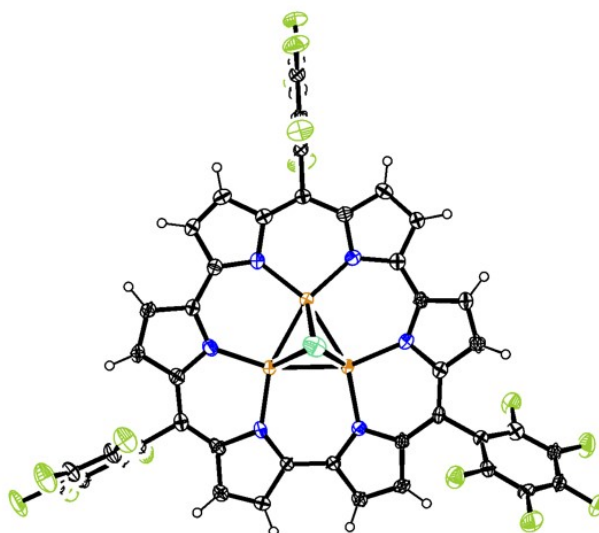


Figure S16. Crystal structure of **2Cu-1**. The thermal ellipsoids represent for 40% probability.

3, Cartesian Coordinates

2Cu-1 Singlet,	29	-0.547427000	1.141737000	-0.059270000
CAM-B3LYP-	29	1.262721000	-0.365631000	0.068384000

D3(BJ)/Def2-SVP	17	-0.127067000	-0.175285000	1.891247000
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2Cu-1 Triplet,	29	-0.669095000	1.084168000	0.017503000
CAM-B3LYP-	29	1.290075000	-0.186815000	0.097956000
D3(BJ)/Def2-	17	-0.167973000	-0.254153000	1.886524000

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2Cu-1 Quintet,	29	1.379075000	0.254188000	0.062057000
CAM-B3LYP-	29	-1.420917000	-0.139227000	0.526376000
D3(BJ)/Def2-	17	-0.007185000	-0.852359000	-1.321402000

SVP	17	-0.091389000	-0.175935000	2.318590000
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	9	4.956840000	-5.591067000	-2.802124000
	9	4.759613000	-8.096118000	-1.781842000
	9	3.089419000	-8.587307000	0.298885000
	9	1.636618000	-6.603062000	1.360509000
	9	5.337618000	3.613908000	-1.186435000
	9	6.691281000	5.928925000	-1.369085000
	9	5.606902000	8.215921000	-0.396352000
	9	3.155644000	8.174204000	0.760487000
	9	1.795066000	5.865560000	0.949738000
	9	-5.899077000	2.378468000	1.462970000
	9	-8.508444000	2.990108000	1.210719000
	9	-10.082092000	1.549568000	-0.462304000
	9	-9.032065000	-0.507170000	-1.883642000
	9	-6.428580000	-1.122420000	-1.640398000
	7	-2.375610000	1.171677000	-0.431208000
	7	-2.952643000	-1.320696000	0.774356000
	7	-0.508888000	-3.056953000	0.991451000
	7	2.450666000	-1.505547000	0.866989000
	7	2.899909000	1.122098000	0.840848000
	7	0.634943000	2.200661000	-0.536950000
	6	3.367013000	-4.809643000	-1.249227000
	6	4.137345000	-5.830148000	-1.791509000
	6	4.035260000	-7.116763000	-1.271468000
	6	3.173738000	-7.367853000	-0.209652000
	6	2.416279000	-6.329804000	0.321627000
	6	2.482979000	-5.031044000	-0.188038000
	6	1.713655000	-3.895205000	0.371883000
	6	0.337402000	-3.994596000	0.448393000
	6	-0.496957000	-5.088185000	0.023636000
	1	-0.143248000	-5.984378000	-0.476895000
	6	-1.793969000	-4.781206000	0.339717000
	1	-2.681121000	-5.369574000	0.119141000
	6	-1.803601000	-3.470195000	0.898185000
	6	-2.954175000	-2.644477000	0.999717000
	6	-4.314541000	-3.111299000	1.132782000
	1	-4.610691000	-4.136486000	1.342911000
	6	-5.120207000	-2.029237000	0.957803000
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	6	-8.263978000	0.191237000	-1.063652000
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	6	-6.649156000	1.659099000	0.643367000
	6	-3.731510000	1.232701000	-0.521448000
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	6	-2.906106000	2.912046000	-1.760555000
	1	-2.815968000	3.782317000	-2.401969000
	6	-1.836788000	2.182115000	-1.161435000
	6	-0.464838000	2.624163000	-1.201204000
	6	-0.182440000	3.865256000	-1.903556000
	1	-0.873384000	4.401775000	-2.544204000
	6	1.070783000	4.234267000	-1.569023000
	1	1.609244000	5.121829000	-1.888961000
	6	1.581155000	3.221150000	-0.676692000
	6	2.785465000	3.375140000	0.005077000
	6	3.519393000	4.663096000	-0.116244000
	6	2.988310000	5.856041000	0.376263000
	6	3.681282000	7.057822000	0.284498000
	6	4.940617000	7.080345000	-0.305764000
	6	5.496199000	5.906144000	-0.802987000
	6	4.785306000	4.715851000	-0.700951000
	6	3.368666000	2.382678000	0.812673000
	6	4.552891000	2.457672000	1.637962000
	1	5.142197000	3.353376000	1.819401000
	6	4.774988000	1.203324000	2.132435000
	1	5.581004000	0.876224000	2.784932000
	6	3.729697000	0.369347000	1.594539000
	6	3.507406000	-1.005221000	1.613669000
	6	4.274780000	-2.056879000	2.184930000
	1	5.150898000	-1.941540000	2.819106000
	6	3.686210000	-3.213737000	1.754777000
	1	3.976738000	-4.236402000	1.983308000
	6	2.547352000	-2.837715000	0.948512000
	1	-0.200423000	-2.190994000	1.441424000
2Cu-1 Triplet	29	-0.547257000	1.188163000	0.044297000
PBE-	29	1.303612000	-0.346859000	0.118673000
D3(BJ)/Def2-	17	-0.190615000	-0.243071000	1.894322000

SVP	17	-0.098414000	-0.286202000	-1.765236000
	9	-5.127824000	-3.895647000	1.995436000
	9	-6.914932000	-5.942454000	1.922688000
	9	-6.894575000	-7.704203000	-0.170387000
	9	-5.080799000	-7.410922000	-2.198818000
	9	-3.287724000	-5.369848000	-2.133082000
	9	-3.110710000	5.522931000	2.033704000
	9	-3.940110000	8.111623000	1.984589000
	9	-3.216473000	9.741288000	-0.091240000
	9	-1.656671000	8.773492000	-2.121284000
	9	-0.821611000	6.187532000	-2.079315000
	9	6.236206000	-0.332666000	-2.097165000
	9	8.901702000	-0.872056000	-2.137449000
	9	10.080044000	-2.105444000	0.002077000
	9	8.583988000	-2.801949000	2.184775000
	9	5.917340000	-2.269924000	2.231433000
	7	2.872789000	0.862395000	0.150437000
	7	2.280021000	-2.036773000	0.099424000
	7	-0.703793000	-2.991936000	0.010905000
	7	-2.935466000	-0.986164000	-0.124422000
	7	-2.309196000	2.009643000	-0.119993000
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	6	-6.028648000	-5.794125000	0.936334000
	6	-6.018175000	-6.701487000	-0.137424000
	6	-5.083101000	-6.553054000	-1.176644000
	6	-4.161987000	-5.494371000	-1.129542000
	6	-4.150977000	-4.570024000	-0.066067000
	6	-3.172491000	-3.442821000	-0.040800000
	6	-1.809036000	-3.816322000	0.102329000
	6	-1.331070000	-5.149896000	0.326379000
	1	-1.967874000	-6.027286000	0.474319000
	6	0.050462000	-5.102470000	0.337729000
	1	0.739575000	-5.936275000	0.499228000
	6	0.441781000	-3.736048000	0.135590000
	6	1.809187000	-3.310538000	0.080467000
	6	2.918875000	-4.245425000	0.003774000
	1	2.839857000	-5.336188000	-0.045018000
	6	4.068530000	-3.492070000	-0.030961000
	1	5.099250000	-3.852483000	-0.111085000
6	3.658596000	-2.104121000	0.045951000	
6	4.533256000	-0.989491000	0.088484000	
6	5.995984000	-1.287807000	0.066944000	
6	6.627189000	-1.924627000	1.152832000	

6	8.003648000	-2.204203000	1.142343000
6	8.773875000	-1.843982000	0.022781000
6	8.168038000	-1.207914000	-1.074786000
6	6.790535000	-0.935213000	-1.041143000
6	4.166971000	0.374889000	0.166343000
6	5.101783000	1.477947000	0.307209000
1	6.191906000	1.391335000	0.362198000
6	4.348058000	2.621741000	0.378500000
1	4.714636000	3.647118000	0.487489000
6	2.952188000	2.213006000	0.274510000
6	1.866389000	3.148913000	0.291742000
6	2.091558000	4.576380000	0.469448000
1	3.059523000	5.059908000	0.632981000
6	0.864345000	5.182129000	0.399971000
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6	-3.811038000	0.018446000	-0.326006000
6	-5.179858000	-0.484085000	-0.539215000
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1	-5.906620000	-2.573530000	-0.567243000
6	-3.684645000	-2.138420000	-0.187564000
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