

Supporting information

Metal-free B₄@g-C₃N₄: a potential electrocatalyst for highly selective and efficient conversion of CO to ethanol

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Table S1: Calculation of the binding energy and molar formation energy of B₄@g-C₃N₄

	Calculation formula	Corresponding value
Binding energy of B ₄ on g-C ₃ N ₄	$E_b = E(\text{B}_4@\text{g-C}_3\text{N}_4) - 4 * E(\text{B in B}_{12}) - E(\text{g-C}_3\text{N}_4)$	-6.51
molar formation energy of B ₄ @g-C ₃ N ₄	$\Delta E_f = [E(\text{B}_4@\text{g-C}_3\text{N}_4) - 4 * E(\text{B atom}) - 24 * E(\text{C in graphene}) - 32 * E(\text{N in N}_2)] / 60$	-6.19
molar formation energy of B ₁₂	$\Delta E_f = [E(\text{B}_{12}) - 12 * E(\text{B})] / 12$	-5.13
molar formation energy of B ₄ @g-C ₃ N ₄	$\Delta E_f = [E(\text{B}_4@\text{g-C}_3\text{N}_4) - 4 * E(\text{B in B}_{12}) - 24 * E(\text{C}) - 32 * E(\text{N})] / 60$	-2.74

We evaluate the thermal stability of B₄@g-C₃N₄ catalyst by calculating the binding energy and molar formation energy.

Binding energy is defined as:

$$E_b = E(\text{B}_4@\text{g-C}_3\text{N}_4) - 4 * E(\text{B}) - E(\text{g-C}_3\text{N}_4) \quad (1),$$

Where $E(\text{B}_4@\text{g-C}_3\text{N}_4)$, $E(\text{B in B}_{12})$ and $E(\text{g-C}_3\text{N}_4)$ are the total energy of B₄@g-C₃N₄ system, B atom (the average B atom energy in the most stable B₁₂ phase), and the original g-C₃N₄, respectively. Note that the more negative the binding energy, the higher the stability. Our calculations show that the binding energy of B₄ on g-C₃N₄ is -6.51 eV, while that of a single B atom is positive (0.42 eV), indicating that doping of B₄ clusters on g-C₃N₄ is easier than single B atom.

A molar formation energy ΔE_f for B₄@g-C₃N₄ can be defined as:

$$E_f = E(\text{B}_4@\text{g-C}_3\text{N}_4) - \sum \chi_i \mu_i \quad (2),$$

where χ_i is the molar fraction of atom i ($i = \text{B, C, and N}$), and μ_i is the chemical potential of the constituent. The B₄@g-C₃N₄ cell contains 4 B, 24 C, and 32 N atoms. If the energy of atom B is defined as the chemical potential of a single B atom, the molar formation energy of the most stable phase B₁₂ and B₄@g-C₃N₄ is -5.13 eV, and

-6.19 eV, which indicates that $B_4@g-C_3N_4$ is thermally stable relative to the most stable phase of B_{12} . If the chemical potential of B is defined as the cohesion energy of each atom on B_{12} . The molar formation energy ΔE_f of $B_4@g-C_3N_4$ is -2.74 eV, which is still negative. All the above data show that the $B_4@g-C_3N_4$ system has higher stability than their corresponding constituents, which indicates the feasibility of its formation.

Table S2 The total adsorption energy, $E_{\text{ads}}(\text{total})$; average adsorption energy, $E_{\text{ads}}(\text{ave})$ and continuous adsorption energy $E_{\text{ads}}(\text{con})$ of CO on $\text{B}_4@\text{g-C}_3\text{N}_4$ catalyst.

	E/eV	$E_{\text{ads}}(\text{total})/\text{eV}$	$E_{\text{ads}}(\text{ave})/\text{eV}$	$E_{\text{ads}}(\text{con})/\text{eV}$	G/eV
CO	-517.73	-1.16	-1.16	-1.16	-0.58
2CO	-532.74	-1.40	-0.70	-0.24	-0.36
3CO	-547.64	-1.53	-0.51	-0.13	0.04
4CO	-562.28	-1.40	-0.35	0.13	0.66

Table S3 Calculated the zero-point energy correction, entropy, enthalpy temperature correction, and the total free energy correction of different adsorption species on the B_{up} site in the process of C1 path are calculated on the B₄@g-C₃N₄, respectively. * is the active site.

Species	$E_{ZPE}(eV)$	$-TS(eV)$	$\int C_{pd}T(eV)$	$G-E_{elec}(eV)$
*C species				
*CO	0.23	-0.09	0.04	0.18
*CHO	0.48	-0.11	0.05	0.43
*COH	0.48	-0.18	0.08	0.39
*CH ₂ O	0.72	-0.17	0.07	0.63
*CHOH	0.83	-0.12	0.07	0.78
*CH ₂ OH	1.10	-0.15	0.08	1.03
*+CH ₃ OH	1.37	-0.27	0.12	1.22
*CH ₂	0.72	-0.04	0.03	0.71
*CH ₃	0.98	-0.12	0.06	0.92
*+CH ₄	1.21	-0.20	0.08	1.09
*O species				
*CO	0.23	-0.09	0.04	0.18
*CHO	0.48	-0.11	0.05	0.43
*COH	0.48	-0.18	0.08	0.39
*OCH ₂	0.77	-0.12	0.07	0.71
*OCH ₃	1.10	-0.14	0.07	1.03
*OHCH ₂	1.04	-0.20	0.10	0.95
*+CH ₃ OH	1.42	-0.20	0.10	1.31
*O+CH ₄	1.32	-0.19	0.09	1.22
*OH+CH ₄	1.60	-0.30	0.14	1.44
*+CH ₄	1.20	-0.22	0.09	1.07
H ₂ (g)	0.27	-0.12	0.05	0.19
CO(g)	0.13	-0.61	0.09	-0.39

Table S4 Free energy change for each possible radical reaction in the electrochemical for the reduction of CO to CH₄ on the B_{up} site of B₄@g-C₃N₄ at U = 0 V for the process of C1 path.

Primitive response	Free energy change ($\Delta G/eV$)
*C species	
* + CO(g) \rightarrow *CO	-0.58
*CO + H ⁺ + e ⁻ \rightarrow *CHO + *CO	0.006
*CO + H ⁺ + e ⁻ \rightarrow *COH + *CO	2.28
*CHO + H ⁺ + e ⁻ \rightarrow *CH ₂ O	0.86
*CHO + H ⁺ + e ⁻ \rightarrow *CHOH	-0.32
*CHOH + H ⁺ + e ⁻ \rightarrow *CH ₂ OH	0.16
*CH ₂ OH + H ⁺ + e ⁻ \rightarrow *+CH ₃ OH	0.23
*CH ₂ OH + H ⁺ + e ⁻ \rightarrow *CH ₂ +H ₂ O	-1.25
*CH ₂ + H ⁺ + e ⁻ \rightarrow *CH ₃	0.13
*CH ₃ + H ⁺ + e ⁻ \rightarrow *CH ₄	0.21
*O species	
* + CO(g) \rightarrow *CO	-0.58
*CO + H ⁺ + e ⁻ \rightarrow *CHO + *CO	0.006
*CO + H ⁺ + e ⁻ \rightarrow *COH + *CO	2.28
*CHO + H ⁺ + e ⁻ \rightarrow *OCH ₂	0.70
*OCH ₂ + H ⁺ + e ⁻ \rightarrow *OCH ₃	-1.04
*OCH ₂ + H ⁺ + e ⁻ \rightarrow *OHCH ₂	1.54
*OCH ₃ + H ⁺ + e ⁻ \rightarrow *+CH ₃ OH	0.53
*OCH ₃ + H ⁺ + e ⁻ \rightarrow *O+CH ₄	-1.44
*O+CH ₄ + H ⁺ + e ⁻ \rightarrow *OH+CH ₄	-2.34
*OH+CH ₄ + H ⁺ + e ⁻ \rightarrow *+CH ₄	-3.79

Table S5 Calculated the zero-point energy correction, entropy, enthalpy temperature correction, and the total free energy correction of different adsorption species on the B_{down} site in the process of C1 path are calculated on the B₄@g-C₃N₄, respectively. * is the active site.

Species	$E_{ZPE}(eV)$	$-TS(eV)$	$\int CpdT(eV)$	$G-Eelec(eV)$
*C species				
*CO	0.21	-0.15	0.06	0.13
*CHO	0.49	-0.15	0.07	0.42
*COH	0.53	-0.10	0.06	0.49
*CH ₂ O	0.74	-0.20	0.09	0.63
*CHOH	0.83	-0.12	0.07	0.72
*CH	0.42	-0.03	0.02	0.41
*CH ₂ OH	1.11	-0.14	0.07	1.04
*+CH ₃ OH	1.37	-0.26	0.12	1.22
*CH ₂	0.72	-0.04	0.03	0.71
*CH ₃	0.98	-0.12	0.06	0.92
*+CH ₄	1.21	-0.20	0.08	1.09
*O species				
*CO	0.21	-0.15	0.06	0.13
*CHO	0.49	-0.15	0.07	0.42
*COH	0.53	-0.10	0.06	0.49
*OCH ₂	0.76	-0.11	0.06	0.72
*OCH ₃	1.12	-0.18	0.09	1.03
*+CH ₃ OH	1.38	-0.27	0.12	1.22
*O+CH ₄	1.30	-0.26	0.12	1.16
*OH+CH ₄	1.60	-0.23	0.12	1.49
*+CH ₄	1.20	-0.20	0.09	1.09
H ₂ (g)	0.27	-0.12	0.05	0.19
CO(g)	0.13	-0.61	0.09	-0.39

Table S6 Free energy change for each possible radical reaction in the electrochemical for the reduction of CO to CH₄ on the B_{down} site B₄@g-C₃N₄ at U = 0 V for the process of C1 path.

Primitive response	Free energy change ($\Delta G/eV$)
*C species	
$* + CO(g) \rightarrow *CO$	0.16
$*CO + H^+ + e^- \rightarrow *CHO + *CO$	-0.51
$*CO + H^+ + e^- \rightarrow *COH + *CO$	0.18
$*CHO + H^+ + e^- \rightarrow *CH_2O$	0.52
$*CHO + H^+ + e^- \rightarrow *CHOH$	-0.58
$*CHOH + H^+ + e^- \rightarrow *CH_2OH$	0.22
$*CHOH + H^+ + e^- \rightarrow *CH$	1.66
$*CH_2OH + H^+ + e^- \rightarrow *+CH_3OH$	0.20
$*CH_2OH + H^+ + e^- \rightarrow *CH_2+H_2O$	-1.24
$*CH_2+ H^+ + e^- \rightarrow *CH_3$	0.08
$*CH_3 + H^+ + e^- \rightarrow *CH_4$	0.23
*O species	
$* + CO(g) \rightarrow *CO$	0.16
$*CO + H^+ + e^- \rightarrow *CHO + *CO$	-0.51
$*CO + H^+ + e^- \rightarrow *COH + *CO$	0.18
$*CHO + H^+ + e^- \rightarrow *OCH_2$	0.48
$*OCH_2 + H^+ + e^- \rightarrow *OCH_3$	-1.62
$*OCH_3 + H^+ + e^- \rightarrow *+CH_3OH$	0.95
	-0.28

$*\text{OCH}_3 + \text{H}^+ + \text{e}^- \rightarrow * \text{O} + \text{CH}_4$	
$* \text{O} + \text{CH}_4 + \text{H}^+ + \text{e}^- \rightarrow * \text{OH} + \text{CH}_4$	-0.51
$* \text{OH} + \text{CH}_4 + \text{H}^+ + \text{e}^- \rightarrow * + \text{CH}_4$	0.60

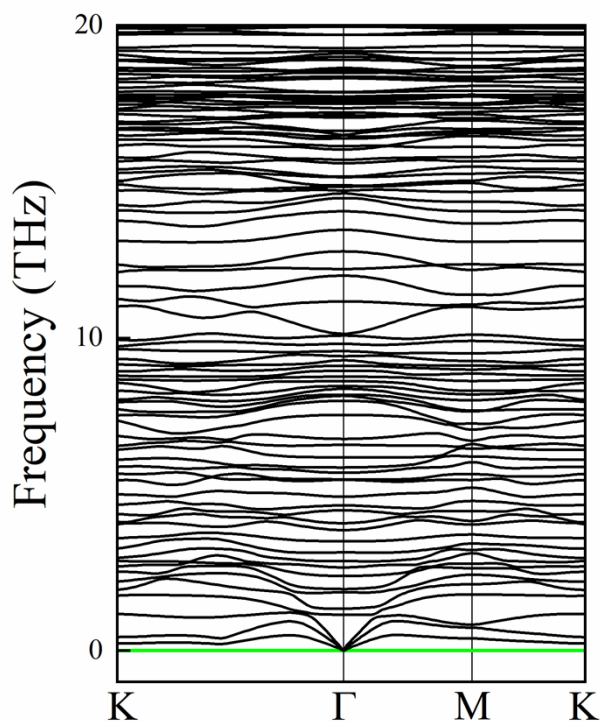
Table S7 Calculated the zero-point energy correction, entropy, enthalpy temperature correction, and the total free energy correction of different adsorption species in the process of ethanol generation are calculated on the B₄@g-C₃N₄, respectively. * is the active site.

Species	$E_{ZPE}(eV)$	$-TS(eV)$	$\int Cp dT(eV)$	$G-E_{elec}(eV)$
*2CO	0.40	-0.27	0.12	0.43
*COCO	0.44	-0.22	0.11	0.33
*CHO+*CO	0.48	-0.11	0.05	0.43
*COH+*CO	0.48	-0.18	0.08	0.39
*COCHO	0.72	-0.24	0.11	0.59
*COHCO	0.76	-0.24	0.12	0.64
*CHOCHO	1.00	-0.31	0.14	0.83
*CH ₂ OCO	1.08	-0.21	0.11	0.98
*CHOHCO	1.02	-0.30	0.14	0.87
*CHOC	0.64	-0.17	0.09	0.56
*CH ₂ OCOH	1.39	-0.16	0.09	1.32
*CHOCHOH	1.33	-0.26	0.13	1.20
*COHCHOH	1.36	-0.30	0.15	1.21
*CCH ₂ O	0.90	-0.16	0.09	0.83
*CH ₂ OHCOH	1.64	-0.25	0.12	1.52
*CH ₂ OCHOH	1.69	-0.25	0.13	1.57
*CHCH ₂ O	1.29	-0.10	0.07	1.25
*CH ₂ OCH ₂ OH	2.03	-0.25	0.13	1.91
*CH ₂ OHCHO	2.00	-0.27	0.15	1.87
H				
*CH ₂ CH ₂ O	1.59	-0.15	0.09	1.53
*CHCH ₂ OH	1.58	-0.15	0.08	1.51
*CHCH ₂	1.12	-0.17	0.08	1.03
*CH ₂ CH ₂ OH	1.90	-0.19	0.10	1.82
*+CH ₂ CH ₂	1.37	-0.14	0.07	1.30
*+CH ₃ CH ₂ OH	2.13	-0.26	0.13	1.99
H ₂ (g)	0.27	-0.12	0.05	0.19
CO(g)	0.13	-0.61	0.09	-0.39

Table S8 Free energy change for each possible radical reaction in the electrochemical for the reduction of CO to CH₃CH₂OH on B₄@g-C₃N₄ at U = 0 V (Bold indicates the optimal primitive reaction)

Primitive response	Free energy change ($\Delta G/eV$)
$* + 2CO(g) \rightarrow *2CO$	-0.36
$*2CO + H^+ + e^- \rightarrow *CHO + *CO$	0.006
$*2CO + H^+ + e^- \rightarrow *COH + *CO$	2.28
$*CO + *CO \rightarrow *COCO$	-0.07
$*COCO + H^+ + e^- \rightarrow *COCHO$	-0.31
$*COCO + H^+ + e^- \rightarrow *COCO H$	0.60
$*COCHO + H^+ + e^- \rightarrow *CHOCHO$	0.60
$*COCHO + H^+ + e^- \rightarrow *COCH_2O$	-1.41
$*COCHO + H^+ + e^- \rightarrow *COCHOH$	0.76
$*COCHO + H^+ + e^- \rightarrow *COHCHO$	-0.61
$*COHCHO + H^+ + e^- \rightarrow *CCHO + H_2O$	0.66
$*COHCHO + H^+ + e^- \rightarrow *COHCH_2O$	-0.39
$*COHCHO + H^+ + e^- \rightarrow *CHOHCHO$	0.34
$*COHCHO + H^+ + e^- \rightarrow *COHCHOH$	0.66
$*COHCH_2O + H^+ + e^- \rightarrow *CCH_2O + H_2O$	1.62
$*COHCH_2O + H^+ + e^- \rightarrow *COHCH_2OH$	1.27
$*COHCH_2O + H^+ + e^- \rightarrow *CHOHCH_2O$	-0.59
$*CHOHCH_2O + H^+ + e^- \rightarrow *CHCH_2O + H_2O$	-0.30
$*CHOHCH_2O + H^+ + e^- \rightarrow *CH_2OHCH_2O$	0.06
$*CHOHCH_2O + H^+ + e^- \rightarrow *CHOHCH_2OH$	0.92
$*CHCH_2O + H^+ + e^- \rightarrow *CH_2CH_2O + H_2O$	-0.70
$*CHCH_2O + H^+ + e^- \rightarrow *CHCH_2OH + H_2O$	0.10
$*CHCH_2OH + H^+ + e^- \rightarrow *CHCH_2 + H_2O$	-0.03
$*CHCH_2OH + H^+ + e^- \rightarrow *CH_2CH_2OH$	0.02
$*CHCH_2 + H^+ + e^- \rightarrow * + CH_2CH_2$	0.53
$*CH_2CH_2OH + H^+ + e^- \rightarrow * + CH_3CH_2OH$	0.19

Figure S1 The phonon spectrum of $B_4@g-C_3N_4$ catalyst computed using a 2×2 supercell within density functional perturbation theory (DFPT) [1] included in the Phonopy program [2].



[1] S. Baroni, S. De Gironcoli, A. Dao Corso, P. Giannozzi, Phonons and related crystal properties from density-functional perturbation theory, *Rev. Mod. Phys.*, 2001, **73**, 515.

[2] A. Togo, F. Oba, I. Tanaka, First-principles calculations of the ferroelastic transition between rutile-type and $CaCl_2$ -type SiO_2 at high pressures, *Phys. Rev. B*, 2008, **78**, 134106.

Figure S2 The unoptimized and optimized structure of CO adsorption on the B-B bridge site.

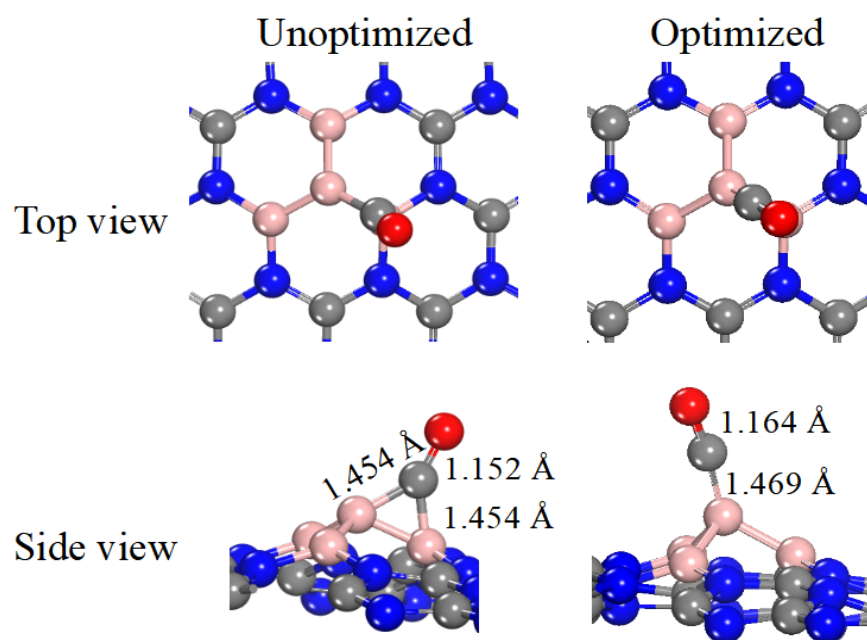


Figure S3 Gibbs free energy change for methane and ethanol products without and with solvation effects.

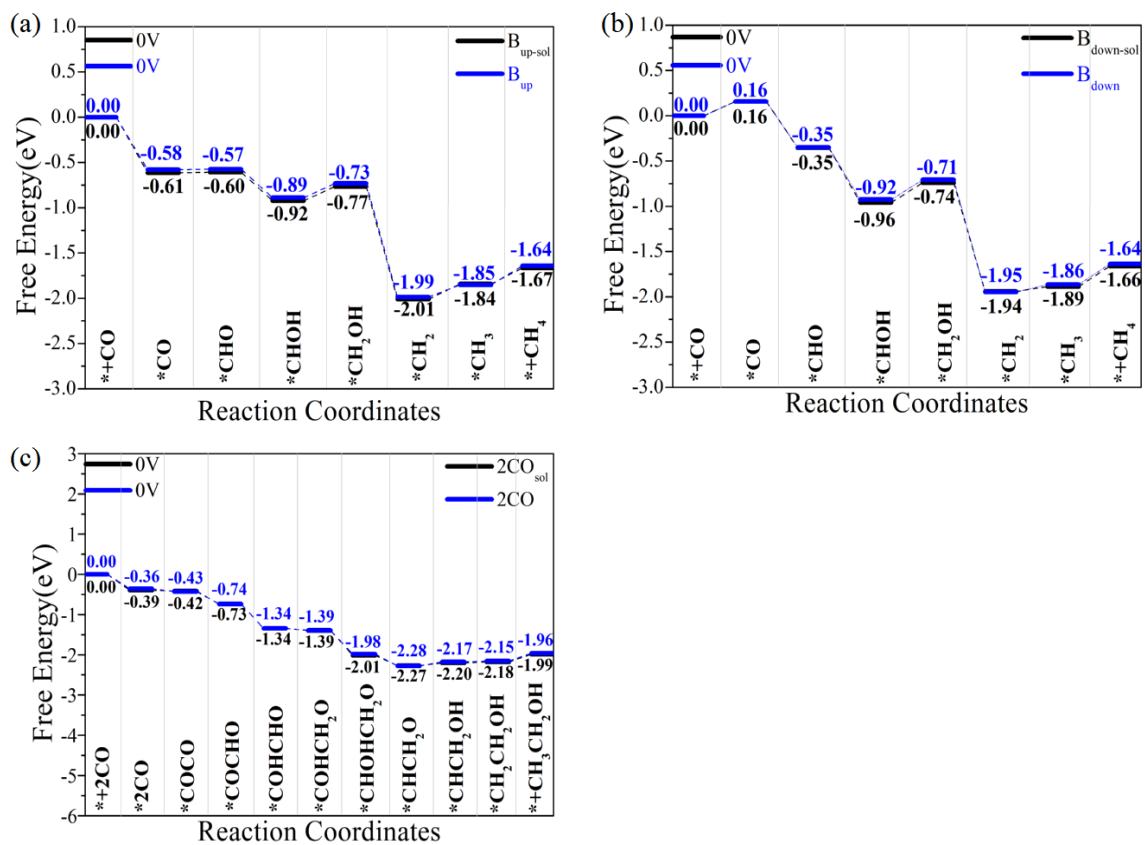


Figure S4 The reaction intermediates in Figure 6.

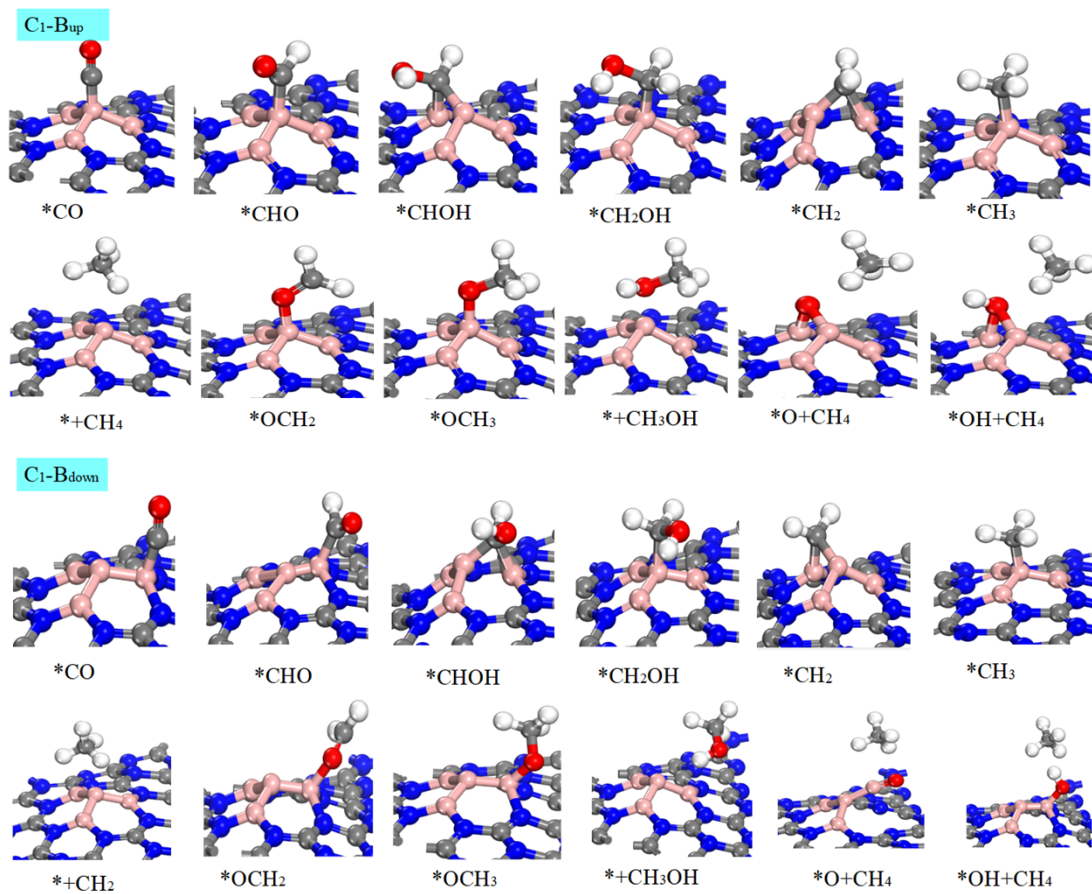


Figure S5 Gibbs free energy change for methane products on (a) B_{up} and (b) B_{down} site.

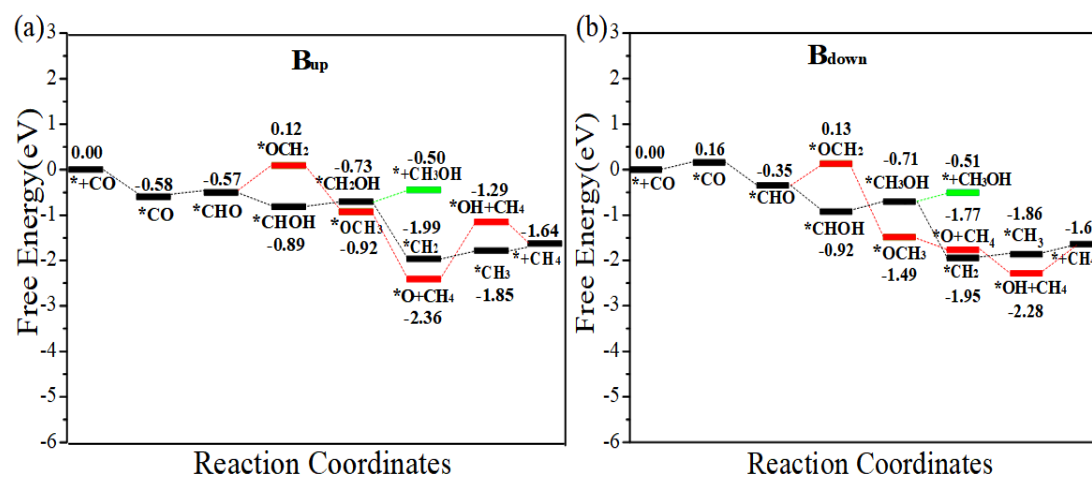


Figure S6 ΔG and some reaction intermediates for the interaction of CH_2 with CO on

$\text{B}_4\text{@g-C}_3\text{N}_4$ at 0 V.

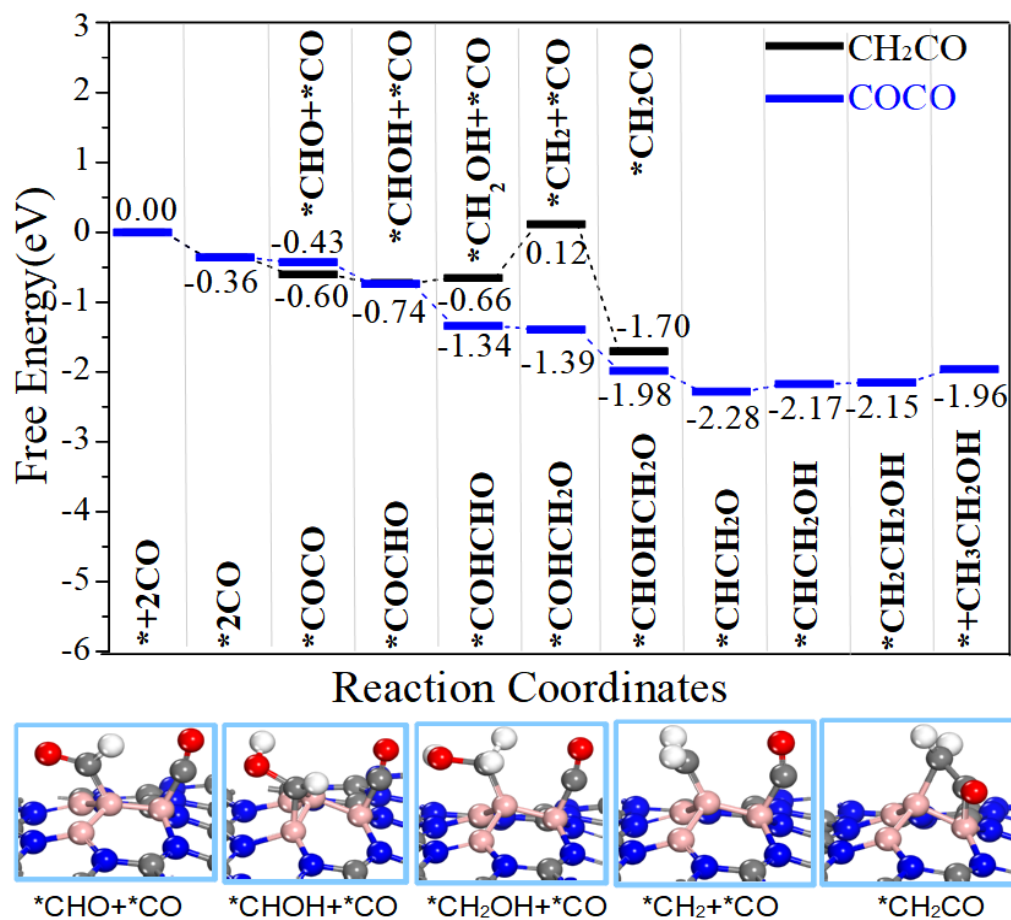
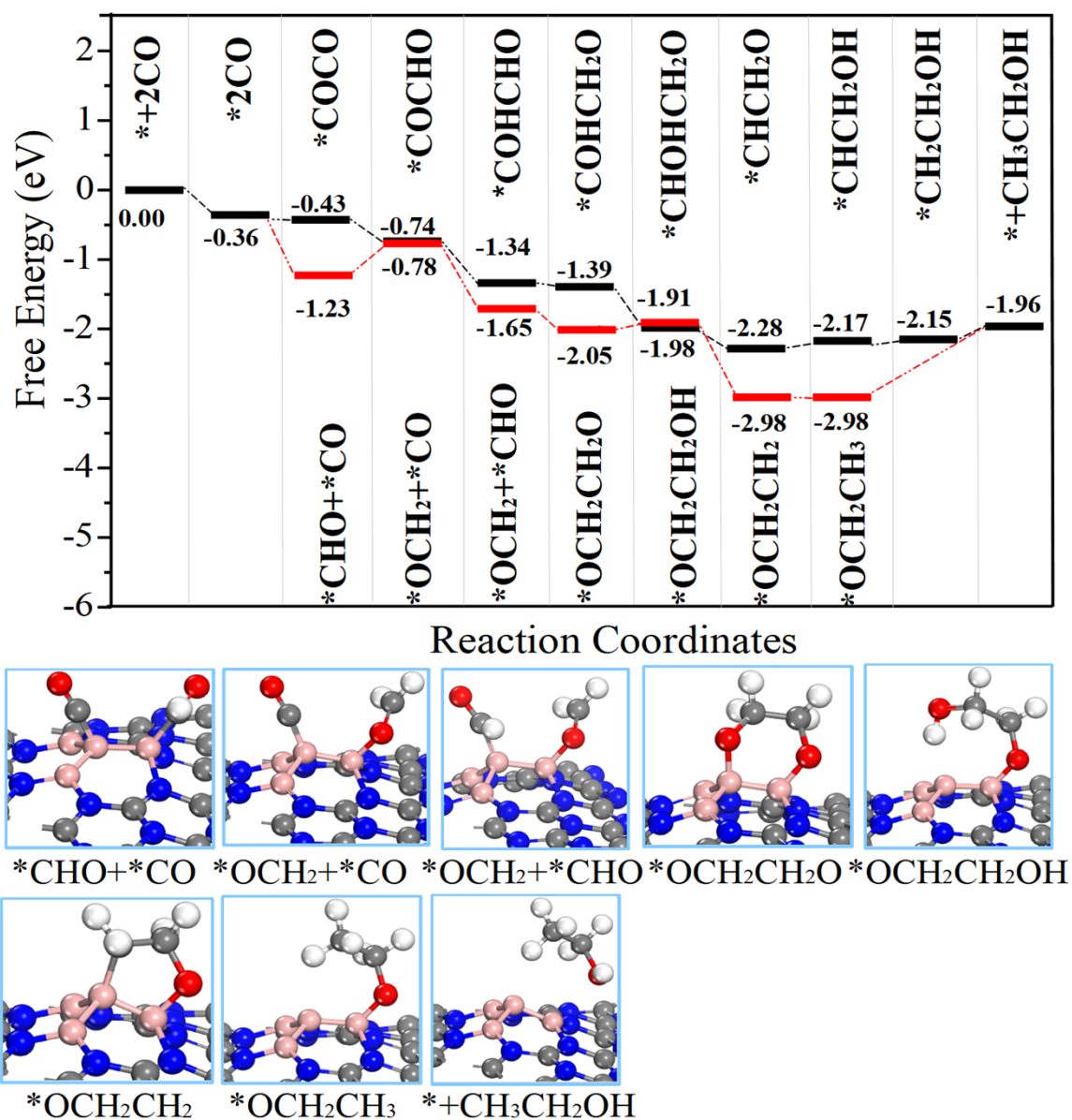


Figure S7 Gibbs free energy change for ethanol products on $B_4@g-C_3N_4$.



Structural coordinate information

B₄@g-C₃N₄, Energy without entropy= -501.81 eV

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   4      24     32
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Direct

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0.8278294018112859	0.8307214691398315	0.4690001848064043
0.6610774621849913	0.9949003651382782	0.4717446758820429
0.8257822670934587	0.9946647219297517	0.4611938023579896
0.6625619850844586	0.6678196655815540	0.4707971064253016
0.5072955871858511	0.8376050004328732	0.5227474332146755
0.5018956574289390	0.4982421700554127	0.4927120616216101
0.6691645520535516	0.8347413820000185	0.5047860884467426

Structural coordinate information of C1 product is generated at the B_{up} site on catalyst B₄@g-C₃N₄

*CO , Energy without entropy=-517.73 eV

1.0000000000000000

14.2659997940000007	0.0000000000000000	0.0000000000000000
-7.1329998970000004	12.3547182319999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.0000000000000000

B	C	N	O
4	25	32	1

Direct

0.3932206221738295	0.6081156600565099	0.5438468329055992
0.2191982930584099	0.6087215039752731	0.5463393728018600
0.3933912710427517	0.7820493582559256	0.5457420756797808
0.3359406013570813	0.6656065916153617	0.5928741528841346
0.0506724447874159	0.2760594568415368	0.4881141336755383
0.2226623671874214	0.2770481184103810	0.4765215918522408
0.2210460129708065	0.4404737607700175	0.5152652722717972
0.0515741687381752	0.4378290673472023	0.5032365835501115

0.0578877266604219	0.1186050575514283	0.4732813629059597
0.5647374464983576	0.2817627336712590	0.4813658615224128
0.7249038440366056	0.2784896737056744	0.5266330930706719
0.7244525101694791	0.4490141122404477	0.5218311641661681
0.5641031057373626	0.4402267244998868	0.4952406591034998
0.5655869782709110	0.1250888434715956	0.5025381703500692
0.8802735522844407	0.4420177968935058	0.5260895501680743
0.0564320272003779	0.7776945981984823	0.4806796336823234
0.2225488267161684	0.7800627669477723	0.5169561517050242
0.2237569489570066	0.9512095945149291	0.5078965905314988
0.0602118687594592	0.9420117298660859	0.4811482683806466
0.0537442903310478	0.6152465045829074	0.5002190262865035
0.3871883347080555	0.9516649886709805	0.5111309552432596
0.5612415061773540	0.7803540258056891	0.5161663473773268
0.7234243900346207	0.7761317795111856	0.4803635208273072
0.7224760767857655	0.9474573524248645	0.4771274986763370
0.5613963674597968	0.9474320198809519	0.4970254615031839
0.5616022035021502	0.6147203184848288	0.4918087354723173
0.8808632434743098	0.9404200741603317	0.4698021173319337
0.3855117941440348	0.4382273295120077	0.4903203616223158
0.3370326140226585	0.6666723648468940	0.6744046956560110
0.0014542887061961	0.1710624563531203	0.4793178532263402
0.3310841503115016	0.3386563063656490	0.4684102930787045
0.1651305048084079	0.4957964644458167	0.5229202703602385
0.3328600813077113	0.4964058943671376	0.5174850871192160
0.1668650840678947	0.1734318236045343	0.4619133902143857
0.0023171390861121	0.3366088688089380	0.4839500008924080
0.9996905514939943	0.0001381698013723	0.4725263892688165
0.1666953493616748	0.3326750212020267	0.5037047197085179
0.5166028508004984	0.1743507444024366	0.4712010390992352
0.8315321205345021	0.3341456997883044	0.5365242431818270
0.6634844002227909	0.4963627769625779	0.5243374338851258
0.8314368052677142	0.5017232028687940	0.5309560740403464
0.6640974411225296	0.1701989697711712	0.5331450743140149
0.5149399743503844	0.3386798687316007	0.4691998310611826
0.5025873457414802	0.0045572017977836	0.5039487690562904
0.6721355389663846	0.3365325042566421	0.5068215317081143
0.0077277263266722	0.6683193821363985	0.4756674222628970
0.3337265727683402	0.8353633059842007	0.5215302776964762
0.1658249846995427	0.9991379889505788	0.5023184954884429
0.3329279662293718	0.0029716387068296	0.5125187442423687
0.1661709167495373	0.6686567088865708	0.5225883225769673
0.0095800990113111	0.8345029436816959	0.4659588241490317
0.9963457828763633	0.4991860401103649	0.5107091953985687

0.1685239001349137	0.8337259138707491	0.5053788360623714
0.5055397062965834	0.6684206251423065	0.5190913287881568
0.8280933681153173	0.8309837438897648	0.4695252449364706
0.6604812536576324	0.9940551813946954	0.4715401920046937
0.8261014710645831	0.9948812266781528	0.4617853882309115
0.6620127322523764	0.6681538261442893	0.4705871219731404
0.5059753016802224	0.8362781241414946	0.5220960762081712
0.5018798510839070	0.4984419664135381	0.4922608790924554
0.6692416913552182	0.8347823765943647	0.5038041522542862
0.3377915623020429	0.6681590990321582	0.7387481982159336

*CHO , Energy without entropy=-521.38 eV

1.0000000000000000

14.2659997940000007 0.0000000000000000 0.0000000000000000

-7.1329998970000004 12.3547182319999997 0.0000000000000000

0.0000000000000000 0.0000000000000000 18.0000000000000000

B C N O H

4 25 32 1 1

Direct

0.3936361017810796	0.6097560624475993	0.5437801558282318
0.2182642415579872	0.6084728571036455	0.5489116961120760
0.3934340927908627	0.7801970775119023	0.5463619758315537
0.3354474422972765	0.6648517617713274	0.5923192249091264
0.0516502989365000	0.2764559548423462	0.4884784989967715
0.2227831093989106	0.2777239357848167	0.4764479816433227
0.2214999954220558	0.4421146022770429	0.5125557111746616
0.0512347566784407	0.4375247795393349	0.5031415310066744
0.0584196241902937	0.1185271792529242	0.4750443829138865
0.5638959027210015	0.2811856187801587	0.4808497753260461
0.7237813860494646	0.2778477870305366	0.5261451534598142
0.7233643590475041	0.4481466746902961	0.5215517532486155
0.5637542652851349	0.4399474648124274	0.4940490330305837
0.5648157956972888	0.1244341327718661	0.5018441679335097
0.8790699990668569	0.4411750595524876	0.5248322659251055
0.0565829026443892	0.7776992132665866	0.4808211455331929
0.2222453474768768	0.7792402887881635	0.5172619352915426
0.2237845359126391	0.9501749441658927	0.5071130621766293
0.0604548966278858	0.9420620379744562	0.4817988701791704
0.0533799529960624	0.6152591031061647	0.5000594823977521
0.3867155777606376	0.9500711710978754	0.5104313976627148
0.5609336320339986	0.7801115516407960	0.5130373403145388
0.7239654489872943	0.7762584373112530	0.4792667123408657
0.7228368222655880	0.9475421026691440	0.4759245444815791
0.5617867300066004	0.9472683099513927	0.4956756347769506
0.5622938217881661	0.6151502095213954	0.4901163392950906

0.8815600167935049	0.9408989204903925	0.4707541214072056
0.3856181250380639	0.4391335820613727	0.4889028319804420
0.3420097471477787	0.6694441810822825	0.6818016868047716
0.0021915575427307	0.1713767054665320	0.4821267293680600
0.3319234856769055	0.3388139673025516	0.4690118507931465
0.1639961258916342	0.4964704172541291	0.5218813339792947
0.3339653543394522	0.4982102139419284	0.5145275133904351
0.1673937340327144	0.1736373956662659	0.4639761991376141
0.0014032274156619	0.3363734083780947	0.4848728234644785
0.0003889639125081	0.0004910166553412	0.4740185004763990
0.1675487547893788	0.3354712208520372	0.4989084293512035
0.5160285963557646	0.1739130124466607	0.4704744361764634
0.8306835163576275	0.3336651058052700	0.5350499746554992
0.6627454672721456	0.4957831734305411	0.5238639328913638
0.8306288432860457	0.5009857167455246	0.5297531217226356
0.6634270450751829	0.1696880593995258	0.5323778951949156
0.5150275002469047	0.3388240587110939	0.4675859402984163
0.5025328782090104	0.0041354436492653	0.5028726436484531
0.6707502927577604	0.3357658110861299	0.5074393660800017
0.0070760156457449	0.6676861854804328	0.4753541516178937
0.3341001394914442	0.8347895757368184	0.5209722198820290
0.1666419095116078	0.9986235678726419	0.5018856483882592
0.3334190962232355	0.0020532422953336	0.5112116087587708
0.1644872595067435	0.6674112925997444	0.5230365504342959
0.0095925277795580	0.8343794133904280	0.4668723884081257
0.9955972204944887	0.4987142646153894	0.5095921319640299
0.1687942713243852	0.8328941357235116	0.5045987852352466
0.5057917702898590	0.6681386166947896	0.5166242507932479
0.8288362522498961	0.8314983123435352	0.4707563919411182
0.6609223081188155	0.9949942149301548	0.4708059544482888
0.8267554652101302	0.9954680436996401	0.4624566370932430
0.6630784470792918	0.6678599807694799	0.4697795054599926
0.5058388303831864	0.8364704067489542	0.5198917473666814
0.5021485964135860	0.4988391913280050	0.4903883666477574
0.6677135960623961	0.8340679037750681	0.4991883919083716
0.2663674087617256	0.6448398210145128	0.7248015952884260
0.4247247128923318	0.6988522258947932	0.7067544957534695

*CHOH , Energy without entropy=-491.61 eV

1.0000000000000000

14.2659997940000007	0.0000000000000000	0.0000000000000000
-7.1329998970000004	12.3547182319999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.0000000000000000

B	C	N	O	H
4	25	32	1	2

Direct

0.3922536165576060	0.6021815144220443	0.5473976553307502
0.2170435901554061	0.6019172260298667	0.5519525569431597
0.3953196352530474	0.7826299931829238	0.5546380119008776
0.3303715333976308	0.6494938293564699	0.5961807281855479
0.0473042372468425	0.2679213776051764	0.4968311329880430
0.2200161902211497	0.2701416178645914	0.4785879478933357
0.2192827506644524	0.4359534719990986	0.5128575238440494
0.0478835042810658	0.4300986248366799	0.5089545187979069
0.0551524751334031	0.1110027616470633	0.4802017591658591
0.5611173101390503	0.2737044031991233	0.4804202721519333
0.7200604143542404	0.2702586919015101	0.5277190238842107
0.7195424799157812	0.4404156136894009	0.5230739464991665
0.5604593077343898	0.4323750043589807	0.4937731156214961
0.5618935737390435	0.1167891226003637	0.5021326923050740
0.8753697585910312	0.4337935639368581	0.5294279655784835
0.0523970204609160	0.7696395602163453	0.4877267969585707
0.2208864257615489	0.7725734175994919	0.5190782637649146
0.2220422245194304	0.9440483579346038	0.5099963805186831
0.0573295250697994	0.9343893343698967	0.4867917645167322
0.0501215047498632	0.6078302986624039	0.5067104341373226
0.3842572776234497	0.9431329599578137	0.5111173866070844
0.5590809400028030	0.7734354782643218	0.5163531374198947
0.7212474117272240	0.7685712603960498	0.4797144122160477
0.7207980459477946	0.9408553191531163	0.4772511424538019
0.5596124509665449	0.9397572624326548	0.4970106551657081
0.5593959639503141	0.6080201804315043	0.4913824188171735
0.8787307630909609	0.9332065728379187	0.4715938322316551
0.3828109150626500	0.4323276040458054	0.4890947593735917
0.3775360187053370	0.7571052847888528	0.6410648599238500
-0.0013379295895705	0.1626503060244657	0.4915765928724357
0.3283222685483682	0.3311300940987679	0.4701401006723292
0.1630876389551174	0.4903746010268299	0.5219269307664172
0.3309546522648925	0.4922335101726302	0.5133330947534521
0.1636169018079796	0.1662658599955970	0.4658871518610873
-0.0027400355072151	0.3269411018872412	0.4953588871408562
-0.0027994347156158	-0.0073132988139150	0.4778718614377185
0.1653341885383277	0.3282099343589662	0.5036400515315365
0.5134158918991140	0.1662885015940623	0.4700822688089677
0.8263907007030827	0.3260299628681957	0.5386125867704222
0.6588120649572279	0.4880185790401501	0.5243860082565449
0.8262852051125525	0.4931567824462070	0.5337064511053710
0.6599089493478696	0.1619192890728394	0.5333674939499092
0.5123529432610420	0.3313971829552139	0.4666160697270434

0.4997213340215837	-0.0036377051971425	0.5033722485485133
0.6674092223178273	0.3281603822684475	0.5078904685087051
0.0026668160187740	0.6604464031506007	0.4841159738015901
0.3308421020303302	0.8271820169252396	0.5186121068480313
0.1643122839467976	0.9921268955652199	0.5055244567191084
0.3311344449013051	-0.0043210154259211	0.5147259959218052
0.1624122125064430	0.6613171690658356	0.5282462994698592
0.0050441599489388	0.8262895220674744	0.4748097140615796
0.9925828045553670	0.4913676134471182	0.5157750679452381
0.1670058444222718	0.8263263209606130	0.5068913805446821
0.5050753719264263	0.6617685891548315	0.5205539536717064
0.8255855763296763	0.8237190339764763	0.4683983851779708
0.6589584834195329	0.9873098155959344	0.4711113883689334
0.8245015393590515	0.9882162228522746	0.4621226367558032
0.6596312588021523	0.6611209259668530	0.4688880889849127
0.5052108409008589	0.8293709201352183	0.5208789653658905
0.4989046347402124	0.4915250948838494	0.4904754098918879
0.6680764122510232	0.8282296111363335	0.5055952870895243
0.3046975586401973	0.7861057275476501	0.6748595380929056
0.4524364892705475	0.7861147873036377	0.6732169281267687
0.2413397800847151	0.7190994081712803	0.6905449682555660

*CH₂OH , Energy without entropy=-528.95 eV

1.0000000000000000

14.2659997940000007	0.0000000000000000	0.0000000000000000
-7.1329998970000004	12.3547182319999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.0000000000000000

B	C	N	O	H
4	25	32	1	3

Direct

0.3906562407128366	0.6011612163023784	0.5464500319924143
0.2183478596762169	0.6010513566654975	0.5550681798750774
0.3916968416393035	0.7742623687324469	0.5519481005222181
0.3367396210647016	0.6584255312072944	0.5978115986264704
0.0485131750215496	0.2676087612678151	0.4960944994448334
0.2193084768124795	0.2691177617795784	0.4797216476808338
0.2189790031726444	0.4335607144061692	0.5175039326149541
0.0490307520161354	0.4294378268042032	0.5101756696913740
0.0547720182060705	0.1098781460980671	0.4798249749834210
0.5618467334697255	0.2737527351978331	0.4804604622886552
0.7206986343243492	0.2703411009674879	0.5283258975779173
0.7207187994865550	0.4406475906017705	0.5223191306217906
0.5611310906656729	0.4322682241711626	0.4937499879121178
0.5619206751480829	0.1169255149660961	0.5030816073984440
0.8763794548555418	0.4335750460812381	0.5289655879718406

0.0538701932161329	0.7693336697080796	0.4866848123800309
0.2201095225480752	0.7719055404576741	0.5235922602803617
0.2208375140766242	0.9425149452512744	0.5110245104875960
0.0568129152162054	0.9332634452478078	0.4860192047913500
0.0520381428930131	0.6074667407842307	0.5062626210047509
0.3838787299334032	0.9429349272224732	0.5137246903628451
0.5568280060217926	0.7720266956870742	0.5132997232650445
0.7198938435678410	0.7682210296611959	0.4794946783774795
0.7193004184515899	0.9395834876446044	0.4773793956583776
0.5585560266879207	0.9397731533097425	0.4976083081560637
0.5582442686384655	0.6070045016245473	0.4899968411038830
0.8779493249493574	0.9326649288975615	0.4731523743426017
0.3823273613936463	0.4305830006750118	0.4906454856807923
0.3454104515909134	0.6559614500115662	0.6890878989356105
0.9987319130536927	0.1623890605531272	0.4897717606079803
0.3281892692038582	0.3302353501111723	0.4705654262839222
0.1622269526253902	0.4884920857245473	0.5278908869812047
0.3313147037210435	0.4893862747734342	0.5179264770489799
0.1632718842014921	0.1651246750398980	0.4666397440489040
0.9985323713266299	0.3276410097320298	0.4934046360574447
0.9965104068824440	0.9916679066397404	0.4778329104785818
0.1647754669510790	0.3266218884714233	0.5046871935447034
0.5137905817424698	0.1663011170757579	0.4705706303192358
0.8271888450410113	0.3260137200653598	0.5394105009183467
0.6598195060297296	0.4880415909556860	0.5239808677813694
0.8276889275533856	0.4933623174399112	0.5323557448126164
0.6598037057327807	0.1622511686504562	0.5346721886458394
0.5127910153570280	0.3312601012217377	0.4669582756427445
0.4995234076369658	0.9967790650840496	0.5048859173555951
0.6685558895391481	0.3283960288093637	0.5073556931049522
0.0054939708431053	0.6596514075618386	0.4813340976908691
0.3319100651663184	0.8283628530153785	0.5266705207837534
0.1634371747801412	0.9905847766489382	0.5048681627253712
0.3306508133908710	0.9950951939347900	0.5135062931274524
0.1633539007848895	0.6599728254165884	0.5296108163870975
0.0062532488558649	0.8254191904386978	0.4722062879189908
0.9936737702648178	0.4909376770803577	0.5157626928544684
0.1660159329881790	0.8251611859728548	0.5110978074406035
0.5015796986008467	0.6599219337555520	0.5164988079720304
0.8249783613573582	0.8233154375533497	0.4719995011946786
0.6576270912699999	0.9876904089417982	0.4726533580959074
0.8234810002351752	0.9877754058408319	0.4648521436697475
0.6591047922740224	0.6597393973224978	0.4698402388288752
0.5025941399234563	0.8291032552698966	0.5218534396811503

0.4988399584739749	0.4907206508302203	0.4905448484996207
0.6634876951852772	0.8257813144978468	0.4988315238185398
0.2826467593749409	0.6947248548871207	0.7283206233669810
0.4291956395685358	0.7092483090663264	0.7079505653105779
0.2073530340149818	0.6465700588060866	0.7148873752271829
0.3214320095922421	0.5733592833794746	0.7088376377445342

*CH₂ , Energy without entropy=-519.06 eV

1.0000000000000000

14.2659997940000007	0.0000000000000000	0.0000000000000000
-7.1329998970000004	12.3547182319999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.0000000000000000

B	C	N	H
4	25	32	2

Direct

0.3953127767642717	0.5983282713253675	0.5628712046430477
0.2151708396716673	0.6039540432800971	0.5555661523977341
0.3901931728836273	0.7779925802296407	0.5522992097375451
0.3271496940899153	0.6690490441561678	0.6004915571833376
0.0462826524146031	0.2693116333140661	0.4982958680806253
0.2188457777618301	0.2710982636131537	0.4848619918278322
0.2175967029962450	0.4351335648374151	0.5249100000300247
0.0477658036047687	0.4312487614841454	0.5120209903492710
0.0538923485792344	0.1122245258959721	0.4814869782927300
0.5596972404887631	0.2756549765139474	0.4835719364350101
0.7199875589551525	0.2719097913610645	0.5277878611790610
0.7193736172759494	0.4421359254400773	0.5249399951224990
0.5592481653579552	0.4341969341539590	0.4990071175397975
0.5608959576233036	0.1186578021668237	0.5030237164528589
0.8753621558273766	0.4353630698081951	0.5295834719716582
0.0520452246947694	0.7704378729404948	0.4828530376214045
0.2204078275385676	0.7725258749511534	0.5117241757327329
0.2211842778683135	0.9447349924864632	0.5075017536751204
0.0559924790274743	0.9350138074834111	0.4854928118412062
0.0497819535878202	0.6085788615555153	0.5036636066364031
0.3834118485444704	0.9442735897414151	0.5106081237929558
0.5567037532004454	0.7744216787031513	0.5203001300452318
0.7189016993226034	0.7695506035716544	0.4837153712822223
0.7185570749408985	0.9416509762855473	0.4795745119512365
0.5581868014921604	0.9417235403598130	0.4997057611818307
0.5572475529698913	0.6094295280798608	0.4970789398264835
0.8765839871911245	0.9338744234004113	0.4738311506337377
0.3805681977522949	0.4326550929410309	0.4979326945335338
0.3823509943895601	0.6157244607002994	0.6469284590610027
0.9973972862968351	0.1643945233424680	0.4890432782752033

0.3267221977041474	0.3328493970641391	0.4757014639870599
0.1602004259622898	0.4889246512774533	0.5336015634062771
0.3283605662907988	0.4897587672820571	0.5258588269638098
0.1630001006122119	0.1678517711266545	0.4695118710815124
0.9981942407000918	0.3296784572073617	0.4933954072119040
0.9956647601697803	0.9934075580815299	0.4785332915528234
0.1631505676164441	0.3269440335159466	0.5138357993155056
0.5115078153855472	0.1683118211073704	0.4726790258219593
0.8264855359253646	0.3274350272971108	0.5382278898552438
0.6586414664376841	0.4897008467487198	0.5280576572344281
0.8262444018148941	0.4946445940591226	0.5348054373121244
0.6596307763381597	0.1636116471628836	0.5331619738756900
0.5100565783304029	0.3330829850766905	0.4722277978269520
0.4986393360669166	-0.0017026031392327	0.5042530526012031
0.6671046187737856	0.3300950527990179	0.5089686601394879
0.0012242417482023	0.6609684519970044	0.4821003412190182
0.3304487286521838	0.8283251239356586	0.5175335313233799
0.1620392379982784	0.9916842683394231	0.5061547809925687
0.3290974562773540	0.9961345142061921	0.5158786928241306
0.1631001544533753	0.6621536926238516	0.5211382314561319
0.0034903203883949	0.8266997081268364	0.4726590153174008
0.9924159678826766	0.4929993567840426	0.5158867485418031
0.1676554470889595	0.8270522635928225	0.4963239788481330
0.5026638665426718	0.6638269415812543	0.5241387622274924
0.8232370282645750	0.8242010114371815	0.4727344504460476
0.6569184928514007	0.9881156563016218	0.4731918002357491
0.8223034804422458	0.9885289412787163	0.4644599349735989
0.6573645140955849	0.6617073035886737	0.4743774685882169
0.5036116547866362	0.8323705706166892	0.5273817512519390
0.4970874119081838	0.4930186810836480	0.4975298168191644
0.6647926345729754	0.8288332278856684	0.5072768418653236
0.4570799791144137	0.6713658898661812	0.6761801834221244
0.3283906556914796	0.5431913779649330	0.6788320571284491

*CH₃ , Energy without entropy=-522.54 eV

1.0000000000000000

14.2659997940000007	0.0000000000000000	0.0000000000000000
-7.1329998970000004	12.3547182319999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.0000000000000000

B	C	N	H
4	25	32	3

Direct

0.3888996440547067	0.6037001634037252	0.5542578711051688
0.2163445951377630	0.6044508333112787	0.5529695998977756
0.3886216339947667	0.7760873872591094	0.5510722745218033

0.3314875655806839	0.6627212270561785	0.5995811703987726
0.0473405570294130	0.2700811911058660	0.4974147462851545
0.2183072770522961	0.2712189333852865	0.4859169593554552
0.2174365028215494	0.4359559603811863	0.5215327258007270
0.0476919603298295	0.4318511894603926	0.5098577085223712
0.0535820705261383	0.1121693628293126	0.4823392699400655
0.5601679711250312	0.2762627307140909	0.4836578873022376
0.7196769133140356	0.2720624181900374	0.5287428368120721
0.7193858205642712	0.4423739551261750	0.5258964510438591
0.5595496549647787	0.4343613458337125	0.4994985994392201
0.5606620814682831	0.1190583800918715	0.5036331476114516
0.8750785785548553	0.4353655902615059	0.5293659415118436
0.0517875432232728	0.7712145076585594	0.4844987098913296
0.2180652625809941	0.7738180497116159	0.5204120501178778
0.2189479802953429	0.9440095458645357	0.5094598343878535
0.0550446129322541	0.9351527957682069	0.4857539624585220
0.0496152473054904	0.6093008914416655	0.5043857608341654
0.3821667936206988	0.9448461531076432	0.5120236081961057
0.5554296034528280	0.7742579730988518	0.5187075198229192
0.7184475622994602	0.7700859821007757	0.4855491043787253
0.7175155301531346	0.9409620456451582	0.4797630439546146
0.5566975916595038	0.9412492099506092	0.4983215357550952
0.5567459987158569	0.6091059915660257	0.4974746240872073
0.8762364459724274	0.9343505739613189	0.4758826158775325
0.3810448782577014	0.4328734437243074	0.4981277040323775
0.3214988631877795	0.6711989030656229	0.6904589577747479
0.9974763492392892	0.1648904462920621	0.4902292359410584
0.3273595267461231	0.3323416310587335	0.4784238511906085
0.1606172209783449	0.4912463676235200	0.5283468502377087
0.3298438111413696	0.4917411851217501	0.5245378098952631
0.1627366142357196	0.1675742040197457	0.4719472600988251
0.9976002512833095	0.3301403533544678	0.4930123043211259
0.9949990858196033	0.9937993321983098	0.4793554846903861
0.1631818214911213	0.3288078589049312	0.5090901011301688
0.5121354072981233	0.1691252370455092	0.4726469894521326
0.8263121068532692	0.3276627446797844	0.5386406548493357
0.6584498463223470	0.4895683998498559	0.5294823675335321
0.8265552226190926	0.4951137632034877	0.5347730682437289
0.6592254961138770	0.1638831807987486	0.5341837538080824
0.5111510336293125	0.3340739112425472	0.4715112365873608
0.4979652609124660	0.9987324056194558	0.5045664353000936
0.6670482292648110	0.3304258695320004	0.5101142735802024
0.0027536567773898	0.6612489826447711	0.4795176116053117
0.3299050952082578	0.8302033214088016	0.5239971895526222

0.1614619764280492	0.9920517960795214	0.5046742765788845
0.3287482759473154	0.9967802481427739	0.5120078492840103
0.1611898620743926	0.6619940087950785	0.5263593068018996
0.0042441560567461	0.8275078694597179	0.4705727299517876
0.9918949271737856	0.4930103927910966	0.5149332185419314
0.1639353526651647	0.8269445019645411	0.5083047531973988
0.5004426485165414	0.6622176199258100	0.5241790048975886
0.8233570162343937	0.8248756539823914	0.4771100658183721
0.6558131736856520	0.9884929418501802	0.4734853143501598
0.8215220087755514	0.9887681843910455	0.4662649123457343
0.6573466890404210	0.6614989300534939	0.4766253234657717
0.5005897027025772	0.8310747075616279	0.5237442951122711
0.4973952349340479	0.4928375195969535	0.4979225322614535
0.6623194464089919	0.8280895400905510	0.5044296654466949
0.4013776847818099	0.7164291762656687	0.7173312985365062
0.2774020387520624	0.5907838466866699	0.7167359851375416
0.2767871717135317	0.7136071976897705	0.7041165861373962

CH₄, Energy without entropy=-525.91 eV

1.0000000000000000

14.2659997940000007 0.0000000000000000 0.0000000000000000

-7.1329998970000004 12.3547182319999997 0.0000000000000000

0.0000000000000000 0.0000000000000000 18.0000000000000000

B C N H

4 25 32 4

Direct

0.3879411545962161	0.6017413509165694	0.5441745495789095
0.2133434030402620	0.6023699713023439	0.5483616834234569
0.3885415083482852	0.7766132634202074	0.5470556840742198
0.3308708723933202	0.6598462755081392	0.5814901835146117
0.0439311780592322	0.2684600649010975	0.4920820449670140
0.2172992090328169	0.2699925386000667	0.4771858083683653
0.2157714885864458	0.4349462041181874	0.5140597142932439
0.0448266289485761	0.4300614530515379	0.5057942018714975
0.0519955342624116	0.1115550788659996	0.4764895182465498
0.5593123849725773	0.2752826511650171	0.4816484783389931
0.7184642458405035	0.2716228580910280	0.5283661026198889
0.7178891963351859	0.4418258479433262	0.5238542315377033
0.5583955381644574	0.4335935025512037	0.4954832836791866
0.5599249939918488	0.1184315145977985	0.5025284769311421
0.8737587601041237	0.4351127246974869	0.5283576253533881
0.0500485727950180	0.7706780248904417	0.4810545936885341
0.2173743219769691	0.7733057452285864	0.5157177404367543
0.2188586272618110	0.9454376716257324	0.5079564874164505
0.0542820676973080	0.9352814032544055	0.4829947791072899

0.0471951126847627	0.6088025173655451	0.5016214927162370
0.3814527100777270	0.9455123213854418	0.5106980224721073
0.5550119106527958	0.7737671606992148	0.5141816267058333
0.7183612382863613	0.7693837064642121	0.4809082593954543
0.7172349822093091	0.9417961391297405	0.4756298445634052
0.5565253929540743	0.9414032299266493	0.4960752445613238
0.5568378042347317	0.6085454231889075	0.4915973410792888
0.8753811284475731	0.9340471459712301	0.4707055014353638
0.3797741928587152	0.4311574119452097	0.4899606087631111
0.3396786373032435	0.6714331225624386	0.7594685703512246
0.9952636615797193	0.1634408173859400	0.4851848025041577
0.3256528399076812	0.3305870124446221	0.4693001414251787
0.1583935300368266	0.4885528755443939	0.5227745216818925
0.3275632520417874	0.4893407989214499	0.5157239050565228
0.1607534468939023	0.1663552816851050	0.4634542537032215
0.9942200348145717	0.3277278490953085	0.4890594545467756
0.9938892475780959	0.9934327625548046	0.4751548138934794
0.1616084101127036	0.3272728734746997	0.5033283564796459
0.5115596032444686	0.1680793945752419	0.4707019994051760
0.8249449464688126	0.3273379960993142	0.5387708639444259
0.6569058143495402	0.4891463838860867	0.5259632106792583
0.8248619223508422	0.4946838716094738	0.5331692601409178
0.6578714514690743	0.1632464344547289	0.5339459466702676
0.5101778038224685	0.3326236365384594	0.4684620544284403
0.4971864524763212	-0.0016554234115388	0.5032189563725529
0.6657291942286453	0.3295812178351056	0.5088558441070966
-0.0000092499725628	0.6612304411456756	0.4775569071329405
0.3283074836248614	0.8303061514836653	0.5207988692090810
0.1599120670770937	0.9923453892040754	0.5045086754211384
0.3276521112933599	0.9976596532977225	0.5133967496439721
0.1591191924327530	0.6622745728721576	0.5228572054814999
0.0032901326101137	0.8277181338143075	0.4677287471734574
0.9899023803316080	0.4922334157844266	0.5125378745912248
0.1642020689611508	0.8271810335284968	0.5020148254325116
0.5011331701884700	0.6622075332500927	0.5172098567608523
0.8229623903842564	0.8246587421443776	0.4711445639570840
0.6557587024683916	0.9887606750642475	0.4699170242224989
0.8207387262077019	0.9884763656968881	0.4602400269728458
0.6581215519141806	0.6615660914450309	0.4712791611447740
0.5016841561130312	0.8313103570331239	0.5205039234735591
0.4964673625225667	0.4918630460646553	0.4917506016195364
0.6635013222068261	0.8285796999269930	0.5031458596855630
0.4257540857659933	0.7309930462353935	0.7517199601135299
0.3176780887111499	0.6026042261880000	0.7222008282820791

0.2907846049814899 0.7086732418864193 0.7452499736562457
0.3247453806854490 0.6438181678732894 0.8174281004960455

Structural coordinate information of C1 product is generated at the B_{down} site on catalyst B₄@g-C₃N₄

*CO , Energy without entropy=-516.94 eV

1.0000000000000000
14.2659997940000007 0.0000000000000000 0.0000000000000000
-7.1329998970000004 12.3547182319999997 0.0000000000000000
0.0000000000000000 0.0000000000000000 18.0000000000000000

B C N O
4 25 32 1

Direct

0.4027804097781172 0.5981440084048033 0.5621762806883496
0.2196492533607508 0.6073755294334249 0.5492346871739681
0.3950512758427215 0.7818041188639795 0.5474432265730973
0.3371061982433033 0.6653596675769148 0.5817553567208433
0.0504514310842739 0.2749743343989743 0.4881631119163901
0.2230790103077556 0.2762659358501470 0.4728743755284532
0.2217929630613853 0.4404684445638855 0.5124672674377996
0.0511439502070615 0.4357938256303086 0.5052519040660358
0.0580664824775452 0.1174389010662229 0.4737836193867463
0.5648505219246743 0.2807545846760782 0.4788066284070965
0.7241272409640036 0.2776858948319615 0.5258885550274803
0.7238626997228489 0.4478402445679390 0.5201279336128439
0.5640617587619592 0.4392601038126748 0.4921231701482270
0.5653758147621006 0.1241227218432062 0.5010638419457263
0.8796725603248287 0.4410724221293011 0.5258180446958052
0.0568742550656299 0.7766812903830591 0.4813959520825486
0.2236273427867562 0.7787205054979255 0.5166845478045609
0.2243640191973279 0.9505790317887541 0.5082532211072630
0.0603606941725167 0.9409043087012853 0.4816868581849656
0.0545271308301481 0.6150207643991475 0.5020058291372023
0.3869508292789574 0.9504072306679703 0.5116636281379966
0.5608237640430683 0.7790930071785952 0.5124365654301218
0.7231472148740165 0.7747936869827142 0.4752596050595345
0.7224138262473315 0.9472065335562335 0.4726562322264167
0.5626313218411835 0.9473053051381722 0.4959311075457226
0.5628296048053794 0.6145539259382941 0.4899138668200361
0.8811055783374202 0.9397409576591147 0.4679281091846122
0.3847981313360658 0.4365168433177203 0.4883307363331664
0.4192578053692174 0.5732903878554967 0.6430390861652538
0.0018766795067200 0.1698620998683781 0.4832778932824164
0.3318912506130838 0.3371383869905557 0.4653216029649385
0.1635157067646277 0.4932311496304870 0.5243099367154400

0.3334738016560801	0.4928400779905881	0.5177532096018892
0.1665795009002637	0.1722549160024093	0.4604498517237288
0.0002745675902829	0.3345139554168589	0.4864610852638521
-0.0003024375739033	0.9989716719231512	0.4728839425443315
0.1679578973401927	0.3352479434128214	0.4958026933602986
0.5169553093775554	0.1732999718150887	0.4686497159760024
0.8306657318320457	0.3334683794942861	0.5363138534652173
0.6629715139143859	0.4951873694421377	0.5220033694023540
0.8308402627159283	0.5007023567212180	0.5297529731241839
0.6634050052716487	0.1695731989189675	0.5324471356206584
0.5156875699727888	0.3380797842316310	0.4655625527290767
0.5027821704807960	0.0038320269823331	0.5031377921988638
0.6715923065133621	0.3355131097516313	0.5055454413903183
0.0075185634683112	0.6672542456623893	0.4770138472443046
0.3341632509257050	0.8353253094760045	0.5217725978589735
0.1660605452162056	0.9982133254439894	0.5029731287467617
0.3333181211841187	0.0028631523453767	0.5136556637829264
0.1657712250417101	0.6678693188205143	0.5238311679627148
0.0096007781230847	0.8330335682758077	0.4667252935567893
0.9965096129594373	0.4982477662274857	0.5118125947476332
0.1693249987454737	0.8328754021487756	0.5047726886977061
0.5099448469039979	0.6678994214221696	0.5206064289646583
0.8279876345386246	0.8301203764290150	0.4672005765880229
0.6611475013385616	0.9952237346583912	0.4690746935042528
0.8265693634078048	0.9947300848374733	0.4596494449998946
0.6621534310138364	0.6662511196496238	0.4657750814857847
0.5084742065982157	0.8377801112416497	0.5214395337770457
0.5018843876928428	0.4975469010384654	0.4893758524761391
0.6661528223504697	0.8325467838363563	0.4942156112467314
0.4188587316073831	0.5613684331796499	0.7071393284478303

*CHO , Energy without entropy=-521.14 eV

1.0000000000000000

14.2659997940000007	0.0000000000000000	0.0000000000000000
-7.1329998970000004	12.3547182319999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.0000000000000000

B	C	N	O	H
4	25	32	1	1

Direct

0.4042591761335276	0.5979440783222555	0.5691416316178060
0.2200618198699115	0.6097717864500989	0.5487699414410403
0.3940044065882566	0.7828962187442277	0.5458290528042692
0.3385017606922340	0.6662173288697416	0.5804852679321738
0.0509145593974000	0.2768367177437978	0.4885228888371331
0.2232759566954522	0.2780665873805475	0.4753778025362793

0.2230548801740818	0.4426866371939616	0.5144039354384214
0.0522371145196648	0.4375627485455011	0.5058628332635347
0.0579578260742422	0.1193097220688747	0.4734220751061092
0.5648859770316541	0.2825832832248698	0.4810064540714291
0.7243065119669290	0.2786634006713598	0.5258378904985983
0.7237845944078659	0.4487761030705993	0.5229389122712971
0.5640089696876970	0.4409090545455938	0.4956944052233246
0.5655914642301161	0.1252702252724616	0.5002833140854643
0.8800184870945755	0.4422175102917272	0.5264830065302759
0.0565454741760005	0.7779819711760516	0.4805695748327132
0.2229933248585155	0.7801754777952774	0.5157407387705729
0.2236757357631202	0.9512053763904689	0.5058667020290845
0.0600395277800319	0.9419839604172280	0.4799596520390579
0.0541749842952214	0.6163894199184701	0.5020825207138788
0.3866014128895637	0.9514560472927417	0.5090268514436906
0.5598417848297818	0.7792078330167993	0.5123439804144175
0.7230256607570315	0.7755073734660354	0.4766047756908059
0.7214780813898113	0.9473766235672602	0.4706731251370001
0.5620613547505923	0.9474059594629871	0.4941534780893000
0.5630328820695447	0.6161069421462959	0.4930872317556904
0.8803196494918141	0.9405725157705926	0.4670806742938405
0.3842984624744066	0.4377091382471295	0.4927572462413375
0.4375786126205954	0.5579248193251383	0.6433734456956696
0.0015565098246867	0.1711509384962354	0.4823824695668379
0.3322918100706359	0.3381703579385120	0.4693115529859091
0.1640637301505612	0.4950108718719760	0.5244634722433679
0.3334749745855958	0.4945732244717199	0.5193213346843040
0.1673877550492892	0.1742600050175727	0.4616183719502545
0.0008607446309932	0.3356913395866354	0.4872978548964910
-0.0005641093931999	0.0006437389825530	0.4716443484237433
0.1680580096163148	0.3361958218276803	0.4973570609126954
0.5170254967219605	0.1752839121533085	0.4695187417646089
0.8310141598977498	0.3343574779366023	0.5356315502159484
0.6628655186521589	0.4961555562752919	0.5257352674602194
0.8310656908938161	0.5016642725132002	0.5316327599113826
0.6640491171505295	0.1701345795817130	0.5308293580649590
0.5159281814449593	0.3402348372582156	0.4682354265444262
0.5025254351488888	0.0046616596855175	0.5010717423827891
0.6712108858772627	0.3366410899438131	0.5080237891713855
0.0070020151149807	0.6681412150831557	0.4767426572631663
0.3338009400666341	0.8367824291937795	0.5204657917467906
0.1656406584177989	0.9992477688293664	0.5004694478379196
0.3328364568312300	0.0036719363396894	0.5098959191606536
0.1652679775537561	0.6691252869801257	0.5237323565362905

0.0091057799465956	0.8342348483626905	0.4652042151870098
0.9965962301136223	0.4995407550898988	0.5122612405493657
0.1682167474769156	0.8339876544817653	0.5040361299467420
0.5093125654152286	0.6692230621380800	0.5213371686882589
0.8279503507561651	0.8307544538890004	0.4684122594530287
0.6607598017791916	0.9953314211691152	0.4668937897292140
0.8259511527672144	0.9949617179308139	0.4571325037450418
0.6626149841345038	0.6668285188402254	0.4688852279326154
0.5078204999704925	0.8385399012031443	0.5198950129455239
0.5019399405781086	0.4989929666502327	0.4932383566105401
0.6659932276444310	0.8333874827812798	0.4939662497898379
0.3883407217197888	0.4655036944649088	0.6688317399391861
0.5088054516815048	0.6222002316440620	0.6757353909552607

*CHOH , Energy without entropy=-525.48 eV

1.0000000000000000

14.2659997940000007	0.0000000000000000	0.0000000000000000
-7.1329998970000004	12.3547182319999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.0000000000000000

B	C	N	O	H
4	25	32	1	2

Direct

0.4049299186586231	0.6019318965351909	0.5481841668502021
0.2261144864746144	0.6056045052817937	0.5511110667265245
0.4020967858241419	0.7797111347736255	0.5472323520178802
0.3407897835033179	0.6689164872686438	0.5939141421793630
0.0554163690627403	0.2703914335289356	0.4993064555791111
0.2277073262138693	0.2736856072185788	0.4767720370680536
0.2276597265673919	0.4382865333984294	0.5158917474494115
0.0553649990471035	0.4318953869649249	0.5122017050129873
0.0633689767633226	0.1141881261263012	0.4794353745011160
0.5690302173776668	0.2784912073903510	0.4774615400697236
0.7270754500596794	0.2751375132708124	0.5269319111868059
0.7273915502945717	0.4454423598316199	0.5201563946700126
0.5684002569292507	0.4374198124381213	0.4899127272515303
0.5697095311598993	0.1216828657643876	0.4996415233235766
0.8830086454184867	0.4381124805884939	0.5289108231885387
0.0610091560630199	0.7724716773749093	0.4843326920732526
0.2299072599257710	0.7750371497057995	0.5124187846100882
0.2309625601792636	0.9474173901623579	0.5061560205587331
0.0652326770434275	0.9371949881464825	0.4844191077675720
0.0587305647772873	0.6104261650847872	0.5042107167024116
0.3933764976066950	0.9466685134942073	0.5082449778629117
0.5674840633082234	0.7775685828565371	0.5107932198543189
0.7289658148026441	0.7727686694753196	0.4721541125282075

0.7297773990710550	0.9460819094008907	0.4738786337787206
0.5690701865874176	0.9455524338674939	0.4948339877438397
0.5670346550891749	0.6127715821427715	0.4844087345309412
0.8870057124112689	0.9371483562088692	0.4674455819280877
0.3898808857457248	0.4357507370145069	0.4860704025622719
0.3918836941341646	0.6081942459729273	0.6349457814314561
0.0069048477954888	0.1647798790857773	0.4934344941540767
0.3358435097955266	0.3347825822198484	0.4665506770900298
0.1699950168914801	0.4915355598511866	0.5279378866273703
0.3381018722109443	0.4942979155321545	0.5112509606239358
0.1715256083527199	0.1699508367854232	0.4631780360979015
0.0048087849881142	0.3287091933919566	0.4985929164157724
0.0054474060989551	-0.0043526772947905	0.4757344132080957
0.1734726987042088	0.3306547016929349	0.5046708168098575
0.5215688165879868	0.1709712289348816	0.4668476094344912
0.8331372826386447	0.3304294196538237	0.5391506261996668
0.6667066766707136	0.4933083356366632	0.5205884333665278
0.8339933362349142	0.4977210675737651	0.5314165895230827
0.6664853348401414	0.1667710444504660	0.5324912997858444
0.5202838828058683	0.3360889296835743	0.4633631207521657
0.5084028903838905	0.0010815165621163	0.5004972739188708
0.6750375829443037	0.3330002348349577	0.5054520941592019
0.0103872618029649	0.6630624023307575	0.4833233810391345
0.3405367963009095	0.8307884525729369	0.5162988027915962
0.1722383847239772	0.9946418903667457	0.5035571875970464
0.3392606238708250	-0.0012476206592053	0.5132302238098790
0.1725827115060630	0.6644297489807706	0.5214011021501461
0.0122621346964967	0.8285037997806284	0.4741080329882524
0.0005419390956197	0.4944559037797303	0.5161114081203857
0.1768235647335469	0.8292818888461807	0.4979623721454586
0.5129249126217547	0.6673210182720974	0.5116612968270351
0.8333560074305471	0.8277941815103410	0.4610891807470593
0.6684130669402065	0.9931940423471227	0.4690669323658366
0.8337648466703502	0.9932817904709926	0.4597808470513358
0.6671822812465139	0.6651930479640671	0.4614337879885663
0.5144707200997604	0.8352454043380318	0.5199704591934819
0.5064657125445789	0.4961529200096005	0.4857133670352779
0.6759903919288054	0.8319961917754682	0.4991202663403668
0.3228115135458648	0.5052444412311490	0.6686958692638542
0.4685167754626098	0.6553494887969983	0.6651265898783998
0.2679697147348903	0.5113714144027699	0.6968448864923330

*CH₂OH , Energy without entropy=-528.93 eV

1.0000000000000000

14.2659997940000007	0.0000000000000000	0.0000000000000000
---------------------	--------------------	--------------------

-7.1329998970000004 12.3547182319999997 0.0000000000000000
0.0000000000000000 0.0000000000000000 18.0000000000000000

B C N O H
4 25 32 1 3

Direct

0.4020398528963872	0.6043431015268758	0.5357041773293200
0.2296911512264911	0.6035705089300505	0.5513214774471071
0.4040081447815708	0.7765223183871289	0.5472813501263013
0.3500655189325427	0.6595683694873445	0.5907745231053863
0.0586802915747962	0.2691303948803879	0.4968151581418686
0.2290726293743187	0.2719476256809111	0.4727474971035673
0.2294601667635912	0.4367202267834194	0.5101567706436868
0.0581204683580485	0.4307227333050506	0.5101117931446495
0.0654936382609761	0.1122181241133775	0.4782327659498216
0.5713219206819691	0.2758635981798730	0.4734649893005340
0.7290760622701039	0.2728707887268603	0.5240216873718035
0.7293576815661548	0.4430483970679719	0.5163742613251425
0.5707427839718460	0.4346981612796446	0.4847555023464890
0.5715494015387784	0.1193346650528982	0.4975848360220709
0.8848273946231395	0.4358226315904551	0.5264718691581483
0.0641311328886864	0.7716258982727985	0.4873992338255466
0.2311676038347032	0.7741084582209402	0.5213101975388418
0.2321176389826081	0.9451252728678735	0.5085890129686788
0.0677828511072118	0.9358731340380754	0.4848732051405282
0.0619057576775764	0.6094442577339054	0.5060252017042666
0.3949356364252152	0.9447467558592872	0.5094731766836273
0.5684621844226224	0.7749734436933736	0.5056938716993006
0.7308572097171659	0.7710113418047320	0.4701611698247083
0.7312949268613852	0.9429840422897797	0.4716152651623667
0.5702335046265020	0.9428231767126356	0.4921216511768536
0.5689644548143795	0.6099041679622977	0.4797115717732998
0.8895085713040333	0.9353045073974956	0.4677942641350359
0.3923046224645839	0.4336361295943945	0.4807262094614892
0.3653129353419748	0.6410154493699435	0.6791326522201446
0.0095702229576436	0.1635728407819512	0.4930200292338255
0.3377865432200622	0.3327717744316944	0.4619617302796108
0.1726970487233715	0.4910679199597491	0.5238609142919451
0.3417989486024756	0.4931458337960329	0.5074823720704513
0.1728406912277471	0.1675776090009311	0.4613459965000639
0.0072060471367253	0.3277676831996898	0.4972688154209649
0.0075700580236408	0.9939441537410851	0.4754919892718543
0.1753675572359028	0.3298630142219999	0.4981006001215541
0.5236397296100327	0.1683003837066304	0.4639873036089884
0.8350806508531636	0.3283286044573125	0.5366669723815781

0.6687429576201424	0.4907358901713442	0.5159452234353020
0.8359851513729842	0.4955237361678267	0.5281464058286033
0.6685400102553626	0.1647911247542764	0.5303279788648477
0.5227394149349471	0.3334049200540986	0.4583411550658039
0.5102902415829376	-0.0010004374061106	0.4995633236172834
0.6773894373740329	0.3307337373981757	0.5016601742465053
0.0150656879331516	0.6620628253253181	0.4826854050194124
0.3432026844589076	0.8302085757650304	0.5227909773403859
0.1749973038343027	0.9935416007114585	0.5023897621980769
0.3418898379896895	0.9970822255434395	0.5100150282786500
0.1740396607928392	0.6622595469616094	0.5276427173627817
0.0163074987696515	0.8275623034066956	0.4734835104659416
0.0030912564345585	0.4928209470745832	0.5153183892685124
0.1771338353181741	0.8277079110606835	0.5097399010902856
0.5129818409416339	0.6628941712908644	0.5071350877719634
0.8360034796342677	0.8259945817572998	0.4633062793739949
0.6695663589117113	0.9912189693570024	0.4674834960522918
0.8357848757351442	0.9913259966552878	0.4602378698263924
0.6696426773675555	0.6626751682365501	0.4589996104946574
0.5144775605077535	0.8320745923420674	0.5159214550404140
0.5088801493954024	0.4934859321651207	0.4801756645417275
0.6749718243131415	0.8285519805473148	0.4911386561624354
0.3162813185974246	0.5268707160662246	0.6979729760390468
0.4514031319779836	0.6758935439056565	0.6937391812204378
0.2402576496226041	0.4935001997703997	0.6843615143601587
0.3326205884435659	0.6800118248109365	0.7159662130226851

*CH₂ , Energy without entropy=-519.02 eV

1.0000000000000000

14.2659997940000007	0.0000000000000000	0.0000000000000000
-7.1329998970000004	12.3547182319999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.0000000000000000

B	C	N	H
4	25	32	2

Direct

0.4008641738251798	0.5970240163536702	0.5424184490988306
0.2268485274270349	0.5977703812744393	0.5492206293743896
0.4065343398602028	0.7811449589468495	0.5582461532274060
0.3392399412119076	0.6423990125425491	0.5933192200488427
0.0569976362654719	0.2649054692193851	0.4923524161544233
0.2295960197822445	0.2673307871178958	0.4706155255453108
0.2289192615922317	0.4332065426962810	0.5053911963703318
0.0572189998569618	0.4267291661481516	0.5053864528221959
0.0651187278914653	0.1080373287283418	0.4759587861301258
0.5704036418479422	0.2703996065474079	0.4784776903358028

0.7294470629315959	0.2679432599730396	0.5271514023427052
0.7296376431854642	0.4382548380082278	0.5183894641508222
0.5700326099297488	0.4295847584484350	0.4891056173821592
0.5712118057328152	0.1140417331245597	0.5021873002857573
0.8851608744385825	0.4311230534947114	0.5270249303775766
0.0622764451293379	0.7666962590110389	0.4861385413110760
0.2302059617534201	0.7694757127882986	0.5200834352626914
0.2313419897501804	0.9414937454009217	0.5103927202041079
0.0668969890315526	0.9314872123609601	0.4852900705909602
0.0602552930559104	0.6048931188685561	0.5047548273521825
0.3935172510496717	0.9405558278294577	0.5126990191201777
0.5676927919047806	0.7697836292060537	0.5134130283894787
0.7304324584837892	0.7659393592759980	0.4762505903481773
0.7300257779968641	0.9382524244633594	0.4760794938204213
0.5687351481072442	0.9368301751285998	0.4968441422034789
0.5686266151652061	0.6051013967428607	0.4860813245168673
0.8882226397039850	0.9307050666003974	0.4700716468033591
0.3923246260011339	0.4292763989384308	0.4813872519283665
0.3934204984722049	0.7489324883975630	0.6419884944595812
0.0087559128929306	0.1595731487422063	0.4883555704441682
0.3378645176665375	0.3283640976287026	0.4613871605597716
0.1729500731655133	0.4874752022677757	0.5158453727936559
0.3404533346132495	0.4888538278835317	0.5058485564748064
0.1729894887062177	0.1629594449519731	0.4591950475091914
0.0060806099200771	0.3231200924496422	0.4928430133733812
0.0067955323356688	0.9898455889770205	0.4757939656866634
0.1750405775659607	0.3253980303662472	0.4961259850094386
0.5226705966122731	0.1627296115856993	0.4693179772633562
0.8357829763597669	0.3237076097458190	0.5386667586528547
0.6692068214649812	0.4861912912782817	0.5183581208436222
0.8363661189576259	0.4908355004805832	0.5288537878337412
0.6687826357872122	0.1598043294080750	0.5341306043622531
0.5209598755351785	0.3272660159812247	0.4643845197728766
0.5089973202167049	0.9934729815812242	0.5039098382886497
0.6772836500025511	0.3255046592951713	0.5049329896537098
0.0135143020598745	0.6578105738546273	0.4811475029901056
0.3402028251190293	0.8251002758091185	0.5230228800496806
0.1734435393102659	0.9893545186905828	0.5048543542908771
0.3403202262016528	0.9932464470388117	0.5148647410167355
0.1721096889195593	0.6582217129744494	0.5277592268234439
0.0152735078857257	0.8234935731641925	0.4725351790380214
0.0024105217294370	0.4882259957834346	0.5133340665242677
0.1761858388160247	0.8232345840554757	0.5081544078163743
0.5140266797619044	0.6580647374874149	0.5164155217612566

0.8351381810529959	0.8212996202740502	0.4663792797289520
0.6682366860853689	0.9850898692653313	0.4710261321130086
0.8338984190165953	0.9859469198123838	0.4616617293824654
0.6690994367195389	0.6587180979016782	0.4642141546089152
0.5144285228638400	0.8263148253236733	0.5204878523384121
0.5084636218089813	0.4885126501892932	0.4843976471822550
0.6762062900264023	0.8245014984782640	0.5013968989853490
0.4681149229268278	0.7688373567696899	0.6716177783366338
0.3385210435094231	0.7664476108678888	0.6737816615334805

*CH₃ , Energy without entropy=-522.56 eV

1.0000000000000000

14.2659997940000007	0.0000000000000000	0.0000000000000000
-7.1329998970000004	12.3547182319999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.0000000000000000

B	C	N	H
4	25	32	3

Direct

0.3990055259128434	0.5984483588154225	0.5460627854967017
0.2270515342010422	0.5996179736476667	0.5467235891126752
0.3993246012673261	0.7717591994037662	0.5485694430354336
0.3417779888609013	0.6555219886953297	0.5939849553416331
0.0569611416823684	0.2655675565974985	0.4912751304768374
0.2278183068703921	0.2665278753542549	0.4775516254795859
0.2274012589971307	0.4312866444543293	0.5137859800405601
0.0574171980669952	0.4273917270344451	0.5042661266348070
0.0631143647263963	0.1075625562897386	0.4765237875840016
0.5699743991917697	0.2716684473549294	0.4778202407624866
0.7293642490621368	0.2684313017434087	0.5244698124189586
0.7294705934675931	0.4388473705660210	0.5186307338818799
0.5695415152679908	0.4303041498967168	0.4911415464130176
0.5703664461452925	0.1148347025729573	0.4998730564894007
0.8850366083153219	0.4316685804380522	0.5242999235667255
0.0622366756976409	0.7672796118868415	0.4811820587877559
0.2285590589475142	0.7695713790142531	0.5168279883548278
0.2290381740679867	0.9401081662060262	0.5077228090342705
0.0651970547641404	0.9311020129937214	0.4825482998266928
0.0600685902370172	0.6052554295877539	0.4999187265604764
0.3922182428595953	0.9408049679655478	0.5101330069340867
0.5653381907449198	0.7696454964771957	0.5122197431725246
0.7278450078913713	0.7658010954265769	0.4763109021214121
0.7273055144634492	0.9369394066963573	0.4747179033401855
0.5667668475333169	0.9373111561768658	0.4947819344445952
0.5662677264896721	0.6047737445540562	0.4879635715902473
0.8860347852621951	0.9302226668422856	0.4699568438583385

0.3907267110762963	0.4281508752904650	0.4889888141503083
0.3279648247973928	0.6480455991342471	0.6852648481910839
0.0071367602929708	0.1602855465314982	0.4849818661061229
0.3368027204691412	0.3277338469120097	0.4689369194990148
0.1707808313720773	0.4866867250552599	0.5216193094655086
0.3398435690749842	0.4868030385290841	0.5162268552889141
0.1719702984228010	0.1625645737479030	0.4645458382468244
0.0069158376663761	0.3254908875694744	0.4877816710152331
0.0047994050880536	0.9893963201205485	0.4746059547456865
0.1730481802618824	0.3242968811046994	0.5012673816026890
0.5217930421002389	0.1641987569168197	0.4679129110371034
0.8360093055726355	0.3241265744531480	0.5348715161668962
0.6687936183364026	0.4864276455527115	0.5204791739092005
0.8364808091651786	0.4915136502200772	0.5282905601003225
0.6686260333557120	0.1603203793856404	0.5309385510144443
0.5206288976866271	0.3289635669659519	0.4649245454432189
0.5078319333364493	0.9945677235339733	0.5017041912535730
0.6770629635682809	0.3264914919964330	0.5039421883499486
0.0131733450029663	0.6575491506811264	0.4758778932505711
0.3402806458853302	0.8260768677120163	0.5214406243585271
0.1713241677703909	0.9880134283512017	0.5028527776805384
0.3388135073871135	0.9928975223098091	0.5114064311983828
0.1718574520672091	0.6576994575996193	0.5215623463789564
0.0146906403824053	0.8236437444256262	0.4675707520421852
0.0019868446899188	0.4888990059895677	0.5099829502250079
0.1745375587834938	0.8229152031975142	0.5048846767042597
0.5102679790917104	0.6574893659276267	0.5161181911439743
0.8328560594540818	0.8207385828398515	0.4683150412906616
0.6657820046352459	0.9849942020253994	0.4696965492977976
0.8314873132673787	0.9852017443891561	0.4620151648019266
0.6665306686286192	0.6574361720250248	0.4663928033736471
0.5110620643539794	0.8268443921067389	0.5199321792171613
0.5071448556365985	0.4884879953912389	0.4884635780925323
0.6717374989648319	0.8233301630538852	0.4967282964500190
0.4065899650880008	0.6898129084781588	0.7141806087123527
0.2803112609776873	0.6849714204123667	0.7043879434719852
0.2851987962952058	0.5632411153721084	0.7044555339633041

CH₄ , Energy without entropy=-525.91 eV

1.0000000000000000

14.2659997940000007	0.0000000000000000	0.0000000000000000
-7.1329998970000004	12.3547182319999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.0000000000000000

B	C	N	H
4	25	32	4

Direct

0.3998550511939676	0.5982353880974414	0.5395082403268817
0.2250220723772782	0.5987567946331528	0.5443281456051935
0.4003595575294721	0.7732025221791722	0.5424101519720254
0.3429008339106193	0.6564059403265667	0.5769430914164204
0.0553277748399076	0.2647031881114949	0.4889598939215231
0.2285524246552252	0.2665670063913434	0.4720257080441042
0.2272337018755507	0.4314212274914390	0.5096273639451536
0.0560660371974505	0.4263166266018229	0.5025496457398425
0.0634068812374482	0.1078892922526165	0.4726066689366755
0.5705603068276223	0.2719297126185529	0.4762650503213817
0.7292443475640982	0.2682963694605927	0.5239470289482221
0.7289940450990913	0.4385502546486979	0.5187081554601657
0.5697055315330783	0.4304031724933747	0.4896143374826754
0.5710298704532185	0.1149828050395496	0.4976350399995956
0.8847796397814642	0.4316480047799451	0.5243636663341107
0.0611716036632465	0.7669769529424542	0.4782893317409431
0.2289056878017920	0.7697415915986557	0.5118319600862427
0.2303860530344916	0.9419825607320980	0.5037453971440984
0.0656290631016048	0.9316816625025017	0.4793898465743994
0.0585902532227802	0.6051335689553550	0.4984065929015093
0.3928231033861636	0.9419447015331481	0.5060675189287415
0.5665790437427743	0.7703938025697724	0.5088105410391669
0.7294450211856466	0.7658802997608548	0.4740747008397156
0.7288271260634599	0.9385584968849113	0.4706020937864519
0.5681910862794628	0.9382010119050669	0.4912824483420092
0.5679908473075992	0.6051770020864796	0.4853435275680461
0.8867997068038522	0.9305464294741529	0.4654164944656449
0.3909638903653322	0.4277148196904448	0.4845373139583621
0.3209675948292203	0.6437226630785168	0.7499415485953140
0.0067533951815398	0.1595632057945288	0.4826539095203515
0.3368805893941448	0.3273363534918230	0.4635040727197073
0.1698882044980108	0.4849907662121089	0.5187949091947409
0.3390829729617696	0.4857788771737318	0.5110897885550961
0.1719168780512480	0.1628910028411293	0.4584915782204640
0.0053067540118628	0.3237539735310050	0.4865653783397164
0.0052431777887105	0.9897283614731989	0.4708320467865438
0.1731888554419293	0.3238387024248822	0.4986761460389900
0.5229235585555360	0.1646631586883056	0.4654754009437985
0.8356612597311247	0.3239464287412506	0.5348154622209187
0.6681954642487002	0.4860790463216244	0.5201128975375096
0.8358794312465617	0.4912365505316681	0.5285941439996503
0.6687340146244993	0.1599592418621419	0.5294294442716441
0.5216058385926592	0.3293477160134846	0.4627357581379657

0.5085298036625167	0.9948563300020696	0.4984715316644542
0.6768119448398769	0.3262952205334654	0.5038199558320855
0.0112151356289602	0.6575444310727790	0.4747794786373846
0.3398844831159685	0.8267728243448108	0.5163528471468757
0.1716147916205577	0.9890520121718884	0.5000916505468531
0.3392501801883754	0.9943222523877389	0.5086081878103436
0.1707448468119757	0.6586459214333125	0.5190485439327641
0.0143235101615390	0.8239172050649204	0.4651266675275603
0.0012825964537888	0.4886169224039071	0.5092392273051705
0.1755299551014389	0.8236185220022116	0.4989050586905506
0.5127531068420732	0.6587773692793474	0.5119456481128219
0.8340402285979311	0.8210979719503788	0.4642518238432638
0.6675623607342475	0.9858088321425831	0.4653461452941152
0.8324836315065760	0.9854451024084079	0.4555667178381609
0.6688540148655284	0.6581052257687069	0.4640484162506587
0.5133584566318934	0.8279690939947673	0.5155003919883262
0.5076682152006151	0.4885420918854111	0.4857443380837858
0.6749261453120897	0.8250293021423569	0.4972124880928341
0.4050530440039135	0.6886153438435297	0.7304511371803744
0.2773193974432664	0.6834136881834630	0.7290463896092028
0.2822604784514743	0.5611124470308481	0.7277987314098393
0.3186152236341498	0.6415246580120284	0.8108923842908566

Structural coordinate information of the C2 product

*2CO , Energy without entropy=-532.74 eV

1.0000000000000000

14.2659997940000007 0.0000000000000000 0.0000000000000000

-7.1329998970000004 12.3547182319999997 0.0000000000000000

0.0000000000000000 0.0000000000000000 18.0000000000000000

B C N O
4 26 32 2

Direct

0.4059085927775978	0.5961546363697110	0.5634462880232968
0.2228553513546352	0.6098535036954402	0.5454124327419738
0.3923764516656691	0.7788221360354410	0.5434882044273804
0.3403911527929147	0.6632748757072036	0.5915552259785134
0.0515579720950976	0.2761176502905268	0.4875922703333377
0.2230185868991922	0.2765336736644576	0.4727479401753640
0.2234405727688505	0.4407868433318557	0.5129581183903945
0.0529775450989168	0.4376042208165504	0.5043767526552472
0.0574376408451351	0.1179530398443009	0.4731494997844850
0.5648914951486329	0.2798801718425239	0.4784626339041547
0.7245252785638994	0.2768942103456472	0.5251607543056029
0.7243828757851949	0.4472872537878221	0.5187732280543930
0.5644551753432113	0.4385936230806073	0.4910003533031619

0.5653642962443056	0.1232052764688794	0.5007983890129708
0.8802241388546466	0.4404001440389655	0.5254393016590813
0.0562497500204291	0.7771877596286019	0.4848100631341832
0.2218896074602816	0.7796436924316201	0.5218633838273378
0.2231932928426431	0.9502586126106588	0.5094856664426536
0.0598627040713214	0.9413333706908616	0.4825830809278587
0.0545573869256209	0.6149886242219786	0.5035496818339754
0.3863887719757869	0.9499132864405293	0.5118127169968723
0.5592152757494337	0.7766812750886414	0.5102779257587160
0.7229026244299124	0.7749060997429905	0.4744345444214254
0.7214562002925964	0.9452469769439485	0.4743046565897500
0.5600939158577382	0.9448579531634081	0.4943649086110498
0.5622853767038569	0.6137638956144128	0.4873294558856492
0.8807877860820842	0.9396925547589382	0.4680819505184700
0.3853666871923103	0.4364227969983304	0.4877343968333492
0.3187179925507695	0.6792486239116451	0.6695144035170434
0.4494839453155594	0.5708565611707754	0.6406119096832199
0.0020323734373144	0.1704637690118079	0.4817560593093163
0.3320619908947444	0.3379602789260840	0.4632892528193875
0.1678170192765951	0.4968208903810810	0.5217076976431424
0.3348007899929355	0.4926153852942404	0.5182368099165825
0.1667700901655301	0.1730249175608640	0.4598402380420036
0.0026696147809384	0.3360704200284294	0.4866508170544337
0.9992415718529678	-0.0005030933653495	0.4727001527799135
0.1686250295202259	0.3351837093034202	0.4971491499413150
0.5167224990921957	0.1724004847531871	0.4688300565599445
0.8311090740724919	0.3326818351364138	0.5359052183731660
0.6636647211780159	0.4949448210149514	0.5202335242205854
0.8311874002622801	0.4999105642733633	0.5286931988006704
0.6636215412623790	0.1686821741309009	0.5318427689497819
0.5153080029205541	0.3368748254829322	0.4654973074159134
0.5020113173693406	0.0026753858977382	0.5026798775918684
0.6720488220330785	0.3348241598212288	0.5043941913633903
0.0086364260886193	0.6679932610388910	0.4788590122533549
0.3336496649354472	0.8349932377817889	0.5250476897632124
0.1661987825303638	0.9989356232555570	0.5020873235743966
0.3329524711552733	0.0018866119265181	0.5115219553057403
0.1663429842377205	0.6681015102399959	0.5270018338838127
0.0092891256371980	0.8336290418295684	0.4690408996369387
0.9973582979437839	0.4984744279944533	0.5121001524982891
0.1675731019463860	0.8332732972772509	0.5111453869535187
0.5065382882460370	0.6655055240945521	0.5159576418093887
0.8278820652055805	0.8301608536824189	0.4654267084912987
0.6597090764260601	0.9930091847711267	0.4702950754739039

0.8258095120642396	0.9943770021015587	0.4615517781364532
0.6620719037604880	0.6663120240738980	0.4643737015157549
0.5040170936916317	0.8331455262699532	0.5173913539613497
0.5022972213999515	0.4969323253631202	0.4878090715515328
0.6665634457617288	0.8316804827291960	0.4954440686811633
0.2944437730428701	0.6980098098410025	0.7269306827222983
0.5161665831067863	0.6131165853405824	0.6865891332753157

*COCO , Energy without entropy=-532.88 eV

1.0000000000000000

14.2659997940000007	0.0000000000000000	0.0000000000000000
-7.1329998970000004	12.3547182319999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.0000000000000000

B	C	N	O
4	26	32	2

Direct

0.4040808590823353	0.6013663853341512	0.5567437092191283
0.2223762737953671	0.6088876328179408	0.5480800372880954
0.3951189166862620	0.7817562039125896	0.5478222178514943
0.3387831072306457	0.6664809525193313	0.5899004578391174
0.0523209106143872	0.2748920850827159	0.4897561908410766
0.2241351493563646	0.2756315624205234	0.4748585891057790
0.2246987329438085	0.4405526993430948	0.5144253297634108
0.0539081252116954	0.4365245276059243	0.5054729793411975
0.0585935463140418	0.1171742567625037	0.4738463843677133
0.5665395597395040	0.2804523695086930	0.4782173726707868
0.7254844834053151	0.2770469445479803	0.5250671745904418
0.7253946945779663	0.4470782753529575	0.5191759498777027
0.5658159163051836	0.4390018317111050	0.4914161578060822
0.5669145050052827	0.1236088418934523	0.4995460552385976
0.8813497221380466	0.4402897353541335	0.5251632627568504
0.0572641933175205	0.7765612866232097	0.4829872313869906
0.2237496785338804	0.7795904324611130	0.5193733995411717
0.2248564810744207	0.9505097354389654	0.5062040906770162
0.0602177955992127	0.9405103525367168	0.4812514550576675
0.0551201371674388	0.6143708487125243	0.5019482463562865
0.3879888819462748	0.9505511421044193	0.5091347491507598
0.5600093699180165	0.7765565632383067	0.5082756628498963
0.7243811720613091	0.7743487101893550	0.4738109477081380
0.7229812967305640	0.9460426192874708	0.4727411545157215
0.5626907546723779	0.9458830330426551	0.4942487071490662
0.5639577443963927	0.6137844261965509	0.4871279767600477
0.8820031640283342	0.9399532372928181	0.4674169965701011
0.3863196374429605	0.4358944868048146	0.4891978902489839
0.3416172636415591	0.6275151256011455	0.6755633014109153

0.4357734704684204	0.6091500397348063	0.6468074443341330
0.0028388155715578	0.1697551504266200	0.4823590865408252
0.3329187063498637	0.3367383637790051	0.4658464687709731
0.1675975489778900	0.4952656500612528	0.5237702678227959
0.3352784604478125	0.4926813218702612	0.5181581817613379
0.1679516875137848	0.1723300281417836	0.4609173095984899
0.0033380048829328	0.3347952339581622	0.4879312713221010
0.9999454275741501	0.9989343577744737	0.4722035314364723
0.1695309212107280	0.3334729698184173	0.5007452286688101
0.5187673026766995	0.1729806658119078	0.4673364888235541
0.8320103612450153	0.3325338900327330	0.5356245545017284
0.6646435454791678	0.4947377741088749	0.5209386859723273
0.8323594075191988	0.4997061455643029	0.5283442829195437
0.6645043663206733	0.1686091363420494	0.5312328895174437
0.5171278645278345	0.3376026452573779	0.4650566200086274
0.5036614413059365	0.0032243490773317	0.5011253181490565
0.6727182318595548	0.3346955654949625	0.5052213190935131
0.0085750339238112	0.6664556862968952	0.4778309538165957
0.3358263512669195	0.8361475200263110	0.5229893105097525
0.1672318584583112	0.9979741720456028	0.4995332701158366
0.3347759557551236	0.0026016805555302	0.5083272161324969
0.1669372447985678	0.6670937344179892	0.5248042078564659
0.0097613154480512	0.8325153913433763	0.4686537113310929
0.9979348255128010	0.4976907791100784	0.5115016298720834
0.1699144454929670	0.8322413629709807	0.5069454903838009
0.5069382049722492	0.6660518843014666	0.5110507850111667
0.8287768163458674	0.8297996932808771	0.4653369614271567
0.6616264262878587	0.9939272929449180	0.4693469525136671
0.8271021427356563	0.9944233473871974	0.4600610301222976
0.6640976485897738	0.6654638385955925	0.4651418657071995
0.5066343343474903	0.8345924938661883	0.5184472534085797
0.5035972003029801	0.4969760870123724	0.4884055890250236
0.6665813826371890	0.8311928512752907	0.4932827649211199
0.2948109340656124	0.6147643428799825	0.7335511909734069
0.5274001581910956	0.6553382297378902	0.6728070296902763

*COCHO , Energy without entropy=-536.86 eV

1.0000000000000000

14.2659997940000007 0.0000000000000000 0.0000000000000000

-7.1329998970000004 12.3547182319999997 0.0000000000000000

0.0000000000000000 0.0000000000000000 18.0000000000000000

B C N O H

4 26 32 2 1

Direct

0.3965594564918137	0.6020743654240737	0.5381500986729826
--------------------	--------------------	--------------------

0.2205797233972469	0.6020279181778889	0.5471383282061250
0.3951006383300664	0.7732768519122696	0.5435022040030728
0.3391472257862853	0.6564656694637075	0.5881380774497335
0.0518650598149235	0.2688215502768242	0.4914276512647416
0.2222601032190459	0.2708782253339352	0.4707651655492882
0.2227392057709621	0.4355955371398413	0.5086556209515990
0.0516388585920604	0.4303563895541648	0.5043837030592335
0.0583558637755786	0.1114210303263876	0.4745698885616199
0.5637119239796939	0.2736491271926779	0.4726325984414588
0.7227066205368702	0.2713367344017453	0.5216156427301086
0.7230621464662897	0.4415590832756932	0.5122648546736326
0.5637917858054657	0.4331186863381437	0.4827847082125389
0.5643595474513250	0.1174073702867940	0.4970369273415531
0.8783893026620581	0.4343014457376679	0.5215879241696310
0.0569920075329855	0.7709495110194007	0.4838449734838825
0.2229890035886958	0.7727607214642509	0.5191364734536225
0.2245049550530185	0.9439539040993691	0.5074943057578580
0.0607623300868967	0.9352194945297966	0.4823396060299977
0.0543612353324157	0.6084710671942849	0.5014461616265993
0.3872437148783274	0.9431506291851820	0.5092364053876530
0.5614438616031536	0.7727547870740470	0.5065478016466165
0.7237456448239881	0.7697617828858297	0.4696576330976613
0.7235707927106455	0.9409884194030290	0.4721854746478066
0.5625071095827137	0.9407203636501751	0.4926116285089118
0.5620595907236876	0.6085893924449346	0.4791499178045732
0.8821022690412436	0.9342068386301279	0.4665148838125069
0.3855685878789666	0.4324916272144066	0.4797759121891884
0.3481140281276080	0.6640970327198401	0.6767254193399002
0.4522323033053806	0.6751568501929421	0.7117359463042275
0.0025186581694546	0.1634690181690635	0.4868554756989779
0.3308922328081271	0.3321238623641156	0.4598791760768166
0.1657908624313834	0.4902839749646326	0.5196373499704261
0.3352823393167696	0.4913544381279156	0.5081598165518481
0.1661687510535404	0.1665937674894993	0.4588929872575015
0.0009239023694330	0.3278979307681791	0.4898512248705224
0.0003806944006533	0.9932191169765229	0.4729413307855312
0.1684423100273680	0.3286532458960859	0.4963138262647035
0.5158386723973780	0.1659265910319254	0.4637585887080860
0.8290984592380792	0.3270187394097660	0.5330405234683014
0.6630013442254760	0.4897823048606351	0.5118878330936795
0.8298296703484126	0.4940580056953960	0.5226096466549607
0.6620411268876965	0.1633889359437550	0.5288469906901371
0.5145241165974375	0.3307992600261432	0.4582097788920189
0.5026837466196099	-0.0029424124711970	0.4997340393827105

0.6705356126037815	0.3288262378313793	0.4992799402430693
0.0081527499043729	0.6613817083746290	0.4777330992432444
0.3350982400259146	0.8282313096363341	0.5214254340501375
0.1676584193517697	0.9926429255680008	0.5008131282973014
0.3343043747988343	-0.0045115548426273	0.5098356952291476
0.1657004779404241	0.6608121025399970	0.5243520224297886
0.0095938966100811	0.8271889614815834	0.4696330109194294
0.9962378475691205	0.4917552247963858	0.5096469893458270
0.1692886421745712	0.8265470693034799	0.5077818946080720
0.5061799729244473	0.6609445465387714	0.5071825238541401
0.8286766081153438	0.8247632315340191	0.4616993539080380
0.6618208672434938	0.9891100818190508	0.4683690702641963
0.8279289827204118	0.9897048306215911	0.4603194600429161
0.6623760822606602	0.6615656757620194	0.4578890790461601
0.5066568963662302	0.8294049485561209	0.5157884564381576
0.5020581501377132	0.4921459196706066	0.4787592303370645
0.6677896356456784	0.8267061959232170	0.4918516414970321
0.2818155625049982	0.6629294423951847	0.7214751563373344
0.5284688649977775	0.6829871849197848	0.6757920886801303
0.4510764428641292	0.6730145947685708	0.7739980814842808

*COHCHO , Energy without entropy=-541.23 eV

1.0000000000000000

14.2659997940000007	0.0000000000000000	0.0000000000000000
-7.1329998970000004	12.3547182319999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.0000000000000000

B	C	N	O	H
4	26	32	2	2

Direct

0.3931245537234133	0.5907454526064431	0.5468889353774469
0.2157711241697982	0.5915859237945502	0.5504393410823329
0.3931490754486606	0.7695161544941752	0.5517327422276722
0.3306449851132643	0.6406768460989627	0.5922493782537082
0.0480118797633211	0.2588901059514278	0.4896600994881997
0.2200491402709544	0.2599272276955941	0.4749139365182656
0.2193873567555224	0.4249897214489279	0.5122947332450821
0.0489326399628076	0.4208425631000039	0.5032299634807020
0.0546434937262124	0.1010273869493684	0.4747986901000352
0.5611462285830620	0.2632209778362231	0.4794233305306124
0.7206673007685849	0.2596374802132270	0.5249396886205615
0.7205328322714772	0.4300860515119991	0.5204016978442164
0.5610285855362133	0.4221845072769740	0.4924827926302965
0.5617392018916785	0.1061024676285788	0.4998990686722197
0.8763091710138154	0.4232212044874757	0.5250290641986499
0.0514316615173784	0.7593987128501865	0.4841330343557679

0.2187081488249459	0.7624533884493836	0.5204640371365338
0.2203587069485367	0.9337924174343653	0.5081768954318927
0.0564221049618739	0.9243424743407178	0.4823275372100756
0.0498039049861153	0.5980018553304975	0.5030502032891337
0.3824353737137554	0.9325890558972185	0.5098921869723089
0.5573217847769613	0.7620480825766192	0.5122916564155884
0.7204673452528088	0.7582892881110833	0.4775868694604053
0.7184430286282812	0.9293812864773900	0.4729264740645074
0.5573811016807921	0.9283038324179116	0.4936150107906838
0.5597129958188372	0.5973207634365629	0.4897793365321428
0.8777940937201504	0.9234399328526839	0.4688400582754216
0.3829493845274740	0.4214588402069107	0.4873156896170104
0.3801644575727087	0.7466346364030725	0.6411397230133663
0.4831552870806423	0.7862830024299113	0.6803137676042831
-0.0012151717374721	0.1540129271466757	0.4829773501476827
0.3287037996171671	0.3215812247961360	0.4659636525136607
0.1630297250930520	0.4801974158295225	0.5202594441982212
0.3314912984126098	0.4803258541856094	0.5143265550646302
0.1635659993426910	0.1563352669022491	0.4618394767168631
-0.0011844581388529	0.3191013217624184	0.4861027383960842
-0.0040847735131050	0.9827149836668517	0.4732907237005436
0.1652327173778136	0.3180455759139628	0.5008314709939794
0.5133614984245142	0.1558910464315108	0.4684590180053881
0.8274635441255218	0.3153679549583904	0.5344057249732411
0.6601819161930609	0.4780705634094392	0.5218227943585770
0.8275273768692106	0.4827652413002958	0.5298051023616299
0.6599817570465413	0.1512416550694066	0.5308714009642083
0.5118214935910637	0.3205801841520082	0.4665641541403202
0.4984318927811199	0.9854832132448891	0.5011076756522808
0.6677536198816098	0.3176168628602664	0.5061811467973738
0.0036312950524073	0.6506098003852109	0.4779118808099351
0.3290226459667352	0.8171714156150486	0.5196639063934988
0.1632792964443737	0.9819844616533552	0.5009652745037035
0.3297030322101580	0.9853095497503511	0.5103979441921088
0.1607486331873864	0.6509288547786207	0.5274844795935871
0.0056430292519314	0.8165780165176125	0.4684206514994590
0.9928879452757676	0.4813251575368819	0.5108016889582556
0.1640815434529273	0.8156923770870701	0.5107972696697168
0.5041950291314866	0.6502115382233254	0.5175619026023870
0.8252556700078688	0.8139268374670400	0.4690699530717719
0.6563562865763258	0.9765220814484944	0.4678398442353554
0.8223537634998835	0.9778694325946494	0.4593838534973344
0.6600795250323429	0.6499945053525822	0.4686247053665452
0.5023388120050071	0.8174882927047790	0.5165425089205512

0.4994526019090103	0.4809002302067276	0.4890554019774540
0.6633419117635546	0.8158400012160699	0.4960666122362705
0.3092139036568017	0.7776159374458465	0.6752617452023527
0.5582434433303392	0.7726324532054852	0.6599672465693883
0.4905022081741552	0.8341371614683109	0.7312928554471844
0.2509401226949014	0.7131489894044544	0.6984359458293338

*COHCH₂O , Energy without entropy=-545.06 eV

1.0000000000000000

14.2659997940000007	0.0000000000000000	0.0000000000000000
-7.1329998970000004	12.3547182319999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.0000000000000000

B	C	N	O	H
4	26	32	2	3

Direct

0.4031897083206109	0.5845494992102381	0.5635448495211792
0.2208733808546977	0.5987767016607660	0.5410994244066228
0.3864266700141502	0.7623356723954248	0.5380403768883066
0.3370102382907260	0.6504060363615950	0.5878139273447812
0.0495659973959166	0.2625935959022325	0.4869101818739837
0.2207190008021994	0.2623819484973107	0.4720808981768523
0.2227123526505526	0.4286866954189074	0.5089987846517414
0.0517042916375820	0.4247640843775096	0.5023237175247747
0.0544505016158281	0.1041219602334355	0.4719641365368806
0.5628582409877999	0.2656888415626383	0.4753411726842329
0.7217336566553637	0.2616930176355498	0.5226660360568436
0.7213073858733838	0.4319324358614368	0.5181880185773128
0.5619430841900540	0.4239114730495283	0.4898380402138313
0.5626114098236519	0.1083830436304827	0.4967006788779922
0.8773801438945965	0.4256511155082171	0.5238304073932569
0.0530194784757825	0.7635512467101032	0.4808905345808187
0.2182565942778288	0.7658318703482107	0.5160383019490334
0.2196524260230271	0.9360149447116024	0.5056467942493816
0.0562895841145050	0.9273920386116123	0.4798393432328680
0.0504543810326372	0.6007757930886150	0.4997727822478081
0.3830163714563930	0.9354845729832425	0.5065279516469111
0.5549986100491958	0.7606193833711375	0.5046106547621892
0.7202647090401383	0.7596071336055297	0.4729024650741619
0.7172266591792955	0.9303799247377745	0.4676756921366352
0.5555274678863557	0.9285405436379496	0.4885849643628418
0.5607289729867868	0.5987849030374889	0.4871550844322810
0.8771881727745895	0.9259786542450612	0.4653584781162209
0.3831025981061689	0.4220664063475009	0.4871722556195779
0.3314969944149976	0.6330514074771550	0.6703692977529816
0.3941875218291396	0.5788095002470099	0.6954907474738612

0.9990505758060605	0.1566668118831441	0.4813451296009004
0.3299629558340014	0.3222706134271170	0.4641635003577317
0.1668133789467524	0.4846238543362699	0.5176714403085759
0.3332943583798726	0.4799411430920359	0.5137652107355510
0.1640785178017692	0.1587688615441708	0.4590979412308527
0.0007147076987529	0.3223837511568340	0.4863129192466019
0.9957689480853611	0.9858683369689467	0.4707006707179337
0.1665767596879991	0.3214256574182960	0.4949975427367784
0.5146340502237605	0.1581869647970711	0.4647271574837499
0.8282364688016909	0.3176311547961311	0.5337350322877340
0.6601935498398454	0.4789483780951788	0.5206607763672100
0.8281254617521877	0.4848530058054202	0.5282963152040229
0.6605421276057801	0.1531269545916194	0.5283343924873524
0.5139609681493370	0.3231528120128166	0.4621763998126370
0.4982436779357385	0.9872939872792323	0.4975901280763453
0.6693874195416571	0.3197986977982469	0.5023678511092728
0.0037818384852864	0.6532742111926162	0.4759779459728718
0.3298578726724970	0.8203995030861995	0.5186155688657677
0.1622846104611079	0.9845584979787430	0.4999120570101084
0.3296654516547899	0.9876443948874187	0.5078122075598901
0.1621567420730189	0.6538210398688769	0.5215454397219568
0.0055451404585184	0.8197016450041109	0.4658900920592975
0.9943695071146553	0.4843690928189499	0.5097445717526952
0.1642037734336804	0.8192655557465773	0.5049142699460070
0.5052363136771874	0.6506835596042997	0.5131726567571763
0.8249090367497076	0.8157179934973486	0.4660376962866363
0.6554237537227813	0.9773531444145983	0.4646260552320861
0.8223157072547168	0.9797624165340176	0.4557648736308573
0.6607344251192858	0.6504679027944356	0.4638645012200519
0.4985538864318431	0.8158015195876699	0.5104277632619942
0.5002910321775935	0.4820799897247617	0.4869173547271672
0.6616793578060868	0.8162746556494995	0.4890284079381844
0.2753389614821435	0.6526293067792616	0.7212003747659409
0.4356003215612876	0.5525972220052567	0.6329783272319744
0.4607867049180313	0.6354125308647702	0.7328306496822755
0.2798298299088786	0.6251749350077455	0.7703058729490428
0.3416952410923812	0.5057755854850551	0.7294750092986240

*CHOHCH₂O , Energy without entropy=-549.30 eV

1.0000000000000000

14.2659997940000007 0.0000000000000000 0.0000000000000000

-7.1329998970000004 12.3547182319999997 0.0000000000000000

0.0000000000000000 0.0000000000000000 18.0000000000000000

B C N O H

4 26 32 2 4

Direct

0.4017923209491429	0.5867007112153687	0.5628135397684955
0.2182117069299309	0.5944407675638683	0.5488180250933326
0.3904550775485407	0.7655064663669616	0.5415492661401041
0.3365169246564025	0.6531696201492736	0.5885056424612509
0.0489250383440675	0.2612784855491994	0.4864381529203275
0.2204522806331113	0.2620624739386476	0.4723150026988935
0.2212815219320194	0.4276019640038625	0.5102197140149139
0.0500576885440557	0.4224282749204837	0.5027763860916844
0.0550542057981412	0.1032305543729130	0.4716330182608894
0.5622456999984602	0.2663411180115016	0.4748865051906742
0.7206387173449686	0.2623297936676692	0.5219831318942921
0.7203664773706590	0.4320929989197449	0.5174372859907764
0.5610897059155360	0.4247743743504322	0.4890159900167206
0.5624889271911341	0.1089108957279436	0.4948685372212486
0.8767780880843252	0.4257544456650169	0.5228767725346950
0.0537315900959612	0.7622667647369141	0.4796205109378289
0.2194945698966422	0.7642827155974531	0.5158812695857039
0.2210358994439375	0.9352813864984122	0.5029573094247553
0.0570013480520799	0.9262807078295284	0.4784347894096134
0.0511917576018386	0.6000521993186383	0.4996847311060036
0.3836581618531514	0.9348238613752995	0.5040493547542252
0.5556442308012803	0.7619451276382192	0.5031668746574627
0.7207481227757744	0.7599573051362694	0.4724388823206289
0.7189597860687135	0.9312612216604964	0.4673298588699680
0.5586181279971124	0.9311024664639397	0.4882281464519476
0.5601779743205316	0.5998990030310410	0.4862799853691682
0.8784566219189978	0.9256772964769687	0.4657946777742418
0.3818537166433397	0.4225432078455094	0.4870206444650511
0.3544926070949236	0.6558934925412951	0.6794803111243214
0.3953711008414661	0.5749968284925010	0.6945627204466873
0.9992638722510836	0.1558660257689812	0.4801401967323394
0.3295719844335616	0.3225860536491035	0.4645507837406538
0.1632398472282148	0.4814759431105818	0.5208958406523871
0.3315482422226118	0.4799438419115841	0.5134501309140022
0.1646910421438373	0.1584096436713693	0.4594712818677330
-0.0009977800567785	0.3206622616775390	0.4852918839039128
0.9966914712372356	0.9850833116534028	0.4701696517696179
0.1657924938449241	0.3207504458749205	0.4950856073603624
0.5147078395303212	0.1589397489047219	0.4630255625954918
0.8271093147901845	0.3177973676003814	0.5328371762018559
0.6593778051750542	0.4794919159696863	0.5195788694234423
0.8275221560057066	0.4849425396176915	0.5267080311653412
0.6596462212679738	0.1536057604218705	0.5271788782266610

0.5132594425325930	0.3238996240385155	0.4615743399356679
0.4994802922145504	0.9883454736781891	0.4953681410378932
0.6678748811601442	0.3200220787830329	0.5027814944860676
0.0046176762041982	0.6518644827569187	0.4747155070111188
0.3316882649860787	0.8206050493581423	0.5169351905442963
0.1637247781466311	0.9832773894768724	0.4972232821369740
0.3309428954437991	0.9874523843799828	0.5049226636172599
0.1620724938742725	0.6518391189011956	0.5230944012283559
0.0063985990045211	0.8183952007038899	0.4649114268341044
0.9933163351581666	0.4831210419417490	0.5090041377319456
0.1658283084925636	0.8174170997085066	0.5033166751529160
0.5039166120022049	0.6520271838632988	0.5102121365778033
0.8254134450990044	0.8152851669219934	0.4669265294013180
0.6579394616430123	0.9797532042985451	0.4640355850962450
0.8236913781405637	0.9797513196313024	0.4563753390134320
0.6605374291084711	0.6504951717972924	0.4643790885820767
0.5018296619522947	0.8199994401398084	0.5117541589992568
0.4993650074501437	0.4829607234576861	0.4859246559058311
0.6614640603939667	0.8164238047945080	0.4865746307902067
0.2558840790576914	0.6263921071156513	0.7203426021515621
0.4400304346857595	0.5571938302596283	0.6284378451710316
0.4590038206487972	0.6046321019471144	0.7377165155894349
0.2752615655193330	0.6469019477246962	0.7721275117495956
0.3257930710108953	0.4981402375251616	0.7142176391737702
0.4172415033501607	0.7374033758991217	0.6979673775321331

*CHCH₂O , Energy without entropy=-538.46 eV

1.0000000000000000

14.2659997940000007	0.0000000000000000	0.0000000000000000
-7.1329998970000004	12.3547182319999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.0000000000000000

B	C	N	O	H
4	26	32	1	3

Direct

0.3919728187456721	0.5728904030349504	0.5677001640111056
0.2109388145808141	0.5858944231788472	0.5442897751388458
0.3882520936311769	0.7618793096173980	0.5581387867016666
0.3177465753436006	0.6285762059495384	0.5889571739983912
0.0448582395297519	0.2539366887572928	0.4783534267246394
0.2155758639683961	0.2515982824949980	0.4736130516956656
0.2157660930075528	0.4162856375829283	0.5133602018914022
0.0479068239436403	0.4157797920389333	0.4946379016267579
0.0491965793704085	0.0945088170368720	0.4687048310743308
0.5559399509322834	0.2558229791309545	0.4842261137061115
0.7186735001314379	0.2537342825990928	0.5234634972512094

0.7183033257380816	0.4240258636789540	0.5173600045586499
0.5568583206444045	0.4156479986208411	0.4953265188988358
0.5573395717908636	0.0994505813362489	0.5050744959794703
0.8747050086236651	0.4173060078780685	0.5181787970821453
0.0494543578563365	0.7550079919603119	0.4783662869219222
0.2143264570756171	0.7566167569309047	0.5199625107406703
0.2145725176583621	0.9277344761562912	0.5109067982511772
0.0515638815279096	0.9181513080187449	0.4811650376067415
0.0470897843948315	0.5931238855483628	0.4955782670355871
0.3769145916559898	0.9270315308566418	0.5171571199128333
0.5443369586282596	0.7500466260553554	0.5020027494809025
0.7121449842064648	0.7500964714762111	0.4744978309933922
0.7103895926794213	0.9209373789657186	0.4747072761844734
0.5500502390121182	0.9201272921721561	0.4971041904833608
0.5516197694639334	0.5895690198735755	0.4888024920302401
0.8703349297112551	0.9158105812709579	0.4698415803195219
0.3765100753633990	0.4097922758619904	0.4930948390714577
0.3938227946470305	0.7205371986043274	0.6415245337342308
0.4806617797736411	0.6907771890813077	0.6635879732865776
0.9947302762606541	0.1491434669331023	0.4684508185944015
0.3242260047645820	0.3130515963370532	0.4647013646297215
0.1606150574486330	0.4729205028243408	0.5148796965749722
0.3254770951049048	0.4627879422551858	0.5261616151053079
0.1593883834914437	0.1481722985296027	0.4596367192405451
-0.0026649543482949	0.3149361636981396	0.4739697825643812
0.9899065646587617	0.9761730501746931	0.4716629942625344
0.1597535736810405	0.3091694412873986	0.4978761887077909
0.5069331291720034	0.1479431314590040	0.4752645629388842
0.8261762461320536	0.3095007410057772	0.5291855975221822
0.6584288229573476	0.4724954466070946	0.5203308361565889
0.8258603872290753	0.4767422885384573	0.5233468874736943
0.6574656848659147	0.1457084726815797	0.5330392975515998
0.5051637338129749	0.3118562652201604	0.4737558125936451
0.4928020729188837	0.9787671167664154	0.5077022775513310
0.6647468430628459	0.3110366392961755	0.5054804373201440
0.0008666193609963	0.6459329977206885	0.4705414244925012
0.3238626145331638	0.8130438887198600	0.5310023465341177
0.1557289834153708	0.9751199236069450	0.5052123617400104
0.3234287840163312	0.9798493812719581	0.5170132676728166
0.1560804918846108	0.6449984807292859	0.5217180471357573
0.0026554443703171	0.8118045450422052	0.4629399275342739
0.9908729159504430	0.4758720954854420	0.5023321229949333
0.1600048914944342	0.8103636056381925	0.5060854047102957
0.4921929470774020	0.6402654734291416	0.5074380701302461

0.8179540078781026	0.8055599435922092	0.4697723755088611
0.6513168333120923	0.9709044560034986	0.4751224217018635
0.8164058788492727	0.9711521512245712	0.4663371243240792
0.6536018102771818	0.6409082742883663	0.4693112039623440
0.4923720416685977	0.8079904938664935	0.5135772405809601
0.4939989392712756	0.4725629750699704	0.4917885150999302
0.6523075056534532	0.8055224203729978	0.4856059741056394
0.4533258263520229	0.5844925880873685	0.6351708016101802
0.5621551879106789	0.7500194395951763	0.6416459791345309
0.4880480492691028	0.6891661257296275	0.7243827205849028
0.3663549146060182	0.7540688511430668	0.6856936672617090

*CH₂OH , Energy without entropy=-542.03 eV

1.0000000000000000

14.2659997940000007 0.0000000000000000 0.0000000000000000

-7.1329998970000004 12.3547182319999997 0.0000000000000000

0.0000000000000000 0.0000000000000000 18.0000000000000000

B	C	N	O	H
4	26	32	1	4

Direct

0.3828237767021646	0.5716994257554825	0.5425067903960958
0.2089767134108587	0.5743919552821478	0.5494333483246854
0.3882904773917469	0.7561880392185563	0.5566601449121401
0.3223945273753845	0.6195482695825839	0.5918437890132245
0.0386879382339884	0.2408662750591886	0.4892352128192521
0.2111575775885489	0.2420649773277308	0.4712865912942560
0.2108056012028230	0.4080297293684622	0.5066799397445788
0.0402826567442988	0.4032702479264209	0.5035832788523764
0.0456792848075011	0.0834100730807682	0.4725428528219550
0.5533047361337285	0.2458293440290426	0.4778313921497190
0.7122633370458993	0.2429181952941514	0.5260635935031014
0.7119597192725460	0.4131089642227939	0.5191707198528296
0.5523756757676849	0.4044887646783102	0.4901430172364261
0.5538432595088958	0.0891562713308893	0.5004497782608581
0.8679113648284309	0.4065532977782308	0.5258808593106342
0.0445597994872993	0.7424491065742993	0.4820709580176956
0.2115900781240893	0.7455444406741957	0.5199261688399129
0.2127412896546269	0.9173784435388630	0.5081047840229205
0.0484621751460703	0.9069637658392503	0.4811347404778787
0.0424193628049466	0.5809631808009503	0.5027274814501932
0.3749866665886188	0.9164631828264221	0.5116922030661316
0.5483492837208747	0.7442220082485278	0.5108649431809148
0.7117118362604230	0.7404111316782773	0.4749337161763806
0.7103179011760052	0.9122586859949937	0.4723161259554894
0.5492086303547210	0.9110785265174732	0.4937815091456942

0.5504596320899642	0.5794647184835302	0.4869527630430799
0.8689766567200407	0.9053633121701349	0.4663990690446323
0.3741997074897916	0.4032812758827419	0.4835283657432449
0.3832065096286220	0.7251467671584253	0.6412090627987396
0.4859560517129656	0.7482975933926066	0.6816966986553642
0.9894159921306980	0.1356105001028816	0.4832263615176456
0.3196924038761263	0.3024990154695442	0.4634034389364886
0.1554871739239150	0.4633350845188023	0.5163485375533607
0.3223185994144969	0.4627320227124889	0.5079196192515693
0.1542393998885840	0.1382181942693459	0.4583793152827353
0.9890999995528632	0.3003858623327546	0.4887370824737058
0.9876877091796989	0.9651004014557181	0.4715939975878118
0.1563837208477272	0.3003838192987018	0.4964739277530618
0.5058387903794480	0.1383390640170190	0.4674760909589297
0.8187450677404603	0.2988894058996476	0.5369728599923032
0.6512536203385076	0.4607256410936509	0.5199341719566705
0.8188935061464574	0.4660468386544388	0.5288823693414546
0.6515462955397575	0.1345043678671490	0.5323837878934254
0.5040313276403035	0.3028990307409452	0.4640159001152224
0.4905353801265412	0.9685748094073425	0.5023448412479982
0.6596443038297869	0.3005127126051481	0.5053339163520026
-0.0037965285726118	0.6334608314516459	0.4771678713394312
0.3216584833797118	0.8014831488446239	0.5240201899183531
0.1544799454955233	0.9648009062023976	0.5019432379914054
0.3217606103627887	0.9692327578512252	0.5123208524595581
0.1534877259158114	0.6342140952501503	0.5274084141789711
-0.0019851699410306	0.7993293900848040	0.4667282708038074
0.9849018917276149	0.4642437231584824	0.5115222603522328
0.1575251632956773	0.7989828529305874	0.5068315232334911
0.4954258311222298	0.6326633268315101	0.5156026440260810
0.8163612676775782	0.7958558369316115	0.4645873602120578
0.6486882385640623	0.9593283935183624	0.4677696225656958
0.8141314389271872	0.9599881710616177	0.4573494000173116
0.6509238092607186	0.6326938816294274	0.4649067308126121
0.4942624645033410	0.8002050598362349	0.5163420299402642
0.4904873279265996	0.4629137156755950	0.4861561596629848
0.6569447397935434	0.7991332833874332	0.4983160261585577
0.4814427119016779	0.6486889917072048	0.7037426846323072
0.5590221021946091	0.7959009391445351	0.6470236775600082
0.4947887078629993	0.7980880782388986	0.7310805355106875
0.3291308154996222	0.7423709469580404	0.6742909163991205
0.5468028395734156	0.6675349841445735	0.7319233249002572

*CH₂CH₂OH , Energy without entropy=-545.72 eV

1.0000000000000000

14.2659997940000007	0.0000000000000000	0.0000000000000000
-7.1329998970000004	12.3547182319999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.0000000000000000

B	C	N	O	H
4	26	32	1	5

Direct

0.3918458821752661	0.5794612396416982	0.5583911695450583
0.2124201300060743	0.5874373936253955	0.5502434248818137
0.3857733867241782	0.7593350354637572	0.5464369980136512
0.3305191486538675	0.6443767561901694	0.5926293204682233
0.0443534293657218	0.2552928169733334	0.4849744914887125
0.2155528933342092	0.2549663062017071	0.4751534566156017
0.2150699858712066	0.4200593443885610	0.5124502551326041
0.0455776590664853	0.4166608306637362	0.5015680410050933
0.0499054981694023	0.0965149939386218	0.4725745781698964
0.5584214271879372	0.2595591808216625	0.4776336890845038
0.7178775425828433	0.2556978941674168	0.5235119404677233
0.7170771028726244	0.4258152255628773	0.5209250890468934
0.5568552898077191	0.4171012123861474	0.4940464455957181
0.5584779169964538	0.1023079181615430	0.4985430860253920
0.8732025634805192	0.4194784428500539	0.5242570433906483
0.0500579186456584	0.7563682071879824	0.4800591236322871
0.2148392096588646	0.7581501214662428	0.5188801485209028
0.2158988844000378	0.9284011348574389	0.5057768556976283
0.0524089753274121	0.9198913417585254	0.4800044340869515
0.0473491097242395	0.5939885464928962	0.4997844582417286
0.3792780075940407	0.9287801490314375	0.5083648839030072
0.5516398658986580	0.7562458175122285	0.5106588875954537
0.7159416775910842	0.7528744899315784	0.4771279054725209
0.7138676685088744	0.9240416354313031	0.4718734239918139
0.5532756042290753	0.9239606722017505	0.4924501791097131
0.5551695181256209	0.5923438543155841	0.4906459248352201
0.8732240731289701	0.9184495312094620	0.4683207143854011
0.3777247300770709	0.4148711609636129	0.4905144494619274
0.3459610640301191	0.6438087286874085	0.6844688337563153
0.4425078037896832	0.6284712555044065	0.6953935046613681
0.9943739926577276	0.1499111547051458	0.4783417059203309
0.3250026077919614	0.3152626797745790	0.4682377835136748
0.1584360056487817	0.4751146013027371	0.5217830152502257
0.3268612456599235	0.4727434737695039	0.5170851323447431
0.1596354497226400	0.1514334066199540	0.4624452696332506
0.9953800096345372	0.3157364426263935	0.4820091262495454
0.9918009333520456	0.9783055627555258	0.4717991285468211
0.1605650974438444	0.3139845668951547	0.4969311199020741

0.5101639264160555	0.1522851052567542	0.4671461644633173
0.8245329876729818	0.3116071175310407	0.5339595184301895
0.6551834897578145	0.4721041282720574	0.5253847998155533
0.8240671972653532	0.4788397912814710	0.5302321888182493
0.6571157122257716	0.1474335911227578	0.5293258908464405
0.5093398131645598	0.3172114123283482	0.4653565829856604
0.4950513773602662	0.9819458764060527	0.5000068765373864
0.6654796491883039	0.3140584925855595	0.5039621680820626
0.0012399449335385	0.6459634384289389	0.4742029191863454
0.3272701012335037	0.8144474207675582	0.5221779508679373
0.1585538462240171	0.9766350036491516	0.4997720745773718
0.3260041022867101	0.9808290842288662	0.5082344494570730
0.1572745006662070	0.6455111759978084	0.5250170235626134
0.0023261805138420	0.8122636136474443	0.4651145771504947
0.9894808717798429	0.4771989271570861	0.5090656957943970
0.1610373623272095	0.8113285692239307	0.5054063154112128
0.4992636349161058	0.6449256352222342	0.5173579346056169
0.8205786796887126	0.8085068008225810	0.4692093080866385
0.6523349708664489	0.9716051037949327	0.4670897064829739
0.8181130996558232	0.9723831585013952	0.4589704611162944
0.6555680345269433	0.6440289653932927	0.4684053567069666
0.4972200241615465	0.8132816330858136	0.5173846201427542
0.4949121223761501	0.4754246427709997	0.4921591702885929
0.6583206534578473	0.8104494354401325	0.4953801665282095
0.4280186975196270	0.5429993495149307	0.6405159650186519
0.5186337888940445	0.7021711962792389	0.6806284225437339
0.4504974313329889	0.5984126963877471	0.7499424236428679
0.3637501335777595	0.7201694347301464	0.7116118174811947
0.2745899447932852	0.5778706188210235	0.7122465999385865
0.4931383432813763	0.5364354033131882	0.6391176407861641

*+CH₃CH₂OH , Energy without entropy=-549.10 eV

1.0000000000000000

14.2659997940000007	0.0000000000000000	0.0000000000000000
-7.1329998970000004	12.3547182319999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.0000000000000000

B	C	N	O	H
4	26	32	1	6

Direct

0.3897098485563605	0.5982114738040013	0.5416482704614575
0.2136990652766224	0.5999787887079936	0.5423821105797041
0.3882339495584149	0.7737249059983480	0.5401437359330276
0.3311434161286470	0.6576383925341940	0.5757141051985084
0.0445099599268434	0.2662152622540800	0.4836451825550606
0.2175521396492207	0.2673494329724128	0.4712073410444849

0.2162515603614090	0.4320574889196294	0.5090068815624014
0.0458855825731521	0.4278596727191653	0.4981535150479047
0.0519505302719732	0.1088979475533097	0.4681223983174340
0.5592406918802234	0.2727042818087320	0.4730894769521565
0.7186869717126307	0.2688159459158315	0.5188971409739385
0.7185542932469391	0.4393580668048251	0.5140862224905517
0.5587070426935281	0.4313123452252516	0.4869227910721353
0.5596458565723936	0.1155788228494019	0.4938459044945990
0.8742156005773968	0.4322373918816404	0.5189927261366583
0.0496148814971133	0.7674578647209321	0.4734433816268743
0.2172088695623701	0.7704341626839531	0.5084472136622624
0.2185149080929865	0.9422085256992353	0.4980586519856852
0.0538698514554236	0.9321338815047775	0.4736472784457200
0.0476618203957414	0.6060493112038822	0.4939591728675568
0.3811413782321859	0.9424294697539958	0.5017575692956480
0.5550723345804282	0.7709518567988071	0.5075737323653318
0.7174565903464841	0.7664542948706845	0.4708275645171469
0.7168315293893839	0.9389303415010923	0.4678769396186016
0.5561747916118630	0.9383562499324074	0.4883904089210507
0.5564216152461652	0.6057838937829795	0.4843271383012112
0.8749147078383384	0.9312016157750374	0.4613016286673653
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