Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

C_2 product formation in the CO_2 electroreduction on boron-doped graphene anchored copper clusters

Supporting Information

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1. Basis set selection

We investigated the effect of the basis size using the CAM-B3LYP functional. We tested the segmentation of the basis sets (DZ, TZ, QZ), and the effect of polarization and diffuse functions. We used the Karlsruhe basis sets (def2-SVP, def2-SVPD, def2-TZVP, def2-TZVPPD, def2-QZVPP, def2-QZVPPD). The computed interaction energies in kJ/mol alongside with the pictures of most stable structures for each basis set are shown in Figure S1.

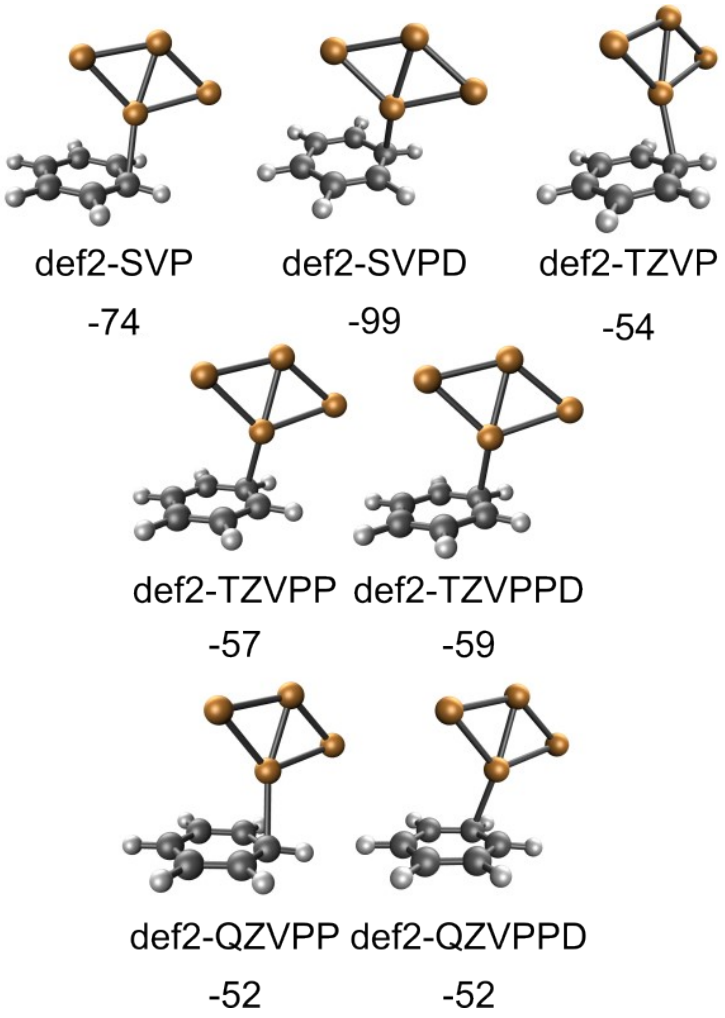


Figure S1. Geometries and interaction energies of Cu_4-benzene adducts with different basis sets. The interaction energies are shown in kJ/mol

It is visible that the interaction energy saturates at around -50 kJ/mol using a triple zeta basis set and further increase of the basis set size does not improve the results. A counterpoise correction was also performed to check the BSSE (Basis Set Superposition Error). The counterpoise-corrected interaction energies are shown in Table S1 Compared to the values in Figure S1, it is visible that starting from def2-TZVP, BSSE is around only a few kJ/mol. These indicate that the def2-TZVP basis set is sufficiently accurate.

Table S1. Counterpoise corrected interaction energies with different basis sets

	$E_{interaction}$ (kJ/mol)
def2-SVP	-37
def2-SVPD	-42
def2-TZVP	-50
def2-TZVPP	-51
def2-TZVPPD	-51
def2-QZVPP	-51
def2-QZVPPD	-

2. Selection of the DFT functional

We also investigated the effect of range-separated functionals, and additional empirical dispersion correction. All functionals were tested against benchmark computations with both CCSD(T) and MP2-based wavefunction methods with def2-TZVPPD (and for MP2 based methods also def2-QZVPPD) basis sets, on both CAM-B3LYP/def2-TZVP and RI-MP2/def2-TZVPPD geometries. The results are available in Table S2 and Figure S2.

Table S2. The results of method testing. Our final choice is shown with green background

		$E_{interaction}$ (kJ/mol)
CAM-B3LYP		-54
ωB97X-D		-76
M11-L		-59
PBE - D2		-98
PBE - D3		-96
BLYP - D3		-82
RI-MP2 (TZ)		-122
MP2 (sp) TZ	On an RI-MP2 TZ geometry	-121
RI-MP2 (sp) QZ		-115
SOS-MP2 (sp) QZ		-64
MOS-MP2 (sp) QZ		-84
SCS-MP2 (sp) QZ		-81
SCS-MI-MP2 (sp) QZ		-81
CCSD(T) (sp) TZ		-118
CCSD(T) (sp) TZ 2	On a CAM-B3LYP geometry	-124
RI-MP2 (sp) TZ 2		-108
CAM-B3LYP-D3 (sp)		-75

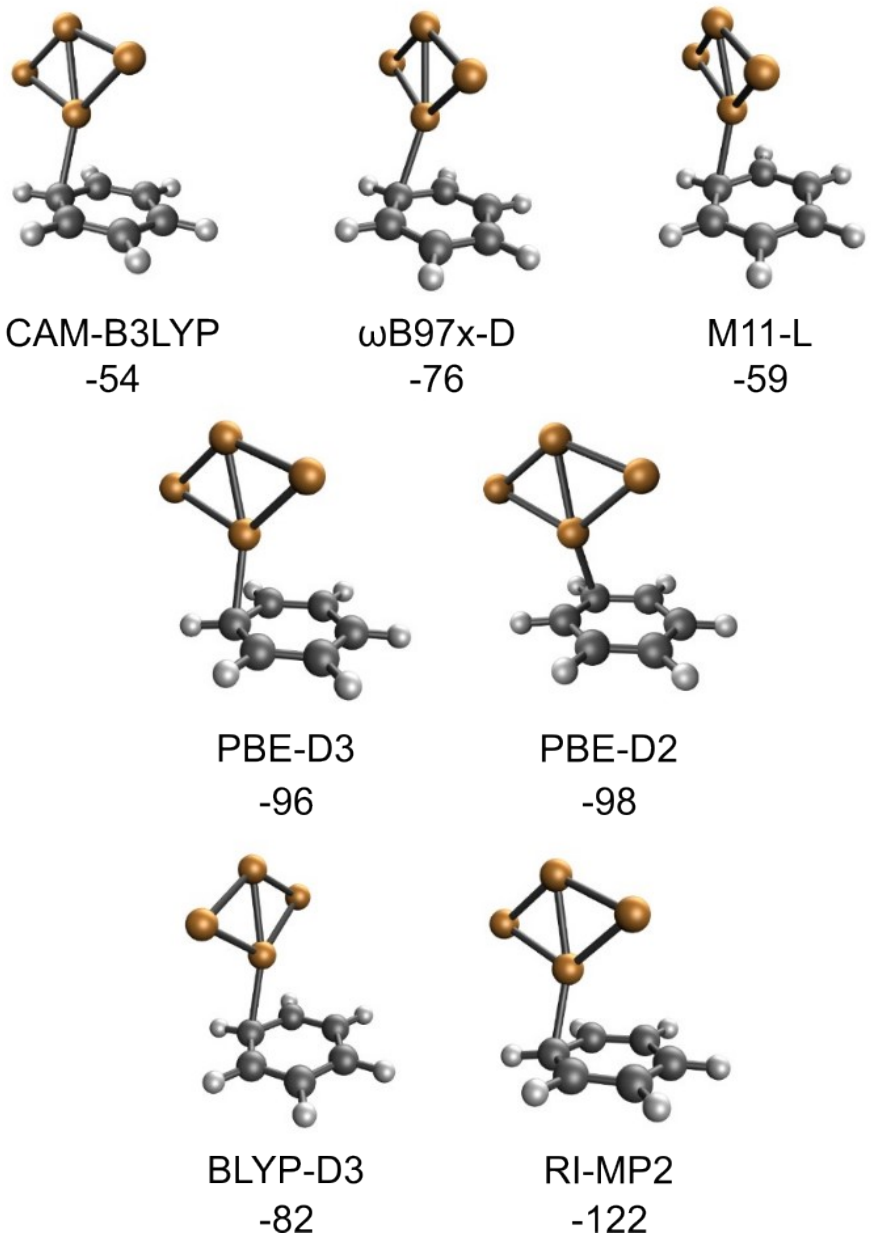


Figure S2. Geometries and interaction energies of Cu_4-benzene adducts with different methods. The interaction energies are shown in kJ/mol

It is visible, that the interaction energies using PBE with additional dispersion correction are closest to those of the CCSD(T) benchmark computations. The effect of the doping was investigated using pyridine (Figure S3). The reference is a CCSD(T) single-point energy on CAM-B3LYP geometry, that is -108 kJ/mol.

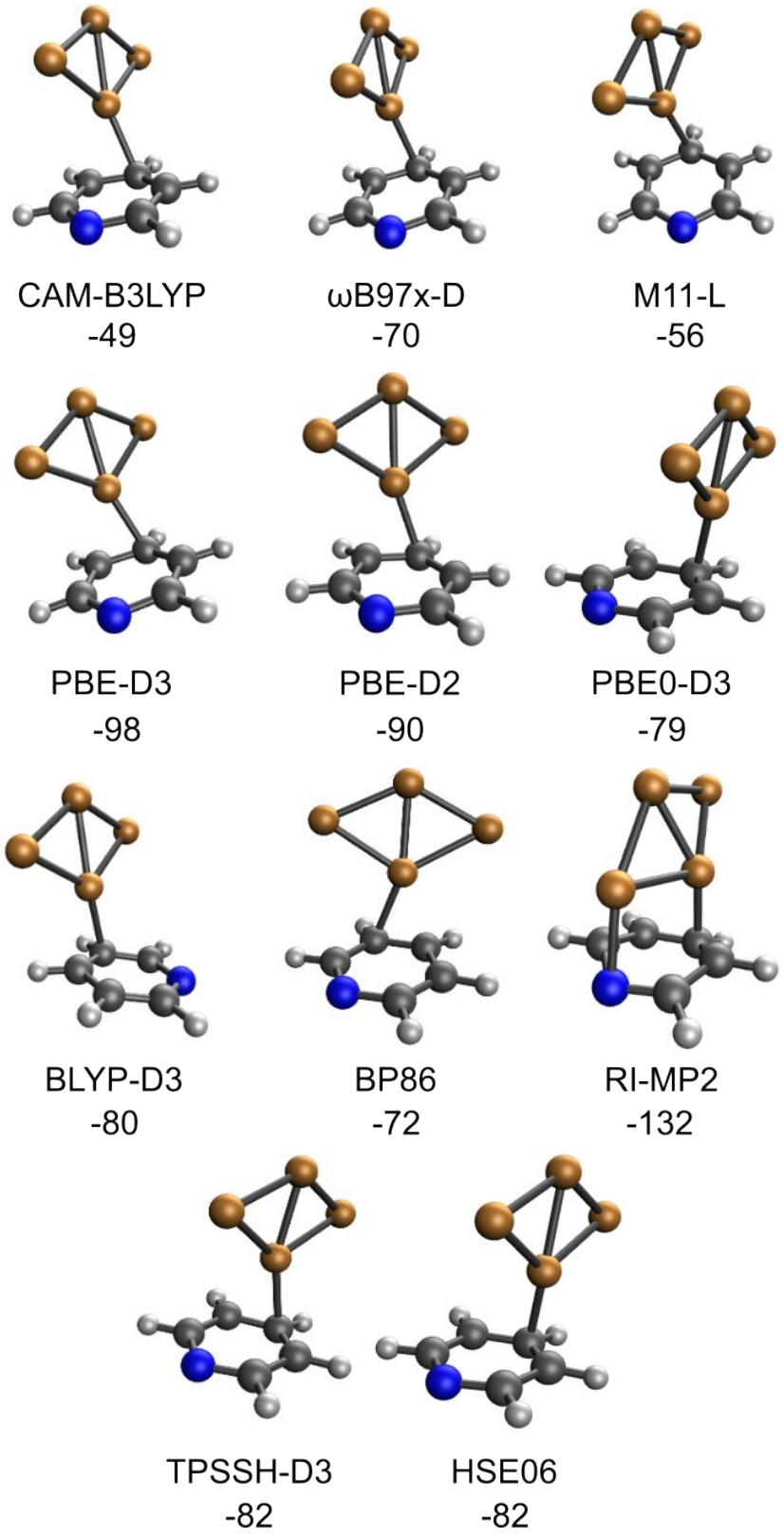


Figure S3. Geometries and interaction energies of Cu_4-pyridine adducts with different methods. The interaction energies are shown in kJ/mol

It is well visible that again, PBE with empirical dispersion correction resulted the closest interaction energy to CCSD(T). We performed single point computations for borabenzene on

a CAM-B3LYP geometry to see if there is any difference but again, PBE with dispersion correction was found to be an appropriate choice. We can clearly see that for all 3 adducts of Cu_4, that D2 and D3 have almost the same results. We finally selected **PBE-D2/def2-TZVP** level of theory for the computations.

Table S3. The results of method testing for the borabenzene adduct of Cu_4

	$E_{interaction}$ (kJ/mol)
CAM-B3LYP	-246
CAM-B3LYP-D3 (sp)	-285
PBE -D2 (sp) (TZVP)	-302
PBE -D3 (sp) (TZVP)	-304
PBE -D3 (sp) (TZVPPD)	-310
RI-MP2 (sp)	-383
CCSD(T) (sp)	-355

We also tested different methods for the CO and CH_3OH adducts of Cu_4, investigating all the different sites of both planar (neutral) and tetrahedral (dicationic) clusters. The results are shown in Figure S4, Figure S5 and Figure S6. It is well visible, that PBE-D2/def2-TZVP is sufficiently accurate.

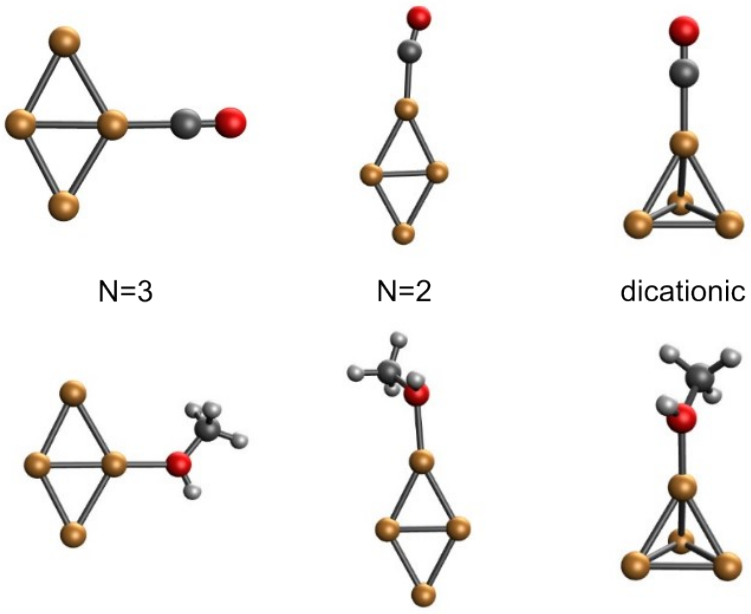


Figure S4. The CO and CH_3OH adducts of planar, neutral and dicationic tetrahedral Cu_4 clusters. N refers to the coordination number of the Cu atom that binds to the reactant molecules

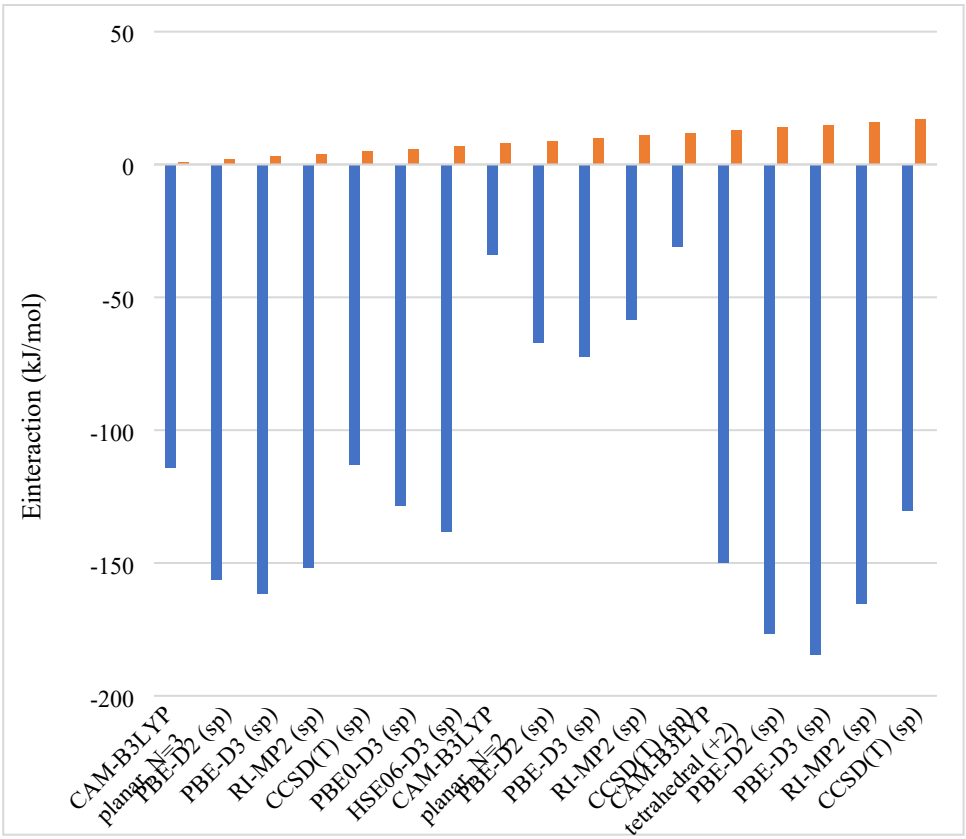


Figure S5. The CO adducts of Cu_4 with different methods.

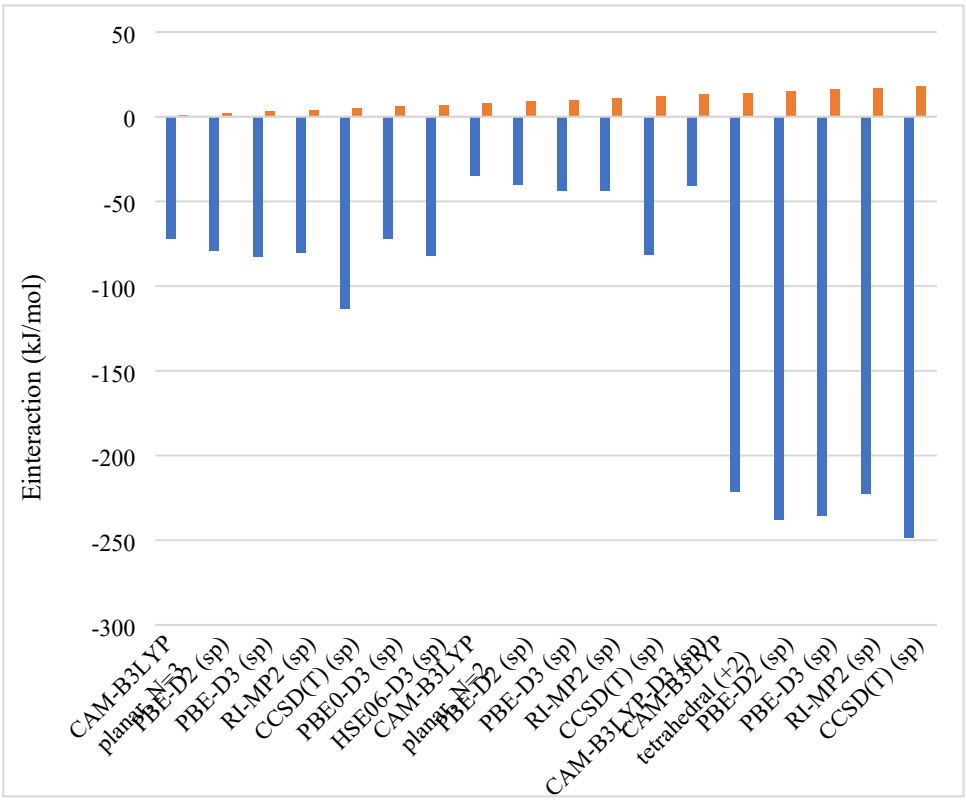


Figure S6. The CH_3OH adducts of Cu_4 with different methods

3. Boron-doping to immobilize copper clusters on graphene

We investigated the interaction of Cu_4 clusters with small aromatic hydrocarbons as a model for the doped graphene. The interaction between aromatic hydrocarbons and Cu_4 clusters can be significantly increased with boron doping: the interaction energy of Cu_4 clusters with borabenzene is much larger than with benzene, and the geometry of the adduct also changes significantly. This shows that boron-doping is a promising method to immobilize copper clusters on graphene.

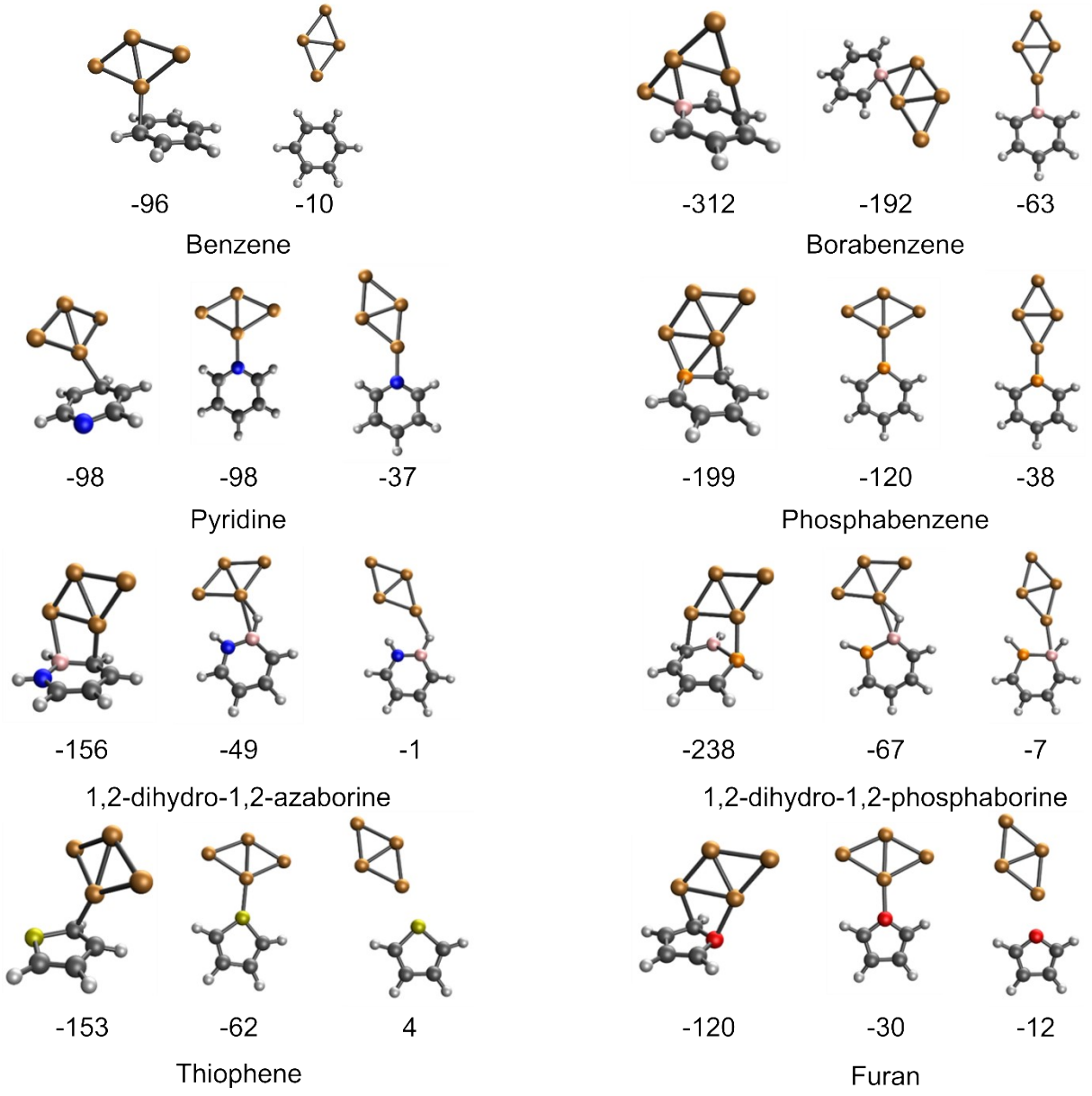


Figure S7. The effect of dopant atoms to the interaction energy and structure. The interaction energies are shown in kJ/mol. For benzene, only two binding modes were observed. (PBE-D3/def2-TZVP)

It was shown in a previous work,[i] that a single Cu atom bound to boron doped graphene in the same dopant pattern as we use, is thermodynamically less stable than the bulk copper metal. This raises questions on the solvent phase synthesizability. Here we propose a different route. According to the above definition, metal clusters are not expected to be stable by their nature, however they can be synthesized[ii-iv] (including Cu clusters[v]) in the gas phase and can be deposited on appropriate support.[iii,iv] The strong interaction with the boron atoms stabilizes the clusters and the large binding energies clearly show that they are immobilized and thus their aggregation is hindered. In line, according to the above definition[i], Au atom is also thermodynamically less stable on defective graphene compared to the bulk metal, but few-atom Au clusters were successfully deposited on graphene several times.[iii,iv] This shows the synthetic potential of our proposed catalyst system.

4. Quantification of the aromaticity

The NICS (0) values of -20.0 ppm (when the ghost atom is placed in the centre of the ring) of our nanoflake model molecule compared to -7.7 ppm of that of the benzene indicates that our model system can be aromatic. However, a relatively large electron density in the center of the ring can lead to low NICS (0) values. The electron density is visualized on Figure S8. It is visible, that in the central trigonal "boron" ring, the electron density is significantly higher than in the centre of other "benzene-like" rings (in the latter, the electron density is non-zero, we only set a higher isosurface value, so that the differences could be easily seen). This excess electron density in the center of the ring is due to the boron-boron interactions, as it is indicated by the Wiberg indices.

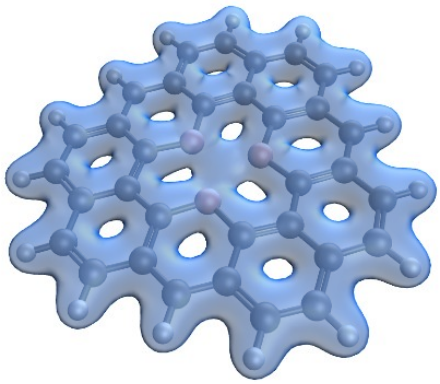


Figure S8. The electron density of the BDG nanoflake

Thus, we also computed the NICS (1) value of the BDG nanoflake, when the ghost atom is placed not in the centre of the ring, but exactly 1 Å higher in z direction. The purpose of

these calculations is that the high electron density of the central ring does not affect the NICS value. For benzene, we got a NICS (1) value of -9,8 ppm, which is lower than the NICS (0) value. For the BDG nanoflake model, we got -8,9 ppm, which is significantly higher than the NICS (0). Here the effect of the high electron density is seen: the absolute value of NICS decreases, but still, -8,9 ppm means that our model molecule is still aromatic.

5. Stability of the investigated boron binding pattern

While the aromaticity suggests the investigated boron doped nanoflake is stable, we also estimated its heat of formation and compared it with that of several reference compounds. The heat of formation was estimated by referencing to the hypothetical formation energy of the different compounds from methane and diborane and also to the experimental heat of formation of these two small molecules.[vi] The results are available in Table S4 and Figure S9.

Table S4. Gas phase heat of formation (at 298K) of BDG, along with several reference compounds

Formula	**Heat of formation (kJ/mol)**	**Remark**
C_6H_6	83.2	Benzene[vii]
$C10H_8$	150.6	Naphthalene[vii]
$C_{14}H_{10}$	202.2	Phenantrene[vii]
$C_{24}H_{12}$	279.7	Coronene[vii]
$C_{12}BH_9$	349[(a)]	Single trivalent boron doped PAH model[(b)]
$C_{33}B_3H_{15}$	937[(a)]	BDG
$C_{48}B_2H_{22}$	934[(a)]	Core of the synthesized boron doped PAH in reference[viii,(b)]
B_{36}	2604[(a)]	Borophene nanoflake[ix,(b)]
C_{60}	2319.7	Buckminsterfullerene[vii]
C_{70}	2501	Fullerene[vii]

[(a)] Computed values in this paper. Method: PBE/def2-TZVP

[(b)] Frequency computation was performed using the LANL2DZ basis.

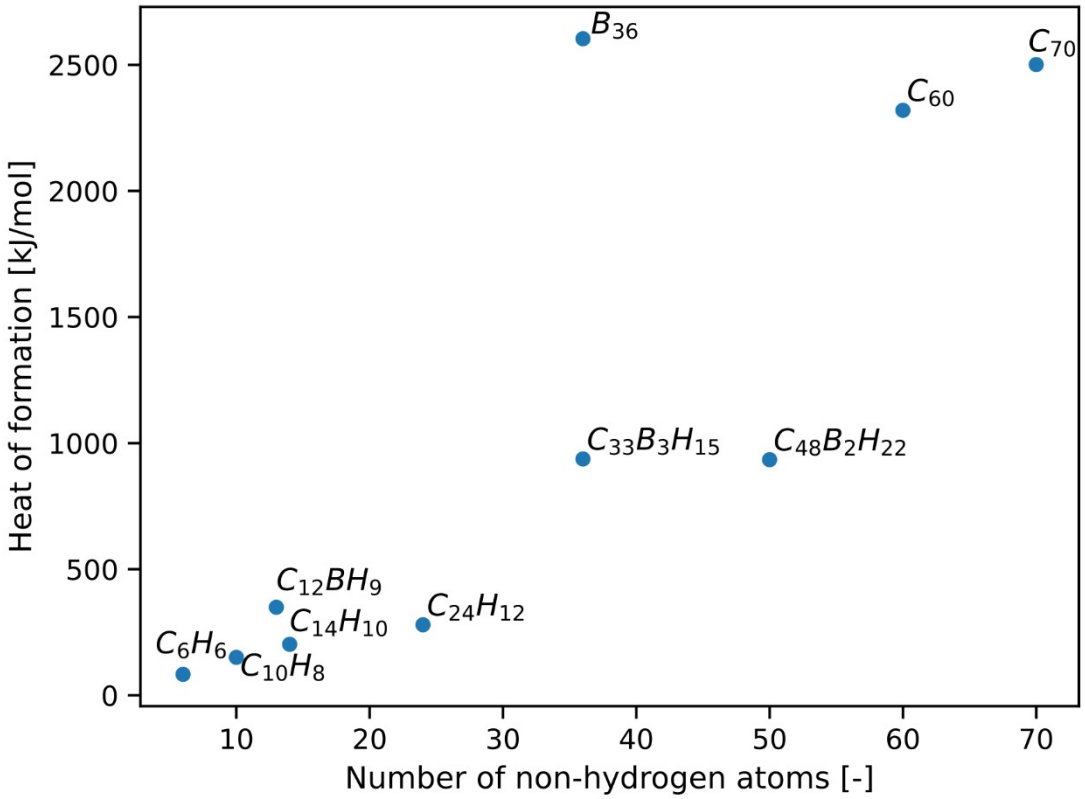


Figure S9. Gas phase heat of formation (at 298K) of BDG ($C_{33}B_3H_{15}$), along with several reference compounds. $C_{12}BH_9$ represents a single, trivalent boron doped small nanoflake, what models the binding mode of the previously synthesized boron doped graphene layer using CVD.[x] $C_{48}B_2H_{22}$ is a PAH doped by two, trivalent boron atoms, which was synthesized using appropriate bulky protecting groups.[viii] B_{36} is a borophene nanoflake, whose anion was first observed in a low pressure cell,[ix] while borophene layer was synthesized later with CVD using well selected substrate materials.[xi-xiv]

These results show that the heat of formation of the BDG nanoflake is in the range of reference compounds of similar size. While polycyclic aromatic hydrocarbons or fullerenes typically have positive heat of formation, these are well known, stable compounds. Thus, based on the heat of formations of BDG and several reference compounds, we expect that systems containing boron in this binding mode can be synthesized using organic or organometallic synthesis methods with appropriate protecting groups or using CVD with well-selected precursors and substrate.

6. The interpretation of the results with ALMO-EDA analysis

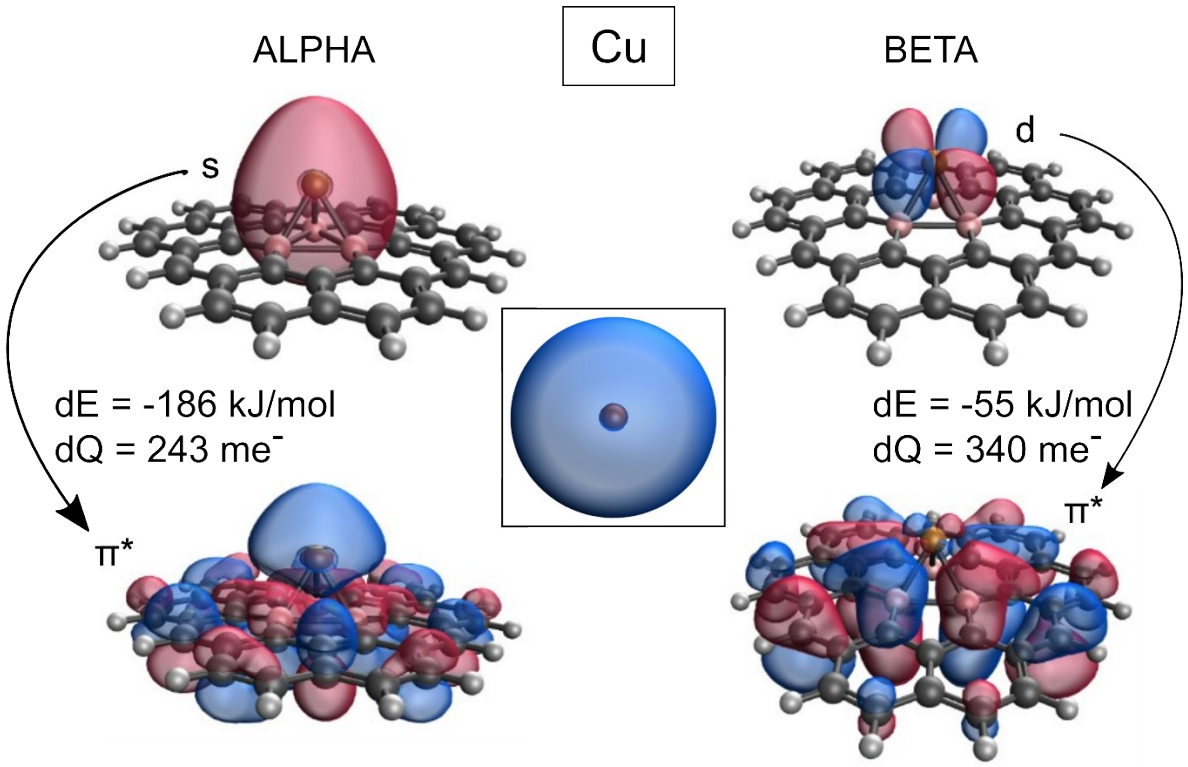


Figure S10. The most relevant COVP pairs of the BDGCu system.

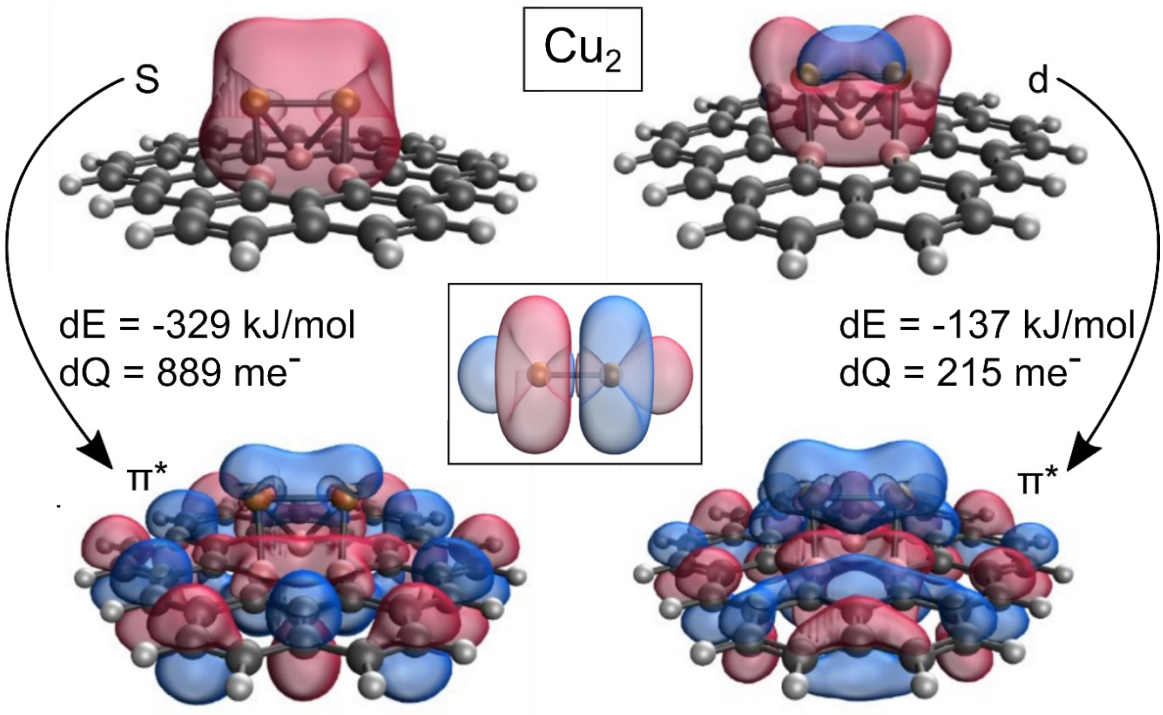


Figure S11. The most relevant COVP pairs of the $BDGCu_2$ system

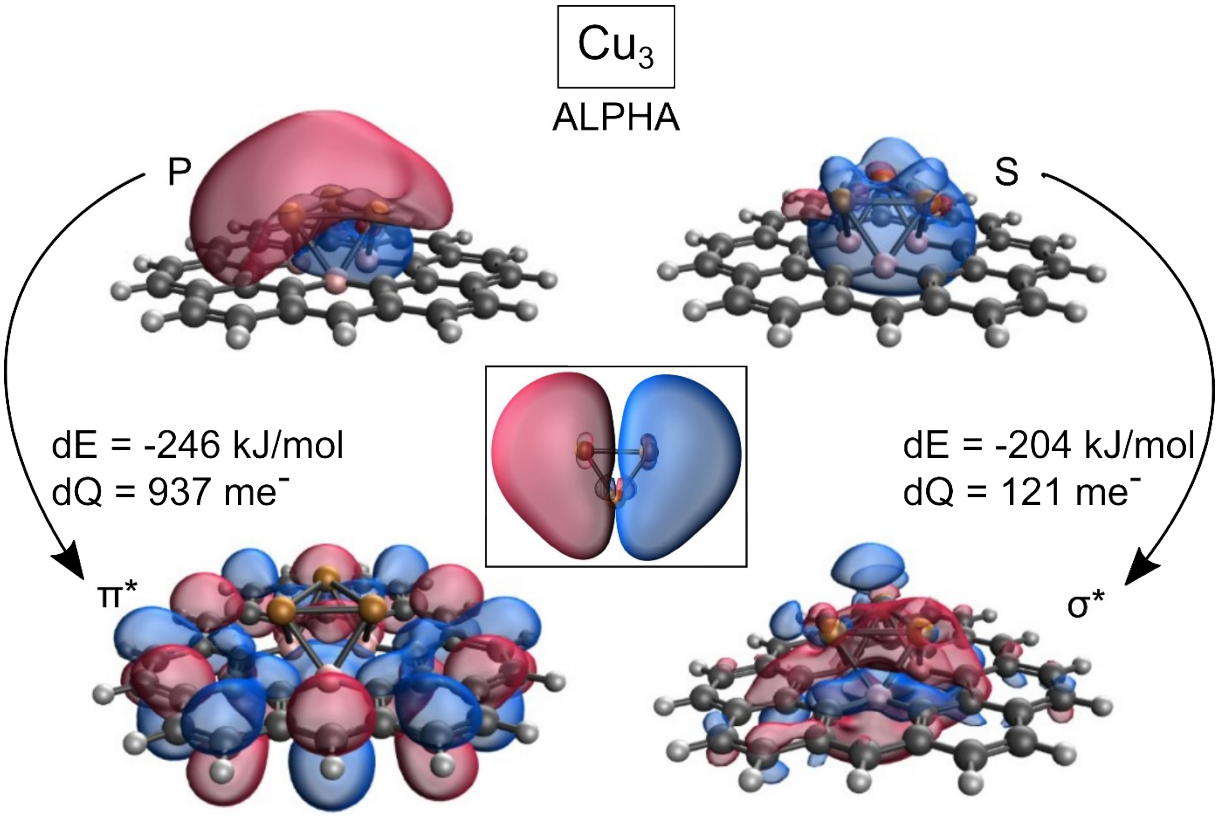


Figure S12. The most relevant COVP pairs of the $BDGCu_3$ system

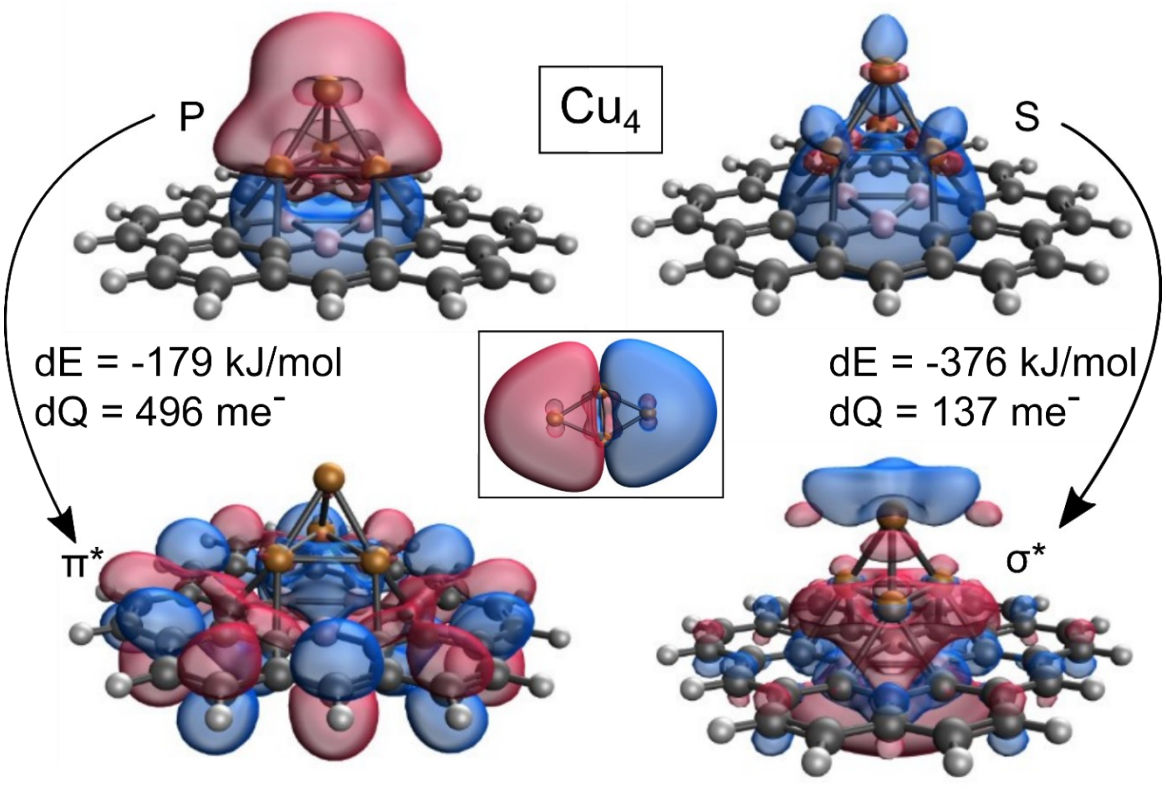


Figure S13. The most relevant COVP pairs of the $BDGCu_4$ system

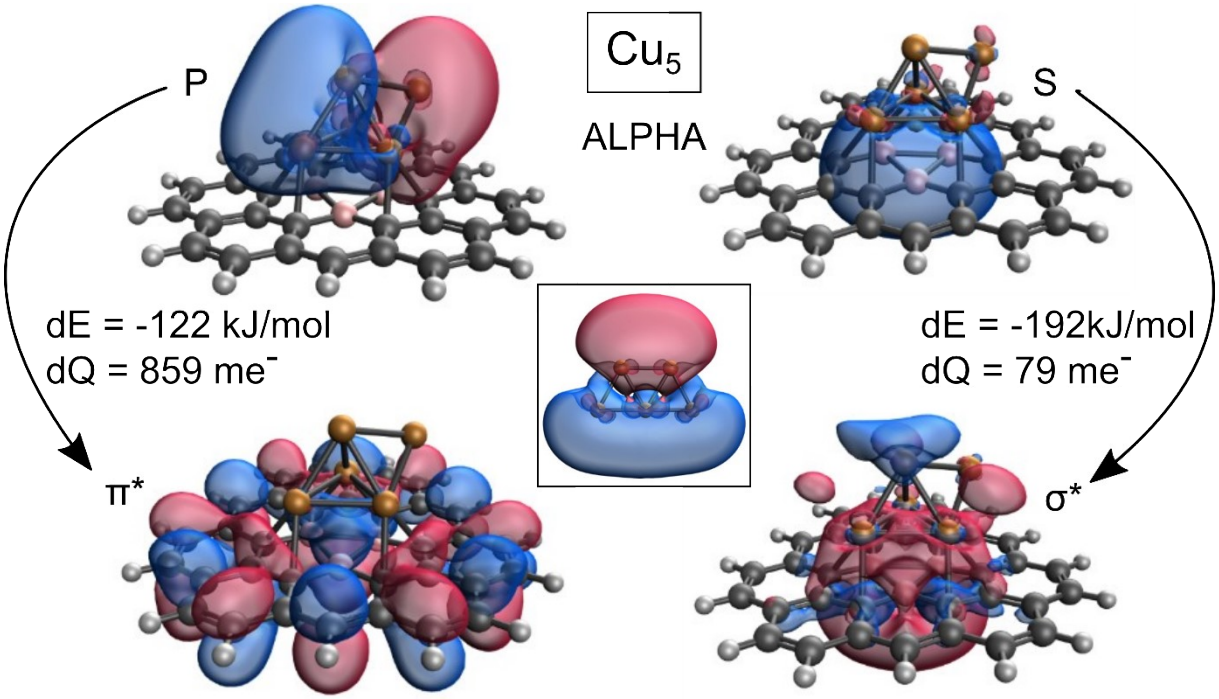


Figure S14. The most relevant COVP pairs of the $BDGCu_5$ system

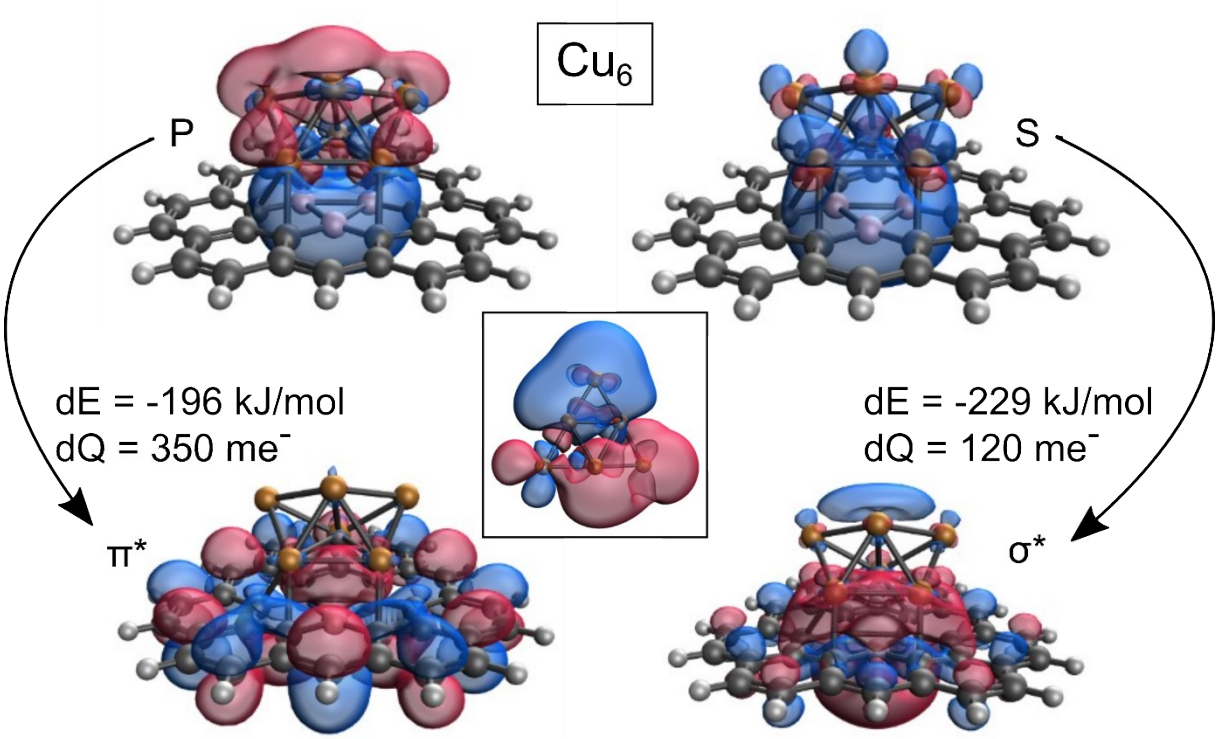


Figure S15. The most relevant COVP pairs of the $BDGCu_6$ system

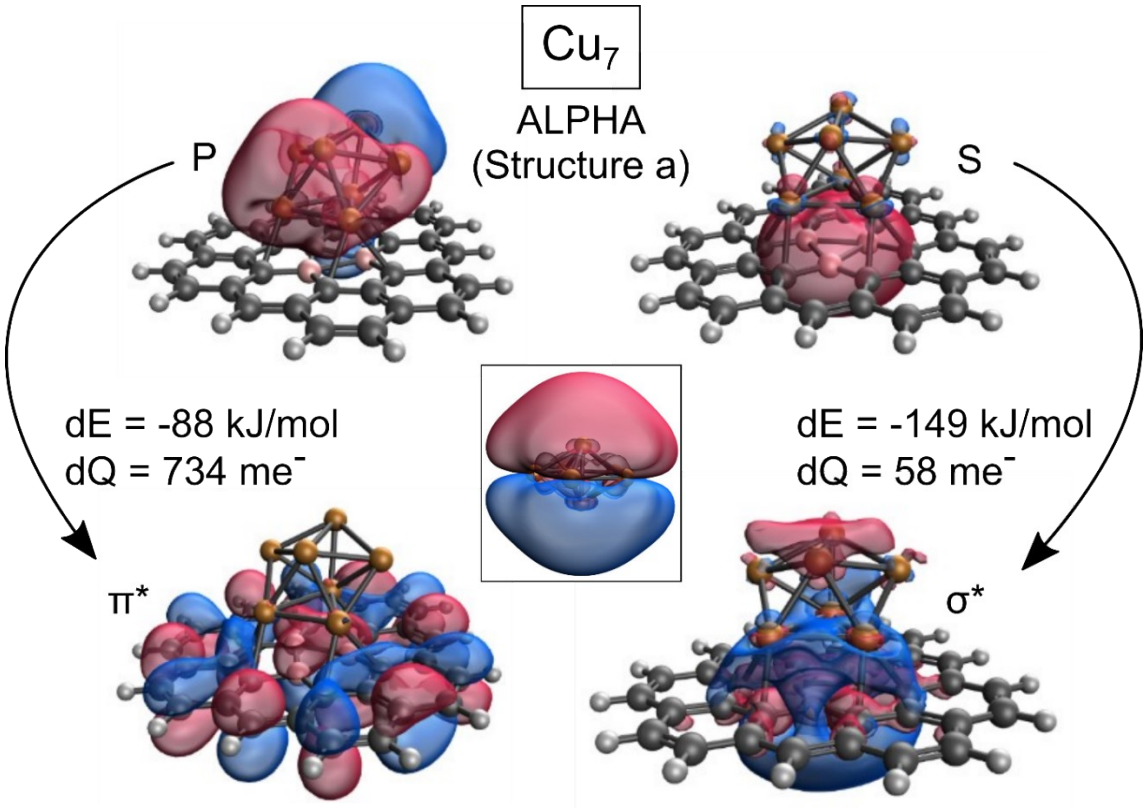


Figure S16. The most relevant COVP pairs of the $BDGCu_7$ system (less stable structure)

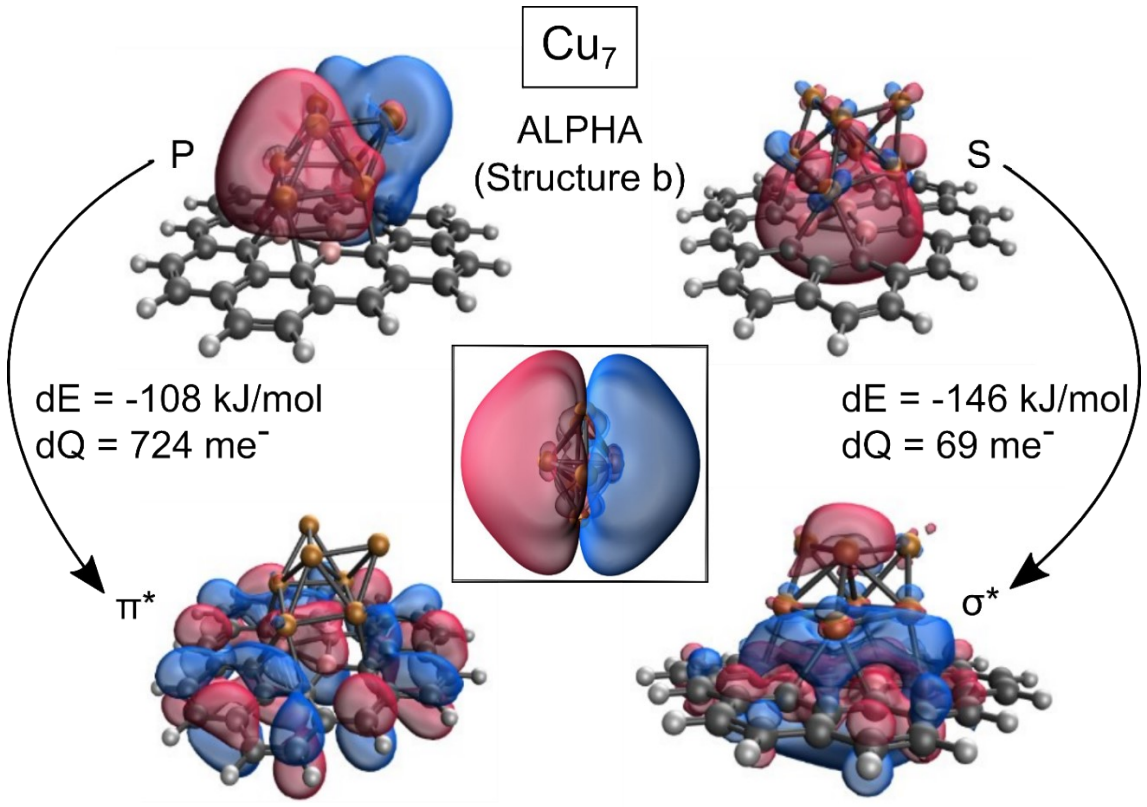


Figure S17. The most relevant COVP pairs of the $BDGCu_7$ system (more stable structure)

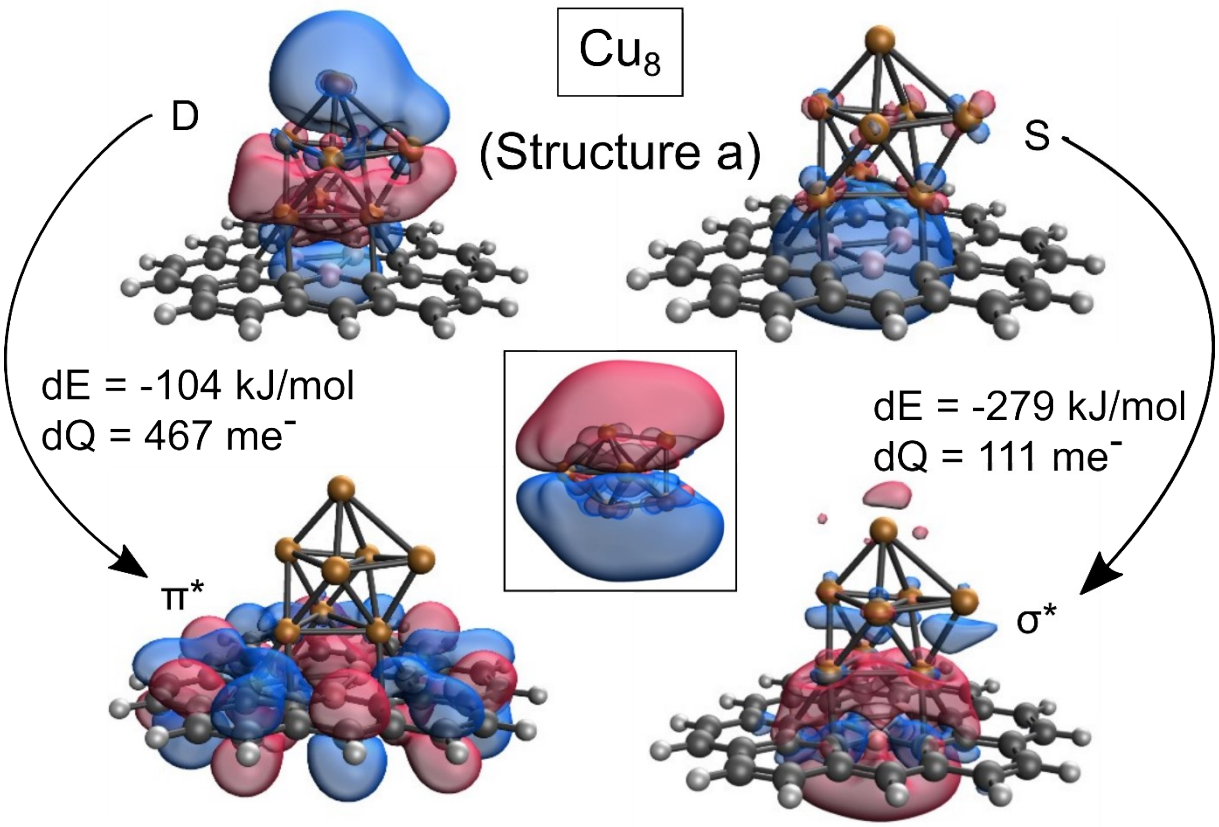


Figure S18. The most relevant COVP pairs of the $BDGCu_8$ system (less stable structure)

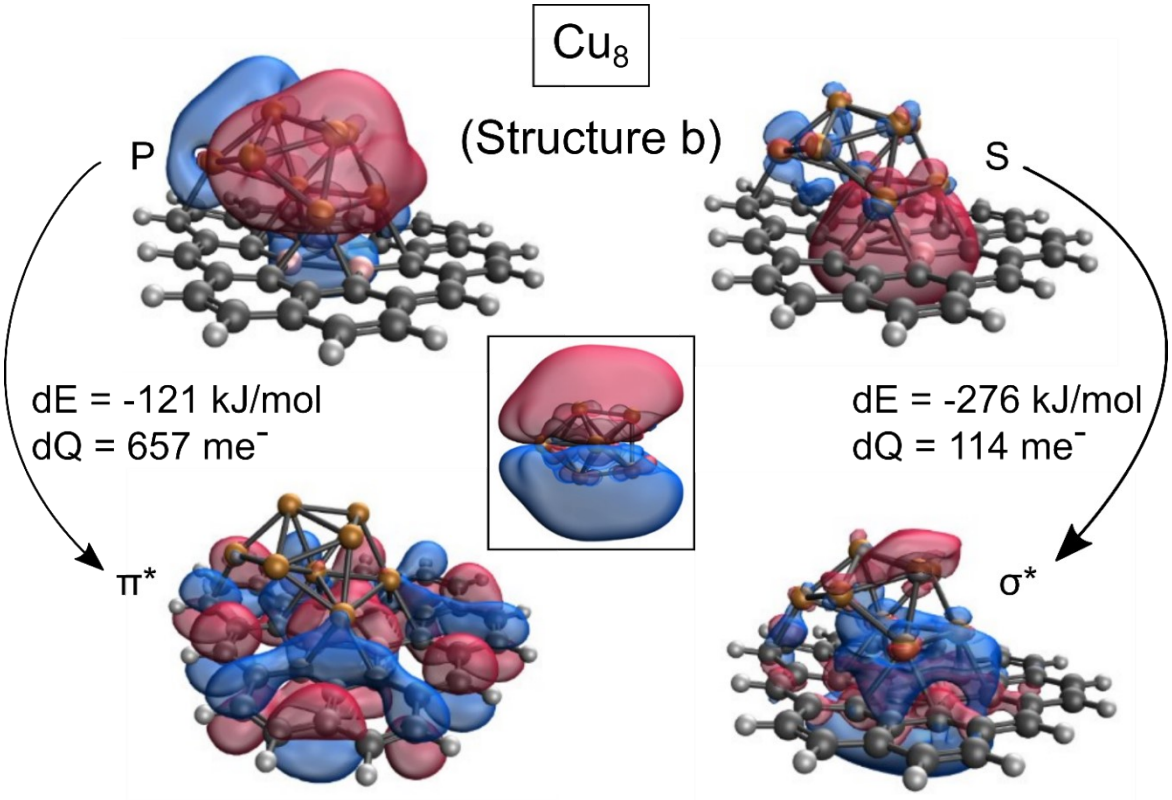


Figure S19. The most relevant COVP pairs of the $BDGCu_8$ system (more stable structure)

7. Investigating various C_1 and C_2 intermediates

a. C_1 intermediates

All possible and relevant intermediates were investigated for BDG bound Cu_4 clusters. Only the most stable (therefore most promising) intermediates were computed in an aqueous solution for Cu_4 and later, on Cu_7 in gas phase and aqueous solution (marked with green background, Table S4).

Table S5. Investigation of various C_1 intermediates. The promising (most stable) intermediates are marked with green, others are marked with red background

METHANOL	Reaction energy (kJ/mol)
* + CO_2 + $4H_2$	0
*CO_2	-95
H* + CO_2	-70
*HCOO	-196
*HCOOH	-137
*H_2COOH	-165
*H_2COHOH	-195
*OH + *CH_2O	-123
*OH + *CH_3O	-287
*H_2O + *CH_3O	-273
*H_2O + *CH_3OH	-303
H_2O + *CH_3O	-151
H_2O + *CH_3OH	-223
H_2O + * + CH_3OH	-80
*H_2O + CH_3OH	-219
CARBON MONOXIDE	**Reaction energy (kJ/mol)**
*COOH	-60
*CO + *OH	-139
CO + *OH	38
CO + *H_2O	-49
*CO + *H_2O	-165
*CO + H_2O	-81
CO + * + H_2O	90
*COHOH	-44
*COH + *OH	49
METHANE	**Reaction energy (kJ/mol)**
H_2O + *O + *CH_3	-223
H_2O + *O + CH_4	-149
H_2O + *OH + *CH_3	-332
H_2O + *H_2O + *CH_3	-272
H_2O + *OH + CH_4	-247
$2H_2O$ + *CH_3	-200
H_2O + *H_2O + *CH_4	-359
*H_2O + *OH + *CH_4	-399
*H_2O + *OH + CH_4	-390
*H_2O + *H_2O + CH_4	-423

H_2O + *H_2O + CH_4	-334
*+ 2H_2O + CH_4	-195
FORMIC ACID	**Reaction energy (kJ/mol)**
*+HCOOH	-13
FORMALDEHYDE	**Reaction energy (kJ/mol)**
*H_2O + *CH_2O	-176
*H_2O + CH_2O	-101
H_2O + *CH_2O	-95
* + H_2O + CH_2O	38
METHANE ALTERNATIVE PATHWAY	**Reaction energy (kJ/mol)**
*H_2O + *COH	73
METHANE + METHANOL ALTERNATIVE PATHWAY	**Reaction energy (kJ/mol)**
*H_2O + *CHO	-112
*H_2O + *CH_2O	-171

Usually, COH species do not form in the gas phase however, the presence of water can promote COH formation instead of CHO.[xv] Therefore, we investigated COH formation in a solvate model as well (Table S5). but still, the reaction through COH on small Cu clusters does not seem to be the most favoured pathway.

Table S6. The reaction energy of COH formation in an aqueous solution

METHANE ALTERNATIVE PATHWAY	Reaction Gibbs free energy (kJ/mol)
*H_2O + *COH	21

b. C_2 intermediates

Here, we divided the reaction pathway into two parts. The first part is the intersection from the CO pathway, and the adsorption of the second CO_2 molecule, until the formation of 2 CO molecules. The second is the formation of OCCOH, and its further reduction until the desired products. For the second part, we made pre-computations (Table S6) for $BDGCu_7$. For the first part of the C_2 pathway, we assumed that the second CO_2 is reduced with the same mechanism as the first one (through *COOH). The most promising reaction paths were also computed for $BDGCu_4$.

Table S7. Our pre-computations for the C_2 pathway. The promising (most stable) intermediates are marked with green, others are marked with red background.

Common pathway	Reaction energy (kJ/mol)
*CO + *CO + 2H_2O	-40
*COCO- + 2H_2O	-216
*COCO + 2H_2O	95
*CO + *COH + 2H_2O	40
*COCOH + 2H_2O	-15
*COHCOH + 2H_2O	105
*CCO + 3H_2O	-45

*CHCO + $3H_2O$	-139
*CCO + *H_2O + $2H_2O$	-102
*CHCO + *H_2O + $2H_2O$	-215
*CHCHO + *H_2O + $2H_2O$	-196
*CH_2CO + *H_2O + $2H_2O$	-188
*$CHCH_2OH$ + *OH + $2H_2O$	-193
*CHCHOH + *H_2O + $2H_2O$	-249
*CH_2CHO + *H_2O + $2H_2O$	-306
ETHYLENE	**Reaction energy (kJ/mol)**
*CH_2CH_2 + *OH + *OH + $2H_2O$	-358
CH_2CH_2 + *OH + *OH + $2H_2O$	-232
*CH_2CH_2 + *H_2O + *OH + $2H_2O$	-391
*CH_2CH_2 + *H_2O + *H_2O + $2H_2O$	-375
CH_2CH_2 + *H_2O + *OH + $2H_2O$	-308
CH_2CH_2 + *H_2O + *H_2O + $2H_2O$	-263
CH_2CH_2 + *H_2O + $3H_2O$	-202
CH_2CH_2 + * +$4H_2O$	-143
ETHYLENE alternative pathway	**Reaction energy (kJ/mol)**
*CHCOH + *H_2O + $2H_2O$	-37
*CCH + *$2H_2O$ + $2H_2O$	-189
*$CHCH_2$ + *OH + *H_2O + $2H_2O$	-340
*$CHCH_2$ + *$2H_2O$ + $2H_2O$	-352
*CH_2CH_2 + *OH + *H_2O + $2H_2O$	-392
*$CHCH_3$ + *OH + *H_2O + $2H_2O$	-355
*CH_2CH_3 + *OH + *H_2O + $2H_2O$	-444
CH_2CH_2 + *H + *OH + *H_2O + $2H_2O$	-344
CH_2CH_2 + *$2H_2O$ + $2H_2O$	-264
ETHANOL	**Reaction energy (kJ/mol)**
*CH_2CHOH + *H_2O + $2H_2O$	-292
*CH_3CHO + *H_2O + $2H_2O$	-295
*CH_2CH_2O + *H_2O + $2H_2O$	-311
*CH_2CH_2OH + *H_2O + $2H_2O$	-355
*CH_3CH_2OH + *OH + $2H_2O$	-380
CH_3CH_2OH + *OH + $2H_2O$	-327
*CH_3CH_2OH + *H_2O + $2H_2O$	-347
CH_3CH_2OH + *H_2O + $2H_2O$	-297
* + CH_3CH_2OH + $3H_2O$	-223

8. Reaction pathways resulting in C_1 products

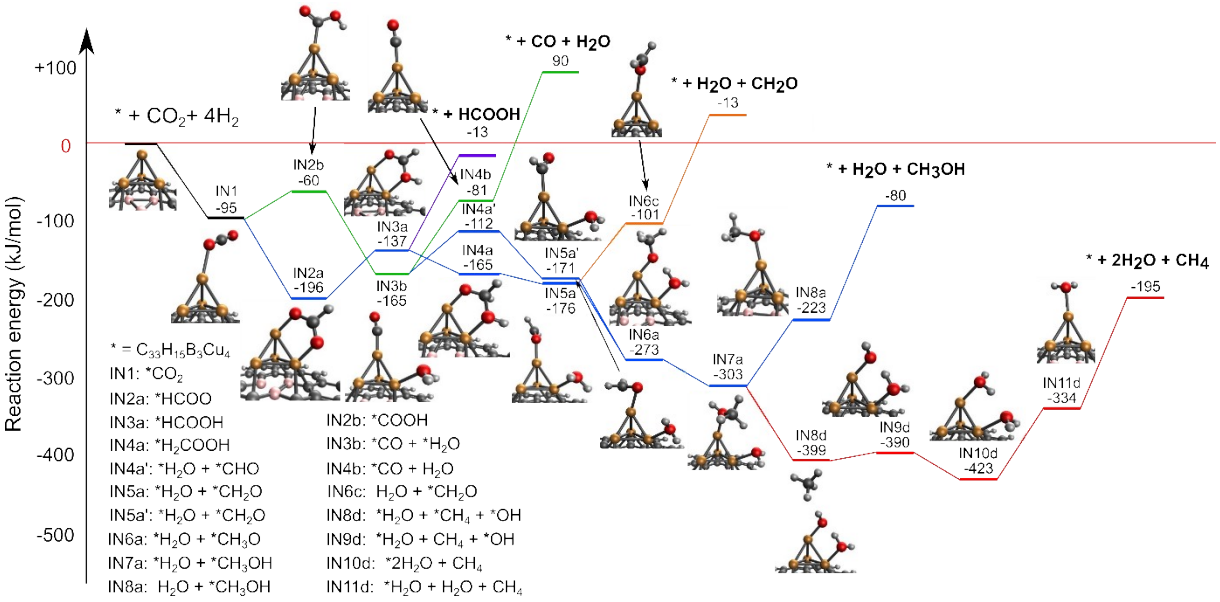


Figure S20. The thermally activated C_1 reaction pathway on a BDG bound Cu_4 cluster

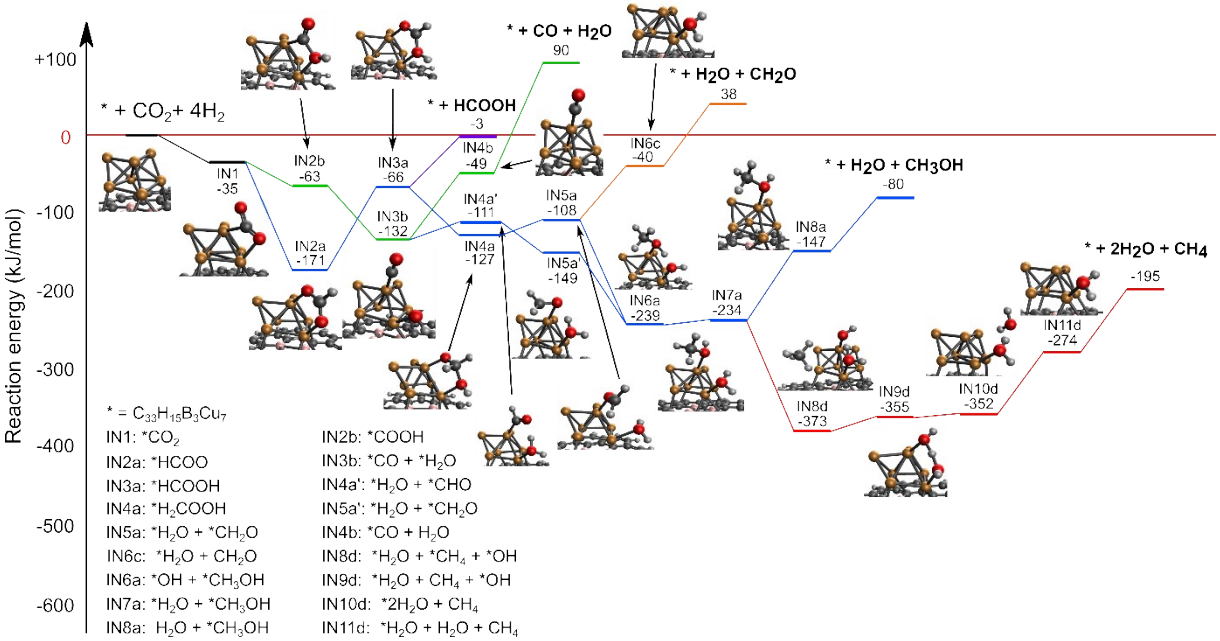


Figure S21. The thermally activated C_1 reaction pathway on a BDG bound Cu_7 cluster

9. Reaction pathways resulting in C_2 products

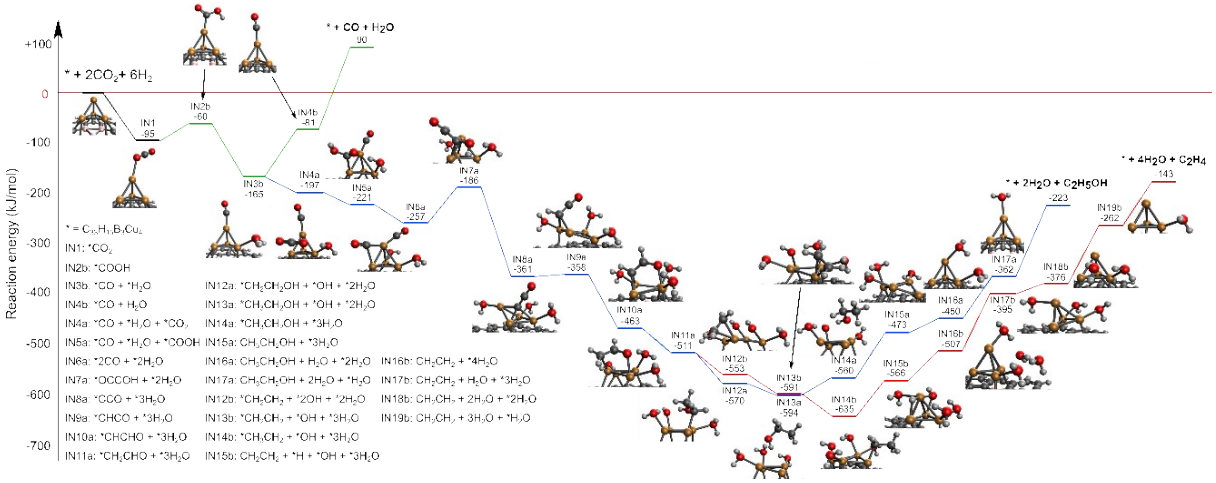


Figure S22. The thermally activated C_2 reaction pathway on a BDG bound Cu_4 cluster

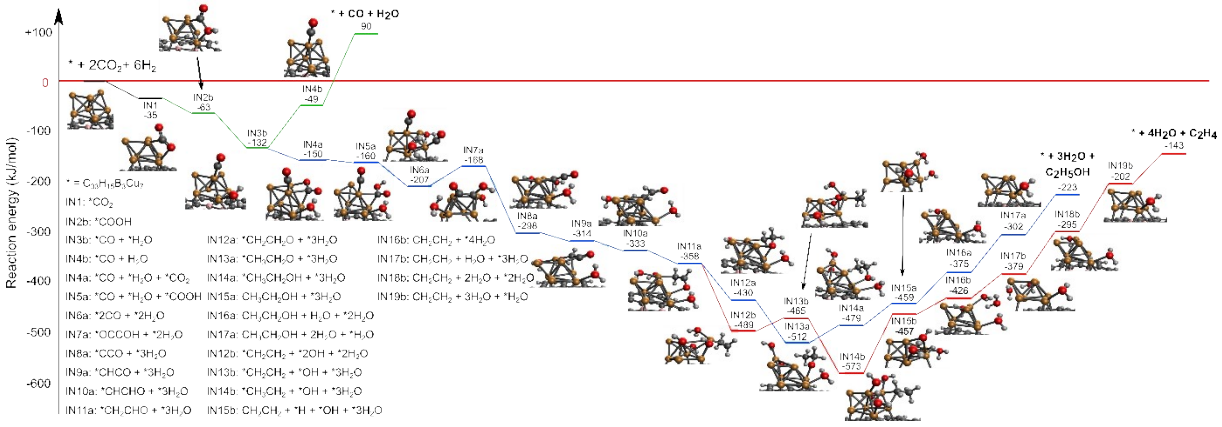


Figure S23. The thermally activated C_2 reaction pathway on a BDG bound Cu_7 cluster

10. The effect of applied overpotential

In Figure S23 the same electrochemical reaction pathway is shown, as in Figure 5. but at applied overpotential of $\phi = -1\ V$, by adding $z \cdot F \cdot \phi$ to the reaction free energy, where z is the number of electrons required for the reaction step, F is the Faraday-constant.[xvi]

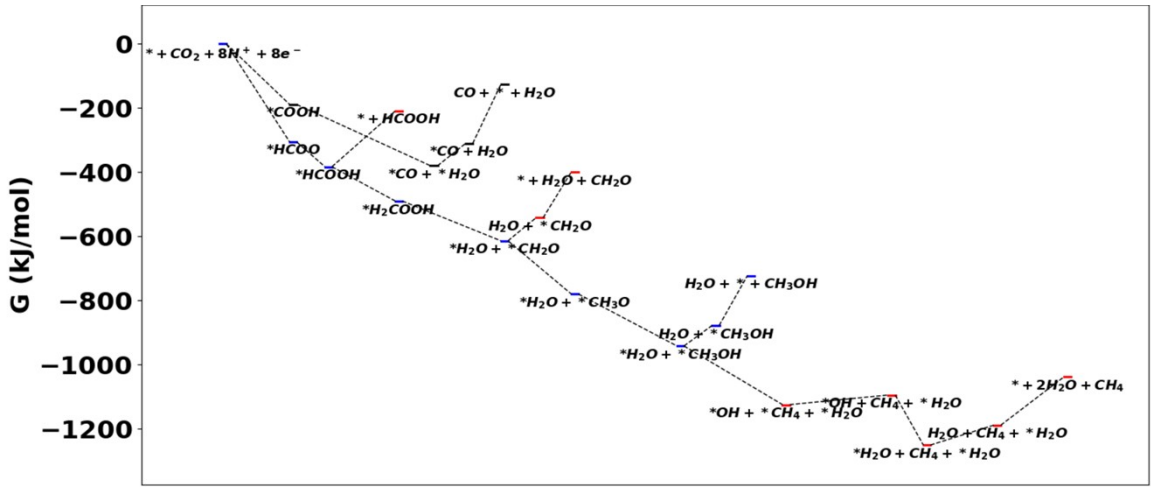


Figure S24. C_1 reaction pathway in an aqueous solution at 298 K, 1 atm on a BDG bound Cu_4 cluster at -1 V overpotential

11. The effect of adsorbed H_2O species

In all reaction pathways presented in the main text, the H_2O byproduct molecules are bound to the cluster. As a comparison, we investigated the opposite limiting case, when all water molecules are dissociated for the onset of the C_2 electroreduction pathway on $BDGCu_7$ (Figure S24). We can clearly see, that despite these endergonic steps, the reaction free energy slopes downwards with the reaction coordinate, with the largest uphill step being only 68 kJs/mol. Thus the adsorbed explicit water molecules do not alter our conclusions.

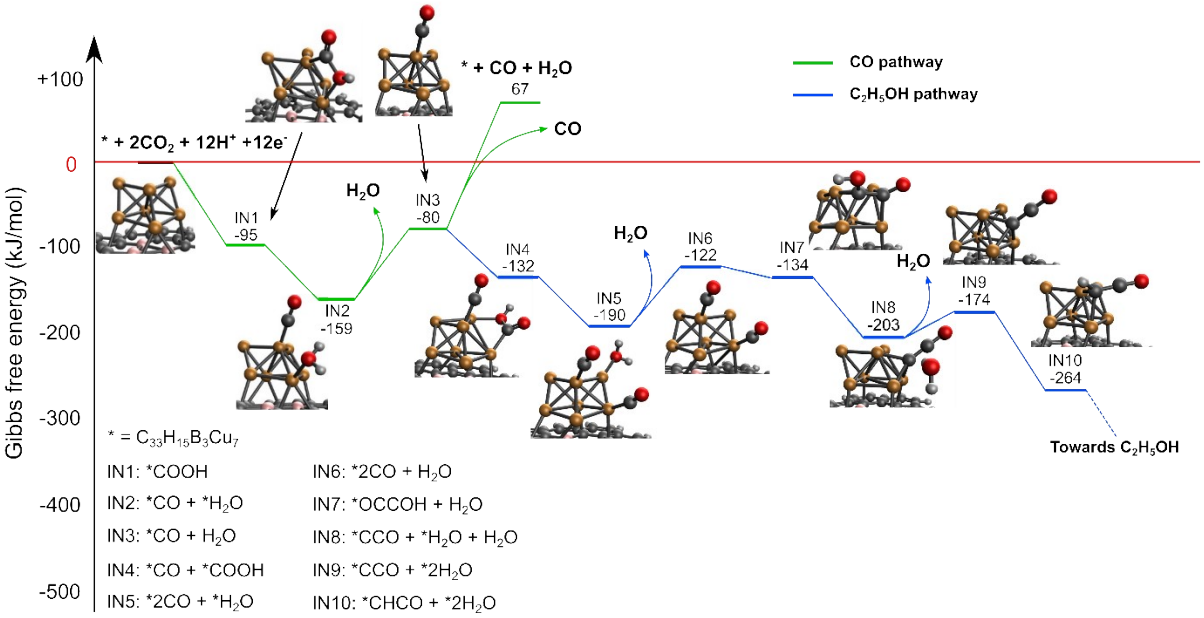
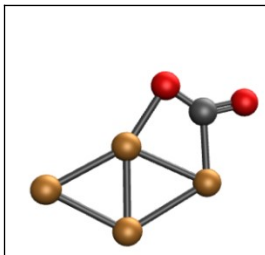
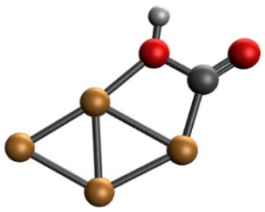
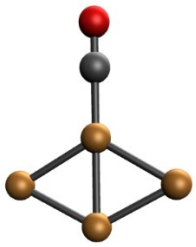
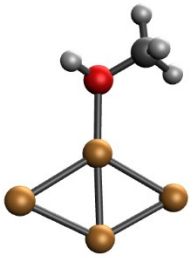


Figure S25. The effect of removing the adsorbed water molecules from the catalyst – in the example of $BDGCu_7$, in an aqueous solution, 298 K, 1 atm

12. The effect of vibrational contributions to the free energies

Table S8. The effect of vibrational contributions on the computed free energies

				
	$Cu_4 + CO_2 = Cu_4CO_2$	$Cu_4 + CO_2 + H^+ + e^- = Cu_4COOH$	$Cu_4 + CO = Cu_4CO$	$Cu_4 + CH_3OH = Cu_4CH_3OH$
$\Delta E + \Delta G_{solv}$ (kJ/mol)	-55	-43	-166	-91
$\Delta E + \Delta H + \Delta G_{solv} + \Delta ZPE - T\Delta S$ (kJ/mol)	-68	-29	-169	-98

In Table S7 the adsorption free energies of CO_2, CO, and CH_3OH on Cu_4 are shown alongside with the reaction free energy of *COOH formation computed using CHE. In the first row only the solvation free energy was added to the gas phase SCF energy. In the second row ZPE was also taken into account as well as the vibrational entropies and enthalpies. It can be seen that the latter two terms do not have any significant effect in the case of CO_2, CO, and CH_3OH adsorption. In the CHE model, H^+ ions are in equilibrium with gas phase H_2 molecules: $\mu(H^+) + \mu(e^-) = \frac{1}{2}\mu(H_2)$, where $\mu(H_2)$ is equal to the gas phase SCF energy. In the gas phase, translational and rotational entropies and enthalpies cannot be neglected. This results a higher difference for *COOH formation (14 kJ/mol) but still, when most reaction free energies for the computed pathways are several hundred kJ/mol, neglecting vibrational contributions does not alter our conclusions.

13.Hydrogen evolution reaction (HER) on $BDGCu_4$ and $BDGCu_7$

According to several previous works,[xvii,xviii] a suitable descriptor for estimating the reactivity of a catalyst in HER is the binding energy of an adsorbed *H species, i.e. the reaction free energy for the $* + H^+ + e^- = *H$ reaction. The results are shown in Table S8.

Table S9. Descriptor for HER, computed on $BDGCu_4$ and $BDGCu_7$

	ΔG_{H^*} (kJ/mol)
$BDGCu_4$	-68
$BDGCu_7$	-86

It is well visible that the *H formation is favoured, but it is also known that the closer this value to 0 kJ/mol, the higher the expected exchange current for hydrogen evolution.[xviii] BDGCu clusters bind hydrogen too strongly for efficient hydrogen evolution reaction (for a commercial Pt catalyst, this descriptor is much closer to 0 kJ/mol,[xvii,xviii] thus HER is less favoured in this case.

14. Proton-electron transfer reaction

We applied the state-of-the-art Joint Density Functional Theory method implemented in the jDFTx program[xix] to explore the proton-electron transfer. We used a similar model to the one that was successfully applied to determine the reaction mechanism (including the proton-electron transfer) of the carbon-dioxide reduction on nickel single atom catalysts on nitrogen doped graphene.[xx] The atomistic model consists of the BDG-Cu_4 system, a CO_2 molecule and a protonated water chain. The full system is embedded in an implicit solvent, modelled using the charge-asymmetric nonlocally determined local-electric (CANDLE) solvation model[xxi] and included 0.1M NaI to consider the ionic strength of the electrolyte. Due to the inclusion of the proton, the total charge of the atomic system is +1, what is balanced by the iodine ions in the solvent. The computed free energies include the solvation contributions, while vibrational terms are neglected.

We used this model to investigate the protonation of the cluster bound CO_2 molecule (Figure S8). The large protonation free-energy clearly shows that at sufficiently acidic conditions, the cluster bound carbon-dioxide is protonated, thus the protonation can precede the reduction step.

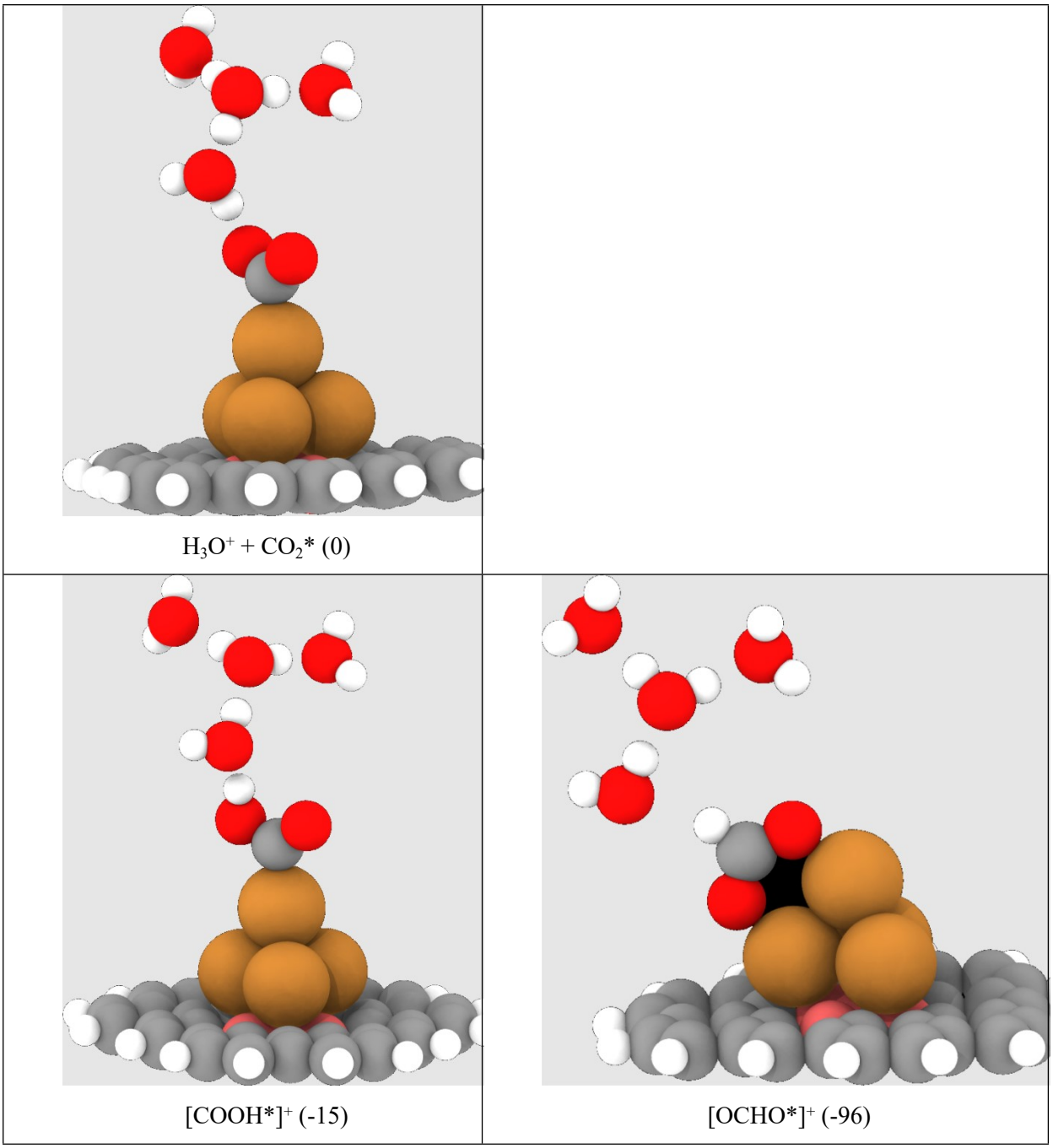


Figure S26. Relative free energies (in parentheses, kJ/mol) of various protonation states of the cluster bound CO2 molecule. Asterisk indicates an adsorbed species.

15. Cartesian coordinates of all reaction intermediates in an aqueous solution

a. Cu_4 cluster – C_1 pathway

*** = $C_{33}H_{15}B_3Cu_4$**

C	-0.22808	-4.87254	0.74118	C	0.03817	-2.42281	0.81255
C	-0.83170	-3.56905	0.83024	C	1.44121	-2.64706	0.67630

C	2.01587	-3.92906	0.55709	C	-2.82188	-2.14144	0.99536
C	1.13020	-5.05124	0.60868	C	-2.01705	-0.94815	0.98564
C	3.43571	-3.99907	0.39805	B	-0.26746	1.13914	0.89492
C	4.19593	-2.85333	0.33589	B	-0.47090	-0.96593	0.92514
C	3.61907	-1.53766	0.42159	C	4.41459	-0.38264	0.33006
C	2.19682	-1.43826	0.61525	C	-2.22401	-3.41217	0.93894
B	1.44820	-0.09026	0.74156	H	5.49443	-0.48887	0.19548
C	2.44041	1.08512	0.57686	H	-1.97333	4.87049	0.83677
C	1.93056	2.41694	0.60967	H	0.23436	5.90201	0.63220
C	2.73935	3.56252	0.46406	H	4.80004	4.22419	0.20183
C	4.14580	3.35507	0.30407	H	5.74901	1.94500	0.13854
C	4.67271	2.08405	0.26853	H	2.68685	5.74091	0.39331
C	3.85535	0.90530	0.38670	H	-4.20453	3.87867	0.98643
C	2.08489	4.83421	0.49021	H	-5.70097	1.91563	1.09369
C	0.71784	4.92184	0.62404	H	-5.95052	-0.68089	1.13897
C	-0.12328	3.75960	0.73951	H	-4.85934	-2.89416	1.09295
C	0.51219	2.46826	0.75114	H	-2.86037	-4.30106	0.95980
C	-1.52005	3.87562	0.84316	H	-0.89000	-5.74171	0.77191
C	-2.35036	2.74488	0.92555	H	1.54747	-6.05836	0.53562
C	-1.78840	1.42070	0.95084	H	3.91146	-4.97952	0.32040
C	-2.68467	0.31247	1.01925	H	5.27891	-2.92571	0.20760
C	-4.08770	0.44959	1.05702	Cu	0.65463	-1.27739	-1.01808
C	-4.61770	1.77825	1.05502	Cu	-1.34686	0.15768	-0.85255
C	-3.78243	2.87065	0.99521	Cu	-0.11034	0.00532	-2.94193
C	-4.86119	-0.75326	1.09599	Cu	0.89132	1.18146	-1.05565
C	-4.25063	-1.98660	1.06940				

***COOH**

C	2.58421	-0.44227	-0.52151	C	4.32520	2.83379	0.10683
C	2.89222	0.94234	-0.39725	C	3.27036	3.68788	-0.13502
C	4.16599	1.41993	-0.00550	C	1.96371	3.21756	-0.50597
C	5.17883	0.44541	0.24376	C	1.78156	1.79897	-0.65330
C	4.91045	-0.90217	0.13040	C	0.89723	4.10640	-0.72971
C	3.61419	-1.40328	-0.23626	C	-0.38853	3.65172	-1.07309

C	-1.47971	4.56538	-1.27550	C	-1.27998	-1.96286	-1.53203
C	-2.75246	4.14186	-1.59384	C	3.35454	-2.78294	-0.32497
C	-3.04810	2.75387	-1.74481	C	-3.65461	-1.48533	-2.03223
C	-1.97658	1.84304	-1.57880	B	0.43529	1.16570	-1.06386
C	-0.65161	2.24831	-1.24421	H	-4.65964	-1.85653	-2.24997
C	-4.33012	2.20426	-2.04726	H	1.06827	5.18040	-0.61716
C	-4.51252	0.84133	-2.14728	H	-1.27707	5.63313	-1.15929
C	-3.44204	-0.09739	-1.95158	H	-5.17452	2.88219	-2.19254
C	-2.13431	0.43086	-1.67221	H	-5.50495	0.44254	-2.37233
B	-0.89887	-0.46938	-1.45040	H	-3.55522	4.87078	-1.72838
Cu	-1.28212	0.80032	0.37182	H	3.41373	4.76701	-0.03763
Cu	-0.68810	-0.14745	2.57495	H	5.29970	3.23486	0.39543
Cu	1.07433	0.38095	0.95130	H	6.17668	0.78210	0.53461
Cu	-0.45109	-1.50637	0.51540	H	5.69939	-1.63103	0.33252
B	1.15402	-0.84598	-0.94188	H	4.15954	-3.48992	-0.10751
C	1.00022	-2.38312	-0.97012	H	2.64272	-5.37291	-0.50368
C	2.08247	-3.27953	-0.66316	H	0.41523	-6.28023	-1.05907
C	1.81794	-4.69068	-0.72434	H	-2.07596	-5.81904	-1.66623
C	0.57463	-5.19961	-1.03511	H	-3.86304	-4.16899	-2.08983
C	-0.52301	-4.33379	-1.32095	O	-1.73412	-0.78683	5.13204
C	-0.27020	-2.93993	-1.29660	C	-1.08499	0.02122	4.47588
C	-1.85301	-4.75019	-1.62794	O	-0.61418	1.13105	5.16376
C	-2.84972	-3.82709	-1.86433	H	-0.12065	1.68885	4.52797
C	-2.61738	-2.41008	-1.81302				

***H_2O + *CO**

C	2.54301	0.24443	0.92895	C	2.16370	-3.51784	0.81953
C	2.79833	-1.15974	0.84095	C	1.80953	-2.19016	0.90389
C	4.14420	-1.56118	0.69587	C	3.86909	-5.30352	0.58903
C	5.23591	-0.64513	0.60880	C	5.19917	-5.72620	0.42108
C	4.94077	0.76518	0.64512	C	5.53658	-7.12473	0.34734
C	3.56958	1.15721	0.83984	C	6.82350	-7.55964	0.13044
C	4.54434	-2.92531	0.56355	C	7.89572	-6.62571	-0.03467
C	3.52711	-3.94235	0.64539	C	7.58679	-5.25843	0.08851

C	6.26692	-4.77156	0.30575	C	5.96201	1.71716	0.48604
C	9.24147	-6.96624	-0.38710	B	8.05401	-2.75127	-0.00666
C	10.17862	-5.98582	-0.61798	Cu	6.87799	-3.73723	-1.70453
C	9.86944	-4.58283	-0.50841	B	6.04941	-3.24213	0.36781
C	8.53115	-4.21595	-0.13406	H	5.71163	2.78059	0.53036
C	10.84102	-3.60082	-0.76756	H	3.07861	-6.05502	0.67008
C	10.54740	-2.23044	-0.67871	H	1.39366	-4.29155	0.87841
C	9.22753	-1.78383	-0.30963	H	1.51350	0.58773	1.05946
C	9.00284	-0.37911	-0.19089	H	3.35055	2.22671	0.89851
C	9.99293	0.59033	-0.45957	H	0.76037	-1.90873	1.02517
C	11.29239	0.11737	-0.82234	H	4.72583	-7.85090	0.45052
C	11.55301	-1.23074	-0.92125	H	7.03790	-8.62895	0.05668
C	9.61217	1.96304	-0.33346	H	9.51026	-8.02055	-0.49021
C	8.32158	2.31261	-0.00597	H	11.19721	-6.26140	-0.90356
C	7.28964	1.33627	0.22554	H	11.85155	-3.91180	-1.04744
C	7.66077	-0.05491	0.16971	H	12.55423	-1.57291	-1.19634
Cu	7.55104	-1.34394	-1.70831	H	12.08295	0.84494	-1.02223
B	6.66145	-1.20437	0.41567	H	10.36088	2.73813	-0.51642
Cu	5.25405	-1.90229	-1.28232	H	8.04837	3.36852	0.06852
Cu	6.13665	-2.16028	-3.56119	O	7.18182	-5.31728	-3.02997
C	5.78762	-2.33851	-5.38007	H	7.40560	-5.01221	-3.93007
O	5.52891	-2.36565	-6.49196	H	7.96498	-5.82667	-2.73747

***CO**

C	-0.10296	2.43708	-0.83910	Cu	-0.75271	1.16546	0.90893
C	-1.52876	2.49190	-0.84644	B	-1.22745	-0.04616	-0.96318
C	-2.25844	3.69470	-0.75983	Cu	-0.71290	-1.26699	0.89318
C	-1.51075	4.91260	-0.69753	B	0.62967	-1.06907	-0.93764
C	-0.13476	4.89768	-0.69054	Cu	1.37484	-0.01289	0.93438
C	0.62401	3.67582	-0.74058	Cu	-0.05958	-0.05878	2.98034
C	-2.13840	1.20198	-0.88547	C	-4.23334	-0.11054	-0.82238
C	-3.57539	1.13111	-0.82691	C	-3.52334	-1.32296	-0.83606
C	-4.30824	2.36879	-0.77473	C	-2.08444	-1.33285	-0.89753
C	-3.68507	3.59531	-0.74101	C	-1.42122	-2.59642	-0.87348

C	-2.09975	-3.82979	-0.79471	B	0.58475	1.05483	-0.92047
C	-3.52920	-3.79043	-0.77003	H	2.55400	4.63983	-0.63308
C	-4.20312	-2.59090	-0.79220	H	2.74907	-4.57214	-0.70338
C	-1.30090	-5.01538	-0.74810	H	4.85250	-3.32354	-0.64834
C	0.07326	-4.94238	-0.74892	H	6.05268	1.40881	-0.56662
C	0.77972	-3.68906	-0.79018	H	4.70902	3.47988	-0.58711
C	0.00109	-2.48107	-0.87159	H	6.10774	-1.19808	-0.59257
C	2.18318	-3.63774	-0.75528	H	0.66705	-5.85915	-0.70268
C	2.87871	-2.41687	-0.75818	H	-1.79883	-5.98700	-0.70207
C	4.31547	-2.37225	-0.68884	H	-4.08381	-4.73101	-0.72282
C	5.01678	-1.18867	-0.65636	H	-5.29579	-2.58097	-0.76171
C	4.33679	0.06935	-0.69205	H	-5.32601	-0.13414	-0.78530
C	2.93144	0.04102	-0.79776	H	-5.39960	2.31222	-0.74721
C	2.17004	-1.16547	-0.83382	H	-4.27892	4.51131	-0.68837
C	2.11989	1.21445	-0.81362	H	-2.04990	5.86167	-0.64456
C	2.77524	2.49311	-0.71635	H	0.41927	5.83806	-0.63120
C	4.21270	2.50758	-0.64455	C	0.00261	-0.07534	4.85001
C	4.96315	1.35421	-0.63215	O	0.07174	-0.08895	5.98794
C	2.02854	3.68315	-0.69924				

***CHO + *H_2O**

C	7.65521	-0.06825	0.08120	C	9.25747	-6.98914	-0.33059
C	9.01082	-0.39871	-0.20678	C	7.90567	-6.64975	-0.01694
C	10.01093	0.57343	-0.45280	C	7.59157	-5.27505	0.08883
C	9.61883	1.94372	-0.37571	C	8.54424	-4.23803	-0.11173
C	8.31340	2.29505	-0.10436	C	6.26969	-4.79387	0.29113
C	7.27942	1.32023	0.11315	C	5.20430	-5.74840	0.42101
C	11.32207	0.09811	-0.75553	C	5.54467	-7.14453	0.35702
C	11.58875	-1.25294	-0.82159	C	6.83479	-7.58023	0.14572
C	10.57958	-2.25212	-0.59972	C	3.87502	-5.32603	0.60693
C	9.24901	-1.80266	-0.28263	C	3.53048	-3.96419	0.66133
C	10.87554	-3.62429	-0.66766	C	4.54099	-2.94562	0.54819
C	9.89356	-4.60594	-0.44057	C	4.14118	-1.58097	0.65180
C	10.20320	-6.00776	-0.53533	C	2.79347	-1.17869	0.82184

C	1.81365	-2.21001	0.93089	H	3.08720	-6.07810	0.70444
C	2.17172	-3.53960	0.85920	H	1.40491	-4.31344	0.94891
C	5.22033	-0.66087	0.51129	H	1.50822	0.56802	1.01905
C	4.92489	0.74758	0.52908	H	3.33426	2.20901	0.77253
C	3.55710	1.13942	0.73611	H	0.76661	-1.93162	1.07364
C	2.53541	0.22407	0.87430	H	4.73648	-7.87232	0.46750
Cu	5.26481	-1.99115	-1.32233	H	7.04929	-8.64995	0.08232
B	6.04301	-3.26626	0.33466	H	9.53084	-8.04320	-0.42230
Cu	6.92478	-3.80394	-1.71759	H	11.22954	-6.28631	-0.78792
O	7.28445	-5.35365	-3.04755	H	11.89441	-3.93725	-0.91164
B	6.64834	-1.21733	0.31271	H	12.60024	-1.59503	-1.05557
Cu	7.60492	-1.41402	-1.73156	H	12.11834	0.82349	-0.93987
B	8.06977	-2.77239	-0.01304	H	10.37046	2.71879	-0.54531
C	5.94616	1.69896	0.35443	H	8.03506	3.35113	-0.05937
Cu	6.18909	-2.18543	-3.56845	H	7.49977	-5.03256	-3.94447
C	5.77633	-1.81688	-5.42240	H	8.08201	-5.84380	-2.75996
O	4.68343	-1.93732	-5.95825	H	6.63065	-1.44604	-6.06156
H	5.69265	2.76214	0.38446				

***CH_2O + *H_2O alternative pathway higher in free energy**

C	2.53999	0.21414	0.81149	C	7.90904	-6.66625	0.05580
C	2.79680	-1.19128	0.75353	C	6.83713	-7.59750	0.22833
C	4.14328	-1.59397	0.61991	C	5.54619	-7.15928	0.41706
C	5.23612	-0.68011	0.52004	C	8.54331	-4.25815	-0.09189
C	4.93891	0.73001	0.52312	C	9.88738	-4.63262	-0.43322
C	3.56673	1.12485	0.70471	C	10.20043	-6.03622	-0.50048
C	1.80871	-2.22094	0.83819	C	9.26058	-7.01318	-0.26140
C	2.16406	-3.54988	0.78360	C	10.86197	-3.65663	-0.70739
C	3.52841	-3.97614	0.62225	C	10.56380	-2.28522	-0.66775
C	4.54443	-2.96006	0.52157	C	11.56844	-1.29030	-0.93252
C	3.87358	-5.33742	0.60023	C	11.30252	0.05934	-0.87829
C	5.20650	-5.76081	0.45256	C	9.99856	0.53843	-0.53995
C	6.27264	-4.80738	0.32433	C	9.00792	-0.42564	-0.25395
C	7.59565	-5.29464	0.13802	C	9.23859	-1.83227	-0.32835

C	9.61420	1.91305	-0.45329	H	1.39487	-4.32292	0.85817
C	8.32032	2.26717	-0.14393	H	1.51042	0.55981	0.93424
C	7.28853	1.29496	0.10452	H	3.34720	2.19531	0.74084
C	7.66147	-0.09632	0.08704	H	0.75948	-1.93737	0.95275
B	6.66416	-1.24308	0.35588	H	4.73554	-7.88439	0.52755
Cu	7.59028	-1.43251	-1.75021	H	7.05378	-8.66776	0.18391
Cu	6.18510	-2.20743	-3.56364	H	9.53319	-8.06894	-0.33412
C	5.56691	-1.23392	-5.27312	H	11.22373	-6.31742	-0.76252
O	5.83699	-2.45333	-5.56307	H	11.87655	-3.97429	-0.96348
C	5.95904	1.68038	0.34782	H	12.57267	-1.63731	-1.18930
B	8.06231	-2.79219	-0.01331	H	12.09163	0.78372	-1.09504
Cu	6.91761	-3.83671	-1.71233	H	10.36299	2.68489	-0.64888
O	7.26530	-5.41299	-3.00332	H	8.04443	3.32397	-0.09675
B	6.05134	-3.27779	0.34434	H	7.48032	-5.12483	-3.91100
Cu	5.27438	-1.99557	-1.33363	H	8.05964	-5.90047	-2.70283
H	5.70663	2.74412	0.36805	H	6.31153	-0.43410	-5.45788
H	3.08428	-6.08865	0.69359	H	4.52075	-0.91905	-5.08722

***HCOO**

C	0.49430	2.47118	1.33527	Cu	0.45032	0.45320	-2.69306
C	1.86622	2.13810	1.49529	O	0.92701	-0.88654	-4.05192
C	2.87856	3.11024	1.69922	C	1.10060	-2.06084	-3.58556
C	2.46969	4.47486	1.76337	O	0.99415	-2.43539	-2.37751
C	1.14526	4.82659	1.60472	C	3.81847	-1.06975	1.47666
C	0.11381	3.85620	1.36726	C	2.83393	-2.05453	1.27813
C	2.13650	0.74178	1.37790	C	1.45414	-1.68982	1.11958
C	3.49780	0.29859	1.52172	C	0.50074	-2.72185	0.89625
C	4.50796	1.29507	1.74799	C	0.84351	-4.09102	0.81945
C	4.21859	2.64088	1.82932	C	2.21679	-4.43030	1.01494
Cu	1.08956	1.29681	-0.51996	C	3.16445	-3.45316	1.23138
B	0.95634	-0.23017	1.14334	C	-0.20748	-5.01148	0.52411
Cu	0.47358	-1.18879	-0.87162	C	-1.49089	-4.56812	0.28831
B	-1.05277	-0.70971	0.74850	C	-1.84625	-3.17525	0.33349
Cu	-1.23934	0.74950	-0.98643	C	-0.81580	-2.23192	0.66515

C	-3.15705	-2.74304	0.06568	H	-5.59283	-1.72049	-0.40502
C	-3.50863	-1.38266	0.10530	H	-5.59806	3.13095	0.12708
C	-4.85570	-0.95379	-0.15313	H	-3.82855	4.75805	0.68303
C	-5.23817	0.36958	-0.09573	H	-6.27201	0.65186	-0.30775
C	-4.29802	1.38852	0.23856	H	-2.27824	-5.28702	0.04779
C	-2.96850	0.97958	0.51598	H	0.02238	-6.07827	0.47095
C	-2.53421	-0.37764	0.43858	H	2.51370	-5.48115	0.97604
C	-1.93055	1.89233	0.84341	H	4.21181	-3.73522	1.36648
C	-2.23335	3.29591	0.88828	H	4.86082	-1.37662	1.59832
C	-3.59018	3.69244	0.63517	H	5.54073	0.95459	1.85871
C	-4.58052	2.78430	0.32286	H	5.01930	3.36511	1.99617
C	-1.22604	4.23934	1.16548	H	3.22500	5.24593	1.93263
B	-0.51390	1.33116	1.08814	H	0.85468	5.87930	1.64728
H	-1.48662	5.30058	1.19772	H	1.37557	-2.84198	-4.32123
H	-3.92201	-3.48313	-0.18416				

***HCOOH**

C	-1.69483	-4.94828	-0.68737	C	-5.63968	-7.81109	-0.00172
C	-2.45672	-3.74164	-0.66847	C	-6.17602	-9.13346	0.19942
C	-1.87874	-2.45924	-0.74400	C	-7.58459	-9.25046	0.47021
C	-0.45722	-2.38854	-0.89467	C	-8.40812	-8.15497	0.59929
C	0.30838	-3.53142	-0.92549	C	-5.34302	-10.26404	0.14207
C	-0.26438	-4.84737	-0.80768	C	-3.95774	-10.14693	-0.06390
C	-2.75792	-1.33644	-0.61952	C	-3.34941	-8.85772	-0.27417
C	-4.10414	-1.51395	-0.39674	C	-1.92893	-8.79994	-0.40166
C	-4.70163	-2.81899	-0.27702	C	-1.09481	-9.93842	-0.35978
C	-3.84678	-3.96589	-0.43878	C	-1.73215	-11.20916	-0.20312
C	-6.07029	-2.97396	-0.00122	C	-3.09828	-11.30165	-0.06345
C	-6.65558	-4.24259	0.15249	C	-1.42939	-7.46929	-0.52734
C	-8.05742	-4.39158	0.44055	C	-0.00711	-7.28470	-0.65382
C	-8.65177	-5.62386	0.59432	C	0.82671	-8.45735	-0.64276
C	-7.89250	-6.82807	0.46144	C	0.31253	-9.72601	-0.49573
C	-6.52125	-6.69896	0.15069	Cu	-2.60386	-7.51174	1.39399
C	-5.86688	-5.43827	0.00652	B	-4.15219	-7.54057	-0.31059

Cu	-4.78950	-6.52160	1.65903	H	1.90568	-8.31548	-0.74757
B	-4.35330	-5.42424	-0.31510	H	-1.11516	-12.11135	-0.18576
Cu	-2.80960	-5.00763	1.26645	H	-7.99684	-10.25595	0.59169
B	-2.43857	-6.29634	-0.53583	H	-9.47030	-8.29008	0.81897
C	0.54074	-5.99879	-0.80295	H	-9.71863	-5.69549	0.82094
O	-2.02723	-3.46096	2.61130	H	-8.65427	-3.48186	0.54571
C	-1.89680	-3.61319	3.93624	H	-6.69442	-2.08273	0.10908
O	-2.25614	-4.64565	4.49292	H	-4.75689	-0.64363	-0.28884
Cu	-3.10144	-6.18949	3.38144	H	-2.34079	-0.32831	-0.68644
H	1.62438	-5.89051	-0.90446	H	0.01778	-1.40694	-0.96925
H	-5.77923	-11.25627	0.28799	H	1.39421	-3.45609	-1.02756
H	-3.56482	-12.28160	0.06880	H	-1.45301	-2.75717	4.46826
H	0.98062	-10.59099	-0.48211	H	-1.70279	-2.58711	2.29622

***H_2COOH**

C	-1.65171	-4.96555	-0.70135	C	-7.55293	-9.23195	0.56628
C	-2.40491	-3.75816	-0.65384	C	-8.37007	-8.12750	0.69059
C	-1.82041	-2.47543	-0.76216	C	-5.32070	-10.25971	0.20853
C	-0.40897	-2.41772	-0.97377	C	-3.93595	-10.15519	-0.02292
C	0.34630	-3.56879	-1.03158	C	-3.31945	-8.87297	-0.22001
C	-0.22983	-4.87810	-0.88424	C	-1.91430	-8.81675	-0.42202
C	-2.68773	-1.34942	-0.61624	C	-1.08869	-9.96977	-0.44148
C	-4.03040	-1.51866	-0.35611	C	-1.72948	-11.23279	-0.27263
C	-4.63270	-2.81753	-0.21748	C	-3.09198	-11.31625	-0.07400
C	-3.78787	-3.96765	-0.38507	C	-1.40689	-7.48988	-0.55301
C	-5.99982	-2.96462	0.07577	C	0.00869	-7.31906	-0.74692
C	-6.58814	-4.23071	0.23769	C	0.82738	-8.49947	-0.78923
C	-7.98931	-4.37183	0.52556	C	0.30943	-9.76849	-0.63891
C	-8.59700	-5.59991	0.67716	Cu	-2.49879	-7.51270	1.41141
C	-7.84859	-6.80742	0.54706	B	-4.11114	-7.54751	-0.19304
C	-6.46916	-6.68631	0.24267	Cu	-4.70299	-6.50964	1.72757
C	-5.80663	-5.43051	0.09513	B	-4.29585	-5.41757	-0.23326
C	-5.60453	-7.80590	0.10836	Cu	-2.68802	-4.96876	1.30940
C	-6.14719	-9.12320	0.29372	B	-2.39662	-6.30273	-0.50705

C	0.56426	-6.03867	-0.91472	H	-9.43306	-8.25546	0.90867
O	-1.85192	-3.58242	2.60110	H	-9.66471	-5.66104	0.90053
C	-2.35444	-3.58329	4.02631	H	-8.58059	-3.45824	0.62701
O	-2.30046	-4.84076	4.54431	H	-6.61895	-2.07084	0.18973
Cu	-2.99154	-6.19409	3.40082	H	-4.67430	-0.64340	-0.23777
H	1.64319	-5.94145	-1.06293	H	-2.26831	-0.34397	-0.70107
H	-5.76361	-11.24994	0.34521	H	0.07152	-1.44148	-1.07433
H	-3.56160	-12.29423	0.05857	H	1.42677	-3.50087	-1.18218
H	0.96979	-10.63827	-0.67112	H	-1.67181	-2.89595	4.56363
H	1.90119	-8.36689	-0.94509	H	-3.37500	-3.15545	3.97985
H	-1.12212	-12.14078	-0.29803	H	-1.97816	-2.67648	2.24877
H	-7.97376	-10.23355	0.68659				

***CH_2O + *H_2O**

C	-1.66928	-4.93483	-0.68749	C	1.90104	3.63423	-1.34534
C	-2.42808	-3.72463	-0.62905	C	2.58469	2.41998	-1.52513
C	-1.73279	-2.51313	-0.83236	C	4.00700	2.38843	-1.75262
C	-0.32254	-2.44591	-1.05184	C	4.70282	1.21098	-1.89519
C	0.41683	-3.68216	-1.09604	C	4.03148	-0.05149	-1.83140
C	-0.31170	-4.90944	-0.91599	C	2.63502	-0.03377	-1.65585
C	-3.83656	-3.63878	-0.39631	C	1.88303	1.16438	-1.48602
C	-4.47100	-2.41842	-0.33972	C	4.67222	-1.33166	-1.86601
C	-3.76876	-1.17279	-0.50435	C	3.94523	-2.48978	-1.71244
C	-2.35848	-1.23145	-0.79375	C	2.51884	-2.48309	-1.51049
C	-4.42789	0.06341	-0.38963	C	1.84924	-1.21046	-1.49070
C	-3.73449	1.28067	-0.50269	Cu	1.47196	-0.00077	0.46603
C	-2.32161	1.30094	-0.78862	Cu	0.23939	-0.01547	2.66165
C	-1.66157	2.56534	-0.82605	O	0.99438	-0.15961	4.49783
C	-2.32417	3.79574	-0.62561	C	2.13539	0.13183	4.86413
C	-3.73504	3.74792	-0.39594	O	3.36331	-0.21677	1.37569
C	-4.40247	2.54530	-0.34037	B	0.33268	-1.05682	-1.24798
C	-0.25483	2.46039	-1.04758	Cu	-0.70046	-1.20018	0.76168
C	0.51767	3.67504	-1.09981	Cu	-0.67574	1.21632	0.77176
C	-0.17695	4.92208	-0.92100	B	0.36276	1.05293	-1.23790
C	-1.53273	4.98447	-0.68835	C	1.80239	-3.67867	-1.32943

B	-1.48626	0.02293	-1.01117	H	0.41029	5.84303	-0.97035
H	2.33990	-4.63072	-1.36344	H	2.46198	4.57217	-1.39219
H	-5.50168	0.07873	-0.18289	H	4.53831	3.34306	-1.79547
H	-5.54657	-2.37383	-0.14834	H	5.78568	1.22716	-2.04385
H	-2.18493	-5.88834	-0.54680	H	5.75599	-1.37764	-2.00084
H	0.25102	-5.84579	-0.95952	H	4.45384	-3.45746	-1.73061
H	-4.40615	-4.56094	-0.25508	H	2.42326	-0.02482	5.92032
H	-5.47940	2.53083	-0.15204	H	2.88241	0.54819	4.16249
H	-4.28044	4.68507	-0.25756	H	3.92203	-0.76070	0.78372
H	-2.02227	5.95204	-0.55026	H	3.30513	-0.72706	2.20596

***CH_2O**

C	1.79339	-1.86442	-0.77818	C	10.78801	-3.93844	-2.03921
C	2.85488	-0.90793	-0.85106	C	9.70842	-4.83755	-2.01448
C	4.14648	-1.39787	-1.13382	C	8.35399	-4.36103	-1.90398
C	4.43960	-2.78261	-1.31587	C	7.30314	-5.32586	-1.84570
C	3.35827	-3.72672	-1.19940	C	7.52564	-6.71812	-1.89437
C	2.03940	-3.20785	-0.94723	C	8.87793	-7.16155	-2.03911
C	5.30419	-0.56582	-1.20888	C	9.91561	-6.25936	-2.09708
C	5.14049	0.84619	-0.97994	C	6.37842	-7.56742	-1.79872
C	3.81035	1.33608	-0.72922	C	5.11893	-7.03788	-1.63310
C	2.71651	0.50355	-0.66443	C	4.88106	-5.62114	-1.54162
C	6.24640	1.71262	-1.00745	C	6.01285	-4.73989	-1.67289
C	7.55197	1.23748	-1.21759	Cu	7.28009	-3.99653	0.04404
C	8.68418	2.12657	-1.20812	Cu	7.29722	-2.78264	2.18309
C	9.97469	1.68022	-1.37967	O	7.57142	-2.67742	4.15667
C	10.25101	0.29140	-1.58207	C	7.29029	-1.75311	4.92223
C	9.14828	-0.58655	-1.62943	B	5.89925	-3.19934	-1.60645
C	7.79707	-0.16117	-1.45456	Cu	5.76840	-2.11306	0.37821
C	11.55163	-0.28220	-1.74388	Cu	8.17395	-1.72062	0.14325
C	11.71007	-1.63959	-1.90540	B	7.98954	-2.86123	-1.81136
C	10.59699	-2.55231	-1.91675	C	3.59026	-5.10618	-1.33182
C	9.27284	-1.99850	-1.79630	B	6.67202	-1.22107	-1.50621

H	2.74794	-5.79842	-1.24745	H	12.71320	-2.06056	-2.01407
H	6.08923	2.78203	-0.84065	H	11.80523	-4.32966	-2.13007
H	3.68514	2.41112	-0.57511	H	10.94388	-6.61804	-2.19260
H	0.77805	-1.51362	-0.57680	H	9.07882	-8.23450	-2.09264
H	1.21651	-3.92413	-0.87773	H	6.51698	-8.65033	-1.85000
H	1.72455	0.91523	-0.46150	H	4.25589	-7.70393	-1.55164
H	8.49383	3.19059	-1.04428	H	7.50922	-1.85525	6.00131
H	10.80852	2.38631	-1.35442	H	6.82297	-0.81947	4.55764
H	12.42456	0.37534	-1.72786				

***CH_3O + *H_2O**

C	-0.76594	-5.11592	-0.63167	C	1.22042	3.94725	-1.30649
C	-1.73445	-4.06885	-0.64824	C	2.12819	2.87750	-1.40659
C	-1.25542	-2.74624	-0.82750	C	1.66867	1.51795	-1.36945
C	0.12939	-2.42297	-0.95241	C	2.63194	0.47336	-1.45844
C	1.08149	-3.50294	-0.93637	C	4.02045	0.70892	-1.57645
C	0.57709	-4.83894	-0.77433	C	4.44964	2.06989	-1.63370
C	-2.10996	-1.61147	-0.84674	C	3.54126	3.10297	-1.55026
C	-3.52103	-1.80561	-0.66539	C	4.87713	-0.43425	-1.58778
C	-3.99494	-3.15317	-0.51603	C	4.36219	-1.70486	-1.44876
C	-3.14356	-4.23855	-0.50605	C	2.95467	-1.95422	-1.28796
C	-4.40079	-0.70672	-0.63598	C	2.06860	-0.82496	-1.31174
C	-3.93662	0.61806	-0.73958	Cu	1.41141	0.35016	0.55001
C	-4.83355	1.73736	-0.66537	Cu	0.06778	0.16510	2.65405
C	-4.39303	3.04318	-0.72667	O	1.39861	0.44990	3.98267
C	-3.00656	3.34491	-0.87270	C	1.75160	-0.59721	4.88315
C	-2.11233	2.24859	-0.97972	B	0.54047	-0.94142	-1.13146
C	-2.53869	0.89481	-0.92209	Cu	-0.57233	-1.23948	0.80170
C	-2.44166	4.65347	-0.92724	Cu	-1.01738	1.16113	0.73663
C	-1.08153	4.83179	-1.06628	B	0.18459	1.12983	-1.19547
C	-0.15969	3.73241	-1.15213	C	2.45408	-3.25688	-1.10955
C	-0.69853	2.39856	-1.10043	B	-1.47173	-0.21661	-1.01664

O	2.93641	0.58933	1.91388	H	1.59847	4.97260	-1.34054
H	3.15093	-4.09925	-1.10023	H	3.89118	4.13792	-1.58220
H	-5.47108	-0.88528	-0.50251	H	5.51674	2.28393	-1.73083
H	-5.07060	-3.30547	-0.39672	H	5.95485	-0.28731	-1.69256
H	-1.10318	-6.14756	-0.50618	H	5.03533	-2.56609	-1.44612
H	1.30203	-5.65688	-0.76630	H	2.58484	-0.26473	5.53184
H	-3.54401	-5.24763	-0.38245	H	2.08064	-1.51194	4.35448
H	-5.89978	1.53032	-0.54367	H	3.33662	1.47505	1.82564
H	-5.10793	3.86651	-0.65665	H	0.90468	-0.87148	5.53833
H	-3.10440	5.51931	-0.85771	H	2.43625	0.57950	2.83189
H	-0.67011	5.84358	-1.10980				

***CH_3OH + *H_2O**

C	2.00176	-0.67679	-1.59741	C	-4.38978	-0.88924	-0.42398
C	2.50462	0.65340	-1.69906	C	-3.47312	-1.93992	-0.60168
C	3.86715	0.95469	-1.88411	C	-2.08798	-1.66798	-0.89107
C	4.76897	-0.14752	-2.03052	C	-1.19040	-2.77377	-0.98344
C	4.31871	-1.44484	-1.94496	C	-1.59550	-4.11865	-0.83293
C	2.93472	-1.76616	-1.70641	C	-2.98561	-4.36053	-0.59976
C	4.24394	2.33506	-1.85343	C	-3.87744	-3.31712	-0.49327
C	3.30984	3.31744	-1.61888	C	0.16612	-2.38146	-1.19593
C	1.91819	3.02005	-1.39477	C	1.16099	-3.41720	-1.30923
C	1.50916	1.64290	-1.45036	C	0.72884	-4.78324	-1.17607
C	0.98946	4.03837	-1.11934	C	-0.58471	-5.12347	-0.94203
C	-0.36455	3.75636	-0.87224	Cu	-0.48192	-1.35885	0.68907
C	-1.31179	4.80545	-0.60281	B	-1.52031	-0.24131	-1.04111
C	-2.64549	4.55363	-0.37056	Cu	-0.96488	0.99970	0.82979
C	-3.15822	3.21969	-0.39937	B	0.05614	1.17800	-1.19551
C	-2.24540	2.18100	-0.68599	Cu	1.41324	0.26664	0.39161
C	-0.85107	2.40057	-0.90454	O	3.20568	0.51355	1.45383
C	-2.61317	0.80474	-0.74608	B	0.49229	-0.87055	-1.31998
C	-3.98269	0.45552	-0.46493	C	2.50469	-3.09725	-1.56907
C	-4.91016	1.52858	-0.21931	Cu	0.29734	-0.06654	2.59876
C	-4.52264	2.84887	-0.18350	O	1.85135	0.01375	3.94346

C	2.41702	-1.24183	4.41757	H	1.33150	5.07694	-1.08931
H	3.23658	-3.90528	-1.65756	H	3.61952	4.36542	-1.58386
H	-5.43720	-1.12312	-0.21400	H	5.29409	2.59998	-2.00205
H	-4.93381	-3.52263	-0.30009	H	5.83105	0.05531	-2.19133
H	-0.86981	-6.17367	-0.83899	H	5.02525	-2.27386	-2.03988
H	1.48667	-5.56669	-1.26121	H	3.38842	-1.04625	4.89248
H	-3.33293	-5.39207	-0.49843	H	2.55161	-1.87694	3.53370
H	-5.95559	1.26523	-0.03707	H	3.63926	1.35207	1.20210
H	-5.25820	3.63157	0.01994	H	1.73002	-1.72404	5.12693
H	-3.33176	5.37848	-0.16196	H	2.98241	0.59813	2.40990
H	-0.93970	5.83327	-0.57918	H	1.74640	0.61461	4.70585

***CH_3OH**

C	2.31659	-1.03648	-0.80978	B	-1.12412	-0.21684	-1.41604
C	2.94422	0.23211	-0.62386	Cu	-1.06285	0.95940	0.53111
C	4.30952	0.38206	-0.30489	Cu	-0.52774	-0.25620	2.60115
C	5.09244	-0.81052	-0.19695	Cu	1.16787	-0.00211	0.84974
C	4.51986	-2.05046	-0.36765	Cu	-0.75678	-1.45924	0.46707
C	3.12042	-2.22109	-0.65791	B	0.80800	-1.07289	-1.13826
C	4.79615	1.71495	-0.12227	C	0.30809	-2.53377	-1.21054
C	3.95088	2.79646	-0.22265	C	1.17787	-3.67059	-1.04675
C	2.54726	2.65729	-0.50859	C	0.59420	-4.98219	-1.15534
C	2.03672	1.32931	-0.73589	C	-0.75107	-5.17728	-1.36972
C	1.69656	3.77419	-0.56833	C	-1.64383	-4.06667	-1.49895
C	0.31976	3.64225	-0.81619	C	-1.08104	-2.77530	-1.42878
C	-0.55177	4.78777	-0.84364	C	-3.05729	-4.15472	-1.70059
C	-1.90718	4.68140	-1.05684	C	-3.83052	-3.02000	-1.79201
C	-2.51944	3.40582	-1.26752	C	-3.27537	-1.69590	-1.68781
C	-1.67288	2.27808	-1.27677	C	-1.85055	-1.57633	-1.51797
C	-0.26403	2.34803	-1.05668	C	2.54922	-3.49800	-0.79520
C	-3.91608	3.17889	-1.47786	C	-4.09142	-0.55390	-1.75466
C	-4.40792	1.90473	-1.64806	B	0.55477	1.03619	-1.07009
C	-3.56181	0.74042	-1.61893	H	-5.16911	-0.67731	-1.89425
C	-2.14644	0.94245	-1.44883	H	2.11450	4.77097	-0.40104

H	-0.10357	5.77085	-0.67636	H	-1.15540	-6.19067	-1.43456
H	-4.59369	4.03626	-1.49397	H	-3.51972	-5.14230	-1.77437
H	-5.47982	1.75025	-1.79805	H	-4.91044	-3.10858	-1.93720
H	-2.53536	5.57590	-1.06000	O	-0.90912	-0.22911	4.58414
H	4.34074	3.80655	-0.07053	C	-0.29733	0.81364	5.39717
H	5.85398	1.86507	0.10811	H	-0.77246	0.82427	6.38822
H	6.15757	-0.72342	0.03214	H	0.78446	0.64330	5.49345
H	5.13200	-2.95087	-0.27055	H	-0.48358	1.76409	4.88335
H	3.18484	-4.38108	-0.68590	H	-0.77188	-1.08368	5.03578
H	1.25808	-5.84439	-1.05036				

***H_2O + *OH + *CH_4**

C	-0.43727	-5.06617	-0.49250	C	0.99969	4.09774	-1.19001
C	-1.46454	-4.07745	-0.46653	C	1.96148	3.08201	-1.33621
C	-1.07273	-2.72992	-0.67554	C	3.35487	3.38717	-1.51688
C	0.28182	-2.32978	-0.88238	C	4.31599	2.40779	-1.64406
C	1.29278	-3.35236	-0.90938	C	3.96526	1.02448	-1.59518
C	0.87836	-4.71271	-0.70600	C	2.59554	0.71027	-1.43991
C	-2.85190	-4.32730	-0.24891	C	1.57863	1.69779	-1.30923
C	-3.76391	-3.29277	-0.21755	C	4.88429	-0.06749	-1.64811
C	-3.37625	-1.92051	-0.39082	C	4.44693	-1.36687	-1.51065
C	-1.98945	-1.64560	-0.64087	C	3.06137	-1.69699	-1.31082
C	-4.31548	-0.87360	-0.31810	C	2.11182	-0.62017	-1.29031
C	-3.93364	0.47583	-0.44242	Cu	1.46314	0.50672	0.60069
C	-2.56351	0.83213	-0.68881	Cu	0.23874	0.25135	2.76312
C	-2.21745	2.20828	-0.75658	O	1.56562	0.59924	4.07976
C	-3.16642	3.25179	-0.60056	C	2.04552	-2.59283	2.37091
C	-4.52558	2.87119	-0.39724	B	0.60077	-0.82805	-1.06010
C	-4.88844	1.54204	-0.32473	Cu	-0.39784	-1.20889	0.93945
C	-0.82107	2.44155	-0.93784	Cu	-0.98261	1.16727	0.89700
C	-0.36055	3.80403	-0.99139	B	0.12630	1.22762	-1.08389
C	-1.33856	4.84817	-0.85575	C	2.64248	-3.02693	-1.12657
C	-2.67985	4.59062	-0.66546	B	-1.43800	-0.21551	-0.83217

O	3.02109	0.88533	1.90991	H	3.64706	4.44011	-1.54419
H	3.38729	-3.82702	-1.13850	H	5.36617	2.68318	-1.76829
H	-5.36599	-1.11304	-0.13309	H	5.94829	0.14184	-1.78268
H	-4.82139	-3.50605	-0.04219	H	5.16744	-2.18838	-1.53785
H	-0.70563	-6.11365	-0.33611	H	2.39969	-1.94121	3.18114
H	1.65054	-5.48612	-0.72284	H	2.23657	-2.11605	1.39919
H	-3.18604	-5.35693	-0.10004	H	3.33516	1.80082	1.78090
H	-5.93487	1.27465	-0.15756	H	0.96482	-2.77379	2.50278
H	-5.28291	3.65167	-0.29110	H	2.56304	0.86929	2.83823
H	-3.38725	5.41653	-0.56012	H	1.39587	1.45555	4.51277
H	-0.98705	5.88214	-0.90313	H	2.56678	-3.56122	2.40741
H	1.31953	5.14276	-1.22228				

***H_2O + *OH**

C	-0.65768	-5.16549	-0.75220	C	-3.02083	-11.14390	0.27430
C	-1.66189	-4.16047	-0.69012	C	-1.70672	-10.73527	-0.02324
C	-1.38438	-2.78102	-0.82684	C	-0.62966	-11.67986	-0.12365
C	-0.02963	-2.40910	-1.08432	C	0.67156	-11.29394	-0.37188
C	0.96398	-3.36128	-1.16133	C	1.01024	-9.91965	-0.54564
C	0.70109	-4.76405	-0.98603	C	-0.04941	-8.97750	-0.48266
C	-2.95339	-4.67277	-0.37355	C	-1.39817	-9.34825	-0.23545
C	-4.02608	-3.73810	-0.17596	C	0.14577	-7.57066	-0.61289
C	-3.73601	-2.33935	-0.34342	C	1.48049	-7.08975	-0.85721
C	-2.47613	-1.87648	-0.65630	C	2.53819	-8.05876	-0.93770
C	-5.31240	-4.18410	0.17786	C	2.32088	-9.41191	-0.78495
C	-5.59237	-5.54668	0.37492	Cu	-0.82435	-7.82664	1.37905
C	-4.56776	-6.54411	0.20432	B	-2.46252	-8.23595	-0.15722
C	-4.92745	-7.91383	0.38653	Cu	-3.17504	-7.30117	1.78084
C	-6.23051	-8.33595	0.75241	B	-3.11414	-6.19628	-0.19482
C	-7.22294	-7.32380	0.91282	Cu	-1.57754	-5.37036	1.30936
C	-6.91233	-5.99375	0.72693	O	-1.21399	-3.82898	2.64448
C	-6.43875	-9.73708	0.91998	B	-1.08296	-6.63176	-0.51991
C	-5.40429	-10.63436	0.75361	C	1.73209	-5.71916	-1.04110
C	-4.07216	-10.21796	0.41368	Cu	-1.49550	-6.69911	3.41513
C	-3.84413	-8.81535	0.21076	O	-1.12212	-5.39976	4.74811

H	2.75723	-5.38760	-1.22661	H	-7.68880	-5.23418	0.84953
H	-3.22543	-12.20748	0.42334	H	-6.11225	-3.45121	0.31411
H	-0.86382	-12.73838	0.01530	H	-4.55510	-1.62938	-0.20242
H	3.15667	-10.11273	-0.84774	H	-2.29614	-0.80380	-0.76116
H	3.55011	-7.69131	-1.12674	H	0.21399	-1.35084	-1.20541
H	1.46334	-12.04452	-0.43113	H	1.99661	-3.05563	-1.34814
H	-5.58611	-11.70336	0.89031	H	-1.98231	-3.22665	2.64203
H	-7.43617	-10.09403	1.18759	H	-1.23048	-4.30584	3.56182
H	-8.23949	-7.61658	1.18587	H	-1.87697	-5.30649	5.35684

***2H_2O**

C	-0.69747	-5.15745	-0.82170	C	-3.02077	-11.12857	0.28510
C	-1.70426	-4.14946	-0.76876	C	-1.70843	-10.71373	-0.00004
C	-1.42995	-2.77450	-0.89459	C	-0.61598	-11.65012	-0.04447
C	-0.07210	-2.39490	-1.14214	C	0.68649	-11.25749	-0.25602
C	0.92458	-3.34069	-1.20864	C	1.01738	-9.88013	-0.45235
C	0.66524	-4.74668	-1.03209	C	-0.04972	-8.95453	-0.45583
C	-2.98896	-4.66554	-0.42761	C	-1.41162	-9.32604	-0.25042
C	-4.06175	-3.73173	-0.21194	C	0.13060	-7.54805	-0.62357
C	-3.77351	-2.32923	-0.36860	C	1.46867	-7.05788	-0.83943
C	-2.51907	-1.86733	-0.69509	C	2.54167	-8.01646	-0.85838
C	-5.34373	-4.17904	0.15237	C	2.33301	-9.36377	-0.66705
C	-5.62339	-5.54194	0.34625	Cu	-0.87688	-7.79210	1.35438
C	-4.59763	-6.53796	0.16255	B	-2.48645	-8.21969	-0.24372
C	-4.95073	-7.90878	0.35150	Cu	-3.20476	-7.27717	1.73523
C	-6.24132	-8.33130	0.73917	B	-3.14431	-6.19313	-0.24948
C	-7.23872	-7.32134	0.90855	Cu	-1.61611	-5.39920	1.26238
C	-6.93978	-5.99163	0.71405	O	-1.10183	-3.65814	2.31988
C	-6.44379	-9.73602	0.91343	B	-1.11690	-6.62770	-0.58645
C	-5.40811	-10.62653	0.74255	C	1.70733	-5.68927	-1.04765
C	-4.07675	-10.20684	0.39014	Cu	-1.54671	-6.67328	3.40675
C	-3.85736	-8.80348	0.15259	O	-1.18687	-5.56910	5.08011

H	2.73299	-5.34738	-1.21351	H	-6.14183	-3.44573	0.29994
H	-3.21895	-12.18991	0.45963	H	-4.58959	-1.62009	-0.20554
H	-0.84481	-12.70728	0.11574	H	-2.33601	-0.79349	-0.78727
H	3.17723	-10.05807	-0.68036	H	0.16765	-1.33443	-1.25581
H	3.55525	-7.64164	-1.02456	H	1.95923	-3.03142	-1.37974
H	1.48823	-12.00048	-0.26914	H	-1.69337	-2.93006	2.04192
H	-5.58128	-11.69573	0.89226	H	-1.27182	-3.77722	3.27556
H	-7.43726	-10.09581	1.19366	H	-1.86097	-5.66304	5.78159
H	-8.25007	-7.61993	1.19648	H	-0.33555	-5.75951	5.52090
H	-7.71686	-5.23413	0.84729				

***H_2O**

C	1.99910	-1.26850	-1.01808	C	-4.30604	0.26981	-1.13518
C	2.84801	-0.12310	-0.95032	C	-3.69014	-0.99306	-1.13693
C	4.24933	-0.19993	-0.81233	C	-2.25542	-1.11165	-1.16952
C	4.83240	-1.50595	-0.77489	C	-1.68796	-2.42166	-1.13875
C	4.04557	-2.63327	-0.83872	C	-2.45919	-3.60091	-1.08103
C	2.61101	-2.57013	-0.94023	C	-3.88196	-3.45317	-1.07923
C	4.96867	1.03373	-0.73055	C	-4.46414	-2.20623	-1.10866
C	4.30818	2.24091	-0.75760	C	-0.26093	-2.41438	-1.11288
C	2.87628	2.33522	-0.86543	C	0.42316	-3.67910	-1.02963
C	2.12883	1.10985	-0.98173	C	-0.37720	-4.87532	-1.01466
C	2.22227	3.57914	-0.86248	C	-1.75299	-4.84435	-1.03445
C	0.82291	3.67743	-0.93777	Cu	-0.91419	-1.15609	0.64480
C	0.15699	4.95316	-0.89899	B	-1.30421	0.10638	-1.20834
C	-1.21362	5.07279	-0.93376	Cu	-0.78869	1.28581	0.67485
C	-2.05057	3.91532	-1.01509	B	0.59049	1.06637	-1.12377
C	-1.41086	2.66051	-1.09153	Cu	1.26020	-0.05001	0.74410
C	0.00656	2.49725	-1.05686	Cu	-0.22209	0.00186	2.70102
C	-2.11589	1.42052	-1.14924	O	-0.27100	-0.00213	4.71598
C	-3.55515	1.45748	-1.12247	B	0.47337	-1.05481	-1.15068
C	-4.19359	2.74705	-1.08264	C	1.82603	-3.73520	-0.96703
C	-3.48095	3.92309	-1.02949	H	2.31797	-4.71049	-0.91766

H	-5.39775	0.33026	-1.12111	H	0.77961	5.84896	-0.82603
H	-5.55335	-2.11344	-1.09567	H	2.81670	4.49345	-0.77915
H	-2.32400	-5.77607	-1.00637	H	4.87438	3.17306	-0.68240
H	0.14438	-5.83494	-0.97160	H	6.05721	1.00498	-0.63818
H	-4.50623	-4.34975	-1.04525	H	5.91789	-1.59815	-0.68782
H	-5.28645	2.77330	-1.08174	H	4.50845	-3.62295	-0.80155
H	-4.00411	4.88179	-0.98759	H	-0.66718	-0.80875	5.10125
H	-1.67957	6.06043	-0.88895	H	-0.78249	0.73785	5.09915

b. Cu_4 cluster – C_2 pathway

***CO + *COOH + *H_2O**

C	4.23072	-3.24113	0.83577	C	-0.82180	-2.17857	1.34389
C	4.18464	-1.81694	0.83893	B	0.36084	-1.18023	1.27694
C	2.91041	-1.20887	1.00008	Cu	-1.18656	-0.81220	-0.41012
C	1.70104	-1.95124	1.12059	Cu	-0.24077	-0.50361	-2.51305
C	1.77627	-3.38791	1.07329	C	0.69701	-0.51538	-4.07509
C	3.07600	-3.98716	0.94726	O	1.44235	-0.52895	-4.94729
C	5.30475	-0.94875	0.68717	C	0.61477	-4.17754	1.15383
C	5.14282	0.42122	0.66749	B	-0.81165	0.54905	1.41590
C	3.85655	1.04936	0.79026	Cu	0.03526	1.43515	-0.60353
C	2.71216	0.19694	0.96555	O	-1.14990	2.50140	-1.89892
C	3.71589	2.44943	0.75416	B	1.26673	0.74711	1.09650
C	2.46093	3.07437	0.88499	Cu	1.37635	-0.62799	-0.65323
C	1.27067	2.29401	1.07298	O	-2.87310	0.47535	-2.41987
C	0.02924	2.96025	1.23721	C	-2.35845	-0.61029	-2.08131
C	-0.09979	4.36756	1.15726	O	-3.02820	-1.76924	-2.36245
C	1.09542	5.12586	0.97488	H	0.70955	-5.26611	1.11502
C	2.32034	4.50385	0.85243	H	4.60731	3.06813	0.61919
C	-1.07424	2.07084	1.39609	H	6.01604	1.06765	0.54613
C	-2.39051	2.64503	1.43978	H	5.19769	-3.73891	0.72976
C	-2.51002	4.07729	1.36568	H	3.13268	-5.07861	0.93069
C	-1.41843	4.90755	1.23442	H	6.30103	-1.38426	0.57811
C	-3.53524	1.83181	1.52312	H	3.22388	5.10343	0.71526
C	-3.44075	0.43290	1.52798	H	1.02625	6.21533	0.92431
C	-4.61271	-0.39760	1.58811	H	-1.55385	5.99012	1.17354
C	-4.55244	-1.77466	1.57403	H	-3.51577	4.50342	1.40677
C	-3.29853	-2.45048	1.49678	H	-4.52222	2.30045	1.55990
C	-2.13326	-1.64582	1.45994	H	-5.58422	0.10051	1.63931
C	-2.15417	-0.21630	1.47850	H	-5.47153	-2.36457	1.61285
C	-3.11291	-3.86397	1.44421	H	-3.99043	-4.51415	1.48182
C	-1.85148	-4.41120	1.33591	H	-1.73254	-5.49688	1.29190
C	-0.66406	-3.60430	1.26854	H	-1.57628	3.21109	-1.37694

H	-1.88592	1.84888	-2.11056	H	-3.88434	-1.53577	-2.79843

***2CO + *2H_2O**

C	1.26400	-2.13614	1.24531	C	4.95975	1.49561	1.02537
C	0.09313	-2.94333	1.26805	Cu	1.26668	0.74776	-0.54587
C	0.12272	-4.35275	1.20944	B	-0.00184	1.20409	1.28251
C	1.40769	-4.98146	1.16455	Cu	-1.25509	0.68360	-0.60852
C	2.56094	-4.23201	1.14775	O	-2.79698	1.52471	-1.75822
C	2.54236	-2.79156	1.16840	B	1.09729	-0.60110	1.26335
C	-1.11151	-2.18460	1.22431	Cu	-0.01156	-1.44498	-0.64173
C	-2.36311	-2.89385	1.15862	C	-0.95344	-0.55104	-3.70196
C	-2.31819	-4.33164	1.11934	O	0.06601	-3.17495	-1.82278
C	-1.13383	-5.03314	1.14023	C	3.73311	-2.04647	1.11146
C	-3.58470	-2.19966	1.13681	B	-1.01445	-0.64156	1.23762
C	-3.63597	-0.79613	1.18558	Cu	0.31072	0.18946	-2.62994
C	-2.42894	-0.01647	1.25605	C	1.92160	1.13010	-2.65431
C	-2.54372	1.40133	1.32201	O	2.92917	1.71122	-2.71334
C	-3.77993	2.08093	1.28247	O	-1.82813	-1.06419	-4.24525
C	-4.96481	1.28293	1.21375	H	4.68951	-2.57439	1.05990
C	-4.89067	-0.09125	1.17076	H	-0.09111	5.30705	1.12943
C	-3.74195	3.51119	1.25161	H	2.35759	5.38064	1.04229
C	-2.54364	4.18563	1.22719	H	5.90965	2.03260	0.96242
C	-1.27510	3.50243	1.22740	H	5.88643	-0.43546	0.98925
C	-1.28518	2.06493	1.28917	H	4.55718	4.26226	0.98282
C	-0.06476	4.21434	1.16754	H	-2.53411	5.27816	1.19039
C	1.17753	3.55884	1.14326	H	-4.68437	4.06499	1.22949
C	2.41385	4.28935	1.07721	H	-5.93736	1.78103	1.18448
C	3.64283	3.66641	1.04470	H	-5.80780	-0.68394	1.11421
C	3.74579	2.24388	1.08065	H	-4.51878	-2.76612	1.08175
C	2.53927	1.51176	1.17335	H	-3.26796	-4.87036	1.06353
C	1.24869	2.12025	1.20424	H	-1.14142	-6.12539	1.09510
C	2.48441	0.08601	1.18405	H	1.46092	-6.07277	1.12832
C	3.72629	-0.64210	1.10462	H	3.53366	-4.72873	1.10014
C	4.94486	0.11771	1.03933	H	-3.54583	1.71984	-1.15590

H	-3.15612	0.89231	-2.40972	H	-0.09750	-3.95339	-1.24989
H	-0.64550	-3.19994	-2.49076				

***OCCOH + *2H_2O**

C	4.21352	2.45700	1.50369	C	2.76931	-2.24871	1.43229
C	2.86734	2.92371	1.42253	C	1.37769	-1.88656	1.39481
C	1.84640	1.94508	1.38095	B	0.88287	-0.42450	1.36591
C	2.09447	0.53863	1.40950	Cu	0.19047	-1.52578	-0.61546
C	3.46600	0.10286	1.45827	Cu	0.23384	0.09661	-2.51534
C	4.49448	1.10806	1.51216	C	3.77644	-1.26745	1.46544
C	0.46506	2.25886	1.23553	B	-1.13243	-0.93844	1.03501
C	0.08872	3.64640	1.14940	Cu	-1.54600	0.28806	-0.80908
C	1.13299	4.63070	1.23003	O	-2.95678	0.99575	-2.16671
C	2.46304	4.29039	1.35887	B	-0.54666	1.08234	1.17712
C	-1.26047	4.00968	1.00652	Cu	0.98962	1.01916	-0.47962
C	-2.28124	3.04364	0.93565	O	1.51356	-2.59571	-1.82236
C	-3.65418	3.43136	0.75873	H	4.82388	-1.57999	1.50104
C	-4.68063	2.51344	0.67440	H	-1.52497	5.06848	0.93705
C	-4.41879	1.11448	0.76332	H	0.84453	5.68383	1.17772
C	-3.06665	0.71853	0.94787	H	5.02613	3.18677	1.54274
C	-1.98433	1.63928	1.03205	H	5.53256	0.76876	1.56183
C	-5.39067	0.08134	0.62669	H	3.22673	5.07112	1.40132
C	-5.02082	-1.24740	0.65089	H	-3.87492	4.49921	0.68071
C	-3.65270	-1.66123	0.79367	H	-5.70901	2.85301	0.52696
C	-2.65473	-0.63802	0.93714	H	-6.43945	0.35700	0.49040
C	-3.29564	-3.02342	0.79713	H	-5.78171	-2.02499	0.54427
C	-1.95899	-3.43998	0.94460	H	-4.07920	-3.77839	0.68761
C	-0.90286	-2.47737	1.08935	H	-2.40520	-5.56708	0.86791
C	0.42204	-2.93984	1.28644	H	-0.06364	-6.32113	1.11157
C	0.76485	-4.31470	1.26211	H	2.45380	-5.69072	1.32251
C	-0.29823	-5.25367	1.11659	H	4.16410	-3.91706	1.45197
C	-1.60343	-4.83145	0.97377	H	-2.55450	1.58208	-2.83599
C	2.15198	-4.64028	1.34006	H	-3.59641	1.56368	-1.68788
C	3.10514	-3.64780	1.41277	H	1.95949	-3.26019	-1.25798

H	2.21250	-1.90488	-1.99876	O	3.11635	-0.34380	-2.00770
C	2.13622	0.68647	-2.14817	O	2.34479	2.71694	-3.60800
C	2.32618	1.73249	-2.94353	H	3.35677	-0.37799	-1.05655

***CCO + *3H_2O**

C	2.31960	-0.04875	-1.16434	C	2.15135	-2.91819	-1.31190
C	2.49094	1.35397	-1.10036	C	2.04385	-4.35609	-1.37716
C	3.74483	1.98814	-1.05968	C	0.83444	-5.00558	-1.36749
C	4.90182	1.15086	-1.05836	Cu	0.16626	-1.47644	0.72178
C	4.77717	-0.22290	-1.13941	C	0.14251	0.12462	2.10484
C	3.49222	-0.87218	-1.20873	O	-0.15352	-3.31754	1.76740
C	3.76698	3.42467	-1.06832	B	0.88624	-0.61666	-1.20240
C	2.60527	4.15242	-1.14673	Cu	0.52256	1.56270	0.80628
C	1.30427	3.52968	-1.19182	O	3.96993	-0.46008	1.84314
C	1.25204	2.07740	-1.11700	C	3.39432	-2.27738	-1.29099
C	0.13078	4.28184	-1.30692	B	-1.18644	-0.48980	-1.01636
C	-1.13989	3.66345	-1.29785	Cu	-1.64005	0.22005	1.02814
C	-2.34765	4.44401	-1.27710	O	-3.25834	0.87442	2.19619
C	-3.59041	3.86621	-1.13529	B	-0.05966	1.27267	-1.24155
C	-3.72538	2.44936	-1.00387	Cu	2.03643	-0.16736	1.83754
C	-2.55450	1.67723	-1.07080	C	-0.30392	0.14390	3.34084
C	-1.26292	2.23472	-1.24314	O	-0.74271	0.15233	4.44671
C	-2.54347	0.25268	-0.91340	H	4.30932	-2.87574	-1.32513
C	-3.81947	-0.43113	-0.81819	H	-4.86735	-2.31336	-0.73992
C	-5.00543	0.38426	-0.70959	H	-3.80374	-4.51934	-0.92790
C	-4.96505	1.75591	-0.78739	H	0.79715	-6.09782	-1.39790
C	-3.89223	-1.82775	-0.83596	H	2.97140	-4.93342	-1.42218
C	-2.73654	-2.62392	-0.99098	H	-1.79820	-5.94395	-1.18451
C	-1.44307	-2.01959	-1.11308	H	-5.96257	-0.12550	-0.57180
C	-0.31693	-2.86950	-1.26949	H	-5.88672	2.33726	-0.70005
C	-0.39905	-4.27322	-1.29421	H	-4.48710	4.49098	-1.10534
C	-1.70052	-4.85525	-1.17378	H	-2.25652	5.53108	-1.35292
C	-2.81672	-4.05992	-1.02814	H	0.19545	5.37264	-1.35209
C	0.92399	-2.15424	-1.26318	H	2.64762	5.24437	-1.18230

H	4.73300	3.93543	-1.03387	H	4.45321	0.05536	2.51800
H	5.89292	1.60937	-1.01193	H	4.39020	-0.22436	0.97924
H	5.67226	-0.85069	-1.16078	H	-0.79531	-3.17549	2.48899
H	-3.97015	1.20344	1.60862	H	-0.60607	-3.92415	1.14475
H	-3.01439	1.63882	2.75215				

***CHCO + *3H_2O**

C	1.49504	-4.76694	-1.24211	C	0.85029	2.28806	-0.83979
C	0.20711	-4.23441	-0.93161	C	4.54052	1.96034	-1.47964
C	0.07989	-2.82505	-0.89208	C	4.62000	0.59287	-1.63195
C	1.16066	-1.94137	-1.15448	C	3.46938	-0.26474	-1.51518
C	2.44861	-2.50077	-1.47443	C	2.19722	0.35944	-1.21211
C	2.56334	-3.93496	-1.50943	B	0.87475	-0.42811	-1.10002
C	-0.97221	-5.00493	-0.70355	Cu	-0.44191	-1.14297	1.19063
C	-2.19504	-4.38691	-0.54432	Cu	2.10090	-0.43077	0.84417
C	-2.34675	-2.95681	-0.58131	O	3.18489	-2.14724	1.49888
C	-1.14973	-2.15814	-0.65345	C	3.56301	-1.66095	-1.68420
C	-3.62266	-2.36503	-0.65855	Cu	0.53098	1.37504	1.18427
C	-3.78725	-0.98423	-0.88559	B	-0.34489	1.27839	-0.82455
C	-2.64754	-0.11513	-0.96907	B	-1.16665	-0.58934	-0.75163
C	-2.87012	1.27457	-1.17195	Cu	-1.81083	0.85841	0.83409
C	-4.16685	1.85324	-1.28395	C	1.73320	0.45539	3.45705
C	-5.27593	0.96055	-1.24006	O	1.29310	-0.13826	4.39240
C	-5.08911	-0.39541	-1.04810	C	2.12302	1.03668	2.35124
C	-1.68225	2.04591	-1.07845	O	0.00091	-2.29792	2.80427
C	-1.78286	3.47591	-1.10711	O	-3.26617	1.52952	2.11031
C	-3.09233	4.04726	-1.26681	H	4.53256	-2.10655	-1.92354
C	-4.23538	3.27433	-1.35196	H	-4.50908	-3.00345	-0.60095
C	-0.62891	4.27760	-0.98523	H	-3.09900	-4.99149	-0.42954
C	0.66019	3.71780	-0.88975	H	1.62524	-5.85179	-1.27986
C	1.83545	4.54395	-0.95350	H	3.53941	-4.36419	-1.75207
C	3.10102	4.01404	-1.09587	H	-0.90301	-6.09594	-0.69796
C	3.29372	2.60396	-1.20603	H	-5.95753	-1.05817	-0.99876
C	2.15312	1.78144	-1.07223	H	-6.28733	1.36459	-1.33572

H	-5.21277	3.75378	-1.45187	H	-3.99861	1.90646	1.58175
H	-3.17362	5.13705	-1.30351	H	-2.95251	2.27179	2.66186
H	-0.73203	5.36607	-1.01857	H	4.06940	-1.88755	1.81996
H	1.69917	5.62868	-0.93134	H	3.36240	-2.68751	0.70024
H	3.96829	4.67581	-1.16703	H	0.40239	-1.77642	3.53258
H	5.43944	2.57420	-1.58244	H	-0.80044	-2.69959	3.19237
H	5.58346	0.12562	-1.85317	H	2.98328	1.70858	2.31727

***CHCHO + *3H_2O**

C	2.43473	-0.08122	-0.86180	C	-0.11053	-4.40328	-1.21946
C	2.55998	1.31648	-1.13509	C	-0.07670	-2.99646	-1.12406
C	3.80038	1.97774	-1.19873	C	-1.24316	-2.18573	-1.05914
C	4.98506	1.18906	-1.02013	C	1.12898	-2.24896	-0.98666
C	4.90703	-0.17659	-0.87127	C	2.37206	-2.96622	-0.96854
C	3.64566	-0.87417	-0.84856	C	2.32664	-4.39949	-1.08076
C	1.31477	1.96969	-1.32923	C	1.14242	-5.09193	-1.20538
C	1.31962	3.39682	-1.51834	Cu	0.01596	-1.57760	0.80363
C	2.59271	4.05762	-1.60168	O	-0.20760	-2.57352	2.56975
C	3.78496	3.38403	-1.45287	B	1.00563	-0.69554	-0.86593
C	0.11083	4.12447	-1.57008	Cu	1.72536	0.24789	1.15642
C	-1.12207	3.49269	-1.36023	C	0.58469	1.36508	2.51729
C	-1.19002	2.05769	-1.12956	C	-0.14513	0.57276	3.38477
C	-2.48081	1.46691	-0.95548	O	-1.18616	-0.18714	3.09446
C	-3.67511	2.19350	-1.01622	C	3.59428	-2.27410	-0.87320
C	-3.58122	3.61127	-1.21727	B	-1.04311	-0.65128	-0.89609
C	-2.36233	4.22422	-1.38004	Cu	-1.89516	-0.00605	1.21698
C	-4.90695	1.45993	-0.92725	O	-3.76602	0.67578	2.10007
C	-4.90867	0.08464	-0.87372	B	0.03122	1.12214	-1.24359
C	-3.69031	-0.68482	-0.87099	Cu	-0.13936	1.81086	0.76302
C	-2.43270	0.04242	-0.79880	O	3.64863	0.55543	2.07981
C	-3.70989	-2.08037	-0.98461	H	4.52899	-2.84206	-0.85817
C	-2.52107	-2.83368	-1.07759	H	-4.67255	-2.59820	-1.02016
C	-2.54768	-4.26654	-1.20218	H	-3.52347	-4.75915	-1.22815
C	-1.39794	-5.02238	-1.27540	H	1.14895	-6.18226	-1.28066

H	3.27469	-4.94366	-1.06093	H	5.82071	-0.77098	-0.78919
H	-1.46074	-6.11029	-1.35949	H	-4.36476	1.01676	1.40358
H	-5.85639	-0.45956	-0.86218	H	-3.57437	1.44741	2.66554
H	-5.85158	2.00911	-0.94668	H	3.60815	1.40971	2.55068
H	-4.50105	4.20029	-1.25832	H	4.32226	0.68569	1.37931
H	-2.31367	5.30321	-1.54970	H	-0.66810	-1.81062	3.03906
H	0.14116	5.20487	-1.73510	H	-0.87944	-3.27790	2.49478
H	2.59788	5.13664	-1.77886	H	1.33671	1.97434	3.04385
H	4.73358	3.92266	-1.52148	H	0.12533	0.54650	4.45774
H	5.95897	1.68435	-1.04102				

***CH_2CHO + *$3H_2O$**

C	0.20704	-5.14593	-0.61837	C	2.28957	3.08812	-1.19921
C	-0.82980	-4.21040	-0.91067	C	1.97097	1.68891	-1.13005
C	-0.49406	-2.83414	-0.87297	C	3.03850	0.74853	-1.14078
C	0.80725	-2.35945	-0.56602	C	4.41109	1.12391	-1.20982
C	1.86621	-3.32783	-0.43451	C	4.69309	2.51490	-1.32798
C	1.49968	-4.71825	-0.39841	C	3.67534	3.44998	-1.32371
C	-1.41873	-1.80403	-1.17913	C	5.37357	0.08503	-1.06451
C	-2.76794	-2.16667	-1.52483	C	4.98303	-1.22021	-0.83026
C	-3.09150	-3.56790	-1.57381	C	3.60333	-1.60454	-0.71219
C	-2.16753	-4.54857	-1.27401	C	2.61147	-0.58093	-0.87613
C	-3.75347	-1.17446	-1.72260	B	1.07324	-0.81550	-0.66762
C	-3.47304	0.18895	-1.51853	B	-0.92375	-0.34498	-1.09464
C	-4.48319	1.20610	-1.64776	Cu	-2.08846	-0.22383	0.78196
C	-4.20117	2.54811	-1.51000	Cu	-0.28959	1.59956	1.12901
C	-2.86925	3.00459	-1.25623	B	0.52530	1.14195	-0.89784
C	-1.86558	2.02608	-1.10026	Cu	1.91132	0.60876	0.83756
C	-2.12808	0.62140	-1.17988	O	3.36795	1.31020	2.08960
C	-2.46043	4.37147	-1.20619	C	3.21957	-2.93681	-0.45625
C	-1.12545	4.70515	-1.10904	Cu	0.29680	-1.15992	1.26886
C	-0.08787	3.71304	-1.03647	O	-0.62803	-1.80227	2.94435
C	-0.49132	2.33114	-0.93761	C	-1.56431	2.60577	2.43143
C	1.27221	4.06257	-1.13593	C	-1.44390	1.35427	3.02542

O	-2.20428	0.28985	2.77436	H	3.92044	4.51339	-1.39336
O	-3.26441	-1.98857	1.46153	H	5.73409	2.84212	-1.39431
H	3.99409	-3.70102	-0.34395	H	6.43624	0.33512	-1.12026
H	-4.77165	-1.47698	-1.98186	H	5.74212	-1.99801	-0.71003
H	-4.11240	-3.84812	-1.84705	H	-3.69290	-2.38959	0.67963
H	-0.02664	-6.21388	-0.61130	H	-3.99907	-1.68042	2.02431
H	2.29439	-5.45145	-0.23501	H	4.21206	1.36363	1.59725
H	-2.45404	-5.60262	-1.31824	H	3.55094	0.70883	2.83667
H	-5.50293	0.88631	-1.87818	H	-1.30199	-1.04229	3.06706
H	-4.99875	3.28699	-1.62431	H	-1.18639	-2.57853	2.73823
H	-3.21672	5.15639	-1.28943	H	-0.70487	1.23149	3.83512
H	-0.82547	5.75640	-1.12978	H	-2.42251	2.83526	1.78979
H	1.54584	5.11968	-1.19953	H	-1.00918	3.43915	2.86849

***CH_2CH_2O + *$3H_2O$**

C	2.40061	-1.06601	-0.92286	C	-4.11424	2.15840	-2.00205
C	3.10091	0.16333	-0.86276	C	-3.54225	3.41178	-2.01318
C	4.50512	0.25412	-0.82331	C	-3.97786	-0.30182	-1.69614
C	5.24576	-0.96992	-0.82961	C	-3.24819	-1.46284	-1.39725
C	4.59508	-2.18228	-0.86717	C	-1.83385	-1.39630	-1.09313
C	3.16029	-2.28130	-0.90607	C	-1.12974	-2.62867	-0.97218
C	5.08510	1.56263	-0.77962	C	-1.74293	-3.88547	-1.05387
C	4.28964	2.68404	-0.81268	C	-3.16414	-3.92013	-1.24545
C	2.85336	2.60658	-0.87952	C	-3.87659	-2.75847	-1.41559
C	2.24069	1.30070	-0.83441	C	0.28661	-2.45325	-0.87325
C	2.07538	3.76306	-1.05462	C	1.11903	-3.64270	-0.88192
C	0.68527	3.69466	-1.24711	C	0.46367	-4.92575	-0.91320
C	-0.09134	4.87206	-1.52874	C	-0.90192	-5.04671	-0.99360
C	-1.44602	4.82306	-1.76607	B	0.85671	-1.00962	-0.94815
C	-2.14768	3.57624	-1.75337	Cu	0.62668	-1.78622	1.05186
C	-1.39595	2.40692	-1.49515	O	0.77930	-1.74247	2.95788
C	0.00060	2.42478	-1.21185	C	2.51769	-3.53710	-0.90432
C	-1.95315	1.10070	-1.47837	B	-1.01365	-0.08490	-1.16105
C	-3.35684	0.96742	-1.72625	Cu	-1.61484	-0.34166	0.87747

O	-3.84340	-0.20581	1.35837	H	0.43003	5.83242	-1.54761
Cu	-0.73023	2.01363	0.71438	H	2.56973	4.73775	-1.08909
C	-1.11539	0.94636	3.50355	H	4.74475	3.67790	-0.80752
O	-1.41410	-0.37662	2.95071	H	6.17273	1.65944	-0.73651
B	0.69939	1.05986	-0.93288	H	6.33741	-0.92968	-0.80000
Cu	1.35935	0.76334	1.06581	H	5.17159	-3.11119	-0.86104
O	2.22808	0.33984	2.82621	H	-4.22671	-0.06054	0.46615
C	-1.46670	2.06429	2.53952	H	-3.92634	0.65645	1.80700
H	3.12213	-4.44852	-0.90417	H	3.17054	0.12138	2.69632
H	-5.04574	-0.38284	-1.91794	H	1.75636	-0.56335	3.04162
H	-4.95315	-2.79990	-1.60111	H	-0.61411	-0.97546	3.13878
H	-1.36497	-6.03568	-1.03501	H	0.99182	-2.58660	3.38992
H	1.09298	-5.81947	-0.89264	H	-0.04294	0.97845	3.74999
H	-3.66927	-4.88837	-1.28774	H	-2.56500	2.18203	2.46913
H	-5.18322	2.04652	-2.20225	H	-1.08164	3.01024	2.96687
H	-4.15070	4.29426	-2.22480	H	-1.68970	1.02401	4.44524
H	-2.00251	5.74114	-1.96978				

***CH_3CH_2OH + *OH + *$2H_2O$**

C	1.83024	-1.79228	-1.07784	C	0.46455	5.14861	-1.34693
C	2.94068	-0.92892	-0.86536	C	1.74067	4.66876	-1.12186
C	4.27984	-1.37992	-0.79450	C	-2.00769	4.64835	-1.60680
C	4.50495	-2.78247	-0.92961	C	-3.01910	3.70759	-1.61827
C	3.44889	-3.65143	-1.10978	C	-2.77055	2.30279	-1.44386
C	2.08264	-3.20566	-1.17055	C	-1.40592	1.88569	-1.26819
C	2.58240	0.43920	-0.72031	C	-3.82030	1.35940	-1.46438
C	3.63341	1.42792	-0.67056	C	-3.59079	-0.02013	-1.32019
C	4.98573	0.95040	-0.56194	C	-4.65210	-0.98724	-1.41108
C	5.29700	-0.39550	-0.60540	C	-4.41306	-2.34779	-1.37367
C	3.33491	2.80003	-0.74711	C	-3.08266	-2.86310	-1.26993
C	2.01991	3.27122	-0.94543	C	-2.03666	-1.93083	-1.13715
C	0.91411	2.35515	-1.01381	C	-2.25259	-0.52574	-1.09464
C	-0.38366	2.87407	-1.27184	C	-0.65080	-2.29259	-1.08996
C	-0.64867	4.26356	-1.41973	C	-0.32064	-3.70592	-1.22124

C	-1.40990	-4.64267	-1.31229	H	-5.24699	-3.04972	-1.45443
C	-2.72899	-4.24852	-1.33349	H	-4.05480	4.02897	-1.75896
B	0.41457	-1.16471	-1.14888	H	-2.24453	5.70801	-1.73479
Cu	0.15500	-1.76094	0.82582	H	0.29744	6.22232	-1.46779
O	0.77766	-1.23231	2.56455	H	2.58088	5.36698	-1.07270
Cu	1.75448	0.17128	1.26058	H	4.15391	3.52362	-0.69939
Cu	-0.26230	1.46475	0.70253	H	5.78431	1.69029	-0.46285
Cu	-1.97700	-0.24472	1.00328	H	6.33793	-0.71901	-0.52251
B	-1.00074	0.39918	-1.02906	H	5.52859	-3.16371	-0.88550
C	1.01586	-4.12522	-1.27762	H	3.63826	-4.72459	-1.20102
B	1.07539	0.80869	-0.80780	H	-4.26086	-1.58969	0.91865
O	3.60195	0.11839	2.37370	H	-3.58747	-1.89625	2.28342
C	-1.32186	1.16454	3.62895	H	3.67603	0.90283	2.94940
O	-1.50988	-0.16464	3.08002	H	4.32059	0.23433	1.71517
C	-2.45607	2.06626	3.19706	H	-0.59566	-0.61904	3.07375
O	-3.81933	-1.16273	1.68325	H	1.36951	-1.84618	3.03503
H	1.23705	-5.19236	-1.36829	H	-1.27593	1.08482	4.72777
H	-4.84453	1.71247	-1.61568	H	-2.30794	3.07702	3.60617
H	-5.67426	-0.61825	-1.52977	H	-2.49529	2.14795	2.09347
H	-3.52314	-4.99487	-1.42035	H	-3.42512	1.68113	3.54816
H	-1.15950	-5.70437	-1.38769	H	-0.34609	1.55997	3.27717

***CH_3CH_2OH + *$3H_2O$**

C	4.58438	1.29285	1.80304	C	-1.53065	3.60858	1.51057
C	3.41791	2.09797	1.60215	C	-2.76981	4.32355	1.65170
C	2.17999	1.43353	1.49407	C	-3.99962	3.69356	1.63421
C	2.05079	0.01313	1.54195	C	-4.10601	2.28115	1.47266
C	3.24576	-0.77771	1.75821	C	-2.88852	1.55112	1.40027
C	4.49763	-0.07800	1.89275	C	-1.60457	2.17275	1.42467
C	0.94439	2.10836	1.31879	C	-5.31320	1.53099	1.36251
C	0.92922	3.55064	1.39045	C	-5.29199	0.16863	1.13533
C	2.20572	4.21643	1.44820	C	-4.06958	-0.57474	0.99261
C	3.39557	3.52887	1.53678	C	-2.83366	0.14406	1.16448
C	-0.28185	4.26333	1.45784	C	-4.06049	-1.95665	0.71117

C	-2.86552	-2.69463	0.64645	H	2.21199	5.31008	1.44758
C	-1.58086	-2.05349	0.80665	H	5.55576	1.78579	1.89711
C	-0.43418	-2.87451	0.97594	H	5.40000	-0.67339	2.05501
C	-0.46383	-4.27935	0.88955	H	4.34048	4.07632	1.59379
C	-1.72854	-4.88770	0.60859	H	-2.72308	5.41167	1.75123
C	-2.87185	-4.12819	0.49900	H	-4.91460	4.28579	1.72433
C	0.76123	-4.98027	1.12142	H	-6.26994	2.05447	1.44339
C	1.92315	-4.30691	1.42744	H	-6.23452	-0.37673	1.03373
C	1.97568	-2.87082	1.51825	H	-5.01336	-2.48084	0.59131
C	0.74950	-2.13660	1.28010	H	-3.83463	-4.61928	0.33050
B	0.63192	-0.59424	1.39376	H	-1.78374	-5.97571	0.51266
Cu	1.60929	-0.95985	-0.45364	H	0.76366	-6.07209	1.05932
Cu	0.54293	1.31389	-0.82962	H	2.84684	-4.86409	1.60468
O	2.30544	2.00833	-1.62999	H	2.98637	2.06397	-0.92594
C	3.17634	-2.18489	1.79312	H	2.68669	1.42070	-2.31152
Cu	-0.86175	-0.98562	-1.07198	H	-0.18871	-1.82310	-3.30618
O	-0.56961	-2.36023	-2.56217	H	-1.41637	-2.71324	-2.89710
B	-1.43059	-0.52244	1.01484	H	0.27461	0.32526	-3.30686
Cu	-1.77573	1.11991	-0.50382	H	2.64167	-2.21945	-2.38133
B	-0.34988	1.26835	1.24239	H	1.49098	-0.59954	-5.73776
O	2.54292	-1.26715	-2.18637	H	2.42244	1.73503	-5.93151
O	0.70634	-0.35859	-3.87427	H	1.71811	2.14463	-4.34403
C	1.09324	0.23415	-5.14307	H	3.02871	0.92459	-4.46159
C	2.12759	1.32400	-4.95343	H	0.19030	0.62145	-5.64058
H	4.09138	-2.75934	1.96177	H	1.93019	-0.91398	-2.91207
H	-0.25097	5.35515	1.52021				

***3H_2O (ethanol pathway)**

C	1.87832	1.13945	-1.18187	C	1.44795	4.85061	-0.73286
C	1.34385	2.44099	-0.94957	C	0.08155	4.88927	-0.56251
C	2.12478	3.61161	-0.97828	C	-0.73603	3.70301	-0.59160
C	3.51577	3.46996	-1.28932	C	-0.05110	2.43691	-0.68743
C	4.06349	2.23440	-1.55019	C	-2.14195	3.77146	-0.58887
C	3.28634	1.02300	-1.49434	C	-2.94316	2.62003	-0.72914

C	-4.37861	2.68485	-0.79806	Cu	-1.92669	0.12704	0.99034
C	-5.17370	1.55721	-0.85990	B	-0.79794	1.08450	-0.71659
C	-4.60431	0.24866	-0.85864	Cu	0.06474	1.31906	1.38019
C	-3.18638	0.16846	-0.86099	O	1.53691	2.55369	2.21512
C	-2.33660	1.31521	-0.80934	O	1.02991	-2.77507	2.31857
C	-2.47531	-1.06688	-0.77644	H	4.94286	-0.31320	-1.90260
C	-3.22471	-2.29217	-0.66754	H	-3.15253	-4.43902	-0.40327
C	-4.65732	-2.19580	-0.74236	H	-1.08600	-5.78216	-0.26232
C	-5.31831	-0.98613	-0.83273	H	3.61361	-4.84433	-1.19111
C	-2.56001	-3.52361	-0.49167	H	4.84567	-2.76928	-1.70226
C	-1.15624	-3.61547	-0.48466	H	1.35345	-5.99288	-0.55038
C	-0.33231	-2.43870	-0.61451	H	-5.23539	-3.12302	-0.69556
C	1.05207	-2.60659	-0.86286	H	-6.41136	-0.96475	-0.86151
C	1.69594	-3.85833	-0.86027	H	-6.26209	1.65981	-0.88721
C	0.88260	-5.00693	-0.58806	H	-4.84559	3.67338	-0.77124
C	-0.47900	-4.88613	-0.42030	H	-2.62490	4.75071	-0.52383
C	1.73300	-1.37714	-1.12235	H	-0.41958	5.85182	-0.42714
C	3.14939	-1.43041	-1.43768	H	2.02831	5.77723	-0.72055
C	3.78043	-2.72529	-1.46044	H	4.14277	4.36495	-1.32589
C	3.09341	-3.88264	-1.17272	H	5.12707	2.14652	-1.78705
B	0.90664	-0.06597	-1.09039	H	1.38347	-3.35525	1.60926
Cu	2.04669	-0.16127	0.68874	H	1.81894	-2.43016	2.78009
O	3.13652	0.26941	2.31039	H	1.25397	3.08766	2.98243
C	3.87639	-0.24579	-1.67085	H	1.84207	3.19779	1.54012
Cu	-0.10254	-1.28902	1.44270	H	2.76780	1.15461	2.56349
B	-0.92446	-1.01378	-0.68367	H	2.93040	-0.31937	3.06344

***C_2H_4 + *2OH + *2H_2O**

C	-0.46161	-2.44173	1.07990	C	-4.20561	-2.68896	1.37618
C	-1.84285	-2.14447	1.18384	C	-4.52045	-1.34997	1.35010
C	-2.84059	-3.12766	1.31957	C	-3.51258	-0.32589	1.23842
C	-2.41966	-4.49187	1.34827	C	-2.14173	-0.74818	1.04121
C	-1.08922	-4.81707	1.19562	C	-3.83296	1.03154	1.34803
C	-0.07031	-3.81830	1.02052	C	-2.83706	2.02749	1.35227

C	-3.16451	3.39981	1.62885	B	-0.95106	0.24033	0.85546
C	-2.19529	4.36272	1.79667	Cu	-1.65824	-0.80514	-0.98407
C	-0.80713	4.02416	1.72837	O	-3.29875	-1.91114	-1.81718
C	-0.47291	2.68647	1.42648	C	-3.39664	1.67281	-1.77410
C	-1.45006	1.69117	1.13087	H	1.53462	-5.24607	0.71107
C	0.85411	2.20275	1.37984	H	4.05851	3.51807	1.46438
C	1.92131	3.14976	1.54039	H	5.74845	1.85716	0.77084
C	1.57690	4.50927	1.85486	H	5.65847	-2.95979	-0.00675
C	0.26986	4.93439	1.95761	H	3.87035	-4.64953	0.17984
C	3.26913	2.77173	1.33528	H	6.37788	-0.46185	0.20986
C	3.60867	1.47713	0.92571	H	2.39337	5.22170	2.00405
C	2.57989	0.46701	0.74102	H	0.04506	5.97564	2.20269
C	3.00378	-0.87297	0.47072	H	-2.47773	5.39651	2.01243
C	4.33780	-1.24427	0.30430	H	-4.22112	3.66246	1.72663
C	5.32805	-0.20382	0.37165	H	-4.87725	1.32453	1.48846
C	4.97568	1.08889	0.68012	H	-5.56365	-1.03258	1.42691
C	1.91884	-1.80651	0.49497	H	-4.99825	-3.43714	1.45602
C	2.24764	-3.22475	0.47715	H	-3.16990	-5.27812	1.46493
C	3.62596	-3.58577	0.24439	H	-0.78391	-5.86696	1.18336
C	4.62263	-2.64607	0.14786	H	3.95803	0.60178	-1.99017
B	0.51451	-1.26061	0.88334	H	3.31312	1.62344	-2.95527
Cu	0.80186	-1.38284	-1.20481	H	-3.84824	-2.23063	-1.07085
O	-0.42568	-1.02928	-2.62404	H	-2.94051	-2.72384	-2.22307
C	1.26798	-4.18577	0.74020	H	0.28872	2.27067	-2.75084
B	1.07263	0.71332	1.04416	H	-0.69371	-1.85208	-3.07753
Cu	1.61500	1.15868	-0.95978	H	-2.16802	1.23790	-3.49206
O	3.12926	0.79544	-2.47221	H	-3.91030	2.45282	-1.20638
Cu	-1.41232	1.70345	-1.06524	H	-3.78766	0.65646	-1.66881
C	-2.52614	2.00066	-2.79346	H	-2.34155	3.04473	-3.06345
O	0.32571	2.36826	-1.78261				

***C_2H_4 + *OH + *3H_2O**

C	1.46887	-4.98372	-1.11638	C	0.18517	-2.93230	-0.90537
C	0.19745	-4.34031	-0.97295	C	1.36757	-2.13175	-1.02005

C	2.64009	-2.81160	-1.20429	C	-1.99850	1.57839	2.59102
C	2.62922	-4.25113	-1.22977	Cu	0.84779	1.21591	1.25302
C	-1.06330	-5.00964	-0.95517	O	1.82309	2.78383	2.39866
C	-2.24208	-4.29336	-0.95957	C	3.82777	-2.07579	-1.34614
C	-2.26512	-2.85698	-0.96598	B	0.12590	1.17731	-0.83482
C	-1.00534	-2.16178	-0.83459	Cu	1.69603	-1.11253	0.82220
C	-3.46853	-2.14467	-1.15883	O	1.73573	-0.29197	2.56558
C	-3.48620	-0.74300	-1.32190	O	-3.09931	-1.80892	1.89374
C	-2.26847	0.01659	-1.24516	H	4.77542	-2.60691	-1.47192
C	-2.34673	1.43253	-1.39617	H	-4.40518	-2.70265	-1.24694
C	-3.56895	2.13131	-1.62586	H	-3.19893	-4.82065	-1.00508
C	-4.74820	1.34434	-1.73898	H	1.50562	-6.07575	-1.15618
C	-4.70523	-0.02895	-1.58669	H	3.58611	-4.76535	-1.35557
C	-1.10293	2.08352	-1.17838	H	-1.08559	-6.10242	-0.98013
C	-1.07787	3.51892	-1.15417	H	-5.62864	-0.60980	-1.65971
C	-2.30994	4.21137	-1.40854	H	-5.70319	1.84301	-1.92456
C	-3.50295	3.55094	-1.64378	H	-4.41765	4.12306	-1.81997
C	0.12376	4.20589	-0.88656	H	-2.29148	5.30470	-1.40377
C	1.34333	3.52310	-0.71515	H	0.11829	5.29944	-0.86177
C	2.58689	4.23340	-0.57529	H	2.54658	5.32185	-0.47959
C	3.80955	3.59131	-0.60419	H	4.73373	4.16722	-0.50766
C	3.88575	2.18178	-0.81459	H	6.04988	1.96624	-0.94395
C	2.66679	1.46657	-0.87954	H	5.99615	-0.47661	-1.31756
C	1.39688	2.08095	-0.73142	H	-3.51949	-1.75146	1.00642
C	5.09276	1.43934	-0.98425	H	-3.38736	-0.99768	2.35093
C	5.06071	0.07676	-1.19646	H	2.34649	3.28848	1.74065
C	3.83089	-0.66718	-1.23920	H	2.49153	2.35534	2.96726
C	2.59680	0.06380	-1.10225	H	0.56787	-1.25477	3.12832
B	1.19201	-0.59136	-1.13521	H	2.61780	-0.06236	2.90734
B	-0.87063	-0.59859	-0.91319	H	-1.27305	2.36331	2.82441
Cu	-0.91987	-1.38184	1.16776	H	-3.93187	1.14921	1.72551
O	-0.30493	-1.77777	3.09683	H	-3.20851	2.81226	1.28872
Cu	-1.55083	0.94526	0.65839	H	-1.98202	0.69460	3.23493
C	-3.08041	1.83561	1.76637	H	-0.04876	-2.71277	3.20682

***CH_3CH_2 + *OH + *3H_2O**

C	2.29081	1.34434	-1.12896	Cu	1.96589	0.07661	1.05337
C	1.59130	2.57680	-1.13244	O	1.40830	1.04701	2.61297
C	2.22312	3.82855	-1.24349	Cu	0.13683	1.83652	1.10557
C	3.64802	3.83966	-1.35316	B	-0.39394	0.98075	-0.92437
C	4.36177	2.66146	-1.32208	Cu	-1.89466	0.49647	0.73720
C	3.72532	1.38075	-1.17799	C	-2.62601	0.18280	2.52259
C	0.17778	2.42486	-0.99577	C	-4.05009	-0.36487	2.31196
C	-0.64247	3.59921	-1.19209	C	4.48682	0.20016	-1.01861
C	0.01833	4.88011	-1.24126	B	-0.27865	-1.07109	-0.82567
C	1.38920	4.99587	-1.24887	Cu	-0.34323	-1.36815	1.31948
C	-2.02432	3.49330	-1.39852	O	-1.74733	-2.98841	2.11688
C	-2.65790	2.24068	-1.49897	O	0.44108	-1.28134	3.29068
C	-1.90776	1.02720	-1.29610	O	0.25663	3.86127	1.94140
C	-2.58595	-0.21811	-1.44838	H	5.57716	0.25318	-1.08212
C	-3.96403	-0.31295	-1.74384	H	-2.07108	-4.77068	-0.91676
C	-4.68251	0.90682	-1.94514	H	0.03595	-5.83649	-0.27001
C	-4.05258	2.12620	-1.82705	H	4.65844	-4.33199	-0.12773
C	-4.52803	-1.62532	-1.79835	H	5.72821	-2.14873	-0.55862
C	-3.75354	-2.73367	-1.53242	H	2.48732	-5.73669	0.02456
C	-2.35602	-2.63871	-1.20543	H	-4.20586	-3.72891	-1.55654
C	-1.75515	-1.33965	-1.19859	H	-5.58858	-1.73990	-2.03611
C	-1.59676	-3.78589	-0.87633	H	-5.74833	0.85948	-2.18202
C	-0.23951	-3.69173	-0.52784	H	-4.61929	3.04953	-1.97194
C	0.55056	-4.87209	-0.28529	H	-2.61314	4.40364	-1.54185
C	1.91399	-4.81849	-0.12692	H	-0.60608	5.77519	-1.30448
C	2.61359	-3.56873	-0.22354	H	1.85721	5.98208	-1.29866
C	1.84902	-2.40779	-0.37196	H	4.16711	4.79626	-1.45309
C	0.42576	-2.40533	-0.46498	H	5.45300	2.68600	-1.38692
C	2.42399	-1.11393	-0.60068	H	-1.97935	-3.44192	1.27768
C	3.87268	-1.01961	-0.70855	H	-2.56484	-2.52213	2.37505
C	4.63899	-2.22297	-0.50122	H	-0.63696	4.11013	2.24563
C	4.04466	-3.43748	-0.26161	H	0.40777	4.43964	1.16399
B	1.46101	0.04763	-0.96939	H	0.86248	-0.36251	3.28693

H	2.04437	1.70843	2.93832	H	-2.04068	-0.49088	3.16718
H	-2.66178	1.15280	3.04828	H	1.19253	-1.89685	3.38254
H	-4.06362	-1.29010	1.71056	H	-4.55218	-0.59325	3.27226
H	-4.68528	0.35736	1.77478				

***H + *OH + *3H_2O**

C	-0.96113	-4.98510	-1.13161	C	5.01192	-0.66488	-1.38120
C	-1.83267	-3.86476	-0.94786	C	4.41014	-1.89923	-1.42588
C	-1.25614	-2.58327	-0.98299	C	2.97988	-2.06162	-1.35654
C	0.12350	-2.34671	-1.19541	C	2.16579	-0.87142	-1.19851
C	0.98565	-3.48544	-1.33964	B	0.61657	-0.87661	-1.19861
C	0.38950	-4.79536	-1.31673	Cu	1.30691	-1.13408	0.75219
C	-1.99767	-1.38832	-0.75523	Cu	-1.30317	-0.85471	1.23224
C	-3.42930	-1.49656	-0.60910	O	-0.92906	-2.59809	2.37136
C	-4.00582	-2.81715	-0.56943	C	2.38355	-3.32771	-1.44695
C	-3.24660	-3.95222	-0.72190	Cu	0.54433	0.47009	2.54892
C	-4.23572	-0.34874	-0.53424	O	2.61053	1.49687	2.00330
C	-3.68910	0.94558	-0.65370	B	0.42762	1.18990	-1.15940
C	-4.52609	2.11490	-0.62262	Cu	-0.64982	1.49920	0.75610
C	-4.01810	3.38722	-0.76618	H	-0.50060	1.67709	2.39381
C	-2.61698	3.59737	-0.95454	B	-1.24104	-0.03382	-0.83411
C	-1.79006	2.45420	-0.99842	O	1.40063	-1.29037	2.70902
C	-2.27771	1.12895	-0.83641	O	-3.00317	-0.07657	2.48347
C	-1.98083	4.87127	-1.09825	H	3.01549	-4.21328	-1.55775
C	-0.61354	4.96664	-1.22438	H	-5.31649	-0.46269	-0.41190
C	0.24943	3.81438	-1.22436	H	-5.08551	-2.89750	-0.41850
C	-0.36798	2.50989	-1.15111	H	-1.37978	-5.99440	-1.11364
C	1.64413	3.94438	-1.28465	H	1.04935	-5.65875	-1.43755
C	2.48356	2.81224	-1.25392	H	-3.71537	-4.93865	-0.68250
C	1.93498	1.48746	-1.18913	H	-5.59968	1.96969	-0.47664
C	2.83087	0.39519	-1.21536	H	-4.68386	4.25307	-0.73229
C	4.22626	0.53266	-1.29386	H	-2.59648	5.77425	-1.08736
C	4.75771	1.86192	-1.32016	H	-0.14514	5.95097	-1.30795
C	3.91654	2.95058	-1.30341	H	2.08796	4.94207	-1.34077

H	4.33024	3.96194	-1.33964	H	2.38961	1.58736	1.04901
H	5.84063	2.00030	-1.37064	H	3.24484	0.75486	2.02236
H	6.10020	-0.58030	-1.43634	H	-0.01299	-2.39297	2.70685
H	5.01928	-2.80203	-1.52070	H	2.30805	-1.24558	3.06351
H	-3.67430	0.16448	1.81075	H	-0.80563	-3.34010	1.74720
H	-2.59756	0.77876	2.73227				

***4H_2O (ethylene pathway)**

C	-1.65629	-1.86716	1.43192	C	4.59582	-1.54747	1.05398
C	-2.88427	-1.15801	1.41309	C	4.62868	-0.17519	0.92216
C	-4.14430	-1.78536	1.49689	C	0.86923	-2.02415	1.31134
C	-4.16187	-3.20859	1.61866	C	0.74922	-3.45923	1.45227
C	-2.98720	-3.92772	1.64886	C	1.96485	-4.23549	1.44623
C	-1.69773	-3.29739	1.55032	C	3.20587	-3.65743	1.32483
C	-5.30315	-0.94184	1.47951	B	-0.34295	-1.05817	1.29243
C	-5.18459	0.42392	1.37853	Cu	0.44877	-1.50109	-0.71982
C	-3.90744	1.08548	1.27929	O	1.72870	-2.39853	-2.10794
C	-2.71740	0.25897	1.29895	Cu	-0.63721	-0.50209	-2.72467
C	-3.81009	2.47912	1.18944	Cu	-1.64849	-0.19029	-0.57440
C	-2.55632	3.12297	1.09140	B	-1.29126	0.84535	1.26154
C	-2.46414	4.55261	0.94469	C	-0.51035	-4.06105	1.57147
C	-1.25696	5.19608	0.79074	Cu	0.44561	0.99310	-1.07924
C	-0.03404	4.45417	0.76188	O	2.07549	1.75161	-2.18399
C	-0.11702	3.05941	0.92247	B	0.81059	0.67898	1.08379
C	-1.33853	2.37118	1.11124	O	3.64234	-0.61922	-2.19214
C	1.01794	2.19360	0.88124	O	0.22222	-1.57746	-4.25126
C	2.32136	2.80175	0.74203	H	-0.57838	-5.14864	1.66677
C	2.38979	4.23401	0.57423	H	4.45968	2.50748	0.63830
C	1.26856	5.02632	0.57742	H	5.58508	0.33815	0.79263
C	3.48747	2.02174	0.76106	H	4.10256	-4.28292	1.31254
C	3.42960	0.62329	0.93514	H	1.87552	-5.32167	1.53600
C	2.17232	-0.04502	1.10029	H	5.52389	-2.12479	1.03196
C	2.18063	-1.45800	1.22850	H	3.37795	4.68427	0.44528
C	3.35189	-2.23447	1.21275	H	1.35901	6.10792	0.44492

H	-1.22112	6.28300	0.67786	H	1.91426	2.19789	-3.03650
H	-3.39299	5.13005	0.94843	H	-0.37464	-2.22810	-4.66832
H	-4.72357	3.08119	1.17870	H	0.84303	-2.10959	-3.68145
H	-6.08235	1.04866	1.36846	H	3.12660	0.22580	-2.22304
H	-6.29210	-1.40281	1.54972	H	2.07812	-3.26674	-1.83029
H	-5.12379	-3.72308	1.69311	H	4.01781	-0.63375	-1.28614
H	-3.01821	-5.01652	1.74522	H	2.53126	-1.76149	-2.15670
H	2.58031	2.38669	-1.63200				

***3H_2O (ethylene pathway)**

C	-3.07398	-3.95989	-1.51251	C	5.26446	-0.76405	-1.15191
C	-3.30896	-2.54547	-1.43249	C	4.15889	-1.67412	-1.20429
C	-2.18370	-1.70300	-1.38495	C	2.86344	-1.11557	-1.23605
C	-0.84443	-2.19824	-1.34664	C	2.60902	0.29335	-1.18996
C	-0.63058	-3.62521	-1.43408	C	4.26036	-3.09781	-1.25483
C	-1.79770	-4.46918	-1.51821	C	3.13137	-3.88479	-1.32794
C	-4.59695	-1.92631	-1.34125	C	1.80518	-3.32821	-1.34286
C	-4.70850	-0.56398	-1.18090	C	1.67710	-1.89776	-1.29290
C	-3.55683	0.29803	-1.11544	B	0.30821	-1.16895	-1.27042
C	-2.25880	-0.29276	-1.25098	Cu	-0.66381	-1.55299	0.72600
C	-3.70025	1.68696	-0.89745	Cu	-0.64960	0.87964	1.00793
C	-2.58260	2.53509	-0.82783	B	-0.94198	0.50759	-1.14940
C	-1.24244	2.00512	-0.92522	C	0.66650	-4.15664	-1.42406
C	-0.15866	2.93789	-0.93597	Cu	1.46661	-0.39045	0.56422
C	-0.33035	4.32571	-0.78985	B	1.15336	0.79646	-1.22307
C	-1.66997	4.81878	-0.64953	O	-2.49940	-1.87377	1.72011
C	-2.74150	3.96002	-0.67139	Cu	0.44396	-0.51406	2.73408
C	1.10600	2.32296	-1.08855	O	0.64260	-0.82787	4.72650
C	2.27549	3.14532	-1.03460	O	-2.62571	0.94940	1.97640
C	2.09384	4.56858	-0.90756	H	0.79976	-5.24095	-1.47673
C	0.84658	5.13983	-0.79316	H	-4.70360	2.11437	-0.81441
C	3.56694	2.57368	-1.07080	H	-5.69647	-0.10511	-1.08783
C	3.74765	1.18647	-1.12046	H	-3.93358	-4.63394	-1.55764
C	5.06251	0.59554	-1.11832	H	-1.64228	-5.54998	-1.57574

H	-5.49187	-2.55320	-1.37907	H	5.25218	-3.55740	-1.23983
H	-3.75868	4.35055	-0.57981	H	3.22809	-4.97298	-1.37239
H	-1.82863	5.89420	-0.53226	H	-3.21467	1.31079	1.27299
H	0.74258	6.22360	-0.69289	H	-2.72849	1.54431	2.74241
H	2.98674	5.19987	-0.89046	H	1.32065	-0.25786	5.14018
H	4.44348	3.22693	-1.02983	H	0.91918	-1.74072	4.94095
H	5.92180	1.27095	-1.07873	H	-3.15450	-2.13910	1.04074
H	6.28026	-1.16837	-1.13863	H	-2.73447	-0.93510	1.93617

For *2H_2O and *H_2O see C_1 pathway.

c. Cu_7 cluster – C_1 pathway

*			=				$C_{33}H_{15}B_3Cu_7$
C	-0.99542	-2.16320	1.24951	C	3.44609	3.74180	0.84091
C	-2.12252	-1.38354	1.62113	C	2.40814	4.58228	1.17491
C	-3.38520	-1.94615	1.89662	C	4.35401	1.45778	0.47343
C	-3.51181	-3.36713	1.79470	C	4.19621	0.05931	0.44212
C	-2.42901	-4.15528	1.47457	C	2.90861	-0.54570	0.65053
C	-1.12869	-3.60046	1.21255	C	2.81803	-1.96417	0.64178
C	-4.42987	-1.05481	2.29502	C	3.93215	-2.81144	0.41754
C	-4.18802	0.29318	2.43473	C	5.19958	-2.18571	0.22323
C	-2.89895	0.87851	2.18099	C	5.31990	-0.81242	0.23738
C	-1.83138	0.00895	1.74890	C	1.49382	-2.45063	0.82058
C	-2.68134	2.25951	2.33462	C	1.27643	-3.87144	0.78611
C	-1.44041	2.84046	2.02301	C	2.41883	-4.71858	0.58179
C	-1.23195	4.25967	2.13237	C	3.69072	-4.21741	0.40339
C	-0.02428	4.85461	1.84718	Cu	1.31435	-1.00444	-0.93440
C	1.09699	4.06987	1.43024	B	0.35095	-1.42135	1.02795
C	0.90287	2.68198	1.29543	Cu	-1.14755	-1.44263	-0.73466
C	-0.33447	2.02347	1.57639	Cu	-2.67614	-0.06949	-2.02245
C	1.94225	1.79071	0.92032	Cu	-0.68448	2.48136	-2.28484
C	3.27113	2.31960	0.72219	Cu	1.13046	1.49254	-1.01558

B	1.61064	0.27498	0.87223	H	6.08006	-2.81182	0.06000
C	-0.00871	-4.41504	0.97342	H	4.44679	4.14821	0.67455
B	-0.38222	0.48129	1.50300	H	2.58008	5.65753	1.26530
Cu	-1.28268	1.07368	-0.35178	H	0.09493	5.93559	1.95275
Cu	-0.29164	0.09669	-2.41337	H	-2.07563	4.87194	2.46138
H	-0.13471	-5.50077	0.95070	H	-3.50293	2.89808	2.66955
H	5.35071	1.88317	0.32886	H	-4.99336	0.96013	2.75320
H	6.30035	-0.35279	0.08811	H	-5.42268	-1.46069	2.50379
H	4.53184	-4.89687	0.24606	H	-4.48367	-3.82513	1.99386
H	2.25458	-5.79907	0.56597	H	-2.53974	-5.24146	1.42564

***COOH**

C	-3.57211	-4.11113	-0.67761	C	3.18500	0.83745	-2.20208
C	-3.79391	-2.70368	-0.76950	C	4.48236	0.22914	-2.32615
C	-2.65680	-1.87872	-0.93749	C	4.69737	-1.11039	-2.09380
C	-1.32769	-2.38150	-0.99347	C	3.61537	-1.96807	-1.71890
C	-1.13189	-3.79857	-0.87677	C	2.34419	-1.38102	-1.57232
C	-2.29552	-4.62855	-0.72710	C	2.07848	-0.00048	-1.80466
C	-5.06378	-2.05620	-0.68524	C	3.72217	-3.38213	-1.52039
C	-5.15906	-0.68272	-0.74637	C	2.61023	-4.14046	-1.23701
C	-4.00912	0.16558	-0.89786	C	1.29983	-3.55920	-1.10562
C	-2.72056	-0.45990	-0.99676	C	1.18372	-2.12309	-1.22081
C	-4.14302	1.56403	-0.98403	B	-0.16959	-1.35374	-1.14048
C	-3.03348	2.39898	-1.19201	Cu	1.22460	-1.36674	0.73500
C	-1.70127	1.84597	-1.27911	Cu	0.32290	0.30091	2.34476
C	-0.64355	2.70658	-1.68291	Cu	1.42599	1.07611	0.20838
C	-0.81619	4.08786	-1.89507	B	0.61990	0.49588	-1.70805
C	-2.13038	4.62930	-1.72051	C	0.15904	-4.35753	-0.92696
C	-3.18953	3.81546	-1.39253	Cu	-0.95511	1.63729	0.68727
C	0.59039	2.02773	-1.88590	B	-1.38419	0.32406	-1.14528
C	1.73278	2.81056	-2.28605	Cu	-1.28901	-0.89199	0.70183
C	1.54646	4.22130	-2.48783	Cu	2.70541	0.03027	2.02158
C	0.32979	4.83965	-2.30420	Cu	0.81481	2.64968	1.97908
C	2.99374	2.20749	-2.45458	H	0.27436	-5.44125	-0.84045

H	-5.14017	2.00727	-0.91854	H	3.84552	2.82065	-2.76031
H	-6.13913	-0.20426	-0.67650	H	5.31686	0.87011	-2.62240
H	-4.43075	-4.77571	-0.55684	H	5.69726	-1.53590	-2.20711
H	-2.14383	-5.70782	-0.64485	H	4.70203	-3.85500	-1.61856
H	-5.96297	-2.66471	-0.56357	H	2.70104	-5.22297	-1.11818
H	-4.19402	4.23448	-1.29543	C	-1.06777	-0.49504	3.43229
H	-2.28469	5.69981	-1.87457	O	-1.85317	-1.37934	2.63308
H	0.22614	5.91347	-2.47698	O	-1.41600	-0.33318	4.58902
H	2.41386	4.80929	-2.79911	H	-2.68916	-1.64533	3.08754

***H_2O + *CO**

C	0.14809	-2.41220	1.37250	C	4.62142	2.34191	1.20807
C	-1.25885	-2.43678	1.55917	C	5.31349	1.14887	1.23841
C	-1.99704	-3.63393	1.68635	C	4.62344	-0.09645	1.30471
C	-1.27460	-4.86366	1.62311	C	3.20486	-0.05139	1.35540
C	0.09565	-4.87468	1.47500	C	2.46393	1.16022	1.30167
C	0.86603	-3.66612	1.37185	C	2.38985	-1.21422	1.34417
C	-1.84346	-1.13711	1.66137	C	3.03094	-2.50103	1.31221
C	-3.26817	-1.05431	1.89969	C	4.46746	-2.53259	1.28341
C	-4.00538	-2.28394	2.00903	C	5.23334	-1.38497	1.27463
C	-3.40430	-3.51891	1.90622	Cu	1.73358	-0.02110	-0.51753
C	-3.90334	0.19433	2.01676	O	3.36535	-0.00845	-1.80823
C	-3.18620	1.39537	1.86585	C	0.82054	-0.04631	-3.90732
C	-1.76044	1.37913	1.63968	O	1.43225	-0.06676	-4.88301
C	-1.09519	2.62909	1.47735	B	0.84893	-1.01929	1.30133
C	-1.75430	3.87813	1.55111	Cu	-0.02421	-1.82786	-0.64392
C	-3.16558	3.86228	1.77094	Cu	-1.86251	-1.63753	-2.22787
C	-3.84382	2.67257	1.92129	Cu	-1.84419	1.60352	-2.25497
C	-0.95280	5.05369	1.43911	Cu	-0.00488	1.80750	-0.67193
C	0.41554	4.96816	1.29643	B	0.91318	1.06253	1.26610
C	1.10376	3.70806	1.24169	C	2.27245	-3.68692	1.31843
C	0.30640	2.50466	1.28793	Cu	-1.68366	-0.00148	-0.39834
C	2.50713	3.63451	1.19118	B	-0.91294	0.09216	1.61772
C	3.18585	2.40170	1.22963	Cu	-0.06328	-0.02599	-2.32075

H	2.78978	-4.64997	1.30510	H	-4.92309	2.68196	2.09526
H	3.08761	4.56003	1.14281	H	-4.98074	0.23372	2.19828
H	5.17034	3.28560	1.15223	H	-5.08170	-2.21549	2.18812
H	6.32342	-1.45394	1.23677	H	-4.00028	-4.42947	2.00663
H	4.95539	-3.51048	1.25755	H	-1.82437	-5.80416	1.71119
H	6.40588	1.14749	1.20256	H	0.63348	-5.82588	1.45177
H	1.01568	5.87998	1.23631	H	4.18269	-0.24499	-1.32355
H	-1.43869	6.03151	1.48526	H	3.28042	-0.68670	-2.50568
H	-3.70339	4.81194	1.83098				

***CO**

C	4.70516	-2.95721	0.71977	C	-4.25287	-0.96621	2.32343
C	4.52227	-1.54298	0.74201	C	-4.07721	-2.32493	2.19152
C	3.20148	-1.06324	0.93107	C	-2.79372	-2.87196	1.87621
C	2.07418	-1.92062	1.06442	C	-1.73454	-1.96407	1.67347
C	2.28451	-3.34296	1.02019	C	-1.87507	-0.54465	1.79118
C	3.63195	-3.81316	0.85331	C	-2.49142	-4.26637	1.78778
C	5.55460	-0.57082	0.59027	C	-1.20844	-4.70243	1.53836
C	5.26632	0.77778	0.60678	C	-0.11305	-3.79160	1.34514
C	3.93108	1.27996	0.77545	C	-0.40784	-2.37802	1.38716
C	2.87193	0.32077	0.94021	B	0.67241	-1.27755	1.22590
C	3.66906	2.66297	0.81049	Cu	-0.59564	-1.80298	-0.64659
C	2.37462	3.16749	1.02607	Cu	-0.25907	-0.00718	-2.32448
C	1.25681	2.26930	1.19242	Cu	-1.62469	0.42819	-0.25390
C	-0.01474	2.81316	1.51536	B	-0.61514	0.33806	1.65282
C	-0.24904	4.20236	1.62124	C	1.20734	-4.24001	1.15606
C	0.86181	5.07568	1.40907	Cu	0.46384	1.72408	-0.69796
C	2.11614	4.57696	1.13193	B	1.38613	0.72377	1.12920
C	-1.01307	1.82504	1.75835	Cu	1.53365	-0.53272	-0.68822
C	-2.33732	2.27747	2.10254	Cu	-2.43022	-1.03612	-2.05331
C	-2.56365	3.69382	2.19915	Cu	-1.50706	2.04364	-2.09929
C	-1.57075	4.62005	1.96681	H	1.40400	-5.31495	1.12675
C	-3.38057	1.35545	2.31263	H	4.49961	3.36385	0.69110
C	-3.17908	-0.02509	2.14645	H	6.07256	1.50626	0.48889

H	5.71342	-3.35822	0.59050	H	-4.37478	1.72235	2.58065
H	3.79425	-4.89381	0.82983	H	-5.23801	-0.56832	2.58043
H	6.58490	-0.90961	0.45655	H	-4.91897	-3.00466	2.34457
H	2.95654	5.26181	0.99302	H	-3.29675	-4.99029	1.93499
H	0.70579	6.15470	1.48411	H	-0.99622	-5.77355	1.49314
H	-1.78299	5.68835	2.05460	C	0.51781	-0.26660	-3.94476
H	-3.56931	4.03002	2.46479	O	1.09344	-0.46108	-4.92394

***CHO + *H_2O**

C	5.31666	-0.86893	1.27498	C	-1.59947	-3.90488	1.62429
C	4.56709	0.34266	1.35711	C	-3.00225	-3.95592	1.89658
C	3.15803	0.23439	1.36289	C	-3.73199	-2.79765	2.04614
C	2.46967	-1.00611	1.26933	C	-0.74825	-5.04798	1.49146
C	3.24663	-2.20933	1.19228	C	0.60517	-4.89917	1.29668
C	4.67839	-2.08790	1.19128	C	1.22835	-3.60553	1.20223
C	2.29093	1.35792	1.32392	C	0.37614	-2.43867	1.24243
C	2.87454	2.66854	1.31293	B	0.91613	-0.97075	1.21713
C	4.30850	2.76817	1.34305	Cu	0.04220	-1.78003	-0.72715
C	5.12415	1.65765	1.36467	Cu	-0.09037	0.04760	-2.35242
C	2.06367	3.81917	1.28850	Cu	-1.72432	-0.00541	-0.39474
C	0.66134	3.73285	1.30140	B	-0.93686	-0.09275	1.61418
C	-0.16192	4.91002	1.39039	C	2.62412	-3.47163	1.14386
C	-1.52683	4.84000	1.54484	Cu	-0.10352	1.89025	-0.72541
C	-2.19039	3.57468	1.63697	B	0.76256	1.08659	1.24985
C	-1.40376	2.41448	1.51304	Cu	1.70780	0.13294	-0.55020
C	0.00034	2.44677	1.29643	O	3.38070	0.17478	-1.74691
C	-3.58918	3.40190	1.88395	Cu	-1.85266	-1.62001	-2.21997
C	-4.12986	2.14342	2.01964	Cu	-1.96094	1.58011	-2.23974
C	-3.33581	0.94879	1.91864	C	1.04559	-0.12214	-3.86742
C	-1.92348	1.09265	1.64856	O	2.26434	-0.21160	-4.07360
C	-3.90863	-0.32469	2.07845	H	3.24469	-4.37084	1.09747
C	-3.13550	-1.49366	1.94595	H	2.53527	4.80537	1.28704
C	-1.72152	-1.41566	1.68799	H	4.74935	3.76828	1.33751
C	-1.00742	-2.63094	1.50861	H	6.40801	-0.81773	1.26397

H	5.26766	-3.00586	1.12203	H	-4.80420	-2.85409	2.25159
H	6.21055	1.77316	1.36933	H	-3.48918	-4.92957	1.99076
H	0.33475	5.88275	1.35605	H	-1.18643	-6.04588	1.56892
H	-2.11988	5.75440	1.62327	H	1.24860	-5.78038	1.23102
H	-4.22284	4.28683	1.97862	H	3.95839	-0.56590	-1.48029
H	-5.19827	2.02723	2.21973	H	3.06490	-0.03695	-2.68714
H	-4.97926	-0.41097	2.28266	H	0.40295	-0.16771	-4.79556

***CH_2O + *H_2O alternative pathway higher in free energy**

C	0.43555	-2.57263	1.10213	C	4.69396	0.12855	1.14839
C	-0.95291	-2.74380	1.33809	C	5.27161	1.42999	1.19051
C	-1.57941	-4.01055	1.37945	C	4.47736	2.55602	1.27375
C	-0.75631	-5.15794	1.17285	C	2.56389	-1.17987	1.13152
C	0.60260	-5.03020	0.98008	C	3.31119	-2.39722	0.97237
C	1.26021	-3.75243	0.96759	C	4.74429	-2.30084	0.92464
C	-2.97866	-4.04028	1.66452	C	5.41009	-1.09470	1.00894
C	-3.67622	-2.87853	1.91297	Cu	1.72693	0.09389	-0.57294
C	-3.05147	-1.58362	1.90326	O	2.99528	0.19839	-2.18672
C	-1.63734	-1.51823	1.60268	B	1.00940	-1.11637	1.15322
C	-3.78369	-0.41400	2.17290	Cu	0.09646	-1.81318	-0.82568
C	-3.18338	0.85591	2.09609	Cu	-1.85719	-1.64321	-2.26883
C	-3.94678	2.05832	2.29318	Cu	-2.11174	1.54591	-1.99653
C	-3.38427	3.31401	2.21742	Cu	-0.16216	1.78761	-0.52674
C	-1.99378	3.47788	1.93764	B	0.89189	0.94984	1.29566
C	-1.23224	2.30639	1.71990	C	2.65954	-3.64250	0.88341
C	-1.77490	0.98784	1.80147	Cu	-1.68928	-0.17477	-0.30424
C	0.16445	2.32654	1.46437	B	-0.81122	-0.21250	1.65875
C	0.85386	3.59644	1.50080	Cu	-0.19870	0.11936	-2.29992
C	0.05880	4.77793	1.69155	C	0.43394	1.58383	-3.65103
C	-1.30380	4.72642	1.89637	O	0.93766	0.41514	-3.94381
C	2.25642	3.65339	1.40801	H	3.25825	-4.55078	0.77227
C	3.04238	2.48800	1.32163	H	2.75092	4.62815	1.43275
C	2.43307	1.18581	1.29635	H	4.94053	3.54594	1.29881
C	3.27746	0.04585	1.22161	H	6.50154	-1.06660	0.95741

H	5.31320	-3.22726	0.80989	H	-3.49150	-5.00501	1.69776
H	6.35912	1.52910	1.14450	H	-1.21644	-6.14915	1.18827
H	0.57237	5.74277	1.69133	H	1.22061	-5.92297	0.85256
H	-1.87021	5.64880	2.04829	H	3.49893	-0.63443	-2.26805
H	-3.99864	4.20239	2.38370	H	2.38199	0.21580	-2.98109
H	-5.01188	1.95127	2.51542	H	-0.42059	1.95629	-4.23997
H	-4.84961	-0.49188	2.40345	H	1.04890	2.32790	-3.11978
H	-4.74503	-2.92549	2.13809				

***HCOO**

C	5.22826	-1.48409	1.09422	C	-3.41398	-3.46172	2.00745
C	4.63961	-0.18444	1.12313	C	-2.01640	-3.59727	1.73901
C	3.22786	-0.11241	1.19947	C	-1.26510	-2.41351	1.59171
C	2.38578	-1.25606	1.22373	C	-1.82016	-1.10918	1.71870
C	3.00434	-2.55060	1.18769	C	-1.31829	-4.84310	1.64947
C	4.43850	-2.61347	1.12438	C	0.04375	-4.87465	1.45912
C	5.35694	1.04730	1.05755	C	0.82820	-3.67608	1.32638
C	4.68659	2.25180	1.05189	C	0.13495	-2.40814	1.34419
C	3.25378	2.33549	1.10860	B	0.84711	-1.02237	1.24458
C	2.50862	1.11185	1.17753	Cu	-0.19276	-1.82675	-0.63699
C	2.59914	3.58192	1.12008	Cu	-0.19500	-0.01289	-2.34908
C	1.20131	3.67784	1.20790	Cu	-1.68029	0.15494	-0.38328
C	0.38192	2.48807	1.24679	B	-0.86867	0.10000	1.62329
C	-1.00854	2.64088	1.49151	C	2.22809	-3.72416	1.23107
C	-1.63350	3.89768	1.61789	Cu	0.05771	1.88501	-0.74097
C	-0.81190	5.06412	1.50821	B	0.95624	1.03579	1.19736
C	0.54589	4.95358	1.31828	Cu	1.68493	-0.07122	-0.59915
C	-1.69282	1.40210	1.65658	Cu	-2.05820	-1.55158	-2.12340
C	-3.10839	1.44495	1.93875	Cu	-1.81706	1.78844	-2.23175
C	-3.73608	2.73387	2.03908	H	2.72837	-4.69588	1.20920
C	-3.03792	3.91069	1.88828	H	3.19509	4.49784	1.07992
C	-3.84376	0.25927	2.11467	H	5.24993	3.18677	0.99653
C	-3.23067	-1.00167	1.99293	H	6.31546	-1.57385	1.03754
C	-3.98724	-2.21561	2.13091	H	4.90309	-3.60238	1.09496

H	6.44772	1.02356	1.00295	H	-4.02068	-4.36229	2.12653
H	1.16662	5.85153	1.26398	H	-1.88198	-5.77320	1.75349
H	-1.27724	6.04844	1.59782	H	0.56797	-5.83252	1.41780
H	-3.54975	4.87077	1.98791	O	2.88102	-0.23478	-2.17628
H	-4.80754	2.76269	2.25362	O	1.21342	-0.19617	-3.72087
H	-4.91356	0.31969	2.33087	C	2.42813	-0.26815	-3.36218
H	-5.05561	-2.12625	2.34436	H	3.17571	-0.37205	-4.17263

***HCOOH**

C	0.03250	-2.42002	1.36615	C	4.51556	-0.10658	1.45673
C	-1.38306	-2.44139	1.46430	C	3.09570	-0.05869	1.43193
C	-2.12956	-3.63661	1.55722	C	2.35887	1.15473	1.35348
C	-1.40574	-4.86692	1.54713	C	2.27715	-1.22061	1.40862
C	-0.02874	-4.88087	1.47820	C	2.91674	-2.50988	1.43489
C	0.74878	-3.67418	1.40973	C	4.35282	-2.54206	1.48695
C	-1.96946	-1.13726	1.51804	C	5.12143	-1.39561	1.49331
C	-3.40473	-1.05073	1.69044	Cu	1.64595	-0.03626	-0.43645
C	-4.14967	-2.27959	1.75839	O	3.08290	-0.09469	-2.01491
C	-3.54701	-3.51655	1.69217	C	2.73330	-0.09448	-3.30962
C	-4.03944	0.19882	1.79178	O	1.55533	-0.06336	-3.64333
C	-3.31193	1.39959	1.68892	Cu	-0.01540	-0.04266	-2.32409
C	-1.87799	1.38256	1.53031	Cu	-1.80182	1.59813	-2.34884
C	-1.20517	2.63314	1.41534	Cu	-0.06403	1.81165	-0.68026
C	-1.86550	3.88389	1.46774	B	0.80555	1.06452	1.27969
C	-3.28488	3.86846	1.61968	B	0.73395	-1.02747	1.32242
C	-3.97027	2.67750	1.72627	Cu	-0.05040	-1.88323	-0.66705
C	-1.05670	5.05735	1.40015	Cu	-1.78439	-1.70476	-2.34272
C	0.31679	4.96979	1.31334	Cu	-1.70510	-0.04907	-0.51747
C	1.00531	3.70894	1.27730	B	-1.02989	0.09120	1.52892
C	0.20352	2.50796	1.28894	C	2.15663	-3.69484	1.43044
C	2.40980	3.63108	1.27692	H	2.67309	-4.65802	1.46336
C	3.08539	2.39651	1.32381	H	2.99381	4.55573	1.26410
C	4.52027	2.33245	1.36928	H	5.07319	3.27545	1.35131
C	5.20851	1.13751	1.42971	H	6.21168	-1.46789	1.52447

H	4.83916	-3.52079	1.51662	H	-5.23405	-2.20858	1.87849
H	6.30134	1.13564	1.45576	H	-4.15125	-4.42485	1.76038
H	0.92001	5.88123	1.28351	H	-1.96034	-5.80672	1.61016
H	-1.54137	6.03648	1.43197	H	0.50733	-5.83328	1.49386
H	-3.82462	4.81813	1.66168	H	3.56989	-0.12531	-4.02403
H	-5.05677	2.68616	1.84775	H	4.05801	-0.12343	-1.89107
H	-5.12438	0.24029	1.92100				

***H_2COOH**

C	5.13559	-1.71438	1.11441	C	-2.15417	-3.73260	1.56035
C	4.56868	-0.40756	1.20893	C	-3.55551	-3.58507	1.79910
C	3.15882	-0.31525	1.28789	C	-4.11261	-2.33448	1.95152
C	2.29750	-1.44492	1.23155	C	-1.47394	-4.98388	1.42339
C	2.89434	-2.74729	1.13693	C	-0.10909	-5.02894	1.25669
C	4.32802	-2.83070	1.08418	C	0.69679	-3.83876	1.19379
C	2.45926	0.92089	1.32797	C	0.02366	-2.56205	1.25966
C	3.22412	2.13450	1.31368	B	0.76124	-1.18673	1.23621
C	4.65552	2.02900	1.25420	Cu	-0.29495	-1.83561	-0.69157
C	5.30571	0.81466	1.20113	Cu	-1.61968	0.25496	-0.43725
C	2.58967	3.39055	1.36248	B	-0.95332	-0.05305	1.58995
C	1.19115	3.50666	1.41002	C	2.09700	-3.90673	1.11362
C	0.54943	4.78835	1.54132	Cu	0.20993	1.88057	-0.69110
C	-0.81280	4.91262	1.68105	B	0.90847	0.87392	1.31320
C	-1.65689	3.75595	1.70415	Cu	1.65682	-0.19916	-0.52328
C	-1.04690	2.49780	1.55024	Cu	-0.09919	0.00348	-2.38814
C	0.35262	2.32958	1.37509	Cu	-2.09312	-1.36954	-2.21502
C	-3.07275	3.78132	1.91254	Cu	-1.60071	1.91372	-2.25677
C	-3.79489	2.61230	1.98625	O	3.05926	-0.12381	-1.99737
C	-3.18337	1.31690	1.86038	C	2.52440	0.46355	-3.27862
C	-1.75803	1.26259	1.61689	O	1.37757	-0.17919	-3.60527
C	-3.93592	0.13852	1.99249	H	2.58035	-4.88522	1.05019
C	-3.33285	-1.12937	1.87682	H	3.20102	4.29708	1.37129
C	-1.91779	-1.25198	1.66113	H	5.23490	2.95575	1.24294
C	-1.38024	-2.55535	1.49039	H	6.22147	-1.81916	1.05736

H	4.77690	-3.82451	1.01004	H	-5.18614	-2.23493	2.13265
H	6.39601	0.77589	1.14459	H	-4.17994	-4.47905	1.86520
H	1.18470	5.67775	1.54779	H	-2.05407	-5.90858	1.47065
H	-1.26702	5.90007	1.79160	H	0.40010	-5.99255	1.17742
H	-3.57348	4.74529	2.03012	H	3.32012	0.28522	-4.02875
H	-4.87308	2.65071	2.16210	H	3.83879	0.40319	-1.72328
H	-5.01193	0.20850	2.17262	H	2.40590	1.54826	-3.07863

***CH_2O + *H_2O**

C	-0.01810	-2.39760	1.39298	C	4.57507	-0.31591	1.39923
C	-1.43185	-2.35201	1.51278	C	5.33087	0.88978	1.33149
C	-2.23588	-3.50602	1.61549	C	4.70331	2.11704	1.26348
C	-1.57571	-4.77266	1.57965	C	2.28070	-1.31340	1.43332
C	-0.20330	-4.85501	1.48461	C	2.85405	-2.63171	1.42056
C	0.63399	-3.68799	1.41640	C	4.28783	-2.73942	1.41233
C	-3.64292	-3.31364	1.78476	C	5.11570	-1.63531	1.40361
C	-4.17950	-2.04917	1.88262	Cu	1.70135	-0.08392	-0.47616
C	-3.37293	-0.85919	1.81194	O	3.24135	-0.69270	-1.74596
C	-1.95038	-1.01915	1.58725	C	2.03992	0.71053	-4.18821
C	-3.93154	0.41863	1.97446	O	1.07030	-0.01493	-3.95632
C	-3.14049	1.58085	1.88592	Cu	-0.07047	-0.04786	-2.30221
C	-3.72860	2.88997	1.97652	Cu	-1.83832	1.63082	-2.22053
C	-2.98659	4.04533	1.85656	Cu	-1.85478	-1.70583	-2.24780
C	-1.57864	3.98932	1.62846	Cu	-1.70602	-0.04643	-0.43775
C	-0.98819	2.70575	1.52795	Cu	-0.01823	1.77080	-0.63251
C	-1.71868	1.49350	1.67714	B	0.92855	1.03229	1.24903
C	0.39923	2.50807	1.30135	B	0.75336	-1.04319	1.35749
C	1.26097	3.66585	1.26561	Cu	-0.05845	-1.87643	-0.64167
C	0.64401	4.96069	1.35322	C	2.03806	-3.77939	1.41353
C	-0.71536	5.12005	1.52064	B	-0.94825	0.15956	1.59610
C	2.65848	3.51857	1.20548	H	2.50636	-4.76727	1.41739
C	3.27309	2.25228	1.24526	H	3.28618	4.41352	1.16939
C	2.48672	1.05022	1.30665	H	5.30210	3.03057	1.21665
C	3.15952	-0.19617	1.41740	H	6.20104	-1.76326	1.38847

H	4.72152	-3.74291	1.40562	H	-4.29073	-4.19096	1.85785
H	6.42234	0.83102	1.32689	H	-2.17630	-5.68375	1.64417
H	1.29282	5.83916	1.29998	H	0.28397	-5.83342	1.48117
H	-1.14518	6.12279	1.58826	H	2.63645	0.54451	-5.10457
H	-3.47213	5.02122	1.93891	H	3.91317	-1.16842	-1.21531
H	-4.80704	2.95315	2.14534	H	2.32708	1.53079	-3.50465
H	-5.00762	0.51618	2.14294	H	2.88729	-1.36893	-2.35610
H	-5.25468	-1.92449	2.03697				

***CH_3OH + *OH**

C	5.09359	-2.11877	1.03081	C	-3.70396	-3.32652	1.74724
C	4.62929	-0.77311	1.12788	C	-2.32432	-3.57369	1.46144
C	3.23063	-0.57168	1.20237	C	-1.46386	-2.46029	1.40038
C	2.28516	-1.63009	1.15689	C	-1.89375	-1.12020	1.63395
C	2.77757	-2.97083	1.03864	C	-1.74637	-4.87069	1.27962
C	4.20022	-3.16746	0.98766	C	-0.39132	-5.01638	1.09561
C	5.45894	0.38824	1.12340	C	0.50421	-3.89063	1.06001
C	4.90293	1.64804	1.17960	C	-0.06751	-2.56603	1.16122
C	3.48295	1.86192	1.24367	B	0.77744	-1.25207	1.18565
C	2.62737	0.71195	1.24376	Cu	-0.29322	-1.82352	-0.79413
C	2.94765	3.16075	1.33693	Cu	-1.72268	0.15268	-0.32173
C	1.56637	3.37924	1.45579	B	-0.82425	-0.00728	1.65691
C	0.64016	2.26977	1.43676	C	1.89420	-4.06623	0.98963
C	-0.72029	2.53202	1.75357	Cu	0.15477	1.75527	-0.54972
C	-1.22446	3.83191	1.96858	B	1.07369	0.77849	1.26351
C	-0.30221	4.92341	1.89677	Cu	1.69571	-0.27200	-0.61707
C	1.03455	4.69987	1.66181	Cu	-0.35995	0.12598	-2.35712
C	-1.51491	1.35660	1.85750	Cu	-2.20166	-1.42461	-2.18386
C	-2.91593	1.51081	2.15335	Cu	-1.78964	2.04761	-1.91317
C	-3.41834	2.84066	2.36160	O	2.81219	-0.37054	-2.23104
C	-2.61505	3.95601	2.27481	O	1.02458	0.26181	-3.77573
C	-3.76823	0.39109	2.21320	C	1.31964	1.59289	-4.23410
C	-3.28689	-0.90300	1.94660	H	2.30100	-5.07820	0.91345
C	-4.15639	-2.04768	1.98203	H	3.62601	4.01823	1.34583

H	5.55065	2.52854	1.17313	H	-5.21104	-1.87779	2.21408
H	6.16836	-2.30735	0.97955	H	-4.39369	-4.17241	1.79522
H	4.56929	-4.19311	0.90683	H	-2.39600	-5.74849	1.31323
H	6.54316	0.26660	1.06783	H	0.04253	-6.01426	0.99288
H	1.73457	5.53888	1.64320	H	3.06195	-1.30201	-2.37012
H	-0.67179	5.93964	2.05295	H	1.89785	-0.06701	-3.14690
H	-3.03418	4.95062	2.44482	H	2.21018	1.56752	-4.88556
H	-4.48069	2.95340	2.59354	H	0.46501	1.97779	-4.80946
H	-4.82675	0.53390	2.44616	H	1.51051	2.27220	-3.38503

***CH_3OH + *H_2O**

C	-0.49135	-2.43325	1.35486	C	5.03842	1.04082	1.58692
C	-1.86588	-2.11973	1.54704	C	5.40630	-0.28819	1.52611
C	-2.88686	-3.10303	1.58601	C	4.42393	-1.31697	1.45130
C	-2.48782	-4.46612	1.46238	C	3.06118	-0.91666	1.46885
C	-1.15796	-4.80576	1.32281	C	2.65319	0.44224	1.50965
C	-0.11119	-3.82278	1.27823	C	1.97639	-1.82946	1.35640
C	-2.11496	-0.72751	1.69114	C	2.27481	-3.23332	1.25511
C	-3.47696	-0.29295	1.83591	C	3.65784	-3.62362	1.23834
C	-4.50283	-1.29879	1.88065	C	4.68932	-2.71149	1.33268
C	-4.22623	-2.64486	1.76157	Cu	1.65985	-0.48071	-0.40342
C	-3.79415	1.07958	1.89922	O	3.02770	-0.83880	-1.90210
C	-2.80213	2.06730	1.78369	B	0.53069	-1.24682	1.33714
C	-1.40606	1.70279	1.61774	B	1.13024	0.74334	1.42925
C	-0.43423	2.75588	1.61210	Cu	0.76453	1.87156	-0.54516
C	-0.76846	4.12117	1.73592	Cu	-0.85655	2.50090	-2.21648
C	-2.15624	4.45113	1.83885	Cu	-0.02435	0.21323	-2.20176
C	-3.12143	3.46969	1.85726	O	1.17515	-0.23166	-3.83953
C	0.30672	5.05967	1.77245	C	1.53199	0.86848	-4.72418
C	1.61809	4.63898	1.71118	C	1.24413	-4.19089	1.20595
C	1.97516	3.25009	1.60476	Cu	-1.52524	0.95637	-0.41892
C	0.90044	2.28667	1.52088	Cu	-2.30156	-0.61500	-2.15095
C	3.31708	2.82642	1.61660	Cu	-0.73698	-1.38818	-0.47334
C	3.66450	1.46183	1.56730	B	-0.90837	0.23626	1.61311

H	1.50597	-5.25060	1.13903	H	-5.53701	-0.96594	2.00405
H	4.11054	3.57669	1.67362	H	-5.03698	-3.37709	1.79766
H	5.80838	1.81502	1.64109	H	-3.25255	-5.24675	1.48856
H	5.72680	-3.05551	1.31477	H	-0.87125	-5.85810	1.24797
H	3.88461	-4.68972	1.15139	H	3.29774	-1.77769	-1.89259
H	6.46375	-0.56513	1.52788	H	2.51642	-0.71845	-2.74646
H	2.42785	5.37186	1.76003	H	2.28866	0.52648	-5.44438
H	0.07671	6.12449	1.86157	H	0.63765	1.23508	-5.24676
H	-2.44453	5.50272	1.91675	H	1.94247	1.65776	-4.08414
H	-4.17453	3.74597	1.95721	H	0.83927	-0.97104	-4.38087
H	-4.83761	1.38382	2.01787				

***CH_3OH**

C	-2.62008	-4.99164	-0.75640	C	2.55369	2.58371	-2.27313
C	-3.13080	-3.67104	-0.92668	C	3.01254	1.28498	-1.99441
C	-2.18587	-2.62346	-1.07250	C	2.08660	0.22779	-1.65780
C	-0.78063	-2.83498	-1.01822	C	2.62816	-1.06852	-1.39749
C	-0.29184	-4.17447	-0.83346	C	4.00513	-1.36791	-1.46170
C	-1.26172	-5.22819	-0.71591	C	4.89723	-0.29528	-1.77440
C	-2.55323	-1.25618	-1.21459	C	4.41577	0.96853	-2.03080
C	-3.95332	-0.92214	-1.22811	C	4.39493	-2.72598	-1.24444
C	-4.89815	-1.99752	-1.10145	C	3.45736	-3.70767	-1.00984
C	-4.51103	-3.31295	-0.95575	C	2.04879	-3.42500	-0.95968
C	-4.38117	0.40989	-1.38798	C	1.64013	-2.04974	-1.12466
C	-3.46843	1.46785	-1.55096	B	0.15424	-1.60356	-1.14001
C	-3.90104	2.81979	-1.77876	Cu	1.30159	-1.25264	0.81986
C	-3.01240	3.84693	-2.01006	B	0.55292	0.40410	-1.66290
C	-1.60326	3.60853	-2.04845	Cu	1.02746	1.17482	0.29315
C	-1.16105	2.29001	-1.81290	Cu	2.35409	0.42105	2.21675
C	-2.04646	1.21648	-1.53449	Cu	-0.06784	0.17812	2.30329
C	-0.60870	4.59370	-2.33803	O	-0.85369	-0.23261	4.15983
C	0.72293	4.25063	-2.41073	C	-1.81322	0.73082	4.67271
C	1.18772	2.90724	-2.19112	C	1.09041	-4.44312	-0.80278
C	0.21068	1.89457	-1.87146	Cu	-1.44372	1.22024	0.50546

Cu	-0.07692	2.59855	1.94994	H	-0.92141	5.62548	-2.51695
B	-1.42691	-0.19229	-1.33251	H	1.46963	5.01353	-2.64609
Cu	-1.17128	-1.25176	0.59551	H	3.27646	3.36436	-2.52500
H	1.42858	-5.47567	-0.67913	H	5.11073	1.77464	-2.28043
H	-5.45310	0.62459	-1.40509	H	5.97060	-0.49486	-1.82262
H	-5.96148	-1.74478	-1.11976	H	5.45676	-2.98217	-1.28283
H	-3.32383	-5.82162	-0.65573	H	3.77727	-4.74346	-0.86952
H	-0.89211	-6.24894	-0.58668	H	-2.22513	0.36411	5.62468
H	-5.26453	-4.09843	-0.85710	H	-1.33838	1.71375	4.81352
H	-4.97575	3.01929	-1.77582	H	-2.60883	0.80853	3.92227
H	-3.38172	4.86118	-2.18182	H	-0.14768	-0.33237	4.82601

***H_2O**		+		***OH**		+	***CH_4**
C	-3.40788	-4.32758	-0.97654	C	3.12989	2.18391	-2.12363
C	-3.65454	-2.92506	-1.07932	C	3.33761	0.81922	-1.86320
C	-2.52814	-2.07324	-1.16815	C	2.22177	-0.05525	-1.56302
C	-1.18929	-2.54179	-1.12987	C	2.49461	-1.44686	-1.38471
C	-0.96869	-3.95474	-1.01867	C	3.78295	-2.00335	-1.46769
C	-2.11879	-4.81390	-0.94721	C	4.87196	-1.10938	-1.72413
C	-2.61951	-0.65693	-1.22028	C	4.65203	0.23559	-1.91186
C	-3.92523	-0.06386	-1.21037	C	3.90660	-3.42214	-1.32028
C	-5.06399	-0.93712	-1.13631	C	2.79416	-4.21052	-1.13976
C	-4.94195	-2.30847	-1.07390	C	1.46631	-3.65798	-1.08190
C	-4.08575	1.33189	-1.28629	C	1.32504	-2.22164	-1.16202
C	-2.98336	2.19074	-1.41174	B	-0.04962	-1.48302	-1.16877
C	-3.16133	3.60685	-1.58409	Cu	1.07835	-1.60489	0.83978
C	-2.10371	4.45765	-1.81203	Cu	2.63973	-0.51138	2.27830
C	-0.76921	3.95320	-1.90767	Cu	1.64457	0.76214	0.41576
C	-0.57737	2.56501	-1.72605	B	0.74842	0.40648	-1.59664
C	-1.64035	1.66840	-1.42201	C	0.33479	-4.48510	-0.99886
C	0.38582	4.73967	-2.20478	Cu	-0.74481	1.44299	0.49188
C	1.62937	4.15269	-2.29627	Cu	0.29943	0.18792	2.41330
C	1.83497	2.74460	-2.09750	O	-0.86853	-0.40222	3.85627
C	0.68536	1.92693	-1.83601	C	-3.39277	1.69637	2.09716

B	-1.29118	0.15430	-1.26181	H	2.50514	4.76869	-2.51673
Cu	-1.36337	-1.01430	0.61400	H	3.98898	2.82474	-2.33808
O	-2.35893	-1.61181	2.25794	H	5.49447	0.89920	-2.12348
Cu	0.83541	2.51575	1.92885	H	5.88501	-1.51409	-1.78551
H	0.46903	-5.56778	-0.92824	H	4.90061	-3.87241	-1.37040
H	-5.09440	1.75320	-1.27215	H	2.89799	-5.29490	-1.05386
H	-6.05657	-0.47980	-1.12527	H	-2.23895	-2.57256	2.37612
H	-4.25671	-5.01227	-0.91178	H	-1.75705	-1.14351	3.02850
H	-1.94609	-5.88982	-0.86222	H	-4.46682	1.87838	2.25254
H	-5.83232	-2.93840	-1.00983	H	-2.93025	1.35946	3.03425
H	-4.18032	3.99890	-1.53904	H	-3.26800	0.92304	1.32474
H	-2.27481	5.52877	-1.94212	H	-0.37944	-1.08052	4.35679
H	0.27095	5.81480	-2.36146	H	-2.91334	2.62941	1.76565

***H_2O + *OH**

C	5.46552	-1.14581	0.62131	C	-3.77779	2.19424	2.25739
C	4.77335	0.09145	0.78399	C	-3.19141	3.43303	2.13829
C	3.36828	0.03622	0.93825	C	-3.64483	-0.28367	2.26603
C	2.62731	-1.17579	0.91042	C	-2.91187	-1.47840	2.11073
C	3.34817	-2.40479	0.74928	C	-3.54686	-2.76138	2.23229
C	4.77581	-2.33901	0.60280	C	-2.87356	-3.94377	2.01482
C	5.38043	1.38401	0.77905	C	-1.49211	-3.93850	1.65091
C	4.61130	2.52171	0.89519	C	-0.85835	-2.68067	1.53647
C	3.18066	2.47522	1.03048	C	-1.51398	-1.44796	1.78655
C	2.54821	1.18812	1.05698	C	-0.70059	-5.10509	1.41197
C	2.42148	3.65526	1.14761	C	0.63601	-4.99678	1.10328
C	1.02458	3.62076	1.29566	C	1.29457	-3.72436	0.97957
C	0.31607	2.36088	1.30515	C	0.50143	-2.53009	1.14369
C	-1.07332	2.37789	1.60226	B	1.07916	-1.07934	1.06082
C	-1.80142	3.56122	1.81886	Cu	-0.26006	-1.66994	-0.63440
C	-1.09224	4.80200	1.73818	Cu	-2.26122	-1.52156	-1.93599
C	0.26111	4.82445	1.49264	Cu	-1.76517	0.27045	-0.33490
C	-1.64243	1.07235	1.71586	B	-0.70547	-0.14956	1.60282
C	-3.04211	0.97125	2.07541	C	2.67864	-3.64257	0.76745

B	1.01203	0.97478	1.15468	H	0.79573	5.77694	1.46034
Cu	0.05496	1.87517	-0.73797	H	-1.63979	5.73461	1.89324
Cu	-0.47031	0.06408	-2.42685	H	-3.78111	4.33818	2.30081
O	0.73867	-0.10945	-3.93913	H	-4.83674	2.11511	2.51628
Cu	1.70089	-0.01958	-0.77032	H	-4.70534	-0.33530	2.52567
O	2.75065	0.10802	-2.47813	H	-4.60718	-2.78306	2.49748
Cu	-1.91097	2.00209	-2.08471	H	-3.39284	-4.89974	2.11571
H	3.25525	-4.56344	0.64418	H	-1.16919	-6.08855	1.49483
H	2.93260	4.62159	1.13555	H	1.23654	-5.89729	0.95157
H	5.08993	3.50432	0.88107	H	3.12732	1.00239	-2.57599
H	6.55136	-1.13514	0.50205	H	0.71423	-1.04139	-4.22257
H	5.31810	-3.27893	0.47240	H	1.94859	0.03450	-3.20079
H	6.46456	1.46140	0.66897				

***2H_2O**

C	5.18338	-1.81497	0.91495	C	-3.38292	3.13328	2.05224
C	4.70642	-0.47290	0.92719	C	-2.60655	4.24635	1.81427
C	3.30475	-0.28329	1.06576	C	-3.67277	0.67898	2.24371
C	2.37959	-1.35839	1.17147	C	-3.17370	-0.63008	2.12453
C	2.88911	-2.70297	1.14653	C	-4.01898	-1.77570	2.33005
C	4.31007	-2.87859	1.01964	C	-3.55085	-3.06812	2.23583
C	5.50790	0.69483	0.77573	C	-2.18011	-3.33067	1.93118
C	4.93258	1.94910	0.73971	C	-1.34133	-2.21628	1.70333
C	3.51332	2.15260	0.84209	C	-1.78747	-0.86277	1.78785
C	2.68112	0.99188	1.00633	C	-1.58388	-4.62639	1.86384
C	2.95424	3.44464	0.80706	C	-0.23567	-4.77483	1.61771
C	1.57083	3.65751	0.95108	C	0.63686	-3.65097	1.41246
C	0.66313	2.54097	1.08664	C	0.04273	-2.33353	1.41700
C	-0.69712	2.80820	1.38773	B	0.86251	-1.01219	1.23738
C	-1.22317	4.11716	1.48414	Cu	-0.25994	-1.81062	-0.59104
C	-0.32252	5.20492	1.27632	Cu	-2.20130	-1.49906	-1.99807
C	1.01465	4.98055	1.02707	Cu	-1.65164	0.23319	-0.33090
C	-1.46481	1.63103	1.64127	B	-0.74272	0.26590	1.62719
C	-2.85798	1.79604	1.98605	C	2.02564	-3.80955	1.25678

Cu	0.17919	1.81754	-0.84271	H	1.69446	5.82750	0.90155
Cu	-0.25393	-0.08595	-2.35276	H	-0.70479	6.22729	1.33573
O	0.89581	-0.40487	-4.05596	H	-3.04229	5.24605	1.88936
B	1.12483	1.04583	1.07316	H	-4.43892	3.25194	2.30979
Cu	1.69104	-0.20258	-0.67120	H	-4.72408	0.83071	2.50392
O	2.97351	-0.49546	-2.26060	H	-5.06889	-1.59448	2.57596
Cu	-1.79168	1.79375	-2.23604	H	-4.22562	-3.91054	2.40882
H	2.44736	-4.81832	1.24607	H	-2.21165	-5.50700	2.02282
H	3.61585	4.30844	0.69745	H	0.20619	-5.77449	1.59231
H	5.56567	2.83270	0.62213	H	3.42020	-1.36085	-2.18463
H	6.25652	-1.99468	0.81073	H	2.38599	-0.56577	-3.05786
H	4.69590	-3.90138	1.00466	H	0.64099	-1.19946	-4.56276
H	6.59104	0.58550	0.67695	H	0.89957	0.33238	-4.69597

***H_2O**

C	5.17410	-1.82995	0.96069	C	11.26345	-0.77394	0.45522
C	4.69202	-0.49435	1.02941	C	9.86364	-0.41280	0.46265
C	3.31900	-0.17234	1.16959	C	11.65658	-2.11852	0.59439
C	2.39984	-1.25737	1.27881	C	10.71492	-3.15083	0.77073
C	2.84036	-2.56373	1.25445	C	11.12601	-4.52094	0.90983
C	4.22795	-2.90662	1.10870	C	10.22409	-5.55356	1.06011
C	5.72006	0.48279	0.92751	C	8.82222	-5.29889	1.10350
C	5.34109	1.86874	0.93873	C	8.40500	-3.94529	1.01411
C	3.94739	2.18355	1.09542	C	9.30693	-2.86556	0.82653
C	2.97545	1.21177	1.20286	C	7.03803	-3.55189	0.99356
C	6.30564	2.88341	0.77784	C	6.03201	-4.57279	1.10563
C	7.65962	2.58209	0.55915	C	6.46853	-5.93870	1.19043
C	8.11351	1.20385	0.50906	C	7.80286	-6.29130	1.18656
C	9.52425	0.96372	0.40855	Cu	7.77645	-2.81881	-0.98896
C	10.47892	1.99483	0.32564	O	7.98465	-4.58264	-2.07252
C	9.99561	3.34211	0.30963	B	6.71587	-2.04254	0.81368
C	8.65212	3.61741	0.41761	Cu	5.76112	-1.18147	-0.98981
C	11.85538	1.61405	0.27882	Cu	7.29288	-1.24115	-2.85798
C	12.22552	0.28868	0.33946	Cu	8.75833	0.61100	-3.38318

Cu	9.26391	-0.84642	-1.51225	H	13.28402	0.01706	0.31949
B	8.70882	-1.44798	0.62338	H	12.61807	2.39312	0.20340
C	4.66479	-4.24121	1.15141	H	10.71614	4.15941	0.22549
Cu	7.30194	0.74972	-1.40482	H	8.30673	4.65447	0.42544
B	7.17486	-0.00716	0.74134	H	5.98954	3.92969	0.80264
Cu	5.40832	0.27966	-2.89486	H	3.66279	3.23888	1.11711
H	3.92575	-5.04109	1.24984	H	1.92580	1.49521	1.31458
H	12.72120	-2.36641	0.57467	H	1.33469	-1.04003	1.39119
H	12.19721	-4.73720	0.87889	H	2.12142	-3.38146	1.35280
H	8.09206	-7.34354	1.24640	H	7.64596	-5.32421	-1.52951
H	5.70234	-6.71515	1.25861	H	7.41267	-4.57148	-2.86407
H	10.57911	-6.58418	1.13914				

d. Cu_7 cluster – C_2 pathway

***CO + *COOH + *H_2O**

C	4.99867	-1.92330	1.21146	C	-1.37249	2.05623	1.66074
C	4.59047	-0.57179	0.99045	C	-2.77250	2.33396	1.86077
C	3.23163	-0.26216	1.18786	C	-3.20423	3.69920	1.77110
C	2.25775	-1.21512	1.58912	C	-2.34844	4.73130	1.44834
C	2.69014	-2.57582	1.77669	C	-3.68420	1.29629	2.13509
C	4.08269	-2.87898	1.58635	C	-3.27039	-0.04230	2.22585
C	5.45710	0.49065	0.57166	C	-4.18984	-1.10222	2.55575
C	4.97837	1.76891	0.40477	C	-3.78195	-2.40341	2.72489
C	3.59447	2.10557	0.61968	C	-2.40613	-2.77307	2.56219
C	2.69107	1.03118	0.96115	C	-1.50235	-1.76158	2.21333
C	3.13425	3.42752	0.50806	C	-1.87952	-0.39996	2.02828
C	1.78822	3.76667	0.74873	C	-1.88391	-4.09696	2.73373
C	0.83137	2.75456	1.10663	C	-0.54282	-4.35130	2.57460
C	-0.51430	3.14804	1.33829	C	0.40107	-3.31603	2.23827
C	-0.96530	4.48528	1.20210	C	-0.10085	-1.97401	2.04387
C	0.00753	5.47096	0.85942	B	0.79971	-0.74527	1.78343
C	1.32555	5.12235	0.65225	Cu	0.44411	-1.57815	-0.14822

C	0.71950	-2.46931	-1.89453	H	5.65846	2.57129	0.10729
O	-0.23026	-3.41154	-2.18443	H	6.04889	-2.19108	1.07092
Cu	-2.59930	-1.31729	-2.13170	H	4.40542	-3.91192	1.74046
Cu	-0.32445	-0.33647	-2.08277	H	6.51375	0.27327	0.39748
C	-0.11369	-0.23878	-3.90929	H	2.05546	5.89155	0.38701
O	0.00731	-0.06663	-5.03989	H	-0.30776	6.51261	0.76137
C	1.77126	-3.58787	2.11410	H	-2.72699	5.75361	1.37352
Cu	-1.84583	-0.36863	-0.05304	H	-4.26224	3.90891	1.94887
B	-0.76051	0.63263	1.72378	H	-4.73864	1.53982	2.28917
Cu	-0.40074	1.63564	-0.37992	H	-5.24106	-0.83726	2.69393
B	1.17118	1.23857	1.19262	H	-4.50875	-3.17592	2.98810
Cu	1.70854	0.59844	-0.91730	H	-2.57001	-4.90494	2.99935
O	3.13095	-0.24534	-2.10846	H	-0.15674	-5.36465	2.71227
Cu	-2.22884	1.12770	-1.92662	H	3.95414	-0.35687	-1.59087
O	1.82706	-2.54942	-2.45042	H	2.76782	-1.17547	-2.24886
H	2.13187	-4.61006	2.25837	H	0.15361	-4.04347	-2.84079
H	3.84202	4.21523	0.23575				

***2CO + *2H_2O**

C	-0.38605	-1.91353	1.76481	C	-1.86890	5.01957	1.31747
C	-1.74686	-1.54165	1.91255	C	-2.83605	4.08690	1.62407
C	-2.78213	-2.46817	2.14270	C	0.56076	5.50328	0.77872
C	-2.41646	-3.84086	2.28538	C	1.84360	5.02575	0.61849
C	-1.09623	-4.23071	2.22052	C	2.16332	3.62937	0.73958
C	-0.03056	-3.29668	1.98400	C	1.07613	2.71033	0.98030
C	-1.95684	-0.12953	1.83254	C	3.49196	3.17130	0.67802
C	-3.30762	0.36624	1.98543	C	3.82135	1.82169	0.90516
C	-4.36230	-0.60142	2.14731	C	5.18614	1.37281	0.89416
C	-4.11683	-1.95542	2.22681	C	5.53381	0.05702	1.12250
C	-3.57153	1.74512	1.96997	C	4.53979	-0.92668	1.39743
C	-2.54534	2.68369	1.74642	C	3.18796	-0.49317	1.43514
C	-1.18117	2.26073	1.57427	C	2.79733	0.84779	1.17160
C	-0.21774	3.24315	1.21536	C	2.08930	-1.37697	1.61159
C	-0.51577	4.62165	1.09657	C	2.36382	-2.77851	1.79378

C	3.73792	-3.19983	1.78145	H	1.55869	-4.75738	2.13238
C	4.78185	-2.31958	1.58502	H	4.29313	3.88920	0.48133
B	0.65609	-0.78098	1.52827	H	5.96433	2.11140	0.68468
Cu	-0.24006	-1.90961	-0.43371	H	5.81117	-2.68633	1.56310
Cu	1.73538	-0.31072	-0.44393	H	3.94489	-4.26387	1.92331
O	3.29359	-1.01207	-1.64937	H	6.58295	-0.24736	1.08711
C	1.31934	-3.70141	1.98206	H	2.66104	5.71978	0.40532
B	1.27318	1.16835	1.15101	H	0.35791	6.57261	0.67766
Cu	0.46240	1.79648	-0.86173	H	-2.13147	6.07750	1.23522
Cu	-1.52765	1.84301	-2.21623	H	-3.87071	4.40817	1.77239
Cu	-1.45854	0.34194	-0.25291	H	-4.60109	2.09529	2.08575
B	-0.72554	0.79431	1.69006	H	-5.38683	-0.22886	2.23066
C	0.73335	-3.27514	-1.23710	H	-4.94402	-2.65433	2.37474
O	1.40757	-3.89567	-1.93501	H	-3.19940	-4.58300	2.46180
Cu	-2.34630	-1.38129	-1.65175	H	-0.83140	-5.28183	2.36085
Cu	-0.23480	-0.19934	-2.24747	H	4.02815	-1.30640	-1.07184
C	0.73761	-0.86571	-3.62050	H	3.05416	-1.80320	-2.16964
O	1.39962	-1.41929	-4.38884	H	-4.41635	-1.80853	-0.27939
O	-4.28240	-1.95301	-1.24317	H	-4.43873	-2.90910	-1.37251

***OCCOH + *2H_2O**

C	5.11380	1.14462	1.57259	C	-3.14937	4.40963	1.14469
C	4.02240	2.01263	1.26414	C	-3.39772	3.02539	1.39221
C	2.72401	1.47146	1.32662	C	-2.28327	2.15811	1.40782
C	2.45130	0.12751	1.70035	C	-0.95342	2.59565	1.13007
C	3.57140	-0.74155	1.95668	C	-4.68345	2.43702	1.60959
C	4.89036	-0.17437	1.90086	C	-4.81117	1.07829	1.78671
C	1.55182	2.22549	1.02669	C	-3.67885	0.18832	1.78466
C	1.69600	3.64613	0.79959	C	-2.37129	0.76196	1.65311
C	3.03241	4.17458	0.70433	C	-3.85543	-1.20914	1.83726
C	4.14697	3.39666	0.91319	C	-2.76384	-2.08677	1.76832
C	0.57888	4.48841	0.71709	C	-1.41085	-1.57790	1.67315
C	-0.72822	4.00138	0.90711	C	-0.34009	-2.50593	1.84081
C	-1.87010	4.87224	0.91828	C	-0.52308	-3.88360	1.98798

C	-1.86946	-4.38079	1.93401	H	3.14458	5.23705	0.47370
C	-2.93658	-3.51673	1.83673	H	6.13229	1.53919	1.53949
C	0.64683	-4.68781	2.20419	H	5.73700	-0.83150	2.11657
C	1.89329	-4.11435	2.28065	H	5.14517	3.83480	0.83692
C	2.10178	-2.69592	2.12792	H	-1.70132	5.93629	0.73321
C	0.93525	-1.86920	1.88345	H	-3.99329	5.10373	1.13162
B	0.98050	-0.33142	1.75403	H	-5.56789	3.07896	1.60895
Cu	1.29603	1.19385	-0.86305	H	-5.80377	0.63744	1.91142
Cu	-0.26943	0.05290	-2.39671	H	-4.86700	-1.61739	1.91202
Cu	1.34129	-1.29209	-0.14668	H	-3.95764	-3.90598	1.84268
Cu	-0.10128	-2.47467	-1.85258	H	-2.03970	-5.45776	2.00479
O	-1.66276	-3.64878	-1.54105	H	0.53110	-5.76807	2.32188
C	3.37898	-2.11960	2.19643	H	2.77156	-4.73968	2.46059
Cu	-1.34302	-0.90104	-0.35719	H	3.43117	2.65123	-1.49442
B	-1.06264	-0.06395	1.62106	H	2.83176	1.73694	-2.65713
Cu	-1.19982	1.49876	-0.63589	H	-2.50137	-3.29776	-1.90454
Cu	-2.65694	0.19205	-2.09271	H	-1.85261	-3.83836	-0.59466
B	0.17798	1.51519	1.15273	O	2.59490	-2.48551	-2.65257
C	1.63651	-1.61418	-2.08949	C	1.70047	-0.25727	-2.53485
O	2.62145	2.48872	-2.01517	O	2.60986	0.22553	-3.30387
H	4.24776	-2.75647	2.38247	H	2.55948	-3.32546	-2.15944
H	0.72990	5.55693	0.54040				

***CCO + *3H_2O**

C	-0.46440	-1.94452	1.67685	C	-3.28668	1.98835	1.90865
C	-1.80258	-1.46202	1.76043	C	-2.16452	2.82635	1.76688
C	-2.91866	-2.28867	1.97040	C	-0.84845	2.27826	1.55965
C	-2.67894	-3.69376	2.10830	C	0.21666	3.18970	1.29745
C	-1.39814	-4.19745	2.08374	C	0.06428	4.60283	1.29508
C	-0.24123	-3.36052	1.89408	C	-1.23857	5.11140	1.56881
C	-1.87852	-0.04078	1.66316	C	-2.30016	4.25816	1.78850
C	-3.17411	0.58877	1.83782	C	1.22389	5.37979	1.01607
C	-4.31761	-0.27774	1.98395	C	2.43929	4.77618	0.75395
C	-4.20019	-1.65149	2.04965	C	2.60706	3.35074	0.74154

C	1.44521	2.54239	1.00283	Cu	0.04447	-1.68896	-0.37821
C	3.86409	2.74941	0.53171	Cu	-2.16694	-1.80650	-1.82912
C	4.05051	1.35818	0.64744	O	-4.04146	-1.38179	-1.21103
C	5.35269	0.76026	0.52883	H	1.20811	-4.94851	2.09275
C	5.57058	-0.58611	0.73835	H	4.73035	3.38454	0.32634
C	4.49936	-1.45397	1.10809	H	6.19246	1.41262	0.27462
C	3.20594	-0.88425	1.20321	H	5.61050	-3.31460	1.31939
C	2.94009	0.48116	0.92457	H	3.61686	-4.68327	1.84782
C	2.04201	-1.63511	1.51491	H	6.57731	-1.00015	0.63712
C	2.18594	-3.05045	1.71992	H	3.31844	5.39396	0.55205
C	3.51038	-3.61049	1.66505	H	1.14271	6.46984	1.01139
C	4.62202	-2.85049	1.36884	H	-1.39319	6.19340	1.58750
B	0.67835	-0.90465	1.53291	H	-3.29649	4.66996	1.97039
B	-0.54116	0.75403	1.51422	H	-4.27367	2.43664	2.05067
Cu	0.13755	1.79439	-0.56242	H	-5.30200	0.18786	2.07599
Cu	1.86262	0.05595	-0.91248	H	-5.09252	-2.26840	2.18239
O	3.26043	-0.81302	-2.14778	H	-3.53030	-4.36294	2.25660
C	1.06153	-3.87682	1.93167	H	-1.23279	-5.26918	2.22291
B	1.45719	0.97188	1.01196	H	4.08367	-0.95920	-1.63699
Cu	-1.78317	0.32013	-0.37655	H	2.96527	-1.70617	-2.41376
Cu	-1.65451	1.96484	-2.19506	H	-4.37449	-0.53129	-1.56111
Cu	-0.26734	-0.00272	-2.24527	H	-4.15885	-1.31429	-0.23405
C	-0.29012	-1.95544	-2.29679	O	-2.97827	-3.65180	-2.78778
C	0.35699	-2.76603	-3.07710	H	-3.51208	-4.13711	-2.13013
O	0.97285	-3.50060	-3.79845	H	-2.18753	-4.20864	-2.92033

***CHCO + *3H_2O**

C	4.49572	-3.00475	1.47587	C	4.06438	1.21094	0.69929
C	4.43535	-1.59187	1.27516	C	5.36519	0.59226	0.70196
C	3.15651	-0.99438	1.29245	C	5.54814	-0.74327	0.97891
C	1.95272	-1.72725	1.47797	C	3.90766	2.58478	0.45035
C	2.03736	-3.15429	1.63951	C	2.65312	3.21524	0.54129
C	3.34675	-3.74773	1.64569	C	2.51818	4.64374	0.44205
C	2.92758	0.37909	0.99732	C	1.32257	5.28711	0.67031

C	0.14902	4.55323	1.03171	Cu	-1.26005	1.95096	-2.37000
C	0.25647	3.15040	1.10600	B	1.46092	0.89663	1.00709
C	1.46031	2.44717	0.81542	Cu	1.71787	-0.61165	-0.63405
C	-1.12021	5.13334	1.34527	O	3.26219	-1.47686	-1.79049
C	-2.18970	4.33969	1.69320	C	-1.02389	-2.26177	-2.31311
C	-2.09147	2.90678	1.76935	H	0.97329	-5.02519	1.87582
C	-0.81166	2.29980	1.50594	H	4.79274	3.19064	0.23723
C	-3.22497	2.11255	2.03097	H	6.22870	1.22258	0.47349
C	-3.15467	0.71269	1.99398	H	5.47131	-3.49788	1.47361
C	-1.88875	0.04343	1.77191	H	3.41584	-4.83052	1.77904
C	-1.87656	-1.38324	1.81776	H	6.55224	-1.17484	0.95860
C	-3.02089	-2.16773	2.01652	H	3.41256	5.22372	0.20007
C	-4.27354	-1.48368	2.15267	H	1.26238	6.37586	0.59557
C	-4.33096	-0.10693	2.15078	H	-1.23280	6.21958	1.30033
C	-2.84752	-3.59007	2.06675	H	-3.15842	4.79577	1.91384
C	-1.59909	-4.15652	1.95946	H	-4.18887	2.59712	2.20850
C	-0.40640	-3.36481	1.78244	H	-5.28989	0.39961	2.28640
C	-0.57064	-1.92931	1.65532	H	-5.18698	-2.07035	2.27891
B	0.61310	-0.94678	1.42640	H	-3.72804	-4.22330	2.20007
Cu	-0.43051	-1.93830	-0.37729	H	-1.48376	-5.24137	2.02529
Cu	-2.51992	-1.18088	-1.65679	H	3.77502	-2.07661	-1.21392
O	-4.18192	-0.14428	-1.14093	H	2.66872	-2.07601	-2.34649
C	0.87562	-3.94133	1.77120	H	-4.07724	0.82715	-1.19234
B	-0.53853	0.78272	1.61026	H	-4.41861	-0.31929	-0.19928
Cu	-1.41666	0.69487	-0.31162	H	-1.52787	-3.11347	-2.80507
Cu	-0.19677	-0.19931	-2.26866	O	-3.82828	-3.02470	-1.12486
C	0.34496	-2.10639	-2.47021	H	-3.15964	-3.59244	-0.69341
O	1.30491	-2.74523	-2.97802	H	-4.39895	-2.74122	-0.38439
Cu	0.76578	1.64839	-1.01849				

***CHCHO + *3H_2O**

C	-0.48364	-1.85862	1.60168	C	-2.78344	-3.45657	2.15268
C	-1.77159	-1.28405	1.79670	C	-1.55513	-4.05479	1.97095
C	-2.92912	-2.03619	2.06388	C	-0.35870	-3.29579	1.71311

C	-4.16200	-1.32199	2.19724	C	0.90051	-3.91304	1.61081
C	-4.20048	0.05408	2.11019	B	1.62906	0.92446	0.95907
C	-3.01589	0.84651	1.88993	Cu	0.36279	1.73926	-0.65356
C	-1.76487	0.13946	1.69137	Cu	-1.47396	2.05531	-2.23230
C	-3.04830	2.25173	1.89165	Cu	-0.15085	0.03698	-2.25270
C	-1.88797	3.01589	1.66284	Cu	-1.69839	0.42846	-0.39894
C	-1.94199	4.45160	1.61020	B	-0.40205	0.85057	1.47475
C	-0.84001	5.22879	1.32027	Cu	-2.68173	-1.64280	-1.61248
C	0.42659	4.63332	1.05134	O	-4.34565	-0.60379	-1.19312
C	0.49907	3.21577	1.11751	H	0.96896	-5.00143	1.68703
C	-0.61148	2.38424	1.44657	H	5.02723	3.13466	0.21521
C	1.69142	2.48643	0.85715	H	6.38757	1.09895	0.26936
C	2.89761	3.22069	0.57563	H	5.47018	-3.64431	0.96100
C	2.80673	4.65216	0.51182	H	3.38121	-4.89974	1.36172
C	1.62565	5.33205	0.73394	H	6.62211	-1.34318	0.55186
C	4.12661	2.55170	0.42692	H	3.71975	5.20986	0.28744
C	4.23751	1.15741	0.58517	H	1.60256	6.42319	0.67504
C	3.08075	0.35304	0.87187	H	-0.93202	6.31744	1.28668
C	3.25528	-1.03900	1.07869	H	-2.90640	4.93028	1.79990
C	4.51068	-1.69050	0.94370	H	-4.00106	2.76356	2.05055
C	5.64036	-0.87356	0.65336	H	-5.14947	0.58146	2.23546
C	5.50640	0.49019	0.48874	H	-5.08208	-1.88370	2.37712
C	2.03602	-1.72870	1.31588	H	-3.66659	-4.06687	2.35697
C	2.07559	-3.16230	1.41139	H	-1.46145	-5.14091	2.04796
C	3.35362	-3.80965	1.28427	H	3.11405	-2.45275	-1.49998
C	4.52189	-3.11036	1.06280	H	2.12105	-2.13258	-2.67548
Cu	1.78381	-0.43275	-0.73429	H	-4.33341	0.33771	-1.45808
O	2.76721	-1.71084	-2.03506	H	-4.56719	-0.60006	-0.23345
B	0.72042	-0.90178	1.35067	H	-0.98148	-3.62272	-1.92344
Cu	-0.35562	-1.72492	-0.49498	H	-0.41705	-1.07403	-3.64512
C	-1.09109	-2.55110	-2.18152	O	-3.87338	-3.48649	-0.80078
C	-0.17264	-2.10736	-3.15329	H	-3.23317	-3.80760	-0.13214
O	0.81765	-2.71458	-3.67679	H	-4.58730	-3.09915	-0.25863

***CH_2CHO + *$3H_2O$**

C	-1.19049	5.36700	-1.26697	Cu	-1.73380	0.12776	0.36154
C	0.10247	4.80486	-1.04916	Cu	-2.19574	-2.17104	1.09694
C	0.21806	3.39600	-1.14655	O	-1.29626	-3.99565	0.98181
C	-0.88240	2.53671	-1.41896	C	-3.31106	2.33085	-1.87046
C	-2.17710	3.13061	-1.61761	Cu	0.20561	-1.59033	0.31994
C	-2.27754	4.56270	-1.54189	B	0.57237	-0.68988	-1.55872
C	1.27642	5.53021	-0.68358	B	1.38206	1.14231	-0.88468
C	2.46030	4.88048	-0.40616	Cu	1.77753	0.14893	1.11573
C	2.58443	3.44777	-0.45237	Cu	-0.26353	-0.10675	2.27386
C	1.41500	2.69546	-0.83029	Cu	1.34936	-1.93541	2.41486
C	3.80142	2.80036	-0.16442	Cu	0.00629	1.86520	0.71129
C	3.94468	1.40633	-0.27458	O	-1.03284	3.37208	1.77101
C	2.81545	0.57151	-0.62730	O	-3.32454	1.87727	1.84660
C	3.04239	-0.81135	-0.88563	C	-2.94980	0.73123	2.22645
C	4.30329	-1.42551	-0.74371	C	-3.34564	-0.53888	1.62778
C	5.38866	-0.59809	-0.31923	H	-4.27860	2.81587	-2.02723
C	5.21378	0.75039	-0.09755	H	4.67199	3.40262	0.10997
C	1.87770	-1.49970	-1.34989	H	3.34473	5.46007	-0.12784
C	2.00354	-2.90831	-1.64955	H	-1.31470	6.45130	-1.20089
C	3.29067	-3.52802	-1.46370	H	-3.26162	5.01335	-1.69580
C	4.39160	-2.82176	-1.03511	H	1.22206	6.62009	-0.61369
C	0.89048	-3.65507	-2.07589	H	6.06656	1.36552	0.20267
C	-0.38839	-3.08077	-2.15452	H	6.37450	-1.05019	-0.18109
C	-1.54576	-3.86249	-2.50743	H	5.35412	-3.32575	-0.91355
C	-2.79930	-3.30261	-2.63226	H	3.37679	-4.59562	-1.68209
C	-3.01343	-1.90873	-2.39227	H	1.01189	-4.71970	-2.29401
C	-1.90418	-1.14256	-1.99110	H	-1.40010	-4.92706	-2.70858
C	-0.58434	-1.67579	-1.86385	H	-3.64972	-3.92559	-2.92285
C	-4.27150	-1.23416	-2.50168	H	-5.15933	-1.81028	-2.77598
C	-4.36790	0.12242	-2.28969	H	-5.33199	0.62385	-2.40902
C	-3.22790	0.93400	-1.94895	H	-1.17463	4.12304	1.15789
C	-1.96880	0.25410	-1.72797	H	-1.93717	2.95482	1.87852
B	-0.64421	1.00236	-1.38181	H	-0.37113	-4.00774	1.31211

H	-1.23778	-4.29675	0.04723	O	-4.01168	-3.24828	0.35916
H	-4.21108	-0.48320	0.95225	H	-4.53097	-2.57559	-0.12360
H	-2.34768	0.64728	3.16660	H	-3.69061	-3.84147	-0.34967
H	-3.47520	-1.29035	2.43944				

***CH_2CH_2O + *$3H_2O$**

C	1.10788	-1.44763	-1.72278	C	-1.22426	-2.41364	-1.44785
C	2.01450	-0.36463	-1.92556	C	-0.66425	-3.71587	-1.67777
C	3.36675	-0.53535	-2.26468	C	-1.54826	-4.84955	-1.61290
C	3.84939	-1.87804	-2.38926	C	-2.88878	-4.72834	-1.31218
C	2.99988	-2.95150	-2.24228	Cu	-1.65543	-1.06815	0.87284
C	1.59771	-2.79373	-1.95238	O	-1.64605	-2.62092	2.20125
C	1.39427	0.91201	-1.77592	B	-0.38640	-1.10675	-1.43812
C	2.19594	2.09688	-2.01955	Cu	0.80717	-1.59363	0.33422
C	3.58684	1.90288	-2.34399	O	0.86927	-1.99949	2.29866
C	4.14782	0.64653	-2.46319	C	2.19229	-2.30480	2.79424
C	1.62221	3.37542	-1.94075	C	3.27485	-1.82628	1.84860
C	0.27057	3.55590	-1.59156	Cu	3.37188	0.04859	1.35970
C	-0.59448	2.42927	-1.35461	Cu	0.32688	-0.08833	2.24907
C	-1.93059	2.69438	-0.93539	Cu	0.61173	2.28411	2.26908
C	-2.46742	4.00237	-0.79198	Cu	-1.06655	1.34948	0.77029
C	-1.59460	5.09382	-1.06930	B	-1.95507	0.13573	-0.86471
C	-0.28692	4.87419	-1.44833	C	0.71458	-3.88589	-1.92871
C	-3.83297	4.10442	-0.40429	B	-0.13042	0.95139	-1.46373
C	-4.59880	2.97448	-0.19346	Cu	1.29265	0.96509	0.31224
C	-4.07135	1.64658	-0.33439	O	4.05951	1.84117	0.80417
C	-2.67930	1.51573	-0.67768	H	1.10611	-4.89277	-2.09766
C	-4.89184	0.50877	-0.21390	H	-5.94831	0.64184	0.03626
C	-4.40562	-0.79023	-0.45959	H	-6.31824	-1.77501	-0.14640
C	-5.26992	-1.93743	-0.41115	H	-3.52379	-5.61695	-1.26454
C	-4.82026	-3.21392	-0.68249	H	-1.12094	-5.83873	-1.79882
C	-3.46242	-3.45128	-1.04339	H	-5.50776	-4.06168	-0.62219
C	-2.60132	-2.32578	-1.11760	H	-5.65311	3.07801	0.07716
C	-3.02302	-1.00860	-0.79646	H	-4.27816	5.09587	-0.28688

H	-1.97398	6.11459	-0.97457	H	3.51244	2.60855	1.06947
H	0.36931	5.72588	-1.64634	H	4.11269	1.89293	-0.18165
H	2.24811	4.25350	-2.12050	H	3.25544	-2.43610	0.92161
H	4.19759	2.79147	-2.52374	H	2.31375	-1.85744	3.79487
H	5.20656	0.54599	-2.71864	H	4.27035	-1.99041	2.31125
H	4.90451	-2.04183	-2.62187	H	2.23666	-3.40628	2.90735
H	3.38142	-3.96797	-2.36995	O	6.00047	-0.69202	0.04180
H	-1.83590	-3.45070	1.72101	H	5.28992	-1.34191	-0.11799
H	-0.65198	-2.64134	2.40446	H	5.74556	0.05807	-0.52749

***CH_3CH_2O + *$3H_2O$**

C	4.73862	-3.02640	0.49752	C	-1.52455	-0.15353	2.18978
C	4.62043	-1.60646	0.40686	C	-1.47148	-1.57993	2.16084
C	3.37894	-1.03359	0.75243	C	-2.53654	-2.40585	2.54390
C	2.25750	-1.79623	1.17642	C	-3.75483	-1.76478	2.94389
C	2.39314	-3.22768	1.22760	C	-3.85725	-0.39117	2.97603
C	3.66925	-3.80025	0.89238	C	-2.32352	-3.82300	2.50065
C	3.11377	0.36103	0.64557	C	-1.09962	-4.34557	2.15596
C	4.19492	1.24894	0.27658	C	0.02621	-3.51279	1.81254
C	5.45573	0.64236	-0.07153	C	-0.18947	-2.07685	1.75945
C	5.65950	-0.71687	-0.01854	B	0.94224	-1.04823	1.49510
C	4.02119	2.64224	0.28250	Cu	0.04599	-1.76479	-0.31320
C	2.81572	3.23943	0.71182	Cu	-1.78092	0.11747	0.16730
C	2.65929	4.66487	0.78213	B	-0.24705	0.63969	1.79662
C	1.48859	5.26518	1.20170	Cu	0.07891	1.71411	-0.29177
C	0.36890	4.48320	1.60862	B	1.70076	0.87430	1.03439
C	0.51997	3.07197	1.57203	Cu	1.77974	0.19167	-1.04894
C	1.70241	2.42967	1.12421	Cu	-0.55666	-0.00341	-1.96215
C	-0.87854	4.99187	2.07612	Cu	-2.09767	1.76654	-1.56891
C	-1.89348	4.14013	2.45877	Cu	-3.58600	-0.11513	-1.39173
C	-1.77002	2.70988	2.39158	O	-4.51837	-1.68336	-0.22161
C	-0.51550	2.16145	1.93997	C	1.29471	-4.05090	1.56007
C	-2.84164	1.86921	2.75140	O	2.47861	-1.14458	-2.46532
C	-2.75244	0.47464	2.63938	O	-0.03063	-1.91963	-2.26997

C	-0.82657	-2.95678	-2.87333	H	-3.14831	-4.48887	2.76701
C	-2.17928	-3.10931	-2.21178	H	-0.94916	-5.42831	2.15555
H	1.43140	-5.13529	1.59433	H	3.10466	-1.76571	-2.04179
H	4.85627	3.28381	-0.01262	H	1.60587	-1.65080	-2.55376
H	6.27125	1.30258	-0.37946	H	-4.45794	-1.39545	0.71668
H	5.69185	-3.49672	0.24109	H	-3.91807	-2.45484	-0.25525
H	3.77074	-4.88754	0.94398	H	-2.06219	-3.31632	-1.13176
H	6.63156	-1.13516	-0.29404	H	-0.95202	-2.71697	-3.94290
H	3.50623	5.28663	0.47878	H	-2.74566	-3.93607	-2.66873
H	1.41138	6.35530	1.22916	H	-0.26100	-3.90176	-2.79380
H	-1.02245	6.07425	2.13090	H	-2.76295	-2.17849	-2.32910
H	-2.84169	4.55185	2.81487	O	-5.11554	-0.21447	-2.82322
H	-3.77902	2.31731	3.09235	H	-5.35847	0.67177	-3.15229
H	-4.79088	0.07745	3.29808	H	-5.93111	-0.55967	-2.41025
H	-4.61103	-2.38265	3.22659				

***CH_3CH_2OH + *$3H_2O$**

C	-0.32848	-1.74639	1.76444	C	1.93617	2.57206	1.01560
C	-1.55835	-1.13471	2.15102	C	3.11183	3.27662	0.58142
C	-2.69401	-1.85448	2.54814	C	3.09287	4.71028	0.67012
C	-2.60700	-3.28669	2.52075	C	2.00358	5.41107	1.14761
C	-1.43280	-3.91601	2.18152	C	4.24429	2.57206	0.12171
C	-0.23827	-3.18826	1.83047	C	4.29336	1.16882	0.13452
C	-3.84347	-1.10267	2.95747	C	3.15085	0.38478	0.55066
C	-3.81344	0.27324	2.99932	C	3.30093	-1.02428	0.69344
C	-2.64358	1.02989	2.63283	C	4.48127	-1.70822	0.33165
C	-1.49241	0.29386	2.15276	C	5.57675	-0.92001	-0.15335
C	-2.59530	2.42763	2.75717	C	5.48626	0.44976	-0.23704
C	-1.45802	3.16406	2.38405	C	2.12761	-1.68075	1.15383
C	-1.44675	4.60273	2.46383	C	2.13836	-3.11839	1.22618
C	-0.35927	5.35561	2.08200	C	3.35889	-3.80257	0.88838
C	0.82822	4.73328	1.58678	C	4.48143	-3.13278	0.45614
C	0.83737	3.31992	1.51897	B	0.87988	-0.82564	1.46135
C	-0.27149	2.50529	1.90133	Cu	-0.06903	-1.36243	-0.39590

O	0.46572	-2.89527	-1.73761	H	3.98337	5.25365	0.34156
C	-0.60889	-3.22263	-2.66375	H	2.03258	6.50311	1.19178
C	-1.81381	-3.62836	-1.84762	H	-0.39610	6.44623	2.14978
C	0.97692	-3.83920	1.57510	H	-2.34831	5.09744	2.83499
B	1.79682	1.02237	0.95341	H	-3.47814	2.95956	3.12296
Cu	1.79045	0.19050	-1.15371	H	-4.69120	0.82744	3.34199
O	2.76500	-1.27398	-2.32660	H	-4.74829	-1.64008	3.25310
Cu	0.28968	1.98444	-0.36566	H	-3.48727	-3.87424	2.79332
Cu	-1.96780	2.20980	-1.57091	H	-1.37769	-5.00788	2.19435
Cu	-2.85714	-0.11099	-1.87757	H	3.04383	-0.96270	-3.20895
O	-4.28438	-1.38977	-2.49972	H	3.58484	-1.57478	-1.87528
B	-0.14926	0.96662	1.74537	H	-4.32499	-1.83471	0.46362
Cu	-1.67225	0.50517	0.09483	H	-4.03362	-3.24468	-0.05824
Cu	-0.44323	0.39523	-2.06855	H	-1.58131	-4.48958	-1.20288
O	-4.69092	-2.52546	-0.12545	H	-0.83173	-2.33404	-3.28077
H	1.02013	-4.93098	1.62017	H	-2.64690	-3.89844	-2.51299
H	5.12549	3.13302	-0.20258	H	-0.26840	-4.03951	-3.31974
H	6.34341	1.03090	-0.58819	H	-2.14643	-2.78701	-1.21062
H	5.38568	-3.68749	0.19122	H	-5.10429	-0.93151	-2.76751
H	3.37074	-4.89331	0.96333	H	-4.51516	-1.88643	-1.64371
H	6.49892	-1.42760	-0.44948	H	1.21292	-2.48192	-2.23243

***3H_2O (ethanol pathway)**

C	-0.29310	-1.66886	1.79134	C	-6.34647	-0.36094	3.93839
C	-1.50810	-1.06258	2.22656	C	-6.22271	-1.79204	3.84431
C	-2.57418	-1.92842	2.58501	C	-7.26537	-2.59599	4.37817
C	-2.49683	-3.34299	2.48398	C	-8.44794	-2.05698	4.94403
C	-1.26909	-3.92767	2.01566	C	-8.55873	-0.63686	4.99778
C	-0.18303	-3.03996	1.69587	C	-7.54875	0.17094	4.51691
C	-1.75595	0.33955	2.29407	C	-7.01832	-3.99163	4.25705
C	-2.98406	0.82282	2.69840	C	-8.04108	-4.90129	4.69580
C	-4.07180	-0.04325	3.06291	C	-9.22687	-4.34367	5.28791
C	-3.85910	-1.46157	2.97048	C	-9.42670	-2.98482	5.41022
C	-5.29695	0.47785	3.52007	C	-7.89331	-6.29231	4.52717

C	-6.76230	-6.84075	3.89968	O	-5.72442	-9.73631	0.17669
C	-6.59002	-8.26558	3.76041	H	-0.18785	-5.73205	1.50803
C	-5.42977	-8.82505	3.27524	H	-5.42039	1.56221	3.59063
C	-4.32969	-8.00644	2.86068	H	-3.15177	1.90186	2.75124
C	-4.49453	-6.61129	2.93864	H	0.55129	-1.03020	1.51951
C	-5.69187	-5.98406	3.42067	H	0.75355	-3.48576	1.34987
C	-3.07687	-8.49402	2.37586	H	-0.95759	1.03316	2.01787
C	-2.06368	-7.62556	2.03113	H	-7.64688	1.25813	4.57743
C	-2.19933	-6.19827	2.15210	H	-9.45857	-0.19123	5.42961
C	-3.47169	-5.68255	2.60760	H	-10.34695	-2.60413	5.86090
B	-3.76926	-4.16873	2.80487	H	-9.99521	-5.03783	5.63902
Cu	-4.36987	-5.12527	0.78941	H	-8.68420	-6.96071	4.87826
Cu	-6.15147	-3.82172	-0.12784	H	-7.40643	-8.91047	4.09591
Cu	-6.69395	-5.34321	1.67803	H	-5.33240	-9.91212	3.21074
B	-5.69878	-4.43989	3.58158	H	-2.93115	-9.57329	2.28067
Cu	-6.78075	-2.87580	2.04851	H	-1.10997	-8.01806	1.66865
Cu	-8.44314	-3.95061	0.65179	H	-4.22949	-1.12253	-0.99266
Cu	-6.07243	-6.20989	-0.58254	H	-3.15739	-0.66060	0.02653
O	-6.58867	-7.90903	-1.53910	H	-6.15942	-9.48578	1.01661
C	-1.13699	-5.32159	1.86330	H	-4.79605	-9.46735	0.32038
B	-4.96854	-2.52100	3.25264	H	-7.55362	-8.00866	-1.64831
Cu	-4.37780	-2.61808	1.12830	H	-6.30564	-8.65901	-0.91443
O	-3.53834	-1.46061	-0.39125				

***C_2H_4 + *2OH + *2H_2O**

C	0.66371	5.51045	-0.89365	C	3.02589	4.83672	-0.26298
C	1.68048	4.54145	-0.63883	C	4.59444	1.43076	-0.15664
C	1.32861	3.18069	-0.79328	C	4.29410	0.08103	-0.41691
C	0.04816	2.73655	-1.21704	C	5.31426	-0.93078	-0.40032
C	-0.95752	3.73792	-1.47070	C	5.05885	-2.24935	-0.71881
C	-0.59730	5.11883	-1.28769	C	3.75023	-2.67759	-1.08341
C	2.24652	2.11262	-0.57284	C	2.72927	-1.68935	-1.10941
C	3.62003	2.44120	-0.24877	C	2.95646	-0.32390	-0.76843
C	3.95069	3.83044	-0.07991	C	3.36990	-4.00851	-1.41826

C	2.06132	-4.31280	-1.73479	O	-1.89100	2.00076	2.10879
C	1.01709	-3.32520	-1.75645	O	-2.85912	-2.25265	0.69435
C	1.37350	-1.96446	-1.45238	H	-2.98688	4.15491	-2.09689
C	-0.30865	-3.66872	-2.08080	H	5.62293	1.70665	0.09212
C	-1.33140	-2.70637	-2.11924	H	4.98172	4.07870	0.18513
C	-1.06328	-1.32472	-1.79170	H	0.89929	6.57162	-0.77775
C	-2.09429	-0.37314	-2.00688	H	-1.36464	5.87321	-1.48281
C	-3.39447	-0.72026	-2.43156	H	3.32020	5.88130	-0.13163
C	-3.66863	-2.10634	-2.64359	H	6.32897	-0.62510	-0.13186
C	-2.67543	-3.05358	-2.50221	H	5.86789	-2.98405	-0.69249
C	-4.32045	0.34383	-2.65185	H	4.12962	-4.79447	-1.41496
C	-3.94026	1.65571	-2.46817	H	1.79054	-5.34313	-1.98116
C	-2.61826	2.02400	-2.03943	H	-0.54562	-4.70916	-2.32055
C	-1.66925	0.96423	-1.78278	H	-2.89245	-4.10545	-2.70634
B	-0.17349	1.20849	-1.42467	H	-4.67392	-2.40745	-2.94967
B	0.34486	-0.79245	-1.40330	H	-5.33647	0.10575	-2.97743
Cu	-1.02733	-1.28811	0.45207	H	-4.65641	2.46069	-2.65494
Cu	-3.09536	0.44331	2.22363	H	1.50480	1.42984	3.71530
C	-4.61605	0.92866	0.94868	H	-1.16889	2.04169	2.77161
C	-5.02581	-0.10248	1.77529	H	-2.84696	-2.85270	1.46366
Cu	-1.09253	1.35195	0.45393	H	-3.04285	-2.81390	-0.08842
Cu	0.03501	-0.12332	2.38556	H	-5.61169	0.10393	2.67721
Cu	0.32960	-2.48270	2.20897	H	-4.24211	0.72668	-0.05943
Cu	1.36284	-0.98322	0.58031	H	-4.87532	1.96810	1.17274
B	1.74275	0.66168	-0.84549	H	-4.98098	-1.14141	1.43933
Cu	1.46283	1.51843	1.21871	O	-2.67223	-1.02555	3.65027
O	0.80412	1.59068	3.05617	H	-3.37062	-1.70470	3.55820
C	-2.25000	3.37310	-1.89191	H	-1.84637	-1.49324	3.37377

***C_2H_4 + *OH + *3H_2O**

C	0.95760	-2.00006	-1.31615	C	2.49673	-3.92110	-1.45927
C	2.05251	-1.17967	-1.71227	C	1.16218	-3.43196	-1.23707
C	3.34359	-1.68304	-1.95933	C	1.68265	0.18496	-1.92909
C	3.54135	-3.09025	-1.80048	C	2.70228	1.09018	-2.42138

C	4.03848	0.57494	-2.58542
C	4.34721	-0.75011	-2.36926
C	2.38444	2.42293	-2.72773
C	1.10360	2.94419	-2.47591
C	0.05003	2.10001	-1.95861
C	-1.19295	2.71856	-1.62827
C	-1.46801	4.08272	-1.85390
C	-0.41614	4.88583	-2.39277
C	0.81448	4.34029	-2.67958
C	-2.78040	4.54747	-1.53184
C	-3.74717	3.68539	-1.06362
C	-3.50055	2.28030	-0.87008
C	-2.14993	1.81023	-1.09277
C	-4.53536	1.38334	-0.55086
C	-4.33297	-0.01084	-0.54384
C	-5.41318	-0.93050	-0.30352
C	-5.23486	-2.29785	-0.29507
C	-3.95405	-2.87741	-0.54152
C	-2.88553	-1.98561	-0.81844
C	-3.03218	-0.57039	-0.80503
C	-1.53702	-2.40782	-0.97021
C	-1.24137	-3.81333	-0.87061
C	-2.34104	-4.71107	-0.63237
C	-3.63581	-4.26812	-0.46739
Cu	-1.53345	-0.89299	0.87584
O	-2.65312	-2.04685	2.24305
B	-0.44131	-1.31740	-1.14907
Cu	0.89633	-1.35467	0.62703
O	1.89346	-0.90955	2.35352
Cu	3.64481	-0.93390	1.37362
O	3.91215	1.02296	0.88776
C	0.07798	-4.29303	-1.00105
B	-1.75629	0.29822	-1.00899
Cu	-1.26232	1.55071	0.81325
Cu	0.25226	0.36433	2.20748
Cu	0.71222	2.75049	1.84946
Cu	1.03911	1.26850	0.01183
B	0.18738	0.56493	-1.77542
C	5.31669	-1.99681	0.92276
C	4.35745	-2.80742	1.51587
H	0.25949	-5.36945	-0.93248
H	-5.54113	1.77533	-0.37386
H	-6.40527	-0.51284	-0.11035
H	-4.43748	-4.98353	-0.26382
H	-2.12067	-5.77969	-0.56260
H	-6.08140	-2.95769	-0.08588
H	-4.75490	4.05855	-0.86101
H	-3.01724	5.60447	-1.68167
H	-0.59961	5.94891	-2.57092
H	1.61135	4.97117	-3.08225
H	3.16662	3.08578	-3.10769
H	4.81261	1.26826	-2.92430
H	5.36808	-1.10837	-2.52625
H	4.54007	-3.50429	-1.96205
H	2.66582	-4.99749	-1.36858
H	-3.15794	-2.69459	1.70274
H	1.79765	-1.66405	2.96658
H	3.18203	1.62441	1.18060
H	3.98877	1.16005	-0.08194
H	6.13367	-1.57203	1.51533
H	3.70131	-3.43008	0.89716
H	4.40247	-3.04094	2.58468
H	5.43411	-1.97525	-0.16436
H	-2.05309	-2.58996	2.78892
O	2.95911	1.10881	4.10978
H	2.58054	0.39033	3.55065
H	3.03384	1.85444	3.48543

***CH_3CH_2 + *OH + *3H_2O**

C	2.87937	-4.71129	0.83129	Cu	-1.33481	-1.26097	-0.41393
C	3.39792	-3.38536	0.80583	C	-2.63730	-1.74358	-1.98782
C	2.47508	-2.32475	1.01475	C	-4.02997	-2.29815	-1.65560
C	1.08287	-2.52934	1.21006	C	-0.78195	-4.14164	1.42755
C	0.58616	-3.87750	1.22292	B	-0.15728	0.74226	1.83233
C	1.53295	-4.94228	1.03120	Cu	-1.09694	1.19555	-0.03357
C	2.83428	-0.95369	0.94459	Cu	-0.48768	2.64447	-1.89271
C	4.20393	-0.61899	0.66830	Cu	-0.37869	0.24853	-2.21876
C	5.13379	-1.70046	0.48985	Cu	1.22511	1.36214	-0.70787
C	4.75242	-3.02593	0.55354	B	1.69902	0.10221	1.11834
C	4.62004	0.72502	0.58852	Cu	1.18138	-1.15982	-0.62340
C	3.72642	1.79081	0.79133	O	1.74997	-2.08858	-2.33509
C	4.17030	3.15758	0.80074	O	0.17042	-0.79097	-3.78418
C	3.33087	4.20560	1.11528	Cu	-2.89536	0.24850	-1.53056
C	1.96621	3.97421	1.46063	O	-3.93815	1.77010	-0.55169
C	1.50191	2.63660	1.42714	H	-1.13023	-5.17828	1.42988
C	2.32715	1.53779	1.05617	H	5.67147	0.94368	0.38204
C	1.03855	4.97756	1.87084	H	6.17759	-1.44687	0.28613
C	-0.25134	4.64513	2.22727	H	3.56227	-5.55119	0.67889
C	-0.73080	3.28955	2.21865	H	1.15440	-5.96804	1.04085
C	0.18841	2.25014	1.82385	H	5.49162	-3.81613	0.39712
C	-2.06344	2.98160	2.55484	H	5.22095	3.35161	0.56905
C	-2.55167	1.66723	2.46208	H	3.71195	5.23003	1.12205
C	-1.67879	0.57608	2.08172	H	1.36583	6.02004	1.90383
C	-2.23982	-0.73387	2.00769	H	-0.94936	5.42849	2.53490
C	-3.59460	-1.02330	2.28309	H	-2.74438	3.78532	2.84726
C	-4.44009	0.07580	2.62251	H	-4.60152	2.18205	2.98768
C	-3.93783	1.35852	2.71080	H	-5.49754	-0.11089	2.82689
C	-4.00250	-2.38909	2.21452	H	-5.04813	-2.63978	2.41055
C	-3.09583	-3.38422	1.92023	H	-3.42103	-4.42753	1.89454
C	-1.71049	-3.10812	1.64948	H	1.48508	-3.02664	-2.29986
C	-1.29168	-1.72369	1.64117	H	-0.57016	-1.38487	-4.00821
B	0.17470	-1.26565	1.35115	H	-3.53298	2.65377	-0.65857

H	-3.97219	1.62704	0.42165	H	1.08683	-1.61544	-3.04288
H	-4.83186	-1.58929	-1.91942	H	-4.21611	-3.22527	-2.22803
H	-1.87145	-2.54026	-1.79940	O	-4.12895	0.75624	-3.26437
H	-2.51704	-1.54463	-3.06550	H	-4.36812	-0.07092	-3.72410
H	-4.12980	-2.53654	-0.58657	H	-4.97778	1.10271	-2.92884

***H + *OH + *3H_2O**

C	0.11634	-2.52601	1.37111	C	5.07084	1.71108	0.95339
C	-1.27000	-2.41321	1.66988	C	2.47025	-1.57525	1.18355
C	-2.12339	-3.53177	1.84804	C	2.96592	-2.92284	1.15876
C	-1.53899	-4.82526	1.72666	C	4.39016	-3.11359	1.10956
C	-0.18850	-4.97013	1.48356	C	5.28100	-2.05926	1.07481
C	0.69570	-3.84772	1.32878	Cu	1.83548	-0.44035	-0.64899
C	-3.49529	-3.26362	2.13478	O	2.70800	-0.72688	-2.42815
C	-3.96245	-1.96553	2.21828	B	0.95333	-1.20464	1.23180
C	-3.10479	-0.82350	2.04297	Cu	-0.42289	-1.53797	-0.43127
C	-1.71022	-1.06661	1.78215	Cu	-2.65420	-1.29703	-1.45419
C	-3.60898	0.49083	2.11247	O	-4.36631	-0.20407	-1.15693
C	-2.77981	1.60873	1.89033	C	2.08423	-4.01997	1.20917
C	-3.29074	2.95172	1.95686	B	1.24736	0.83288	1.11626
C	-2.48746	4.05820	1.78493	Cu	0.51454	1.63388	-0.87979
C	-1.09367	3.92484	1.50590	Cu	-0.51016	-0.11750	-2.41719
C	-0.57417	2.61432	1.40211	O	0.70704	-0.50565	-3.90744
C	-1.36743	1.44099	1.60358	B	-0.66003	0.05866	1.57847
C	0.78961	2.33143	1.12640	Cu	-1.62022	0.69094	-0.35873
C	1.71233	3.44368	1.04516	Cu	-1.40230	2.15845	-2.28127
C	1.16355	4.77050	1.12235	H	-1.17071	-1.77711	-1.94493
C	-0.17781	5.00614	1.33828	H	2.49411	-5.03372	1.19144
C	3.09939	3.22288	0.95822	H	3.77022	4.08414	0.89425
C	3.64996	1.92555	0.99203	H	5.71638	2.59112	0.88708
C	2.80524	0.76924	1.09578	H	6.35641	-2.25091	1.03493
C	3.41232	-0.51110	1.14057	H	4.76434	-4.14075	1.10033
C	4.81832	-0.71284	1.07697	H	6.72138	0.33622	0.95548
C	5.63506	0.45112	0.99485	H	1.85501	5.61239	1.03185

H	-0.55141	6.03149	1.39991	H	3.05169	-1.63774	-2.48411
H	-2.91657	5.06075	1.86013	H	0.49364	-1.39867	-4.23323
H	-4.35521	3.07958	2.17021	H	-4.25633	0.73455	-1.41264
H	-4.66994	0.64709	2.32635	H	-4.59663	-0.17552	-0.20282
H	-5.01901	-1.78229	2.43086	H	1.86938	-0.67941	-3.12677
H	-4.18037	-4.10234	2.28362	O	-3.74714	-3.10425	-1.03165
H	-2.17288	-5.70790	1.84396	H	-3.10618	-3.84122	-1.01535
H	0.24750	-5.97094	1.42321	H	-4.02613	-3.02809	-0.09108

***4H_2O (ethylene pathway)**

C	-0.02394	-2.15564	1.71354	C	3.39002	-0.46483	1.08182
C	-1.41226	-1.89877	1.88364	C	4.75641	-0.80033	0.88483
C	-2.36387	-2.90880	2.12331	C	5.65146	0.26285	0.57276
C	-1.88852	-4.25317	2.20225	C	5.19790	1.56134	0.46073
C	-0.54892	-4.54267	2.05139	C	2.37914	-1.42564	1.36085
C	0.43678	-3.52302	1.80875	C	2.75901	-2.81064	1.43789
C	-3.72933	-2.50291	2.26906	C	4.14782	-3.13466	1.24930
C	-4.08391	-1.17145	2.23274	C	5.10595	-2.17860	0.98359
C	-3.11554	-0.11595	2.06174	Cu	1.73020	-0.24617	-0.63675
C	-1.73799	-0.50459	1.81878	O	2.88353	-1.22689	-2.04727
C	-3.46893	1.24087	2.16970	B	0.91183	-0.94052	1.46337
C	-2.51662	2.26487	1.99544	Cu	-0.21097	-1.87842	-0.34682
C	-2.89898	3.65063	2.04058	Cu	-2.09458	-1.87206	-1.91361
C	-2.01140	4.67451	1.78496	O	-4.03204	-2.43014	-1.14006
C	-0.65049	4.39689	1.45712	C	1.80465	-3.82047	1.67231
C	-0.25613	3.03438	1.43102	B	1.34629	1.07121	1.07908
C	-1.13904	1.95539	1.71958	Cu	-0.01330	1.64527	-0.53156
C	1.05269	2.61165	1.07710	Cu	-0.31634	-0.21940	-2.07983
C	2.04775	3.61543	0.80467	Cu	-1.88355	1.63403	-2.06524
C	1.63562	4.99082	0.84094	Cu	-1.85705	-0.02296	-0.23884
C	0.34392	5.36930	1.14833	B	-0.58373	0.51313	1.63026
C	3.38540	3.25071	0.55990	O	1.08573	-2.80091	-3.34214
C	3.81469	1.91162	0.63394	H	2.13561	-4.86108	1.73398
C	2.88674	0.85206	0.92264	H	4.11984	4.03242	0.34567

H	5.90282	2.36466	0.22990	H	-2.60540	-5.05793	2.38391
H	6.14827	-2.47432	0.83719	H	-0.20385	-5.57770	2.12229
H	4.43845	-4.18700	1.31154	H	3.47476	-1.82874	-1.55193
H	6.71001	0.03740	0.41879	H	0.86741	-2.38149	-4.19697
H	2.38662	5.75368	0.61829	H	-4.72876	-1.85991	-1.51875
H	0.07197	6.42799	1.16106	H	-4.04085	-2.21697	-0.18186
H	-2.34746	5.71401	1.82164	H	2.26768	-1.83199	-2.56726
H	-3.94208	3.88179	2.27297	H	0.32319	-2.53907	-2.75486
H	-4.51172	1.50503	2.36453	O	-2.39043	-2.98349	-3.71936
H	-5.12855	-0.88380	2.37678	H	-1.53482	-2.99942	-4.19152
H	-4.49506	-3.26679	2.42717	H	-2.99908	-2.52551	-4.33074

***3H_2O (ethylene pathway)**

C	4.69248	-2.99758	0.60826	C	-3.21217	1.56449	2.39102
C	4.55159	-1.57775	0.61409	C	-3.06985	0.18089	2.19673
C	3.25405	-1.05650	0.85573	C	-4.16928	-0.72619	2.40081
C	2.10803	-1.87541	1.05750	C	-4.03130	-2.09408	2.29270
C	2.27737	-3.30331	1.03419	C	-2.76724	-2.68443	1.96770
C	3.60220	-3.81757	0.81305	C	-1.69363	-1.80970	1.70649
C	5.59337	-0.64038	0.35083	C	-1.79590	-0.38333	1.79467
C	5.33430	0.71413	0.31698	C	-2.50147	-4.08751	1.91832
C	4.01762	1.25227	0.52489	C	-1.23358	-4.55825	1.65533
C	2.94884	0.32728	0.78089	C	-0.12037	-3.67964	1.41239
C	3.78195	2.64099	0.49768	C	-0.37765	-2.25634	1.40900
C	2.50946	3.18127	0.75989	B	0.72767	-1.17873	1.19665
C	1.37704	2.31734	0.99555	Cu	-0.64591	-1.77856	-0.61579
C	0.15500	2.90721	1.41308	Cu	-1.63386	0.48425	-0.23472
C	-0.02997	4.30488	1.51984	B	-0.50618	0.45624	1.61858
C	1.08415	5.14233	1.21230	C	1.18209	-4.16995	1.21304
C	2.30040	4.59968	0.85588	Cu	0.48124	1.70226	-0.82663
C	-0.85594	1.95562	1.73623	Cu	-1.53072	2.07889	-2.11080
C	-2.14643	2.45141	2.14145	Cu	-0.40224	-0.06264	-2.27860
C	-2.32135	3.87579	2.24216	Cu	-2.56237	-1.09025	-1.96915
C	-1.31317	4.76697	1.94477	O	-4.37899	-1.72961	-0.98769

B	1.45660	0.75114	0.94714	H	-4.18226	1.96437	2.69880
Cu	1.57973	-0.57431	-0.82373	H	-5.13773	-0.29919	2.67444
O	2.85563	-1.39620	-2.25796	H	-4.88898	-2.74604	2.47638
H	1.34923	-5.25056	1.20261	H	-3.31966	-4.78756	2.10587
H	4.61949	3.31878	0.31024	H	-1.04503	-5.63503	1.64208
H	6.14718	1.41731	0.11696	H	3.52156	-1.94580	-1.79441
H	5.67958	-3.43174	0.42921	H	-5.11612	-1.12667	-1.20458
H	3.73072	-4.90326	0.79904	H	-4.26640	-1.64114	-0.01648
H	6.60616	-1.01005	0.16990	H	2.36274	-2.02102	-2.82426
H	3.15083	5.25510	0.65000	O	-3.74428	-0.69023	-3.71591
H	0.96564	6.22702	1.27854	H	-4.62827	-0.37784	-3.44091
H	-1.48572	5.84263	2.03506	H	-3.34488	0.07741	-4.16867
H	-3.29912	4.24735	2.56070				

***2H_2O (both pathways)**

C	-0.35088	-2.25866	1.39082	C	2.32375	4.59769	0.85254
C	-1.67624	-1.81095	1.63872	C	1.10747	5.13732	1.21187
C	-2.76889	-2.68458	1.81307	C	3.80905	2.64058	0.49917
C	-2.50442	-4.08739	1.75241	C	4.04773	1.25268	0.53510
C	-1.22465	-4.55943	1.55447	C	2.97808	0.32729	0.78642
C	-0.09772	-3.68249	1.37909	C	3.28444	-1.05520	0.87905
C	-4.04670	-2.09139	2.06793	C	4.58621	-1.57570	0.66001
C	-4.17936	-0.72620	2.21293	C	5.62894	-0.63851	0.39962
C	-3.06295	0.17701	2.10665	C	5.36748	0.71511	0.34793
C	-1.77376	-0.38610	1.75876	C	2.13924	-1.87437	1.08019
C	-3.20427	1.55766	2.32617	C	2.30967	-3.30211	1.06638
C	-2.12823	2.44296	2.11874	C	3.63892	-3.81544	0.87121
C	-2.30092	3.86636	2.22875	C	4.73046	-2.99492	0.67451
C	-1.28934	4.75765	1.94397	Cu	1.61953	-0.58418	-0.82743
C	-0.00590	4.29716	1.51743	O	2.90868	-1.39865	-2.24548
C	0.17948	2.90119	1.40356	B	0.75782	-1.17842	1.20359
C	-0.83070	1.94747	1.72658	Cu	-0.59062	-1.76059	-0.61144
C	1.39985	2.31470	0.97938	Cu	-2.61534	-1.04090	-1.73709
C	2.53372	3.17952	0.75204	O	-4.58007	-1.40229	-1.25904

C	1.21086	-4.17032	1.21787	H	3.17403	5.25448	0.65077
B	1.48669	0.75183	0.93495	H	0.98774	6.22149	1.28324
Cu	0.58955	1.70579	-0.90116	H	-1.46099	5.83285	2.04045
Cu	-0.43420	-0.07093	-2.27284	H	-3.28107	4.23745	2.54020
Cu	-1.44442	2.13717	-2.13315	H	-4.18302	1.95870	2.60317
Cu	-1.53726	0.58899	-0.22592	H	-5.15999	-0.29855	2.43807
B	-0.47477	0.44697	1.63083	H	-4.92005	-2.73947	2.17747
H	1.37890	-5.25066	1.20326	H	-3.33440	-4.78753	1.87690
H	4.64678	3.31967	0.31775	H	-1.04000	-5.63668	1.53250
H	6.18166	1.41782	0.15183	H	3.58433	-1.93520	-1.78100
H	5.72113	-3.42857	0.51551	H	-5.16961	-0.65736	-1.49031
H	3.76975	-4.90087	0.86841	H	-4.62709	-1.45707	-0.27741
H	6.64484	-1.00769	0.23634	H	2.43326	-2.03247	-2.81666

For *H_2O see C_1 pathway.

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