

Supplementary Materials

First Principles Prediction of CH₄ Reactivities with Co₃O₄ Nanocatalysts of Different Morphologies

Shibin Wang,^{a,b,c} Chengcheng Zhao,^{a,b,c} Shenggang Li,^{a,c,*} and Yuhan Sun,^{a,c}

^a *CAS Key Laboratory of Low-Carbon Conversion Science and Engineering, Shanghai Advanced Research Institute, Chinese Academy of Sciences, 100 Haike Road, Shanghai 201210, China*

^b *University of Chinese Academy of Sciences, 19 Yuquan Road, Shijingshan District, Beijing 100049, China*

^c *School of Physical Science and Technology, ShanghaiTech University, 100 Haike Road, Shanghai 201210, China*

*E-mail: lisg@sari.ac.cn

This supplementary information is briefly summarized below.

Table S1. Fractional Coordinates of the Slab Models Shown in Figure 1.

Table S2. Fractional Coordinates of the Stationary States Shown in Figure 2.

Table S3. Fractional Coordinates of the Stationary States Shown in Figure 3.

Table S4. Fractional Coordinates of the Stationary States Shown in Figure 4.

Table S5. Energy Barriers for CH₄ Activation at the Different Co-O Pair Sites and the Calculated Bader Charges at the Co and O Sites on the Clean Surface, and That on the H Atom in the Transition State.

Table S6. The Ratio of CH₄ Reaction Rates (r) and Rate Constants (k) at the Reaction Temperature of 300, 400, and 500 °C for the Nanoparticle, Nanorod, and Nanoplate Catalysts.

Table S1. Fractional Coordinates of the Slab Models Shown in Figure 1.

(001) -A: Co₈O₁₂

Co	O				
1.0000000000000000					
5.7629999999999999	0.0000000000000000	0.0000000000000000			
0.0000000000000000	5.7629999999999999	0.0000000000000000			
0.0000000000000000	0.0000000000000000	21.1119999999999983			
Co	O				
8	12				
Selective dynamics					
Direct					
0.7386777719937498	0.9611313551969474	0.4517336112163690	F	F	F
0.2387512587644072	0.9611028800142899	0.5533986326923241	T	T	T
0.4888079125455462	0.4612181155648116	0.5000000000000000	F	F	F
0.9887211521776820	0.4612181155648116	0.5000000000000000	F	F	F
0.2387645323616141	0.2111747353808795	0.4035145888594158	F	F	F
0.7387661179762023	0.7127795206839083	0.5978931122074835	T	T	T
0.7387647123817516	0.2099212765663742	0.5979309259584131	T	T	T
0.2387645323616141	0.7110879750130152	0.4035145888594158	F	F	F
0.0163109491584237	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.6834981780322735	0.4946949602122004	F	F	F
0.4612181155648116	0.9611313551969474	0.3981621826449384	F	F	F
0.9529766641883576	0.4614352793172720	0.5938556535284600	T	T	T
0.5244841241449878	0.4614343709192658	0.5938612739654984	T	T	T
0.7386777719937498	0.2387645323616141	0.5053050397877996	F	F	F
0.0163109491584237	0.9611313551969474	0.3981621826449384	F	F	F
0.7386777719937498	0.6834981780322735	0.5053050397877996	F	F	F
0.5241400059999719	0.9613624801758093	0.6022854581733841	T	T	T
0.9533090019633931	0.9613633268948579	0.6022721724064564	T	T	T
0.4612181155648116	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.2387645323616141	0.4946949602122004	F	F	F

(001) -A: Co₁₄O₂₀

Co	O				
14	20				
Selective dynamics					
Direct					
0.7690439007461407	0.3716814159292028	0.4351128658484242	F	F	F
0.2709207881581619	0.8703626201102430	0.6152343662875113	T	T	T
0.2757077905034827	0.3707860756434962	0.5210243013989263	T	T	T
0.7690439007461407	0.8684712823182394	0.3482104540382807	F	F	F
0.5207357279194866	0.8684712823182394	0.4785426143678677	F	F	F
0.7716427291607356	0.1201001027061987	0.5648787015020688	T	T	T
0.2722540343571040	0.1233732431025487	0.3916402025577170	F	F	F
0.7716811092216826	0.6210909568194775	0.5650193599616368	T	T	T
0.0239458615304500	0.3716814159292028	0.3047807055188372	F	F	F
0.0219392257468724	0.3704068098687646	0.6490147368261761	T	T	T

0.0239458615304500	0.8684712823182394	0.4785426143678677	F	F	F
0.2722540343571040	0.6201631094915854	0.3916402025577170	F	F	F
0.5207357279194866	0.3716814159292028	0.3047807055188372	F	F	F
0.5168034762322196	0.3704066805248251	0.6508087414526963	T	T	T
0.4957487419746656	0.8684712823182394	0.3960175092266738	F	F	F
0.2722540343571040	0.0982127364219991	0.4741653076989110	F	F	F
0.7690439007461407	0.1483602290473698	0.3004033988498875	F	F	F
0.7733881448179949	0.1589466738720265	0.6474892164873576	T	T	T
0.5540158135280410	0.3707507813157523	0.5653121247847674	T	T	T
0.7690439007461407	0.5950026028110358	0.3004033988498875	F	F	F
0.7734986301596112	0.5819544609159375	0.6475392175678881	T	T	T
0.0489328474752710	0.8684712823182394	0.3960175092266738	F	F	F
0.5466225905045652	0.8703223033328588	0.5620337741292752	T	T	T
0.7690439007461407	0.0982127364219991	0.4829199210368174	F	F	F
0.2722540343571040	0.1483602290473698	0.3091580121877939	F	F	F
0.2635478623279594	0.1593177753186909	0.6573690831641222	T	T	T
0.7690439007461407	0.6451500954364064	0.4829199210368174	F	F	F
0.4957487419746656	0.3716814159292028	0.3872628958887674	F	F	F
0.2722540343571040	0.5950026028110358	0.3091580121877939	F	F	F
0.2638120898572622	0.5815243781225853	0.6574154636066023	T	T	T
0.9962887989208579	0.8703134608759867	0.5614746017681512	T	T	T
0.0489328474752710	0.3716814159292028	0.3872628958887674	F	F	F
0.9896358631450755	0.3707105167994015	0.5641334539059160	T	T	T
0.2722540343571040	0.6451500954364064	0.4741653076989110	F	F	F

(001) -B: Co₁₀O₁₂

Co O

1.0000000000000000		
5.7629999999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.7629999999999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.1119999999999983

Co O

10 12

Selective dynamics

Direct

0.7386777719937498	0.9611313551969474	0.4517336112163690	F	F	F
0.2389032671178627	0.2784819551103609	0.6183098813818612	T	T	T
0.7386777719937498	0.4612181155648116	0.3552482000757848	F	F	F
0.2378472789300888	0.9459719064685247	0.5478151585052297	T	T	T
0.4888079125455462	0.4612181155648116	0.5000000000000000	F	F	F
0.9887211521776820	0.4612181155648116	0.5000000000000000	F	F	F
0.2387645323616141	0.2111747353808795	0.4035145888594158	F	F	F
0.7371770467885299	0.7490091468753018	0.6001471257314702	T	T	T
0.7384811537640437	0.2254004224922480	0.5947300731150671	T	T	T
0.2387645323616141	0.7110879750130152	0.4035145888594158	F	F	F
0.0163109491584237	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.6834981780322735	0.4946949602122004	F	F	F
0.4612181155648116	0.9611313551969474	0.3981621826449384	F	F	F
0.9698754378253938	0.4626940156654471	0.5928738790814643	T	T	T
0.5072040954948602	0.4647126334739135	0.5929618084059023	T	T	T
0.7386777719937498	0.2387645323616141	0.5053050397877996	F	F	F
0.0163109491584237	0.9611313551969474	0.3981621826449384	F	F	F
0.7386777719937498	0.6834981780322735	0.5053050397877996	F	F	F
0.4955334268798281	0.0099837630919993	0.6098319928695080	T	T	T

0.9796290914935383	0.0066830243941378	0.6095375374324319	T	T	T
0.4612181155648116	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.2387645323616141	0.4946949602122004	F	F	F

(011)-A: Co₁₄O₂₀

Co O

1.0000000000000000

8.1500000000000004	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.7629999999999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.0139999999999993

Co O

14 20

Selective dynamics

Direct

0.6741170659422053	0.2499126790080339	0.4081088797944261	F	F	F
0.1865717639648270	0.7499225214837195	0.5494283150764955	T	T	T
0.9240553223018040	0.7499126790080339	0.4081088797944261	F	F	F
0.4116006242791824	0.2499225214837196	0.5494283150764955	T	T	T
0.2990861941220047	0.0000000000000000	0.4081088797944261	F	F	F
0.5482545341111966	0.7498936068676444	0.6102174806091387	T	T	T
0.0491479377624131	0.2499126790080339	0.3399638336347195	F	F	F
0.0499178541328198	0.2498936068676445	0.6102174806091387	T	T	T
0.5490244504816033	0.7499126790080339	0.4762063386313855	F	F	F
0.7990741706202363	-0.0001303356517913	0.5450450873530291	T	T	T
0.5490244504816033	0.7499126790080339	0.3399638336347195	F	F	F
0.2990861941220047	0.5000000000000000	0.4081088797944261	F	F	F
0.7990982176237730	0.4998696643482087	0.5450450873530291	T	T	T
0.0491479377624131	0.2499126790080339	0.4762063386313855	F	F	F
0.5612889433313465	0.9850811727538453	0.5415502312829223	T	T	T
0.0617436404050409	0.4748515543136591	0.4081088797944261	F	F	F
0.2602889851508301	0.2498895824942118	0.6201813909230588	T	T	T
0.7864904914793769	0.7499126790080339	0.3331112591605603	F	F	F
0.0617436404050409	0.0251484456863409	0.4081088797944261	F	F	F
0.5613019269846691	0.5147411968204103	0.5415499487249696	T	T	T
0.7769856330115561	0.7498511570508772	0.6059729099808616	T	T	T
0.2864904914793769	0.2499126790080339	0.3468164081088787	F	F	F
0.2864904914793769	0.2499126790080339	0.4693537641572263	F	F	F
0.3116818967646324	0.7499126790080339	0.4693537641572263	F	F	F
0.8116818967646324	0.2499126790080339	0.4830589131055518	F	F	F
0.3116818967646324	0.7499126790080339	0.3468164081088787	F	F	F
0.8211867552324532	0.2498511570508772	0.6059729099808616	T	T	T
0.8116818967646324	0.2499126790080339	0.3331112591605603	F	F	F
0.3378834030931792	0.7498895824942118	0.6201813909230588	T	T	T
0.5364287478389755	0.9748515543136591	0.4081088797944261	F	F	F
0.0368704612593475	0.0147411968204104	0.5415499487249696	T	T	T
0.5364287478389755	0.5251484456863409	0.4081088797944261	F	F	F
0.0368834449126696	0.4850811727538452	0.5415502312829223	T	T	T
0.7864904914793769	0.7499126790080339	0.4830589131055518	F	F	F

(011)-B: Co₁₆O₂₀

Co O

1.0000000000000000

8.1500000000000004	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.7599999999999998	0.0000000000000000

```

0.0000000000000000 0.0000000000000000 20.7259999999999991
Co O
16 20
Selective dynamics
Direct
0.9560385280316126 0.0064617534055174 0.5008684743800060 F F F
0.4321066577212632 0.5110586368752209 0.6307813832448413 T T T
0.4528278587305508 0.5031435557107926 0.3618643250024149 F F F
0.2012842677204247 0.5031435557107926 0.5008684743800060 F F F
0.7044949370214866 0.0064617534055174 0.3618643250024149 F F F
0.7302279724777120 0.0008617735979631 0.6289670518578612 T T T
0.5786613978760187 0.7548026545581550 0.5008684743800060 F F F
0.8302049888861447 0.5031435557107926 0.4313905239795446 F F F
0.3298732278416596 0.0037868537147244 0.5727129723961729 T T T
0.3271178068658926 0.0064617534055174 0.4313905239795446 F F F
0.8265904724311981 0.5047150730883313 0.5723701414355106 T T T
0.0789297519841002 0.7561156362951473 0.6373651500118446 T T T
0.0754507285749568 0.7548026545581550 0.3618643250024149 F F F
0.0781618163071571 0.2566671059210536 0.6321288406700371 T T T
0.0754507285749568 0.2516590988473624 0.3618643250024149 F F F
0.5786613978760187 0.2516590988473624 0.5008684743800060 F F F
0.3409483823166184 0.2238910234020253 0.5008684743800060 F F F
0.5648308224252929 0.0000000000000000 0.4390620476695943 F F F
0.5655264067201452 0.0025589351642667 0.5632719021860981 T T T
0.0616201531242311 0.5031435557107926 0.4237190002894948 F F F
0.8530554990644669 0.2703212189281295 0.6391844828795626 T T T
0.8441590516176802 0.2794271742926995 0.3618643250024149 F F F
0.8441590516176802 0.7270345791128179 0.3618643250024149 F F F
0.8163744134354189 0.2794271742926995 0.5008684743800060 F F F
0.5913295136497186 0.5014703690330562 0.5630549680616731 T T T
0.0894047913064924 0.0064617534055174 0.4237190002894948 F F F
0.3131637441343571 0.2238910234020253 0.3618643250024149 F F F
0.3061627408748127 0.2423444729219756 0.6373224793422521 T T T
0.0966112814322499 0.0048198320917170 0.5751644494306877 T T T
0.5924919733267444 0.5031435557107926 0.4390620476695943 F F F
0.3131637441343571 0.7825707300034921 0.3618643250024149 F F F
0.3134665163821861 0.7807312687898876 0.6431445321619305 T T T
0.8163744134354189 0.7270345791128179 0.5008684743800060 F F F
0.8414756185882223 0.7269451703845045 0.6427619405900585 T T T
0.0595200691131340 0.5064382163734187 0.5749653061063127 T T T
0.3409483823166184 0.7825707300034921 0.5008684743800060 F F F

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(112): Co₁₈O₂₆

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Co3O4
1.0000000000000000
5.7629999999999999 0.0000000000000000 0.0000000000000000
0.0000000000000000 14.1150000000000002 0.0000000000000000
0.0000000000000000 0.0000000000000000 19.1189999999999998
Co O
18 26
Selective dynamics
Direct
0.3678639597431896 0.4704923839886632 0.4918667294314574 F F F
0.8677771993753254 0.8038257173219989 0.4048328887494108 F F F

```

0.8696688609202216	0.1335459713267411	0.5739040351176964	T	T	T
0.8663551801223395	0.3700345809189777	0.5865172515425870	T	T	T
0.3678639597431896	0.7205100956429362	0.4918667294314574	F	F	F
0.8677771993753254	0.0538434289762648	0.4048328887494108	F	F	F
0.3678639597431896	0.0955012398157962	0.4918667294314574	F	F	F
0.8677771993753254	0.5955366631243351	0.4918667294314574	F	F	F
0.5705776323800428	0.5718310481803078	0.5996550840897259	T	T	T
0.3678639597431896	0.9288699964576708	0.4048328887494108	F	F	F
0.1178205795592575	0.2622033297909994	0.4483498090904305	F	F	F
0.8677771993753254	0.4288345731491319	0.4048328887494108	F	F	F
0.1660476998983755	0.5718731545051275	0.5992247105286382	T	T	T
0.3657367838967263	0.2610762244343018	0.5821719347640287	T	T	T
0.8671319114705026	0.7727906863528843	0.5792843587462241	T	T	T
0.1187336923837402	0.9299690992128288	0.5396213984178152	T	T	T
0.6179073399271218	0.2622033297909994	0.4483498090904305	F	F	F
0.6158689097588622	0.9295022605970412	0.5371176459884149	T	T	T
0.3678639597431896	0.8592986184909677	0.4918667294314574	F	F	F
0.8677771993753254	0.3409139213602543	0.4822427951252664	F	F	F
0.0902307825785158	0.3409139213602543	0.3661279355614866	F	F	F
0.1185604676022481	0.3187079599519256	0.6229372344126606	T	T	T
0.6077732775028456	0.3200300104005762	0.6224534784721568	T	T	T
0.3686582470290121	0.0062912449078894	0.5691790066453258	T	T	T
0.6478775382646199	0.6758361310292523	0.5422303807818232	T	T	T
0.8677771993753254	0.1926319518243034	0.4048328887494108	F	F	F
0.6454971369078635	0.3409139213602543	0.3661279355614866	F	F	F
0.3678639597431896	0.6742472546935900	0.3952089544432269	F	F	F
0.8683027106700895	0.5151991303233098	0.5819613619339716	T	T	T
0.5903175429463801	0.0075805880269186	0.4531617762435260	F	F	F
0.8677771993753254	0.8500885582713451	0.5014383597468495	F	F	F
0.3678639597431896	0.3317038611406318	0.4918667294314574	F	F	F
0.8677771993753254	0.6650371944739604	0.4048328887494108	F	F	F
0.1079918847042264	0.8434960972068234	0.6065329923373739	T	T	T
0.5891173700058960	0.1800981479047495	0.5315234945546987	T	T	T
0.6454971369078635	0.5167552249380094	0.4435378419373421	F	F	F
0.8737886037613994	0.0022156453843862	0.5714451335879016	T	T	T
0.3678639597431896	0.1834218916046737	0.4144568230556018	F	F	F
0.3674900370126868	0.5111897694434230	0.6497753224635102	T	T	T
0.6466278210241327	0.8442905272736091	0.6097032535925850	T	T	T
0.1494627529296987	0.1797973703031048	0.5327516969756352	T	T	T
0.0902307825785158	0.5167552249380094	0.4435378419373421	F	F	F
0.1454103765399992	0.0075805880269186	0.4531617762435260	F	F	F
0.0882699739534506	0.6756242725033872	0.5419572256658182	T	T	T

Table S2. Fractional Coordinates of the Stationary States Shown in Figure 2.

(001)-A: Co₈O₁₂

α pair site:

Physisorption

Co	O	C	H			
1.0000000000000000						
5.7629999999999999	0.0000000000000000					0.0000000000000000
0.0000000000000000	5.7629999999999999					0.0000000000000000
0.0000000000000000	0.0000000000000000					21.1119999999999983

Co	O	C	H	
8	12	1	4	

Selective dynamics

Direct

0.7386777719937498	0.9611313551969474	0.4517336112163690	F	F	F
0.2382135645648931	0.9595414398724981	0.5556494807214282	T	T	T
0.4888079125455462	0.4612181155648116	0.5000000000000000	F	F	F
0.9887211521776820	0.4612181155648116	0.5000000000000000	F	F	F
0.2387645323616141	0.2111747353808795	0.4035145888594158	F	F	F
0.7394435996679971	0.7081477566003719	0.5921487234316799	T	T	T
0.7392207992812745	0.2142620645639070	0.5919734816708396	T	T	T
0.2387645323616141	0.7110879750130152	0.4035145888594158	F	F	F
0.0163109491584237	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.6834981780322735	0.4946949602122004	F	F	F
0.4612181155648116	0.9611313551969474	0.3981621826449384	F	F	F
0.9516133038242118	0.4615456430584583	0.5912107662214532	T	T	T
0.5267771276168507	0.4617829856026656	0.5912332038373297	T	T	T
0.7386777719937498	0.2387645323616141	0.5053050397877996	F	F	F
0.0163109491584237	0.9611313551969474	0.3981621826449384	F	F	F
0.7386777719937498	0.6834981780322735	0.5053050397877996	F	F	F
0.5201034007274800	0.9622438159972584	0.5941637483741425	T	T	T
0.9585837930915443	0.9616813510007025	0.5957892637426145	T	T	T
0.4612181155648116	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.2387645323616141	0.4946949602122004	F	F	F
0.6490350157183473	0.8862552183633404	0.7481668804276148	T	T	T
0.5423398569898450	0.9983580929921694	0.7179735092379473	T	T	T
0.6217567526632242	0.9320905172336740	0.7979623638255616	T	T	T
0.5968825989961044	0.7052155407723837	0.7406293042014912	T	T	T
0.8331935719113177	0.9078629244215874	0.7362629400009121	T	T	T

Transition state

Co	O	C	H			
1.0000000000000000						
5.7629999999999999	0.0000000000000000					0.0000000000000000
0.0000000000000000	5.7629999999999999					0.0000000000000000
0.0000000000000000	0.0000000000000000					21.1119999999999983

Co	O	C	H	
8	12	1	4	

Selective dynamics

Direct

0.7386777719937498	0.9611313551969474	0.4517336112163690	F	F	F
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0.2160285514687079	0.9644103450546544	0.5508136203969891	T	T	T
0.4888079125455462	0.4612181155648116	0.5000000000000000	F	F	F
0.9887211521776820	0.4612181155648116	0.5000000000000000	F	F	F
0.2387645323616141	0.2111747353808795	0.4035145888594158	F	F	F
0.7500462450039208	0.7084365134767674	0.5993473891370504	T	T	T
0.7365282376033635	0.2197752821944179	0.5989678768305547	T	T	T
0.2387645323616141	0.7110879750130152	0.4035145888594158	F	F	F
0.0163109491584237	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.6834981780322735	0.4946949602122004	F	F	F
0.4612181155648116	0.9611313551969474	0.3981621826449384	F	F	F
0.9678475887690047	0.4489825559509012	0.5912681266012458	T	T	T
0.5282735693348655	0.4662116630343810	0.5975702966407719	T	T	T
0.7386777719937498	0.2387645323616141	0.5053050397877996	F	F	F
0.0163109491584237	0.9611313551969474	0.3981621826449384	F	F	F
0.7386777719937498	0.6834981780322735	0.5053050397877996	F	F	F
0.4916794109563543	0.9757419757704862	0.6103942019360691	T	T	T
0.9426968977047718	0.9659339350836703	0.6059844484120792	T	T	T
0.4612181155648116	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.2387645323616141	0.4946949602122004	F	F	F
0.6497954018300991	0.7761687316686197	0.7431104726135938	T	T	T
0.4457899036434362	-0.0404652078268916	0.6548626135489297	T	T	T
0.4700253593548873	0.8200000694582915	0.7533232424679894	T	T	T
0.7000262713994945	0.5962415333829343	0.7422580430521271	T	T	T
0.7810701814649825	0.9106046467193892	0.7449702439951433	T	T	T

Chemisorption

Co3O4

1.0000000000000000		
5.7629999999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.7629999999999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.1119999999999983

Co O C H
8 12 1 4

Selective dynamics

Direct

0.7386777719937498	0.9611313551969474	0.4517336112163690	F	F	F
0.2202704879708889	0.9570445021940330	0.5481671222090744	T	T	T
0.4888079125455462	0.4612181155648116	0.5000000000000000	F	F	F
0.9887211521776820	0.4612181155648116	0.5000000000000000	F	F	F
0.2387645323616141	0.2111747353808795	0.4035145888594158	F	F	F
0.7467545542639631	0.7033089365935510	0.6024443403725570	T	T	T
0.7407667039129721	0.2142887758102454	0.5976419168023328	T	T	T
0.2387645323616141	0.7110879750130152	0.4035145888594158	F	F	F
0.0163109491584237	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.6834981780322735	0.4946949602122004	F	F	F
0.4612181155648116	0.9611313551969474	0.3981621826449384	F	F	F
0.9607458478993156	0.4611687782978280	0.5910182540875364	T	T	T
0.5315399268063916	0.4599822588607584	0.5954500569460109	T	T	T
0.7386777719937498	0.2387645323616141	0.5053050397877996	F	F	F
0.0163109491584237	0.9611313551969474	0.3981621826449384	F	F	F
0.7386777719937498	0.6834981780322735	0.5053050397877996	F	F	F
0.5036146021856425	0.9593173483752450	0.6080462459228900	T	T	T
0.9472266879266725	0.9613324814760650	0.6021278747303694	T	T	T
0.4612181155648116	0.4612181155648116	0.4088196286472154	F	F	F

0.2387645323616141	0.2387645323616141	0.4946949602122004	F	F	F
0.7439665616289536	0.6817042583250901	0.6954704298045342	T	T	T
0.4387686358657358	0.9600660963330313	0.6507481261686553	T	T	T
0.5653116968302827	0.6400516845713551	0.7093221120840593	T	T	T
0.8650128609260775	0.5419043337709638	0.7077218808194856	T	T	T
0.8039991830034939	0.8488811282680443	0.7138922850634309	T	T	T

(001)-A: Co₈O₁₂

β pair site:

Physisorption

Co	O	C	H			
1.0000000000000000						
5.7629999999999999	0.0000000000000000					0.0000000000000000
0.0000000000000000	5.7629999999999999					0.0000000000000000
0.0000000000000000	0.0000000000000000					21.1119999999999983

Co	O	C	H	
8	12	1	4	

Selective dynamics

Direct

0.7386777719937498	0.9611313551969474	0.4517336112163690	F	F	F
0.2384689853617093	0.9618182848490062	0.5558864707649701	T	T	T
0.4888079125455462	0.4612181155648116	0.5000000000000000	F	F	F
0.9887211521776820	0.4612181155648116	0.5000000000000000	F	F	F
0.2387645323616141	0.2111747353808795	0.4035145888594158	F	F	F
0.7384432507500553	0.7076076265341543	0.5920813496602821	T	T	T
0.7388344888767230	0.2133615411386151	0.5918408536554884	T	T	T
0.2387645323616141	0.7110879750130152	0.4035145888594158	F	F	F
0.0163109491584237	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.6834981780322735	0.4946949602122004	F	F	F
0.4612181155648116	0.9611313551969474	0.3981621826449384	F	F	F
0.9506676086396277	0.4600838525706701	0.5911404975865027	T	T	T
0.5261540145544616	0.4595799438491347	0.5905780946823794	T	T	T
0.7386777719937498	0.2387645323616141	0.5053050397877996	F	F	F
0.0163109491584237	0.9611313551969474	0.3981621826449384	F	F	F
0.7386777719937498	0.6834981780322735	0.5053050397877996	F	F	F
0.5200552971500287	0.9607508374007294	0.5952769791693819	T	T	T
0.9571078337525309	0.9600727791691163	0.5955396089529109	T	T	T
0.4612181155648116	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.2387645323616141	0.4946949602122004	F	F	F
0.5413755472908719	0.6248212113554898	0.7437394478943737	T	T	T
0.4681341572661203	0.5239588331651800	0.7044640437057855	T	T	T
0.5024865447829853	0.8090746285545193	0.7362934617024189	T	T	T
0.4632805717198868	0.5672928388195294	0.7883765038839067	T	T	T
0.7299519894218920	0.5995093319104225	0.7462118113122840	T	T	T

Transition state

Co	O	C	H			
1.0000000000000000						
5.7629999999999999	0.0000000000000000					0.0000000000000000
0.0000000000000000	5.7629999999999999					0.0000000000000000
0.0000000000000000	0.0000000000000000					21.1119999999999983

Co	O	C	H	
8	12	1	4	

Selective dynamics

Direct

0.7386777719937500	0.9611313551969470	0.4517336112163690	F	F	F
0.2434378227208570	0.9581144442739600	0.5523604786820679	T	T	T
0.4888079125455460	0.4612181155648120	0.5000000000000000	F	F	F
0.9887211521776820	0.4612181155648120	0.5000000000000000	F	F	F
0.2387645323616140	0.2111747353808790	0.4035145888594160	F	F	F

0.7450520705608810	0.7121052120671510	0.6010826931757191	T	T	T
0.7469634753034100	0.2029325316965610	0.5973727357605370	T	T	T
0.2387645323616140	0.7110879750130150	0.4035145888594160	F	F	F
0.0163109491584237	0.4612181155648120	0.4088196286472150	F	F	F
0.2387645323616140	0.6834981780322740	0.4946949602122000	F	F	F
0.4612181155648120	0.9611313551969470	0.3981621826449380	F	F	F
0.9579672662244580	0.4595053467115660	0.5941277209597760	T	T	T
0.5212468128713250	0.4583003206708510	0.5938101219558120	T	T	T
0.7386777719937500	0.2387645323616140	0.5053050397877999	F	F	F
0.0163109491584237	0.9611313551969470	0.3981621826449380	F	F	F
0.7386777719937500	0.6834981780322740	0.5053050397877999	F	F	F
0.5334153411128710	0.9581154749791740	0.6024356640878350	T	T	T
0.9617285665195890	0.9602729721869570	0.6032332155599390	T	T	T
0.4612181155648120	0.4612181155648120	0.4088196286472150	F	F	F
0.2387645323616140	0.2387645323616140	0.4946949602122000	F	F	F
0.6691752164052360	0.6703640334890080	0.7172489269286469	T	T	T
0.4039216369204370	0.4841827829852430	0.6535941348845780	T	T	T
0.5489557664479821	0.7741599758350260	0.7230457611101641	T	T	T
0.6678405058554520	0.5411950096548070	0.7432798169425890	T	T	T
0.8240332220953090	0.7337494174173070	0.7261132072626850	T	T	T

Chemisorption

Co3O4

1.0000000000000000		
5.7629999999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.7629999999999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.1119999999999983

Co	O	C	H
8	12	1	4

Selective dynamics

Direct

0.7386777719937498	0.9611313551969474	0.4517336112163690	F	F	F
0.2473364979767866	0.9559895402982628	0.5518580656390135	T	T	T
0.4888079125455462	0.4612181155648116	0.5000000000000000	F	F	F
0.9887211521776820	0.4612181155648116	0.5000000000000000	F	F	F
0.2387645323616141	0.2111747353808795	0.4035145888594158	F	F	F
0.7498933130088244	0.7117937291729031	0.6031238749321511	T	T	T
0.7527834283673639	0.1985562040666633	0.5971310062475601	T	T	T
0.2387645323616141	0.7110879750130152	0.4035145888594158	F	F	F
0.0163109491584237	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.6834981780322735	0.4946949602122004	F	F	F
0.4612181155648116	0.9611313551969474	0.3981621826449384	F	F	F
0.9621452623543465	0.4584599289604216	0.5942467904289901	T	T	T
0.5200207486221901	0.4567922265370946	0.5941820168414556	T	T	T
0.7386777719937498	0.2387645323616141	0.5053050397877996	F	F	F
0.0163109491584237	0.9611313551969474	0.3981621826449384	F	F	F
0.7386777719937498	0.6834981780322735	0.5053050397877996	F	F	F
0.5399307778565895	0.9556901836921249	0.6027668330466681	T	T	T
0.9675895621322205	0.9595778252863170	0.6037636763475729	T	T	T
0.4612181155648116	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.2387645323616141	0.4946949602122004	F	F	F
0.7556640587193353	0.6999572276654378	0.6964942118726918	T	T	T
0.3685097519345352	0.4573854470512091	0.6155461556084380	T	T	T
0.5805923169225113	0.7501223458350902	0.7110955474359100	T	T	T

0.7994671830568332	0.5212285015438718	0.7091813330950829	T	T	T
0.8880427048492954	0.8240031777569146	0.7114879513771221	T	T	T

**(001)-A: Co₁₄O₂₀
 α pair site:**

Physisorption

Co14O20

1.0000000000000000		
5.7629999999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.7629999999999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5470000000000006

Co	O	C	H	
14	20	1	4	

Selective dynamics

Direct

0.7690439007461407	0.3716814159292028	0.3819263946962010	F	F	F
0.2696336588321049	0.8725798733090141	0.5384295770369824	T	T	T
0.2705164703276571	0.3707755769470761	0.4577544513957162	T	T	T
0.7690439007461407	0.8684712823182394	0.3056465890684450	F	F	F
0.5207357279194866	0.8684712823182394	0.4200474629901692	F	F	F
0.7699333089524187	0.1225097050504309	0.4960989491674265	T	T	T
0.2722540343571040	0.1233732431025487	0.3437676573624131	F	F	F
0.7699529352329709	0.6194159785031659	0.4962191251831453	T	T	T
0.0239458615304500	0.3716814159292028	0.2675255207744769	F	F	F
0.0214042434801674	0.3718219029291672	0.5711683557983681	T	T	T
0.0239458615304500	0.8684712823182394	0.4200474629901692	F	F	F
0.2722540343571040	0.6201631094915854	0.3437676573624131	F	F	F
0.5207357279194866	0.3716814159292028	0.2675255207744769	F	F	F
0.5179913694108144	0.3719634486072228	0.5716707067729202	T	T	T
0.4957487419746656	0.8684712823182394	0.3476098994236665	F	F	F
0.2722540343571040	0.0982127364219991	0.4162052209289158	F	F	F
0.7690439007461407	0.1483602290473698	0.2636832787132235	F	F	F
0.7699842966609323	0.1569515351151468	0.5682345954644242	T	T	T
0.5520363369446611	0.3708931935154005	0.4955381346616498	T	T	T
0.7690439007461407	0.5950026028110358	0.2636832787132235	F	F	F
0.7699947293281380	0.5867878163120288	0.5682915507158102	T	T	T
0.0489328474752710	0.8684712823182394	0.3476098994236665	F	F	F
0.5443004228882818	0.8707057335916703	0.4930847693947320	T	T	T
0.7690439007461407	0.0982127364219991	0.4238897050514154	F	F	F
0.2722540343571040	0.1483602290473698	0.2713677628357232	F	F	F
0.2690660231949493	0.1569737604602484	0.5755048321093010	T	T	T
0.7690439007461407	0.6451500954364064	0.4238897050514154	F	F	F
0.4957487419746656	0.3716814159292028	0.3399254153011668	F	F	F
0.2722540343571040	0.5950026028110358	0.2713677628357232	F	F	F
0.2688195009613322	0.5868366807739990	0.5750035723759481	T	T	T
0.9963021399899042	0.8707244186142130	0.4929736624172969	T	T	T
0.0489328474752710	0.3716814159292028	0.3399254153011668	F	F	F
0.9878047033624132	0.3709133302825441	0.4952361573732423	T	T	T
0.2722540343571040	0.6451500954364064	0.4162052209289158	F	F	F
0.4817873812665066	0.4002594306373439	0.6916353434112646	T	T	T
0.5864059888356855	0.2760955295383666	0.6699127312991231	T	T	T
0.4111152897484096	0.5360089730299151	0.6670274819083265	T	T	T
0.3384993870528922	0.3059347757853226	0.7094238772635999	T	T	T
0.5913887790640068	0.4809507234638098	0.7204094997453571	T	T	T

Transition state

Co	O	C	H
1.0000000000000000			
5.7629999999999999		0.0000000000000000	0.0000000000000000
0.0000000000000000		5.7629999999999999	0.0000000000000000
0.0000000000000000		0.0000000000000000	26.1311999999999998

Co	O	C	H
14	20	1	4

Selective dynamics

Direct

0.7690439007461406	0.3716814159292027	0.3871194482482849	F	F	F
0.2700899716237328	0.8718544423013848	0.5466857538831841	T	T	T
0.2692728720725102	0.3717896405899192	0.4647113134797605	T	T	T
0.7690439007461406	0.8684712823182394	0.3098024660308312	F	F	F
0.5207357279194866	0.8684712823182394	0.4257588487441240	F	F	F
0.7697638238716182	0.1191039016693378	0.5035171299938721	T	T	T
0.2722540343571040	0.1233732431025487	0.3484418665266631	F	F	F
0.7711577210722983	0.6178468711261540	0.5044837697204890	T	T	T
0.0239458615304500	0.3716814159292027	0.2711630655349992	F	F	F
0.0211392212961625	0.3725576789615959	0.5802848140570617	T	T	T
0.0239458615304500	0.8684712823182394	0.4257588487441240	F	F	F
0.2722540343571040	0.6201631094915854	0.3484418665266631	F	F	F
0.5207357279194866	0.3716814159292027	0.2711630655349992	F	F	F
0.5217273390358363	0.3663951839561882	0.5819593047813970	T	T	T
0.4957487419746656	0.8684712823182394	0.3523363515568789	F	F	F
0.2722540343571040	0.0982127364219991	0.4218643637139081	F	F	F
0.7690439007461406	0.1483602290473698	0.2672685805047834	F	F	F
0.7678203122465588	0.1531697797045599	0.5755872322151299	T	T	T
0.5471915224283063	0.3698895856188359	0.5074059807469485	T	T	T
0.7690439007461406	0.5950026028110358	0.2672685805047834	F	F	F
0.7710427024514810	0.5823307400677898	0.5789937883806893	T	T	T
0.0489328474752710	0.8684712823182394	0.3523363515568789	F	F	F
0.5470246179613951	0.8677358027550173	0.5007385911601736	T	T	T
0.7690439007461406	0.0982127364219991	0.4296533337743327	F	F	F
0.2722540343571040	0.1483602290473698	0.2750575505652080	F	F	F
0.2685209843295714	0.1620153747026759	0.5827537450615978	T	T	T
0.7690439007461406	0.6451500954364064	0.4296533337743327	F	F	F
0.4957487419746656	0.3716814159292027	0.3445473814964544	F	F	F
0.2722540343571040	0.5950026028110358	0.2750575505652080	F	F	F
0.2699355555782844	0.5971258946284866	0.5916906455384442	T	T	T
0.9943646127761199	0.8670313479300596	0.5000007986970444	T	T	T
0.0489328474752710	0.3716814159292027	0.3445473814964544	F	F	F
0.9890774661661340	0.3676799254455734	0.5033347759570395	T	T	T
0.2722540343571040	0.6451500954364064	0.4218643637139081	F	F	F
0.4922009602013344	0.3738349407215850	0.6652704108720560	T	T	T
0.6352646374868574	0.2487351353085789	0.6629065586555507	T	T	T
0.5460580363437449	0.5175123338098440	0.6901420298832407	T	T	T
0.3397442384913126	0.2804815464183264	0.6799602590066969	T	T	T
0.3841317599630422	0.5101354219014150	0.6330021798753698	T	T	T

Chemisorption

Co14O20			
1.0000000000000000			
5.7629999999999999	0.0000000000000000	0.0000000000000000	

0.0000000000000000	5.762999999999999	0.0000000000000000			
0.0000000000000000	0.0000000000000000	25.853999999999992			
Co	O	C	H		
14	20	1	4		

Selective dynamics

Direct

0.7690439007461407	0.3716814159292028	0.3921636884041177	F	F	F
0.2709968982484098	0.8898884234204606	0.5490273911969820	T	T	T
0.2734928270147757	0.3710894541940593	0.4702587519028436	T	T	T
0.7690439007461407	0.8684712823182394	0.3138392511797008	F	F	F
0.5207357279194866	0.8684712823182394	0.4313065676491092	F	F	F
0.7690463277912177	0.1225199025236125	0.5096117748566332	T	T	T
0.2722540343571040	0.1233732431025487	0.3529821304246923	F	F	F
0.7702797171817450	0.6189051853398193	0.5099459418787726	T	T	T
0.0239458615304500	0.3716814159292028	0.2746963719347093	F	F	F
0.0185912794126045	0.3696909636283684	0.5866011940645210	T	T	T
0.0239458615304500	0.8684712823182394	0.4313065676491092	F	F	F
0.2722540343571040	0.6201631094915854	0.3529821304246923	F	F	F
0.5207357279194866	0.3716814159292028	0.2746963719347093	F	F	F
0.5278868415487349	0.3643124900860155	0.5917371478946937	T	T	T
0.4957487419746656	0.8684712823182394	0.3569273613367372	F	F	F
0.2722540343571040	0.0982127364219991	0.4273613367370643	F	F	F
0.7690439007461407	0.1483602290473698	0.2707511410226644	F	F	F
0.7705931641120133	0.1503158136530228	0.5828378958418249	T	T	T
0.5480974198533113	0.3725474282558237	0.5125593417292760	T	T	T
0.7690439007461407	0.5950026028110358	0.2707511410226644	F	F	F
0.7728640871992787	0.5782969274846287	0.5859457176078029	T	T	T
0.0489328474752710	0.8684712823182394	0.3569273613367372	F	F	F
0.5481987593489720	0.8701673647955740	0.5059753749067341	T	T	T
0.7690439007461407	0.0982127364219991	0.4352517985611541	F	F	F
0.2722540343571040	0.1483602290473698	0.2786416028467542	F	F	F
0.2707463763156133	0.1669941782340963	0.5914666927780979	T	T	T
0.7690439007461407	0.6451500954364064	0.4352517985611541	F	F	F
0.4957487419746656	0.3716814159292028	0.3490368995126474	F	F	F
0.2722540343571040	0.5950026028110358	0.2786416028467542	F	F	F
0.2725504648478781	0.6064414393552947	0.5963500303749805	T	T	T
0.9932929779738391	0.8706302108561129	0.5057740989236311	T	T	T
0.0489328474752710	0.3716814159292028	0.3490368995126474	F	F	F
0.9906981480416166	0.3702146919074993	0.5095910402351068	T	T	T
0.2722540343571040	0.6451500954364064	0.4273613367370643	F	F	F
0.5472632002989301	0.3703689138893973	0.6675711025687018	T	T	T
0.6659797170355508	0.2302488002983745	0.6785689285627199	T	T	T
0.6153358821213017	0.5416361185693378	0.6780697607095446	T	T	T
0.3724740010729618	0.3392708146752659	0.6828742328974524	T	T	T
0.2698768624914881	0.6662036735539416	0.6316485333711357	T	T	T

(001)-A: Co₁₄O₂₀
β pair site:

Physisorption

Co14O20

1.0000000000000000
 5.7629999999999999 0.0000000000000000 0.0000000000000000
 0.0000000000000000 5.7629999999999999 0.0000000000000000
 0.0228085615966845 0.0460477931420283 27.0631424491152544

Co O C H
 14 20 1 4

Selective dynamics

Direct

0.7690439007461407	0.3716814159292028	0.3819263946962010	F	F	F
0.2691616719951436	0.8692639322299450	0.5398402512143050	T	T	T
0.2706072728415448	0.3700253250519616	0.4559905449097525	T	T	T
0.7690439007461407	0.8684712823182394	0.3056465890684450	F	F	F
0.5207357279194866	0.8684712823182394	0.4200474629901692	F	F	F
0.7697643824919159	0.1180958968170973	0.4951796804373642	T	T	T
0.2722540343571040	0.1233732431025487	0.3437676573624131	F	F	F
0.7697806603074296	0.6201370628622399	0.4952729792630245	T	T	T
0.0239458615304500	0.3716814159292028	0.2675255207744769	F	F	F
0.0212824796688907	0.3676858883881241	0.5696186746743510	T	T	T
0.0239458615304500	0.8684712823182394	0.4200474629901692	F	F	F
0.2722540343571040	0.6201631094915854	0.3437676573624131	F	F	F
0.5207357279194866	0.3716814159292028	0.2675255207744769	F	F	F
0.5184863668069654	0.3679158208866364	0.5702410559624065	T	T	T
0.4957487419746656	0.8684712823182394	0.3476098994236665	F	F	F
0.2722540343571040	0.0982127364219991	0.4162052209289158	F	F	F
0.7690439007461407	0.1483602290473698	0.2636832787132235	F	F	F
0.7698502218101609	0.1505388736934067	0.5658890373433607	T	T	T
0.5441798429845094	0.3689767256292165	0.4951824082491404	T	T	T
0.7690439007461407	0.5950026028110358	0.2636832787132235	F	F	F
0.7701294607420568	0.5852681604887985	0.5657394414063690	T	T	T
0.0489328474752710	0.8684712823182394	0.3476098994236665	F	F	F
0.5420100588888742	0.8689666166002012	0.4916239494468939	T	T	T
0.7690439007461407	0.0982127364219991	0.4238897050514154	F	F	F
0.2722540343571040	0.1483602290473698	0.2713677628357232	F	F	F
0.2692421366940377	0.1530978248899927	0.5768730528192010	T	T	T
0.7690439007461407	0.6451500954364064	0.4238897050514154	F	F	F
0.4957487419746656	0.3716814159292028	0.3399254153011668	F	F	F
0.2722540343571040	0.5950026028110358	0.2713677628357232	F	F	F
0.2688521685964577	0.5825736678399203	0.5761312624964969	T	T	T
-0.0018278805249948	0.8690807121390722	0.4915167121078688	T	T	T
0.0489328474752710	0.3716814159292028	0.3399254153011668	F	F	F
0.9951162629443271	0.3692867329437578	0.4948107867476594	T	T	T
0.2722540343571040	0.6451500954364064	0.4162052209289158	F	F	F
0.5538443318467609	0.4110857127545424	0.6904935041115191	T	T	T
0.4292694259613019	0.2985631429695687	0.6703784377201978	T	T	T
0.6622608719943424	0.3016173055497797	0.7149570395579743	T	T	T
0.4536405349788885	0.5393152021019785	0.7121345399694957	T	T	T
0.6695091439255000	0.5063374094849934	0.6646394367307399	T	T	T

Transition state

Co	O	C	H
1.0000000000000000			
5.7629999999999999		0.0000000000000000	0.0000000000000000
0.0000000000000000		5.7629999999999999	0.0000000000000000
0.0048139138326937		-0.0003325900304718	26.2352849453928982

Co	O	C	H
14	20	1	4

Selective dynamics

Direct

0.7690439007461405	0.3716814159292028	0.3852600736668430	F	F	F
0.2708599724452367	0.8684795537970139	0.5455055403351687	T	T	T
0.2761102318650376	0.3706735046626492	0.4622872368208129	T	T	T
0.7690439007461407	0.8684712823182394	0.3083144528782711	F	F	F
0.5207357279194865	0.8684712823182394	0.4237138851424262	F	F	F
0.7749746913804756	0.1213955272695619	0.5011833126869460	T	T	T
0.2722540343571040	0.1233732431025459	0.3467682643538481	F	F	F
0.7703853541204506	0.6217401819002255	0.5008964501465353	T	T	T
0.0239458615304500	0.3716814159292027	0.2698606414027011	F	F	F
0.0348894659506362	0.3626432101090029	0.5749976779515271	T	T	T
0.0239458615304499	0.8684712823182249	0.4237138851424261	F	F	F
0.2722540343571040	0.6201631094915853	0.3467682643538481	F	F	F
0.5207357279194764	0.3716814159291954	0.2698606414027011	F	F	F
0.5344360490653894	0.3670020525991282	0.5777918020964592	T	T	T
0.4957487419746656	0.8684712823182394	0.3506440437713464	F	F	F
0.2722540343571040	0.0982127364219991	0.4198381057249134	F	F	F
0.7690439007461407	0.1483602290473698	0.2659848619851957	F	F	F
0.7871174201570538	0.1523959857897114	0.5738729304800484	T	T	T
0.5529199661088361	0.3672731523374118	0.5036938669059112	T	T	T
0.7690439007461407	0.5950026028110360	0.2659848619851957	F	F	F
0.7886496507882936	0.5920652774228615	0.5765329610523728	T	T	T
0.0489328474752710	0.8684712823182394	0.3506440437713402	F	F	F
0.5429131553165728	0.8708719450977351	0.4978539200975690	T	T	T
0.7690439007461407	0.0982127364219973	0.4275896645599113	F	F	F
0.2722540343570978	0.1483602290473698	0.2737364208201996	F	F	F
0.2830219439673849	0.1443937642781454	0.5799907679289131	T	T	T
0.7690439007461405	0.6451500954364066	0.4275896645599175	F	F	F
0.4957487419746656	0.3716814159292028	0.3428924849363497	F	F	F
0.2722540343570938	0.5950026028110358	0.2737364208201996	F	F	F
0.2759189925985863	0.5845505949477362	0.5782082498871510	T	T	T
1.0023643689963060	0.8697957660052150	0.4971589698282377	T	T	T
0.0489328474752706	0.3716814159291957	0.3428924849363435	F	F	F
0.9898524861124134	0.3748240213357638	0.4995894980683074	T	T	T
0.2722540343571040	0.6451500954364064	0.4198381057249206	F	F	F
0.5734796528333864	0.4168831003042358	0.6561342032870581	T	T	T
0.5653244232309018	0.5891333559847799	0.6747479408202695	T	T	T
0.7151657757359601	0.3100612932144868	0.6718553707715988	T	T	T
0.4050789707475957	0.3318697872641162	0.6630952671041418	T	T	T
0.6883806362936881	0.5539215952627520	0.6157869958993036	T	T	T

Chemisorption

Co14O20

1.0000000000000000		
5.7629999999999999	0.0000000000000000	0.0000000000000000

0.0000000000000000	5.762999999999999	0.0000000000000000			
0.0000000000000000	0.0000000000000000	26.036999999999990			
Co	O	C	H		
14	20	1	4		

Selective dynamics

Direct

0.7690439007461407	0.3716814159292028	0.3894073818028190	F	F	F
0.2722914617286344	0.8651778092559720	0.5484013509685126	T	T	T
0.2725113579946245	0.3697850620325189	0.4674573654503000	T	T	T
0.7690439007461407	0.8684712823182394	0.3116334447132942	F	F	F
0.5207357279194866	0.8684712823182394	0.4282751469063228	F	F	F
0.7672103173585715	0.1216209402636721	0.5061798573367933	T	T	T
0.2722540343571040	0.1233732431025487	0.3505012098167981	F	F	F
0.7680789628514851	0.6221783185691691	0.5050708403263465	T	T	T
0.0239458615304500	0.3716814159292028	0.2727656796097833	F	F	F
0.0278207086078503	0.3607213344579172	0.5801625699964078	T	T	T
0.0239458615304500	0.8684712823182394	0.4282751469063228	F	F	F
0.2722540343571040	0.6201631094915854	0.3505012098167981	F	F	F
0.5207357279194866	0.3716814159292028	0.2727656796097833	F	F	F
0.5129059065946951	0.3638917132618973	0.5873094323005326	T	T	T
0.4957487419746656	0.8684712823182394	0.3544187118331621	F	F	F
0.2722540343571040	0.0982127364219991	0.4243576448899660	F	F	F
0.7690439007461407	0.1483602290473698	0.2688481775934264	F	F	F
0.7681994900861147	0.1515014651919584	0.5802252642695797	T	T	T
0.5492577428412394	0.3718570177023829	0.5083125506366259	T	T	T
0.7690439007461407	0.5950026028110358	0.2688481775934264	F	F	F
0.7697562943098758	0.5931455633822668	0.5798458321132207	T	T	T
0.0489328474752710	0.8684712823182394	0.3544187118331621	F	F	F
0.5465552252136000	0.8701449941485995	0.5019871839052268	T	T	T
0.7690439007461407	0.0982127364219991	0.4321926489226868	F	F	F
0.2722540343571040	0.1483602290473698	0.2766831816261472	F	F	F
0.2648894456896945	0.1486202982435909	0.5873018568460392	T	T	T
0.7690439007461407	0.6451500954364064	0.4321926489226868	F	F	F
0.4957487419746656	0.3716814159292028	0.3465837078004412	F	F	F
0.2722540343571040	0.5950026028110358	0.2766831816261472	F	F	F
0.2706865393876555	0.5715195889065474	0.5863673658408758	T	T	T
0.9936167737176479	0.8701691266813154	0.5023442831621429	T	T	T
0.0489328474752710	0.3716814159292028	0.3465837078004412	F	F	F
0.9875233236869914	0.3727942842508881	0.5084151289653370	T	T	T
0.2722540343571040	0.6451500954364064	0.4243576448899660	F	F	F
0.5190272813633648	0.3537333071437012	0.6626904498095434	T	T	T
0.5970356106803598	0.5178277886808182	0.6751347188998391	T	T	T
0.6251235591255340	0.2022675802963984	0.6721765333148549	T	T	T
0.3397989241456902	0.3350391987527932	0.6757561923298577	T	T	T
0.7741583123352181	0.7454568524210140	0.5968611266394116	T	T	T

**(001)-B: Co₁₀O₁₂
 α pair site:**

Physisorption

Co O
 1.0000000000000000
 5.7629999999999999 0.0000000000000000 0.0000000000000000
 0.0000000000000000 5.7629999999999999 0.0000000000000000
 0.0000000000000000 0.0000000000000000 21.1119999999999983

Co O C H
 10 12 1 4

Selective dynamics

Direct

0.7386777719937498	0.9611313551969474	0.4517336112163690	F	F	F
0.2388294452475382	0.2777648066924384	0.6187894854941046	T	T	T
0.7386777719937498	0.4612181155648116	0.3552482000757848	F	F	F
0.2410572953363320	0.9444079889810496	0.5480004164071871	T	T	T
0.4888079125455462	0.4612181155648116	0.5000000000000000	F	F	F
0.9887211521776820	0.4612181155648116	0.5000000000000000	F	F	F
0.2387645323616141	0.2111747353808795	0.4035145888594158	F	F	F
0.7391628887852629	0.7455055945199892	0.5997350138310528	T	T	T
0.7392079283377497	0.2253519946652583	0.5948471789586673	T	T	T
0.2387645323616141	0.7110879750130152	0.4035145888594158	F	F	F
0.0163109491584237	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.6834981780322735	0.4946949602122004	F	F	F
0.4612181155648116	0.9611313551969474	0.3981621826449384	F	F	F
0.9713056142998090	0.4632334124593596	0.5930654360153343	T	T	T
0.5066629230460048	0.4632760049078118	0.5931923411449770	T	T	T
0.7386777719937498	0.2387645323616141	0.5053050397877996	F	F	F
0.0163109491584237	0.9611313551969474	0.3981621826449384	F	F	F
0.7386777719937498	0.6834981780322735	0.5053050397877996	F	F	F
0.4966498678710747	0.0078873031723820	0.6092075718565021	T	T	T
0.9823827920605298	0.0072249616535117	0.6085224066041240	T	T	T
0.4612181155648116	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.2387645323616141	0.4946949602122004	F	F	F
0.7386678564127643	0.2518265809022600	0.7538774887665141	T	T	T
0.8441460047429082	0.3514015510922380	0.7874876011680628	T	T	T
0.6180496508846670	0.1392233135988733	0.7796199287506909	T	T	T
0.6399908799718537	0.3720500158423052	0.7238599976263662	T	T	T
0.8520859013010070	0.1438132356702701	0.7242538879309766	T	T	T

Transition state

Co O C H
 1.0000000000000000
 5.7629999999999999 0.0000000000000000 0.0000000000000000
 0.0000000000000000 5.7629999999999999 0.0000000000000000
 0.0000000000000000 0.0000000000000000 21.1119999999999983

Co O C H
 10 12 1 4

Selective dynamics

Direct

0.7386777719937500	0.9611313551969470	0.4517336112163690	F	F	F
0.2341090642582050	0.2896262844110110	0.6172524442715360	T	T	T
0.7386777719937500	0.4612181155648120	0.3552482000757850	F	F	F

0.2273664868513370	0.9467107785518040	0.5461285015661460	T	T	T
0.4888079125455460	0.4612181155648120	0.5000000000000000	F	F	F
0.9887211521776820	0.4612181155648120	0.5000000000000000	F	F	F
0.2387645323616140	0.2111747353808790	0.4035145888594160	F	F	F
0.7523920191155100	0.7471687578530630	0.5986728853624450	T	T	T
0.7423334497635360	0.2351235015414580	0.6013792082708770	T	T	T
0.2387645323616140	0.7110879750130150	0.4035145888594160	F	F	F
0.0163109491584237	0.4612181155648120	0.4088196286472150	F	F	F
0.2387645323616140	0.6834981780322740	0.4946949602122000	F	F	F
0.4612181155648120	0.9611313551969470	0.3981621826449380	F	F	F
0.9705537180946370	0.4706807732597860	0.5921549063400759	T	T	T
0.5051449224354370	0.4652612013347100	0.5931539727301000	T	T	T
0.7386777719937500	0.2387645323616140	0.5053050397877999	F	F	F
0.0163109491584237	0.9611313551969470	0.3981621826449380	F	F	F
0.7386777719937500	0.6834981780322740	0.5053050397877999	F	F	F
0.4988554771816470	0.9984451868277000	0.6116632946213960	T	T	T
0.9929988499577500	0.0131480066814156	0.6110895968492890	T	T	T
0.4612181155648120	0.4612181155648120	0.4088196286472150	F	F	F
0.2387645323616140	0.2387645323616140	0.4946949602122000	F	F	F
0.7441553119735130	0.2673102553228550	0.7198216633653970	T	T	T
0.8788046896142220	0.3673977381185730	0.7421321306137650	T	T	T
0.6107979948496510	0.3709440794205280	0.7180911188660590	T	T	T
0.7948612909032680	0.1204954363807530	0.7218082354667550	T	T	T
0.5187044079175051	0.0267759767068539	0.7051212678323850	T	T	T

Chemisorption

Co O

1.0000000000000000		
5.7629999999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.7629999999999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.1119999999999983

Co O C H
10 12 1 4

Selective dynamics

Direct

0.7386777719937498	0.9611313551969474	0.4517336112163690	F	F	F
0.2310285113439856	0.2973671658854888	0.6162493606585486	T	T	T
0.7386777719937498	0.4612181155648116	0.3552482000757848	F	F	F
0.2184317716087144	0.9482135947734133	0.5449068771396889	T	T	T
0.4888079125455462	0.4612181155648116	0.5000000000000000	F	F	F
0.9887211521776820	0.4612181155648116	0.5000000000000000	F	F	F
0.2387645323616141	0.2111747353808795	0.4035145888594158	F	F	F
0.7610254400371455	0.7482541496178611	0.5979797330604132	T	T	T
0.7443731864200519	0.2415004537518292	0.6056420552696488	T	T	T
0.2387645323616141	0.7110879750130152	0.4035145888594158	F	F	F
0.0163109491584237	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.6834981780322735	0.4946949602122004	F	F	F
0.4612181155648116	0.9611313551969474	0.3981621826449384	F	F	F
0.9700630254892573	0.4755409718473134	0.5915606884472954	T	T	T
0.5041542648560423	0.4665567540987711	0.5931289332401719	T	T	T
0.7386777719937498	0.2387645323616141	0.5053050397877996	F	F	F
0.0163109491584237	0.9611313551969474	0.3981621826449384	F	F	F
0.7386777719937498	0.6834981780322735	0.5053050397877996	F	F	F
0.5002948729009035	-0.0077168028692543	0.6132659160913617	T	T	T

-0.0000730380600553	0.0170134263716910	0.6127649627591373	T	T	T
0.4612181155648116	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.2387645323616141	0.4946949602122004	F	F	F
0.7477364629987031	0.2774150071356549	0.6975965988160503	T	T	T
0.9014231843764948	0.3778369591627237	0.7125328403642264	T	T	T
0.5917465183817923	0.3702223377486846	0.7143263091363092	T	T	T
0.7575161188241581	0.1052780811043933	0.7202121859438871	T	T	T
0.4538710229794042	-0.0466079243259636	0.6565029322540501	T	T	T

(001)-B: Co₁₀O₁₂
β pair site:

Physisorption

Co O
 1.0000000000000000
 5.7629999999999999 0.0000000000000000 0.0000000000000000
 0.0000000000000000 5.7629999999999999 0.0000000000000000
 0.0000000000000000 0.0000000000000000 21.1119999999999983

Co O C H
 10 12 1 4

Selective dynamics

Direct

0.7386777719937498	0.9611313551969474	0.4517336112163690	F	F	F
0.2384405649815444	0.2803801957560805	0.6169711991003091	T	T	T
0.7386777719937498	0.4612181155648116	0.3552482000757848	F	F	F
0.2389653350104674	0.9457502371015820	0.5479124288161173	T	T	T
0.4888079125455462	0.4612181155648116	0.5000000000000000	F	F	F
0.9887211521776820	0.4612181155648116	0.5000000000000000	F	F	F
0.2387645323616141	0.2111747353808795	0.4035145888594158	F	F	F
0.7384212281172234	0.7457827765611501	0.5996519274034994	T	T	T
0.7381100710814698	0.2240480677815620	0.5949128786553883	T	T	T
0.2387645323616141	0.7110879750130152	0.4035145888594158	F	F	F
0.0163109491584237	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.6834981780322735	0.4946949602122004	F	F	F
0.4612181155648116	0.9611313551969474	0.3981621826449384	F	F	F
0.9693898299997107	0.4633871484879648	0.5924184952771666	T	T	T
0.5076071318817394	0.4639381421125632	0.5927418330069344	T	T	T
0.7386777719937498	0.2387645323616141	0.5053050397877996	F	F	F
0.0163109491584237	0.9611313551969474	0.3981621826449384	F	F	F
0.7386777719937498	0.6834981780322735	0.5053050397877996	F	F	F
0.4958489386625334	0.0065706653012886	0.6086496553027239	T	T	T
0.9805576657519737	0.0061753826711420	0.6086531686893036	T	T	T
0.4612181155648116	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.2387645323616141	0.4946949602122004	F	F	F
0.7145737338623031	0.2480085497332769	0.7424897953873177	T	T	T
0.5729277530865907	0.1389720244286475	0.7602415350420032	T	T	T
0.6427591289469357	0.3806412613421763	0.7107431276554224	T	T	T
0.8037509041448522	0.3343061103428378	0.7818481673490290	T	T	T
0.8379649567575578	0.1379608974502844	0.7165750806139783	T	T	T

Transition state

Co O C H
 1.0000000000000000
 5.7629999999999999 0.0000000000000000 0.0000000000000000
 0.0000000000000000 5.7629999999999999 0.0000000000000000
 0.0000000000000000 0.0000000000000000 21.1119999999999983

Co O C H
 10 12 1 4

Selective dynamics

Direct

0.7386777719937500	0.9611313551969470	0.4517336112163690	F	F	F
0.2287688148026110	0.2696024331223130	0.6215128676691580	T	T	T
0.7386777719937500	0.4612181155648120	0.3552482000757850	F	F	F

0.2578867592238690	0.9492219483945150	0.5465058877302190	T	T	T
0.4888079125455460	0.4612181155648120	0.5000000000000000	F	F	F
0.9887211521776820	0.4612181155648120	0.5000000000000000	F	F	F
0.2387645323616140	0.2111747353808790	0.4035145888594160	F	F	F
0.7710801335235110	0.7587352715447130	0.5966034442050721	T	T	T
0.7440514577025090	0.2279847511705630	0.6007575322514320	T	T	T
0.2387645323616140	0.7110879750130150	0.4035145888594160	F	F	F
0.0163109491584237	0.4612181155648120	0.4088196286472150	F	F	F
0.2387645323616140	0.6834981780322740	0.4946949602122000	F	F	F
0.4612181155648120	0.9611313551969470	0.3981621826449380	F	F	F
0.9728432563036440	0.4685137747191460	0.5934405526549060	T	T	T
0.4934140778822870	0.4560314846032970	0.5945901340585170	T	T	T
0.7386777719937500	0.2387645323616140	0.5053050397877999	F	F	F
0.0163109491584237	0.9611313551969470	0.3981621826449380	F	F	F
0.7386777719937500	0.6834981780322740	0.5053050397877999	F	F	F
0.5090442573774280	0.9897398374204980	0.6092395839538620	T	T	T
0.9966737651797430	0.0112094223767356	0.6098562418107150	T	T	T
0.4612181155648120	0.4612181155648120	0.4088196286472150	F	F	F
0.2387645323616140	0.2387645323616140	0.4946949602122000	F	F	F
0.7326342781986860	0.2554959504141940	0.7182762234950780	T	T	T
0.7999892711635960	0.3918766709904610	0.7435537704008870	T	T	T
0.5725387330824671	0.1847661008944320	0.7361085025961830	T	T	T
0.8549083974231840	0.1372515488835700	0.7179017734827110	T	T	T
0.5505994018745100	0.5027965666255270	0.6594382767030290	T	T	T

Chemisorption

Co O

1.0000000000000000		
5.7629999999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.7629999999999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.1119999999999983

Co O C H
10 12 1 4

Selective dynamics

Direct

0.7386777719937498	0.9611313551969474	0.4517336112163690	F	F	F
0.2207277965949904	0.2601185596457014	0.6255851830273585	T	T	T
0.7386777719937498	0.4612181155648116	0.3552482000757848	F	F	F
0.2738272716154382	0.9536275343328627	0.5456207088340785	T	T	T
0.4888079125455462	0.4612181155648116	0.5000000000000000	F	F	F
0.9887211521776820	0.4612181155648116	0.5000000000000000	F	F	F
0.2387645323616141	0.2111747353808795	0.4035145888594158	F	F	F
0.7982954799094887	0.7684685541034556	0.5937018493623559	T	T	T
0.7488857644035057	0.2315024358512810	0.6058972771705187	T	T	T
0.2387645323616141	0.7110879750130152	0.4035145888594158	F	F	F
0.0163109491584237	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.6834981780322735	0.4946949602122004	F	F	F
0.4612181155648116	0.9611313551969474	0.3981621826449384	F	F	F
0.9755756132582830	0.4729186667147591	0.5943054014464181	T	T	T
0.4818436029612747	0.4493932020908195	0.5963131515738689	T	T	T
0.7386777719937498	0.2387645323616141	0.5053050397877996	F	F	F
0.0163109491584237	0.9611313551969474	0.3981621826449384	F	F	F
0.7386777719937498	0.6834981780322735	0.5053050397877996	F	F	F
0.5190803717174584	-0.0236822871310407	0.6096872658010335	T	T	T

0.0108058784204484	0.0161949862420640	0.6108402788304339	T	T	T
0.4612181155648116	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.2387645323616141	0.4946949602122004	F	F	F
0.7475341766907275	0.2620076165973896	0.6979201074619885	T	T	T
0.7968403148393406	0.4399038691024409	0.7114750105293403	T	T	T
0.5722323676122678	0.2229804423007500	0.7158784820766581	T	T	T
0.8691619091403940	0.1365336019917091	0.7189205925566462	T	T	T
0.4736749205984968	0.6045409869910251	0.6165405914130732	T	T	T

(001)-B: Co₁₀O₁₂
γ pair site:

Physisorption

Co O
 1.0000000000000000
 5.7629999999999999 0.0000000000000000 0.0000000000000000
 0.0000000000000000 5.7629999999999999 0.0000000000000000
 0.0000000000000000 0.0000000000000000 21.1119999999999983

Co O C H
 10 12 1 4

Selective dynamics

Direct

0.7386777719937498	0.9611313551969474	0.4517336112163690	F	F	F
0.2373911220891601	0.2822566604124623	0.6200561717506228	T	T	T
0.7386777719937498	0.4612181155648116	0.3552482000757848	F	F	F
0.2430674386084074	0.9437308370680606	0.5487996619520327	T	T	T
0.4888079125455462	0.4612181155648116	0.5000000000000000	F	F	F
0.9887211521776820	0.4612181155648116	0.5000000000000000	F	F	F
0.2387645323616141	0.2111747353808795	0.4035145888594158	F	F	F
0.7425864894731055	0.7424683569392208	0.5997706919844763	T	T	T
0.7413262314768583	0.2212546322347508	0.5947154474271800	T	T	T
0.2387645323616141	0.7110879750130152	0.4035145888594158	F	F	F
0.0163109491584237	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.6834981780322735	0.4946949602122004	F	F	F
0.4612181155648116	0.9611313551969474	0.3981621826449384	F	F	F
0.9701763012025167	0.4632732847659302	0.5933158829820401	T	T	T
0.5071186806133896	0.4582637285614103	0.5925499481290175	T	T	T
0.7386777719937498	0.2387645323616141	0.5053050397877996	F	F	F
0.0163109491584237	0.9611313551969474	0.3981621826449384	F	F	F
0.7386777719937498	0.6834981780322735	0.5053050397877996	F	F	F
0.5039377011195448	0.0006887999300973	0.6091919280555901	T	T	T
0.9850003723763173	0.0070993956766948	0.6095336258485800	T	T	T
0.4612181155648116	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.2387645323616141	0.4946949602122004	F	F	F
0.2852063153464096	0.2411331403606539	0.7473878417576334	T	T	T
0.3346237069441894	0.1664991553241572	0.7932414673310282	T	T	T
0.0953389863322925	0.2488245161712614	0.7446115199133126	T	T	T
0.3605323213732489	0.4153384210439918	0.7433156087397361	T	T	T
0.3561468613553750	0.1236976891403303	0.7108086145370568	T	T	T

Transition state

Co O C H
 1.0000000000000000
 5.7629999999999999 0.0000000000000000 0.0000000000000000
 0.0000000000000000 5.7629999999999999 0.0000000000000000
 0.0000000000000000 0.0000000000000000 21.1119999999999983

Co O C H
 10 12 1 4

Selective dynamics

Direct

0.7386777719937498	0.9611313551969474	0.4517336112163690	F	F	F
0.2251866665289869	0.2705985693025623	0.6399296457789196	T	T	T
0.7386777719937498	0.4612181155648116	0.3552482000757848	F	F	F

0.1968517775612289	0.9356024512300518	0.5469795645091289	T	T	T
0.4888079125455462	0.4612181155648116	0.4999999999999999	F	F	F
0.9887211521776819	0.4612181155648116	0.4999999999999999	F	F	F
0.2387645323616141	0.2111747353808795	0.4035145888594156	F	F	F
0.7907351959970249	0.7768174765912099	0.5935561067732386	T	T	T
0.7693294755243156	0.3069559357428386	0.5912472501766552	T	T	T
0.2387645323616141	0.7110879750130152	0.4035145888594156	F	F	F
0.0163109491584237	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.6834981780322734	0.4946949602121994	F	F	F
0.4612181155648116	0.9611313551969474	0.3981621826449384	F	F	F
1.0353043257276247	0.5184088107490477	0.5868268898803580	T	T	T
0.4996562186018103	0.4564619094390436	0.5970887439582276	T	T	T
0.7386777719937498	0.2387645323616141	0.5053050397877995	F	F	F
0.0163109491584237	0.9611313551969474	0.3981621826449384	F	F	F
0.7386777719937498	0.6834981780322734	0.5053050397877995	F	F	F
0.4668954847395396	0.8864539717996539	0.5980972506022137	T	T	T
0.9459072979232592	1.0577920252090049	0.6022123376682467	T	T	T
0.4612181155648116	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.2387645323616141	0.4946949602121994	F	F	F
0.2361200088545113	0.2909282842785363	0.7501666425637382	T	T	T
0.3225320850440578	0.4618781501165205	0.7281420757393827	T	T	T
0.0312204728486916	0.3252458075471578	0.7514241345173723	T	T	T
0.2564193228332359	0.4441270216569559	0.8164392511727530	T	T	T
0.4088034658193404	-0.0844288398320503	0.6448870324222242	T	T	T

Chemisorption

Co O

1.0000000000000000		
5.7629999999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.7629999999999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.1119999999999983

Co O C H
10 12 1 4

Selective dynamics

Direct

0.7386777719937498	0.9611313551969474	0.4517336112163690	F	F	F
0.2382930287882903	0.3830800153975866	0.6410748297777416	T	T	T
0.7386777719937498	0.4612181155648116	0.3552482000757848	F	F	F
0.2182060009693117	0.9612950423511168	0.5482816600214877	T	T	T
0.4888079125455462	0.4612181155648116	0.5000000000000000	F	F	F
0.9887211521776820	0.4612181155648116	0.5000000000000000	F	F	F
0.2387645323616141	0.2111747353808795	0.4035145888594158	F	F	F
0.7466034896588424	0.7243109291207176	0.6006125795847465	T	T	T
0.7430493170649455	0.2147964725489518	0.5958099962616735	T	T	T
0.2387645323616141	0.7110879750130152	0.4035145888594158	F	F	F
0.0163109491584237	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.6834981780322735	0.4946949602122004	F	F	F
0.4612181155648116	0.9611313551969474	0.3981621826449384	F	F	F
0.9683793800089681	0.4519756773698697	0.5912039350932503	T	T	T
0.5135864466738467	0.4538917817020395	0.5928993792958411	T	T	T
0.7386777719937498	0.2387645323616141	0.5053050397877996	F	F	F
0.0163109491584237	0.9611313551969474	0.3981621826449384	F	F	F
0.7386777719937498	0.6834981780322735	0.5053050397877996	F	F	F
0.4966155131263043	-0.0237320382502779	0.6111389317523495	T	T	T

0.9634744478024995	-0.0131770370857375	0.6078184896913138	T	T	T
0.4612181155648116	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.2387645323616141	0.4946949602122004	F	F	F
0.2487386892953337	0.3540149763427741	0.7354549968011445	T	T	T
0.3882672617025457	0.4577118266658425	0.7570238076523700	T	T	T
0.0828705701038723	0.4194178123383925	0.7543917724272073	T	T	T
0.2669799848708045	0.1737842841029763	0.7522699323347469	T	T	T
0.4353015414172376	-0.0074978849680038	0.6541796431066471	T	T	T

**(001)-B: Co₁₀O₁₂
 δ pair site:**

Physisorption

CoO

1.0000000000000000		
5.7629999999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.7629999999999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.1119999999999983

Co	O	C	H
10	12	1	4

Selective dynamics

Direct

0.7386777719937498	0.9611313551969474	0.4517336112163690	F	F	F
0.2382383061751443	0.2850533361524950	0.6198285006172144	T	T	T
0.7386777719937498	0.4612181155648116	0.3552482000757848	F	F	F
0.2404143335542659	0.9434581421869521	0.5489611344205004	T	T	T
0.4888079125455462	0.4612181155648116	0.5000000000000000	F	F	F
0.9887211521776820	0.4612181155648116	0.5000000000000000	F	F	F
0.2387645323616141	0.2111747353808795	0.4035145888594158	F	F	F
0.7403384693210164	0.7449647185111598	0.5997189472659842	T	T	T
0.7396275197928994	0.2225762852728433	0.5950104286230787	T	T	T
0.2387645323616141	0.7110879750130152	0.4035145888594158	F	F	F
0.0163109491584237	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.6834981780322735	0.4946949602122004	F	F	F
0.4612181155648116	0.9611313551969474	0.3981621826449384	F	F	F
0.9697844670900525	0.4633395377331522	0.5928043685153294	T	T	T
0.5074838611045907	0.4615958497713941	0.5922711564955928	T	T	T
0.7386777719937498	0.2387645323616141	0.5053050397877996	F	F	F
0.0163109491584237	0.9611313551969474	0.3981621826449384	F	F	F
0.7386777719937498	0.6834981780322735	0.5053050397877996	F	F	F
0.5001174805230952	0.0047631711016947	0.6097801077907926	T	T	T
0.9815871826249997	0.0072050013901038	0.6100157460063885	T	T	T
0.4612181155648116	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.2387645323616141	0.4946949602122004	F	F	F
0.2762754562307149	0.3422490958818719	0.7472117081860640	T	T	T
0.2186118361014350	0.1847122538341424	0.7218245481324459	T	T	T
0.3741909833100702	0.4614023274454259	0.7165272668977191	T	T	T
0.1243294353064219	0.4326542425341726	0.7661771956138339	T	T	T
0.3908165652514425	0.2851993416962995	0.7856623353684193	T	T	T

Transition state

Co

O	C	H
1.0000000000000000		
5.7629999999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.7629999999999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.1119999999999983

Co	O	C	H
10	12	1	4

Selective dynamics

Direct

0.7386777719937498	0.9611313551969474	0.4517336112163690	F	F	F
0.1955549875933939	0.2385437782661312	0.6332112845090205	T	T	T
0.7386777719937498	0.4612181155648116	0.3552482000757848	F	F	F

0.2466123202145692	0.9485167082672284	0.5484375178698067	T	T	T
0.4888079125455462	0.4612181155648116	0.4999999999999999	F	F	F
0.9887211521776819	0.4612181155648116	0.4999999999999999	F	F	F
0.2387645323616141	0.2111747353808795	0.4035145888594156	F	F	F
0.7401467031331888	0.7260768284179651	0.6037842811849495	T	T	T
0.7307969602337614	0.2132390918963650	0.5956153512435181	T	T	T
0.2387645323616141	0.7110879750130152	0.4035145888594156	F	F	F
0.0163109491584237	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.6834981780322734	0.4946949602121994	F	F	F
0.4612181155648116	0.9611313551969474	0.3981621826449384	F	F	F
0.9644306534102683	0.4533658487437480	0.5925111339110637	T	T	T
0.5114220348583802	0.4567012287507767	0.6131639971749409	T	T	T
0.7386777719937498	0.2387645323616141	0.5053050397877995	F	F	F
0.0163109491584237	0.9611313551969474	0.3981621826449384	F	F	F
0.7386777719937498	0.6834981780322734	0.5053050397877995	F	F	F
0.5029505152193442	0.9859381255726025	0.6079497255989114	T	T	T
0.9712692927802197	0.9889711565533283	0.6047071929349168	T	T	T
0.4612181155648116	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.2387645323616141	0.4946949602121994	F	F	F
0.2834182694983414	0.3448078621414540	0.7261674267621404	T	T	T
0.1472407218535703	0.2119604531822388	0.7382968327131578	T	T	T
0.2212358670104922	0.5101334161359543	0.7447882693022865	T	T	T
0.4378736198606457	0.2876060223779757	0.7530617924054084	T	T	T
0.4230590823728318	0.4262409872892815	0.6642862442221475	T	T	T

Chemisorption

Co O

1.0000000000000000		
5.7629999999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.7629999999999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.1119999999999983

Co O C H
10 12 1 4

Selective dynamics

Direct

0.7386777719937498	0.9611313551969474	0.4517336112163690	F	F	F
0.2593992584312376	0.0554636837730981	0.6732319725946140	T	T	T
0.7386777719937498	0.4612181155648116	0.3552482000757848	F	F	F
0.2547934479012004	0.9586543418687837	0.5503554987189100	T	T	T
0.4888079125455462	0.4612181155648116	0.5000000000000000	F	F	F
0.9887211521776820	0.4612181155648116	0.5000000000000000	F	F	F
0.2387645323616141	0.2111747353808795	0.4035145888594158	F	F	F
0.7602262474311798	0.7235488642864722	0.6014014259703601	T	T	T
0.7617868261978550	0.2074667430554936	0.5999569941016933	T	T	T
0.2387645323616141	0.7110879750130152	0.4035145888594158	F	F	F
0.0163109491584237	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.6834981780322735	0.4946949602122004	F	F	F
0.4612181155648116	0.9611313551969474	0.3981621826449384	F	F	F
0.9827143051297536	0.4543455885967824	0.5917718106792081	T	T	T
0.5003061511381183	0.4643724399809837	0.5907493277799897	T	T	T
0.7386777719937498	0.2387645323616141	0.5053050397877996	F	F	F
0.0163109491584237	0.9611313551969474	0.3981621826449384	F	F	F
0.7386777719937498	0.6834981780322735	0.5053050397877996	F	F	F
0.5160924057777638	-0.0247583730521046	0.6147101933462360	T	T	T

0.0019020030678586	-0.0283999726336225	0.6160688550179549	T	T	T
0.4612181155648116	0.4612181155648116	0.4088196286472154	F	F	F
0.2387645323616141	0.2387645323616141	0.4946949602122004	F	F	F
0.2657281678568542	0.2571562388400826	0.7488946703922714	T	T	T
0.1275608691271327	0.2154578439856609	0.7830217218914952	T	T	T
0.2403693144273524	0.4380493030729777	0.7331099163494895	T	T	T
0.4333173617930672	0.2471314789086300	0.7737791572290058	T	T	T
0.3385992928181328	0.4585431213655617	0.6065988497848689	T	T	T

Table S3. Fractional Coordinates of the Stationary States Shown in Figure 3.

**(011)-A: Co₁₄O₂₀
α pair site:**

Physisorption

Co	O	C	H			
1.0000000000000000						
8.1500000000000004				0.0000000000000000		0.0000000000000000
0.0000000000000000				5.7260000000000000		0.0000000000000000
0.0000000000000000				0.0000000000000000		21.0139999999999993

Co	O	C	H	
14	20	1	4	

Selective dynamics

Direct

0.6741170659422053	0.2499126790080339	0.4081088797944261	F	F	F
0.1865738280992613	0.7500335291442433	0.5477197921952282	T	T	T
0.9240553223018040	0.7499126790080339	0.4081088797944261	F	F	F
0.4110217174801963	0.2497598186888064	0.5502422834524477	T	T	T
0.2990861941220047	0.0000000000000000	0.4081088797944261	F	F	F
0.5394159004018384	0.7495784801784524	0.6094819636431421	T	T	T
0.0491479377624131	0.2499126790080339	0.3399638336347195	F	F	F
0.0544011186071860	0.2499191056879048	0.6111972073173753	T	T	T
0.5490244504816033	0.7499126790080339	0.4762063386313855	F	F	F
0.8005912380703357	-0.0007490097574044	0.5456866413550636	T	T	T
0.5490244504816033	0.7499126790080339	0.3399638336347195	F	F	F
0.2990861941220047	0.5000000000000000	0.4081088797944261	F	F	F
0.8006337183973559	0.5004815393668098	0.5456757074341261	T	T	T
0.0491479377624131	0.2499126790080339	0.4762063386313855	F	F	F
0.5636188882733507	0.9858169865680837	0.5432803513161297	T	T	T
0.0617436404050409	0.4748515543136591	0.4081088797944261	F	F	F
0.2660299585409076	0.2498661471209173	0.6224079164790960	T	T	T
0.7864904914793769	0.7499126790080339	0.3331112591605603	F	F	F
0.0617436404050409	0.0251484456863409	0.4081088797944261	F	F	F
0.5635482853789795	0.5138875611354733	0.5432500878892398	T	T	T
0.7784628116464448	0.7499803189753678	0.6047565102435838	T	T	T
0.2864904914793769	0.2499126790080339	0.3468164081088787	F	F	F
0.2864904914793769	0.2499126790080339	0.4693537641572263	F	F	F
0.3116818967646324	0.7499126790080339	0.4693537641572263	F	F	F
0.8116818967646324	0.2499126790080339	0.4830589131055518	F	F	F
0.3116818967646324	0.7499126790080339	0.3468164081088787	F	F	F
0.8230330852510249	0.2499155177145319	0.6061498695406490	T	T	T
0.8116818967646324	0.2499126790080339	0.3331112591605603	F	F	F
0.3122676800242097	0.7497903044827234	0.6180204109680683	T	T	T
0.5364287478389755	0.9748515543136591	0.4081088797944261	F	F	F
0.0382300657320343	0.0122849654069121	0.5412711690655231	T	T	T
0.5364287478389755	0.5251484456863409	0.4081088797944261	F	F	F
0.0382466996872511	0.4875296334498531	0.5412786661839339	T	T	T
0.7864904914793769	0.7499126790080339	0.4830589131055518	F	F	F
0.5561240818011810	0.7409887386858840	0.7522243619353793	T	T	T
0.5630748234006563	0.5864186065300270	0.7828564205096120	T	T	T
0.5704343514819310	0.9004822688438368	0.7805001812080641	T	T	T
0.6591188451910404	0.7323770300993319	0.7179449691149368	T	T	T

0.4348479773481056 0.7438677515350164 0.7287609529077959 T T T

Transition state

Co	O	C	H
1.0000000000000000			
8.1500000000000004	0.0000000000000000	0.0000000000000000	
0.0000000000000000	5.7599999999999998	0.0000000000000000	
0.0000000000000000	0.0000000000000000	21.0139999999999993	

Co	O	C	H
14	20	1	4

Selective dynamics

Direct

0.6741170659422053	0.2499126790080385	0.4081088797944261	F	F	F
0.1854446782980312	0.7496267482144560	0.5480909959537932	T	T	T
0.9240553223018040	0.7499126790080342	0.4081088797944261	F	F	F
0.4148079938102294	0.2526471658623169	0.5495674270026445	T	T	T
0.2990861941220047	0.0000000000000000	0.4081088797944261	F	F	F
0.5464978207278869	0.7619173131169663	0.6150507024403500	T	T	T
0.0491479377624131	0.2499126790080385	0.3399638336347195	F	F	F
0.0507103702037799	0.2514948988390531	0.6087328601117837	T	T	T
0.5490244504816033	0.7499126790080342	0.4762063386313855	F	F	F
0.7984989468798878	0.9981257379673382	0.5454912976376777	T	T	T
0.5490244504816033	0.7499126790080342	0.3399638336347195	F	F	F
0.2990861941220047	0.5000000000000001	0.4081088797944261	F	F	F
0.7965659999511002	0.5037443858297513	0.5459213578253422	T	T	T
0.0491479377624131	0.2499126790080385	0.4762063386313855	F	F	F
0.5618316463575583	0.9800227122292857	0.5423368312395622	T	T	T
0.0617436404050409	0.4748515543136682	0.4081088797944261	F	F	F
0.2585201256974129	0.2608843190171372	0.6206735699830945	T	T	T
0.7864904914793769	0.7499126790080342	0.3331112591605603	F	F	F
0.0617436404050409	0.0251484456863409	0.4081088797944261	F	F	F
0.5604714343355973	0.5222841698873357	0.5431059874108788	T	T	T
0.7808647794155618	0.7519352364560283	0.6063605296350929	T	T	T
0.2864904914793769	0.2499126790080385	0.3468164081088787	F	F	F
0.2864904914793769	0.2499126790080385	0.4693537641572263	F	F	F
0.3116818967646324	0.7499126790080342	0.4693537641572263	F	F	F
0.8116818967646324	0.2499126790080385	0.4830589131055518	F	F	F
0.3116818967646324	0.7499126790080342	0.3468164081088787	F	F	F
0.8241656250016559	0.2509292513783517	0.6060960774066904	T	T	T
0.8116818967646324	0.2499126790080385	0.3331112591605603	F	F	F
0.3222170225294566	0.7698734448086346	0.6216319147323950	T	T	T
0.5364287478389755	0.9748515543136774	0.4081088797944261	F	F	F
0.0382902582835627	0.0166991163461976	0.5418436746538309	T	T	T
0.5364287478389755	0.5251484456863411	0.4081088797944261	F	F	F
0.0365207222114099	0.4847026953606762	0.5412984133324356	T	T	T
0.7864904914793769	0.7499126790080342	0.4830589131055518	F	F	F
0.5174804069878866	0.7079192767877535	0.7169073701283224	T	T	T
0.4184183406319552	0.6294926810317620	0.7466603500137298	T	T	T
0.6265042881480336	0.5950960153073825	0.7203474712167739	T	T	T
0.5420528575109536	0.8839737413781505	0.7350576359744716	T	T	T
0.3952383213718783	0.7143706476249558	0.6732829677771579	T	T	T

Chemisorption

Co	O	C	H
----	---	---	---

```

1.0000000000000000
 8.1500000000000004  0.0000000000000000  0.0000000000000000
 0.0000000000000000  5.7599999999999998  0.0000000000000000
 0.0000000000000000  0.0000000000000000  21.0139999999999993
Co   O   C   H
 14  20  1   4
Selective dynamics
Direct
0.6741170659422053  0.2499126790080339  0.4081088797944261  F  F  F
0.1797071954733845  0.7498569813444974  0.5467073665140060  T  T  T
0.9240553223018040  0.7499126790080339  0.4081088797944261  F  F  F
0.4134646764061969  0.2502722560292810  0.5506752971371058  T  T  T
0.2990861941220047  0.0000000000000000  0.4081088797944261  F  F  F
0.5611156577066557  0.7511434052005972  0.6163852887445544  T  T  T
0.0491479377624131  0.2499126790080339  0.3399638336347195  F  F  F
0.0473514631997892  0.2498222859273816  0.6093646868880681  T  T  T
0.5490244504816033  0.7499126790080339  0.4762063386313855  F  F  F
0.7975784994477673 -0.0016756493245440  0.5450237660728252  T  T  T
0.5490244504816033  0.7499126790080339  0.3399638336347195  F  F  F
0.2990861941220047  0.5000000000000000  0.4081088797944261  F  F  F
0.7976298150113614  0.5016526480875056  0.5450542862847221  T  T  T
0.0491479377624131  0.2499126790080339  0.4762063386313855  F  F  F
0.5616870907769081  0.9814445321455713  0.5420824018743955  T  T  T
0.0617436404050409  0.4748515543136591  0.4081088797944261  F  F  F
0.2568370366522460  0.2491349147793987  0.6222453580273243  T  T  T
0.7864904914793769  0.7499126790080339  0.3331112591605603  F  F  F
0.0617436404050409  0.0251484456863409  0.4081088797944261  F  F  F
0.5617218200976314  0.5189300854454046  0.5423122605848690  T  T  T
0.7892242856627117  0.7496876721521771  0.6056699387129575  T  T  T
0.2864904914793769  0.2499126790080339  0.3468164081088787  F  F  F
0.2864904914793769  0.2499126790080339  0.4693537641572263  F  F  F
0.3116818967646324  0.7499126790080339  0.4693537641572263  F  F  F
0.8116818967646324  0.2499126790080339  0.4830589131055518  F  F  F
0.3116818967646324  0.7499126790080339  0.3468164081088787  F  F  F
0.8196970410271234  0.2499063236761231  0.6063434816458277  T  T  T
0.8116818967646324  0.2499126790080339  0.3331112591605603  F  F  F
0.3301171168332585  0.7494351155796495  0.6200653693933541  T  T  T
0.5364287478389755  0.9748515543136591  0.4081088797944261  F  F  F
0.0357512559560398  0.0159848616493967  0.5409175170183153  T  T  T
0.5364287478389755  0.5251484456863409  0.4081088797944261  F  F  F
0.0358538236949870  0.4837370314190683  0.5409455129944418  T  T  T
0.7864904914793769  0.7499126790080339  0.4830589131055518  F  F  F
0.5752990627261074  0.7595731032995110  0.7095017391465849  T  T  T
0.4874045748542809  0.6302944910344974  0.7279673054323422  T  T  T
0.7023576526485765  0.7230838379362686  0.7238557894865816  T  T  T
0.5377298959013277  0.9391551967088851  0.7209749156513739  T  T  T
0.2825214544921450  0.7559848156534357  0.6624793556476427  T  T  T

```

(011)-A: Co₁₄O₂₀
β pair site:

Physisorption

Co	O	C	H			
1.0000000000000000						
8.1500000000000004	0.0000000000000000					
0.0000000000000000	5.7260000000000000					
0.0000000000000000	0.0000000000000000					21.0139999999999993

Co	O	C	H	
14	20	1	4	

Selective dynamics

Direct

0.6741170659422053	0.2499126790080339	0.4081088797944261	F	F	F
0.1865738280992613	0.7500335291442433	0.5477197921952282	T	T	T
0.9240553223018040	0.7499126790080339	0.4081088797944261	F	F	F
0.4110217174801963	0.2497598186888064	0.5502422834524477	T	T	T
0.2990861941220047	0.0000000000000000	0.4081088797944261	F	F	F
0.5394159004018384	0.7495784801784524	0.6094819636431421	T	T	T
0.0491479377624131	0.2499126790080339	0.3399638336347195	F	F	F
0.0544011186071860	0.2499191056879048	0.6111972073173753	T	T	T
0.5490244504816033	0.7499126790080339	0.4762063386313855	F	F	F
0.8005912380703357	-0.0007490097574044	0.5456866413550636	T	T	T
0.5490244504816033	0.7499126790080339	0.3399638336347195	F	F	F
0.2990861941220047	0.5000000000000000	0.4081088797944261	F	F	F
0.8006337183973559	0.5004815393668098	0.5456757074341261	T	T	T
0.0491479377624131	0.2499126790080339	0.4762063386313855	F	F	F
0.5636188882733507	0.9858169865680837	0.5432803513161297	T	T	T
0.0617436404050409	0.4748515543136591	0.4081088797944261	F	F	F
0.2660299585409076	0.2498661471209173	0.6224079164790960	T	T	T
0.7864904914793769	0.7499126790080339	0.3331112591605603	F	F	F
0.0617436404050409	0.0251484456863409	0.4081088797944261	F	F	F
0.5635482853789795	0.5138875611354733	0.5432500878892398	T	T	T
0.7784628116464448	0.7499803189753678	0.6047565102435838	T	T	T
0.2864904914793769	0.2499126790080339	0.3468164081088787	F	F	F
0.2864904914793769	0.2499126790080339	0.4693537641572263	F	F	F
0.3116818967646324	0.7499126790080339	0.4693537641572263	F	F	F
0.8116818967646324	0.2499126790080339	0.4830589131055518	F	F	F
0.3116818967646324	0.7499126790080339	0.3468164081088787	F	F	F
0.8230330852510249	0.2499155177145319	0.6061498695406490	T	T	T
0.8116818967646324	0.2499126790080339	0.3331112591605603	F	F	F
0.3122676800242097	0.7497903044827234	0.6180204109680683	T	T	T
0.5364287478389755	0.9748515543136591	0.4081088797944261	F	F	F
0.0382300657320343	0.0122849654069121	0.5412711690655231	T	T	T
0.5364287478389755	0.5251484456863409	0.4081088797944261	F	F	F
0.0382466996872511	0.4875296334498531	0.5412786661839339	T	T	T
0.7864904914793769	0.7499126790080339	0.4830589131055518	F	F	F
0.5561240818011810	0.7409887386858840	0.7522243619353793	T	T	T
0.5630748234006563	0.5864186065300270	0.7828564205096120	T	T	T
0.5704343514819310	0.9004822688438368	0.7805001812080641	T	T	T
0.6591188451910404	0.7323770300993319	0.7179449691149368	T	T	T
0.4348479773481056	0.7438677515350164	0.7287609529077959	T	T	T

Transition state

Co	O	C	H
1.0000000000000000			
8.1500000000000004	0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.7599999999999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0000000000000000	21.0139999999999993

Co	O	C	H
14	20	1	4

Selective dynamics

Direct

0.6741170659422053	0.2499126790080376	0.4081088797944261	F	F	F
0.1785876396967025	0.7518876984596019	0.5454513252885710	T	T	T
0.9240553223018040	0.7499126790080342	0.4081088797944261	F	F	F
0.4153307560280415	0.2499140261898830	0.5496215857736853	T	T	T
0.2990861941220047	0.0000000000000000	0.4081088797944261	F	F	F
0.5090479615486090	0.7485300202761253	0.6097571204270883	T	T	T
0.0491479377624131	0.2499126790080376	0.3399638336347195	F	F	F
0.0587510529085903	0.2528425628579876	0.6115555755356052	T	T	T
0.5490244504816033	0.7499126790080342	0.4762063386313855	F	F	F
0.8032778390305383	0.0000738908240035	0.5458984753521373	T	T	T
0.5490244504816033	0.7499126790080342	0.3399638336347195	F	F	F
0.2990861941220047	0.5000000000000001	0.4081088797944261	F	F	F
0.8030523940904595	0.5012353847117235	0.5457891190111103	T	T	T
0.0491479377624131	0.2499126790080376	0.4762063386313855	F	F	F
0.5643926446020932	0.9792505307017777	0.5458944176330117	T	T	T
0.0617436404050409	0.4748515543136664	0.4081088797944261	F	F	F
0.2705731300725324	0.2545004264316217	0.6222736867115204	T	T	T
0.7864904914793769	0.7499126790080342	0.3331112591605603	F	F	F
0.0617436404050409	0.0251484456863409	0.4081088797944261	F	F	F
0.5655936819640490	0.5196049942251393	0.5458872948131328	T	T	T
0.8112023343578805	0.7500654372695789	0.6038700812705683	T	T	T
0.2864904914793769	0.2499126790080376	0.3468164081088787	F	F	F
0.2864904914793769	0.2499126790080376	0.4693537641572263	F	F	F
0.3116818967646324	0.7499126790080342	0.4693537641572263	F	F	F
0.8116818967646324	0.2499126790080376	0.4830589131055518	F	F	F
0.3116818967646324	0.7499126790080342	0.3468164081088787	F	F	F
0.8264441610251912	0.2511216171509355	0.6064285706094771	T	T	T
0.8116818967646324	0.2499126790080376	0.3331112591605603	F	F	F
0.2829124091196530	0.7547167437274155	0.6201212230167558	T	T	T
0.5364287478389755	0.9748515543136739	0.4081088797944261	F	F	F
0.0387217300260456	0.0172792870267434	0.5404706267440761	T	T	T
0.5364287478389755	0.5251484456863411	0.4081088797944261	F	F	F
0.0387022657915285	0.4852577450782277	0.5399859084655509	T	T	T
0.7864904914793769	0.7499126790080342	0.4830589131055518	F	F	F
0.6149766643486119	0.7437738505329754	0.7045691374645533	T	T	T
0.4825450518232271	0.7780834281644244	0.7131970380459441	T	T	T
0.6841723964949873	0.8829757561803839	0.7285898475075371	T	T	T
0.6456474743477673	0.5718127962129319	0.7241816975408382	T	T	T
0.7096725011482916	0.7498191241894253	0.6530618152155443	T	T	T

Chemisorption

Co	O	C	H
1.0000000000000000			
8.1500000000000004	0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.7599999999999998	0.0000000000000000	0.0000000000000000

```

0.00000000000000000000 0.00000000000000000000 21.01399999999999993
Co O C H
14 20 1 4
Selective dynamics
Direct
0.6741170659422053 0.2499126790080339 0.4081088797944261 F F F
0.1874035662032840 0.7501088012275163 0.5456381485120507 T T T
0.9240553223018040 0.7499126790080339 0.4081088797944261 F F F
0.4137710356949477 0.2481572229156786 0.5507882860798147 T T T
0.2990861941220047 0.000000000000000000 0.4081088797944261 F F F
0.5237113404163698 0.7454577671769540 0.6133937693542654 T T T
0.0491479377624131 0.2499126790080339 0.3399638336347195 F F F
0.0579328072539612 0.2508605889096429 0.6101563097554110 T T T
0.5490244504816033 0.7499126790080339 0.4762063386313855 F F F
0.7990070814495021 0.0033027611338624 0.5448141021981572 T T T
0.5490244504816033 0.7499126790080339 0.3399638336347195 F F F
0.2990861941220047 0.500000000000000000 0.4081088797944261 F F F
0.7995008654843896 0.4970656254287528 0.5447700458721760 T T T
0.0491479377624131 0.2499126790080339 0.4762063386313855 F F F
0.5623114002371298 0.9817323518947979 0.5431628810453102 T T T
0.0617436404050409 0.4748515543136591 0.4081088797944261 F F F
0.2679823090153045 0.2535471755664499 0.6238230787309337 T T T
0.7864904914793769 0.7499126790080339 0.3331112591605603 F F F
0.0617436404050409 0.0251484456863409 0.4081088797944261 F F F
0.5626420266269960 0.5183072756253978 0.5436861205656690 T T T
0.7738589245881751 0.7498633582706637 0.6062192019258084 T T T
0.2864904914793769 0.2499126790080339 0.3468164081088787 F F F
0.2864904914793769 0.2499126790080339 0.4693537641572263 F F F
0.3116818967646324 0.7499126790080339 0.4693537641572263 F F F
0.8116818967646324 0.2499126790080339 0.4830589131055518 F F F
0.3116818967646324 0.7499126790080339 0.3468164081088787 F F F
0.8221404183332682 0.2503188301447007 0.6064118863601714 T T T
0.8116818967646324 0.2499126790080339 0.3331112591605603 F F F
0.3026541694456132 0.7549925914866308 0.6165747238476925 T T T
0.5364287478389755 0.9748515543136591 0.4081088797944261 F F F
0.0365578874557698 0.0126536735345876 0.5413611681252042 T T T
0.5364287478389755 0.5251484456863409 0.4081088797944261 F F F
0.0366258746253069 0.4885833027052066 0.5411398348280790 T T T
0.7864904914793769 0.7499126790080339 0.4830589131055518 F F F
0.5407082649142878 0.7370851563080197 0.7055193052017443 T T T
0.4181101429557673 0.7653509248163775 0.7258305524899713 T T T
0.6284531430522476 0.8736794277874100 0.7199101388908352 T T T
0.5876372302418158 0.5607090242801022 0.7156569517982334 T T T
0.8409308215951361 0.7504636906363292 0.6446695177044397 T T T

```

(011)-B: Co₁₆O₂₀
a pair site:

Physisorption

Co O
 1.0000000000000000
 8.1500000000000004 0.0000000000000000 0.0000000000000000
 0.0000000000000000 5.7599999999999998 0.0000000000000000
 0.0000000000000000 0.0000000000000000 20.7259999999999991

Co O C H
 16 20 1 4

Selective dynamics

Direct

0.9560385280316126	0.0064617534055174	0.5008684743800060	F	F	F
0.4252180413256444	0.5155254711664656	0.6279197529289494	T	T	T
0.4528278587305508	0.5031435557107926	0.3618643250024149	F	F	F
0.2012842677204247	0.5031435557107926	0.5008684743800060	F	F	F
0.7044949370214866	0.0064617534055174	0.3618643250024149	F	F	F
0.7344906697973171	0.0056897834436053	0.6275489650672182	T	T	T
0.5786613978760187	0.7548026545581550	0.5008684743800060	F	F	F
0.8302049888861447	0.5031435557107926	0.4313905239795446	F	F	F
0.3309187265670525	0.0049275246063951	0.5721632728612670	T	T	T
0.3271178068658926	0.0064617534055174	0.4313905239795446	F	F	F
0.8267593287266266	0.5053935959013535	0.5721117295088962	T	T	T
0.0786494256221806	0.7598956053283735	0.6371285361800809	T	T	T
0.0754507285749568	0.7548026545581550	0.3618643250024149	F	F	F
0.0808918364144405	0.2598995158644402	0.6314156786698083	T	T	T
0.0754507285749568	0.2516590988473624	0.3618643250024149	F	F	F
0.5786613978760187	0.2516590988473624	0.5008684743800060	F	F	F
0.3409483823166184	0.2238910234020253	0.5008684743800060	F	F	F
0.5648308224252929	0.0000000000000000	0.4390620476695943	F	F	F
0.5653417694205071	0.0024449267439045	0.5633550729631990	T	T	T
0.0616201531242311	0.5031435557107926	0.4237190002894948	F	F	F
0.8545527281958616	0.2764007020198138	0.6394314032763271	T	T	T
0.8441590516176802	0.2794271742926995	0.3618643250024149	F	F	F
0.8441590516176802	0.7270345791128179	0.3618643250024149	F	F	F
0.8163744134354189	0.2794271742926995	0.5008684743800060	F	F	F
0.5919123144808676	0.5021797934875829	0.5631080232767901	T	T	T
0.0894047913064924	0.0064617534055174	0.4237190002894948	F	F	F
0.3131637441343571	0.2238910234020253	0.3618643250024149	F	F	F
0.3076619833376781	0.2411164125988172	0.6364949919925920	T	T	T
0.0968192672230680	0.0104202723336212	0.5767180558867351	T	T	T
0.5924919733267444	0.5031435557107926	0.4390620476695943	F	F	F
0.3131637441343571	0.7825707300034921	0.3618643250024149	F	F	F
0.3077825582651247	0.7841742329427692	0.6418689513623740	T	T	T
0.8163744134354189	0.7270345791128179	0.5008684743800060	F	F	F
0.8476966928182238	0.7323928939609590	0.6396550536599221	T	T	T
0.0604813184132541	0.5065829070456959	0.5762171195777740	T	T	T
0.3409483823166184	0.7825707300034921	0.5008684743800060	F	F	F
0.1284940535846714	0.2961734210048280	0.7868057152562927	T	T	T
0.0771501397249602	0.4628321431790865	0.7696966970413356	T	T	T
0.1519105919154471	0.3093255365502229	0.8388196041483076	T	T	T
0.2440935575053918	0.2573919118774409	0.7615041294034032	T	T	T
0.0386214414253538	0.1566473821737083	0.7779667327427042	T	T	T

Transition state

Co	O	C	H
1.0000000000000000			
8.1500000000000004		0.0000000000000000	0.0000000000000000
0.0000000000000000		5.7599999999999998	0.0000000000000000
0.0000000000000000		0.0000000000000000	20.7259999999999991

Co	O	C	H
16	20	1	4

Selective dynamics

Direct

0.9560385280316136	0.0064617534055173	0.5008684743800060	F	F	F
0.4366561378555990	0.5221479308094907	0.6310087025422663	T	T	T
0.4528278587305508	0.5031435557107925	0.3618643250024149	F	F	F
0.2012842677204247	0.5031435557107925	0.5008684743800060	F	F	F
0.7044949370214866	0.0064617534055173	0.3618643250024149	F	F	F
0.7353845052101171	0.9973916447840548	0.6253361187633456	T	T	T
0.5786613978760187	0.7548026545581492	0.5008684743800060	F	F	F
0.8302049888861455	0.5031435557107925	0.4313905239795445	F	F	F
0.3295224625467898	0.0048972020976473	0.5730501745205667	T	T	T
0.3271178068658926	0.0064617534055173	0.4313905239795445	F	F	F
0.8264034925329348	0.5028524218247913	0.5717330830026053	T	T	T
0.0768309869434051	0.7532045627146084	0.6354348717598231	T	T	T
0.0754507285749568	0.7548026545581492	0.3618643250024149	F	F	F
0.0712369954646496	0.2578466696874548	0.6379254800950035	T	T	T
0.0754507285749568	0.2516590988473623	0.3618643250024149	F	F	F
0.5786613978760187	0.2516590988473623	0.5008684743800060	F	F	F
0.3409483823166184	0.2238910234020227	0.5008684743800060	F	F	F
0.5648308224252934	0.0000000000000000	0.4390620476695943	F	F	F
0.5642980544069895	0.0022847811234456	0.5632144211181797	T	T	T
0.0616201531242311	0.5031435557107925	0.4237190002894948	F	F	F
0.8415381557956430	0.2749169752148379	0.6391010585817665	T	T	T
0.8441590516176802	0.2794271742926990	0.3618643250024149	F	F	F
0.8441590516176802	0.7270345791128178	0.3618643250024149	F	F	F
0.8163744134354189	0.2794271742926990	0.5008684743800060	F	F	F
0.5919275437928860	0.5017422847709425	0.5626439676108778	T	T	T
0.0894047913064924	0.0064617534055173	0.4237190002894948	F	F	F
0.3131637441343571	0.2238910234020227	0.3618643250024149	F	F	F
0.3168643000362373	0.2403666299250831	0.6421098589572121	T	T	T
0.0959973859574052	0.0107688303651242	0.5772107604580419	T	T	T
0.5924919733267444	0.5031435557107925	0.4390620476695943	F	F	F
0.3131637441343571	0.7825707300034889	0.3618643250024149	F	F	F
0.3068557978279008	0.7818784774846002	0.6417936342811655	T	T	T
0.8163744134354189	0.7270345791128178	0.5008684743800060	F	F	F
0.8443849392041839	0.7257882638662351	0.6409980403250150	T	T	T
0.0613780867615666	0.4994313761491769	0.5760825342575460	T	T	T
0.3409483823166184	0.7825707300034889	0.5008684743800060	F	F	F
0.1046203204831177	0.2283372912490515	0.7398626580349303	T	T	T
0.9743849603020189	0.2798422958414137	0.7405664224706167	T	T	T
0.1730997737017598	0.3585561346608024	0.7684350909334474	T	T	T
0.2319235903431437	0.2175661292155363	0.6933037510837083	T	T	T
0.1159876308445013	0.0538976388540303	0.7615268978018140	T	T	T

Chemisorption

Co O

1.0000000000000000
 8.15000000000000004 0.0000000000000000 0.0000000000000000
 0.0000000000000000 5.7599999999999998 0.0000000000000000
 0.0000000000000000 0.0000000000000000 20.7259999999999991

Co O C H
 16 20 1 4

Selective dynamics

Direct

0.9560385280316126	0.0064617534055174	0.5008684743800060	F	F	F
0.4423317362443154	0.5304343908859108	0.6325512002366733	T	T	T
0.4528278587305508	0.5031435557107926	0.3618643250024149	F	F	F
0.2012842677204247	0.5031435557107926	0.5008684743800060	F	F	F
0.7044949370214866	0.0064617534055174	0.3618643250024149	F	F	F
0.7405505781144944	-0.0059047416281930	0.6235440291767700	T	T	T
0.5786613978760187	0.7548026545581550	0.5008684743800060	F	F	F
0.8302049888861447	0.5031435557107926	0.4313905239795446	F	F	F
0.3289658202494839	0.0044380214339594	0.5711004230434772	T	T	T
0.3271178068658926	0.0064617534055174	0.4313905239795446	F	F	F
0.8286684025394943	0.5014249266876293	0.5720842686882119	T	T	T
0.0772613179214127	0.7555424104513034	0.6366520476856509	T	T	T
0.0754507285749568	0.7548026545581550	0.3618643250024149	F	F	F
0.0653418195633269	0.2545502903219486	0.6427939178163823	T	T	T
0.0754507285749568	0.2516590988473624	0.3618643250024149	F	F	F
0.5786613978760187	0.2516590988473624	0.5008684743800060	F	F	F
0.3409483823166184	0.2238910234020253	0.5008684743800060	F	F	F
0.5648308224252929	0.0000000000000000	0.4390620476695943	F	F	F
0.5642215410669514	0.0035458804859446	0.5630717103485935	T	T	T
0.0616201531242311	0.5031435557107926	0.4237190002894948	F	F	F
0.8358583587106959	0.2785053707277736	0.6401984402642124	T	T	T
0.8441590516176802	0.2794271742926995	0.3618643250024149	F	F	F
0.8441590516176802	0.7270345791128179	0.3618643250024149	F	F	F
0.8163744134354189	0.2794271742926995	0.5008684743800060	F	F	F
0.5926226749089557	0.5029404714265784	0.5629021096471469	T	T	T
0.0894047913064924	0.0064617534055174	0.4237190002894948	F	F	F
0.3131637441343571	0.2238910234020253	0.3618643250024149	F	F	F
0.3176980585222217	0.2372372012155811	0.6427309850942725	T	T	T
0.0975055137984846	0.0153586723872550	0.5757020019055399	T	T	T
0.5924919733267444	0.5031435557107926	0.4390620476695943	F	F	F
0.3131637441343571	0.7825707300034921	0.3618643250024149	F	F	F
0.3181696006675639	0.7945990288821084	0.6463139926043372	T	T	T
0.8163744134354189	0.7270345791128179	0.5008684743800060	F	F	F
0.8410135763499442	0.7227732153339933	0.6430871505754233	T	T	T
0.0643064909072556	0.4955934046094789	0.5762589536221326	T	T	T
0.3409483823166184	0.7825707300034921	0.5008684743800060	F	F	F
0.0704394845997143	0.2297026516814315	0.7374795144226250	T	T	T
0.9457522856472897	0.2627318896804611	0.7558013593698383	T	T	T
0.1582037394022677	0.3613158234219133	0.7555128986598550	T	T	T
0.3470329031878631	0.1208212973664673	0.6758745897321239	T	T	T
0.1136062602802730	0.0546567313385282	0.7516220903672404	T	T	T

(011)-B: Co₁₆O₂₀
β pair site:

Physisorption

Co O

1.0000000000000000		
8.15000000000000004	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.7599999999999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.7259999999999991

Co	O	C	H
16	20	1	4

Selective dynamics

Direct

0.9560385280316126	0.0064617534055174	0.5008684743800060	F	F	F
0.4306812206738115	0.5060280919839908	0.6310090242180476	T	T	T
0.4528278587305508	0.5031435557107926	0.3618643250024149	F	F	F
0.2012842677204247	0.5031435557107926	0.5008684743800060	F	F	F
0.7044949370214866	0.0064617534055174	0.3618643250024149	F	F	F
0.7392659788935813	0.0004076895877197	0.6247626624506077	T	T	T
0.5786613978760187	0.7548026545581550	0.5008684743800060	F	F	F
0.8302049888861447	0.5031435557107926	0.4313905239795446	F	F	F
0.3295642992885753	0.0024015053229313	0.5726756458226070	T	T	T
0.3271178068658926	0.0064617534055174	0.4313905239795446	F	F	F
0.8270776566298943	0.5043579386853705	0.5721089372062417	T	T	T
0.0789798425168128	0.7514486687293425	0.6374067846108833	T	T	T
0.0754507285749568	0.7548026545581550	0.3618643250024149	F	F	F
0.0798846681929786	0.2557724103410018	0.6311566778271819	T	T	T
0.0754507285749568	0.2516590988473624	0.3618643250024149	F	F	F
0.5786613978760187	0.2516590988473624	0.5008684743800060	F	F	F
0.3409483823166184	0.2238910234020253	0.5008684743800060	F	F	F
0.5648308224252929	0.0000000000000000	0.4390620476695943	F	F	F
0.5643004085731493	0.0040188431159735	0.5634566395896782	T	T	T
0.0616201531242311	0.5031435557107926	0.4237190002894948	F	F	F
0.8523716172092693	0.2751903118320452	0.6393614857224639	T	T	T
0.8441590516176802	0.2794271742926995	0.3618643250024149	F	F	F
0.8441590516176802	0.7270345791128179	0.3618643250024149	F	F	F
0.8163744134354189	0.2794271742926995	0.5008684743800060	F	F	F
0.5921197894398168	0.5030605650626601	0.5632709671342957	T	T	T
0.0894047913064924	0.0064617534055174	0.4237190002894948	F	F	F
0.3131637441343571	0.2238910234020253	0.3618643250024149	F	F	F
0.3032239365487397	0.2332318912831681	0.6390512387022811	T	T	T
0.0958184401771855	0.0039154343413734	0.5771166345556860	T	T	T
0.5924919733267444	0.5031435557107926	0.4390620476695943	F	F	F
0.3131637441343571	0.7825707300034921	0.3618643250024149	F	F	F
0.3091328917108323	0.7783958107880371	0.6406507554029554	T	T	T
0.8163744134354189	0.7270345791128179	0.5008684743800060	F	F	F
0.8471259807279751	0.7274537763932594	0.6414427558947825	T	T	T
0.0611427712813706	0.5039942912277448	0.5764626741572374	T	T	T
0.3409483823166184	0.7825707300034921	0.5008684743800060	F	F	F
0.4772555050851354	0.5171057825083879	0.7784956435195710	T	T	T
0.4144233492365436	0.6803492857037458	0.7658491164484609	T	T	T
0.4758972408643867	0.4949384185457553	0.8310951271956771	T	T	T
0.6059628304249517	0.5225305396637693	0.7618877945091566	T	T	T
0.4126221486214954	0.3679235772035022	0.7566746494750503	T	T	T

Transition state

```
Co   O   C   H
    1.0000000000000000
    8.1500000000000004    0.0000000000000000    0.0000000000000000
    0.0000000000000000    5.7599999999999998    0.0000000000000000
    0.0000000000000000    0.0000000000000000    20.7259999999999991
```

```
Co   O   C   H
16  20  1   4
```

Selective dynamics

Direct

```
0.9560385280316130  0.0064617534055174  0.5008684743800060  F F F
0.4389449388589660  0.5215552617262650  0.6362711973054850  T T T
0.4528278587305510  0.5031435557107929  0.3618643250024150  F F F
0.2012842677204250  0.5031435557107929  0.5008684743800060  F F F
0.7044949370214870  0.0064617534055174  0.3618643250024150  F F F
0.7411990029843660  0.9966267871261451  0.6233557269722390  T T T
0.5786613978760190  0.7548026545581550  0.5008684743800060  F F F
0.8302049888861450  0.5031435557107929  0.4313905239795450  F F F
0.3304692236518410  0.0014380211793135  0.5708488865351440  T T T
0.3271178068658930  0.0064617534055174  0.4313905239795450  F F F
0.8276123040396510  0.5027039701776070  0.5717695254322940  T T T
0.0821872036283379  0.7498538777796260  0.6361320889722190  T T T
0.0754507285749568  0.7548026545581550  0.3618643250024150  F F F
0.0706515422906880  0.2468552387474290  0.6361417732529300  T T T
0.0754507285749568  0.2516590988473620  0.3618643250024150  F F F
0.5786613978760190  0.2516590988473620  0.5008684743800060  F F F
0.3409483823166180  0.2238910234020250  0.5008684743800060  F F F
0.5648308224252930  0.0000000000000000  0.4390620476695940  F F F
0.5657434929740490  0.0034941113699312  0.5631966934301660  T T T
0.0616201531242311  0.5031435557107929  0.4237190002894950  F F F
0.8421222649297940  0.2749595581966340  0.6398374573646139  T T T
0.8441590516176800  0.2794271742926990  0.3618643250024150  F F F
0.8441590516176800  0.7270345791128180  0.3618643250024150  F F F
0.8163744134354191  0.2794271742926990  0.5008684743800060  F F F
0.5896688929175190  0.5031632793559290  0.5637868746539030  T T T
0.0894047913064924  0.0064617534055174  0.4237190002894950  F F F
0.3131637441343570  0.2238910234020250  0.3618643250024150  F F F
0.3157138283987130  0.2292243384312510  0.6420341137451741  T T T
0.0986447848071531  0.0010854353046268  0.5754150809385140  T T T
0.5924919733267440  0.5031435557107929  0.4390620476695940  F F F
0.3131637441343570  0.7825707300034920  0.3618643250024150  F F F
0.3119799869095290  0.7864172811648830  0.6426409458450960  T T T
0.8163744134354191  0.7270345791128180  0.5008684743800060  F F F
0.8505040787190520  0.7285306931231100  0.6399794920263741  T T T
0.0625628222030751  0.4996829833178830  0.5763417060783820  T T T
0.3409483823166180  0.7825707300034920  0.5008684743800060  F F F
0.5056680780083380  0.5325940608749730  0.7393524485114310  T T T
0.4165236758606750  0.5291684546573771  0.7734034338941980  T T T
0.5504547234011500  0.6913006127264050  0.7421544881932460  T T T
0.3619235752347620  0.1687324711936570  0.6932937757774700  T T T
0.5913723726075890  0.4090741501765030  0.7406126285087971  T T T
```

Chemisorption

```
Co   O
```

1.0000000000000000
 8.15000000000000004 0.0000000000000000 0.0000000000000000
 0.0000000000000000 5.7599999999999998 0.0000000000000000
 0.0000000000000000 0.0000000000000000 20.7259999999999991

Co O C H
 16 20 1 4

Selective dynamics

Direct

0.9560385280316126	0.0064617534055174	0.5008684743800060	F	F	F
0.4427689010683682	0.5262438376439206	0.6384733950611717	T	T	T
0.4528278587305508	0.5031435557107926	0.3618643250024149	F	F	F
0.2012842677204247	0.5031435557107926	0.5008684743800060	F	F	F
0.7044949370214866	0.0064617534055174	0.3618643250024149	F	F	F
0.7430939881086808	-0.0047722985507506	0.6224632728188889	T	T	T
0.5786613978760187	0.7548026545581550	0.5008684743800060	F	F	F
0.8302049888861447	0.5031435557107926	0.4313905239795446	F	F	F
0.3311190952472166	0.0008119727239179	0.5704032749169051	T	T	T
0.3271178068658926	0.0064617534055174	0.4313905239795446	F	F	F
0.8277032773205201	0.5027393121843999	0.5719442907372955	T	T	T
0.0828969445621474	0.7483107390067854	0.6361052238346396	T	T	T
0.0754507285749568	0.7548026545581550	0.3618643250024149	F	F	F
0.0682208158063498	0.2451795525661653	0.6364209078816442	T	T	T
0.0754507285749568	0.2516590988473624	0.3618643250024149	F	F	F
0.5786613978760187	0.2516590988473624	0.5008684743800060	F	F	F
0.3409483823166184	0.2238910234020253	0.5008684743800060	F	F	F
0.5648308224252929	0.0000000000000000	0.4390620476695943	F	F	F
0.5652703817126605	0.0035514798201115	0.5628225006009241	T	T	T
0.0616201531242311	0.5031435557107926	0.4237190002894948	F	F	F
0.8414175704583073	0.2767006600519308	0.6402425858953518	T	T	T
0.8441590516176802	0.2794271742926995	0.3618643250024149	F	F	F
0.8441590516176802	0.7270345791128179	0.3618643250024149	F	F	F
0.8163744134354189	0.2794271742926995	0.5008684743800060	F	F	F
0.5890052923919126	0.5032757637011799	0.5640100175698345	T	T	T
0.0894047913064924	0.0064617534055174	0.4237190002894948	F	F	F
0.3131637441343571	0.2238910234020253	0.3618643250024149	F	F	F
0.3179806793175090	0.2289994372797263	0.6424655432967162	T	T	T
0.0992040777363144	0.0004218914188656	0.5757902654547371	T	T	T
0.5924919733267444	0.5031435557107926	0.4390620476695943	F	F	F
0.3131637441343571	0.7825707300034921	0.3618643250024149	F	F	F
0.3136810594498439	0.7885707678520909	0.6430256412404339	T	T	T
0.8163744134354189	0.7270345791128179	0.5008684743800060	F	F	F
0.8515691920136109	0.7263520005961694	0.6403631101114284	T	T	T
0.0632891650328020	0.4981146124948571	0.5763621441758497	T	T	T
0.3409483823166184	0.7825707300034921	0.5008684743800060	F	F	F
0.5131759891686829	0.5369602285662551	0.7284912782463762	T	T	T
0.3995940557944062	0.5384296711404161	0.7574232432561815	T	T	T
0.5877203372832088	0.6944564931669768	0.7355938405389715	T	T	T
0.3476038074550976	0.1139204872038006	0.6757677785551111	T	T	T
0.5871133638081251	0.3778574858851975	0.7347892238681296	T	T	T

Table S4. Fractional Coordinates of the Stationary States Shown in Figure 4.

(112)

α pair site:

Physisorption

Co3O4

1.0000000000000000		
5.7629999999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.115000000000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.1189999999999998

Co	O	C	H	
18	26	1	4	

Selective dynamics

Direct

0.3678639597431896	0.4704923839886632	0.4918667294314574	F	F	F
0.8677771993753254	0.8038257173219989	0.4048328887494108	F	F	F
0.8724568235237135	0.1346607728107894	0.5730368631680079	T	T	T
0.8841500894604670	0.3624566786733863	0.5870338601639303	T	T	T
0.3678639597431896	0.7205100956429362	0.4918667294314574	F	F	F
0.8677771993753254	0.0538434289762648	0.4048328887494108	F	F	F
0.3678639597431896	0.0955012398157962	0.4918667294314574	F	F	F
0.8677771993753254	0.5955366631243351	0.4918667294314574	F	F	F
0.6330640650099483	0.5745892471233754	0.6146214832032060	T	T	T
0.3678639597431896	0.9288699964576708	0.4048328887494108	F	F	F
0.1178205795592575	0.2622033297909994	0.4483498090904305	F	F	F
0.8677771993753254	0.4288345731491319	0.4048328887494108	F	F	F
0.1798662217182720	0.5757197010427604	0.5893558852140305	T	T	T
0.3783051120660100	0.2601271330490934	0.5813208348989063	T	T	T
0.8642480784003795	0.7746902173863552	0.5797450807286557	T	T	T
0.1187409560667118	0.9303727218249944	0.5395283989355100	T	T	T
0.6179073399271218	0.2622033297909994	0.4483498090904305	F	F	F
0.6151652266130595	0.9301640898443356	0.5371096062857170	T	T	T
0.3678639597431896	0.8592986184909677	0.4918667294314574	F	F	F
0.8677771993753254	0.3409139213602543	0.4822427951252664	F	F	F
0.0902307825785158	0.3409139213602543	0.3661279355614866	F	F	F
0.1404347192232935	0.3156286327084438	0.6265422417951400	T	T	T
0.6323372452830397	0.3120888784776525	0.6244013026099808	T	T	T
0.3680511566752003	0.0062820118754739	0.5694390606171500	T	T	T
0.6458161728484241	0.6753578511763513	0.5462548653943915	T	T	T
0.8677771993753254	0.1926319518243034	0.4048328887494108	F	F	F
0.6454971369078635	0.3409139213602543	0.3661279355614866	F	F	F
0.3678639597431896	0.6742472546935900	0.3952089544432269	F	F	F
0.8996543887200725	0.5120334518152638	0.5806027639067972	T	T	T
0.5903175429463801	0.0075805880269186	0.4531617762435260	F	F	F
0.8677771993753254	0.8500885582713451	0.5014383597468495	F	F	F
0.3678639597431896	0.3317038611406318	0.4918667294314574	F	F	F
0.8677771993753254	0.6650371944739604	0.4048328887494108	F	F	F
0.1065174878478706	0.8435166435535888	0.6070555329536245	T	T	T
0.5899104749474295	0.1791562554613835	0.5314199069996287	T	T	T
0.6454971369078635	0.5167552249380094	0.4435378419373421	F	F	F
0.8745898147651026	0.0027051917029186	0.5713786577090659	T	T	T
0.3678639597431896	0.1834218916046737	0.4144568230556018	F	F	F

0.3951585552767217	0.4882648374980422	0.5937377988723692	T	T	T
0.6435354586322231	0.8449217041771495	0.6103536700180915	T	T	T
0.1506777623439289	0.1815210348071160	0.5309181035351459	T	T	T
0.0902307825785158	0.5167552249380094	0.4435378419373421	F	F	F
0.1454103765399992	0.0075805880269186	0.4531617762435260	F	F	F
0.0799403092717499	0.6793999594157821	0.5406242916527428	T	T	T
0.6809973492348367	0.5795735564839508	0.7467347528641296	T	T	T
0.5600816860610549	0.5298538094754838	0.7206485563490188	T	T	T
0.8529103033809896	0.5472257721601638	0.7511083536649963	T	T	T
0.6921460086699029	0.6498738402533940	0.7214852393227921	T	T	T
0.6078790752557960	0.5919009524249940	0.7989272046817636	T	T	T

Transition state

Co	O	C	H
1.0000000000000000			
5.7629999999999999	0.0000000000000000	0.0000000000000000	
0.0000000000000000	14.1150000000000002	0.0000000000000000	
0.0000000000000000	0.0000000000000000	19.1189999999999998	

Co	O	C	H
18	26	1	4

Selective dynamics

Direct

0.3678639597431896	0.4704923839886630	0.4918667294314574	F	F	F
0.8677771993753254	0.8038257173219987	0.4048328887494108	F	F	F
0.8691541503404966	0.1317560677573128	0.5726098451211081	T	T	T
0.8673727027707271	0.3696184881921721	0.5846254172228840	T	T	T
0.3678639597431896	0.7205100956429360	0.4918667294314574	F	F	F
0.8677771993753254	0.0538434289762648	0.4048328887494108	F	F	F
0.3678639597431896	0.0955012398157962	0.4918667294314574	F	F	F
0.8677771993753254	0.5955366631243351	0.4918667294314574	F	F	F
0.6413758292603577	0.5851966483611687	0.6263803911710273	T	T	T
0.3678639597431896	0.9288699964576708	0.4048328887494108	F	F	F
0.1178205795592575	0.2622033297909994	0.4483498090904305	F	F	F
0.8677771993753254	0.4288345731491316	0.4048328887494108	F	F	F
0.1570646694854855	0.5680031546267506	0.6008743015342574	T	T	T
0.3673957218023873	0.2645605148859838	0.5827371652381214	T	T	T
0.8635728239649301	0.7689988865099758	0.5843667907089067	T	T	T
0.1177622622896243	0.9275865131180780	0.5403452509985320	T	T	T
0.6179073399271218	0.2622033297909994	0.4483498090904305	F	F	F
0.6179987663356409	0.9278634143625133	0.5381101512814053	T	T	T
0.3678639597431896	0.8592986184909673	0.4918667294314574	F	F	F
0.8677771993753254	0.3409139213602543	0.4822427951252664	F	F	F
0.0902307825785158	0.3409139213602543	0.3661279355614866	F	F	F
0.1193150991541366	0.3201045251367238	0.6230118432997028	T	T	T
0.6084958890607070	0.3246188581569557	0.6218639256473387	T	T	T
0.3682255845525804	0.0059493461646588	0.5691921419389152	T	T	T
0.6402196048582918	0.6715458143964805	0.5448097548389016	T	T	T
0.8677771993753254	0.1926319518243033	0.4048328887494108	F	F	F
0.6454971369078635	0.3409139213602543	0.3661279355614866	F	F	F
0.3678639597431896	0.6742472546935900	0.3952089544432269	F	F	F
0.8718551335139769	0.5100445104963665	0.5764598469559777	T	T	T
0.5903175429463801	0.0075805880269186	0.4531617762435261	F	F	F
0.8677771993753254	0.8500885582713448	0.5014383597468495	F	F	F
0.3678639597431896	0.3317038611406317	0.4918667294314574	F	F	F

0.8677771993753254	0.6650371944739604	0.4048328887494108	F	F	F
0.1073442947257456	0.8452862688731620	0.6090821103767154	T	T	T
0.5881227974694153	0.1810182681242372	0.5327242547651596	T	T	T
0.6454971369078635	0.5167552249380094	0.4435378419373422	F	F	F
0.8723370960971745	0.0011590894528004	0.5710062220718238	T	T	T
0.3678639597431896	0.1834218916046737	0.4144568230556018	F	F	F
0.3534069709240645	0.5299707182305033	0.6651223884413298	T	T	T
0.6455286959163717	0.8449997214058521	0.6124207250022180	T	T	T
0.1497933487143643	0.1809256150668737	0.5324554044022869	T	T	T
0.0902307825785158	0.5167552249380094	0.4435378419373422	F	F	F
0.1454103765399992	0.0075805880269186	0.4531617762435261	F	F	F
0.0961012270151410	0.6731288367796595	0.5422733562058691	T	T	T
0.7053060184784546	0.5855287837848197	0.7396315563243177	T	T	T
0.4913578736566691	0.5530951376810108	0.7070686947469066	T	T	T
0.8507352641593340	0.5355581313089854	0.7431982071025416	T	T	T
0.7625557247518566	0.6592576775425451	0.7455135515119858	T	T	T
0.5898358860643830	0.5711022757515845	0.7846278868488474	T	T	T

Chemisorption

Co3O4

1.0000000000000000		
5.7629999999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.1150000000000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.1189999999999998

Co O C H
18 26 1 4

Selective dynamics

Direct

0.3678639597431896	0.4704923839886632	0.4918667294314574	F	F	F
0.8677771993753254	0.8038257173219989	0.4048328887494108	F	F	F
0.8679519108086269	0.1315684660645478	0.5713595868738283	T	T	T
0.8598677501151833	0.3716644676703249	0.5836056920871635	T	T	T
0.3678639597431896	0.7205100956429362	0.4918667294314574	F	F	F
0.8677771993753254	0.0538434289762648	0.4048328887494108	F	F	F
0.3678639597431896	0.0955012398157962	0.4918667294314574	F	F	F
0.8677771993753254	0.5955366631243351	0.4918667294314574	F	F	F
0.6353182235706373	0.5879079255969509	0.6189069480860895	T	T	T
0.3678639597431896	0.9288699964576708	0.4048328887494108	F	F	F
0.1178205795592575	0.2622033297909994	0.4483498090904305	F	F	F
0.8677771993753254	0.4288345731491319	0.4048328887494108	F	F	F
0.0760701116490905	0.5908949133436966	0.6248917344401047	T	T	T
0.3604529467521282	0.2670058439408590	0.5780449087969646	T	T	T
0.8750418736806236	0.7675420739757115	0.5813928212650052	T	T	T
0.1178855990338419	0.9277248001737665	0.5380693282309297	T	T	T
0.6179073399271218	0.2622033297909994	0.4483498090904305	F	F	F
0.6179427693543526	0.9271505924696278	0.5403840406104924	T	T	T
0.3678639597431896	0.8592986184909677	0.4918667294314574	F	F	F
0.8677771993753254	0.3409139213602543	0.4822427951252664	F	F	F
0.0902307825785158	0.3409139213602543	0.3661279355614866	F	F	F
0.1169836710147741	0.3236021489811464	0.6207928212566903	T	T	T
0.5871593171451520	0.3372278308061502	0.6199622418599510	T	T	T
0.3673619051010638	0.0060209909398745	0.5691910121341228	T	T	T
0.6418019459085034	0.6763514953627978	0.5401875743711352	T	T	T
0.8677771993753254	0.1926319518243034	0.4048328887494108	F	F	F

0.6454971369078635	0.3409139213602543	0.3661279355614866	F	F	F
0.3678639597431896	0.6742472546935900	0.3952089544432269	F	F	F
0.8682497855779112	0.5091062760249461	0.5752241196640648	T	T	T
0.5903175429463801	0.0075805880269186	0.4531617762435260	F	F	F
0.8677771993753254	0.8500885582713451	0.5014383597468495	F	F	F
0.3678639597431896	0.3317038611406318	0.4918667294314574	F	F	F
0.8677771993753254	0.6650371944739604	0.4048328887494108	F	F	F
0.0933500515779894	0.8432184326414689	0.6114755306791837	T	T	T
0.5879237588583307	0.1835576865088307	0.5323377400472000	T	T	T
0.6454971369078635	0.5167552249380094	0.4435378419373421	F	F	F
0.8632231738325661	0.0010699291066942	0.5712973949487573	T	T	T
0.3678639597431896	0.1834218916046737	0.4144568230556018	F	F	F
0.3525519684596051	0.5146611598077802	0.5986054713644450	T	T	T
0.6311223194180043	0.8447624818664912	0.6088679729600682	T	T	T
0.1481041021905100	0.1812521520061756	0.5317195404909318	T	T	T
0.0902307825785158	0.5167552249380094	0.4435378419373421	F	F	F
0.1454103765399992	0.0075805880269186	0.4531617762435260	F	F	F
0.0953584099847656	0.6743809203165930	0.5402327862496480	T	T	T
0.8612738127016548	0.6480045208613168	0.6985720901322926	T	T	T
-0.0324827587257336	0.6100593646139579	0.7381821196830367	T	T	T
0.8790408260698198	0.7244282358137314	0.7082703968122698	T	T	T
0.6793723025971855	0.6315470578914500	0.7166116739780579	T	T	T
0.3623653173145659	0.4512614703980248	0.6211778096806485	T	T	T

(112)

β pair site:

Physisorption

Co3O4

1.0000000000000000		
5.7629999999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.115000000000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.1189999999999998

Co	O	C	H
18	26	1	4

Selective dynamics

Direct

0.3678639597431896	0.4704923839886632	0.4918667294314574	F	F	F
0.8677771993753254	0.8038257173219989	0.4048328887494108	F	F	F
0.8658566691077136	0.1331677872526761	0.5744590527127279	T	T	T
0.8634582106598893	0.3616179117561825	0.5985301555714265	T	T	T
0.3678639597431896	0.7205100956429362	0.4918667294314574	F	F	F
0.8677771993753254	0.0538434289762648	0.4048328887494108	F	F	F
0.3678639597431896	0.0955012398157962	0.4918667294314574	F	F	F
0.8677771993753254	0.5955366631243351	0.4918667294314574	F	F	F
0.6137992810290235	0.5758465241281004	0.6119144530572919	T	T	T
0.3678639597431896	0.9288699964576708	0.4048328887494108	F	F	F
0.1178205795592575	0.2622033297909994	0.4483498090904305	F	F	F
0.8677771993753254	0.4288345731491319	0.4048328887494108	F	F	F
0.0860163188604048	0.5621739925938531	0.6009930377293480	T	T	T
0.3654787318585681	0.2588536858693329	0.5826492343445054	T	T	T
0.8705514111944420	0.7712263072314594	0.5853652146191457	T	T	T
0.1174900379638175	0.9280521376174723	0.5379367242181353	T	T	T
0.6179073399271218	0.2622033297909994	0.4483498090904305	F	F	F
0.6183029529342022	0.9285263183511665	0.5407414845279991	T	T	T
0.3678639597431896	0.8592986184909677	0.4918667294314574	F	F	F
0.8677771993753254	0.3409139213602543	0.4822427951252664	F	F	F
0.0902307825785158	0.3409139213602543	0.3661279355614866	F	F	F
0.1181911811338591	0.3042385615732268	0.6275018058366654	T	T	T
0.6099635666006041	0.3039055147876492	0.6282733483493432	T	T	T
0.3669071467609051	0.0061147540032894	0.5691975783266906	T	T	T
0.6450959626269742	0.6734329785449502	0.5437902412119273	T	T	T
0.8677771993753254	0.1926319518243034	0.4048328887494108	F	F	F
0.6454971369078635	0.3409139213602543	0.3661279355614866	F	F	F
0.3678639597431896	0.6742472546935900	0.3952089544432269	F	F	F
0.8575129792816173	0.4914543099022496	0.6369401478338528	T	T	T
0.5903175429463801	0.0075805880269186	0.4531617762435260	F	F	F
0.8677771993753254	0.8500885582713451	0.5014383597468495	F	F	F
0.3678639597431896	0.3317038611406318	0.4918667294314574	F	F	F
0.8677771993753254	0.6650371944739604	0.4048328887494108	F	F	F
0.0946218931281339	0.8442065801664057	0.6122491021237110	T	T	T
0.5870140634259932	0.1802275332141281	0.5309012041667838	T	T	T
0.6454971369078635	0.5167552249380094	0.4435378419373421	F	F	F
0.8635280721728870	0.0022825180514547	0.5706245533293060	T	T	T
0.3678639597431896	0.1834218916046737	0.4144568230556018	F	F	F
0.3613580821449641	0.5016488322926829	0.5888236739339525	T	T	T
0.6284807736338901	0.8456240101443937	0.6095140925339219	T	T	T
0.1466468088561350	0.1796930706255842	0.5308285444811396	T	T	T

0.0902307825785158	0.5167552249380094	0.4435378419373421	F	F	F
0.1454103765399992	0.0075805880269186	0.4531617762435260	F	F	F
0.0921014901548089	0.6707877952831598	0.5435355186675264	T	T	T
0.3715040832245478	0.1699453104431176	0.7707164330616656	T	T	T
0.5494622222518997	0.1839968985041739	0.7531623963845069	T	T	T
0.3677128649327526	0.1670719910467973	0.8279773167613966	T	T	T
0.3121812345387393	0.1020545041727258	0.7493906359742586	T	T	T
0.2584466849417020	0.2272764355521061	0.7523244217987638	T	T	T

Transition state

Co	O	C	H
1.0000000000000000			
5.7629999999999999	0.0000000000000000	0.0000000000000000	
0.0000000000000000	14.1150000000000002	0.0000000000000000	
0.0000000000000000	0.0000000000000000	19.1189999999999998	

Co	O	C	H
18	26	1	4

Selective dynamics

Direct

0.3678639597431896	0.4704923839886632	0.4918667294314574	F	F	F
0.8677771993753254	0.8038257173219989	0.4048328887494108	F	F	F
0.8723339295472664	0.1283094480671983	0.5699580957718010	T	T	T
0.8734732947737186	0.3649613244338603	0.5891194564058853	T	T	T
0.3678639597431896	0.7205100956429362	0.4918667294314574	F	F	F
0.8677771993753254	0.0538434289762648	0.4048328887494108	F	F	F
0.3678639597431896	0.0955012398157962	0.4918667294314574	F	F	F
0.8677771993753254	0.5955366631243351	0.4918667294314574	F	F	F
0.6222167159248833	0.5641283703013000	0.6110373024190534	T	T	T
0.3678639597431896	0.9288699964576708	0.4048328887494108	F	F	F
0.1178205795592575	0.2622033297909994	0.4483498090904305	F	F	F
0.8677771993753254	0.4288345731491319	0.4048328887494108	F	F	F
0.0796717774719767	0.5669171789081919	0.6061972982597265	T	T	T
0.3912794290292587	0.2510180829401116	0.5842132817782512	T	T	T
0.8690262023584885	0.7694350447390722	0.5840499697079040	T	T	T
0.1179923195608992	0.9270210883667530	0.5380628419390326	T	T	T
0.6179073399271218	0.2622033297909994	0.4483498090904305	F	F	F
0.6168019160016807	0.9263685996386288	0.5401125989930953	T	T	T
0.3678639597431896	0.8592986184909677	0.4918667294314574	F	F	F
0.8677771993753254	0.3409139213602543	0.4822427951252664	F	F	F
0.0902307825785158	0.3409139213602543	0.3661279355614866	F	F	F
0.1623204374654133	0.3180328316815315	0.6321998192835048	T	T	T
0.6121882794994651	0.3107381092635268	0.6268410120828813	T	T	T
0.3676466415048271	0.0041307253552364	0.5689559899928847	T	T	T
0.6430994821173593	0.6684194887458152	0.5464814028132380	T	T	T
0.8677771993753254	0.1926319518243034	0.4048328887494108	F	F	F
0.6454971369078635	0.3409139213602543	0.3661279355614866	F	F	F
0.3678639597431896	0.6742472546935900	0.3952089544432269	F	F	F
0.8617065573159959	0.4895301188787833	0.6431601845487325	T	T	T
0.5903175429463801	0.0075805880269186	0.4531617762435260	F	F	F
0.8677771993753254	0.8500885582713451	0.5014383597468495	F	F	F
0.3678639597431896	0.3317038611406318	0.4918667294314574	F	F	F
0.8677771993753254	0.6650371944739604	0.4048328887494108	F	F	F
0.0954449551043872	0.8418307509003472	0.6106492597621345	T	T	T
0.5955454036383258	0.1782165966798420	0.5289904598676809	T	T	T

0.6454971369078635	0.5167552249380094	0.4435378419373421	F	F	F
0.8635584931329965	0.9981001482856187	0.5728659919365442	T	T	T
0.3678639597431896	0.1834218916046737	0.4144568230556018	F	F	F
0.3509982512596331	0.5067507133499451	0.5864278787586565	T	T	T
0.6261222661027147	0.8417392777244231	0.6077625523383596	T	T	T
0.1496771447631161	0.1817820970237979	0.5322293545116608	T	T	T
0.0902307825785158	0.5167552249380094	0.4435378419373421	F	F	F
0.1454103765399992	0.0075805880269186	0.4531617762435260	F	F	F
0.0933569673381640	0.6712342670232937	0.5447433136742472	T	T	T
0.3752768083559704	0.1655938752451331	0.6677863128604845	T	T	T
0.5153660714159966	0.1137793997901655	0.6642916306081711	T	T	T
0.3935357742738159	0.2102413186296048	0.7147772528361725	T	T	T
0.2076592284236110	0.1285115342648014	0.6660368492298466	T	T	T
0.2172465280472687	0.2653899101598482	0.6643552423061057	T	T	T

Chemisorption

Co3O4

1.0000000000000000		
5.7629999999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.1150000000000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.1189999999999998

Co O C H
18 26 1 4

Selective dynamics

Direct

0.3678639597431896	0.4704923839886632	0.4918667294314574	F	F	F
0.8677771993753254	0.8038257173219989	0.4048328887494108	F	F	F
0.8703208339741904	0.1273336044755265	0.5705308186139874	T	T	T
0.8649004436805821	0.3657502405839524	0.5875541923366768	T	T	T
0.3678639597431896	0.7205100956429362	0.4918667294314574	F	F	F
0.8677771993753254	0.0538434289762648	0.4048328887494108	F	F	F
0.3678639597431896	0.0955012398157962	0.4918667294314574	F	F	F
0.8677771993753254	0.5955366631243351	0.4918667294314574	F	F	F
0.6171407164182988	0.5631065751141601	0.6115561066433572	T	T	T
0.3678639597431896	0.9288699964576708	0.4048328887494108	F	F	F
0.1178205795592575	0.2622033297909994	0.4483498090904305	F	F	F
0.8677771993753254	0.4288345731491319	0.4048328887494108	F	F	F
0.0888650088738474	0.5683774537852344	0.6093890251314498	T	T	T
0.3845414256401295	0.2506397274746234	0.5868868921420519	T	T	T
0.8693845487311895	0.7664951057812204	0.5860230793526454	T	T	T
0.1179560311371319	0.9265553096971472	0.5378359762804493	T	T	T
0.6179073399271218	0.2622033297909994	0.4483498090904305	F	F	F
0.6180851400289926	0.9266364615392801	0.5397686844582293	T	T	T
0.3678639597431896	0.8592986184909677	0.4918667294314574	F	F	F
0.8677771993753254	0.3409139213602543	0.4822427951252664	F	F	F
0.0902307825785158	0.3409139213602543	0.3661279355614866	F	F	F
0.1527761246266515	0.3240040610444090	0.6301902197935778	T	T	T
0.6014443905143900	0.3145591412887942	0.6267937640885735	T	T	T
0.3679833686523160	0.0042480621515540	0.5686220367857623	T	T	T
0.6443889844416784	0.6657283880368849	0.5482122662441083	T	T	T
0.8677771993753254	0.1926319518243034	0.4048328887494108	F	F	F
0.6454971369078635	0.3409139213602543	0.3661279355614866	F	F	F
0.3678639597431896	0.6742472546935900	0.3952089544432269	F	F	F
0.8636260370458744	0.4904478488994363	0.6449882095113155	T	T	T

0.5903175429463801	0.0075805880269186	0.4531617762435260	F	F	F
0.8677771993753254	0.8500885582713451	0.5014383597468495	F	F	F
0.3678639597431896	0.3317038611406318	0.4918667294314574	F	F	F
0.8677771993753254	0.6650371944739604	0.4048328887494108	F	F	F
0.0931731264877548	0.8422465543386871	0.6114820058034294	T	T	T
0.5931964751590275	0.1788944075837935	0.5302752758798018	T	T	T
0.6454971369078635	0.5167552249380094	0.4435378419373421	F	F	F
0.8632057650496122	-0.0024102627368971	0.5724856891808869	T	T	T
0.3678639597431896	0.1834218916046737	0.4144568230556018	F	F	F
0.3512928429171442	0.5019293415742067	0.5847213787054765	T	T	T
0.6248467809062810	0.8417501474016750	0.6082058022116434	T	T	T
0.1479164159664225	0.1817459076778229	0.5333163117358782	T	T	T
0.0902307825785158	0.5167552249380094	0.4435378419373421	F	F	F
0.1454103765399992	0.0075805880269186	0.4531617762435260	F	F	F
0.0880084650491250	0.6689119552884223	0.5457939800766404	T	T	T
0.3721030235437920	0.1667578341278122	0.6689959392728505	T	T	T
0.5125395898284020	0.1149176234839080	0.6645950029357603	T	T	T
0.3878124587099180	0.2134941415039688	0.7144613210606351	T	T	T
0.2039709544409301	0.1308681931381106	0.6665349742761383	T	T	T
0.2424387053983099	0.3776871735496773	0.6483017296666963	T	T	T

(112)

γ pair site:

Physisorption

Co3O4

1.0000000000000000		
5.7629999999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.115000000000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.1189999999999998

Co	O	C	H
18	26	1	4

Selective dynamics

Direct

0.3678639597431896	0.4704923839886632	0.4918667294314574	F	F	F
0.8677771993753254	0.8038257173219989	0.4048328887494108	F	F	F
0.8628733592947314	0.1444473409390097	0.5802187851565418	T	T	T
0.9203503436670391	0.3546774788628814	0.6485322740240338	T	T	T
0.3678639597431896	0.7205100956429362	0.4918667294314574	F	F	F
0.8677771993753254	0.0538434289762648	0.4048328887494108	F	F	F
0.3678639597431896	0.0955012398157962	0.4918667294314574	F	F	F
0.8677771993753254	0.5955366631243351	0.4918667294314574	F	F	F
0.6484525873437127	0.5596679315436403	0.6087486834490519	T	T	T
0.3678639597431896	0.9288699964576708	0.4048328887494108	F	F	F
0.1178205795592575	0.2622033297909994	0.4483498090904305	F	F	F
0.8677771993753254	0.4288345731491319	0.4048328887494108	F	F	F
0.1041776970346735	0.5621837054074073	0.6083048098447509	T	T	T
0.4099044402866875	0.2573130181196232	0.5878295472385520	T	T	T
0.8663863038271392	0.7684679673245877	0.5802225980149139	T	T	T
0.1153398544990325	0.9299609124782077	0.5398118071208834	T	T	T
0.6179073399271218	0.2622033297909994	0.4483498090904305	F	F	F
0.6211244140604492	0.9305051160076695	0.5395815403986804	T	T	T
0.3678639597431896	0.8592986184909677	0.4918667294314574	F	F	F
0.8677771993753254	0.3409139213602543	0.4822427951252664	F	F	F
0.0902307825785158	0.3409139213602543	0.3661279355614866	F	F	F
0.2063456205620524	0.3189290863934724	0.6474171642115600	T	T	T
0.7326433629931798	0.2562592617204205	0.6341438337586867	T	T	T
0.3686180870085835	0.0066476636088651	0.5698504869022428	T	T	T
0.6461136552123070	0.6679195738732788	0.5483006178710530	T	T	T
0.8677771993753254	0.1926319518243034	0.4048328887494108	F	F	F
0.6454971369078635	0.3409139213602543	0.3661279355614866	F	F	F
0.3678639597431896	0.6742472546935900	0.3952089544432269	F	F	F
0.8770686718465442	0.4868392347908688	0.6524690564054169	T	T	T
0.5903175429463801	0.0075805880269186	0.4531617762435260	F	F	F
0.8677771993753254	0.8500885582713451	0.5014383597468495	F	F	F
0.3678639597431896	0.3317038611406318	0.4918667294314574	F	F	F
0.8677771993753254	0.6650371944739604	0.4048328887494108	F	F	F
0.1028822766779946	0.8456281313829038	0.6072311612337967	T	T	T
0.5940898115663172	0.1773818080573807	0.5248172123571446	T	T	T
0.6454971369078635	0.5167552249380094	0.4435378419373421	F	F	F
0.8694112974818112	0.0062550805002543	0.5690237530966910	T	T	T
0.3678639597431896	0.1834218916046737	0.4144568230556018	F	F	F
0.3760432595054888	0.4994026950830231	0.5888250078816796	T	T	T
0.6344487207883384	0.8460997786431295	0.6071687289441634	T	T	T
0.1482224972312538	0.1821108453837644	0.5321590884181437	T	T	T

0.0902307825785158	0.5167552249380094	0.4435378419373421	F	F	F
0.1454103765399992	0.0075805880269186	0.4531617762435260	F	F	F
0.0891273947701873	0.6689552204180600	0.5472300445710071	T	T	T
0.8462142012148162	0.7268556853045149	0.7665702358009139	T	T	T
0.9799117566691106	0.7693484400116706	0.7926003551957941	T	T	T
0.7868729798829832	0.6700835464314810	0.8013072827400920	T	T	T
0.7007596955147325	0.7724890465843472	0.7515732159880438	T	T	T
0.9235799712807149	0.6949445656354606	0.7194494791203591	T	T	T

Transition state

Co	O	C	H
1.0000000000000000			
5.7629999999999999	0.0000000000000000	0.0000000000000000	
0.0000000000000000	14.1150000000000002	0.0000000000000000	
0.0000000000000000	0.0000000000000000	19.1189999999999998	

Co	O	C	H
18	26	1	4

Selective dynamics

Direct

0.3678639597431896	0.4704923839886632	0.4918667294314574	F	F	F
0.8677771993753254	0.8038257173219989	0.4048328887494108	F	F	F
0.8621141283838887	0.1407540388688840	0.5780718258834748	T	T	T
0.9139802430089273	0.3549688482834287	0.5979433961106234	T	T	T
0.3678639597431896	0.7205100956429362	0.4918667294314574	F	F	F
0.8677771993753254	0.0538434289762648	0.4048328887494108	F	F	F
0.3678639597431896	0.0955012398157962	0.4918667294314574	F	F	F
0.8677771993753254	0.5955366631243351	0.4918667294314574	F	F	F
0.6344301353558675	0.5665050841337974	0.6011271786394865	T	T	T
0.3678639597431896	0.9288699964576708	0.4048328887494108	F	F	F
0.1178205795592575	0.2622033297909994	0.4483498090904305	F	F	F
0.8677771993753254	0.4288345731491319	0.4048328887494108	F	F	F
0.0688429328513772	0.5787140121420404	0.6083438028311605	T	T	T
0.4078675345047312	0.2598601408903367	0.5820868853403586	T	T	T
0.8868183266783927	0.7634667410837106	0.5790156830406001	T	T	T
0.1165944669844094	0.9297489401665673	0.5402644039951227	T	T	T
0.6179073399271218	0.2622033297909994	0.4483498090904305	F	F	F
0.6186063472688311	0.9307023529603360	0.5369362910299060	T	T	T
0.3678639597431896	0.8592986184909677	0.4918667294314574	F	F	F
0.8677771993753254	0.3409139213602543	0.4822427951252664	F	F	F
0.0902307825785158	0.3409139213602543	0.3661279355614866	F	F	F
0.2016592130051626	0.3243625964665206	0.6301652526575868	T	T	T
0.7171839648316756	0.2625272365426278	0.6237892491132339	T	T	T
0.3704503818549567	0.0064462305827512	0.5693021623323495	T	T	T
0.6462843072698350	0.6715521775294049	0.5407984847502691	T	T	T
0.8677771993753254	0.1926319518243034	0.4048328887494108	F	F	F
0.6454971369078635	0.3409139213602543	0.3661279355614866	F	F	F
0.3678639597431896	0.6742472546935900	0.3952089544432269	F	F	F
0.8627526922493403	0.4814616511798005	0.6270061204062382	T	T	T
0.5903175429463801	0.0075805880269186	0.4531617762435260	F	F	F
0.8677771993753254	0.8500885582713451	0.5014383597468495	F	F	F
0.3678639597431896	0.3317038611406318	0.4918667294314574	F	F	F
0.8677771993753254	0.6650371944739604	0.4048328887494108	F	F	F
0.1088886681622874	0.8439842215230211	0.6078085647520272	T	T	T
0.5903893677202444	0.1763056830044782	0.5252076259614571	T	T	T

0.6454971369078635	0.5167552249380094	0.4435378419373421	F	F	F
0.8732390773269370	0.0040837466327274	0.5706063776856010	T	T	T
0.3678639597431896	0.1834218916046737	0.4144568230556018	F	F	F
0.3461896198672321	0.5169674254638424	0.5871776869448811	T	T	T
0.6497593581011324	0.8349975481491840	0.6175609534946133	T	T	T
0.1509509618750035	0.1824423573371008	0.5331066257442298	T	T	T
0.0902307825785158	0.5167552249380094	0.4435378419373421	F	F	F
0.1454103765399992	0.0075805880269186	0.4531617762435260	F	F	F
0.0925883727070918	0.6739065611609265	0.5390655143836832	T	T	T
0.8710919942847756	0.6965639578730108	0.6802574982208403	T	T	T
0.9301698733360936	0.7597297190297501	0.7086941710832217	T	T	T
0.6938197247973024	0.6767180840728024	0.6974085720864488	T	T	T
0.9878564206282590	0.6401832772076514	0.6998815921179340	T	T	T
0.7109331815469171	0.7788045928462050	0.6482187243252648	T	T	T

Chemisorption

Co3O4

1.0000000000000000		
5.7629999999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.1150000000000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.1189999999999998

Co	O	C	H
18	26	1	4

Selective dynamics

Direct

0.3678639597431896	0.4704923839886632	0.4918667294314574	F	F	F
0.8677771993753254	0.8038257173219989	0.4048328887494108	F	F	F
0.8642000071759420	0.1393901127881199	0.5771265839143125	T	T	T
0.9142157395640891	0.3543656609949526	0.5988383463824110	T	T	T
0.3678639597431896	0.7205100956429362	0.4918667294314574	F	F	F
0.8677771993753254	0.0538434289762648	0.4048328887494108	F	F	F
0.3678639597431896	0.0955012398157962	0.4918667294314574	F	F	F
0.8677771993753254	0.5955366631243351	0.4918667294314574	F	F	F
0.6301311837314701	0.5677848874692480	0.6029307995237365	T	T	T
0.3678639597431896	0.9288699964576708	0.4048328887494108	F	F	F
0.1178205795592575	0.2622033297909994	0.4483498090904305	F	F	F
0.8677771993753254	0.4288345731491319	0.4048328887494108	F	F	F
0.0682334904484412	0.5811339776418534	0.6086535541457385	T	T	T
0.4083720070160115	0.2631312760296999	0.5857252053785204	T	T	T
0.8774590792231037	0.7624575198571272	0.5818254027359453	T	T	T
0.1164125897088205	0.9281168816183686	0.5408960896537305	T	T	T
0.6179073399271218	0.2622033297909994	0.4483498090904305	F	F	F
0.618938622236616	0.9309117229444546	0.5363451173316192	T	T	T
0.3678639597431896	0.8592986184909677	0.4918667294314574	F	F	F
0.8677771993753254	0.3409139213602543	0.4822427951252664	F	F	F
0.0902307825785158	0.3409139213602543	0.3661279355614866	F	F	F
0.1995159638744966	0.3265488143789831	0.6304927949185681	T	T	T
0.7201164009499841	0.2622278036921935	0.6237165240016285	T	T	T
0.3703401116980997	0.0067988252236103	0.5692619885592489	T	T	T
0.6433805880004395	0.6737238503277478	0.5399238244410817	T	T	T
0.8677771993753254	0.1926319518243034	0.4048328887494108	F	F	F
0.6454971369078635	0.3409139213602543	0.3661279355614866	F	F	F
0.3678639597431896	0.6742472546935900	0.3952089544432269	F	F	F
0.8657600249276115	0.4819888305149780	0.6270225713357914	T	T	T

0.5903175429463801	0.0075805880269186	0.4531617762435260	F	F	F
0.8677771993753254	0.8500885582713451	0.5014383597468495	F	F	F
0.3678639597431896	0.3317038611406318	0.4918667294314574	F	F	F
0.8677771993753254	0.6650371944739604	0.4048328887494108	F	F	F
0.1065830372299569	0.8454356362759512	0.6090043269425727	T	T	T
0.5920950293995116	0.1758005540813753	0.5240882529896600	T	T	T
0.6454971369078635	0.5167552249380094	0.4435378419373421	F	F	F
0.8715672607194082	0.0044471602204903	0.5713423808487343	T	T	T
0.3678639597431896	0.1834218916046737	0.4144568230556018	F	F	F
0.3382401490598209	0.5181434508486537	0.5869676053660338	T	T	T
0.6384823581650194	0.8466701696059111	0.6145085039917688	T	T	T
0.1513888704529674	0.1819173444946710	0.5320329565738573	T	T	T
0.0902307825785158	0.5167552249380094	0.4435378419373421	F	F	F
0.1454103765399992	0.0075805880269186	0.4531617762435260	F	F	F
0.0900370845332256	0.6739687587989542	0.5396821624329262	T	T	T
0.8729879793627833	0.6937996812020906	0.6781973456432512	T	T	T
0.9266471674204916	0.7595964812288711	0.7042307514804690	T	T	T
0.6926905866282858	0.6784269915790844	0.6942650705110641	T	T	T
0.9871910883346958	0.6395651112568418	0.7027179196175435	T	T	T
0.7046386681318252	0.8860376355710931	0.6516054774875168	T	T	T

Table S5. Energy Barriers for CH₄ Activation at the Different Co-O Pair Sites and the Calculated Bader Charges at the Co and O Sites on the Clean Surface, and That on the H Atom in the Transition State.

Surface	E _a (eV)	Co	O	H
(001)-A (α site)	0.96	+1.39	-0.95	+0.59
(001)-A (β site)	1.22	+1.39	-0.83	+0.64
(011)-A (α site)	0.90	+1.24	-0.82	+0.41
(011)-A (β site)	1.14	+1.24	-0.84	+0.33
(112) (α site)	0.79	+0.95	-0.79	+0.49

Table S6. The Ratio of CH₄ Reaction Rates (r) and Rate Constants (k) at the Reaction Temperature of 300, 400, and 500 °C for the Nanoparticle, Nanorod, and Nanoplate Catalysts.

Temperature (°C)	k	r
300	1.0 : 1.8 : 31.3	1.0 : 1.3 : 2.6
400	1.0 : 1.7 : 18.7	1.0 : 1.2 : 1.5
500	1.0 : 1.6 : 12.8	1.0 : 1.1 : 1.1