

Supporting Information for

The Importance of Grand-Canonical Quantum Mechanical Methods to Describe the Effect of Electrode Potential on the Stability of Intermediates Involved in both Electrochemical CO₂ Reduction and Hydrogen Evolution

Haochen Zhang,^a William A. Goddard,^b Qi Lu,^{a,*} and Mu-Jeng Cheng^{c,*}

^a*Department of Chemical Engineering, Tsinghua University, Beijing 100084, China*

^b*Materials and Process Simulation Center, California Institute of Technology, Pasadena, California 91125, USA*

^c*Department of Chemistry, National Cheng-Kung University, Tainan 701, Taiwan*

*Email: luqicheme@mail.tsinghua.edu.cn, and mjcheng@mail.ncku.edu.tw

Correction for the electronic energy of gas-phase CO₂.

The electronic energies of gas-phase thermochemical reactions containing CO₂ calculated with the RPBE functional were found to be inconsistent with experimental data.¹ However, the accuracy of calculated electronic energy of gas-phase CO₂ was critical in this study. According to the procedure proposed by Peterson et al², to quantify the error, a sensitivity analysis of 21 reactions (Table S1) was performed.

The calculated enthalpy change of each reaction was compared with the experimental data from the CRC handbook.³ A systematic deviation was found for COO-motif-contained molecules (i.e., CO₂, HCOOH, CH₃COOH and HCOOCH₃). The absolute mean error for COO-motif free reactions is 0.05 eV while that of COO-motif-containing reactions is 0.32 eV. To minimize the deviation, a correction must be added to the electronic energy of these molecules. For example, No.1 reaction has one CO₂ molecule as the product. Therefore a correction by a factor of -1 needs to be added to the overall reaction enthalpy change. However, for No.19 reaction, the COO-motif-containing molecule, i.e., CH₃COOH, serves as the product with the stoichiometric number of 0.5, which requires for a correction by the factor of 0.5 to be added to the enthalpy change of the reaction. The factor of each reaction is also listed in Table S1.

Table S1 Gas phase reactions for sensitivity analysis.

No.	Stoichiometry	Factor
1	CO ₂ + H ₂ → CO + H ₂ O	-1.0
2	CO ₂ + 4 H ₂ → CH ₄ + 2 H ₂ O	-1.0
3	CO + 3 H ₂ → CH ₄ + H ₂ O	0.0
4	CO ₂ + H ₂ → HCOOH	0.0
5	CO + H ₂ O → HCOOH	1.0
6	CO ₂ + 3 H ₂ → CH ₃ OH + H ₂ O	-1.0
7	CO + 2 H ₂ → CH ₃ OH	0.0
8	CO ₂ + 3 H ₂ → 1/2 C ₂ H ₅ OH + 3/2 H ₂ O	-1.0
9	CO + 2 H ₂ → 1/2 C ₂ H ₅ OH + 1/2 H ₂ O	0.0
10	CO ₂ + 10/3 H ₂ → 1/3 C ₃ H ₈ + 2 H ₂ O	-1.0
11	CO + 7/3 H ₂ → 1/3 C ₃ H ₈ + H ₂ O	0.0
12	CO ₂ + 7/2 H ₂ → 1/2 C ₂ H ₆ + 2 H ₂ O	-1.0
13	CO + 5/2 H ₂ → 1/2 C ₂ H ₆ + H ₂ O	0.0
14	CO ₂ + 3 H ₂ → 1/2 C ₂ H ₄ + 2 H ₂ O	-1.0
15	CO + 2 H ₂ → 1/2 C ₂ H ₄ + H ₂ O	0.0
16	CO ₂ + 11/4 H ₂ → 1/4 C ₄ H ₆ + 2 H ₂ O	-1.0
17	CO + 7/4 H ₂ → 1/4 C ₄ H ₆ + H ₂ O	0.0
18	CO ₂ + 2 H ₂ → 1/2 CH ₃ COOH + H ₂ O	-0.5
19	CO + H ₂ → 1/2 CH ₃ COOH	0.5
20	CO ₂ + 2 H ₂ → 1/2 HCOOCH ₃ + H ₂ O	-0.5
21	CO + H ₂ → 1/2 HCOOCH ₃	0.5

The corrected calculated enthalpy was also compared with the experimental value. The mean absolute error of all COO-motif-containing was plotted against the correction in Figure S1. A correction of 0.372 eV was found to minimize the mean absolute error of these reactions. The mean absolute error of COO-motif-containing reactions decreased from 0.320 eV to 0.130 eV when a correction of 0.372 eV was added to the electronic energy of corresponding molecules. The mean absolute error of all these 21 reactions decreased to only 0.100 eV after correction.

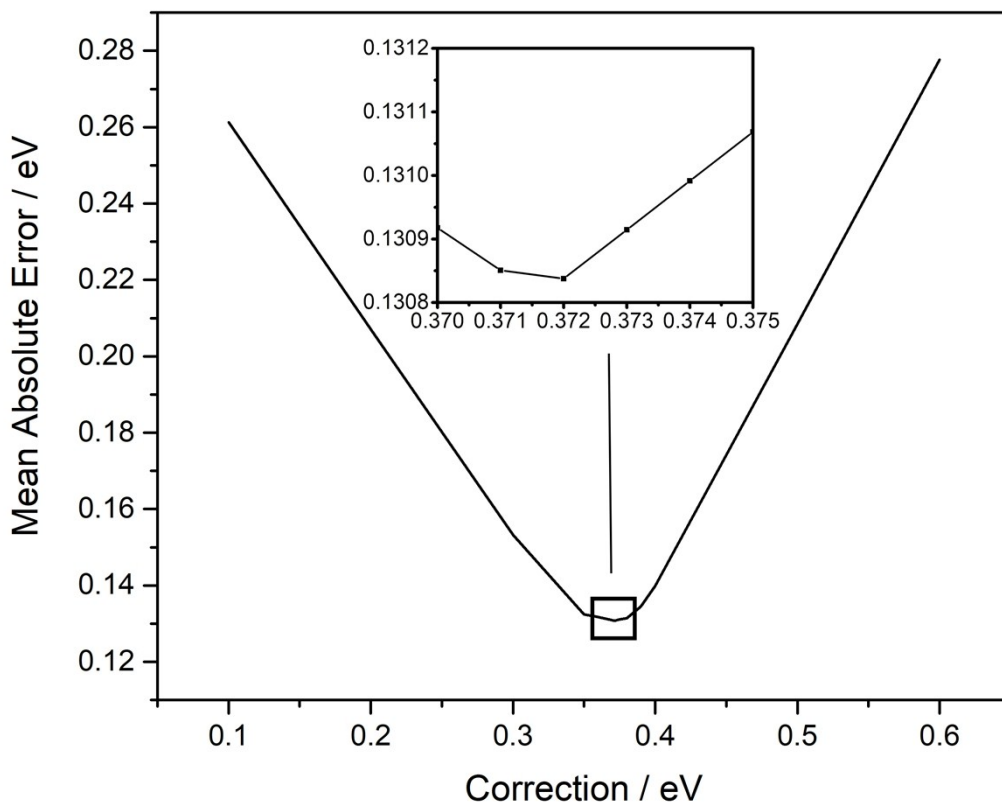


Figure S1 Sensitivity analysis for COO-motif-containing molecules.

Fractional coordinates for the adsorbates on Cu(111).

Cu $E_0 = -139.873$ eV

cu111

1.0000000000000000		
7.6679000854000003	0.0000000000000000	0.0000000000000000
-3.8339500427000002	6.6405962677000003	0.0000000000000000
0.0000000000000000	0.0000000000000000	58.3478012085000017

Cu
45

Selective Dynamics

Direct

-0.0000031809555234	0.0000031910965102	0.4635503013484916	T	T	T
-0.0000001230505084	0.0000003934364459	0.5727173947531549	T	T	T
0.2221345504335284	0.1110726768741272	0.4272639020164266	T	T	T

0.2221111703586517	0.1110581082928867	0.5364220226922831	T	T	T
0.1111100018365576	0.2222200036731223	0.499999999957154	F	F	F
0.3331662538541215	0.0000451630013955	0.4636223337228392	T	T	T
0.3332734657527062	-0.0000153710627698	0.5726361533595213	T	T	T
0.5555477421089756	0.1111041003863716	0.4274795062009548	T	T	T
0.5554632964591819	0.1109344045912075	0.5363625054475661	T	T	T
0.4444400072531138	0.2222200036731223	0.499999999957154	F	F	F
0.6668713585047297	0.0000404413668558	0.4636230138445830	T	T	T
0.6667178310110455	-0.0000178083750967	0.5726312592213499	T	T	T
0.8889266964714734	0.1110730912894989	0.4272670238896639	T	T	T
0.8889498402504712	0.1110503282948611	0.5364188290428225	T	T	T
0.7777799964982535	0.2222200036731223	0.499999999957154	F	F	F
-0.0000406202865688	0.3331283573327044	0.4636230592340497	T	T	T
0.0000176981313541	0.3332822049666601	0.5726312844486757	T	T	T
0.222150832365191	0.4443217027293523	0.4274236223521913	T	T	T
0.2221291520642844	0.4442547980713260	0.5363557288000161	T	T	T
0.1111100018021958	0.5555599928495241	0.499999999957154	F	F	F
0.3331659384710659	0.3331315471439260	0.4636211598768876	T	T	T
0.3332740704627261	0.3332867737824283	0.5726402438813036	T	T	T
0.5555426107209941	0.4444573954380593	0.4274763143680298	T	T	T
0.5554576589576821	0.4445424466804488	0.5363641483844921	T	T	T
0.4444400072187520	0.5555599928495241	0.499999999957154	F	F	F
0.6666639309560246	0.3333357771210830	0.4636994028270602	T	T	T
0.6666675751425617	0.3333317657741511	0.5725020268693610	T	T	T
0.8888966743191287	0.4444526933757702	0.4274795225399604	T	T	T
0.8890654610905615	0.4445366326393510	0.5363625339723341	T	T	T
0.7777799964638845	0.5555599928495241	0.499999999957154	F	F	F
-0.0000450340485447	0.6668340493104873	0.4636223555613887	T	T	T
0.0000153728409824	0.6667267683405267	0.5726360412085830	T	T	T
0.2221589006031051	0.7778417216332366	0.4274256428188468	T	T	T
0.2221282657096214	0.7778715685253539	0.5363567122113083	T	T	T
0.1111100017117366	0.8888900279499197	0.499999999957154	F	F	F
0.3333310149609160	0.6666692258115263	0.4636328042384469	T	T	T
0.3333392332120191	0.6666600945450289	0.5724848829009584	T	T	T
0.5556781192794074	0.7778493961739325	0.4274235640634353	T	T	T
0.5557450783177211	0.7778706701984887	0.5363556651247583	T	T	T
0.4444400071282928	0.8888900279499197	0.499999999957154	F	F	F
0.6668682893553400	0.6668341985088152	0.4636211360988213	T	T	T
0.6667134600597548	0.6667262304211650	0.5726402038144033	T	T	T
0.8889269882476819	0.7778650995176806	0.4272639227275034	T	T	T
0.8889419394732232	0.7778888991751508	0.5364219986380460	T	T	T
0.7777799963734253	0.8888900279499197	0.499999999957154	F	F	F

*H $E_0 = -147.205$ eV

Cu111-H

1.0000000000000000

7.6679000854000003 0.0000000000000000 0.0000000000000000

-3.8339500427000002 6.6405962677000003 0.0000000000000000

0.0000000000000000 0.0000000000000000 58.3478012085000017

Cu H

45 2

Selective Dynamics

Direct

0.9999517485643525	0.0000486576252468	0.4631997065541731	T	T	T
0.0000572973128778	0.9999421349824196	0.5731272176449711	T	T	T
0.2213526319319683	0.1094463971828782	0.4268952444230927	T	T	T
0.2228482700698391	0.1124351492695636	0.5369199538866982	T	T	T
0.1111100018365576	0.2222200036731223	0.499999999957154	F	F	F
0.3333274242637017	0.0001061457313457	0.4632036887949006	T	T	T
0.3333143227491510	0.9999952750650070	0.5731034804475392	T	T	T
0.5556137372335026	0.1111751145605339	0.4269324290508024	T	T	T
0.5553456222147730	0.1109141620437163	0.5367853261211901	T	T	T
0.4444400072531138	0.2222200036731223	0.499999999957154	F	F	F
0.6661638629105679	0.9986589713221536	0.4630814328950329	T	T	T
0.6675157069757863	0.0016363410540920	0.5730618698011883	T	T	T
0.8888718033152263	0.1111273177273725	0.4268676178813128	T	T	T
0.8889743113236493	0.1110247015030279	0.5368022859007164	T	T	T
0.7777799964982535	0.2222200036731223	0.499999999957154	F	F	F
0.0013395913807241	0.3338347474823538	0.4630813434944535	T	T	T
0.9983629014995500	0.3324828624728706	0.5730621028392749	T	T	T

0.2221882600312669	0.4442528853330165	0.4264136485459656	T	T	T
0.2217256789254417	0.4442136562896293	0.5363140459373010	T	T	T
0.1111100018021958	0.555599928495241	0.4999999999957154	F	F	F
0.3330284880150842	0.3327822208516069	0.4636822480393983	T	T	T
0.3333218932043682	0.3332998770551422	0.5735900760534146	T	T	T
0.5554541045831252	0.4445443472794982	0.4264162506646764	T	T	T
0.5558324974709494	0.4441664808072429	0.5363111195127209	T	T	T
0.4444400072187520	0.555599928495241	0.4999999999957154	F	F	F
0.6658973335914001	0.3341010212040370	0.4630798811796275	T	T	T
0.6675886958503578	0.3324094750180157	0.5730543063160970	T	T	T
0.8888255263803558	0.4443885140440048	0.4269323729253798	T	T	T
0.8890856157953416	0.4446547967450910	0.5367852652974530	T	T	T
0.7777799964638845	0.555599928495241	0.4999999999957154	F	F	F
0.9998933304899663	0.6666713156714921	0.4632036994592091	T	T	T
0.0000031165619529	0.6666827053205915	0.5731033404456447	T	T	T
0.2213106439185630	0.7786902359176232	0.4269243148212306	T	T	T
0.2228977670995272	0.7771036127786862	0.5369317646070706	T	T	T
0.1111100017117366	0.8888900279499197	0.4999999999957154	F	F	F
0.3329961842328643	0.6670038487811042	0.4636872719254102	T	T	T
0.3333388637476207	0.6666614077487549	0.5736049340450822	T	T	T
0.5557452094168464	0.7778101408958873	0.4264135450153202	T	T	T
0.5557848073764875	0.7782718376240143	0.5363138839239578	T	T	T
0.4444400071282928	0.8888900279499197	0.4999999999957154	F	F	F
0.6672196713390249	0.6669724932512550	0.4636821249538068	T	T	T
0.6667002311502066	0.6666783543597842	0.5735898594650105	T	T	T
0.8905529276464752	0.7786474127499786	0.4268950319336959	T	T	T
0.8875655208980946	0.7771525603781414	0.5369199698545262	T	T	T
0.7777799963734253	0.8888900279499197	0.4999999999957154	F	F	F
0.4444579153566490	0.5555436016975170	0.5891373193935315	T	T	T
0.4444231577117462	0.5555747735557264	0.4108626232417686	T	T	T

*COOH $E_0 = -190.581$ eV

Cu111-COOH

1.0000000000000000

7.6679000854000003	0.0000000000000000	0.0000000000000000
-3.8339500427000002	6.6405962677000003	0.0000000000000000
0.0000000000000000	0.0000000000000000	58.3478012085000017

Cu	C	O	H
45	2	4	2

Selective Dynamics

Direct

0.9956868150119460	0.9986507550086737	0.4633928435140333	T	T	T
0.0032705358011499	0.9980872516533431	0.5725423671257509	T	T	T
0.2180999654278579	0.1113188851775002	0.4275114336664246	T	T	T
0.2267465807645827	0.1143286863251388	0.5370642224074050	T	T	T
0.1111100018365576	0.2222200036731223	0.4999999999957154	F	F	F
0.3309232328430652	-0.0003215327246934	0.4637618429854490	T	T	T
0.3385204348687291	0.9987873121087808	0.5727136146120689	T	T	T
0.5503849971026276	0.1122014981157647	0.4273093476669818	T	T	T
0.5578627467941234	0.1113120600667219	0.5362460260240547	T	T	T
0.4444400072531138	0.2222200036731223	0.4999999999957154	F	F	F
0.6620316739200197	0.9969764680322938	0.4629442050959389	T	T	T
0.6708141972888387	0.9995337956199092	0.5724858067582005	T	T	T
0.8855207464911762	0.1128521960406875	0.4274596530614719	T	T	T
0.8931354472651596	0.1124726687234248	0.5366091309846037	T	T	T
0.7777799964982535	0.2222200036731223	0.4999999999957154	F	F	F
0.9971089863981882	0.3327945706210669	0.4635958610906930	T	T	T
0.0034475999198500	0.3333274732673027	0.57301122457666722	T	T	T
0.2165559188317178	0.4416448982107174	0.4274138932551875	T	T	T
0.2262669086251072	0.4434211794824277	0.5371399081720797	T	T	T
0.1111100018021958	0.555599928495241	0.4999999999957154	F	F	F
0.3306702816825652	0.3336263644614660	0.4637372713342633	T	T	T
0.3446222500668466	0.3344381472004082	0.5757641689093549	T	T	T
0.5484049120814765	0.4407070898947054	0.4275332802537624	T	T	T
0.5564196956452553	0.4440752141286926	0.5367496466430290	T	T	T
0.4444400072187520	0.555599928495241	0.4999999999957154	F	F	F
0.6633804942072041	0.3326140447313564	0.4636024110226332	T	T	T
0.6748122482943648	0.3332637790435745	0.5719398443793866	T	T	T
0.8832490053976496	0.4426743384963583	0.4276471962140623	T	T	T
0.8931057133321306	0.4452641788211149	0.5364500415799516	T	T	T

0.7777799964638845	0.555599928495241	0.499999999957154	F	F	F
0.9957385655833628	0.6658979931921111	0.4635509448239535	T	T	T
0.0057841220948384	0.6683755312248676	0.5723549774368397	T	T	T
0.2140505678951063	0.7776685054047093	0.4280573995783885	T	T	T
0.2255540395988028	0.7785902244609092	0.5364078134826127	T	T	T
0.1111100017117366	0.8888900279499197	0.499999999957154	F	F	F
0.3323552183046674	0.6669684989818179	0.4632310320806826	T	T	T
0.3406016481167862	0.6701946143997928	0.5724670454798733	T	T	T
0.5443272370274796	0.7764456928730264	0.4242352721614047	T	T	T
0.5582228055708743	0.7774263156157717	0.5362510886340834	T	T	T
0.4444400071282928	0.8888900279499197	0.499999999957154	F	F	F
0.6624544538415574	0.6679090511378933	0.4628523267715021	T	T	T
0.6723479278059987	0.6692145736700088	0.5725574309792887	T	T	T
0.8854768091578438	0.7776523368508071	0.4269857804977391	T	T	T
0.8917544180889589	0.7782941908526870	0.5363890319815208	T	T	T
0.7777799963734253	0.8888900279499197	0.499999999957154	F	F	F
0.3099122644518991	0.3345102067900461	0.6095355012761767	T	T	T
0.5791757961677714	0.7768435636347820	0.3904636795037706	T	T	T
0.444907382683920	0.3390129545495223	0.6251216961701657	T	T	T
0.1575383450081453	0.3302942906412046	0.6171746913748508	T	T	T
0.4442474141885334	0.7724179438509476	0.3748796922561605	T	T	T
0.7317131963007352	0.7812893075111029	0.3828112120785346	T	T	T
0.5596451103772934	0.3419687589808398	0.6174190108856915	T	T	T
0.3294052193385603	0.7693182066890545	0.3825910618681654	T	T	T

*OCHO E₀ = -191.825 eV

Cu111-OCHO

1.0000000000000000

7.6679000854000003	0.0000000000000000	0.0000000000000000
-3.8339500427000002	6.6405962677000003	0.0000000000000000
0.0000000000000000	0.0000000000000000	58.3478012085000017

Cu C O H
45 2 4 2

Selective Dynamics

Direct

0.9925111134971707	0.9995219275243273	0.4638937047703484	T	T	T
0.0156021678704892	0.0056073047408371	0.5722080399438022	T	T	T
0.2070201486439076	0.1034091193028857	0.4279255154242471	T	T	T
0.2299223203217291	0.1125608721484748	0.5360176620191869	T	T	T
0.1111100018365576	0.2222200036731223	0.499999999957154	F	F	F
0.3260795188859723	0.9996387224978507	0.4638815080059889	T	T	T
0.3454025796727219	0.0050847077592765	0.5722212311362785	T	T	T
0.5433951737509739	0.1064656846355465	0.4277776456984639	T	T	T
0.5628148219622996	0.1115661781300775	0.5360982190815359	T	T	T
0.4444400072531138	0.2222200036731223	0.499999999957154	F	F	F
0.6589637916688591	0.9987267523434625	0.4639713506818045	T	T	T
0.6816277643432149	0.0081227593664667	0.5720903180214554	T	T	T
0.8730856836520997	0.1057592031036679	0.4277946209692139	T	T	T
0.8963080312513759	0.1116368514609988	0.5361175583321929	T	T	T
0.7777799964982535	0.2222200036731223	0.499999999957154	F	F	F
0.9945818113530241	0.3333811982635982	0.4630845953012155	T	T	T
0.0107766735012299	0.3343426095401835	0.5724261470478533	T	T	T
0.2059201841632350	0.4421502144583621	0.4252154727422870	T	T	T
0.2319154804327403	0.4486574548265089	0.5370001919688090	T	T	T
0.1111100018021958	0.555599928495241	0.499999999957154	F	F	F
0.3263093511417370	0.3342221023591206	0.4624995931253336	T	T	T
0.3435382377073437	0.3318610214425596	0.5721965549229300	T	T	T
0.5428959876974211	0.4419798131979529	0.4246981573313688	T	T	T
0.5645932328560030	0.4484787929081256	0.5368913027989094	T	T	T
0.4444400072187520	0.555599928495241	0.499999999957154	F	F	F
0.6569445376716578	0.3335217763528400	0.4631163492419839	T	T	T
0.6792559111733169	0.3336702777135532	0.5723167497460532	T	T	T
0.8755731270255117	0.4439420023020280	0.4278576990449734	T	T	T
0.8969319121724612	0.4459446885536418	0.5363543834294073	T	T	T
0.7777799964638845	0.555599928495241	0.499999999957154	F	F	F
0.9918621311823383	0.6652460319030449	0.4636461892626522	T	T	T
0.0130082912230895	0.6675045753555152	0.5721342649442576	T	T	T
0.2095222929804719	0.7777241397733802	0.4276874789501628	T	T	T
0.2318783041884118	0.7778227821473189	0.5368962349084428	T	T	T
0.1111100017117366	0.8888900279499197	0.499999999957154	F	F	F

0.3242234628682950	0.6627344884886961	0.4630994622211422	T	T	T
0.3457927587046491	0.6694487984621218	0.5752904208397540	T	T	T
0.5451020185586816	0.7795089668858127	0.4277911015381266	T	T	T
0.5625629460985723	0.7769947607134446	0.5375021215447822	T	T	T
0.4444400071282928	0.8888900279499197	0.499999999957154	F	F	F
0.6568426003218306	0.6626375839779142	0.4630036220993433	T	T	T
0.6826579283571464	0.6692828031753012	0.5747813345845739	T	T	T
0.8779459979887697	0.7770005407236155	0.4275778832769010	T	T	T
0.8942333146749364	0.7777869681362709	0.5368975246516680	T	T	T
0.7777799963734253	0.8888900279499197	0.499999999957154	F	F	F
0.5312542215889247	0.6825045429061697	0.6197534083799238	T	T	T
0.3571085168178064	0.4279366535438981	0.3802387583388615	T	T	T
0.6776227247311138	0.6790308096462820	0.6097417863739582	T	T	T
0.3813004215731194	0.6832639132415781	0.6103581026414265	T	T	T
0.2109409975251037	0.4317916886516737	0.3902512586006364	T	T	T
0.5071373841537448	0.4273009176750854	0.3896308828123319	T	T	T
0.5353609214070716	0.6850124624078545	0.6386969876679182	T	T	T
0.3527267334773300	0.4249028029204440	0.3612958347587989	T	T	T

*CO E₀ = -170.186 eV

Cu111-CO

1.0000000000000000		
7.6679000854000003	0.0000000000000000	0.0000000000000000
-3.8339500427000002	6.6405962677000003	0.0000000000000000
0.0000000000000000	0.0000000000000000	58.3478012085000017

Cu C O
45 2 2

Selective Dynamics

Direct

-0.0001242092068880	0.0001242092068882	0.4637202854026244	T	T	T
0.0001524805535019	0.9998475194464980	0.5726343017320000	T	T	T
0.2219173036111168	0.1110165473149638	0.4275124803299670	T	T	T
0.2235343787946606	0.1124139907798476	0.5368228164691231	T	T	T
0.1111100018365576	0.2222200036731223	0.499999999957154	F	F	F
0.3325853601997206	0.9976693868050729	0.4632314800163910	T	T	T
0.3318835977418926	0.9965943619537772	0.5726524584654921	T	T	T
0.5569925124198876	0.1144707748352954	0.4273808853848168	T	T	T
0.5561677893470003	0.1134663091655656	0.5367640832223144	T	T	T
0.4444400072531138	0.2222200036731223	0.499999999957154	F	F	F
0.6653655858415944	0.9986514373553649	0.4631873568527862	T	T	T
0.6670597137406407	-0.0000116944421516	0.5724608580093278	T	T	T
0.8887490569855750	0.1112509726954361	0.4273543323540483	T	T	T
0.8889857518805825	0.1110142778004288	0.5362524496634985	T	T	T
0.7777799964982535	0.2222200036731223	0.499999999957154	F	F	F
0.0013485627187591	0.3346344439888300	0.4631873568527862	T	T	T
0.0000116945162754	0.3329403160897836	0.5724608580093278	T	T	T
0.2218063224700902	0.4428516241827559	0.4261521219478951	T	T	T
0.2238821821248921	0.4438321463971874	0.5366104023974549	T	T	T
0.1111100018021958	0.5555599928495241	0.499999999957154	F	F	F
0.3326862764249635	0.3350041979616614	0.4633812567888734	T	T	T
0.3318324424221795	0.3328005277668821	0.5738490037042004	T	T	T
0.5564377941180351	0.4435622059205757	0.4275451748962933	T	T	T
0.5556699575556960	0.4443300424829149	0.5358502592155593	T	T	T
0.4444400072187520	0.5555599928495241	0.499999999957154	F	F	F
0.6666812777028940	0.3333187522016470	0.4637884307985884	T	T	T
0.6680259675061728	0.3319740623983681	0.5742207263532653	T	T	T
0.8855292549198398	0.4430074875446067	0.4273808853848168	T	T	T
0.8865337205895696	0.4438322106174938	0.5367640832223144	T	T	T
0.7777799964638845	0.5555599928495241	0.499999999957154	F	F	F
0.0023306131453952	0.6674146696442252	0.4632314800163910	T	T	T
0.0034056379966909	0.6681164321020533	0.5726524584654921	T	T	T
0.2208667334976624	0.7791332664378630	0.4257860159163713	T	T	T
0.2222178462698290	0.7777821536656820	0.5362361757146925	T	T	T
0.1111100017117366	0.8888900279499197	0.499999999957154	F	F	F
0.3331248722031345	0.6668751575912796	0.4641560858272457	T	T	T
0.3324850185884505	0.6675150112059636	0.5724616960774307	T	T	T
0.5571483758214931	0.7781936774997898	0.4261521219478951	T	T	T
0.5561678536070614	0.7761178178449881	0.5366104023974549	T	T	T
0.4444400071282928	0.8888900279499197	0.499999999957154	F	F	F
0.6649958319496442	0.6673137533626933	0.4633812567888734	T	T	T

0.6671995021444234	0.6681675873654771	0.5738490037042004	T	T	T
0.8889834824058026	0.7780826962846393	0.4275124803299670	T	T	T
0.8875860389409186	0.7764656211010957	0.5368228164691231	T	T	T
0.7777799963734253	0.8888900279499197	0.4999999999957154	F	F	F
0.5561667888533101	0.4438332111853009	0.5979626072757959	T	T	T
0.3327266904134550	0.6672733393809591	0.4020178180017943	T	T	T
0.5538992371386725	0.4461007628999383	0.6184308963520596	T	T	T
0.3350239033241270	0.6649761264702870	0.3815470905420237	T	T	T

*CHO E₀ = -175.730 eV

Cu111-CHO

1.0000000000000000

7.6679000854000003 0.0000000000000000 0.0000000000000000

-3.8339500427000002 6.6405962677000003 0.0000000000000000

0.0000000000000000 0.0000000000000000 58.3478012085000017

Cu C O H
45 2 2 2

Selective Dynamics

Direct

0.0000415506761018	0.9999530489436993	0.4634187261343419	T	T	T
0.0001213434234367	0.0012824891262548	0.5732114642311252	T	T	T
0.2222652911430012	0.1085885229844166	0.4276144974494691	T	T	T
0.2216117331377819	0.1119636437385887	0.5367434017369402	T	T	T
0.1111100018365576	0.222200036731223	0.4999999999957154	F	F	F
0.3341376325918314	0.9996252270160197	0.4635227680682532	T	T	T
0.3321967389145618	0.0002380432246647	0.5726359208140025	T	T	T
0.5565272572166580	0.1108324158695535	0.4273812885604080	T	T	T
0.5548244714918169	0.1114270986981097	0.5364915061426211	T	T	T
0.4444400072531138	0.222200036731223	0.4999999999957154	F	F	F
0.6673814210246848	0.9991938439890761	0.4632579619705526	T	T	T
0.6664587078785130	0.0025750119604332	0.5724178697828908	T	T	T
0.8887116121320413	0.1098380810010868	0.4267637957945303	T	T	T
0.8888225440221904	0.1110675318986972	0.5365802701012932	T	T	T
0.7777799964982535	0.222200036731223	0.4999999999957154	F	F	F
0.0023124925931227	0.3334969877365798	0.4628168431112737	T	T	T
0.0004267025190373	0.3341958311840303	0.5729137485699693	T	T	T
0.2237515221506281	0.4444308905074949	0.4235505416590163	T	T	T
0.2228101731425024	0.4452965547391651	0.5364921489123778	T	T	T
0.1111100018021958	0.5555599928495241	0.4999999999957154	F	F	F
0.3327622352827442	0.3339088661713781	0.4630556965763497	T	T	T
0.3311599281975742	0.3339337196999660	0.5730615343428839	T	T	T
0.5578725429863485	0.4453075628238413	0.4270635685369349	T	T	T
0.5563822650162209	0.4470553576884927	0.5370423157796027	T	T	T
0.4444400072187520	0.5555599928495241	0.4999999999957154	F	F	F
0.6672503323291077	0.3332568223437837	0.4633786915193275	T	T	T
0.6664610303727808	0.3313312519579923	0.5725318612525131	T	T	T
0.8882256892482888	0.4437375619368116	0.4270802601943163	T	T	T
0.8885606686595745	0.4454958302170033	0.5366094630141686	T	T	T
0.7777799964638845	0.5555599928495241	0.4999999999957154	F	F	F
0.0003641414930525	0.6656126532751306	0.4633927032804286	T	T	T
0.0006677215796231	0.6674090540163305	0.5729287066890927	T	T	T
0.2223170410823337	0.7798280646494790	0.4274748794219806	T	T	T
0.2216867162941707	0.7778768232668325	0.5366206306304079	T	T	T
0.1111100017117366	0.8888900279499197	0.4999999999957154	F	F	F
0.3325381346519767	0.6640070786847694	0.4629568635962795	T	T	T
0.3309734227094073	0.6657932000032388	0.5729267271783797	T	T	T
0.5576885784047982	0.7772310694670861	0.4269421715790310	T	T	T
0.5561833755968517	0.7771556340493233	0.5369515723036320	T	T	T
0.4444400071282928	0.8888900279499197	0.4999999999957154	F	F	F
0.6661013673843749	0.6658427868440321	0.4634988265906083	T	T	T
0.6652077312338194	0.6667857976109254	0.5764559698711709	T	T	T
0.8883848556635007	0.7769081052950622	0.4270433404259975	T	T	T
0.8867079930917440	0.7774861757916384	0.5371784609937421	T	T	T
0.7777799963734253	0.8888900279499197	0.4999999999957154	F	F	F
0.6643046481575200	0.6550744753960919	0.6104369189924906	T	T	T
0.2245825348543176	0.4562064534162569	0.3895779457515797	T	T	T
0.6786205156694060	0.5300806354060703	0.6220244547378384	T	T	T
0.2103199392385847	0.5811676806590110	0.3779980401464494	T	T	T
0.6498995839025991	0.7768077821048398	0.6191693000225765	T	T	T
0.2389050433165899	0.3344493956849744	0.3808347175108205	T	T	T

*COH E₀ = -175.443 eV

Cu111-COH

1.0000000000000000		
7.6679000854000003	0.0000000000000000	0.0000000000000000
-3.8339500427000002	6.6405962677000003	0.0000000000000000
0.0000000000000000	0.0000000000000000	58.3478012085000017

Cu	H	O	C
45	2	2	2

Selective Dynamics

Direct

0.9995495813558047	0.0001965643295502	0.4634245988339612	T	T	T
0.0005682058982606	0.9995857539301931	0.5730609331354873	T	T	T
0.2208045668335627	0.1123910624994099	0.4268803652201113	T	T	T
0.2239273997880738	0.1127737277412130	0.5371032062430610	T	T	T
0.1111100018365576	0.2222200036731223	0.4999999999957154	F	F	F
0.3314679853561783	0.9978353106163196	0.4628976204970451	T	T	T
0.3337640733292242	0.9975969308664072	0.5732634361646055	T	T	T
0.5550269673542138	0.1134380324615050	0.4267202839969438	T	T	T
0.5573927718800568	0.1133696716458499	0.5371067799489051	T	T	T
0.4444400072531138	0.2222200036731223	0.4999999999957154	F	F	F
0.6649380362615916	0.9982979576477479	0.4628907574964549	T	T	T
0.6680808520571335	0.9986579003762889	0.5731236043110872	T	T	T
0.8883375950304457	0.1114833348561375	0.4269326200443175	T	T	T
0.8893175772634904	0.1109302562938468	0.5365784597931843	T	T	T
0.7777799964982535	0.2222200036731223	0.4999999999957154	F	F	F
0.0014116481749649	0.3347845497128473	0.4629089812413292	T	T	T
0.0015599957847041	0.3322028055841087	0.5730695041186933	T	T	T
0.2212362382455983	0.4423215337143162	0.4249766375364895	T	T	T
0.2233926521356464	0.4431790840903375	0.5368459605894503	T	T	T
0.1111100018021958	0.5555599928495241	0.4999999999957154	F	F	F
0.3317840146171256	0.3342147232445584	0.4631368776183922	T	T	T
0.3310903477474154	0.3327706570392446	0.5750109043912184	T	T	T
0.5560729986221793	0.4433719662973303	0.4267584707641691	T	T	T
0.5563305886285472	0.4439164427564289	0.5362500577040765	T	T	T
0.4444400072187520	0.5555599928495241	0.4999999999957154	F	F	F
0.6661528169992925	0.3334946195060134	0.4633226611594087	T	T	T
0.6718953960785640	0.3290912521922572	0.5753730384106327	T	T	T
0.8857531615010494	0.4442240955049584	0.4267624758671975	T	T	T
0.8870239953894045	0.4430192311385588	0.5370836681727241	T	T	T
0.7777799964638845	0.5555599928495241	0.4999999999957154	F	F	F
0.0018239121156544	0.6681725576809147	0.4629157786165628	T	T	T
0.0031088434507012	0.6668842648473796	0.5732273921290341	T	T	T
0.2169973303316905	0.7819646823306409	0.4246443047837880	T	T	T
0.2227966756562486	0.7775736261567440	0.5366670205904411	T	T	T
0.1111100017117366	0.8888900279499197	0.4999999999957154	F	F	F
0.3325455484494870	0.6672139648239515	0.4637573482162206	T	T	T
0.3327289725568134	0.6677501729870247	0.5732557417135400	T	T	T
0.5578223529850189	0.7782918096502479	0.4249785104283022	T	T	T
0.5571194037738249	0.7768841155796592	0.5368654969269602	T	T	T
0.4444400071282928	0.8888900279499197	0.4999999999957154	F	F	F
0.6654916042344068	0.6679063923236523	0.4631569063811847	T	T	T
0.6676630010583109	0.6687359215813717	0.5750094390463300	T	T	T
0.8873323272870620	0.7788579979193053	0.4269358404493893	T	T	T
0.8875145741017705	0.7763288965496353	0.5370876488509871	T	T	T
0.7777799963734253	0.8888900279499197	0.4999999999957154	F	F	F
0.6235798249327754	0.3924329866304586	0.6270612695597004	T	T	T
0.2652003321011345	0.7187840499139635	0.3729389019892632	T	T	T
0.5492167641336723	0.4489637542499269	0.6193033974431787	T	T	T
0.3396442706844174	0.6622319688827832	0.3807042019404445	T	T	T
0.5589334671127361	0.4390183493798887	0.5964697205200833	T	T	T
0.3299174964724274	0.6721390448923642	0.4035290513472597	T	T	T

*CHOH E₀ = -182.591 eV

Cu111-CHOH

1.0000000000000000		
7.6679000854000003	0.0000000000000000	0.0000000000000000
-3.8339500427000002	6.6405962677000003	0.0000000000000000

```

0.0000000000000000    0.0000000000000000    58.3478012085000017
Cu   H   C   O
45   4   2   2
Selective Dynamics
Direct
0.9977838038652846  0.9984406798693837  0.4635728534794644  T   T   T
0.0039021306629376  0.0032528326082301  0.5731975683202810  T   T   T
0.2186534378364140  0.1108177418573325  0.4277208850879269  T   T   T
0.2250828655123052  0.1157931029087674  0.5371443890661991  T   T   T
0.1111100018365576  0.2222200036731223  0.4999999999957154  F   F   F
0.3318689085163939  0.9978835944421420  0.4635237922695327  T   T   T
0.3361925940556585  0.0021111240182843  0.5724635021733153  T   T   T
0.5526200092799091  0.1086411796263277  0.4275218335418480  T   T   T
0.5569651715475753  0.1131104837570284  0.5364460227421314  T   T   T
0.4444400072531138  0.2222200036731223  0.4999999999957154  F   F   F
0.6638343535867941  0.9951112854680574  0.4628359382988911  T   T   T
0.6699880089466640  -0.0000233839236121  0.5722754603985186  T   T   T
0.8849134408345291  0.1075974069819556  0.4268114965120627  T   T   T
0.8910883938322657  0.1125596058374163  0.5364305271407100  T   T   T
0.7777799964982535  0.2222200036731223  0.4999999999957154  F   F   F
0.0009079940373198  0.3322584406993705  0.4628890968171150  T   T   T
0.0048276204514208  0.3345407362102519  0.5725274138546397  T   T   T
0.2173707539529711  0.4461717836272986  0.4248846183427455  T   T   T
0.2251768328663278  0.4448050818418950  0.5365791851423526  T   T   T
0.1111100018021958  0.5555599928495241  0.4999999999957154  F   F   F
0.3300049104821653  0.3332941096938552  0.4633152460119314  T   T   T
0.340317059526568  0.3396653240906081  0.5759563433645298  T   T   T
0.5565347503728767  0.4388730890321487  0.4286651333901044  T   T   T
0.5568741502591030  0.4456827446562495  0.5366095627055759  T   T   T
0.4444400072187520  0.5555599928495241  0.4999999999957154  F   F   F
0.6659452947751417  0.3305659358182022  0.4640110965465682  T   T   T
0.6745026691950734  0.3311801624716754  0.5721922731116590  T   T   T
0.8844881809502565  0.4416297203231966  0.4273790185324295  T   T   T
0.8908188981462298  0.4466032697002917  0.5364484975830944  T   T   T
0.7777799964638845  0.5555599928495241  0.4999999999957154  F   F   F
0.9980005357389636  0.6643189008615024  0.4635708173162075  T   T   T
0.0042067975161321  0.6692777714205591  0.5726348484411966  T   T   T
0.2139012179601867  0.7796897906682112  0.4278099343464227  T   T   T
0.2228415360908706  0.7803055277018565  0.5359566156834823  T   T   T
0.1111100017117366  0.8888900279499197  0.4999999999957154  F   F   F
0.3320447046475819  0.6653464915782358  0.4633582121998435  T   T   T
0.3321395007374424  0.6720328771083031  0.5713264354963639  T   T   T
0.5483468616926840  0.7713376593251611  0.4240844974564781  T   T   T
0.5588521260704352  0.7776860927697700  0.5366349717978721  T   T   T
0.4444400071282928  0.8888900279499197  0.4999999999957154  F   F   F
0.6635845019932448  0.6661878487380887  0.4633893105854733  T   T   T
0.6715062586819630  0.6650772952545313  0.5751440475861290  T   T   T
0.8841685678474002  0.7764897338064501  0.4274905424390118  T   T   T
0.8880137977370969  0.7786681748318807  0.5371047968947663  T   T   T
0.7777799963734253  0.8888900279499197  0.4999999999957154  F   F   F
0.5823413442710889  0.4074287666398260  0.6121605455729910  T   T   T
0.4323680828138489  0.6756865563222638  0.6134273654637038  T   T   T
0.3062522913876735  0.7043335588701976  0.3878653668514229  T   T   T
0.4562248163458645  0.4361407902166498  0.3864799349709638  T   T   T
0.5285849035847213  0.4968092858157689  0.6029057849742649  T   T   T
0.3601263975444835  0.6149343171050188  0.3971018796273389  T   T   T
0.4762988062650648  0.5855342141989562  0.6198670936624771  T   T   T
0.4121479383253917  0.5263749369172419  0.3800965599741717  T   T   T

```

```

*C   E0 = -152.079 eV
cu111-c
1.0000000000000000
7.6679000854000003    0.0000000000000000    0.0000000000000000
-3.8339500427000002    6.6405962677000003    0.0000000000000000
0.0000000000000000    0.0000000000000000    58.3478012085000017
Cu   C
45   2
Selective Dynamics
Direct

```

0.9997774380549428	0.0002223546026687	0.4636811845861483	T	T	T
0.0010459768368835	0.9989550432346672	0.5724387001779708	T	T	T
0.2212964354446165	0.1095561731152669	0.4274427395258500	T	T	T
0.2226623332642901	0.1119000435679551	0.5364620886739869	T	T	T
0.1111100018365576	0.2222200036731223	0.499999999957154	F	F	F
0.3336094489672050	0.0002575807780466	0.4637092716091319	T	T	T
0.3316461065861408	0.9989207156156762	0.5724044970789186	T	T	T
0.5573129443479529	0.1120768418585958	0.4276145142058445	T	T	T
0.5552140044418202	0.1108059557025064	0.5362911138774623	T	T	T
0.4444400072531138	0.2222200036731223	0.499999999957154	F	F	F
0.6662034887136223	0.9991955005472692	0.4635586853210029	T	T	T
0.6677417921078794	0.0014467087372169	0.5725237236364028	T	T	T
0.8879490031108148	0.1120508721794990	0.4275844265229314	T	T	T
0.8891500408572705	0.1108496862024528	0.5363051991605424	T	T	T
0.7777799964982535	0.2222200036731223	0.499999999957154	F	F	F
0.0008035299605466	0.3337953540055288	0.4635586710983461	T	T	T
0.9985509569308516	0.3322565294949659	0.5725232456052912	T	T	T
0.2110068305500532	0.4390701481124406	0.4257722865578829	T	T	T
0.2233248357185656	0.4449139964361234	0.5366561766589465	T	T	T
0.1111100018021958	0.5555599928495241	0.499999999957154	F	F	F
0.3337845996696099	0.3343924396278290	0.4633213791908720	T	T	T
0.3280636937163967	0.3220502578192002	0.5742195278643142	T	T	T
0.5609781696687623	0.4390220615127683	0.4257706789811105	T	T	T
0.5550977470086466	0.4449032644656002	0.5366567477218318	T	T	T
0.4444400072187520	0.5555599928495241	0.499999999957154	F	F	F
0.6661601797949011	0.3338401504397190	0.4635717872539493	T	T	T
0.6677737574508245	0.3322246413260502	0.5724982911303759	T	T	T
0.8879238372827409	0.4426880743767074	0.4276148877375780	T	T	T
0.8891916924137427	0.4447836876529173	0.5362905576443867	T	T	T
0.7777799964638845	0.5555599928495241	0.499999999957154	F	F	F
0.9997427897314289	0.6663918102487940	0.4637095118702762	T	T	T
0.0010787148276055	0.6683527364558811	0.5724041102364459	T	T	T
0.2212137633187608	0.7787872113478587	0.4274801161227968	T	T	T
0.2227220755526836	0.7772779455491926	0.5364457494721302	T	T	T
0.1111100017117366	0.8888900279499197	0.499999999957154	F	F	F
0.3337932393873691	0.6662062915240410	0.4633288910334162	T	T	T
0.3279438179020125	0.6720559395946257	0.5742026204065546	T	T	T
0.5609281173134608	0.7889900829388469	0.4257722416765575	T	T	T
0.5550867265569837	0.7766756615443209	0.5366563122700777	T	T	T
0.4444400071282928	0.8888900279499197	0.499999999957154	F	F	F
0.6656077775849645	0.6662146156939063	0.4633215161320113	T	T	T
0.6779489354330218	0.6719363549970915	0.5742198566481197	T	T	T
0.8904439594076893	0.7787030441600229	0.4274429744031623	T	T	T
0.8881008818533135	0.7773382682815239	0.5364620804614416	T	T	T
0.7777799963734253	0.8888900279499197	0.499999999957154	F	F	F
0.4445757137771512	0.5554260503064695	0.5917023521775223	T	T	T
0.4443056627632021	0.5556966683024284	0.4082965026691301	T	T	T

*OCH₃ E₀ = -192.314 eV

cu111-och3

1.0000000000000000

7.6679000854000003

-3.8339500427000002

0.0000000000000000

0.0000000000000000

6.6405962677000003

0.0000000000000000

0.0000000000000000

0.0000000000000000

58.3478012085000017

Cu C O H
45 2 2 6

Selective Dynamics

Direct

0.0000229845499932	0.0002632833421585	0.4637266980277288	T	T	T
0.9994188928406528	0.0000752403241563	0.5728246361710584	T	T	T
0.2216132002538765	0.1115185777311898	0.4273557777061366	T	T	T
0.2226598642701061	0.1127986218770542	0.5369184773180263	T	T	T
0.1111100018365576	0.2222200036731223	0.499999999957154	F	F	F
0.3321001020140779	0.9976704530451991	0.4632233686153525	T	T	T
0.3311230142732601	0.9946369261366924	0.5722570932425306	T	T	T
0.5577859720484070	0.1164038332118638	0.4277502023839375	T	T	T
0.5567490789774673	0.1134773716226833	0.5367679743396454	T	T	T
0.4444400072531138	0.2222200036731223	0.499999999957154	F	F	F
0.6663233101509483	0.9982684536260904	0.4630863347592624	T	T	T
0.6673431773208010	0.9995942131234331	0.5726155753325417	T	T	T

0.8895468936303579	0.1109914447621579	0.4271637734383782	T	T	T
0.8889017411079595	0.1107680401017386	0.5362605776141214	T	T	T
0.7777799964982535	0.2222200036731223	0.4999999999957154	F	F	F
0.0020012624507567	0.3339639025497368	0.4630785858830865	T	T	T
0.9996427605319930	0.3321446704991218	0.5726041931373043	T	T	T
0.2183446549420540	0.4361800965002922	0.4256531498460219	T	T	T
0.2231605256855540	0.4431256126648589	0.5367498946299356	T	T	T
0.1111100018021958	0.5555599928495241	0.4999999999957154	F	F	F
0.3322910488445998	0.3346317333272641	0.4632308969279589	T	T	T
0.3244778440509024	0.3293582440680009	0.5742755030865159	T	T	T
0.5577367371384464	0.4426324718136069	0.4277333598642028	T	T	T
0.5554172764525177	0.4442452434931161	0.5372858834922845	T	T	T
0.4444400072187520	0.5555599928495241	0.4999999999957154	F	F	F
0.6668575823157776	0.3334658138924173	0.4640916220252843	T	T	T
0.670986052685511	0.3279805301887381	0.5743605368122331	T	T	T
0.8841752944086992	0.4428640537612225	0.4277447686517664	T	T	T
0.8860803225608804	0.4429000054193403	0.5367723670245850	T	T	T
0.7777799964638845	0.5555599928495241	0.4999999999957154	F	F	F
0.0027152788048727	0.6682098739474229	0.4632200523585486	T	T	T
0.0047425581592192	0.6682373634225296	0.5722598396493004	T	T	T
0.2179532908018420	0.7831386311729526	0.4256690656683739	T	T	T
0.2219891625271692	0.7776924774258485	0.5359051732252738	T	T	T
0.1111100017117366	0.8888900279499197	0.4999999999957154	F	F	F
0.3333921311610642	0.6668781044438238	0.4627098775530759	T	T	T
0.3312099878292949	0.6684451618521347	0.5722556822243873	T	T	T
0.5645777279367407	0.7818289952845920	0.4257234153511694	T	T	T
0.5566080272958377	0.7764379209391979	0.5367586970132857	T	T	T
0.4444400071282928	0.8888900279499197	0.4999999999957154	F	F	F
0.6657330659538940	0.6679617602265291	0.4632405784457307	T	T	T
0.6704915404455130	0.6748345773590960	0.5743354009862476	T	T	T
0.88929833684859538	0.7789376217900366	0.4273649194276935	T	T	T
0.8869169320480104	0.7770245790946830	0.5369239193534173	T	T	T
0.7777799963734253	0.8888900279499197	0.4999999999957154	F	F	F
0.5542444409041840	0.4403780191644484	0.6228643250451391	T	T	T
0.3347121816277275	0.6708124316040261	0.3771629991574867	T	T	T
0.5553536336405884	0.4426207442348246	0.5981121227495207	T	T	T
0.3336191230684374	0.6685233603965978	0.4019099738457781	T	T	T
0.5044063195530889	0.5430962272339659	0.6293967402467295	T	T	T
0.7067882598788250	0.4892557314267087	0.6293392927968152	T	T	T
0.4506062309558163	0.2869394730016997	0.6290956458701942	T	T	T
0.3844993541456163	0.5681266395568341	0.3706288668330655	T	T	T
0.1821384483254631	0.6219505276856461	0.3706978556136886	T	T	T
0.4383007396041025	0.8242392438640228	0.3709389702998057	T	T	T

*CH₂OH E₀ = -190.856 eV

cu111-CH2OH

1.0000000000000000

7.6679000854000003

-3.8339500427000002

0.0000000000000000

0.0000000000000000

6.6405962677000003

0.0000000000000000

0.0000000000000000

0.0000000000000000

58.3478012085000017

Cu C O H
45 2 2 6

Selective Dynamics

Direct

0.9994966041540007	0.9984898644369622	0.4634037351065002	T	T	T
0.9976024708547351	0.0003209333078921	0.5729575729559413	T	T	T
0.2229354574041473	0.1106720994445284	0.4270850683359344	T	T	T
0.2233790966850457	0.1143883347700846	0.5372918062295624	T	T	T
0.1111100018365576	0.2222200036731223	0.4999999999957154	F	F	F
0.3341631152184039	0.9988693685087953	0.4634480049796225	T	T	T
0.3339010098302319	0.0004533220722326	0.5729986073463810	T	T	T
0.5549402130859159	0.1107321334871141	0.4270093309861581	T	T	T
0.5548062711166161	0.1122061487535559	0.5365634650739559	T	T	T
0.4444400072531138	0.2222200036731223	0.4999999999957154	F	F	F
0.6656001903421513	0.9965783230142393	0.4627056140764521	T	T	T
0.6659002016595639	0.0004713771330000	0.5728915275174296	T	T	T
0.8912903175794197	0.1108186095144186	0.4270326472989323	T	T	T
0.8894517867966073	0.1125408363925030	0.5365969468491526	T	T	T
0.7777799964982535	0.2222200036731223	0.4999999999957154	F	F	F
0.0002888098184446	0.3319068108338509	0.4633964787251348	T	T	T

0.9989274670547368	0.3349789913910460	0.5729400603421368	T	T	T
0.2219489078136415	0.4417070554097457	0.4271457331031114	T	T	T
0.2230520199495527	0.4440557281564015	0.5370545470263233	T	T	T
0.1111100018021958	0.5555599928495241	0.499999999957154	F	F	F
0.3338446823895236	0.3332615020042058	0.4634620939707220	T	T	T
0.3309935394632245	0.3356981715149372	0.5774222561001450	T	T	T
0.5549633822971870	0.4412840818530762	0.4271176601268847	T	T	T
0.5523248230596859	0.4439418077677846	0.5370316380231481	T	T	T
0.4444400072187520	0.5555599928495241	0.499999999957154	F	F	F
0.6665906462330508	0.3319625006871501	0.4632900607043697	T	T	T
0.6686330374452633	0.3354878354874115	0.5721606006948172	T	T	T
0.8889363656497878	0.4421438587301430	0.4272240815054818	T	T	T
0.8897316175425385	0.4458572281984176	0.5365124762330142	T	T	T
0.7777799964638845	0.5555599928495241	0.499999999957154	F	F	F
0.9992208950195752	0.6651081021695001	0.4634886305456819	T	T	T
0.9999662701909124	0.6690647327262103	0.5727676378968194	T	T	T
0.2202202442404389	0.7759137736691282	0.4278400093523627	T	T	T
0.2222844717848472	0.7790637060344902	0.5367149332039561	T	T	T
0.1111100017117366	0.8888900279499197	0.499999999957154	F	F	F
0.3366171355977677	0.6670867409621748	0.4629610884383007	T	T	T
0.3339172494670261	0.6698436606910332	0.5728897891009308	T	T	T
0.5577807423545263	0.7756039873993339	0.4225934653169303	T	T	T
0.5549985615638537	0.7777975184479307	0.5365358256898453	T	T	T
0.4444400071282928	0.8888900279499197	0.499999999957154	F	F	F
0.6659697251713754	0.6669466629045360	0.4629461939741897	T	T	T
0.6669191211682205	0.6694991873126380	0.5728542308804768	T	T	T
0.8898286446131267	0.7760810524890095	0.4270599608033868	T	T	T
0.8886090271851134	0.7791248635706893	0.5366002060333785	T	T	T
0.7777799963734253	0.8888900279499197	0.499999999957154	F	F	F
0.3256993858130183	0.3308508991388897	0.6127557055665748	T	T	T
0.5630374766970720	0.7804157881317150	0.3872421518440676	T	T	T
0.3969061720242451	0.2061630841384931	0.6217223006857799	T	T	T
0.4920395120940387	0.9049381466508586	0.3783027556270769	T	T	T
0.1701592014522562	0.2693787502767848	0.6184754995771133	T	T	T
0.4194978888578996	0.4876619351824348	0.6180323610232920	T	T	T
0.5421313814873768	0.2685473196584848	0.6188849281447976	T	T	T
0.7185405033131138	0.8418672459416797	0.3815461381148600	T	T	T
0.4694239919121383	0.6237894114540190	0.3819887310080219	T	T	T
0.3464950757733030	0.8426112586901051	0.3811343680025195	T	T	T

*CH $E_0 = -161.671$ eV

cu111-CH

1.0000000000000000

7.6679000854000003	0.0000000000000000	0.0000000000000000
-3.8339500427000002	6.6405962677000003	0.0000000000000000
0.0000000000000000	0.0000000000000000	58.3478012085000017

Cu C H
45 2 2

Selective Dynamics

Direct

0.0002412041193004	0.0000871956742852	0.4630430848206648	T	T	T
0.0001734934249919	0.9991847103946281	0.5732915698781704	T	T	T
0.2218519109267590	0.1102144241548074	0.4265125489572325	T	T	T
0.2228601751650019	0.1125526715191383	0.5371088311641239	T	T	T
0.1111100018365576	0.2222200036731223	0.499999999957154	F	F	F
0.3333168717612561	0.0001206400437265	0.4630464166134935	T	T	T
0.3319707360980593	0.9992325826167184	0.5732822056340374	T	T	T
0.5569032880009094	0.1118747198503171	0.4267485656925430	T	T	T
0.5554760374250158	0.1109029032675037	0.5369442143175810	T	T	T
0.4444400072531138	0.2222200036731223	0.499999999957154	F	F	F
0.6661635209519674	0.9985033280126926	0.4628915016141865	T	T	T
0.6671324135889916	0.0008470339545335	0.5734826729885089	T	T	T
0.8887431265659966	0.1118952103703805	0.4266914915040713	T	T	T
0.8886895689270213	0.11099326271105571	0.5369623666458324	T	T	T
0.7777799964982535	0.2222200036731223	0.499999999957154	F	F	F
0.0018634326062002	0.3341707049321347	0.4628753007697607	T	T	T
0.9986658317960819	0.3323716074886383	0.5734766647938180	T	T	T
0.2156528205819759	0.4413719746563077	0.4246398817085943	T	T	T
0.2231030733497917	0.4447701735885016	0.5367619138409805	T	T	T
0.1111100018021958	0.5555599928495241	0.499999999957154	F	F	F

0.3339637884213414	0.3345153190215537	0.4632221800564493	T	T	T
0.3297000662734805	0.3261803611238718	0.5752588074201680	T	T	T
0.5593219707586080	0.4412793142997397	0.4247065302122353	T	T	T
0.5549460462820065	0.4448316098726505	0.5367792366107282	T	T	T
0.4444400072187520	0.5555599928495241	0.499999999957154	F	F	F
0.6659626708992863	0.3344269553075869	0.4628852288355307	T	T	T
0.6671788116987887	0.3323030843399254	0.5734688978872456	T	T	T
0.8887589488131937	0.4437006010835945	0.4267333025055000	T	T	T
0.8887728756699191	0.4442031049724113	0.5369448895534222	T	T	T
0.7777799964638845	0.5555599928495241	0.499999999957154	F	F	F
0.0002208595722938	0.6670177306978645	0.4630444611640901	T	T	T
0.0001591635872667	0.6675067322670742	0.5732926717056217	T	T	T
0.2217717037743217	0.7787634398747667	0.4265267844671846	T	T	T
0.2229538321634268	0.7767021399454732	0.5371187701115469	T	T	T
0.1111100017117366	0.8888900279499197	0.499999999957154	F	F	F
0.3339509530344250	0.6662569585156359	0.4632275969370786	T	T	T
0.3295261777826289	0.6698847369601737	0.5752943798529800	T	T	T
0.5592305713666931	0.7849745171084183	0.4247387230337578	T	T	T
0.5549580272113847	0.7765499721704545	0.5367742646757779	T	T	T
0.4444400071282928	0.8888900279499197	0.499999999957154	F	F	F
0.66583166645115426	0.6663304462357856	0.4632349365944859	T	T	T
0.6732092381088497	0.6697024763264718	0.5753669117402841	T	T	T
0.8902830667723876	0.7786668275246861	0.4265178435986334	T	T	T
0.8870877457841645	0.7767986441728627	0.5371232928687908	T	T	T
0.7777799963734253	0.8888900279499197	0.499999999957154	F	F	F
0.4436288502392443	0.5549953370807900	0.5953983639646540	T	T	T
0.4451624605040271	0.5561654220930924	0.4046141507794984	T	T	T
0.4430932064004420	0.5545507202438096	0.6141738256999237	T	T	T
0.4456793017153541	0.5566370098575859	0.3858247036199678	T	T	T

*O E₀ = -152.654 eV

cu111-o

1.0000000000000000		
7.6679000854000003	0.0000000000000000	0.0000000000000000
-3.8339500427000002	6.6405962677000003	0.0000000000000000
0.0000000000000000	0.0000000000000000	58.3478012085000017

Cu 0
45 2

Selective Dynamics

Direct

0.0001393569215887	0.0001835854815188	0.4638529865965365	T	T	T
0.0001042246889945	0.9994731798210416	0.5721396468011580	T	T	T
0.2201527691550479	0.1072290699872466	0.4278401558776436	T	T	T
0.2234340415801677	0.1134969042623705	0.5367600329098020	T	T	T
0.1111100018365576	0.2222200036731223	0.499999999957154	F	F	F
0.3333713486270562	0.0001532951804303	0.4638316620682276	T	T	T
0.3326892747749640	0.9994956228784050	0.5721368097281679	T	T	T
0.5560882501240741	0.1116010492205868	0.4278802813209860	T	T	T
0.5554716038179084	0.1109141452226718	0.5361780941730656	T	T	T
0.4444400072531138	0.2222200036731223	0.499999999957154	F	F	F
0.6654989994801623	0.9975144198315170	0.4632448332958969	T	T	T
0.6687417194738041	0.0039349622666359	0.5721425037781344	T	T	T
0.8887526431197946	0.1115785723825873	0.4278643824245731	T	T	T
0.8888059740129299	0.1108959752644012	0.5361355918661243	T	T	T
0.7777799964982535	0.2222200036731223	0.499999999957154	F	F	F
0.0028124114353583	0.3348262089199653	0.4632489414242699	T	T	T
0.9955819413695047	0.3308243172500833	0.5721478266353962	T	T	T
0.2137679578306989	0.4405594311802872	0.4256105350644804	T	T	T
0.2239713581770968	0.4451255657127560	0.5366900815759482	T	T	T
0.1111100018021958	0.5555599928495241	0.499999999957154	F	F	F
0.3344024900586701	0.3353949478668485	0.4633105297963998	T	T	T
0.3289596557686738	0.3243224335041395	0.5743715066805671	T	T	T
0.5599670658474858	0.4404395800875611	0.4255929469550424	T	T	T
0.5545944886229299	0.4450729827691836	0.5366990352924311	T	T	T
0.4444400072187520	0.5555599928495241	0.499999999957154	F	F	F
0.6654505478180489	0.3348705612496814	0.4632388862833441	T	T	T
0.6687788658161566	0.3307920150330882	0.5721621653029195	T	T	T
0.8887839390411035	0.4443692667472203	0.4278827042445144	T	T	T
0.8888059313046847	0.4442237487424036	0.5361780029657017	T	T	T
0.7777799964638845	0.5555599928495241	0.499999999957154	F	F	F

0.0001482214790054	0.6669361248683893	0.4638322282750179	T	T	T
0.0000876633845226	0.6668909246323500	0.5721357170765748	T	T	T
0.2200802884140490	0.7803934612829768	0.4278311911765189	T	T	T
0.2235125166420682	0.7761813518726394	0.5367563394501993	T	T	T
0.1111100017117366	0.8888900279499197	0.4999999999957154	F	F	F
0.3343571825723581	0.6659995547804566	0.4632946066436527	T	T	T
0.3288904353189944	0.6706697848800811	0.5744081038541625	T	T	T
0.5599437342432673	0.7868747301390444	0.4256161017350038	T	T	T
0.5545390435977535	0.7756936363499806	0.5366880009205552	T	T	T
0.4444400071282928	0.8888900279499197	0.4999999999957154	F	F	F
0.6649478514114677	0.6659472475256729	0.4633094211857901	T	T	T
0.6750684816702937	0.6705084708980670	0.5743786459451314	T	T	T
0.8932202935258488	0.7803147413805666	0.4278388994759810	T	T	T
0.8861637804340989	0.7762383924113285	0.5367559773545714	T	T	T
0.7777799963734253	0.8888900279499197	0.4999999999957154	F	F	F
0.4442832610507798	0.5552599827771835	0.5942626918345322	T	T	T
0.4443909325073567	0.5558634920702225	0.4057321296892590	T	T	T

*CH₂ E₀ = -169.484 eV

cu111-CH₂

1.0000000000000000

7.6679000854000003

-3.8339500427000002

0.0000000000000000

0.0000000000000000

6.6405962677000003

0.0000000000000000

0.0000000000000000

0.0000000000000000

58.3478012085000017

Cu C H
45 2 4

Selective Dynamics

Direct

0.9999690854542356	0.9997439776821319	0.4634573510802007	T	T	T
0.0000946426918249	0.0009594141586398	0.5731772333452073	T	T	T
0.2207663516897656	0.1086189845691012	0.4270514524751802	T	T	T
0.2228799186773671	0.1135230027722869	0.5371592275619658	T	T	T
0.1111100018365576	0.2222200036731223	0.4999999999957154	F	F	F
0.3332739516570872	0.9989748615535794	0.4632631386897026	T	T	T
0.3334375538875021	0.9976800154599712	0.5727546220351367	T	T	T
0.5554217804065263	0.1134626799464875	0.4272490433750720	T	T	T
0.5556166706689606	0.1120907981739924	0.5367344359398332	T	T	T
0.4444400072531138	0.2222200036731223	0.4999999999957154	F	F	F
0.6661191771452388	0.9974801357174791	0.4628381363689997	T	T	T
0.6681110942181568	0.0025409681623665	0.5729483289524858	T	T	T
0.8887724170298179	0.1101696934949616	0.4268146816751985	T	T	T
0.8889760572027304	0.1113281303091127	0.5365462562383903	T	T	T
0.7777799964982535	0.2222200036731223	0.4999999999957154	F	F	F
0.0019684758153192	0.3334112905869775	0.4628692030365438	T	T	T
0.9981093412676673	0.3324229924978331	0.5730551357867382	T	T	T
0.2173790580020606	0.4409452362579729	0.4244912347441330	T	T	T
0.2227298741955990	0.4436069250917897	0.5367825486005428	T	T	T
0.1111100018021958	0.5555599928495241	0.4999999999957154	F	F	F
0.3322736999286370	0.3337463540289680	0.4632051557932449	T	T	T
0.3302133834396033	0.3305389629517826	0.5757398065343330	T	T	T
0.5557523592066251	0.4442316222295350	0.4271672473981437	T	T	T
0.5545186502232342	0.4455306039639292	0.5369784055656608	T	T	T
0.4444400072187520	0.5555599928495241	0.4999999999957154	F	F	F
0.6662297279868343	0.3336556225004360	0.4634677508290543	T	T	T
0.6685379607727269	0.3321779005549212	0.5729898299595302	T	T	T
0.8857964130990761	0.4439057557363099	0.4271783710591869	T	T	T
0.8882856456700912	0.4446144951168457	0.5367385812839360	T	T	T
0.7777799964638845	0.5555599928495241	0.4999999999957154	F	F	F
0.0006572949776414	0.6664968973369815	0.4632593698758642	T	T	T
0.0030902853894515	0.6672678161351709	0.5728225069873846	T	T	T
0.2203521173604727	0.7789562936085778	0.4270100975548183	T	T	T
0.2227118078083742	0.7774042594150551	0.5365293660950253	T	T	T
0.1111100017117366	0.8888900279499197	0.4999999999957154	F	F	F
0.3344034289792954	0.6655364034137659	0.4630237738228642	T	T	T
0.3331292637811883	0.6669084886010149	0.5728218044434955	T	T	T
0.5586239421451087	0.7805393623861463	0.4242714620746107	T	T	T
0.5566616406716686	0.7773393573014850	0.5367918633579393	T	T	T
0.4444400071282928	0.8888900279499197	0.4999999999957154	F	F	F
0.6661999519373220	0.6674566749610142	0.4632155178075727	T	T	T
0.6714712631770735	0.6701995995591324	0.5755136514867900	T	T	T

0.8907849676702371	0.7787458160343648	0.4269445562046439	T	T	T
0.8869978370281053	0.7775780024716763	0.5371296041157294	T	T	T
0.7777799963734253	0.8888900279499197	0.4999999999957154	F	F	F
0.4996449242292098	0.5039592546314680	0.6010961369453158	T	T	T
0.3891057103633271	0.6072964372585558	0.3989234798492569	T	T	T
0.4394425117863426	0.5752638003464281	0.6124407373180714	T	T	T
0.5638240768438604	0.4311486847263509	0.6118771214249840	T	T	T
0.4494139613727131	0.5358245818822280	0.3875531056899998	T	T	T
0.3250109990676527	0.6800227313324295	0.3881286327158018	T	T	T

*OH E₀ = -160.845 eV

cu111-oh

1.0000000000000000		
7.6679000854000003	0.0000000000000000	0.0000000000000000
-3.8339500427000002	6.6405962677000003	0.0000000000000000
0.0000000000000000	0.0000000000000000	58.3478012085000017

Cu O H
45 2 2

Selective Dynamics

Direct

0.9998676466495596	-0.0000437628187365	0.4637001190699750	T	T	T
0.9997359486955379	0.0009041218283352	0.5728993305376097	T	T	T
0.2210725554394001	0.1105528355987197	0.4272667712171316	T	T	T
0.2228447786185699	0.1132121223988145	0.5370129035805231	T	T	T
0.1111100018365576	0.2222200036731223	0.4999999999957154	F	F	F
0.3317282800292287	0.9971289217324468	0.4631067163641870	T	T	T
0.3314330585888302	0.9952407241670741	0.5722540259976293	T	T	T
0.5574016318487929	0.1158976933110712	0.4277551917943617	T	T	T
0.5571260909107112	0.1140904391628735	0.5368876636577484	T	T	T
0.4444400072531138	0.2222200036731223	0.4999999999957154	F	F	F
0.6661721167190759	0.9978319750762443	0.4629888109878079	T	T	T
0.6677854320419760	0.0006010653879426	0.5727148115485521	T	T	T
0.8891648045397105	0.1101797513493402	0.4270869019818408	T	T	T
0.8890628605695717	0.1111246918233192	0.5362916101276517	T	T	T
0.7777799964982535	0.2222200036731223	0.4999999999957154	F	F	F
0.0019281873171857	0.3335898769376678	0.4630000893537708	T	T	T
0.9998836649621191	0.3325924420232680	0.5727325950556281	T	T	T
0.2173698845884068	0.4337472202901586	0.4255233296405879	T	T	T
0.2233145317482749	0.4432165814869460	0.5368457026424680	T	T	T
0.1111100018021958	0.5555599928495241	0.4999999999957154	F	F	F
0.3320041017748468	0.3342173992346703	0.4631605356833336	T	T	T
0.3231788701492819	0.3291077402190617	0.5745647606421749	T	T	T
0.5576577087611867	0.4420246650051677	0.4277161070900234	T	T	T
0.5555716261148682	0.4445903005445224	0.5374535355828999	T	T	T
0.4444400072187520	0.5555599928495241	0.4999999999957154	F	F	F
0.6666909667232528	0.3331245615268482	0.4640909395790196	T	T	T
0.6721831413785301	0.3282519658774052	0.5746061779292980	T	T	T
0.8836369966837636	0.4421883492548193	0.4277653037800438	T	T	T
0.8861609082326233	0.4430778898257134	0.5368806969168086	T	T	T
0.7777799964638845	0.5555599928495241	0.4999999999957154	F	F	F
0.0026551415655421	0.6681009728513427	0.4631114716906743	T	T	T
0.0052701774157045	0.6689684604979973	0.5722432282949116	T	T	T
0.2166268619073562	0.7828686160675205	0.4253996685520314	T	T	T
0.2221923817965343	0.7780151162947510	0.5359066743111397	T	T	T
0.1111100017117366	0.8888900279499197	0.4999999999957154	F	F	F
0.3332657167209971	0.6665850622894083	0.4625560405769972	T	T	T
0.3312603531231003	0.6690551698174373	0.5722716332228504	T	T	T
0.5655203418048446	0.7820473729957631	0.4254509755985603	T	T	T
0.5569570750929722	0.7768893796644981	0.5368382327438089	T	T	T
0.4444400071282928	0.8888900279499197	0.4999999999957154	F	F	F
0.6655961725194763	0.6678322781675795	0.4631508695463348	T	T	T
0.6714495289097984	0.6774708490434722	0.5745015717688547	T	T	T
0.8889369479489869	0.7785595034641334	0.4272446639864581	T	T	T
0.8870168414572335	0.7774006528389770	0.53700466761563648	T	T	T
0.7777799963734253	0.8888900279499197	0.4999999999957154	F	F	F
0.5568442506902546	0.4454312798038538	0.5976818901988737	T	T	T
0.3319801058306085	0.6656529524336098	0.4023124882291864	T	T	T
0.5591194835680424	0.4476174879541717	0.6143792649688568	T	T	T
0.3297747676132984	0.6634215535546101	0.3856452025198877	T	T	T

*CH₃ E₀ = -178.547 eV

cu111-CH3

1.0000000000000000	0.0000000000000000	0.0000000000000000
7.6679000854000003	0.0000000000000000	0.0000000000000000
-3.8339500427000002	6.6405962677000003	0.0000000000000000
0.0000000000000000	0.0000000000000000	58.3478012085000017

Cu C H
45 2 6

Selective Dynamics

Direct

0.0002401642763108	0.9995632847567902	0.4633756458818502	T	T	T
0.0005562666716910	0.9996592249533064	0.5729284947090072	T	T	T
0.2220369001970250	0.1124311718291274	0.4271080007068085	T	T	T
0.2234483004958494	0.1119499109098188	0.5365825670365211	T	T	T
0.1111100018365576	0.2222200036731223	0.4999999999957154	F	F	F
0.3322558974402965	0.9975961197282004	0.4629956655886546	T	T	T
0.3313574474295094	0.9978554842945061	0.5730428694954705	T	T	T
0.5575905429869875	0.1131474315574283	0.4269695008818055	T	T	T
0.5564812658965286	0.1136705784469278	0.5370008600741689	T	T	T
0.4444400072531138	0.2222200036731223	0.4999999999957154	F	F	F
0.6653691735089209	0.9991699806216612	0.4634327400608332	T	T	T
0.6669151527890783	0.9986229119249582	0.5728836461878262	T	T	T
0.8884056925405273	0.1113932923979684	0.4270776562594252	T	T	T
0.8885742648506152	0.1116115175857829	0.5366276633148671	T	T	T
0.7777799964982535	0.2222200036731223	0.4999999999957154	F	F	F
0.0007100434117180	0.3344996342485752	0.4634385211799151	T	T	T
0.0019800662629127	0.3333819181143122	0.5729015207802947	T	T	T
0.2217564615063059	0.4421096383040344	0.4270653319204194	T	T	T
0.2223173036159775	0.4445955335076251	0.5366725728835429	T	T	T
0.1111100018021958	0.5555599928495241	0.4999999999957154	F	F	F
0.3332875433058474	0.3332549876456853	0.4633304883509338	T	T	T
0.3316903947560936	0.3331607682747919	0.5729160737384956	T	T	T
0.5558121943447514	0.4439698795640477	0.4268466505921197	T	T	T
0.5567427356940058	0.4435836916875344	0.5370620454581801	T	T	T
0.4444400072187520	0.5555599928495241	0.4999999999957154	F	F	F
0.6667732399449439	0.3330800599904511	0.4633166858204816	T	T	T
0.6665958509644423	0.3331501083336422	0.5764166833146134	T	T	T
0.8869527325253234	0.4425220119183304	0.4270247267519456	T	T	T
0.8863738074571170	0.4434596314406006	0.5370036882199631	T	T	T
0.7777799964638845	0.5555599928495241	0.4999999999957154	F	F	F
0.0023771338071478	0.6678080433731127	0.4629926786262940	T	T	T
0.0020300983817657	0.6685285017050135	0.5729878607959699	T	T	T
0.2223244337569266	0.7779323931116096	0.4235842437208709	T	T	T
0.2220972302758273	0.7780601381932718	0.5366874715544131	T	T	T
0.1111100017117366	0.8888900279499197	0.4999999999957154	F	F	F
0.3319936959063834	0.6677351780065169	0.4629217959706745	T	T	T
0.3331443044945417	0.6670600705027544	0.5731603469031648	T	T	T
0.5573066791967080	0.7778891409810680	0.4270831199906617	T	T	T
0.5555651734075773	0.7779187260817141	0.5366686436452348	T	T	T
0.4444400071282928	0.8888900279499197	0.4999999999957154	F	F	F
0.6665168235759158	0.6665583049684899	0.4633260095798993	T	T	T
0.6672504048903789	0.6689555942861368	0.5729367141062218	T	T	T
0.8869797249722305	0.7776667051852608	0.4270898127228233	T	T	T
0.8881883684884735	0.7766965265456740	0.5365768113508637	T	T	T
0.7777799963734253	0.8888900279499197	0.4999999999957154	F	F	F
0.6620249163930856	0.3318329076965418	0.6109380342755060	T	T	T
0.2268838307672672	0.7792338829692775	0.3890601989849686	T	T	T
0.5382430526532189	0.3532150537386275	0.6169599983373368	T	T	T
0.8063123917438992	0.4551833835354328	0.6171905059846726	T	T	T
0.6399921178815307	0.1870598083780599	0.6171761850399439	T	T	T
0.3506625363915757	0.7578236142484929	0.3830320982637949	T	T	T
0.0825603710223151	0.6558567131437238	0.3828038318431699	T	T	T
0.2489225354270550	0.9240214608472493	0.3828162761670558	T	T	T

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