

Supporting Information

**Dynamic Confinement of Cu₃ Clusters in
T-C₃N₂ Pores: An Adaptive Interface for
Selective CO Electroreduction to C₃ Products**

List of Figures and Tables

Figure S1 Comparison of the structures and unit cell parameters, Cu–Cu bond lengths, Cu–N bond lengths, and binding energies of Cu ₃ with the substrates for Cu ₃ @g-C ₃ N ₄ , Cu ₃ @g-C ₄ N ₃ , Cu ₃ @g-CN, Cu ₃ @C ₂ N, Cu ₃ @C ₉ N ₄ , and Cu ₃ @T-C ₃ N ₂	3
Figure S2 (a-d) The optimized structures of Cu _n @T-C ₃ N ₂ (n = 1-4) and (e) the interaction energy between Cu clusters and the substrate	4
Figure S3 Kinetic energy barriers (<i>G</i> _b), Gibbs free energy changes (ΔG), and the main C-C bond lengths for the formation of *COCOCO from different configurations of CO coupling.	5
Figure S4 Kinetic energy barrier (<i>G</i> _b), the change in Gibbs free energy (ΔG) of the 3*CO coupling reaction on the Cu(111) surface to form *COCOCO, as well as the main C-C bond length.	6
Figure S5 PDOS of (a) Cu(111), (b) Cu(111) catalyst with three adjacent CO molecules, as well as the d-band center of the Cu site; (c) ICOHP analysis of the C-O bond and Cu-C bond; (d) Charge difference density map of CO adsorption, with the interface value being 0.002 e/Å ³	7
Figure S6 Gibbs free energy diagram and intermediate structures for the lowest energy pathway of CO reduction to C ₁ products.....	8
Figure S7 Gibbs free energy diagram and intermediate structures for the lowest energy pathway of CO reduction to C ₂ products.....	9
Table S1 Changes in Cu-Cu, Cu-N bond lengths, the distances between the three Cu sites and the T-C ₃ N ₂ sheet, and the CO adsorption energy (eV/CO) during continuous CO adsorption.	10
Table S2 Changes in Cu-Cu, Cu-N bond lengths, and the distances between the three Cu sites and the T-C ₃ N ₂ sheet during the C-C coupling process.	11

Table S3 The reaction path for the formation of the C ₃ product of the Cu ₃ @T-C ₃ N ₂ catalyst and the relative free energy ($\Delta G/eV$)	12
Table S4 Cu-Cu, Cu-N bond lengths, and the distances between the three Cu sites and the T-C ₃ N ₂ sheet during the progress for C ₃ products.....	13
Table S5 The reaction path for the formation of the C ₁ product of the Cu ₃ @T-C ₃ N ₂ catalyst and the relative free energy ($\Delta G/eV$)	14
Table S6 The reaction path for the formation of the C ₂ product of the Cu ₃ @T-C ₃ N ₂ catalyst and the relative free energy ($\Delta G/eV$)	15
Table S7 Optimized energy and CONTCAR,,,.....	17

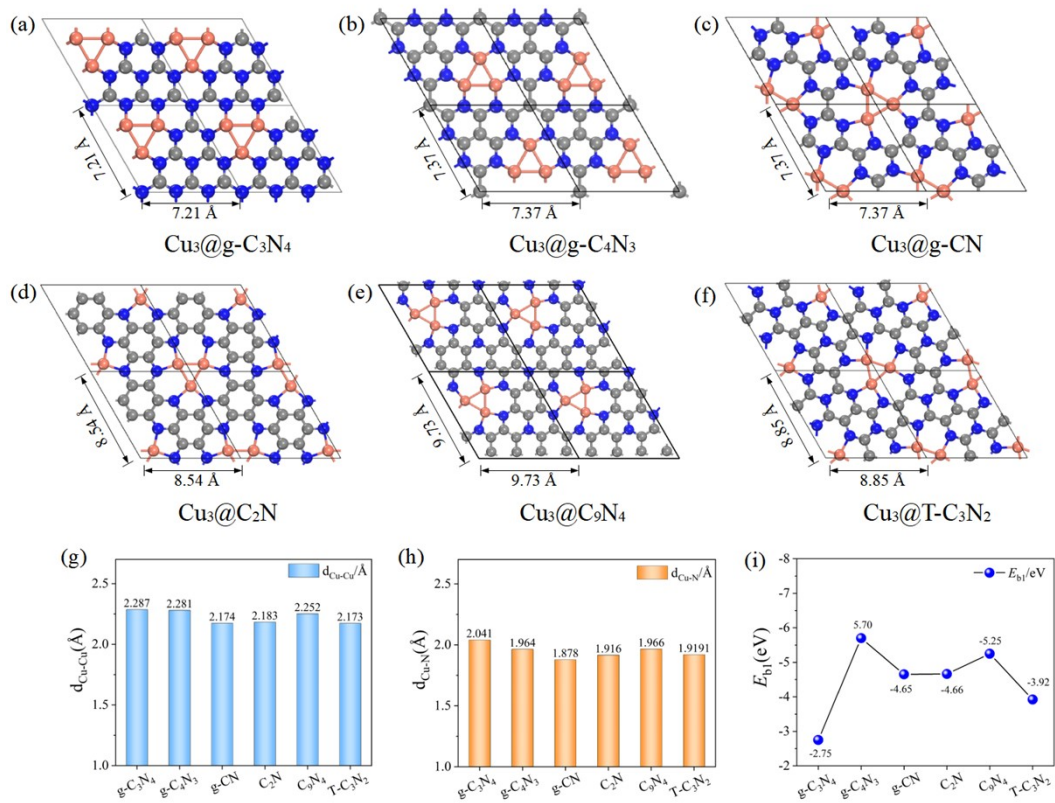


Figure S1 Comparison of the structures and unit cell parameters, Cu–Cu bond lengths, Cu–N bond lengths, and binding energies of Cu₃ with the substrates for Cu₃@g-C₃N₄, Cu₃@g-C₄N₃, Cu₃@g-CN, Cu₃@C₂N, Cu₃@C₉N₄, and Cu₃@T-C₃N₂.

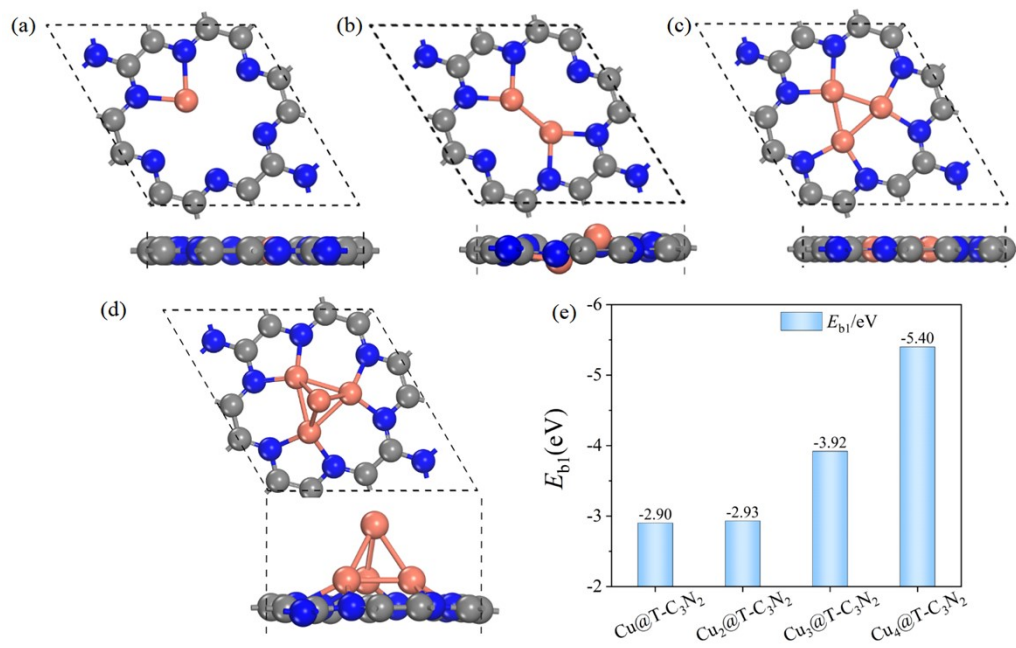


Figure S2 (a-d) The optimized structures of Cu_n@T-C₃N₂ (n = 1-4) and (e) the interaction energy (E_{b1}) between Cu clusters and the substrate

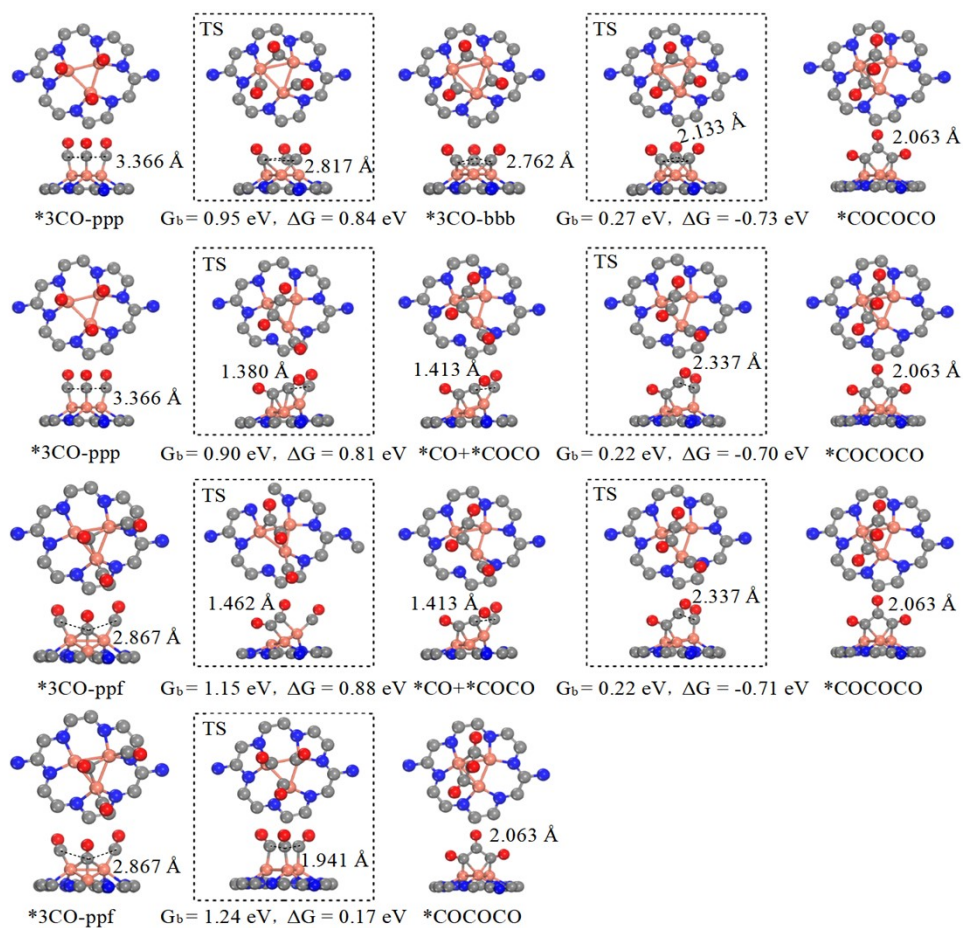


Figure S3 Kinetic energy barriers (G_b), Gibbs free energy changes (ΔG), and the main C-C bond lengths for the formation of *COCOCO from different configurations of CO coupling.

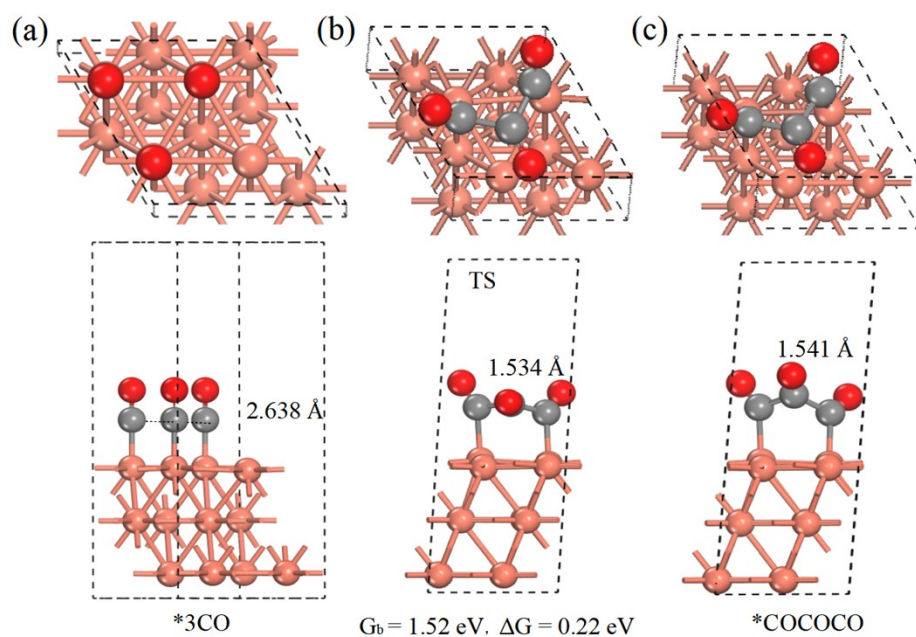


Figure S4 Kinetic energy barrier (G_b), the change in Gibbs free energy (ΔG) of the $3*CO$ coupling reaction on the Cu(111) surface to form $*\text{COCOCO}$, as well as the main C-C bond length.

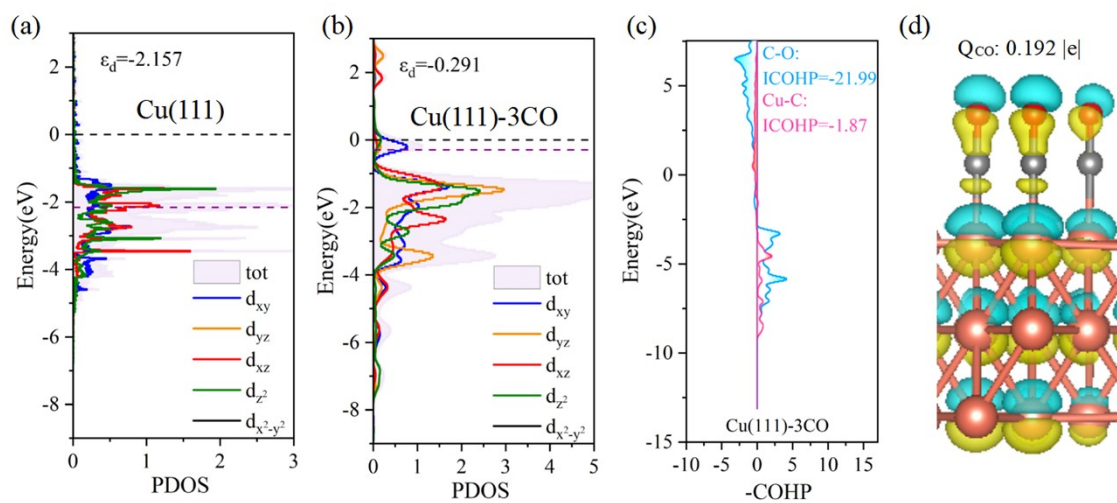


Figure S5 PDOS of (a) Cu(111), (b) Cu(111) catalyst with three adjacent CO molecules, as well as the d-band center of the Cu site (ϵ_d); (c) ICOHP analysis of the C-O bond and Cu-C bond; (d) Charge difference density map of CO adsorption, with the interface value being $0.002 \text{ e}/\text{\AA}^3$.

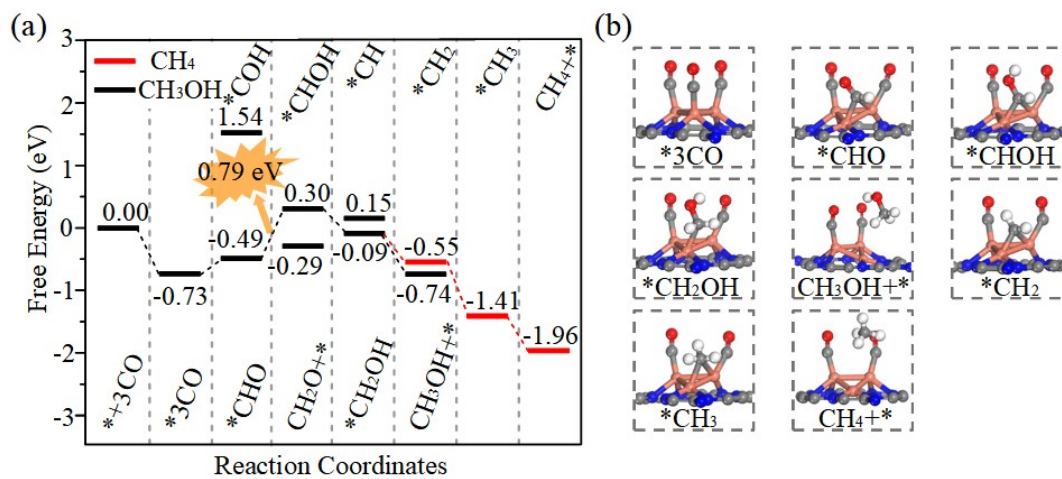


Figure S6 Gibbs free energy diagram and intermediate structures for the lowest energy pathway of CO reduction to C₁ products.

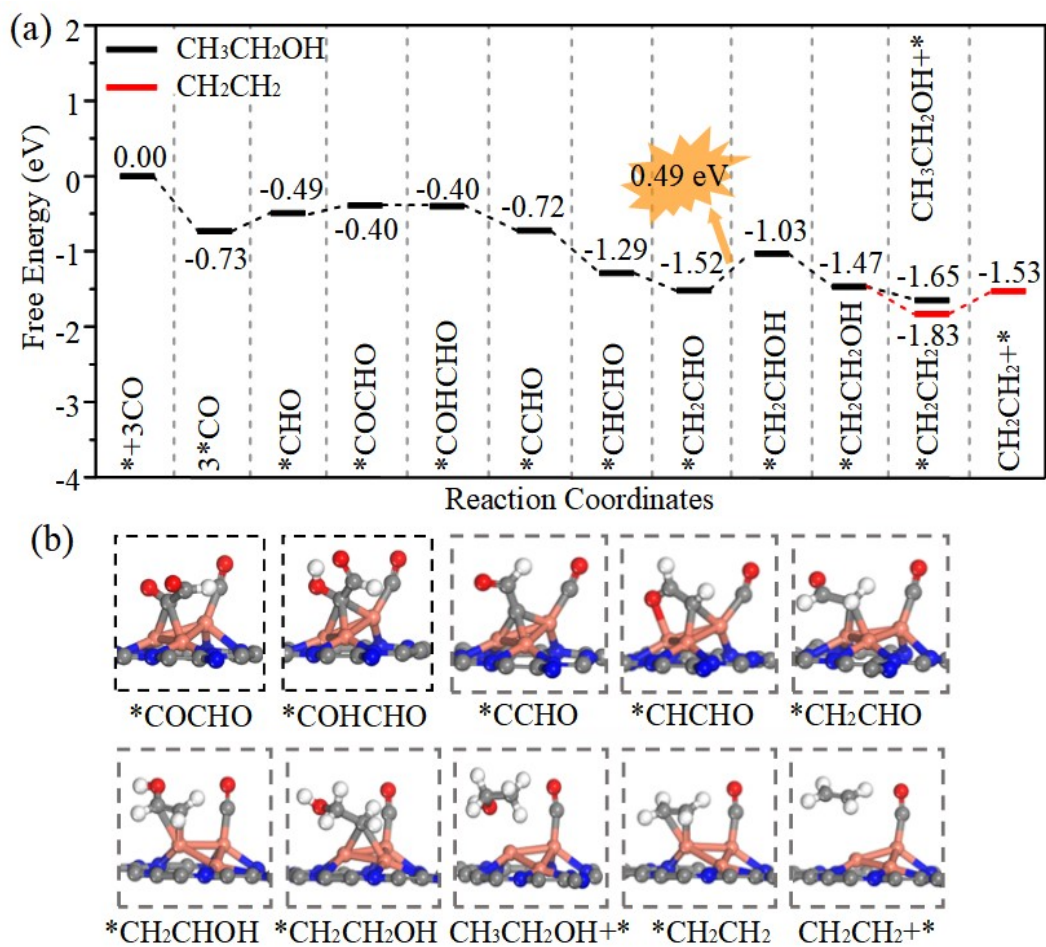


Figure S7 Gibbs free energy diagram and intermediate structures for the lowest energy pathway of CO reduction to C₂ products.

Table S1 Changes in Cu-Cu, Cu-N bond lengths, the distances between the three Cu sites and the T-C₃N₂ sheet, and the CO adsorption energy (eV/CO) during continuous CO adsorption.

Pathway 1						
	Cu-Cu/Å	Cu-N/Å	h _{Cu1} /Å	h _{Cu2} /Å	h _{Cu3} /Å	E _{ads} /eV
*+3CO	2.1730	1.9191	0	0	0	
*CO-p+2CO	2.2405	2.0704	0.5362	1.2922	0.6369	-0.44
*2CO-pp+CO	2.3785	2.1713	0.4594	1.3405	1.3394	-0.39
*3CO-ppp ^a	2.4926	2.1189	1.3582	1.3574	1.3506	-0.24
Pathway 2						
	Cu-Cu/Å	Cu-N/Å	h _{Cu1} /Å	h _{Cu2} /Å	h _{Cu3} /Å	E _{ads} /eV
*+3CO	2.1730	1.9191	0	0	0	
*CO-f+2CO	2.3447	1.9646	0.9293	0.8625	0.8659	-1.41
*2CO-pf+CO	2.5120	2.0180	0.7753	1.4604	0.7909	-0.64
*3CO-ppf	2.4870	2.1497	0.5376	1.4206	1.3926	-0.27

^a The p represents a point position, b represents a bridge position, and f represents a face position.

Table S2 Changes in Cu-Cu, Cu-N bond lengths, and the distances between the three Cu sites and the T-C₃N₂ sheet during the C-C coupling process.

	Cu-Cu/Å	Cu-N/Å	h _{Cu1} /Å	h _{Cu2} /Å	h _{Cu3} /Å
3*CO-ppp ^a	2.4926	2.1189	1.3582	1.3574	1.3506
TS1	2.6193	2.0887	1.3345	1.3282	1.3305
3*CO-bbb	2.6735	2.0402	1.3220	1.3224	1.3222
TS2	2.5297	2.0634	1.2645	1.2150	1.2499
*COCOCO	2.3965	2.0538	1.2282	1.0854	1.0478
3*CO-ppp	2.4926	2.1189	1.3582	1.3574	1.3506
TS1	2.3202	2.0618	0.9000	1.5985	0.9452
*COCO+*CO	2.2887	2.0710	0.8671	1.6442	0.8515
TS2	2.3306	2.0926	1.0020	1.3563	0.9894
*COCOCO	2.3965	2.0538	1.2282	1.0854	1.0478
3*CO-ppf	2.4870	2.1497	0.5376	1.4206	1.3926
TS1	2.3375	2.1756	1.0749	1.7747	0.8207
*COCO+*CO	2.2887	2.0710	0.8671	1.6442	0.8515
TS2	2.3306	2.0926	1.0020	1.3563	0.9894
*COCOCO	2.3965	2.0538	1.2282	1.0854	1.0478
3*CO-ppf	2.4870	2.1497	0.5376	1.4206	1.3926
TS	2.5099	2.0841	1.1979	1.2626	1.2197
*COCOCO	2.3965	2.0538	1.2282	1.0854	1.0478

^a The p represents a point position, b represents a bridge position, and f represents a face position.

Table S3 The reaction path for the formation of the C₃ product of the Cu₃@T-C₃N₂ catalyst and the relative free energy ($\Delta G/eV$)

Primitive response	Free energy change ($\Delta G/eV$)
* +3CO(g) \rightarrow 3*CO	-0.73
3*CO \rightarrow *COCOCO	0.10
*COCOCO + H ⁺ + e ⁻ \rightarrow *COCO _H CO	-0.25
*COCO _H CO + H ⁺ + e ⁻ \rightarrow *COCCO+H ₂ O	-0.18
*COCCO + H ⁺ + e ⁻ \rightarrow *CHCOCO	-0.14
*CHCOCO + H ⁺ + e ⁻ \rightarrow *CHCO _H CO	-0.20
*CHCO _H CO + H ⁺ + e ⁻ \rightarrow *CHCO _H CHO	-0.28
*CHCO _H CHO + H ⁺ + e ⁻ \rightarrow *CHCCHO+H ₂ O	0.18
*CHCCHO + H ⁺ + e ⁻ \rightarrow *CH ₂ CCHO	-0.43
*CH ₂ CCHO + H ⁺ + e ⁻ \rightarrow *CH ₂ CHCHO	0.09
*CH ₂ CHCHO + H ⁺ + e ⁻ \rightarrow *CH ₂ CHCHO _H	0.09
*CH ₂ CHCHO _H + H ⁺ + e ⁻ \rightarrow *CH ₂ CHCH+H ₂ O	-0.03
*CH ₂ CHCHO _H + H ⁺ + e ⁻ \rightarrow *CH ₃ CHCHO _H	0.03
*CH ₂ CHCH + H ⁺ + e ⁻ \rightarrow *CH ₂ CHCH ₂	-0.86
*CH ₃ CHCHO _H + H ⁺ + e ⁻ \rightarrow *CH ₃ CH ₂ CHO _H	-0.61
*CH ₂ CHCH ₂ + H ⁺ + e ⁻ \rightarrow CH ₃ CHCH ₂	0.24
*CH ₃ CH ₂ CHO _H + H ⁺ + e ⁻ \rightarrow CH ₃ CH ₂ CH ₂ OH	0.14

Table S4 Cu-Cu, Cu-N bond lengths, and the distances between the three Cu sites and the T-C₃N₂ sheet during the progress for C₃ products.

	Cu-Cu/Å	Cu-N/Å	h _{Cu1} /Å	h _{Cu2} /Å	h _{Cu3} /Å
*+3CO	2.1730	1.9191	0.0000	0.0000	0.0000
*3CO	2.4926	2.1189	1.3582	1.3574	1.3506
*COCOCO	2.3965	2.0538	1.2282	1.0854	1.0478
*COCOHC	2.3264	2.0759	1.1318	1.0621	1.0467
*COCCO	2.4138	2.0378	1.0662	1.0590	1.1880
*CHCOCO	2.3600	2.0903	1.1085	1.1134	1.1158
*CHCOHC	2.4391	2.1668	1.1128	1.2262	1.2153
*CHCOHCHO	2.3435	2.2154	1.1076	0.2428	1.2237
*CHCCHO	2.4832	2.0112	1.1361	1.1438	1.1107
*CH ₂ CCHO	2.5251	2.0040	0.1141	1.1894	1.1660
*CH ₂ CHCHO	2.4172	2.2024	0.9729	1.3647	1.1453
*CH ₂ CHCHOH	2.3309	2.1121	1.0638	1.0093	1.1077
*CH ₃ CHCHOH	2.5250	2.0518	0.0000	0.0000	0.9068
*CH ₃ CH ₂ CHOH	2.2975	1.9526	0.9714	1.1906	0.2610
*CH ₃ CH ₂ CH ₂ OH	2.2209	1.9539	0.6586	0.6977	0.6626

Table S5 The reaction path for the formation of the C₁ product of the Cu₃@T-C₃N₂ catalyst and the relative free energy ($\Delta G/eV$)

Primitive response	Free energy change ($\Delta G/eV$)
*+3CO(g)→3*CO	-0.73
3*CO+H ⁺ +e ⁻ →*CHO+2*CO	0.24
3*CO+H ⁺ +e ⁻ →*COH+2*CO	2.27
*CHO+2*CO+H ⁺ +e ⁻ →*CHOH+2*CO	0.79
*CHO+2*CO+H ⁺ +e ⁻ →*CH ₂ O+2*CO	0.20
*CHOH+2*CO+H ⁺ +e ⁻ →*CH ₂ OH+2*CO	-0.39
*CHOH+2*CO+H ⁺ +e ⁻ →*CH+2*CO	-0.15
*CH ₂ OH+2*CO+H ⁺ +e ⁻ →*CH ₃ OH+2*CO	-0.65
*CH ₂ OH+2*CO+H ⁺ +e ⁻ →*CH ₂ +2*CO	-0.46
*CH ₂ +2*CO+H ⁺ +e ⁻ →*CH ₃ +2*CO	-0.86
*CH ₃ +2*CO+H ⁺ +e ⁻ →*CH ₄ +2*CO	-0.55

Table S6 The reaction path for the formation of the C₂ product of the Cu₃@T-C₃N₂ catalyst and the relative free energy ($\Delta G/eV$)

Primitive response	Free energy change ($\Delta G/eV$)
*+3CO(g)→3*CO	-0.73
3*CO+H ⁺ +e ⁻ →*CHO+2*CO	0.24
*CHO+2*CO→*COCHO+*CO	0.09
*COCHO+*CO+H ⁺ +e ⁻ →*COHCHO+*CO	0.00
*COHCHO+*CO+H ⁺ +e ⁻ →*CCHO+*CO+H ₂ O	-0.32
*CCHO+*CO+H ⁺ +e ⁻ →*CHCHO+*CO	-0.57
*CHCHO+*CO+H ⁺ +e ⁻ →*CH ₂ CHO+*CO	-0.23
*CH ₂ CHO+*CO+H ⁺ +e ⁻ →*CH ₂ CHOH+*CO	0.49
*CH ₂ CHOH+*CO+H ⁺ +e ⁻ →*CH ₂ CH ₂ OH+*CO	-0.44
*CH ₂ CH ₂ OH+*CO+H ⁺ +e ⁻ →CH ₃ CH ₂ OH+*CO	-0.18
*CH ₂ CH ₂ OH+*CO+H ⁺ +e ⁻ →*CH ₂ CH ₂ +*CO+H ₂ O	-0.36
*CH ₂ CH ₂ +*CO→CH ₂ CH ₂ +*CO	0.30

Table S7 Optimized energy and CONTCAR

	Structure	Energy
Adsorption	$\text{Cu}_3@T\text{-C}_3\text{N}_2$	-181.14226485
	*CO-p	-196.96757572
	*2CO-pp	-212.61634141
	*3CO-ppp	-227.92162500
	*CO-f	-197.96212000
	*2CO-pf	-213.22065000
	*3CO-ppf	-228.10627299
TS	TS1 from 3*CO-ppp to 3*CO-bbb	-227.01163784
	3*CO-bbb	-227.19550669
	TS2 from 3*CO-bbb to *COCOCO	-226.895296
	*COCOCO	-228.01356096
	TS1 from 3*CO-ppp to *COCO+*CO	-227.09346670
	*COCO+*CO	-227.19663000
	TS2 from *COCO+*CO to *COCOCO	-226.9451288
	3*CO-ppf	-228.10627299
	TS1 from 3*CO-ppf to *COCO+*CO	-226.96372172
	*COCO+*CO	-227.19663000
	TS from 3*CO-ppf to *COCOCO	-226.86343535
C ₃ path	*COCO HCO	-232.0038137
	*COCCO	-221.02736974
	*CHCOCO	-224.9759038
	*CHCO HCO	-228.9325488
	*CHCO HCHO	-232.92928745
	*CHCCHO	-221.54947233
	*CH ₂ CCHO	-225.76503233
	*CH ₂ CHCHO	-229.398671
	*CH ₂ CHCHOH	-233.0363195
	*CH ₂ CHCH	-221.9060828
	*CH ₃ CHCHOH	-236.7936818
	*CH ₂ CHCH ₂	-226.4972252
	*CH ₃ CH ₂ CHOH	-241.1434035
	CH ₃ CHCH ₂	-229.9743444
	CH ₃ CH ₂ CH ₂ OH	-244.7360426
C ₁ path	*CHO+2*CO	-231.4834829

	*COH+2*CO	-229.4693639
	*CHOH+2*CO	-234.4203718
	CH ₂ O+2*CO	-234.893457
	*CH ₂ OH+2*CO	-238.5545784
	*CH+2*CO	-223.4810031
	*CH ₂ +2*CO	-227.8247217
	*CH ₃ OH+2*CO	-242.8715262
	*CH ₃ +2*CO	-232.4196046
	*CH ₄ +2*CO	-236.6091254
C ₂ path	*COCHO+*CO	-231.3604608
	*COHCHO+*CO	-235.2001934
	*CCHO+*CO	-224.3806900
	*CHCHO+*CO	-228.6842368
	*CH ₂ CHO+*CO	-232.7006568
	*CH ₂ CHOH+*CO	-235.920168
	*CH ₂ CH ₂ OH+*CO	-240.1307666
	*CH ₃ CH ₂ OH+*CO	-244.0166579
	*CH ₂ CH ₂ +*CO	-229.3380316
	CH ₂ CH ₂ +*CO	-228.9519672

Cu₃@T-C₃N₂

C12Cu3N8

1.00000000000000

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-4.4239698369999658 7.6625187567800541 0.0000028950696540

-0.0000083164190687 0.0000029202282706 19.5595854150194626

C N Cu

12 8 3

Direct

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0.9758086660034886 0.4205822981821677 0.5000000349075365

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0.8777356518871637	0.8445583408863574	0.5000000740754373
0.1554409324867988	0.0331788577052001	0.4999996270079801

*CO-p

C13Cu3N8O1

1.0000000000000000

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-4.4239634595000004	7.6624988503000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.5596008300999991

C	N	Cu	O
13	8	3	1

Direct

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0.7889225680192141	0.2772939999233663	0.4890761963715043
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0.4365842406586138	0.0194411433301096	0.4900226213533386
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0.8863024971879594	0.6324373280999173	0.4998894433970971
0.3597608551407777	0.2501491599038373	0.4906616859475774
0.3296439387484940	0.6621533258600073	0.4925310359832414
0.6627282308089369	0.3303015587703658	0.4872583481585683
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*2CO-pp

C14Cu3N8O2

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  0.0000000000000000    0.0000000000000000    19.5596008300999991
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```
  C    N    Cu    O
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Direct

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0.5176912588419486  0.7909791080486421  0.4876588326257976
0.7925295747074442  0.2789918976234313  0.4841005646450401
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0.0212862483563596  0.5944759315798508  0.4913360373737106
0.4045332085897260  0.4267248923011381  0.4860877833209133
0.5720110791026618  0.9772563585034315  0.4860329470908730
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0.4382276857710857  0.0229323660374972  0.4875792455269878
0.7996586130035740  0.7924580253140769  0.6417148658590264
0.2336677580044639  0.0904544177890336  0.6421845145377197
0.2650272584564907  0.8985939334970119  0.4942684917382885
0.1007745682585554  0.3658206331458742  0.4854697360556564
0.6325538125376928  0.7343977381958419  0.4884121049200387
0.7449830686098321  0.1083148254607743  0.4850441872129218
0.8901811561312142  0.6355667284127999  0.4945339061077391
0.3631875588069890  0.2546850460902686  0.4879662158207849
0.3321159426829592  0.6660060598108195  0.4881215800841389
0.6662369397987271  0.3332007921258388  0.4830963074520389
0.9672720239921031  0.1057130084145683  0.5065808084069259
0.8630745024256279  0.8206843761803276  0.5516288221716218
0.1799012265932227  0.0433163166196033  0.5515734156180764
0.7797282000771577  0.8174518289999007  0.6983614046039563
0.2319748927172774  0.1232710044098820  0.6995527901591638
```

*3CO-ppp

C15Cu3N8O3

```
1.0000000000000000
  8.8479003905999996    0.0000000000000000    0.0000000000000000
 -4.4239634595000004    7.6624988503000004    0.0000000000000000
  0.0000000000000000    0.0000000000000000    19.5596008300999991
```

C	N	Cu	O
15	8	3	3
Direct			
0.2067965964141081	0.7278250880969498	0.4856847982942851	
0.2713636719341668	0.4820722252677201	0.4856833885611912	
0.5170777289900581	0.7923716457513356	0.4858092702710953	
0.7914745702449979	0.2798615719127081	0.4812244028308618	
0.7193718820463121	0.5146907535077004	0.4811091565599982	
0.4845659388610116	0.2077831769488692	0.4813118735782375	
0.0203834677345140	0.5957073765580310	0.4842924504249713	
0.4034558196775394	0.4276868341592695	0.4844308194631022	
0.5714711918174127	0.9788306304413902	0.4845874255076939	
0.9750431745089820	0.4161082989336331	0.4828150189271649	
0.5830539875095564	0.5619433353760838	0.4828827975277628	
0.4372680983860208	0.0241971693471003	0.4830527639424780	
0.8148501437141359	0.7596239858657042	0.6370214094315444	
0.2330569719263015	0.0575285296097533	0.6372926415998947	
0.9417470041939960	0.1872812580559289	0.6367330435573574	
0.2634107494731856	0.8995309373331966	0.4874268146316225	
0.0996894589096956	0.3669810705914439	0.4872492406078334	
0.6321611860545333	0.7356993206052638	0.4873884337972459	
0.7438146440680841	0.1097424909861324	0.4866597122495209	
0.8894727512619328	0.6371809316064667	0.4863541521876633	
0.3620288400611979	0.2552954892903606	0.4866280666098681	
0.3317561384007887	0.6674178968031743	0.4841532511542440	
0.6651151860226356	0.3340811255530650	0.4767516800195411	
0.9545334901112127	0.1369243481747608	0.5461903309114179	
0.8618440116858814	0.8203488016263978	0.5461502714105819	
0.1781342050796645	0.0441137830132193	0.5458017025744804	
0.8155062558591717	0.7613428317286196	0.6963004766097270	
0.2267930233311190	0.0573466055389498	0.6965307830316543	
0.9435398667217576	0.1896425503168138	0.6959937557269895	

*CO-f

C13Cu3N8O1

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239634600000004 7.6624988500000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

C	N	O	Cu
13	8	1	3

Direct

0.6959063245111952 0.2260072210050544 0.4918012712763198

0.7618415241357527 0.9816865782679303 0.4924473435922874

0.0059607064650794	0.2920087339804321	0.4920426626595036
0.2821057500993164	0.7824647155692033	0.4879156437405415
0.2053987099330292	0.0114454151651864	0.4871109463969080
0.9766980992991892	0.7060336421823227	0.4873622236790299
0.5112063917781497	0.0977348949070511	0.4901292195889190
0.8902489433901107	0.9254030730346722	0.4904140360671104
0.0627564653829341	0.4768433726448574	0.4907819316689325
0.4632289440438794	0.9173544700997989	0.4897192837792337
0.0704273541434271	0.0577394738332206	0.4890589738534607
0.9304613267419605	0.5248492462462993	0.4892091199226800
0.4889915932576891	0.4956154256899754	0.5980998644494399
0.7564327782424136	0.4000499541870784	0.4934904058710174
0.5878648246676016	0.8681454129308089	0.4950776948138548
0.1194227200305121	0.2315523682930194	0.4936853055152381
0.2350426814060641	0.6106934998705166	0.4931059387210348
0.3773213012296055	0.1361801192319933	0.4913641738566840
0.8520222468600177	0.7532487072486236	0.4918470500000787
0.8211534502930022	0.1665591187509613	0.4908189087453015
0.1547111148423782	0.8332697556206546	0.4837025603398255
0.4898383943833114	0.4899908517467119	0.6591935307180582
0.4493338495300511	0.6305586569098427	0.5312150840471458
0.3576814579476577	0.3316030837206730	0.5277967345395853
0.6565460673856781	0.5388231388631073	0.5279699521578278

*2CO-pf

C14Cu3N8O2

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239634600000004 7.6624988500000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

C N O Cu

14 8 2 3

Direct

0.6948023413137074 0.2336086523626810 0.4896081354058984

0.7601361647256563 0.9891379974252784 0.4892230902760460

0.0056570632794039 0.3002708966773852 0.4905387170949791

0.2803329192381514 0.7908226018600411 0.4850578078317184

0.2064232473804833 0.0223285977103450 0.4873650274667751

0.9746115588496578 0.7147663514614271 0.4849249080803824

0.5097517192908082 0.1054494767222180 0.4890384439068680

0.8900200656908734 0.9344139007312717 0.4880597612600510

0.0600123253194198 0.4847012343849423 0.4880534316549396

0.4617563993382974 0.9246664356757837 0.4866529633153129

0.0710912672187049 0.0686258795688377 0.4889832576005825

0.9283382294950152	0.5331158610331987	0.4867763285961162
0.2592781009311282	0.1962522040940536	0.6391220785018734
0.5195407440982746	0.5536931286611330	0.5977366906298689
0.7539906630230305	0.4074218322737359	0.4907791972510602
0.5861435744915467	0.8746416847820390	0.4900541830145542
0.1205614985726874	0.2425204156368768	0.4943397339863402
0.2324711189302125	0.6182361797661138	0.4887013475275812
0.3780990082420532	0.1462858608979057	0.4927213626869224
0.8500766583813313	0.7613795527903403	0.4885298485341376
0.8199257631124978	0.1741454896493420	0.4885550650654997
0.1536379955327244	0.8427983650562254	0.4823641431273612
0.2204945480505096	0.1281378417901285	0.6915009606307583
0.5539655502306783	0.6018250276377011	0.6558141707546119
0.4399240521141118	0.6264601105606366	0.5220024210425965
0.3450079682454257	0.3201581729175765	0.5570284871237978
0.6464095849035872	0.5367408078727576	0.5227988676333689

*3CO-ppf

C15Cu3N8O3

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239634600000004 7.6624988500000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

C N O Cu

15 8 3 3

Direct

0.7076137971514511	0.2447198881841833	0.4900768120598673
0.7741795045001960	0.0003011909042522	0.4864679314210876
0.0187092886839443	0.3106105447514343	0.4883020341748867
0.2938368709818863	0.7999117156385885	0.4818216030149663
0.2196277332926939	0.0320845627847434	0.4874746213755161
0.9865820774199029	0.7250870710399709	0.4853558568292710
0.5228465147306685	0.1150727180840816	0.4890797677342795
0.9039492045562485	0.9451823150930685	0.4872355652577536
0.0729256383554678	0.4950912980315761	0.4852390664524766
0.4751865184906199	0.9344478714784066	0.4837733922337568
0.0849183382058842	0.0793484591310724	0.4881107524741795
0.9397154495725593	0.5424875617812240	0.4868156932795836
0.2693036620432686	0.2123705177641447	0.6379143155353790
0.4889284285877827	0.5692682506340621	0.5980035397761613
0.8060999895958514	0.5496996854520938	0.6317766611806040
0.7659500949440603	0.4179808855484934	0.4927259078285394
0.6005122802590395	0.8846149704732112	0.4844960328871954
0.1342581163737750	0.2536719289988310	0.4917329561868899

0.2463195579219080	0.6275103990815831	0.4830315840257047
0.3910527996104358	0.1555804580550851	0.4935325701650745
0.8624888730071529	0.7722626454444093	0.4900673111946961
0.8330023502193894	0.1847491877333705	0.4874543780534922
0.1660198731057627	0.8519011594287587	0.4815491093379201
0.2417617538243199	0.1678682499901107	0.6941253884949125
0.4762496671148890	0.6202450635516875	0.6531478857030548
0.8541927871107838	0.4971323324058600	0.6755942123075501
0.4650770770496980	0.6338125508057422	0.5090318593858593
0.3622691444779172	0.3328669941725816	0.5541772443284557
0.6840264888124484	0.5587357235573716	0.5527449873008949

3*CO-ppp

C15Cu3N8O3

1.0000000000000000

8.8479003905999996 0.0000000000000000 0.0000000000000000

-4.4239634595000004 7.6624988503000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300999991

C N Cu O

15 8 3 3

Direct

0.6960600020000030	0.2353700399999994	0.4856800140000033
0.7606300120000000	0.9896199699999997	0.4856800140000033
0.0063499999999976	0.2999199630000007	0.4858100120000017
0.2807399929999974	0.7874100209999995	0.4812200069999975
0.2086399940000021	0.0222300289999993	0.4811100069999981
0.9738299850000018	0.7153300049999984	0.4813100100000014
0.5096499919999999	0.1032500270000014	0.4842900040000018
0.8927199840000029	0.9352300170000021	0.4844299849999985
0.0607400009999992	0.4863699670000017	0.4845899939999967
0.4643099899999967	0.9236500259999971	0.4828099910000034
0.0723199990000012	0.0694899559999982	0.4828799960000012
0.9265400170000007	0.5317400100000000	0.4830499890000013
0.3041200039999978	0.2671699520000033	0.6370199919999990
0.7223199609999966	0.5650699729999999	0.6372900009999967
0.4310100080000012	0.6948199870000025	0.6367300149999977
0.7526800039999983	0.4070700409999972	0.4874300059999968
0.5889599919999995	0.8745200039999972	0.4872500000000031
0.1214300019999968	0.2432399989999965	0.4873900119999988
0.2330800000000011	0.6172900199999987	0.4866600040000009
0.3787400129999980	0.1447199580000031	0.4863500000000016
0.8513000009999985	0.7628399729999984	0.4866299930000011
0.8210200070000013	0.1749600169999965	0.4841499919999990
0.1543799940000028	0.8416200280000012	0.4767499860000015

0.4438000020000032	0.6444699760000034	0.5461900230000012
0.3511100110000029	0.3278900379999996	0.5461500290000032
0.6674000020000008	0.5516600010000019	0.5457999710000010
0.3047699930000007	0.2688900229999973	0.6963000300000033
0.7160600420000023	0.5648900269999970	0.6965299840000014
0.4328100090000007	0.6971899870000016	0.6959900259999969

TS1 from 3*CO-ppp to 3*CO-bbb

C15N8Cu3O3

1.0000000000000000

8.8479003905999996	0.0000000000000000	0.0000000000000000
-4.4239539850714298	7.6625043203714300	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.5596008300999991

C	N	Cu	O
15	8	3	3

Direct

0.6939096276025045	0.2209548722752488	0.4886424549551986
0.7613447261985047	0.9773720295198870	0.4886184210028435
0.0049346140782531	0.2883866844549804	0.4886538776180848
0.2802454299882461	0.7763923671326959	0.4804619301446564
0.2058402803072287	0.0082323339651452	0.4804294164560406
0.9739925401852918	0.7019948421634163	0.4804461484774857
0.5097232582504498	0.0916529865469019	0.4848852326155156
0.8906142215840106	0.9224624692735680	0.4848879520275811
0.0598260520074292	0.4725707587752032	0.4849439300301114
0.4618660623759908	0.9109123934241012	0.4843114091489515
0.0714009781177451	0.0553809335161739	0.4842868993209991
0.9268865339128054	0.5204030065528731	0.4843155821774633
0.4879810685088069	0.3126318518391490	0.6135416924484611
0.6686462517163370	0.6801932859663423	0.6133790526063208
0.3020133885761985	0.4944039518252678	0.6137029979541517
0.7528351147264173	0.3953642525501587	0.4928729346733617
0.5869039468799898	0.8619036661003928	0.4928295562825291
0.1204078477674738	0.2294076418678342	0.4928774476319389
0.2326020004841912	0.6049245752577784	0.4849634440354566
0.3773583519763566	0.1320682454121569	0.4848873902912538
0.8501931894215690	0.7496824016024997	0.4849367153145943
0.8200741717903917	0.1622417574386285	0.4860130534315212
0.1533667751006587	0.8288855446266012	0.4761867765116921
0.4449684045197765	0.6419304510185886	0.5444116684873386
0.3408098379070106	0.3074022213066498	0.5440924808622368
0.6747639832369831	0.5375626696876791	0.5442083133624401
0.5399218954451680	0.2649084485713509	0.6585614458800155
0.7166059000109521	0.7786237902997097	0.6588346090998626

0.2030672907822099 0.4421836523307455 0.6589187884687925

3*CO-bbb

C15N8Cu3O3

1.0000000000000000

8.8479003905999996 0.0000000000000000 0.0000000000000000

-4.4239501952999998 7.6625065083999999 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300999991

C N Cu O

15 8 3 3

Direct

0.6944299940000036 0.2190599440000014 0.4870199860000000

0.7602199909999996 0.9742699860000030 0.4870199860000000

0.0050200000000018 0.2848399880000017 0.4870199860000000

0.2805500030000019 0.7745400069999988 0.4825899900000010

0.2047400029999977 0.0049099920000018 0.4825899900000010

0.9743700029999971 0.6987199779999997 0.4825899900000010

0.5096600059999972 0.0903099780000005 0.4855599999999995

0.8889700169999983 0.9182500240000024 0.4855599999999995

0.0610300000000024 0.4696300029999989 0.4855599999999995

0.4620400069999988 0.9096800089999988 0.4841800029999987

0.0695900019999982 0.0512599950000023 0.4841899870000006

0.9280199999999965 0.5172500010000007 0.4841800029999987

0.5347399710000005 0.3415199519999987 0.6068500279999967

0.6377600430000001 0.6920999880000025 0.6068400139999994

0.2871499959999966 0.4445500369999991 0.6068500279999967

0.7539200189999988 0.3930499550000022 0.4892300070000033

0.5862200259999995 0.8597699999999975 0.4892300070000033

0.1194999960000018 0.2253799439999966 0.4892300070000033

0.2338999959999981 0.6029199959999971 0.4878500100000025

0.3763599990000017 0.1298899649999967 0.4878500100000025

0.8493900300000021 0.7453899980000003 0.4878399970000018

0.8198800090000020 0.1593999859999968 0.4851599930000035

0.1532099989999978 0.8260700109999988 0.4784100059999972

0.4411099849999971 0.6399599909999978 0.5460000039999997

0.3393099899999967 0.3000400069999998 0.5460199709999998

0.6792299749999984 0.5381600259999999 0.5460100170000004

0.5568699840000022 0.2647299770000018 0.6510599850000034

0.7145500179999971 0.7910199760000012 0.6510499720000027

0.1882299930000002 0.4224400519999989 0.6510499720000027

TS2 from 3*CO-bbb to *COCOCO

C15N8Cu3O3

1.0000000000000000

8.8479003905999996	0.0000000000000000	0.0000000000000000
-4.4239501952999998	7.6625065083999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.5596008300999991

C	N	Cu	O
15	8	3	3

Direct

0.6950379105057936	0.2218169758325197	0.4877602639243864
0.7601815507726382	0.9762774314483352	0.4869071272587746
0.0056492465341280	0.2868549636632567	0.4869953591359572
0.2805171174462355	0.7756593685074874	0.4827085866030943
0.2064466882002081	0.0080851001825864	0.4830616423994016
0.9739443351616028	0.7014454757655882	0.4828764252090376
0.5094718199079575	0.0917286548458925	0.4862834571322296
0.8904115565357773	0.9208075487134401	0.4856289454877198
0.0611336570526259	0.4725812307178173	0.4857261366680374
0.4631646854321448	0.9117401888932821	0.4843210281324371
0.0704418450086712	0.0546220494558160	0.4843421080013406
0.9273729105039079	0.5188683596779932	0.4847722923907120
0.5195740082166124	0.3887790521659795	0.6220916220919944
0.6132810247840459	0.6621827133168022	0.6157996479100528
0.3285931526329733	0.4573465463265706	0.6173371147644446
0.7534880274952964	0.3945664569650106	0.4896398041788089
0.5874174387762942	0.8621055108911470	0.4882104955951120
0.1199840232177124	0.2285253771133079	0.4882527021002769
0.2337255348099027	0.6049466700406836	0.4869882891715127
0.3770624204720064	0.1318907647745093	0.4879214406626036
0.8501918029291911	0.7482085038547002	0.4870355201121818
0.8203341605682147	0.1617068041116631	0.4858873884475176
0.1537070796499611	0.8283867773101145	0.4796683595551733
0.4428443918498604	0.6382670173503897	0.5443171476188455
0.3483026910839543	0.3137559595759991	0.5417866039820135
0.6702566810448929	0.5378884779149137	0.5435691366883434
0.5410517660713364	0.3070776835770062	0.6656339952616543
0.7000960920929074	0.7701808063230651	0.6567904904902940
0.2164799139264218	0.4263485341891098	0.6579549520263140

TS1 from 3*CO-ppp to*COCO+*CO

C15N8O3Cu3

1.0000000000000000		
8.8479003899999995	0.0000000000000000	0.0000000000000000
-4.4239634600000004	7.6624988500000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.5596008300000008

C	N	O	Cu
15	8	3	3

Direct

0.6921116789201599	0.2458227112425200	0.4941799595216272
0.7569171415106548	0.0008129906769095	0.4915888143679528
0.0028043748357736	0.3110540242123380	0.4963638653650277
0.2777663376283844	0.8013392958152676	0.4892332991865371
0.2050090334284072	0.0346309860473677	0.4910870750229459
0.9710731501804541	0.7275686775453464	0.4886587047128023
0.5066125606514510	0.1158318376974625	0.4928330000799705
0.8889798272212124	0.9464062147953953	0.4907921409714095
0.0574769490702678	0.4975108537867157	0.4940388133775634
0.4599377866771339	0.9360292142448532	0.4894220196886491
0.0687020784228063	0.0812462334839876	0.4932578171735952
0.9242180294293538	0.5436600241929854	0.4918051640194006
0.2740578597273833	0.1839057370716952	0.6464563483714516
0.4076416659892814	0.5485380058983889	0.6390809132223350
0.5763523314067951	0.6482419887897944	0.6153585162978938
0.7508013318103879	0.4191526379121290	0.4959122291000526
0.5847182610934910	0.8860169849043290	0.4907137161101658
0.1175310932294047	0.2545886271120010	0.4998304566439413
0.2300206646196334	0.6298381103643437	0.4946297850000586
0.3751442840780846	0.1567614883229476	0.4964057088435113
0.8478609807441237	0.7741480192170336	0.4898693570430811
0.8173556073485289	0.1861913844292038	0.4928484424480609
0.1505073742946154	0.8538162352315658	0.4865667794397974
0.2629615439879650	0.1136291002962097	0.6972246734444185
0.2823642414008637	0.5153324776793887	0.6749430566224622
0.7242414522097587	0.7535164586140455	0.6398875868106767
0.4391900821381258	0.6404824883021955	0.5325801335645766
0.3492427161722976	0.3291128208881428	0.5682911232132376
0.6393750745733411	0.5438955459875393	0.5348887631925757

*COCO+*CO

C15Cu3N8O3

1.0000000000000000		
8.8479003899999995	0.0000000000000000	0.0000000000000000
-4.4239634600000004	7.6624988500000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.5596008300000008

C	N	O	Cu
15	8	3	3

Direct

0.6925885218332325	0.2474536285870433	0.4942759377539775
0.7575025868451504	0.0028439081060405	0.4908451395425548
0.0032026938142274	0.3125316492811017	0.4963465518899542
0.2784299517707053	0.8030749967580106	0.4896939896683740

0.2057143295234072	0.0363297784780720	0.4916165973156255
0.9718863519318559	0.7293655145315778	0.4885448829192729
0.5074273370264696	0.1175572626505761	0.4933328442726263
0.8896879800428386	0.9481727387150501	0.4902972080566835
0.0580879100087417	0.4991964569472632	0.4941107070220621
0.4606249453488567	0.9379522804003397	0.4895851226894595
0.0691244276935720	0.0831972676669422	0.4934911092617114
0.9248331154376672	0.5453070772892663	0.4916394107554137
0.2677527732661575	0.1713261020124050	0.6468109224783011
0.4060275035263264	0.5300743245418283	0.6400265495642379
0.5725878791497414	0.6540932835024493	0.6151585884545939
0.7517627306642963	0.4207973183749461	0.4956458272613712
0.5856522556439600	0.8881754562332641	0.4896738966250360
0.1177780569492445	0.2560760664742457	0.4995486097010193
0.2302383672823285	0.6315349717636962	0.4950235468901885
0.3755772239182575	0.1585185911273323	0.4972433641686130
0.8484213507891462	0.7759015688737422	0.4891035110638848
0.8180739986885387	0.1878307558851184	0.4928915021955834
0.1511335567015188	0.8559514407710223	0.4870526410121003
0.2611771189911874	0.1074731034416547	0.6987690708476685
0.2821071397878489	0.5098629567882529	0.6745648413081620
0.7199024400543179	0.7510124355386879	0.6400480046570100
0.4398669146966056	0.6410815565969041	0.5313816407585616
0.3547757351535161	0.3284090617331877	0.5711116757552843
0.6379547534602641	0.5465372469299761	0.5305858961106801

TS2 from *COCO+*CO to *COCOCO

C15N8O3Cu3

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239634600000004 7.6624988500000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

C N O Cu

15 8 3 3

Direct

0.6827221980069446	0.2425102612722303	0.4930656150549522
0.7478908508264049	0.9978431604497009	0.4908765604819362
0.9933794618176816	0.3077006878716020	0.4958429454643586
0.2690393913988114	0.7973892706352126	0.4896955761683161
0.1948524255748824	0.0292403415935562	0.4885400550765009
0.9616509888990540	0.7235941019881366	0.4873652086589313
0.4975989653543925	0.1124410252420639	0.4914172040202903
0.8795562891334996	0.9425301538047101	0.4889026965197315
0.0486122918011668	0.4939783327805533	0.4944086852217220

0.4513760852931861	0.9325459224909112	0.4895501655849967
0.0586676583073596	0.0759206347896392	0.4908327273979087
0.9149723981136063	0.5400428791996881	0.4911199268606912
0.3482286589914110	0.2617800961136179	0.6428831112095529
0.4462686725558316	0.5539910293631436	0.6692303367961231
0.5733123097307481	0.6503723832809093	0.6152658600873707
0.7414039518986703	0.4157492385524089	0.4951838210950704
0.5761861882625453	0.8837380098147143	0.4913338629842464
0.1077413655922255	0.2497552305237572	0.4991245916518759
0.2213151958268524	0.6260021401712136	0.4967213973557495
0.3649326948368927	0.1519999561527917	0.4934753651013757
0.8388098613872004	0.7706325501139357	0.4883270417470161
0.8087467713245008	0.1831445903156168	0.4916326687176231
0.1415091981255703	0.8490790462436633	0.4849557467708954
0.3673780570969023	0.1824483617518377	0.6860603433225095
0.3545142424903783	0.5538701627912882	0.7132129747476708
0.7212825246243164	0.7716971812106119	0.6343794780673200
0.4294492951833913	0.6372961209605223	0.5361855687643117
0.3299843029771414	0.3251583269756251	0.5542959579585907
0.6318886839678051	0.5419292797862059	0.5355403803736917

TS1 from 3*CO-ppf to *COCO+*CO

C15N8O3Cu3

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239634600000004 7.6624988500000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

C N O Cu

15 8 3 3

Direct

0.6841047008884763	0.2461559806848692	0.4903648181204621
0.7483559412266981	1.0011433039329138	0.4880358345466895
0.9942750089128960	0.3105942789405224	0.4924486905252225
0.2697615896584387	0.8006014327626789	0.4877545146631102
0.1983089983838492	0.0360735648677327	0.4893200802722025
0.9632917389518834	0.7279103314033031	0.4865018477824805
0.4986148381889711	0.1152452694661382	0.4901776100891800
0.8815847560894712	0.9473703548684895	0.4878521162916846
0.0488007256623746	0.4977527049980214	0.4914681412275442
0.4527567841709459	0.9357559544515627	0.4868968287287306
0.0609105676704129	0.0827375816324725	0.4901271132621214
0.9157979930996563	0.5434878391443153	0.4883960242144609
0.2230909272418924	0.1628566873353492	0.6403255285791877
0.5194616622551466	0.5249710194533872	0.6513291907310024

0.5854295185578858	0.6919762395388901	0.6161112477589717
0.7419599096260339	0.4189098022449584	0.4905250732793353
0.5774864213171027	0.8864711085832980	0.4863891456451429
0.1094028020686757	0.2558269654842312	0.4941076101562610
0.2213089053669828	0.6292195023333125	0.4940818366016838
0.3679147176622996	0.1573215074904187	0.4946819028604300
0.8400663478128755	0.7745694711752223	0.4879166097081307
0.8091817556645583	0.1864322804117573	0.4900288767078766
0.1430109754805694	0.8543047148285002	0.4849624938033824
0.1688162549092990	0.0672191265176939	0.6853413387368584
0.4773193504261263	0.4737902584064542	0.7095646641738080
0.7228351741296389	0.8310646102086207	0.6269223684770668
0.4240285283332865	0.6400387475557064	0.5399162999907663
0.3655711985908269	0.3340257987661601	0.5756932839914233
0.6291017054014043	0.5491120309300326	0.5269219693175803

TS from 3*CO-ppf to *COCOCO

C15N8O3Cu3

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239634600000004 7.6624988500000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

C N O Cu

15 8 3 3

Direct

0.7124498407367821	0.2318615424581588	0.4861419386097514
0.7770514709750330	0.9866674115869668	0.4851114034969365
0.0225360215544949	0.2968244865725677	0.4856262276607937
0.2969475586357083	0.7844326016124802	0.4816562088775306
0.2245954778316907	0.0189413110944944	0.4828211768961010
0.9901607572481916	0.7121995422600192	0.4820084336151033
0.5262006485363881	0.1002252327886318	0.4852495538833835
0.9088504958945365	0.9323195701672478	0.4843476498038759
0.0766186373248877	0.4827122148295054	0.4843507019243226
0.4806283510707433	0.9208069625121892	0.4829425318792572
0.0883453210831254	0.0664153024627636	0.4837156792981098
0.9428863255157705	0.5283601340506483	0.4832949784385533
0.3619760073271295	0.3743140058556179	0.6399179501048841
0.4921602611031395	0.6275300133571533	0.6398878744005284
0.6505892643364304	0.5413016301069282	0.6405333054149711
0.7688765338131643	0.4039345967456884	0.4871476679503237
0.6051236772233994	0.8709240874777300	0.4858322058276693
0.1380319732297020	0.2404451875388286	0.4867951223856334
0.2498033592060035	0.6141523238142871	0.4855963062177626

0.3951379913334491	0.1420441548483410	0.4875088587250267
0.8668127353700552	0.7592890826868629	0.4856529698165278
0.8370851711717682	0.1717565362794829	0.4851822822189593
0.1704871703064918	0.8386011650452011	0.4798031424972918
0.2634234482336070	0.2996203821690409	0.6850427908399261
0.4944207916222473	0.7204908339649575	0.6847434333885745
0.7391600916951464	0.5506366169967098	0.6874927911207386
0.4587143795152011	0.6411741034442815	0.5410483556913073
0.3693492563573863	0.3223266505352571	0.5443523099872473
0.6841964509028315	0.5481608148813397	0.5421624526114319

C₃ path

*COCOCO

C15N8Cu3O3

1.0000000000000000

8.8479003905999996 0.0000000000000000 0.0000000000000000

-4.4239501952999998 7.6625065083999999 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300999991

C N Cu O

15 8 3 3

Direct

0.6967512104207482	0.2221358969268586	0.4907397264795893
0.7613924414574849	0.9763832053865812	0.4897896037851838
0.0070034734955820	0.2866887011130015	0.4898701982582452
0.2826166993398329	0.7760886323754467	0.4877464480345999
0.2082667085980063	0.0086586843833224	0.4862000147752637
0.9759933975761201	0.7026516127082383	0.4848959924437649
0.5113386175896183	0.0918378924620935	0.4899340539885201
0.8926737652909114	0.9215129905746043	0.4867639563249991
0.0628368349455022	0.4733516362956193	0.4896394870967277
0.4647798885911467	0.9119848966705595	0.4892811187283939
0.0718122532183024	0.0554178112985562	0.4864764778790861
0.9294084318886902	0.5195219349991190	0.4877450732321045
0.4919046501560264	0.5213038424243474	0.6673898823136747
0.6308184518554196	0.6511889407629247	0.6186605993571533
0.3298103822982547	0.4341114840658831	0.6220460834064893
0.7550896657724833	0.3950424910284853	0.4921350285963405
0.5893446324498091	0.8622529448370206	0.4929162997997263
0.1207416406182436	0.2286635668934598	0.4899851150425089
0.2354311604825924	0.6054977862444615	0.4924939410121108
0.3788262799460029	0.1324900654720391	0.4916218180919319
0.8531332260693180	0.7497174311898627	0.4866011698916171
0.8219698840296663	0.1621612898817165	0.4889313478626987
0.1559047492785305	0.8292708765971754	0.4829627361685013

0.4491225302484583	0.6277287454775662	0.5426866438999164
0.3616957430084210	0.3238882423354815	0.5384544091174125
0.6588555781713807	0.5321351104002120	0.5365306867331793
0.5014927753728566	0.5089336883605280	0.7289624877214066
0.7668562537542979	0.7839295961437336	0.6331271838270970
0.1769888100762675	0.3609097636910919	0.6396523721317752

*COCO HCO

C15Cu3H1N8O3

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239502000000002 7.6625065100000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

H C N O Cu

1 15 8 3 3

Direct

0.4846944765730174	0.5069363775977971	0.7595702744965246
0.6994835885263136	0.2200081097200057	0.4921140808421554
0.7649921545904220	0.9754413765815834	0.4916337722049844
0.0099223196912898	0.2853667470164364	0.4904911250945501
0.2858344724513807	0.7751778712194179	0.4890615549347112
0.2109250020273095	0.0067701413697282	0.4871879336093684
0.9790426190592889	0.7009469176816815	0.4861998768424459
0.5148319234443285	0.0906498358302165	0.4911320242378757
0.8954353737974277	0.9199034284044996	0.4886331403819991
0.0659932075141850	0.4715397668485565	0.4904677077345521
0.4673946879717040	0.9104275125235544	0.4906862912428760
0.0747874546369383	0.0538461566368322	0.4875907267115307
0.9326071487494433	0.5182172631155400	0.4888267468423466
0.4770790872031359	0.5441198070011777	0.6622234726262400
0.6324553241740871	0.6360670103310208	0.6225104275048964
0.3283390312477577	0.4271442014775846	0.6227324688217259
0.7586781708042752	0.3936944136842711	0.4935636273687329
0.5922732499315125	0.8609908128465661	0.4951164718844616
0.1241438127140160	0.2271596448980478	0.4902366126693807
0.2383170466906784	0.6039195367711729	0.4936900395550075
0.3816051754613528	0.1306537299447030	0.4926281381566719
0.8553185307658792	0.7477886965453104	0.4883490558982768
0.8249477062102726	0.1603036028933136	0.4899169581818280
0.1585865022097393	0.8277258439870575	0.4839297654619256
0.4665062776812862	0.5840288779470986	0.7292105014586557
0.7805993995750973	0.7502890466596609	0.6383328136236728
0.1743022042777938	0.3343683681085764	0.6387808601290671
0.4521167103356847	0.6250698337542600	0.5417924808279024

0.3642668218621026	0.3227289033061045	0.5382289783652853
0.6603878398222784	0.5287909152982279	0.5374424622903534

*COCCO

C15Cu3N8O2

1.00000000000000		
8.8479003899999995	0.0000000000000000	0.0000000000000000
-4.4239502000000002	7.6625065100000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.5596008300000008
C	N	O
15	8	2
		Cu
		3

Direct

0.7111617462403637	0.2285383153540888	0.4881338883757707
0.7767504875813832	0.9838453471576127	0.4860102494060599
0.0219623346177516	0.2940771853506399	0.4856506726499843
0.2972056488064208	0.7833396249238267	0.4823369441291950
0.2221044325694044	0.0147494595998646	0.4819878164186944
0.9902524030643183	0.7088498788963448	0.4831765218191204
0.5262575950350820	0.0988585625456821	0.4860460768224368
0.9069665122680703	0.9280373085164090	0.4848866864929705
0.0776704736985336	0.4797080519441632	0.4849933325014972
0.4793530166868625	0.9189159432996445	0.4838579752804581
0.0867885024102494	0.0616858960826754	0.4829524234893185
0.9440492579734195	0.5266815730695047	0.4853390223624857
0.5675153200057231	0.5872398382559164	0.6166404495690962
0.6677161675277565	0.6813117017289327	0.6682580567490362
0.3842214695772185	0.4522577802230396	0.6162251163758216
0.7701995354396484	0.4018246158625535	0.4912023060871999
0.6040940392067887	0.8694620093874098	0.4873663339085620
0.1363053453226576	0.2358920785420325	0.4857166144664661
0.2501476923623369	0.6121904771551721	0.4866757472178455
0.3930445699887821	0.1383349528391490	0.4880392412187222
0.8666204130816902	0.7560002307664876	0.4873431898798520
0.8366912770285058	0.1689476949847143	0.4854828621054013
0.1697473294613632	0.8353269254081980	0.4786597825024020
0.7661228191178663	0.7619108314032074	0.7120214215277890
0.2638487083504578	0.4071987735590602	0.6570022189696080
0.4638581337809675	0.6363718340152994	0.5331691083356416
0.3700898078606796	0.3257208588829710	0.5328021718678957
0.6779652809357132	0.5346182202453941	0.5393989094706600

*CHCOCO

C15Cu3H1N8O2

1.00000000000000

8.8479003899999995	0.0000000000000000	0.0000000000000000
-4.4239502000000002	7.6625065100000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.5596008300000008

H	C	N	O	Cu
1	15	8	2	3

Direct

0.7135149709578874	0.7565626582997665	0.6296941006326254
0.7047964753979958	0.2246424793218525	0.4928685561764398
0.7692766508133324	0.9790391377688146	0.4902966422892219
0.0152128103723529	0.2897060745266358	0.4910891017420381
0.2900089729022778	0.7787370887203166	0.4874156120504421
0.2158274082386261	0.0108827276432182	0.4879644933958232
0.9833061092597501	0.7041326942555859	0.4883357202864820
0.5189399968423105	0.0945846477023943	0.4911344215165012
0.8997794651337466	0.9232693014666933	0.4897651344402427
0.0702586685722774	0.4750186373155762	0.4905312964575065
0.4731714097252817	0.9148635004440046	0.4883440986110587
0.0796916841334895	0.0572960706755825	0.4886525329862347
0.9372847762151219	0.5222189509949108	0.4903267122403436
0.4825065474794998	0.5283201597457322	0.6665978758051065
0.5998944065125061	0.6323898887909811	0.6134104948937148
0.3099171230239199	0.3984729945794071	0.6285431702861158
0.7627819150198086	0.3973694109349171	0.4957885656357136
0.5968779047179247	0.8652913703911410	0.4907428483376783
0.1286933629718129	0.2308021669363923	0.4914212264579508
0.2431958335069017	0.6082001122876636	0.4925142293647717
0.3867222726430484	0.1346279304348257	0.4935944104161447
0.8601094336128325	0.7512480608230234	0.4920242660744374
0.8294034064583865	0.1648207717311913	0.4902012419790832
0.1636126942016752	0.8313477628803499	0.4840780023823635
0.4891296966680842	0.5423676450786056	0.7289468419484514
0.1598961594333449	0.3296690309210362	0.6458935644714928
0.4492954122021763	0.6286959411156655	0.5407484427905924
0.3636117209045944	0.3234741029960043	0.5409990888097689
0.6649387920790336	0.5293053312177154	0.5411218375216693

*CHCOHCO

C15Cu3H2N8O2

1.0000000000000000

8.8479003899999995	0.0000000000000000	0.0000000000000000
-4.4239502000000002	7.6625065100000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.5596008300000008

H	C	N	O	Cu
2	15	8	2	3

Direct

0.7133681259800001	0.7618139773727484	0.6348165431861995
0.3304741553195621	0.5062370475731156	0.7379379981218798
0.7053182410678204	0.2216366688392909	0.4928103583403202
0.7703516916890657	0.9767095257896370	0.4886068424978747
0.0162689017990711	0.2867344440982167	0.4892220114411107
0.2915028717295350	0.7755795838529256	0.4868667349454217
0.2171932069570071	0.0081233875989253	0.4862563249214892
0.9839349497713257	0.7020277772676852	0.4861997792489569
0.5201541398283300	0.0912027936880358	0.4909547081529259
0.9019182276476998	0.9213215388510335	0.4868770224429549
0.0713470092393846	0.4728231855223279	0.4891861370632694
0.4740059669191392	0.9114763890571043	0.4880692617460602
0.0813255421745333	0.0553777806933913	0.4862338884467182
0.9377213861422692	0.5194447123239395	0.4894264531494583
0.4676233829645416	0.5429860133461304	0.6600343072176700
0.6082044139100662	0.6345293702579389	0.6169337148299610
0.3169634745255165	0.3814769399694222	0.6326797107780884
0.7635444903348654	0.3946994273930596	0.4961527991982186
0.5985009189809152	0.8617955415800522	0.4900874915135760
0.1310394180209367	0.2297179330342749	0.4889465014092553
0.2442853869334067	0.6045654750574155	0.4915507592595926
0.3873433222818517	0.1312348440903637	0.4936051268723688
0.8606372704490776	0.7491078608258180	0.4881996962620574
0.8303976882938942	0.1617927978469541	0.4891431783385567
0.1643317039856955	0.8282830275638531	0.4827259268223787
0.4499899379335435	0.5930348895349750	0.7233876766758954
0.1775088161642311	0.3094032638876138	0.6646932713832876
0.4544478213596216	0.6238091219810707	0.5396178205804865
0.3572195268479940	0.3092149213264371	0.5454171871952944
0.6678954607490918	0.5245790397762449	0.5448598479586595

*CHCOHCHO

C15Cu3H3N8O2

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239502000000002 7.6625065100000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

H	C	N	O	Cu
3	15	8	2	3

Direct

0.6998566764820390	0.7413903739852232	0.6275565952204358
0.3751339699640509	0.5371137576078064	0.7532206987584514
0.2830713055039168	0.2952260835153602	0.6129176363798980

0.7006512993784578	0.2226952907672708	0.4881259657690047
0.7664672009863656	0.9778290158231272	0.4882619812990080
0.0102530525098286	0.2883237908286750	0.4853804786816222
0.2871149242563617	0.7773988715491571	0.4855497048899206
0.2128410541892397	0.0099098696298760	0.4814352733007772
0.9796170632203129	0.7043839291116949	0.4857444536365609
0.5160954961429038	0.0925850202884691	0.4847685514842953
0.8974614796006304	0.9234753718239995	0.4867379501931984
0.0663702640976344	0.4747841927394839	0.4870960777914184
0.4697697053453940	0.9123957414534031	0.4864004918131527
0.0772197843272079	0.0568357805252447	0.4826869509499020
0.9327081661100015	0.5209547672935531	0.4873090479461151
0.4637775900953789	0.5410307311187001	0.6660905724344180
0.5853203333922083	0.6145324046728834	0.6143689319939614
0.3018994677486484	0.3706561709606186	0.6607329341178410
0.7589838903518236	0.3960316307872373	0.4922643940970725
0.5941430530741465	0.8639400914174471	0.4911972650855217
0.1246674159294521	0.2309658608348756	0.4827886600639197
0.2392351511553819	0.6060815546614765	0.4904593968922183
0.3842633999366562	0.1324209528692042	0.4820434837201588
0.8572564384119340	0.7513422728686044	0.4889271107743094
0.8263523597376932	0.1639613935791139	0.4858633236754655
0.1598483494214672	0.8294548720606993	0.4817443258430298
0.4816619124757990	0.6190125758403048	0.7273611719848150
0.1959259349130247	0.3168110773613820	0.7083498973283816
0.4471955451130516	0.6234579843161920	0.5383704833849756
0.3790838406444713	0.3497486463917936	0.4941588195421758
0.6568934254845123	0.5154642533171365	0.5427718809479744

*CHCCHO

C15Cu3H2N8O1

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239502000000002 7.6625065100000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

H C N O Cu

2 15 8 1 3

Direct

0.6252069483063705	0.7003873435387946	0.6550275776543962
0.5372720293376981	0.3894282981935301	0.7251134322647658
0.6902025571750016	0.2280738301248759	0.4894223780042012
0.7547102783940326	0.9820911746426746	0.4894006604129359
0.0004988240604655	0.2931204428454938	0.4908429415448583
0.2758300011910039	0.7824418632040333	0.4857953821768605

0.2015256471022567	0.0141323123708268	0.4852377395328314
0.9695701742264691	0.7072700624974209	0.4856459695517755
0.5042097687003985	0.0977517883926195	0.4878654596967972
0.8849127481055805	0.9265875823602678	0.4880625864445804
0.0560221078850465	0.4782651452615840	0.4892717385918861
0.4582558222711418	0.9181068409049108	0.4871884778474144
0.0653779904692426	0.0601238537799931	0.4872142562270539
0.9230996932130209	0.5254435688644650	0.4873367770029911
0.4944579381778993	0.4259154315846724	0.6183345467146629
0.5477215766707701	0.6005640347838492	0.6164723829349279
0.5132420924045940	0.3239961200818113	0.6739367819557325
0.7486367913801022	0.4008459601406520	0.4915117025234035
0.5823077271172072	0.8680137471200712	0.4907000701425515
0.1144646655309174	0.2338382546436593	0.4932374143411501
0.2287706411077960	0.6117092164556164	0.4918980527994934
0.3723510043106387	0.1384198979434658	0.4890402077083154
0.8453665256874699	0.7541079114262288	0.4902408249597460
0.8152657299063367	0.1681260774966333	0.4884946780835089
0.1490550340472939	0.8347449491262722	0.4816956901252195
0.4999917841613774	0.1794916005545424	0.6687838341456956
0.4339679566534700	0.6331516768108729	0.5397779062378936
0.3416662112498837	0.3252979287796698	0.5401750841816023
0.6587306211565408	0.5417369960705030	0.5384784761927621

*CH₂CCHO

C15Cu3H3N8O1

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239502000000002 7.6625065100000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

H C N O Cu

3 15 8 1 3

Direct

0.6615204041580878	0.6539768759258859	0.6855710179956112
0.5815573753409080	0.3769993101726842	0.7158985131582193
0.5371673060954965	0.7045757302691146	0.6226201909122805
0.6800386755301212	0.2237545446438029	0.4932503172368578
0.7473051338446991	0.9798933412528670	0.4893851686829981
0.9911841864983845	0.2894268820936973	0.4911814940634894
0.2668939797917503	0.7771128362836546	0.4854902745438401
0.1946353202062764	0.0105702894221784	0.4893181134162802
0.9604089827175646	0.7034798199153344	0.4897754516282087
0.4952017894737767	0.0925509686278123	0.4910694755792730
0.8782055891814745	0.9241687847919132	0.4907678478655814

0.0455599875421826	0.4738444522033301	0.4882103059894025
0.4490977216325759	0.9126026066905036	0.4870939083099093
0.0577786842199215	0.0577148643885542	0.4901802201423649
0.9120717077256801	0.5208016561712607	0.4910804757046603
0.4845230672275285	0.4353259422478392	0.6220867698649680
0.5717899747513562	0.6100321205780286	0.6417197758372885
0.5185481893828090	0.3174694024653607	0.6655166594216102
0.7388536450553987	0.3966726276082385	0.4974470940626513
0.5755937133206801	0.8645698715355195	0.4870760922676418
0.1065762389784213	0.2311465333026159	0.4943145841851722
0.2174709966574358	0.6053874399713933	0.4851728785113589
0.3635437805733819	0.1331596347569048	0.4925621757125012
0.8371393652722348	0.7517186223299169	0.4945059474429944
0.8063893580769027	0.1637848943866149	0.4898834850574061
0.1397496514837055	0.8305298925259749	0.4858935684229630
0.4802315904393282	0.1667869416700434	0.6522575300543284
0.4404189833257987	0.6067888745481121	0.4917254330629433
0.3268004648693603	0.3306839187440555	0.5467024853734236
0.6502482866267800	0.5469576804767958	0.5455076554938232

*CH₂CHCHO

C15Cu3H4N8O1

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239502000000002 7.6625065100000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

H C N O Cu

4 15 8 1 3

Direct

0.5570142779487819	0.7329921273652960	0.6160494241960628
0.3429269453633177	0.3292746413884032	0.7480141716533221
0.7430681937339696	0.7198273531970638	0.6257035151325087
0.5940404650577128	0.6079845903162090	0.7332234074799341
0.7124191066444685	0.2292201246536382	0.4929198115052360
0.7775069079679102	0.9840652293525942	0.4876899707531361
0.0234238301482035	0.2940988709960716	0.4915461832508824
0.2992807633795166	0.7831510996831799	0.4870714930827288
0.2258737866185375	0.0167695285008608	0.4877506556240078
0.9913384527088476	0.7102047237407562	0.4866777295149461
0.5275019636539454	0.0985560435824689	0.4912549231252541
0.9099739061529099	0.9295393330918192	0.4867468427079058
0.0783870415819287	0.4807551779593406	0.4906957093800847
0.4816622538141641	0.9187327778121868	0.4873627226508075
0.0890588500753602	0.0638072999346396	0.4880652802399378

0.9448031076432404	0.5266554360168620	0.4903199525137096
0.5291263420280944	0.5373090700454350	0.6865055344014843
0.5995655927080183	0.6320958366778783	0.6210504305575242
0.3860204148378327	0.3741883140363851	0.6952057207819053
0.7710214939294958	0.4022398614303405	0.4966625746969617
0.6065881801690898	0.8695115266486693	0.4876253790316650
0.1381725281628482	0.2374689649542775	0.4931965395466455
0.2510773197968315	0.6117429629806023	0.4921129796973072
0.3951405402262333	0.1391332576739493	0.4943374883215721
0.8684535120203331	0.7569716566573489	0.4879585941952033
0.8382567314204885	0.1697681373966995	0.4893158224566284
0.1718765788711123	0.8361400048811765	0.4835751124441776
0.2927285372894768	0.2633394690991177	0.6474572372570800
0.4557577169888288	0.6154731681806702	0.5333136816787774
0.3596439729528811	0.3105510879951095	0.5533456140212643
0.6652664561056223	0.5263247437509510	0.5421289181013300

*CH₂CHCHOH

C15Cu3H5N8O1

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239502000000002 7.6625065100000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

H C N O Cu

5 15 8 1 3

Direct

0.5874405218129873	0.7529169746487895	0.6228964112371128
0.3454781821148999	0.3256245756570546	0.7518064902273985
0.7389953835034864	0.6874891564519712	0.6257078623075319
0.5693420939351695	0.6137381372259622	0.7344806595203468
0.2026876403841169	0.1478805381514791	0.6676215506320694
0.7110178857173183	0.2286309243142526	0.4922957825240853
0.7765074171482268	0.9837003227376302	0.4884808418678266
0.0214573078639020	0.2939487419697701	0.4911906852077660
0.2975022225626858	0.7824769269234625	0.4870126442483228
0.2234589708879617	0.0148540163871890	0.4870637676084001
0.9898244773912087	0.7086846392600414	0.4867841385939718
0.5262364550824923	0.0978131704797675	0.4903001788769975
0.9075616835576927	0.9283477897138785	0.4874884753459266
0.0767062520969075	0.4794411279983513	0.4905171498603850
0.4802181793971044	0.9177677328662155	0.4874226232721407
0.0874642414768368	0.0623598455845981	0.4877380612595711
0.9431167919025520	0.5262633697254492	0.4899173599656651
0.5159379509234856	0.5361715874286594	0.6878151671142535

0.5942020603056192	0.6297632834167390	0.6220034385507983
0.3885068669968553	0.3727740677682068	0.6998663955699425
0.7692574925387198	0.4016296590784658	0.4959377916742026
0.6049321254686514	0.8689958783165386	0.4889717226871022
0.1354779047238412	0.2355555586424332	0.4924464765692420
0.2495690119964459	0.6115336101116744	0.4925971811708758
0.3936563958422847	0.1370646869046779	0.4925884554081038
0.8670347824872499	0.7563518992752611	0.4892629206326040
0.8365607298473762	0.1692167620946069	0.4890915126659039
0.1703019123761048	0.8349837517960664	0.4830191760259913
0.3041206651298210	0.2500949739929025	0.6488873948655894
0.4551925658971645	0.6237368096617570	0.5374053939841956
0.3716652915808984	0.3296545080550077	0.5346190662022151
0.6685156070499544	0.5345541733611379	0.5396530743234652

*CH₂CHCH

C15Cu3H4N8

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239502000000002 7.6625065100000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

H C N Cu

4 15 8 3

Direct

0.6215529638770388	0.7814102135897795	0.6303852437615527
0.3005195353318720	0.2642669791578435	0.6939880476936259
0.7606501235309414	0.6976307963896833	0.6302440937343785
0.5307071031390572	0.5582769411959789	0.7302691736365305
0.7125833650715141	0.2331313615765456	0.4960075683610498
0.7773308212228089	0.9881141912431559	0.4906291675341501
0.0236583436129926	0.2981935528712537	0.4960075636167088
0.2988425819415344	0.7866638612894569	0.4919636841592612
0.2252979924288261	0.0201021620329725	0.4907518757416556
0.9913040879114347	0.7136084267835086	0.4891439426712973
0.5269422058136648	0.1018645259193381	0.4944380707861394
0.9096875742926188	0.9335306796742520	0.4890265552278784
0.0781037985412492	0.4841997160628891	0.4956688867988977
0.4816533836476586	0.9223159921645107	0.4915315698332435
0.0891025059662624	0.0675481274931093	0.4917101915540347
0.9445090676685005	0.5306681347764519	0.4934468602156675
0.5071397160360479	0.5213063820448489	0.6758716235425488
0.6197705530977465	0.6556417687306451	0.6239254777405951
0.3829754601179750	0.3618719735516321	0.6556584284484981
0.7700763997407908	0.4058836630376875	0.4988139386776388

0.6062893138838855	0.8729339260811817	0.4909724006183547
0.1384019785524627	0.2412118616279423	0.4982122175766416
0.2508432447766383	0.6157672505239900	0.4982826498780059
0.3950373776983806	0.1428150163669968	0.4973979158630159
0.8680930984459623	0.7609717725834795	0.4889713455388180
0.8378425364105782	0.1737681051719886	0.4931433821273666
0.1717823267625532	0.8397928576535919	0.4870605045120530
0.4549428151519624	0.6230148591094398	0.5428512856160401
0.3612406028671007	0.3109260773626273	0.5599773295484932
0.6661696424599389	0.5377651039332314	0.5400748249858419

*CH₃CHCHOH

C15Cu3H6N8O1

1.0000000000000000

8.8479003899999995	0.0000000000000000	0.0000000000000000
-4.4239502000000002	7.6625065100000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.5596008300000008

H	C	N	O	Cu
6	15	8	1	3

Direct

0.7378988634408254	0.8410883951480478	0.6446090173084308
0.6031863218501651	0.3693364787522083	0.6591361353769786
0.8006463758167388	0.6933707040764967	0.6782852113255170
0.6582179812948549	0.7424775464321729	0.7250438613582932
0.3290202306421199	0.1742366974611763	0.6063471982518299
0.4199959711142063	0.5841950628834587	0.6323373751637533
0.6656809947790863	0.2038371782215439	0.5054715846513890
0.7331436761966694	0.9619514735046226	0.5008857228411455
0.9761767749004097	0.2702649102574924	0.4979927874517846
0.2505800883915691	0.7574688732523547	0.4987275840767993
0.1756212047846915	0.9886328422794392	0.5024439583402718
0.9429076292468790	0.6832161413935562	0.5031492229995574
0.4811335947750578	0.0727158767117183	0.5039354336361785
0.8613155804013943	0.9045712132217684	0.5033392856707427
0.0304435294078543	0.4549785792857636	0.4975763139445340
0.4337790540258104	0.8933700227733810	0.5005391583184087
0.0416954364264117	0.0378244921484303	0.5007414411184655
0.8962706832578811	0.5015337861829646	0.5029801351424666
0.5339778413702951	0.5688144265873568	0.6405828046963324
0.6917433548822450	0.7190947066433718	0.6732697876199558
0.5025034615095980	0.3986861631562105	0.6413454484017568
0.7229525490758086	0.3768232217636889	0.5096335226078408
0.5607868123948905	0.8480859734524312	0.4985761797718100
0.0897457741706682	0.2108922379333458	0.4960750188387582

0.2026995039557730	0.5863453964327731	0.4955898369979566
0.3485233705499271	0.1116910771111945	0.5043675452405477
0.8195817782188850	0.7317705549786581	0.5078006988561697
0.7917693184701209	0.1459172779322960	0.5009212625856263
0.1228414712046770	0.8098287125817407	0.5000469021279978
0.3342269033514185	0.2597721538062180	0.6396557787255045
0.4366878371972152	0.6047477705598009	0.4741032790710217
0.3461320428462137	0.3190315576189828	0.4733870548260369
0.6082805300496344	0.5120761754553443	0.5464097926561226

*CH₂CHCH₂

C15Cu3H5N8

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239502000000002 7.6625065100000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

H C N Cu

5 15 8 3

Direct

0.5902998040075161	0.7452143564676593	0.6363963632745844
0.2825012611371684	0.2812329768230070	0.7313255647233211
0.7370234881023673	0.6736383795030066	0.6336807695002943
0.5736669676374987	0.5318499305036889	0.7336149123535514
0.2604607122453193	0.3184536641898175	0.6385370745653535
0.7158219247635026	0.2388410469728905	0.4936803270622026
0.7810579396854447	0.9933011986829970	0.4921678186282697
0.0255715521829878	0.3038932211621028	0.4924664691017256
0.3021373350030737	0.7924641249405076	0.4907717528344365
0.2274942192928288	0.0247355920476990	0.4880635247606347
0.9948324016153767	0.7189801847932071	0.4899312238675199
0.5309233398279680	0.1080912365058236	0.4912536621641463
0.9117727312940180	0.9383234207639466	0.4907841768364400
0.0817945002119561	0.4898906335508262	0.4932085919086019
0.4848676099011783	0.9279489830079566	0.4911020880535669
0.0916106548156967	0.0716295802810681	0.4891284569403113
0.9481402766378563	0.5362801968005851	0.4922394872650058
0.5000012451688137	0.4983147645207972	0.6854118303214584
0.5933425318381894	0.6215942394136496	0.6275464395000100
0.3395455398354662	0.3588257359973544	0.6852119109271870
0.7742206383074083	0.4119190330106239	0.4971926219274792
0.6090677884692673	0.8791450410266349	0.4942061975555178
0.1391489879028332	0.2453302278068500	0.4921439888078502
0.2548249231844404	0.6217695400036156	0.4965822697696417
0.3985607697119691	0.1473191343220769	0.4910623864306981

0.8720312218331048	0.7662679981116716	0.4927845667981853
0.8411221535872495	0.1795253129020204	0.4911553958300455
0.1749468922985740	0.8445691875615338	0.4862088123556749
0.4631988278548245	0.6377447449738501	0.5441459117464199
0.3871956157958452	0.3555135595690591	0.5153967037260144
0.6753813758502545	0.5456205237834663	0.5430729004638460

*CH₃CH₂CHOH

C₁₅Cu₃H₇N₈O₁

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239502000000002 7.6625065100000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

H C N O Cu

7 15 8 1 3

Direct

0.5898214648678551	0.7779840653892959	0.6936764833939982
0.3361790796962855	0.5503037372150824	0.6324229259981218
0.7269597541291629	0.7470295553663110	0.6353843146079887
0.4597466307296721	0.4688350507325708	0.7335942703510110
0.1367488593047988	0.2660326424179964	0.6231381808241591
0.7541429094142702	0.7368344773855122	0.7250569633533307
0.5960423703422316	0.4342837053233292	0.6771508330263434
0.7040039737231574	0.2051692104638854	0.4906204975793181
0.7684167166482014	0.9597012636566724	0.4918310914538206
0.0141738386870255	0.2711947235508211	0.4918203033124169
0.2880425311384612	0.7598424308510809	0.4900965784285118
0.2151103311070633	-0.0061760988435947	0.4914571838350352
0.9829218808472772	0.6864129967296186	0.4856697033270475
0.5179390457031409	0.0754111252084339	0.4931152574823940
0.8995714896923841	0.9064703120846030	0.4888530210699958
0.0686386764337389	0.4567817201130153	0.4901373263475916
0.4714824193162903	0.8953959227707198	0.4918642392862742
0.0802038699987310	0.0414212254707375	0.4909372731905839
0.9359214714100215	0.5035063223305549	0.4868711903274845
0.5267289399152224	0.5076302488294350	0.6836488383906761
0.6569465309615017	0.7035092226057162	0.6843636971459079
0.3862433431589011	0.4565954208736643	0.6290225157649258
0.7622491204575775	0.3771247185831366	0.4882691208965220
0.5951860215022606	0.8452842520710442	0.4953641323318002
0.1285428017239959	0.2139315829097811	0.4945376332053754
0.2405732429304761	0.5894716511155520	0.4924000963063728
0.3864518896522537	0.1164985728351901	0.4978968854558996
0.8601575184686585	0.7348297621777272	0.4860538420205981

0.8276644896642346	0.1448619777184829	0.4901753140771475
0.1630737755183946	0.8143343585716422	0.4867185617544348
0.2405474341214622	0.2832618580000483	0.6475649270244764
0.4547356940324465	0.6019334954465957	0.5363815191260931
0.3843804087498958	0.3091112307096237	0.5475882036039462
0.6450935159529400	0.5130411893357082	0.5000643657003532

CH₃CHCH₂

C15Cu3H6N8

1.0000000000000000		
8.8479003899999995	0.0000000000000000	0.0000000000000000
-4.4239502000000002	7.6625065100000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.5596008300000008

H	C	N	Cu
6	15	8	3

Direct

0.5859651864824039	0.6971199312203387	0.6526873852373661
0.2805156794184891	0.2713660049853580	0.7370765075781474
0.7686581657452053	0.6843772320010539	0.6833935045759461
0.5755892056985031	0.4728914212469393	0.7770924111021550
0.3081755631500729	0.4227202093996800	0.6655300887855291
0.6814982161545621	0.7873436906914565	0.7341331395892946
0.7101940136656654	0.2328901284302403	0.4776141318697832
0.7746293040816231	0.9875578779168582	0.4773221021062318
0.0201086385466721	0.2973845015498338	0.4777232464082651
0.2954231029693503	0.7883415030622022	0.4748604467899248
0.2194118731909461	0.0174921411531515	0.4748835033748401
0.9901754759860086	0.7121738467829321	0.4748132752851386
0.5241170106027913	0.1041183215476696	0.4767825065543065
0.9035342833243375	0.9302814932499112	0.4767094238965517
0.0773258757790188	0.4834725135484903	0.4768188425625095
0.4775445445871155	0.9247525446010834	0.4756202408827116
0.0829466281618548	0.0632267243272575	0.4759546810986037
0.9444498061107773	0.5299975846563053	0.4757635254737189
0.5244356887593135	0.5064145528184064	0.7320843142165526
0.6453500871414944	0.6774282032605643	0.6987522840517554
0.3626594135001410	0.3944820462625934	0.7106843579595691
0.7717296614828274	0.4058891056319021	0.4787987658863334
0.6016349087181774	0.8759655806348455	0.4785953703640762
0.1316265073625596	0.2359668654204347	0.4791637621493299
0.2487140334428393	0.6176829209632161	0.4778601986712465
0.3899931066202647	0.1413838840526204	0.4782878274718984
0.8662168591704430	0.7588479541844434	0.4777678613892247
0.8349966784885273	0.1725722038173262	0.4762944949563370

0.1683379701153824	0.8393961345346536	0.4727099860455730
0.4658009373184939	0.6290032510662289	0.5053182261066881
0.3778223879107993	0.3462524798619170	0.5073627588670726
0.6605545163133553	0.5411974471200833	0.5058757886933237

CH₃CH₂CH₂OH

C15Cu3H8N8O1

1.0000000000000000

8.8479003899999995	0.0000000000000000	0.0000000000000000
-4.4239502000000002	7.6625065100000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.5596008300000008

H	C	N	O	Cu
8	15	8	1	3

Direct

0.4772750001626219	0.6168541390844579	0.7395105185733298
0.2862409893266348	0.3256314955108567	0.6397038856397087
0.5803001221890044	0.5964530071299171	0.6647337284907855
0.4379357050373514	0.3206689930857272	0.7801015829035214
0.0757573356038488	0.0377991332508255	0.6804642103308198
0.6773774695590672	0.6165307836948656	0.7464372509552731
0.5255927633419876	0.3041591441394307	0.7009619888293589
0.1889081214226103	0.3163107441763488	0.7209924938998581
0.7126925595222441	0.2197365317447446	0.4869318037836809
0.7769415107375176	0.9744172071392180	0.4865155695205239
0.0226210658497765	0.2844250420229553	0.4870892406531191
0.2975739400831651	0.7752864203862101	0.4841000266089022
0.2216478394178958	0.0042903464968005	0.4848633868126873
0.9924094313556654	0.6989580386495449	0.4840231236440546
0.5261528846090040	0.0908906570795214	0.4864961289352870
0.9057628770116021	0.9170474436353161	0.4859021303390559
0.0797838625836750	0.4705297888092258	0.4860735603023364
0.4798877593286129	0.9116832331740052	0.4849808800808763
0.0853242160096024	0.0499892484993188	0.4856003064783372
0.9468336289274052	0.5169262667925145	0.4849821139247052
0.4526108670681371	0.3597197164992341	0.7259449648833557
0.5524809739862417	0.5586436491734620	0.7189267754374584
0.2729644725094007	0.2775027245532211	0.6931110731732679
0.7739688505555180	0.3925195566129732	0.4883046603624485
0.6039328334483082	0.8629292561647757	0.4877248935150784
0.1339220853763644	0.2227257697859386	0.4890296239313862
0.2512676375272271	0.6048088853835032	0.4872519004369210
0.3923291784263305	0.1283121829855392	0.4883810072852850
0.8682509781962112	0.7455105598584599	0.4869472872519909
0.8372731192701978	0.1595005279827551	0.4852556873663875

0.1706752398652557	0.8262548606102140	0.4819695373743125
0.1974488940408603	0.0907320421850936	0.6939927263462857
0.4683108852528473	0.6163991843947023	0.5156423948921377
0.3801416238324823	0.3331153258824250	0.5176421146021170
0.6632673685653387	0.5282400434258933	0.5158429324353129

C₁ path

*CHO+2*CO

C15Cu3H1N8O3

1.0000000000000000		
8.8479003899999995	0.0000000000000000	0.0000000000000000
-4.4239634600000004	7.6624988500000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.5596008300000008

H	C	N	O	Cu
1	15	8	3	3

Direct

0.2170809312635618	0.4947266570242103	0.6101785727272924
0.6985608778709052	0.2397687205578511	0.4914051405632617
0.7637409081866803	0.9941120269047026	0.4889046705592573
0.0092080234996881	0.3052203971999239	0.4895896226691355
0.2830315401126547	0.7934428295362062	0.4835073977243661
0.2111769541538902	0.0284572069804227	0.4884446528529328
0.9763312323162229	0.7201051907750925	0.4861559746090453
0.5123589932403148	0.1085687604189434	0.4908672374802490
0.8948126678779335	0.9405429813204957	0.4892805875097406
0.0628011858744468	0.4905452826492021	0.4863101884203382
0.4665329097349609	0.9285150744495650	0.4862303697293603
0.0758144374868582	0.0756120842707125	0.4894021876424747
0.9290657293400637	0.5369744645424146	0.4874254289335124
0.2885482332749825	0.1990840797027670	0.6411686912059952
0.7351256437614919	0.5609446416644217	0.6433167175958777
0.3617394181494048	0.5439041041974048	0.6117541318725260
0.7557119634577218	0.4118038986250079	0.4935282953581011
0.5905814521538199	0.8780779625212484	0.4882440192730280
0.1242718302341977	0.2489252739206070	0.4928820756043244
0.2354611056490710	0.6229037501730715	0.4844172888523127
0.3818685448513862	0.1505130187242651	0.4948184711265102
0.8538857611096807	0.7680146664278784	0.4915864036560537
0.8226278617558584	0.1791308019807645	0.4882988749693702
0.1572647312264331	0.8477188780069271	0.4825506409704913
0.2737732873304649	0.1427049021327325	0.6954128124583058
0.7608856901856530	0.5477566337149040	0.7002017624419198
0.4447278489940780	0.6292685342243427	0.6614943288204439
0.4554684466365276	0.6238356761454489	0.5182725443782024

0.3606355585954256	0.3339158899653422	0.5607996715995933
0.6787101016756200	0.5582201212431180	0.5529337483960095

*COH+2*CO

C15Cu3H1N8O3

1.0000000000000000		
8.8478999999999992	0.0000000000000000	0.0000000000000000
-4.4239633700000001	7.6624984500000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.559599999999997

H	C	N	O	Cu
1	15	8	3	3

Direct

0.8099178728028263	0.7568962747512696	0.7261564373399712
0.1919632648941395	0.7111926298482458	0.4871481258754823
0.2574086902534916	0.4658734726395007	0.4875592445280594
0.5032974188579040	0.7767664123953931	0.4863014176347286
0.7779090484073289	0.2636642158173959	0.4834735693768147
0.7043061764429912	0.4973660667827232	0.4818357966277002
0.4696956246974698	0.1904254710749544	0.4834958731183069
0.0070150197228127	0.5800614521542123	0.4853228740244859
0.3885036854100539	0.4106076687820928	0.4861852730737884
0.5574765112477483	0.9617528231090755	0.4859965647607815
0.9605538194280336	0.3995009743410569	0.4849727719277910
0.5685997777595100	0.5451149867489345	0.4833505464219727
0.4228372863232026	0.0081434914819547	0.4850904663876017
0.8232575511214453	0.7759503967895937	0.6301068611648066
0.2411994118112814	0.0571625594089842	0.6392021182125066
0.9371946926078680	0.1882178552908657	0.6391903367255650
0.2491447798319595	0.8833211204115747	0.4898593017854638
0.0854612221711694	0.3504827826415067	0.4899828399675503
0.6184370022378927	0.7189571128139735	0.4868415122153059
0.7300275553100870	0.0932812509247001	0.4888753334871277
0.8749000104176129	0.6211616775430339	0.4860850569661749
0.3468843778131873	0.2383806758261960	0.4889317398913173
0.3178271829154434	0.6507391938951286	0.4850424761859929
0.6507023915921404	0.3176627677598479	0.4788530999460039
0.8756254442623067	0.8430009172567642	0.6901580824952698
0.2516180903353274	0.0686843754402810	0.6982725493598753
0.9454585297257102	0.2029216634389676	0.6981979842907007
0.9389208544947442	0.1214439108003157	0.5501713996935359
0.8505750480663767	0.8087536135493785	0.5399902303055207
0.1656833490379726	0.0267115162821073	0.5498318362098020

*CHOH+2*CO

C15Cu3H2N8O3

1.0000000000000000

8.8479003899999995	0.0000000000000000	0.0000000000000000
-4.4239634600000004	7.6624988500000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.5596008300000008

H	C	N	O	Cu
2	15	8	3	3

Direct

0.2186740210462574	0.4743874284554536	0.6121792181947734
0.3576724026376241	0.5564685668084279	0.7066430637316812
0.6968355929280523	0.2406239721032580	0.4899346830099503
0.7627849754523073	0.9954678604641195	0.4882834479980356
0.0080697158446725	0.3061623176491394	0.4876456013889310
0.2822990046793002	0.7942875999079940	0.4817441035377011
0.2095526808514321	0.0284626464482148	0.4855789543349806
0.9754185576174766	0.7209113330099638	0.4852216921511475
0.5118201934333176	0.1096567019739985	0.4886427825557300
0.8934790287975093	0.9410710812289950	0.4882861062120355
0.0618698403066420	0.4913936248743576	0.4849900504116695
0.4647677271869701	0.9294053184967156	0.4846888577511562
0.0741124866793608	0.0760728625207383	0.4868393581878538
0.9280279476231841	0.5380828672791040	0.4862804045191143
0.2826051574027101	0.1812803865985834	0.6393646641449342
0.7410209067249185	0.5577709296601621	0.6434055423807137
0.3586142431697008	0.5144891690590163	0.6088180797209972
0.7543462570240541	0.4132223773057728	0.4924557542742202
0.5896161906375583	0.8788674356317032	0.4888052182013226
0.1232229537066266	0.2493199169236007	0.4898851707317363
0.2347880825460976	0.6237668859438660	0.4836846835126998
0.3802384734426759	0.1510861531928137	0.4919669548824308
0.8522386613897134	0.7685659593565271	0.4914805788423263
0.8216297815376992	0.1799675905619081	0.4869437155953832
0.1555555281379338	0.8485903784030833	0.4807010604849158
0.2873774748715233	0.1821849240460230	0.6987593331538118
0.7727062397918636	0.5431474178673033	0.6994408304626802
0.4427183086315802	0.5783843646588613	0.6707268643521075
0.4578824195315252	0.6383611868814645	0.5260438155318973
0.3613756627088448	0.3262363272952988	0.5562241772548973
0.6812640336608854	0.5608284153935567	0.5538535124881662

CH₂O+2*CO

C15Cu3H2N8O3

1.0000000000000000

8.8479003899999995	0.0000000000000000	0.0000000000000000
--------------------	--------------------	--------------------

-4.4239634600000004	7.6624988500000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.5596008300000008

H	C	N	O	Cu
2	15	8	3	3

Direct

0.2873024353374944	0.6065569566417729	0.6477863734432117
0.4967587915078799	0.6476555939472456	0.6895445551500372
0.6994098523382598	0.2080692505110728	0.4878841390472419
0.7637057908526651	0.9627612484291678	0.4842951082045918
0.0089954573662734	0.2725292859482247	0.4856649512119336
0.2833126010112307	0.7603151842428961	0.4815183392843526
0.2119200862021352	0.9953301341121372	0.4843739285117544
0.9763156339022598	0.6884434733481506	0.4827323637588663
0.5122550056980829	0.0753797320065882	0.4870963671608338
0.8960509829087827	0.9086129738963964	0.4841581244053645
0.0627694595773313	0.4587369198035198	0.4838544777290226
0.4676410999748604	0.8967313973005244	0.4828584560217871
0.0757472006774529	0.0432327413365114	0.4841886392566729
0.9289881621321563	0.5042065809155365	0.4845085867039360
0.3035494031727619	0.2475922856991702	0.6415729463202002
0.7425977636127709	0.5446145332262781	0.6399660057048219
0.4250813367353900	0.7022217754686627	0.6617664330093228
0.7555816444725836	0.3794962919378757	0.4893618555711273
0.5918351113503647	0.8470139263059336	0.4829462213318313
0.1241472415863988	0.2163203982949086	0.4867722633640966
0.2361103260277319	0.5901231638506025	0.4829214533912610
0.3819826865548644	0.1173261021344077	0.4897488956619100
0.8544099762861158	0.7364636987764516	0.4856909036363889
0.8230744038429629	0.1472158919852145	0.4857028800585106
0.1575720028235081	0.8148319162014042	0.4806742930227605
0.3070163728951962	0.2624852547028889	0.7006082606861606
0.7431003319896027	0.5453265176816747	0.6993129608457646
0.4902820259021216	0.8577779615021145	0.6492749861075038
0.4576416410662513	0.5866222405812090	0.5071776596335119
0.3564093269734700	0.3017812712689234	0.5509525393064133
0.6711098352211001	0.5254311479425493	0.5507846724588147

*CH₂OH+2*CO

C15Cu3H3N8O3

1.0000000000000000		
8.8479003899999995	0.0000000000000000	0.0000000000000000
-4.4239634600000004	7.6624988500000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.5596008300000008
H	C	N
	O	Cu

3 15 8 3 3

Direct

0.2087259675055732	0.4701335704318668	0.6207869741586182
0.3931903319815559	0.4829863716566598	0.7057307438214712
0.3584074329414462	0.6977300553361780	0.6084461165911924
0.6979440349322836	0.2402929595510571	0.4888595410230285
0.7638066344589486	0.9948222672752736	0.4868261801467866
0.0086188224540918	0.3055049117083851	0.4870146881292053
0.2833599696110934	0.7935061739768489	0.4808208655653191
0.2114601165460404	0.0292406218948748	0.4851109329381431
0.9765772200133858	0.7211936641872364	0.4842126141129829
0.5126205406737295	0.1092966106208278	0.4876467138780917
0.8951399097178204	0.9413373712945636	0.4871128779613698
0.0629467683924008	0.4917453362836842	0.4838833871853529
0.4662523067280204	0.9285222329159504	0.4836462192666775
0.0757176194221186	0.0759371854851233	0.4865317856886206
0.9286102347182141	0.5373380329120452	0.4853872051490994
0.2963977065223309	0.2031673362809687	0.6375213642131304
0.7337635237417702	0.5576154577007678	0.6424811623233314
0.3481104354575467	0.5703376152215635	0.6203011154589884
0.7554422576692635	0.4129564982217708	0.4915726863053023
0.5911437811273362	0.8787568063300280	0.4867870459957827
0.1240511869711859	0.2496002484245526	0.4903924893768410
0.2351297630356884	0.6225555570848349	0.4821050986881523
0.3819553181660939	0.1512594402842443	0.4907823484020644
0.8538982921762427	0.7685091247572668	0.4898848840985998
0.8231505501290759	0.1803827916893509	0.4857335046050306
0.1567415718231063	0.8478152222256889	0.4798218106018777
0.2993419832959064	0.1552898791944291	0.6923592485937675
0.7441869131385742	0.5392092182829401	0.7005230560208061
0.4283672218011567	0.5953236444789446	0.6843824903112782
0.4573126156441487	0.6316026416711896	0.5255743335729868
0.3531425867228824	0.3332109530542122	0.5570092778575483
0.6790683724809971	0.5581219895666619	0.5525524079585648

*CH+2*CO

C15Cu3H1N8O2

1.0000000000000000		
8.8479003899999995	0.0000000000000000	0.0000000000000000
-4.4239634600000004	7.6624988500000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.5596008300000008

H C N O Cu
1 15 8 2 3

Direct

0.4604128880771430	0.5548135399081202	0.6571106503741733
0.6821345758945027	0.2349955396895989	0.4885222761999894
0.7473268717939544	0.9897395101257415	0.4845085431005849
0.9936800773334651	0.3001882976004729	0.4856515118137957
0.2679164301252520	0.7894971367608926	0.4801825522770723
0.1941271921910571	0.0218413648479264	0.4840251632060534
0.9596006961406092	0.7154224711579763	0.4824623681232576
0.4974132470865092	0.1046929907394142	0.4868352488266453
0.8788835530381321	0.9347827471695082	0.4843370661115696
0.0482646450319122	0.4862535155216771	0.4834872436107145
0.4500832947042869	0.9247453686829232	0.4821401187799668
0.0584467483364170	0.0701375331838494	0.4846373623498955
0.9142354670265908	0.5325810871157999	0.4849439514936865
0.2426181607207438	0.1870113932089844	0.6399648795992258
0.7917116514861882	0.5889202247123090	0.6407694745346916
0.4676281481860841	0.5338461304054777	0.6023012110888055
0.7412238451329338	0.4078938652371491	0.4924046908567090
0.5744921635478107	0.8741513823896709	0.4848585014875809
0.1086353104524842	0.2438284315599570	0.4877042810841096
0.2213579888258768	0.6186393071361223	0.4833153811292211
0.3642854426501531	0.1442474005039522	0.4909316995102583
0.8362801415261317	0.7622048208094447	0.4861238533765298
0.8075731328530504	0.1744957843185411	0.4848148699066346
0.1398559376808202	0.8423288626014028	0.4786317059573031
0.2392075433680242	0.1564674653758754	0.6976795255835166
0.8116498773444890	0.5905534083404859	0.6993159686056789
0.4344671829181019	0.6347293085958781	0.5267440008367347
0.3479070309547265	0.3116340553426925	0.5586475435899692
0.6607745955725794	0.5330281469580728	0.5590966865855964

*CH₂+2*CO

C15Cu3H2N8O2

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239634600000004 7.6624988500000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

H C N O Cu

2 15 8 2 3

Direct

0.2345519319973730	0.4865231092502821	0.6127504081694969
0.4423306390735364	0.5680830198714886	0.6551081488014262
0.6902158401274363	0.2444340673926758	0.4872911968962422
0.7557026038829195	-0.0006056574513444	0.4844465349006853
0.0010553100153220	0.3092992669349195	0.4841300199851286

0.2748778312138386	0.7975252588586826	0.4784344964769505
0.2024678689159975	0.0319196602711771	0.4827994720509526
0.9683018593502036	0.7248161582273803	0.4827422249138227
0.5045060355982716	0.1127942217769136	0.4857441421051831
0.8868187631728421	0.9449079319326859	0.4850469249291735
0.0549950107383919	0.4955409058218271	0.4819552562111692
0.4577780033593017	0.9331724197075333	0.4808888048444601
0.0669621809377707	0.0798242691230834	0.4836885355613378
0.9206658275724440	0.5411693485378724	0.4839367820133043
0.2870237724673675	0.1842498305155753	0.6395296551398076
0.7301876222157384	0.5635351665611787	0.6429118556680047
0.3729596308039699	0.5230795067787277	0.6064818227590474
0.7472937474178016	0.4168349460090220	0.4902405462257500
0.5828084232104983	0.8825796115850835	0.4845658567206146
0.1158333433032806	0.2529280852587313	0.4858432819908403
0.2278565303290228	0.6273907491644617	0.4803321117316443
0.3731643667027859	0.1542991357690199	0.4895717747515868
0.8450857323358417	0.7722530477112202	0.4886808076227306
0.8147142709957478	0.1839718652932832	0.4838395574783056
0.1479386946032883	0.8518140689713330	0.4781769400985810
0.3082933038688378	0.1765842880464116	0.6976521444760537
0.7367956896060649	0.5499491670393799	0.7014135691559998
0.4548588924877768	0.6455376011796428	0.5234658726335960
0.3587013522538931	0.3266222696337474	0.5565970743783204
0.6724808614424453	0.5666026202280319	0.5528595113097887

*CH₃OH+2*CO

C₁₅Cu₃H₄N₈O₃

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239634600000004 7.6624988500000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

H C N O Cu

4 15 8 3 3

Direct

0.2109302851112811	0.5473369739635668	0.6564697246042666
0.4055026827667570	0.5528390475119561	0.7409656870266671
0.2672256592739558	0.7586057802584492	0.6885049027303154
0.4275881552209895	0.7272625875965129	0.6448763222355307
0.7083770019626542	0.2169982110031789	0.4791187162796662
0.7733371533464675	0.9716527980596740	0.4754095410442060
0.0182718724403187	0.2812990051057115	0.4765782388177660
0.2932148700375609	0.7693412822947300	0.4729989347045486
0.2212270586080378	0.0039783281501138	0.4754277272428805

0.9862382122573298	0.6973171549566815	0.4742942915621069
0.5220099687115572	0.0848451989970402	0.4783526415675185
0.9052867568115471	0.9171265072045069	0.4753544568693655
0.0726518920789723	0.4676122791421368	0.4750258568521280
0.4766634969911918	0.9055494004071070	0.4743722281769368
0.0848350377927415	0.0515688778310889	0.4751166243087955
0.9387943755787244	0.5131475211103850	0.4760089022834949
0.3171096173118885	0.2570932215547502	0.6306243493201746
0.7269333890558082	0.5607544291765364	0.6319273492957114
0.3156679695283231	0.6672406655817988	0.6806102952702449
0.7654456463639336	0.3888853039200106	0.4813791310101665
0.6014102264425729	0.8561134661214002	0.4746887625324359
0.1333083884090533	0.2247814724968506	0.4777368001391319
0.2455376455576927	0.5986002354487039	0.4742848930493496
0.3911198731021091	0.1262445926757846	0.4807272746746905
0.8638914338157766	0.7449936685003604	0.4773163896919184
0.8328744059485703	0.1563059235331201	0.4763330310179441
0.1667942491852526	0.8234718182397537	0.4719448504503247
0.3245797383022884	0.2658933857735549	0.6899160618173228
0.7105913783156514	0.5675134563864956	0.6905843286834090
0.3630526747683050	0.6346004486796792	0.7462173022334633
0.4673136809687023	0.5959949460254098	0.4957309432199127
0.3638116625391257	0.3111184036639821	0.5399824958762582
0.6802310213948842	0.5339615586289941	0.5401162654113244

*CH₃+2*CO

C15Cu3H3N8O2

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239634600000004 7.6624988500000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

H	C	N	O	Cu
3	15	8	2	3

Direct

0.2285816295747922	0.4896057654391391	0.6222393273048917
0.4247589839373965	0.6952921585380060	0.6184041779340552
0.4255973161106147	0.5250242996288338	0.6627209147589734
0.6960746333046143	0.2462743440654012	0.4870175421576581
0.7619209513324933	0.0009273944468132	0.4844737112719045
0.0067623236847925	0.3114392106323727	0.4850715478483837
0.2815323896461378	0.7997582958972980	0.4794847483402297
0.2094474387365001	0.0354029603930273	0.4831462194767168
0.9747608886108918	0.7273555950364607	0.4819986206425343
0.5109602666938984	0.1155629145794267	0.4860454416108709

0.8930813761884409	0.9474487073653262	0.4846371911496629
0.0613126805822827	0.4978837097255628	0.4822967203043164
0.4643830880001827	0.9346691282808035	0.4818673428709887
0.0738757553014028	0.0821603631074544	0.4841402800803729
0.9269372608087146	0.5436066589956556	0.4833160788827639
0.2909629629636339	0.1883584385127041	0.6340924678314875
0.7374386861974516	0.5677646806715699	0.6406008315897977
0.3711023849479955	0.5515998720741307	0.6171256753617436
0.7536034448190558	0.4190399566654447	0.4894684921649196
0.5892064213868553	0.8848305450541308	0.4843395287720391
0.1220502063472729	0.2555451995380469	0.4878476092793381
0.2332735152168025	0.6289111469059466	0.4812193581726428
0.3800686127571680	0.1576034943995435	0.4894102778936357
0.8519680943787420	0.7746197579882288	0.4873874715091556
0.8211776230891434	0.1864841750014269	0.4839162348842105
0.1549439784410794	0.8540616785404972	0.4780140665773072
0.3004533903791952	0.1347010402304573	0.6867351036361682
0.7444624683169921	0.5550637955048537	0.6992803245516911
0.4559541322174896	0.6364639536587664	0.5205527987528279
0.3547210573247722	0.3382971144885872	0.5558234908362324
0.6793702487031822	0.5650731546340931	0.5506370235524686

*CH₄+2*CO

C15Cu3H4N8O2

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239634600000004 7.6624988500000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

H C N O Cu

4 15 8 2 3

Direct

0.1870482253881275	0.5104095267227188	0.7020201326532028
0.3264479286085452	0.6628595590245646	0.7651378665071962
0.4102469442534992	0.5645669800083830	0.7078419097518208
0.3578167799394584	0.7224783699230329	0.6766016069171804
0.6972066791945121	0.2231120149301133	0.4827850828685940
0.7620940701805956	0.9777750995129697	0.4798503821551866
0.0070511401353103	0.2874677912414178	0.4809916356724590
0.2819129048463513	0.7752480351158570	0.4772907884644256
0.2103872807068086	0.0104598178461226	0.4786567099020335
0.9748107251926219	0.7035316894063587	0.4785304230805986
0.5107467484968617	0.0905951026547017	0.4816898855386237
0.8945309277923541	0.9236310051750533	0.4796082095509455
0.0612567279004511	0.4738530173987592	0.4794444171725769

0.4655156150888697	0.9113124367822263	0.4786513923762518
0.0739759910578641	0.0581551621927647	0.4789698886183062
0.9271455210052643	0.5191401756074979	0.4800581771614849
0.3085271685051074	0.2305703946124352	0.6339323979208971
0.7330966603916187	0.5605851902351520	0.6360842653920740
0.3203653636545970	0.6151388584983307	0.7129376173893788
0.7538386771901010	0.3948904141356188	0.4846119672170028
0.5902679843854205	0.8617610798136331	0.4792656645751606
0.1224215725171292	0.2313621571211169	0.4819584195071392
0.2342817726050133	0.6045857449875262	0.4787932975584379
0.3803717736951286	0.1325973572598784	0.4829047398405797
0.8526812788762893	0.7513769236231856	0.4815565062001806
0.8216750925121205	0.1623720583335609	0.4808574036327218
0.1555204853836726	0.8294901138723225	0.4761693665832885
0.3219939718294137	0.2103253138585378	0.6917156938510260
0.7294231840920680	0.5627771992226640	0.6953869249345400
0.4558873543870611	0.6007082464297224	0.5014905044212469
0.3525796723748298	0.3162179325016533	0.5462855405914292
0.6688940878129320	0.5399428419521457	0.5459603319939942

C₂ path

*COCHO+*CO

C15Cu3H1N8O3

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239634600000004 7.6624988500000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

H C N O Cu

1 15 8 3 3

Direct

0.2763933076759690	0.5392235245310445	0.6484145064107446
0.6952428323529330	0.2291244699370783	0.4928696073880088
0.7603841894358365	0.9848019541634536	0.4901431717383448
0.0064696659842379	0.2953901363369089	0.4932060173233269
0.2810440474834324	0.7849907964934586	0.4873357575647255
0.2083288495145577	0.0178928941491775	0.4900884647473044
0.9743926646516429	0.7106726146887946	0.4876514192457281
0.5099202360651196	0.0995419125817876	0.4921613683642140
0.8919476203580420	0.9299929329420935	0.4896350597941833
0.0604402063626272	0.4804884044760503	0.4907881671558700
0.4633681113756535	0.9197137249440500	0.4883995113289760
0.0721210060927402	0.0651116729167855	0.4913462875121740
0.9275480948659537	0.5275029767287415	0.4899304634089228
0.2794507665293983	0.2065941503487836	0.6455580371303682

0.5414007631206659	0.5892243649626158	0.6135477178894670
0.4154238773416265	0.6462541118724837	0.6431258072494269
0.7544552384567722	0.4022759052827422	0.4946025247594702
0.5880593810257745	0.8703283122504735	0.4895075334685856
0.1210997254604492	0.2380441837593156	0.4967018938910247
0.2327000634398700	0.6134555980441823	0.4906939742269494
0.3781503007680578	0.1400004855569296	0.4957698311787667
0.8514711207068103	0.7580634348112026	0.4899415707974963
0.8204668227133427	0.1693567205195509	0.4905858720184551
0.1543563446067762	0.8379294374797147	0.4852318606846713
0.2534228507738001	0.1470561702292433	0.6996084109484526
0.6724899261796928	0.6170575889758960	0.6465339794429605
0.4634745289738493	0.7974922413234554	0.6591190516801133
0.4423000837115597	0.6149980227604598	0.5211284730866420
0.3507771827558365	0.3174377358901143	0.5620236377139005
0.6428524112169581	0.5287992810434248	0.5283793418507093

*COHCHO+*CO

C15Cu3H2N8O3

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239634600000004 7.6624988500000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

H	C	N	O	Cu
2	15	8	3	3

Direct

0.2606837659121575	0.5481874742710812	0.6405716568248827
0.6577635773752188	0.6807703233202396	0.6850326509389092
0.7017294201706525	0.2382274986223788	0.4903250663298512
0.7665717238913247	0.9939426669699882	0.4873346482454270
0.0125717169250253	0.3039691541396032	0.4918010544370439
0.2867745939368606	0.7942431937312817	0.4851577533198860
0.2140307629647297	0.0272270470133694	0.4889280487151788
0.9803702939596528	0.7199137541465986	0.4847955508772653
0.5161904135131180	0.1087341332390558	0.4902338392225081
0.8978530014248116	0.9391963520506724	0.4869100123890443
0.0669184639869929	0.4900872485056015	0.4889927082060826
0.4693703765882510	0.9290936686554341	0.4856755955113337
0.0780763494517070	0.0741404704693445	0.4902633456391323
0.9336673897574174	0.5362877152098919	0.4871344263683480
0.2674461621452622	0.1948851620709054	0.6460289703374518
0.5114136679383774	0.5642161265157236	0.6106122893822326
0.3991781100684719	0.6002826659296714	0.6547695207431845
0.7607590112776097	0.4113562550918974	0.4911331537147467

0.5941160901430649	0.8792730428689521	0.4864483708012508
0.1271368748231809	0.2473775306550488	0.4957894064277031
0.2389199245633347	0.6227096404580502	0.4894059977756223
0.3846484455490907	0.1496143459370450	0.4952927473780254
0.8563454644113361	0.7663870052333542	0.4857757901436864
0.8269111628748286	0.1789338301582548	0.4887396209438870
0.1598065897552009	0.8470297118282999	0.4835771381871193
0.2384748068777329	0.1506235640438885	0.7022912217850192
0.6726267771479245	0.6278032298275216	0.6416675264318586
0.4618865536333632	0.6872534864559628	0.7084536943535431
0.4497737426992049	0.6339142567685793	0.5250404266530336
0.3691058302867428	0.3229660230274701	0.5660479939935046
0.6443887959473508	0.5374836727848372	0.5193472639232369

*CCHO+*CO

C15Cu3H1N8O2

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239634600000004 7.6624988500000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

H C N O Cu

1 15 8 2 3

Direct

0.4525796777026130	0.5697923752943105	0.7049864483425737
0.6777357258991706	0.2298847517814291	0.4882119047805545
0.7416971177918336	0.9837739780248289	0.4870030146157192
0.9879211322282833	0.2945601966434688	0.4874857909103965
0.2630696490132658	0.7855959445203040	0.4821113201101007
0.1897235123382026	0.0187763429792928	0.4886028508130556
0.9579032923388600	0.7111877021610645	0.4830301055785556
0.4922192989173229	0.1001642458782955	0.4893284013138482
0.8734033318743049	0.9302339610832934	0.4875211844017787
0.0430619917628300	0.4810730467092451	0.4839406466096009
0.4453375233529861	0.9199246006585011	0.4844667467026629
0.0535961976273109	0.0657059438459841	0.4889915576271037
0.9110764845990054	0.5283842747255824	0.4833027199748670
0.2480787316424788	0.2004652350546901	0.6468359319586120
0.5049548220691470	0.5545622902230800	0.5978652697896708
0.5418954740190443	0.6438315423289556	0.6615566054685020
0.7371870890270616	0.4032280455633035	0.4882493212168763
0.5689501825983729	0.8691792141739265	0.4863037018343822
0.1026179983676914	0.2388435778500881	0.4908330983820482
0.2146486835351308	0.6138652765034766	0.4842644032613563
0.3605944953135647	0.1407896587198670	0.4959225197794710

0.8335224795903168	0.7571209026046396	0.4877628218092511
0.8020931900425904	0.1697616242314829	0.4865726783348459
0.1366227843580537	0.8392364389667973	0.4811031450561611
0.1975320851102861	0.1444181144506833	0.7003855526188649
0.6642286322397865	0.7966722416008785	0.6696618940803301
0.4162548340211592	0.6196642574794253	0.5252192094342281
0.3597661992769747	0.3147247799462760	0.5672837377398846
0.6391896833423842	0.5363375959968314	0.5286927474547369

*CHCHO+*CO

C15Cu3H2N8O2

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239634600000004 7.6624988500000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

H	C	N	O	Cu
2	15	8	2	3

Direct

0.6047031605238488	0.6380983474747074	0.7136100884566999
0.3278669557245719	0.5214641864399140	0.6547906590944135
0.6853824223095248	0.2265011534759340	0.4883598738509925
0.7496177801775893	0.9809150438307878	0.4864764577537251
0.9957880414538479	0.2914453417928768	0.4886329621594671
0.2699336113676754	0.7803861314072233	0.4844491468484031
0.1989009635750384	0.0159355290340266	0.4862807314392169
0.9637902677922208	0.7083423279843879	0.4816156880140351
0.4991287529726706	0.0952793010579118	0.4889534594152516
0.8828616912802834	0.9279233648847094	0.4846958906007069
0.0498414155247299	0.4781939283502332	0.4862979637082890
0.4534346966341108	0.9158660192924877	0.4859289242637123
0.0623640110810854	0.0632426174302625	0.4869655090859616
0.9165495471637659	0.5240359812477244	0.4837146669427778
0.2373766229992279	0.1546952036555292	0.6415312301249796
0.4374926418086575	0.5337247153821977	0.6237757773105351
0.5965487830817154	0.5985694951633361	0.6592279645338488
0.7428350937178221	0.3988941449258644	0.4884515554605846
0.5774988952888802	0.8649121344383789	0.4880804003334159
0.1109766401005067	0.2362720963233024	0.4915298075795193
0.2225773321369063	0.6100722089255776	0.4882848837824058
0.3688055661469948	0.1379190312776647	0.4931972448580245
0.8408366314107846	0.7553988981271279	0.4832654940649088
0.8097917178190305	0.1662287039853304	0.4866109809700955
0.1442562639801886	0.8354347577504340	0.4813645600771161
0.2060814011096453	0.1073562511974814	0.6974591711857421

0.7363423362244043	0.6154433548398096	0.6324086328577504
0.4336605570302631	0.6192173045777972	0.5328747183813327
0.3511478359411186	0.3113483124203303	0.5680952462295988
0.6495994836228658	0.5343559933066481	0.5338211706164951

*CH₂CHO+*CO

C15Cu3H3N8O2

1.0000000000000000

8.8479003899999995	0.0000000000000000	0.0000000000000000
-4.4239634600000004	7.6624988500000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.5596008300000008

H	C	N	O	Cu
3	15	8	2	3

Direct

0.8048006098161132	0.8281217421086682	0.6204587979614105
0.4941787579831767	0.6958636188781721	0.6293258633315562
0.4710220397083152	0.4968992153064024	0.6636269049974785
0.6551289850735270	0.2030120902926236	0.4944249179086000
0.7208708795129847	0.9579612925818114	0.4905705417159256
0.9656711332236253	0.2683892958486624	0.4949048550289186
0.2417776621457552	0.7573224422440261	0.4904063968615352
0.1684619638336121	0.9912282180212993	0.4896054221560797
0.9345400522631164	0.6844368832555979	0.4879031947425920
0.4703475232745569	0.0728582830612366	0.4932297138789173
0.8523833528998340	0.9041575896609354	0.4885193072240012
0.0204389355012460	0.4544688561873599	0.4938814079605075
0.4244008259159290	0.8922169321700045	0.4906398974749746
0.0327770410477851	0.0381129727706697	0.4904322615602381
0.8869681098622695	0.5007723210222839	0.4916932618764604
0.2455014514584623	0.1909789688579033	0.6486489632065394
0.5388947851379507	0.5985453770711207	0.6252599677187823
0.7304815362009153	0.6902321322072368	0.6388569934483427
0.7131707307028826	0.3764234147302922	0.4971775061750241
0.5489911262332678	0.8434429283660330	0.4919628505574112
0.0808193917330816	0.2116189924701705	0.4974800237646886
0.1930736744226760	0.5856224998150981	0.4961677031330357
0.3388021062361740	0.1135512628954115	0.4959169219001896
0.8117637420160826	0.7314231917886926	0.4890724886658068
0.7811906128229036	0.1444684666556157	0.4913086620142325
0.1149238363206086	0.8100558648991588	0.4855235978346878
0.2308086295443335	0.1471564938536234	0.7050043885379673
0.8065858955487886	0.6264954427720411	0.6699767464989488
0.3975260687256930	0.5897350477572626	0.5371442732891177
0.2977755195185241	0.2788666949685179	0.5614010904896688

0.6082547713157892 0.5046078474820287 0.5399387480863428

*CH₂CHOH+*CO

C15Cu3H4N8O2

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239634600000004 7.6624988500000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

H	C	N	O	Cu
4	15	8	2	3

Direct

0.8947076695402258 0.6847807906734570 0.6338291523807817

0.6787015084568215 0.7838594475224143 0.6191441570058380

0.5197715351218241 0.6005463067421808 0.6731557014644940

0.8279355644996467 0.4566216611290891 0.6982810457432957

0.6361993978270342 0.2017512578697443 0.4956237041529822

0.7018924420412955 0.9571212073123541 0.4865292810170083

0.9465627529545156 0.2672533707519383 0.4906235460252017

0.2214210011377148 0.7546845375371362 0.4855059144656649

0.1484109872470224 0.9886948905546706 0.4885472810498592

0.9132394379182505 0.6819588037196954 0.4855466949568780

0.4499733417197267 0.0700853170625715 0.4938363545752277

0.8332018044988330 0.9026508254420219 0.4854417736350248

0.0005899119913212 0.4527062199286211 0.4886902340041216

0.4049335987843310 0.8907015345988035 0.4872162763954182

0.0136788524974240 0.0368967327028116 0.4874885373481249

0.8671047327526717 0.4993307224811778 0.4905638790084487

0.2577213939501617 0.2740899650577971 0.6436857613944307

0.6359348365142751 0.6554495705561613 0.6411413174533824

0.7610112318816504 0.6078594847027881 0.6528547628349959

0.6939253430986917 0.3743225577475521 0.5004621263275895

0.5295551106835197 0.8415532386765366 0.4857849773025810

0.0613828893413971 0.2099500876061617 0.4922645493956166

0.1739439782249257 0.5837054428799034 0.4868801164167859

0.3188267025067097 0.1107568330057846 0.4966926740112965

0.7917109641456008 0.7307465489641318 0.4864523499577577

0.7606582020100781 0.1422072039675965 0.4894460887574226

0.0954146801410273 0.8084949631876265 0.4837010442970633

0.2632302253451695 0.3010832866211645 0.7021990864347284

0.7304559685101885 0.4783021494912602 0.6987500354421889

0.3976747367931287 0.5809384345935764 0.5048092644621985

0.2882290846174692 0.2938336723049308 0.5518289160090503

0.6046151632473669 0.5108760746083786 0.5544704062745415

*CH₂CH₂OH+*CO

C15Cu3H5N8O2

1.0000000000000000

8.8479003899999995 0.0000000000000000 0.0000000000000000

-4.4239634600000004 7.6624988500000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.5596008300000008

H C N O Cu

5 15 8 2 3

Direct

0.8179950523515800 0.8075065997987170 0.6261238314149047

0.5064658601957239 0.7148017344033512 0.6197540708735558

0.4479087438742828 0.5163069345213745 0.6606349903656584

0.8798345940508739 0.6121904234563319 0.6888708400608936

0.7145715728964576 0.7435591156030978 0.7076402166946971

0.6534289231027877 0.2014940794260342 0.4934792332225459

0.7195462690415847 0.9567318952799857 0.4887247327037400

0.9642289386463361 0.2670075655298542 0.4934295633250018

0.2402843644376918 0.7554964242354152 0.4884307241138405

0.1666942928015838 0.9892444935772039 0.4883460143030274

0.9321327495183698 0.6824715322061338 0.4877666808036126

0.4687024534833757 0.0712922372159919 0.4917010677270496

0.8508130173051268 0.9022778131161150 0.4878020983611548

0.0189417311640338 0.4528355889756906 0.4924544858869319

0.4227620886030470 0.8907586642807434 0.4883178814817298

0.0311554871392690 0.0363464430185293 0.4892128051874570

0.8848650540365072 0.4990235340135011 0.4913551386076811

0.2492916002346879 0.1945752203758083 0.6464330869334580

0.5397986295129023 0.6093708767436611 0.6234541414088296

0.7209864552881425 0.6951102769816208 0.6561823457008421

0.7112276956311395 0.3747347317119205 0.4972319694910817

0.5476846979879354 0.8423534023489671 0.4888541078607423

0.0793350891998632 0.2099508032283507 0.4957721555255291

0.1919731130391453 0.5838577611579389 0.4937001935123410

0.3370510070483689 0.1117648464185381 0.4944121536822934

0.8096712411062276 0.7297717979548878 0.4893187800545648

0.7796866024645875 0.1429258038803535 0.4899628704323697

0.1128859509561039 0.8080646596099255 0.4845047336270671

0.2412620817759896 0.1534926809439692 0.7031575925987487

0.7721663618456797 0.5638849700385127 0.6624895405778293

0.4024058347281956 0.5872005435868393 0.5291184279149724

0.2966815593399441 0.2792149633194937 0.5593400493383789

0.6057033471924640 0.4979660830411418 0.5445143262074704

*CH₃CH₂OH+*CO

C15Cu3H6N8O2

1.0000000000000000

8.8479003899999995	0.0000000000000000	0.0000000000000000
-4.4239634600000004	7.6624988500000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.5596008300000008

H	C	N	O	Cu
6	15	8	2	3

Direct

0.8615918544686255	0.8528118858523016	0.6490665129555722
0.5316355188915893	0.7036236241009092	0.6359426497269887
0.5088069610768620	0.6297793079366304	0.7220466528717373
0.8471237877354240	0.5717567413195591	0.6572287717024451
0.8297707544641719	0.7562559422207745	0.7318268113977501
0.6132909606436481	0.8582734677329149	0.7044115661400547
0.6379923243985814	0.1759821975312890	0.4863385715204349
0.7032431256754317	0.9315962800289455	0.4805235960341230
0.9481302039235733	0.2413142288597963	0.4835457090772001
0.2233962508074921	0.7300341170618622	0.4786359917205985
0.1508079562552598	0.9639081918116523	0.4827738988894590
0.9161565029458439	0.6571349210252605	0.4809384367130877
0.4520050394134235	0.0452292190023438	0.4851984710680716
0.8349085115384450	0.8772805545816391	0.4813395127894380
0.0027017950598652	0.4273120800729040	0.4814131545905806
0.4060675053233365	0.8655567859305641	0.47975309255585435
0.0146488408014181	0.0113797247372757	0.4822679721873043
0.8688571897635921	0.4730873008438254	0.4828622224073353
0.2708616362869739	0.2430475014082152	0.6384033463307321
0.5954218230609891	0.7326879266126861	0.6863656346781376
0.7701725727613741	0.7410642698843896	0.6809053168749659
0.6962198327431840	0.3486067794744475	0.4887394120162352
0.5312951457020867	0.8165369853727353	0.4787173154932960
0.0632348922514225	0.1845294112995472	0.4853017172103254
0.1752010148161847	0.5585482797677946	0.4792954107307317
0.3208260948688378	0.0862405064905341	0.4880356882893360
0.7934142191774050	0.7047959446418385	0.4832764763087196
0.7628983210768054	0.1162393862979807	0.4830972979017844
0.0963365869932187	0.7833630646521714	0.4791984810920746
0.2907159037332274	0.2657470999255565	0.6971947320279894
0.7423357621991972	0.5795252398552301	0.6501536430288453
0.3924991310000153	0.5547059726527986	0.4973626768613452
0.2933782050408321	0.2732776491265539	0.5465040587685343
0.5992673851016496	0.4884565518870594	0.5348889180362342

*CH₂CH₂+*CO

C15Cu3H4N8O1

1.0000000000000000

8.8479003899999995	0.0000000000000000	0.0000000000000000
-4.4239634600000004	7.6624988500000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.5596008300000008

H	C	N	O	Cu
4	15	8	1	3

Direct

0.8908350948523578	0.6953811194334070	0.6323141989370578
0.6559426247579543	0.7752601676085379	0.6327910611217369
0.5095269936260509	0.5713644112801919	0.6784993741456375
0.7426944422117239	0.4883026973668743	0.6769322135640751
0.6329981188131029	0.2072029810876822	0.4962502319203652
0.6983073679240018	0.9623977915500541	0.4882055096302828
0.9431250562277687	0.2723075631461012	0.4911029613451358
0.2178486918398047	0.7595047705539257	0.4864363883048027
0.1454689973178932	0.9938270166143230	0.4888789903368554
0.9095598994257212	0.6873076199671335	0.4869838364021878
0.4465030111997143	0.0748789519105739	0.4941571634401331
0.8302461122557516	0.9077530316150012	0.4870749400347261
0.9970851995930492	0.4581787229093842	0.4892941281973062
0.4015853010624395	0.8957986281979270	0.4884808634226626
0.0100851450520069	0.0422508525322213	0.4881101722956059
0.8634878502584020	0.5042988210559755	0.4915090911505424
0.2469200032450167	0.2545229102247586	0.6442083348952009
0.6273715317052957	0.6448595814704806	0.6481236247048895
0.7585413878960475	0.6018068818515612	0.6487841615313000
0.6903446271186332	0.3794238004643349	0.5011049115704341
0.5263876557256931	0.8464796242899764	0.4878524424740723
0.0580845782307918	0.2153075998706362	0.4921562237012905
0.1706966851544776	0.5890273019943378	0.4875541349595676
0.3155911955932730	0.1160038486677894	0.4959507580916647
0.7883086582487435	0.7360353088081394	0.4882725437074094
0.7574057734058282	0.1471421885649739	0.4906750674075889
0.0916656214051896	0.8136553004105559	0.4849217291598908
0.2578825594623093	0.2688254361264811	0.7034790767558432
0.3961704383964684	0.5865385193385337	0.5091146699620619
0.2847197514646706	0.2991396428429190	0.5531039128141625
0.6007511165298238	0.5127259882452103	0.5588077540155075

CH₂CH₂+*CO

C15Cu3H4N8O1

1.0000000000000000

8.8479003899999995	0.0000000000000000	0.0000000000000000
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-4.4239634600000004	7.6624988500000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.5596008300000008

H	C	N	O	Cu
4	15	8	1	3

Direct

0.9306497932151919	0.7567010189983605	0.6889633943011787
0.6630385405056128	0.7788684974979478	0.6750071431953449
0.5322673265960794	0.5633073394573223	0.7168095970953207
0.7988545879711907	0.5402915617839718	0.7305312580576649
0.6327307077743147	0.2002358112744586	0.4940324695045907
0.6970877811160169	0.9555611393096396	0.4904451399702444
0.9423784103566802	0.2658055131971610	0.4927548941958825
0.2170389620584610	0.7551112727959846	0.4882805479798786
0.1458173697750228	0.9896453899313988	0.4911979780482544
0.9110401442901646	0.6823583816960023	0.4893227967434463
0.4461908294380311	0.0695916384256565	0.4933454339860681
0.8295011339605028	0.9018998269203961	0.4906360330312947
0.9965390320956539	0.4521926471601798	0.4907614851532289
0.4005324621131816	0.8902857116398345	0.4893064329243335
0.0090912881458462	0.0367071105645610	0.4914251841686687
0.8636622379170377	0.4979059455026920	0.4907220576702053
0.2411501327966578	0.2347735563905995	0.6500043587458283
0.6594128974117492	0.6655134937170774	0.6988102339137927
0.8030206546490429	0.6535251551986454	0.7063217567623887
0.6909197920704934	0.3726549982008280	0.4949391887531686
0.5251054045701196	0.8405493742648167	0.4892340354057554
0.0576612675292615	0.2097492611299240	0.4944287791190446
0.1683946317813002	0.5841009010984344	0.4902060024346573
0.3156651907419004	0.1113746075284013	0.4958278732259409
0.7882132145153877	0.7294440705766150	0.4916538515605414
0.7570732262966245	0.1404675343457028	0.4922922650988265
0.0908350113985094	0.8088162017099868	0.4877799641795817
0.2487205898750640	0.2404363792829540	0.7093790964582192
0.3793706183038399	0.5799321199036954	0.5144189027121341
0.2873079493622239	0.2967047217734777	0.5603723346172318
0.5826480713688452	0.5029979087232993	0.5322166709872942