

Supporting Information

A Computational Study of K Promotion of CO Dissociation on Hägg carbide

Xianxuan Ren,^a Rozemarijn D.E. Krösschell,^a Zhuowu Men,^b Peng Wang,^{a,b} Ivo A. W. Filot^{a,*}
and Emiel J. M. Hensen^{a,*}

^a Laboratory of Inorganic Materials and Catalysis, Department of Chemistry and Chemical Engineering, Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands

^b National Institute of Clean-and-Low-Carbon Energy, Future Science and Technology City, Changping District, Beijing 102211, People's Republic of China

CONTCAR files for the optimized configurations

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Fe3C2(510)
1.0000000000000000
10.1180000000000003 0.0000000000000000 0.0000000000000000
-0.7809265139842700 12.8064770233652006 0.0000000000000000
0.0000000000000000 -0.00000000000000600 17.4192900000000002
Fe C
60 24
Selective dynamics

Direct
0.2394699999999972 0.26026000000000024 0.0193299999999965 F F F
0.7394699999999972 0.26026000000000024 0.0193299999999965 F F F
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0.85242000000000022 0.86413000000000030 0.0267499999999998 F F F
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0.2651299999999992 0.65990000000000004 0.03052000000000028 F F F
0.7651299999999992 0.65990000000000004 0.03052000000000028 F F F
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0.7917699999999996 0.0723199999999977 0.0369999999999990 F F F
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0.92483000000000000 0.4166799999999995 0.04867000000000013 F F F
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0.2155791749650179 0.9388466664200296 0.1337132564304916 T T T
0.7155794745934726 0.9388468835519787 0.1337134169686988 T T T
0.3388175556543681 0.5350705197458738 0.1399472872259149 T T T
0.8388178592702695 0.5350702122343353 0.1399466913335005 T T T
0.1357447403290867 0.1436456464823797 0.1463162478501974 T T T
0.6357431824266031 0.1436453466037221 0.1463165431851225 T T T
0.2258864544020466 0.3430504044568526 0.1428286583220073 T T T
0.7258846691859829 0.3430492334425344 0.1428275109676510 T T T
0.2853476701818202 0.7513015203043244 0.1491454315378236 T T T
0.7853481442372557 0.7513017525538278 0.1491454268676252 T T T
0.4624738662474814 0.8827088210204506 0.1530073421800585 T T T
0.9624742939399208 0.8827095371439430 0.1530072148130349 T T T
0.4712239545995901 0.2942539554341868 0.1630733989348515 T T T
0.9712278880008319 0.2942561404540960 0.1630730708882391 T T T
0.0773924885384019 0.4890945329276314 0.1603927383240293 T T T
0.5773923005195898 0.4890939531183804 0.1603930297853820 T T T
0.3940721109124656 0.0948100614573140 0.1637784691076950 T T T
0.8940729152292265 0.0948105278988109 0.1637783343107422 T T T
0.0389471694544336 0.6925773970442861 0.1661771945027513 T T T
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0.5389467537077118	0.6925770994474563	0.1661772711362822	T	T	T
0.2036565715176731	0.6212278075557680	0.2521194034479172	T	T	T
0.7036575115265198	0.6212294135970574	0.2521203326750439	T	T	T
0.2898967113099961	0.2257809824074688	0.2547134807100339	T	T	T
0.7898982036563227	0.2257811093180753	0.2547121621438092	T	T	T
0.1345594582245159	0.8248179787176551	0.2549199328596545	T	T	T
0.6345592459048870	0.8248184240080948	0.2549198653157093	T	T	T
0.2135612121226208	0.0217017030922648	0.2592817274640155	T	T	T
0.7135611016934181	0.0217018275460055	0.2592816325753254	T	T	T
0.2399060221326208	0.4302257831465102	0.2690369500583480	T	T	T
0.7399085971870587	0.4302253781258701	0.2690363808721954	T	T	T
0.4430816040408703	0.5623988352391011	0.2679107630477543	T	T	T
0.9430812637636390	0.5623992757807486	0.2679108025027211	T	T	T
0.4560627100744860	0.9755476991356662	0.2717084415541344	T	T	T
0.9560629833330011	0.9755485313591346	0.2717080533788148	T	T	T
0.0377827273547981	0.1727521050113321	0.2735038115832681	T	T	T
0.5377840240993491	0.1727515308909132	0.2735031118781735	T	T	T
0.3900208000307229	0.7625133243240975	0.2729141768474825	T	T	T
0.8900211115561383	0.7625141837923043	0.2729139786905581	T	T	T
0.4866641250373546	0.3734027495173166	0.2920030223402428	T	T	T
0.9866661191826587	0.3734035175806194	0.2920032957562717	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
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0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0654122556469604	0.0088681986366892	0.1833685129977307	T	T	T
0.5654126943329264	0.0088680468374081	0.1833685241800153	T	T	T
0.3953393080500801	0.4238307468597896	0.2039307781524363	T	T	T
0.8953434174520514	0.4238312380037231	0.2039296432846560	T	T	T
0.3079007103710192	0.8876166031878506	0.2313330206458192	T	T	T
0.8079009840568185	0.8876168453874592	0.2313332283648269	T	T	T
0.1287661673422958	0.3039296488896111	0.2448902837271188	T	T	T
0.6287674677396581	0.3039304835876510	0.2448923568046588	T	T	T
0.0497394620529417	0.6904572556579187	0.2816296332689791	T	T	T
0.5497380489443242	0.6904576978416929	0.2816297664007100	T	T	T
0.3689308920676152	0.1010440207818554	0.2867058435239837	T	T	T
0.8689313114480601	0.1010447219476860	0.2867056187395565	T	T	T

Fe₅C₂(111)

1.000000000000000

12.3812999725000008	0.0000000000000000	0.0000000000000000
-2.0391083097000000	13.2888646689000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.8052997588999986

Fe C

80 32

Selective dynamics

Direct

0.8393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.7319762979070614	0.2192300578232861	0.4670120702077448	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999985	F	F	F
0.5598104024855430	0.0974160285790886	0.4376348749871939	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000003	F	F	F
0.5946308418996568	0.2769379749247988	0.3884279572465876	T	T	T
0.8070399759999987	0.3298200070000021	0.3692500000000010	F	F	F
0.6872590939259122	0.0422679260690059	0.5099130848593751	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.2319759311683288	0.2192317233565735	0.4670111703354827	T	T	T
0.1632599980000009	0.3849500119999973	0.2899999919999985	F	F	F
0.0598116559282322	0.0974167840668554	0.4376316986826443	T	T	T
0.1955399960000008	0.0652299970000030	0.2403199970000003	F	F	F
0.0946306521954124	0.2769383031151740	0.3884281074609128	T	T	T
0.3070400060000011	0.3298200070000021	0.3692500000000010	F	F	F
0.1872571752184251	0.0422679868281426	0.5099118339218560	T	T	T
0.0044699999999978	0.4602699880000003	0.2462999970000013	F	F	F
0.9045338630952970	0.1724479976334810	0.3940455163067200	T	T	T

0.4981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.4041957463136257	0.1523430715042890	0.5053336596657355	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999982	F	F	F
0.4351354418670121	0.3249999145948612	0.4624860457676757	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F
0.8788682943778074	0.4896422385193612	0.4489647536045228	T	T	T
0.5044699910000006	0.4602699880000003	0.2462999970000013	F	F	F
0.4045346522391059	0.1724499014611756	0.3940494144319999	T	T	T
0.9981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.9041949299177455	0.1523425977773460	0.5053334212456074	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999982	F	F	F
0.9351381757353288	0.3250011268737411	0.4624856350752891	T	T	T
0.4722500150000002	0.2798599899999985	0.2958799900000031	F	F	F
0.3788663177627593	0.4896419166907997	0.4489642919668341	T	T	T
0.7199699880000026	0.1401900050000009	0.3529999849999967	F	F	F
0.6315887256089240	0.3596835187253049	0.4914064791852804	T	T	T
0.7826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.6901692592034482	0.4673302618550201	0.4026752673903595	T	T	T
0.2199700030000002	0.1401900050000009	0.3529999849999967	F	F	F
0.1315890107963557	0.3596829855947962	0.4914055398323921	T	T	T
0.2826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.1901675516214610	0.4673298265514771	0.4026755911570225	T	T	T
0.8393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.7319788962116572	0.7192247503862588	0.4670129225209748	T	T	T
0.6632599830000032	0.8849499820000020	0.2899999919999985	F	F	F
0.5598139068996385	0.5974092661128182	0.4376438391658499	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000003	F	F	F
0.5946379834935207	0.7769479025643662	0.3884266646815759	T	T	T
0.8070399759999987	0.8298199769999997	0.3692500000000010	F	F	F
0.6872590025319388	0.5422595992791484	0.5099177834622095	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.2319771627690402	0.7192262316336111	0.4670129057715145	T	T	T
0.1632599800000009	0.8849499820000020	0.2899999919999985	F	F	F
0.0598143888158197	0.5974092359353309	0.4376430047967491	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000003	F	F	F
0.0946375864796423	0.7769480681699004	0.3884267877525788	T	T	T
0.3070400060000011	0.8298199769999997	0.3692500000000010	F	F	F
0.1872573133020973	0.5422563960441009	0.5099164190750661	T	T	T
0.0044699999999978	0.9602699880000003	0.2462999970000013	F	F	F
0.9045359267283445	0.6724537352140200	0.3940534046612300	T	T	T
0.4981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.4041941333223467	0.6523430116357082	0.5053402753395160	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999982	F	F	F
0.4351307878204057	0.8250098470835343	0.4624853331439193	T	T	T
0.9722499849999977	0.7798600200000010	0.2958799900000031	F	F	F
0.8788709861493044	0.9896537898271407	0.4489610507135687	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000013	F	F	F
0.4045333108792856	0.6724545101695862	0.3940546905869911	T	T	T
0.9981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.9041951035299004	0.6523435399081201	0.5053401228326264	T	T	T
0.0303299999999993	0.6151900289999972	0.3136900069999982	F	F	F
0.9351346260237406	0.8250112103874164	0.4624852731483592	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3788694136936592	0.9896532402766810	0.4489616595019822	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999967	F	F	F
0.6315894094238813	0.8596942273190864	0.4914038447265819	T	T	T
0.7826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.6901754812000537	0.9673451065203954	0.4026688313831186	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999967	F	F	F
0.1315899713489714	0.8596948546089078	0.4914033896588483	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.1901741735814951	0.9673448152090887	0.4026692635456887	T	T	T
0.8641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.7796018304031193	0.3652973596256544	0.4622169226880072	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999986	F	F	F
0.5389270546878955	0.4540456359255156	0.4618429392355979	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999985	F	F	F
0.5497531414481602	0.2280751428133042	0.4789666317793458	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000016	F	F	F
0.7804917251879838	0.0927697322703952	0.4381768482230252	T	T	T
0.3641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.2795998684881359	0.3652968279136894	0.4622168803490846	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999986	F	F	F
0.0389242530253521	0.4540453697370364	0.4618438668422916	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999985	F	F	F

0.0497505448910415	0.2280759563509294	0.4789651226792480	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000016	F	F	F
0.2804928213722022	0.0927700933908894	0.4381767325125296	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.7796077439543964	0.8653017766376022	0.4622141002836530	T	T	T
0.6384199860000024	0.7358700039999988	0.3038099999999986	F	F	F
0.5389218443773549	0.9540509800651168	0.4618439390406389	T	T	T
0.6260200139999981	0.5126500129999982	0.3228900129999985	F	F	F
0.5497460733512434	0.7280712429601338	0.4789681297718967	T	T	T
0.8765599729999991	0.8823999760000021	0.2866800130000016	F	F	F
0.7804903488015349	0.5927675968850726	0.4381771579502086	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.2796062444732958	0.8653011548560327	0.4622140941902432	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999986	F	F	F
0.0389212641249225	0.9540536929348885	0.4618441307450191	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999985	F	F	F
0.0497481285375950	0.7280727580866018	0.4789684270254736	T	T	T
0.3765600030000016	0.8823999760000021	0.2866800130000016	F	F	F
0.2804903087929853	0.5927680010969703	0.4381773795854291	T	T	T

Fe₅C₂(010)

1.000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C
40 16

Selective dynamics

Direct

0.0371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4786528431799858	0.3743131211570990	0.4045567741279271	T	T	T
0.9786599556864115	0.3742534661473370	0.4045107701664763	T	T	T
0.1561994128621159	0.5634848665451477	0.4044572010673037	T	T	T
0.6561811403420637	0.5634076253610815	0.4045338266966650	T	T	T
0.0389006550071692	0.7473114640717610	0.4086186685730461	T	T	T
0.5389623670914935	0.7472849559817295	0.4086333530131558	T	T	T
0.0957978673426308	0.1903367809197846	0.4086440915206922	T	T	T
0.5958329588150486	0.1904237640484154	0.4086524677054225	T	T	T
0.5674072292844605	0.9688541126379656	0.4121693668483944	T	T	T
0.0673672518387465	0.9688441829082862	0.4122545665666170	T	T	T
0.8174457975155737	0.9689248848663264	0.4355274283845125	T	T	T
0.3173918081272038	0.9687554744995032	0.4355060909023168	T	T	T
0.7835138444584065	0.7424915449671201	0.4446922338595605	T	T	T
0.3511844778729838	0.1952228860257339	0.4446340447107358	T	T	T
0.2833226884071769	0.7424445898818006	0.4447621494234572	T	T	T
0.8514057358033982	0.1952479888308872	0.4447624102664514	T	T	T
0.8987786092338200	0.5599534439968186	0.4461374908703881	T	T	T
0.3986819616282313	0.5600231939505480	0.4461072529916615	T	T	T
0.2361549343159136	0.3778659073908553	0.4461035450458128	T	T	T
0.7362710920104136	0.3777879439862988	0.4461015176796977	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999966	0.3528200000000012	F	F	F

0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9063573265368939	0.8505720073509391	0.3835170130492154	T	T	T
0.2283356154752202	0.0870254202819991	0.3834724810445833	T	T	T
0.7285186372836129	0.0872868333886090	0.3835751934321670	T	T	T
0.4062822212720157	0.8503576511982539	0.3835864181451603	T	T	T
0.6671417757217784	0.8549977589256051	0.4528454495614239	T	T	T
0.4676070078298594	0.0827216591018254	0.4528162611944154	T	T	T
0.1669530684381017	0.8549532585733560	0.4529661761997141	T	T	T
0.9678105352882495	0.0827385015317487	0.4530590941816835	T	T	T

Fe₅C₂(010*)

1.000000000000000

9.9837999344000004 0.0000000000000000 0.0000000000000000

-1.5315638797000000 11.4316603084999997 0.0000000000000000

0.0000000000000000 0.0000000000000000 18.9298000335999994

Fe C

40 15

Selective dynamics

Direct

0.0371499999999996	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4797040679859896	0.3718238032062758	0.4050615400900664	T	T	T
0.9779186869894271	0.3709830714371891	0.4045110424492678	T	T	T
0.1549747120836144	0.5621550168320235	0.4055074606081180	T	T	T
0.6562398027830545	0.5646447038391941	0.4039191261455832	T	T	T
0.0364985322368098	0.7469612974913841	0.4099850420993352	T	T	T
0.5448514249559075	0.7511552793553875	0.4057076703708151	T	T	T
0.0954269420971845	0.1879272080740397	0.4087510591160898	T	T	T
0.5950471468663685	0.1878116948042005	0.4094795135863606	T	T	T
0.5667623259375069	0.9697194825874160	0.4081852434442660	T	T	T
0.0697296473119023	0.9674689061710273	0.4107578163828126	T	T	T
0.8197056466711593	0.9642733974898583	0.4351718960083149	T	T	T
0.3187973551670603	0.9673561679053672	0.4367397038643646	T	T	T
0.7690507683384689	0.7462919712314102	0.4454864117466463	T	T	T
0.3539503222043821	0.1918509102892638	0.4429739831410172	T	T	T
0.2824146358520625	0.7427431102955653	0.4430417968557354	T	T	T
0.8500343589729422	0.1914656391565333	0.4429616201822421	T	T	T
0.8979940499727570	0.5608401070250189	0.4449222088568564	T	T	T
0.4000137376042139	0.5611920868697334	0.4440449562633846	T	T	T
0.2372647764973145	0.3751420820535749	0.4444575944854278	T	T	T
0.7356494145504173	0.3751029891366747	0.4452266953184580	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.8994632090094632	0.8463088026901999	0.3825773896284008	T	T	T
0.2289463123739670	0.0856385286153726	0.3833842148787054	T	T	T
0.7278472894437373	0.0825940380780888	0.3822437015030786	T	T	T

0.4062188422425306	0.8515566522441104	0.3848479085113812	T	T	T
0.4698329595921806	0.0794465296920850	0.4553976749796280	T	T	T
0.1663016660125659	0.8560605854034272	0.4529343756461554	T	T	T
0.9660794191503173	0.0776701082005389	0.4505397814970787	T	T	T

K₂O-Fe₅C₂(510)

1.000000000000000

10.1180000000000003	0.000000000000000	0.000000000000000
-0.7809265139842700	12.8064770233652006	0.000000000000000
0.000000000000000	-0.000000000000600	17.419290000000002

Fe C O K

60 24 1 2

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2162180767976957	0.9386947002555442	0.1330342527909587	T	T	T
0.7165991540513672	0.9393114745990652	0.1338954031295556	T	T	T
0.3386946453436447	0.5361084576105317	0.1433548545509740	T	T	T
0.8388772239546233	0.5351274345786033	0.1388292747122440	T	T	T
0.1345477558609472	0.1448647319500486	0.1462015971041633	T	T	T
0.6350549091997560	0.1466913627176382	0.1514290201594792	T	T	T
0.2322087726084993	0.3464124471968350	0.1387637754709367	T	T	T
0.7230198721141773	0.3443096396891214	0.1389620106233394	T	T	T
0.2857356211125509	0.7506750430643178	0.1498047238123865	T	T	T
0.7845725429627336	0.7518723421209816	0.1492233571227804	T	T	T
0.4630295294908751	0.8820545835454301	0.1527144568619237	T	T	T
0.9636852362423863	0.8816287275449075	0.1533830138920994	T	T	T
0.4714306788565408	0.2967191879859533	0.1633364531696118	T	T	T
0.9625618758972831	0.2951067138226051	0.1594543979369527	T	T	T
0.0797690501016126	0.4861293413353251	0.1619262322856692	T	T	T
0.5763690959670822	0.4896480721833676	0.1603209902430897	T	T	T
0.3957770188685374	0.0950987371083572	0.1645878955848051	T	T	T
0.8950041252548346	0.0945658940517451	0.1635849279263376	T	T	T
0.0392688315595097	0.6902921516795227	0.1671228710014512	T	T	T
0.5376975260590908	0.6915640121953153	0.1669299285186346	T	T	T
0.2065405211286067	0.6188788034769575	0.2540278181928736	T	T	T
0.7072257050156283	0.6206975778578880	0.2513646901197880	T	T	T
0.2796878940540060	0.2261647268767678	0.2501120088760850	T	T	T
0.7939047550147991	0.2255952862597121	0.2506959505884602	T	T	T
0.1356623509365002	0.8218972959937785	0.2557251883359170	T	T	T
0.6353183104151653	0.8246285495214563	0.2553045679946160	T	T	T
0.2115901994340748	0.0194237412008002	0.2575785756399385	T	T	T
0.7115197761193526	0.0228737329863162	0.2600770336920210	T	T	T
0.2405082726121514	0.4237668567172212	0.2684028881628442	T	T	T
0.7387037526054530	0.4280062310441397	0.2642109449803848	T	T	T
0.4496862861928763	0.5591681589163958	0.2697096060628890	T	T	T
0.9440668519805009	0.5592514838130015	0.2690591950437619	T	T	T
0.4557620699722658	0.9747177788771311	0.2705677530603522	T	T	T
0.9555467801358213	0.9756734611241384	0.2714247857814446	T	T	T
0.0378693692555150	0.1777029234145373	0.2737693905742526	T	T	T
0.5316177754023064	0.1776905551905687	0.2855996661668367	T	T	T
0.3917135116311437	0.7606509644780727	0.2728267897548081	T	T	T
0.8908413037490903	0.7608557157363990	0.2727686131766248	T	T	T

0.4865913878634032	0.3606423907620635	0.2975521741043745	T	T	T
0.9892070175695596	0.3667067726164444	0.2886902522306307	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0644541757618524	0.0094967416335353	0.1814498076024011	T	T	T
0.5657236946631712	0.0088537257524522	0.1816770051250429	T	T	T
0.4003780965218539	0.4240887700495190	0.2064354662402962	T	T	T
0.9010235075251356	0.4265719070965042	0.2028697263889255	T	T	T
0.3077024678525639	0.8854221309406370	0.2312366474135071	T	T	T
0.8088057540467456	0.8867419674271851	0.2315526488361432	T	T	T
0.1457316667075078	0.2990654499080981	0.3023176185291233	T	T	T
0.6289298250222013	0.2967055463028440	0.2347324878472388	T	T	T
0.0499027173733239	0.6876560971566620	0.2826221073057516	T	T	T
0.5525658286430052	0.6891674762334733	0.2824816040391098	T	T	T
0.3660619192891748	0.0998538575164142	0.2823513821415917	T	T	T
0.8698313006685722	0.1023091634438646	0.2862868900133796	T	T	T
0.5161250884971686	0.2667673776180147	0.3762042116399577	T	T	T
0.7537614691455522	0.2598332186280496	0.4260513400855633	T	T	T
0.2922537939023461	0.1911054007557494	0.4282104888442919	T	T	T

K₂O-Fe₅C₂(111)

1.0000000000000000

12.3812999725000008 0.0000000000000000 0.0000000000000000

-2.0391083097000000 13.2888646689000005 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.8052997588999986

Fe C O K

80 32 1 2

Selective dynamics

Direct

0.8393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.7323958039899588	0.2193378195308735	0.4662908500549227	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999985	F	F	F
0.5607686472312590	0.0974539779713640	0.4383318168223879	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000003	F	F	F
0.5955694716147986	0.2769605101929500	0.3884259764290680	T	T	T
0.8070399759999987	0.3298200070000021	0.3692500000000010	F	F	F
0.6903000475593136	0.0414637611688356	0.5098577512908185	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.2335376639453698	0.2202726824220817	0.4676158412892069	T	T	T
0.1632599980000009	0.3849500119999973	0.2899999919999985	F	F	F
0.0601495327002199	0.0976402672542244	0.4383884991980240	T	T	T
0.1955399960000008	0.0652299970000030	0.2403199970000003	F	F	F
0.0946937274004538	0.2765561820557534	0.3888431375909573	T	T	T
0.3070400060000011	0.3298200070000021	0.3692500000000010	F	F	F
0.1882204299880034	0.0430660842915316	0.5100719576234106	T	T	T
0.0044699999999978	0.4602699880000003	0.2462999970000013	F	F	F
0.9051756026763342	0.1727128828720376	0.3939980444692722	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.4038724101114572	0.1539577436413504	0.5052433057885745	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999982	F	F	F
0.4360343693385790	0.3244127768215180	0.4612502439871051	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F
0.8788103809924578	0.4902610129932057	0.4484524838081576	T	T	T
0.5044699910000006	0.4602699880000003	0.2462999970000013	F	F	F
0.4048815524854759	0.1715907210927584	0.3938767734127548	T	T	T
0.9981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.9039474619974127	0.1511120648863798	0.5048260656354095	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999982	F	F	F
0.9351392708197963	0.3255136897375258	0.4629926280079644	T	T	T
0.4722500150000002	0.2798599899999985	0.2958799900000031	F	F	F
0.3787373046053706	0.4908030392609934	0.4466158652137825	T	T	T
0.7199699880000026	0.1401900050000009	0.3529999849999967	F	F	F
0.6325825505090208	0.3587724499234887	0.4913329132455345	T	T	T

0.7826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.6897925081709037	0.4683029281933039	0.4034750363728014	T	T	T
0.2199700030000002	0.1401900050000009	0.3529999849999967	F	F	F
0.1322402661923575	0.3596890609464311	0.4917033916706558	T	T	T
0.2826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.1896029614290853	0.4675369306790730	0.4028526619645795	T	T	T
0.8393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.7342276490024414	0.7205258350541371	0.4658226388629758	T	T	T
0.6632599830000032	0.8849499820000020	0.2899999919999985	F	F	F
0.5624328596195736	0.5975087551558393	0.4399720560940001	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000003	F	F	F
0.5943343839876605	0.7754822899359445	0.3885915800531993	T	T	T
0.8070399759999987	0.8298199769999997	0.3692500000000010	F	F	F
0.6917294968636055	0.5382353687958087	0.5177927132147092	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.2330656607159641	0.7195090171082184	0.4672665585701050	T	T	T
0.1632599880000009	0.8849499820000020	0.2899999919999985	F	F	F
0.0601642309054106	0.5969146752728273	0.4379375886604099	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000003	F	F	F
0.09453243400576783	0.7766389485576461	0.3886824269648875	T	T	T
0.3070400060000011	0.8298199769999997	0.3692500000000010	F	F	F
0.1899746480494102	0.5419346655873459	0.5106012258209440	T	T	T
0.0044699999999978	0.9602699880000003	0.2462999970000013	F	F	F
0.9031590275466210	0.6712013687491771	0.3942970452566482	T	T	T
0.4981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.4037291558143891	0.6529074970387201	0.5044380684480354	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999982	F	F	F
0.4356485650446600	0.8254133023778374	0.4632969173237761	T	T	T
0.9722499849999977	0.7798600200000010	0.2958799900000031	F	F	F
0.8794487968819147	0.9889542094275936	0.4499230688386744	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000013	F	F	F
0.4056400132492979	0.6720478379353929	0.3938198400373196	T	T	T
0.9981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.9051528890901590	0.6504120994089174	0.5047546252378565	T	T	T
0.0303299999999993	0.6151900289999972	0.3136900069999982	F	F	F
0.9359707430220618	0.8242123773309079	0.4632454884452675	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3792398795000790	0.9902408628397029	0.4485541519406014	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999967	F	F	F
0.6327083175773217	0.8608002868066238	0.4901681866878908	T	T	T
0.7826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.6906352671761968	0.9684277669988978	0.4020443072172771	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999967	F	F	F
0.1322064892023261	0.8598803897644351	0.4916021432704529	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.1899383563496988	0.9677101239029617	0.4028010869353884	T	T	T
0.8641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.7813836808677439	0.3660005158267065	0.4626360417264327	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999986	F	F	F
0.5396990535356209	0.4515952779254896	0.4575729299774815	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999985	F	F	F
0.5492089366502921	0.2285596147275303	0.4787351089693756	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000016	F	F	F
0.7813599524444899	0.0922606672011057	0.4369482395118165	T	T	T
0.3641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.2809159184715024	0.3667392235675733	0.4623015783157832	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999986	F	F	F
0.0395852045039826	0.4540924452451218	0.4621503016251975	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999985	F	F	F
0.0489787540260549	0.2287249358875711	0.4794893762020942	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000016	F	F	F
0.2806134869846331	0.0930704134620499	0.4378195556407901	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.7820380700502207	0.8648700545454189	0.4642629923506696	T	T	T
0.6384199860000024	0.7358700039999988	0.3038099999999986	F	F	F
0.5391957093961626	0.9542166647230435	0.4613702499239729	T	T	T
0.6260200139999981	0.5126500129999982	0.3228900129999985	F	F	F
0.5504539547378758	0.7299496541303141	0.4806787385307243	T	T	T
0.8765599729999991	0.8823999760000021	0.2866800130000016	F	F	F
0.7769869247613908	0.5925168474902864	0.4388689057907417	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.2802042300269156	0.8654836670672437	0.4623307299423778	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999986	F	F	F
0.0392530566738675	0.9537253493265221	0.4621451720928838	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999985	F	F	F

0.0508716396810976	0.7277866957643069	0.4795353529448719	T	T	T
0.3765600030000016	0.8823999760000021	0.2866800130000016	F	F	F
0.2808988243969624	0.5928162973323005	0.4378693122772294	T	T	T
0.6475661627446083	0.5474436038092336	0.5955454168820739	T	T	T
0.6751712465814979	0.7337122165762625	0.6189303007440058	T	T	T
0.4531768339680589	0.4379428190492419	0.6003892739276964	T	T	T

K₂O-Fe₃C₂(010)

1.000000000000000

9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O K

40 16 1 2

Selective dynamics

Direct

0.03714999999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.09747999999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.53714999999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.59747999999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.48413999999999965	0.8711600000000033	0.28837999999999965	F	F	F
0.15048999999999978	0.06642999999999969	0.28837999999999965	F	F	F
0.98413999999999965	0.8711600000000033	0.28837999999999965	F	F	F
0.65048999999999978	0.06642999999999969	0.28837999999999965	F	F	F
0.06730999999999991	0.4688000000000017	0.29153999999999977	F	F	F
0.56730999999999991	0.4688000000000017	0.29153999999999977	F	F	F
0.31730999999999991	0.4688000000000017	0.32540999999999980	F	F	F
0.81730999999999991	0.4688000000000017	0.32540999999999980	F	F	F
0.40048999999999978	0.06642999999999969	0.3285800000000023	F	F	F
0.23413999999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.90048999999999978	0.06642999999999969	0.3285800000000023	F	F	F
0.73413999999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.34747999999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.28714999999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.84747999999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.78714999999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4795119629744818	0.3709749870728479	0.4008993248872221	T	T	T
0.9815590705612510	0.3745142735780996	0.4064345582700469	T	T	T
0.1549851888598768	0.5666386138422674	0.4010220555175587	T	T	T
0.6528289585842381	0.5629694103889156	0.4065333592729760	T	T	T
0.0381972942396547	0.7480892408431523	0.4111125139458391	T	T	T
0.5387493388774581	0.7480005374465796	0.4088706084934353	T	T	T
0.0958769811589562	0.1895006970942904	0.4089305783164401	T	T	T
0.5963866902008346	0.1894323964722470	0.4111187733737038	T	T	T
0.5680356218008916	0.9693131890329278	0.4126567658157047	T	T	T
0.0665849691418429	0.9682679728600196	0.4125940848881567	T	T	T
0.8173903480542143	0.9687867731641094	0.4357725353224438	T	T	T
0.3174379028311122	0.9687763365106048	0.4360362254293187	T	T	T
0.7829900253077428	0.7426034391213913	0.4452517014194852	T	T	T
0.3505360161646828	0.1914548464079803	0.4412348262545669	T	T	T
0.2841410793794799	0.7458040318053089	0.4415144150704323	T	T	T
0.8515580236876465	0.1949950632857512	0.4452464338438974	T	T	T
0.8932485603555731	0.5590502309441273	0.4428281395295195	T	T	T
0.3969749505442748	0.5603356017982788	0.4484778494144525	T	T	T
0.2375645223311038	0.3769649546282073	0.4482923106777943	T	T	T
0.7410686650507711	0.3786933040684056	0.4430182906446062	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9055280329575788	0.8506712228529384	0.3836551532133932	T	T	T
0.2269814262954083	0.0842652929274602	0.3829417545615877	T	T	T
0.7291147070793732	0.0868255657617870	0.3836278244746347	T	T	T
0.4075828158266157	0.8531167576065466	0.3829820178337380	T	T	T
0.6669514033664246	0.8554752402002770	0.4538566721630277	T	T	T
0.4676439694481603	0.0816168191562759	0.4556098974781206	T	T	T
0.1671269015096107	0.8559311940696183	0.4553059536431908	T	T	T
0.9676469734408882	0.0820851174299664	0.4539311137170752	T	T	T
0.3163844371891057	0.4687996876219239	0.5230800960781000	T	T	T
0.1116937837250796	0.5622859815434466	0.5729503354636157	T	T	T

0.5150931472590823 0.3668200778846945 0.5726325901395298 T T T

K₂O-Fe₅C₂(010*)

1.00000000000000

9.9837999344000004 0.000000000000000 0.000000000000000
-1.5315638797000000 11.4316603084999997 0.000000000000000
0.000000000000000 0.000000000000000 18.9298000335999994

Fe C O K
40 15 1 2

Selective dynamics

Direct

0.0371499999999969 0.2536300000000011 0.2882999999999996 F F F
0.0974799999999973 0.6839700000000022 0.2882999999999996 F F F
0.5371499999999969 0.2536300000000011 0.2882999999999996 F F F
0.5974799999999973 0.6839700000000022 0.2882999999999996 F F F
0.4841399999999965 0.8711600000000033 0.2883799999999965 F F F
0.1504899999999978 0.0664299999999969 0.2883799999999965 F F F
0.9841399999999965 0.8711600000000033 0.2883799999999965 F F F
0.6504899999999978 0.0664299999999969 0.2883799999999965 F F F
0.0673099999999991 0.4688000000000017 0.2915399999999977 F F F
0.5673099999999991 0.4688000000000017 0.2915399999999977 F F F
0.3173099999999991 0.4688000000000017 0.3254099999999980 F F F
0.8173099999999991 0.4688000000000017 0.3254099999999980 F F F
0.4004899999999978 0.0664299999999969 0.3285800000000023 F F F
0.2341399999999965 0.8711600000000033 0.3285800000000023 F F F
0.9004899999999978 0.0664299999999969 0.3285800000000023 F F F
0.7341399999999965 0.8711600000000033 0.3285800000000023 F F F
0.3474799999999973 0.6839700000000022 0.3286500000000032 F F F
0.2871499999999969 0.2536300000000011 0.3286500000000032 F F F
0.8474799999999973 0.6839700000000022 0.3286500000000032 F F F
0.7871499999999969 0.2536300000000011 0.3286500000000032 F F F
0.4817174528562674 0.3715159395248622 0.4051262185271315 T T T
0.9813038624176845 0.3734683176927302 0.4070323122953877 T T T
0.1549444880153763 0.5656711442321829 0.4047256159804632 T T T
0.6572036640391330 0.5628304168846062 0.4028529302181977 T T T
0.0368409660626184 0.7473031320050988 0.4094862444629019 T T T
0.5434233387427355 0.7471856294247264 0.4101013882166826 T T T
0.0956387448080232 0.1896767463709340 0.4093851285322097 T T T
0.5958599447783787 0.1864504468051809 0.4109243647129687 T T T
0.5653844424903840 0.9698589666406924 0.4060798546049763 T T T
0.0705664630407224 0.9684600294834257 0.4108910030432360 T T T
0.8215722151246934 0.9653140073345344 0.4354815298159788 T T T
0.3181641684943932 0.9692522207867911 0.4360358485917064 T T T
0.7703915029187981 0.7467089077968226 0.4438799857012644 T T T
0.3572442002610509 0.1920238191974621 0.4446382523071986 T T T
0.2854104980697820 0.7458697516958936 0.4493343452087727 T T T
0.8513653756631500 0.1918220097823910 0.4424376655083125 T T T
0.8941212114910357 0.5601287830364677 0.4450822719073145 T T T
0.3942010395700728 0.5604940119440969 0.4431520977245650 T T T
0.2407586094937901 0.3748112411566127 0.4445067635081167 T T T
0.7393033265284045 0.3740397334270208 0.4437294578112441 T T T
0.2320300000000017 0.5823099999999997 0.2641300000000015 F F F
0.4025999999999996 0.3552899999999966 0.2641300000000015 F F F
0.7320300000000017 0.5823099999999997 0.2641300000000015 F F F
0.9025999999999996 0.3552899999999966 0.2641300000000015 F F F
0.1525999999999996 0.3552899999999966 0.3528200000000012 F F F
0.4820300000000017 0.5823099999999997 0.3528200000000012 F F F
0.6525999999999996 0.3552899999999966 0.3528200000000012 F F F
0.9820300000000017 0.5823099999999997 0.3528200000000012 F F F
0.8998379634962602 0.8469063231911725 0.3827081183869799 T T T
0.2308248301206034 0.0889354555538167 0.3844671136205811 T T T
0.7288137760143588 0.0808438226120922 0.3826563205345335 T T T
0.4044863899083465 0.8520567136961418 0.3835598157515152 T T T
0.4704699947266360 0.0771729240325915 0.4582115517019128 T T T
0.1672077943903577 0.8560187333608992 0.4536266575787414 T T T
0.9663888429518668 0.0778540160367225 0.4525392967615219 T T T
0.4287691385712126 0.6904689733193117 0.5034737213566747 T T T
0.5260011993225040 0.8928527557951103 0.5654553387026066 T T T
0.5678385796513283 0.5019308546070550 0.5700778476318819 T T T

CO dissociation on Fe₅C₂(510)

Fe₅C₂(510)-CO (IS) (Initial state)

1.000000000000000

10.1180000000000003 0.000000000000000 0.000000000000000
 -0.7809265139842700 12.8064770233652006 0.0000000000000000
 0.0000000000000000 -0.0000000000000600 17.4192900000000002

Fe C O

60 25 1

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2156043565080224	0.9388673988896989	0.1336779453375163	T	T	T
0.7160557002584148	0.9389182794704611	0.1336268924346063	T	T	T
0.3399309900387017	0.5358374343703454	0.1414536561352753	T	T	T
0.8379966003643033	0.5354286893734213	0.1414522921269293	T	T	T
0.1360663767177638	0.1433579619642498	0.1452032407588787	T	T	T
0.6362762525583844	0.1434724158385493	0.1471237329725320	T	T	T
0.2258065743761381	0.3428631252159651	0.1427936216537894	T	T	T
0.7270627442321727	0.3437477025325408	0.1407104577262943	T	T	T
0.2856965737262844	0.7511733428204712	0.1491105951060017	T	T	T
0.7857964525879069	0.7505814144571021	0.1499990720204385	T	T	T
0.4627782828692825	0.8823346486536913	0.1529743499141133	T	T	T
0.9627149196345012	0.8825130648833929	0.1527944247441093	T	T	T
0.4721678811572773	0.2946537272729554	0.1633645847576623	T	T	T
0.9703086923230833	0.2946373523919870	0.1633840141243660	T	T	T
0.0773056533441374	0.4879823581837119	0.1602358853832583	T	T	T
0.5780002019994871	0.4892015726997954	0.1583720846139739	T	T	T
0.3937621938671895	0.0943890747430553	0.1636842911537955	T	T	T
0.8945365162531890	0.0948932812598640	0.1636696767406504	T	T	T
0.0384095124093839	0.6923209912132122	0.1662743197991736	T	T	T
0.5404965651708229	0.6919106328095485	0.1664130715562932	T	T	T
0.2041006430836435	0.6216822850151311	0.2517888441251246	T	T	T
0.7034618171890942	0.6200880963282008	0.2547259878949685	T	T	T
0.2908709893538621	0.2269226125090559	0.2553541111268534	T	T	T
0.7906932140549987	0.2235241643775071	0.2532496851278573	T	T	T
0.1346748033948913	0.8245557317738087	0.2548899109177354	T	T	T
0.6350804292870911	0.8247893323349613	0.2549828128487658	T	T	T
0.2135376959496764	0.0218412792472423	0.2592057100509714	T	T	T
0.7138942222358448	0.0211469391530206	0.2594505829037460	T	T	T
0.2424772263955760	0.4310742510382982	0.2681166201755616	T	T	T
0.7362473069512855	0.4257654716475046	0.2673235712017584	T	T	T
0.4411409229262687	0.5638751603600151	0.2686193274813909	T	T	T
0.9473235084652440	0.5605105502267490	0.2682772618930996	T	T	T
0.4560638727764055	0.9752320804982623	0.2717069682880472	T	T	T
0.9566602920911877	0.9741624871160577	0.2716700014744480	T	T	T
0.0407527399999827	0.1711171890111772	0.2714391301418090	T	T	T
0.5385149680345285	0.1701159983159600	0.2740769058345303	T	T	T
0.3894640060055387	0.7631591135512058	0.2732896291946577	T	T	T
0.8906316980956551	0.7624378039209507	0.2734348449023407	T	T	T
0.4988564625476337	0.3784169961910163	0.2903422688221122	T	T	T
0.9765400224821952	0.3679517053337120	0.2936584474742361	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F

0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0653398008444163	0.0091049266521063	0.1834123170825955	T	T	T
0.5655516321259152	0.0085431107686413	0.1833305242085894	T	T	T
0.3958594800485749	0.4227937745186715	0.2047647944676108	T	T	T
0.8971439960350348	0.4244371499728483	0.2045680255886992	T	T	T
0.3078294903114906	0.8875329321987457	0.2309103307297664	T	T	T
0.8086630583756458	0.8870753844139483	0.2309067875473118	T	T	T
0.1306741475688246	0.3055756293812987	0.2563551638410912	T	T	T
0.6278637445237860	0.2990655028290365	0.2386176396968435	T	T	T
0.0502379903057546	0.6903530535265473	0.2818056835700769	T	T	T
0.5481953282082219	0.6922112152060732	0.2808760175931113	T	T	T
0.3688195580286685	0.1007478035456065	0.2867257826657085	T	T	T
0.8711727345761585	0.1002347240955716	0.2861573137078293	T	T	T
0.6269383729321160	0.4730806734943382	0.3496597367098299	T	T	T
0.6255538309017367	0.5049579047558773	0.4142586277042666	T	T	T

Fe₅C₂(510)-C+O (TS) (transition state)

1.0000000000000000
10.1180000000000003 0.0000000000000000 0.0000000000000000
-0.7809265139842700 12.8064770233652006 0.0000000000000000
0.0000000000000000 -0.0000000000000600 17.4192900000000002
Fe C O
60 25 1

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2144677848480665	0.9388988054149084	0.1334333501038115	T	T	T
0.7158198519961603	0.9396589493721069	0.1334719239328529	T	T	T
0.3414698091783241	0.5370125814906928	0.1447097440309683	T	T	T
0.8407209572913278	0.5378676062931609	0.1424970792677676	T	T	T
0.1371356348613399	0.1434045784122033	0.1454364460291426	T	T	T
0.6374333266345650	0.1428782119506689	0.1467859242078255	T	T	T
0.2271013233050582	0.3437846152155934	0.1430939041778225	T	T	T
0.7268988866529646	0.3428455420971784	0.1407595824126134	T	T	T
0.2839970090993347	0.7509936124805662	0.1488631058539922	T	T	T
0.7846020000609920	0.7515364041925112	0.1496337559269666	T	T	T
0.4616702378041902	0.8829565329732054	0.1524288550147392	T	T	T
0.9621890152204434	0.8829119921605092	0.1522424446988200	T	T	T
0.4727403341838610	0.2915441299877474	0.1616735269702347	T	T	T
0.9721642651834091	0.2928464938869502	0.1621416475796105	T	T	T
0.0781886049643600	0.4896471127971709	0.1628037169575964	T	T	T
0.5800483065793869	0.4899551016454508	0.1620698152973448	T	T	T
0.3934452470974766	0.0938061911756340	0.1633385518451682	T	T	T
0.8945670757212848	0.0939429057003016	0.1632767574185237	T	T	T
0.0372954277727104	0.6913760411501804	0.1670919523358310	T	T	T
0.5383314148578283	0.6935877074155490	0.1661595178256201	T	T	T

0.2011993731897312	0.6212046674707604	0.2538995577514386	T	T	T
0.6946348379496387	0.6265843382759687	0.2565035877978555	T	T	T
0.2949685501377194	0.2285928711213608	0.2547136068176916	T	T	T
0.7948493237940429	0.2245679455459851	0.2531280331282804	T	T	T
0.1331333690152902	0.8250147065083828	0.2552667842764254	T	T	T
0.6338216048940909	0.8305822333248896	0.2531047870740994	T	T	T
0.2132767008624293	0.0235406685292934	0.2589610566704950	T	T	T
0.7145226493060601	0.0232607967082554	0.2593108884736250	T	T	T
0.2428075583508858	0.4308008551962385	0.2700486346436394	T	T	T
0.7463934705562003	0.4185055057276865	0.2670143255858756	T	T	T
0.4438058328201229	0.5703277290802835	0.2726321159181390	T	T	T
0.9349296873400296	0.5647162565016999	0.2736200196109097	T	T	T
0.4551627985035916	0.9748956861024364	0.2718761118273217	T	T	T
0.9575441038753673	0.9742355279262159	0.2717174240856262	T	T	T
0.0402795564573429	0.1706759519617498	0.2713227764059987	T	T	T
0.5393415219914535	0.1676116461185379	0.2724450677194505	T	T	T
0.3837158271915915	0.7669192888417649	0.2728316723689462	T	T	T
0.8891048197197489	0.7654719596846763	0.2722162335875981	T	T	T
0.4979854227017403	0.3778591247060920	0.2854597708913949	T	T	T
0.9914196776087463	0.3739867381843688	0.2888374220638935	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0649240724086396	0.0096052144084453	0.1830277242112333	T	T	T
0.5650447040736299	0.0089175942194961	0.1840234699207526	T	T	T
0.3910749472952774	0.4175795884461473	0.2016146664509737	T	T	T
0.8991801020161038	0.4221576230961829	0.1997625185074743	T	T	T
0.3053503827114579	0.8906189438769642	0.2306467772344788	T	T	T
0.8087152593152361	0.8899529818018237	0.2302912972877877	T	T	T
0.1332794568899384	0.3019725992914887	0.2485163097073325	T	T	T
0.6296612669964308	0.2959902734127057	0.2402987155159259	T	T	T
0.0474426133976936	0.6913468155083489	0.2820409158256509	T	T	T
0.5438953910322862	0.7031503461041285	0.2806769202652956	T	T	T
0.3691412935967184	0.1014731255153493	0.2865904994393323	T	T	T
0.8725880119925832	0.1002778066821803	0.2864892536296915	T	T	T
0.6045670351314525	0.5010284893684487	0.2968517388419529	T	T	T
0.7552336521314726	0.5345467801537648	0.3394139898232952	T	T	T

Fe₅C₂(510)C+O (FS) (final state)

1.0000000000000000		
10.1180000000000003	0.0000000000000000	0.0000000000000000
-0.7809265139842700	12.8064770233652006	0.0000000000000000
0.0000000000000000	-0.00000000000000600	17.4192900000000002

Fe C O

60 25 1

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F

0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2152295008330027	0.9393064159562630	0.1337780896909971	T	T	T
0.7165922728526037	0.9397600869857389	0.1340634741551909	T	T	T
0.3391364352178910	0.5345600833626695	0.1425158543552057	T	T	T
0.8396858882213744	0.5350779346778273	0.1417277246575816	T	T	T
0.1361897631229153	0.1428461588875606	0.1448195823084444	T	T	T
0.6372949039817876	0.1436151859262763	0.1477263531000395	T	T	T
0.2247741590544203	0.3416790747485468	0.1430888599085162	T	T	T
0.7289048002844042	0.3446957601340612	0.1483828989163833	T	T	T
0.2844469877843412	0.7521884579463701	0.1485164136861051	T	T	T
0.7861884846674033	0.7530362488932054	0.1479846179612137	T	T	T
0.4626143111475011	0.8830826746618418	0.1522319321648984	T	T	T
0.9638257988959774	0.8818737058044395	0.1532682002399626	T	T	T
0.4712042540618929	0.2898422295314070	0.1601453369319600	T	T	T
0.9694087274550659	0.2927961112911481	0.1628689398594519	T	T	T
0.0763270964555808	0.4879615338316087	0.1586311665809077	T	T	T
0.5753396084744778	0.4883967593471061	0.1592992840207466	T	T	T
0.3931759545207898	0.0929495667940231	0.1632509742687938	T	T	T
0.8931759818807340	0.0943478051302375	0.1641660577494921	T	T	T
0.0395190708389816	0.6911478650610499	0.1666417059506575	T	T	T
0.5286050669049602	0.6892450251105330	0.1665123752202518	T	T	T
0.2123641196947385	0.6204628321934382	0.2503597501427207	T	T	T
0.7034175450321599	0.6340605399719601	0.2469665244711290	T	T	T
0.2916890838290212	0.2261930291878775	0.2545515581258501	T	T	T
0.7919751200044619	0.2261162978993429	0.2562256517747700	T	T	T
0.1364359321823991	0.8248669263868179	0.2552420548648963	T	T	T
0.6346163428788548	0.8286824197364754	0.2530817147677469	T	T	T
0.2133085372647566	0.0216497353538973	0.2593237340657707	T	T	T
0.7133826863816497	0.0223857940165570	0.2602547824729367	T	T	T
0.2362871608327483	0.4314050897591488	0.2672469646226254	T	T	T
0.7285708658670639	0.4457758069039567	0.2784937749524419	T	T	T
0.4613791237964607	0.5606399477588478	0.2765119745823074	T	T	T
0.9536701665980269	0.5608170640203637	0.2719768457669338	T	T	T
0.4563052027693812	0.9749203377107620	0.2712083250981552	T	T	T
0.9555060188264796	0.9724423587846612	0.2718760276725906	T	T	T
0.0400444136925750	0.1677130370599710	0.2712787464574479	T	T	T
0.5368202578014568	0.1693215310640997	0.2738133732167033	T	T	T
0.3894127185527627	0.7640453484885164	0.2729092718774080	T	T	T
0.8925624711677632	0.7569701794919211	0.2752801419459459	T	T	T
0.4895058950548903	0.3696833151447979	0.2845693381808087	T	T	T
0.9915846467005833	0.3755945275792211	0.2891492240306203	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0645771683304394	0.0098481352905213	0.1841963787742789	T	T	T
0.5661788478017837	0.0090747636502213	0.1836773736581525	T	T	T
0.3911579846463236	0.4171575006952083	0.2009494630768864	T	T	T
0.8887928008369199	0.4210079804851490	0.2058049390971721	T	T	T
0.3081114273152300	0.8882328975726519	0.2300430577635530	T	T	T
0.8099534955419463	0.8844797499193869	0.2307630471700646	T	T	T
0.1281745579661015	0.3002377505154000	0.2459646183876120	T	T	T
0.6268107132379835	0.2974083558461652	0.2388271312838650	T	T	T
0.0594007430936183	0.6895243242110917	0.2798899567379176	T	T	T
0.5500057226660765	0.6969677148082620	0.2803494519256731	T	T	T
0.3684901503452068	0.1000472829511811	0.2870609962402318	T	T	T
0.8711496216670406	0.0997665941274662	0.2871494726021255	T	T	T
0.8037215495040978	0.5798694793098860	0.3188312846893468	T	T	T
0.5605939070435014	0.4745882355608696	0.3412750837515873	T	T	T

HCO formation and dissociation on Fe₅C₂(510)

Fe₅C₂(510)-CO+H (IS)

```

1.000000000000000
10.118000000000003 0.000000000000000 0.000000000000000
-0.7809265139842700 12.8064770233652006 0.000000000000000
0.000000000000000 -0.0000000000000600 17.419290000000002
Fe C O H
60 25 1 1
Selective dynamics

Direct
0.2394699999999972 0.2602600000000024 0.0193299999999965 F F F
0.7394699999999972 0.2602600000000024 0.0193299999999965 F F F
0.3524200000000022 0.8641300000000030 0.0267499999999998 F F F
0.8524200000000022 0.8641300000000030 0.0267499999999998 F F F
0.1786799999999999 0.4665400000000020 0.0302900000000008 F F F
0.6786799999999999 0.4665400000000020 0.0302900000000008 F F F
0.2651299999999992 0.6599000000000004 0.0305200000000028 F F F
0.7651299999999992 0.6599000000000004 0.0305200000000028 F F F
0.2917699999999996 0.0723199999999977 0.0369999999999990 F F F
0.7917699999999996 0.0723199999999977 0.0369999999999990 F F F
0.4854800000000026 0.2084899999999976 0.0384200000000021 F F F
0.9854800000000026 0.2084899999999976 0.0384200000000021 F F F
0.0121200000000030 0.6209100000000021 0.0448999999999984 F F F
0.5121200000000030 0.6209100000000021 0.0448999999999984 F F F
0.0985700000000023 0.8142700000000005 0.0451300000000003 F F F
0.5985700000000023 0.8142700000000005 0.0451300000000003 F F F
0.4248300000000000 0.4166799999999995 0.0486700000000013 F F F
0.9248300000000000 0.4166799999999995 0.0486700000000013 F F F
0.0377799999999979 0.0205500000000001 0.0560899999999975 F F F
0.5377799999999979 0.0205500000000001 0.0560899999999975 F F F
0.2150856145887532 0.9386801297179201 0.1340847903241666 T T T
0.7155254176313891 0.9386616033637099 0.1338135210395472 T T T
0.3389288245433145 0.5353154135009255 0.1394465023020557 T T T
0.8388633531405273 0.5361930768279345 0.1397469243335620 T T T
0.1359534237098683 0.1431639634946641 0.1455059503907692 T T T
0.6362481278279077 0.1437471305041619 0.1464305859980752 T T T
0.2239460786788372 0.3421373954206028 0.1422275092185437 T T T
0.7260776450470916 0.3426774916698668 0.1435177472071055 T T T
0.2855814480016725 0.7517032790311678 0.1489790870925167 T T T
0.7870028369351415 0.7499603454928019 0.1498664411163927 T T T
0.4639637219516492 0.8818924821110989 0.1533678290170739 T T T
0.9628438359401633 0.8829067169587840 0.1527837952379359 T T T
0.4711407390315907 0.2943620285579123 0.1626108931658830 T T T
0.9676146043025258 0.2917360756843970 0.1619617823792189 T T T
0.0766347006861886 0.4886854975911529 0.1612955534923949 T T T
0.5779140262428285 0.4879137174016258 0.1605540652036300 T T T
0.3937594196797992 0.0941308342503880 0.1635809506933376 T T T
0.8926973883879893 0.0953884609245019 0.1646951349984051 T T T
0.0383672045223661 0.6923242780877982 0.1663816376031966 T T T
0.5413854163029563 0.6915244992598831 0.1662953789082604 T T T
0.2065540073991352 0.6224395511933382 0.2511759583129562 T T T
0.7015781440642221 0.6193125321468467 0.2551301637302759 T T T
0.2900754532346463 0.2253385139232207 0.2542014019039912 T T T
0.7897971833069902 0.2275463275542202 0.2606909033901224 T T T
0.1352216630528934 0.8247647728172517 0.2551268697062070 T T T
0.6357732233371864 0.8241191029099281 0.2545469255195490 T T T
0.2136239555219253 0.0219917549494333 0.2593923218417485 T T T
0.7136819805621276 0.0219663975469523 0.2594015743567779 T T T
0.2392591736578014 0.4311532419332932 0.2666194189198202 T T T
0.7433431324150110 0.4285455890537305 0.2692523860304239 T T T
0.4421641496971928 0.5614552717050718 0.2673067579069955 T T T
0.9473844903945515 0.5608209751785334 0.2697290088889874 T T T
0.4563689554070141 0.9753496500382081 0.2716440712225481 T T T
0.9558418698428254 0.9735348033458834 0.2721865659956623 T T T
0.0392152591261314 0.1694761261362960 0.2713431510837546 T T T
0.5395511854959477 0.1723307519658071 0.2729341838768070 T T T
0.3917594267199209 0.7626121553133703 0.2732338973870567 T T T
0.8900093370434546 0.7607408024946165 0.2731833427360125 T T T
0.4781443058607970 0.3693939683928594 0.2919128628261052 T T T
0.9832430214101034 0.3710970826640264 0.2888002519467844 T T T
0.3220200000000020 0.5286800000000014 0.0000000000000000 F F F
0.8220200000000020 0.5286800000000014 0.0000000000000000 F F F
0.2192900000000009 0.9343099999999964 0.0082499999999968 F F F
0.7192900000000009 0.9343099999999964 0.0082499999999968 F F F
0.0579600000000013 0.3464999999999989 0.0671699999999973 F F F
0.5579600000000013 0.3464999999999989 0.0671699999999973 F F F
0.4552300000000002 0.7521300000000011 0.0754200000000012 F F F

```

0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0646591893908985	0.0096059336064239	0.1840262623011789	T	T	T
0.5653921959489087	0.0093131819394638	0.1832980705808934	T	T	T
0.3951352122275827	0.4232345579780947	0.2022225116899735	T	T	T
0.8941675612024294	0.4234073241189639	0.2001903907333372	T	T	T
0.3086123832134264	0.8870790177426020	0.2310967260508062	T	T	T
0.8086822653478689	0.8864954767384851	0.2304466945124987	T	T	T
0.1308274284814376	0.3027203444604438	0.2527230720014070	T	T	T
0.6255902778809599	0.3061159042024568	0.2445153916571074	T	T	T
0.0526624302633136	0.6904489813444853	0.2813198728659408	T	T	T
0.5500520962609429	0.6895127683680340	0.2814117320952094	T	T	T
0.3701018138061696	0.1009861682570389	0.2862657728415579	T	T	T
0.8696658836184095	0.1000413187137962	0.2872175040632686	T	T	T
0.7661410209742014	0.5680912616949881	0.3442948218192162	T	T	T
0.7809457248632984	0.5605939552561060	0.4120743906235563	T	T	T
0.8306036758871567	0.3354279049813458	0.3269047768360256	T	T	T

Fe₅C₂(510)-HCO (TS)

1.000000000000000		
10.118000000000003	0.000000000000000	0.000000000000000
-0.7809265139842700	12.8064770233652006	0.000000000000000
0.000000000000000	-0.0000000000000600	17.419290000000002
Fe	C	O
60	25	1

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2151406150353707	0.9392044327348027	0.1337300266195530	T	T	T
0.7156909185391311	0.9385074657747094	0.1335860395755866	T	T	T
0.3388481530381241	0.5350125386385571	0.1384940912887604	T	T	T
0.8395451525140436	0.5366770081802099	0.1430373896637213	T	T	T
0.1363864875164492	0.1434168883356343	0.1465092776167961	T	T	T
0.6358839061570852	0.1431577638633651	0.1453701295518213	T	T	T
0.2253068628195653	0.3425327507648691	0.1414270894092882	T	T	T
0.7267832197633416	0.3426361159053873	0.1453085170953534	T	T	T
0.2845584858597736	0.7521174071728591	0.1483678094806971	T	T	T
0.7869755667991443	0.7498800071715273	0.1505598417923002	T	T	T
0.4629262595354772	0.8822780693190825	0.1530655888237171	T	T	T
0.9620885108607249	0.8825209287987980	0.1527065166885790	T	T	T
0.4714491343828683	0.2945676185684188	0.1626766375448959	T	T	T
0.9708385075810330	0.2920288711466840	0.1625544165424244	T	T	T
0.0768834221744174	0.4885648156823449	0.1601338857256877	T	T	T
0.5789196050815535	0.4882825736483119	0.1608907020277373	T	T	T
0.3942798544946907	0.0946603586414956	0.1633373509818307	T	T	T
0.8934605897728662	0.0934723253177200	0.1635736637630674	T	T	T
0.0375362920556834	0.6924446501452041	0.1665012587027612	T	T	T
0.540899832413823	0.6920541210149778	0.1660628127975319	T	T	T
0.2056759971966623	0.6215946473234291	0.2499946194961871	T	T	T
0.6989431022761663	0.6226745687396070	0.2554285096279054	T	T	T
0.2911211202353596	0.2249581164281655	0.2540992795694630	T	T	T

0.7897624101415682	0.2247623876460115	0.2550002388431021	T	T	T
0.1341564444995398	0.8259785267127762	0.2543884956037745	T	T	T
0.6332726864400503	0.8251899936511097	0.2546265228431893	T	T	T
0.2134800993016449	0.0222780298704479	0.2592592150584084	T	T	T
0.7133608502301352	0.0210644878366768	0.2590005179985720	T	T	T
0.2371635151147818	0.4284881744206195	0.2677450262980183	T	T	T
0.7485415724961539	0.4301139718224662	0.2712090300096170	T	T	T
0.4382502464194390	0.5627597553317301	0.2666829829079220	T	T	T
0.9485273940189474	0.5619962528448773	0.2696930156856228	T	T	T
0.4561610744058383	0.9753609466261277	0.2715915226578262	T	T	T
0.9555158148663153	0.9741026600400712	0.2715652064563848	T	T	T
0.0379513473639608	0.1702682779698198	0.2734350942924062	T	T	T
0.5393064288941615	0.1727234679011068	0.2713409755318015	T	T	T
0.3866963340296067	0.7639925721122233	0.2730461043362096	T	T	T
0.8897850227880780	0.7614324196774601	0.2756772336312556	T	T	T
0.4786464957816867	0.3709970071390714	0.2904827694450841	T	T	T
0.9947609267371853	0.3745432185586388	0.2897392538193782	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0649992574116341	0.0089341351077466	0.1833379190948820	T	T	T
0.5650804522203924	0.0090506734735107	0.1831988430404079	T	T	T
0.3949611692179880	0.4246720470198946	0.2023079929497253	T	T	T
0.8956238393325336	0.4203547926594867	0.2015586158915590	T	T	T
0.3074182342879173	0.8887497289564797	0.2304360046494390	T	T	T
0.8077136748946973	0.8860125810191537	0.2304646827903356	T	T	T
0.1291395801676996	0.2994281085379079	0.2420440797141116	T	T	T
0.6302928709611576	0.3066438582773707	0.2498605348327721	T	T	T
0.0543740607844200	0.6915519633374014	0.2805556579230612	T	T	T
0.5430432694976581	0.6916509004438122	0.2802216369455321	T	T	T
0.3702986561586620	0.1012920117198968	0.2862085851592026	T	T	T
0.8691530688079652	0.0997102604607831	0.2869898810667529	T	T	T
0.7762399241506673	0.5340605317709789	0.3448467098132600	T	T	T
0.7911173645666830	0.6217476778540700	0.3766195778993740	T	T	T
0.7405700981251848	0.4614263575011494	0.3824068448526313	T	T	T

Fe₅C₂(510)-HCO (FS)

```

1.000000000000000
 10.1180000000000003  0.0000000000000000  0.0000000000000000
-0.7809265139842700  12.8064770233652006  0.0000000000000000
 0.0000000000000000 -0.0000000000000060  17.4192900000000002
Fe  C  O  H
60 25  1  1

```

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F

0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2156628732607928	0.9388273768923201	0.1338208616181525	T	T	T
0.7154319336234282	0.9390009438312649	0.1336220953640275	T	T	T
0.3390805025362089	0.5351084194531254	0.1389515165263147	T	T	T
0.8408558920823280	0.5390151848687773	0.1415455482069329	T	T	T
0.1368212988253180	0.1432700428511032	0.1454365052215948	T	T	T
0.6355924520265099	0.1430445291394981	0.1451092028015312	T	T	T
0.2259632400183175	0.3432884745710562	0.1423241927505974	T	T	T
0.7243914304418683	0.3425650340617949	0.1393837245129028	T	T	T
0.2853610195649376	0.7515208667602378	0.1487103403165460	T	T	T
0.7850705694989381	0.7507195116708227	0.1504758215460610	T	T	T
0.4636793957312762	0.8823602180603054	0.1531837756655330	T	T	T
0.9622348762505745	0.8832670986281604	0.1522047517351065	T	T	T
0.4722497153592450	0.2947882343774809	0.1633870055050186	T	T	T
0.9709276397169604	0.2915739596167421	0.1621527780882572	T	T	T
0.0760388116252897	0.4895572571183433	0.1607627480117149	T	T	T
0.5786681073461658	0.4898148335382482	0.1606016744650175	T	T	T
0.3937455647864243	0.0949987323614752	0.1636827355776312	T	T	T
0.8945125855431969	0.0939999219984286	0.1634104110498196	T	T	T
0.0373530877720646	0.6922262345826764	0.1664217988687381	T	T	T
0.5423618228434295	0.6923144757497210	0.1666611996996137	T	T	T
0.2035755143507879	0.6220242892277448	0.2511297024432394	T	T	T
0.7014152806476679	0.6196863015797847	0.2581259756947741	T	T	T
0.2896846841666576	0.2286029575005019	0.2547256686026571	T	T	T
0.7894415743445378	0.2247505244188711	0.2513771282808523	T	T	T
0.1349368958764157	0.8272985381543699	0.2541296562750874	T	T	T
0.6339989460993593	0.8256908396840084	0.2553912179079139	T	T	T
0.2137590029964524	0.0234932838765103	0.2590327196903404	T	T	T
0.7136054685946064	0.0225007278554786	0.2590030255303805	T	T	T
0.2421053222053532	0.4325829444077251	0.2671988643419236	T	T	T
0.7451582779846506	0.4254089352500121	0.2647152171833185	T	T	T
0.4372839122362543	0.5649001130439117	0.2664810368765803	T	T	T
0.9415902316101991	0.5679867879780028	0.2731271972922221	T	T	T
0.4564731956563965	0.9767769543966758	0.2716503072116019	T	T	T
0.9560323891530256	0.9751667219344040	0.2714771216611130	T	T	T
0.0386763800430439	0.1730651641567677	0.2705372126119570	T	T	T
0.5385539969410827	0.1738023482328639	0.2722445545988426	T	T	T
0.3895470642954638	0.7641056357246747	0.2728080359504103	T	T	T
0.8919811287215450	0.7657191342371190	0.2725684655253118	T	T	T
0.4952259459765052	0.3816461860877519	0.2918049480866997	T	T	T
0.9831974884138955	0.3811575560846073	0.2880299114819042	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0655023235702696	0.0092864029639927	0.1832520308535155	T	T	T
0.5648052029478253	0.0095125240348764	0.1829572868465416	T	T	T
0.3954038836510474	0.4236748561158767	0.2031859046774696	T	T	T
0.8923774878412853	0.4189590904742981	0.1945276153713314	T	T	T
0.3085359726428042	0.8888706314346559	0.2310893936953213	T	T	T
0.8071684918299983	0.8885906469154004	0.2305448082572291	T	T	T
0.1298139447713522	0.3070771250691290	0.2560281280936915	T	T	T
0.6295083343864563	0.3051859890272872	0.2414742076546936	T	T	T
0.0545204399181218	0.6942559394752001	0.2806933158106490	T	T	T
0.5467501810326943	0.6911736507240559	0.2814266027864104	T	T	T
0.3693943327738370	0.1028339889887098	0.2859115592389041	T	T	T
0.8703728063348423	0.1017486398648294	0.2857733486864799	T	T	T
0.8124800175838520	0.4917140466345367	0.3547865140002306	T	T	T
0.8018566729813950	0.5957481534445711	0.3576748826683855	T	T	T
0.8366989953448734	0.4580817564156408	0.4112517919952223	T	T	T

Fe₅C₂(510)-CH+O (TS)

```

1.000000000000000
10.118000000000003 0.000000000000000 0.000000000000000
-0.7809265139842700 12.8064770233652006 0.000000000000000
0.000000000000000 -0.0000000000000600 17.419290000000002
Fe C O H
60 25 1 1

```

Selective dynamics

Direct

```

0.2394699999999972 0.2602600000000024 0.0193299999999965 F F F
0.7394699999999972 0.2602600000000024 0.0193299999999965 F F F
0.3524200000000022 0.8641300000000030 0.0267499999999998 F F F
0.8524200000000022 0.8641300000000030 0.0267499999999998 F F F
0.1786799999999999 0.4665400000000020 0.0302900000000008 F F F
0.6786799999999999 0.4665400000000020 0.0302900000000008 F F F
0.2651299999999992 0.6599000000000004 0.0305200000000028 F F F
0.7651299999999992 0.6599000000000004 0.0305200000000028 F F F
0.2917699999999996 0.0723199999999977 0.0369999999999990 F F F
0.7917699999999996 0.0723199999999977 0.0369999999999990 F F F
0.4854800000000026 0.2084899999999976 0.0384200000000021 F F F
0.9854800000000026 0.2084899999999976 0.0384200000000021 F F F
0.0121200000000030 0.6209100000000021 0.0448999999999984 F F F
0.5121200000000030 0.6209100000000021 0.0448999999999984 F F F
0.0985700000000023 0.8142700000000005 0.0451300000000003 F F F
0.5985700000000023 0.8142700000000005 0.0451300000000003 F F F
0.4248300000000000 0.4166799999999995 0.0486700000000013 F F F
0.9248300000000000 0.4166799999999995 0.0486700000000013 F F F
0.0377799999999979 0.0205500000000001 0.0560899999999975 F F F
0.5377799999999979 0.0205500000000001 0.0560899999999975 F F F
0.2147709283251809 0.9390752012239008 0.1339136644033962 T T T
0.7163960139312007 0.9384184249260373 0.1337110590653595 T T T
0.3389031319597175 0.5353148907934464 0.1391360327371669 T T T
0.8411071514087634 0.5394004390117744 0.1412456925437245 T T T
0.1366411793063603 0.1428365327941291 0.1447359207596690 T T T
0.6361837332162044 0.1424955896002669 0.1451913597097952 T T T
0.2259180145278597 0.3429504119467535 0.1422402158821776 T T T
0.7259184504353853 0.3429860516896348 0.1419617664139536 T T T
0.2845590923509627 0.7520478720857562 0.1481631556865821 T T T
0.7855850923316080 0.7492154851197871 0.1522785057977158 T T T
0.4632392929435347 0.8818597870073686 0.1529777115597794 T T T
0.9620107925581777 0.8810461063033607 0.1539483759395155 T T T
0.4717832668501214 0.2935219255460859 0.1625620205652703 T T T
0.9711347657376844 0.2918614660853230 0.1625180211609099 T T T
0.0776599967410075 0.4890315922644043 0.1585907538393029 T T T
0.5783276672566734 0.4889592557999297 0.1607710848290728 T T T
0.3940743495637941 0.0945281331462451 0.1632689496782572 T T T
0.8939658746709777 0.0937334433296913 0.1638801981697962 T T T
0.0374705585790148 0.6929151523902586 0.1658328367346559 T T T
0.5414129775781212 0.6911237586014987 0.1660305913594662 T T T
0.2055303812323211 0.6213181431234396 0.2507284475587641 T T T
0.6974964024758373 0.6240248401899653 0.2618001485480408 T T T
0.2884678610871853 0.2267657490867565 0.2539077173534145 T T T
0.7887956427357261 0.2260749129975939 0.2529232608551541 T T T
0.1338434998282868 0.8264678614013999 0.2544103175715283 T T T
0.6317533115431372 0.8271881910890941 0.2541684989949449 T T T
0.2132906333277164 0.0236083612172481 0.2587504908394144 T T T
0.7133001247408206 0.0221521293276523 0.2588888018348118 T T T
0.2386160499609186 0.4315763831865062 0.2666002282285967 T T T
0.7442632895259478 0.4324116374520880 0.2663904133819875 T T T
0.4406138613687252 0.5626574702247187 0.2657466604200531 T T T
0.9512977243083033 0.5607283780738711 0.2690259180926536 T T T
0.4560718483053748 0.9766890672803598 0.2713930060556903 T T T
0.9551103375301351 0.9732449497000489 0.2725784074222466 T T T
0.0385555105809724 0.1700105602577766 0.2700401100964232 T T T
0.5394163589427032 0.1744857807854486 0.2709797424095104 T T T
0.3859831743961655 0.7649267358956545 0.2724564916030658 T T T
0.8897397644886794 0.7604866793248342 0.2810080156006699 T T T
0.4809620788465724 0.3755986432629452 0.2907101752591846 T T T
0.9863005406869377 0.3805020344739014 0.2875691727772139 T T T
0.3220200000000020 0.5286800000000014 0.0000000000000000 F F F
0.8220200000000020 0.5286800000000014 0.0000000000000000 F F F
0.2192900000000009 0.9343099999999964 0.0082499999999968 F F F
0.7192900000000009 0.9343099999999964 0.0082499999999968 F F F
0.0579600000000013 0.3464999999999989 0.0671699999999973 F F F

```

0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0639632455720087	0.0091064262472606	0.1837013814320110	T	T	T
0.5651037629605027	0.0086599532914358	0.1829528991795421	T	T	T
0.3929544337771479	0.4216907103642424	0.2008488663250988	T	T	T
0.8910280211136595	0.4199935447573624	0.1961554045039837	T	T	T
0.3071166553283803	0.8897715287104729	0.2307200354825380	T	T	T
0.8082192654929774	0.8851404375971059	0.2305503062722128	T	T	T
0.1273501570465433	0.3039082574253741	0.2505297119678421	T	T	T
0.6302743505492321	0.3089258303953829	0.2503893484619543	T	T	T
0.0545151981804595	0.6922264297641523	0.2791397786077451	T	T	T
0.5400673354538950	0.6929196633257271	0.2797761555358427	T	T	T
0.3702408186714908	0.1028426082567749	0.2854188231467858	T	T	T
0.8696173316054269	0.1011704735581169	0.2859934745109489	T	T	T
0.8153362865825305	0.5295759609321219	0.3407405487892328	T	T	T
0.7917468949223885	0.6739219295460838	0.3483614036436811	T	T	T
0.8016861461880115	0.5223363669238567	0.4029319474801267	T	T	T

Fe₅C₂(510)-CH+O (FS)

1.000000000000000		
10.1180000000000003	0.0000000000000000	0.0000000000000000
-0.7809265139842700	12.8064770233652006	0.0000000000000000
0.0000000000000000	-0.0000000000000600	17.4192900000000002
Fe	C	O
60	25	1

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2155408223341976	0.9385092212601783	0.1340092911792505	T	T	T
0.7132025235729070	0.9372446557492070	0.1340938331216659	T	T	T
0.3389541134197747	0.5353570246847349	0.1392152179658258	T	T	T
0.8410230563505449	0.5405455547295807	0.1430256508757702	T	T	T
0.1369217030971187	0.1426673379091256	0.1442689256437799	T	T	T
0.6355674337759201	0.1429058146577045	0.1442833118731495	T	T	T
0.2250247383784535	0.3435842722221691	0.1413884935014898	T	T	T
0.7263328687136290	0.3429100449879410	0.1405081891013701	T	T	T
0.2850180538510377	0.7510635500971712	0.1485187662693923	T	T	T
0.7866565964972713	0.7482511112754511	0.1522137017677091	T	T	T
0.4639710274465477	0.8816141165848778	0.1535445401021050	T	T	T
0.9625809956578785	0.8827803837927313	0.1523805864450038	T	T	T
0.4696180985200051	0.2933604924791347	0.1619833340075596	T	T	T
0.9735048682173006	0.2928463850487047	0.1634806482474893	T	T	T
0.0775603882009536	0.4904984504141324	0.1605826161905467	T	T	T
0.5806946631179823	0.4889812806637904	0.1632078339685547	T	T	T
0.3937273416251842	0.0938709174232059	0.1633736365437202	T	T	T
0.8940696470318015	0.0941741221273643	0.1632167095488110	T	T	T
0.0371812164548793	0.6932579188492617	0.1660793398264854	T	T	T

0.5429226553148635	0.6907410596707474	0.1673074823875914	T	T	T
0.1990802329674215	0.6204549753193316	0.2524968708620873	T	T	T
0.6976438535991383	0.6236192835566398	0.2715551163109274	T	T	T
0.2889337112064105	0.2248776146994114	0.2529143420986934	T	T	T
0.7891666374829265	0.2254648228749974	0.2511530263646097	T	T	T
0.1344514785828940	0.8267449762997163	0.2550426508524487	T	T	T
0.6420582278069107	0.8208610004257332	0.2652665956000305	T	T	T
0.2143762133929610	0.0229195156503802	0.2590083678144580	T	T	T
0.7135436480898745	0.0232813789608616	0.2580354275458122	T	T	T
0.2407423572120816	0.4275746926438179	0.2673263677839069	T	T	T
0.7457451020783947	0.4294784286633103	0.2659728594023407	T	T	T
0.4352483334290824	0.5591478623740198	0.2664472202849397	T	T	T
0.9394925118620157	0.5677663484685748	0.2722197070074311	T	T	T
0.4575448449894716	0.9752974539004032	0.2723357348469204	T	T	T
0.9567362962077192	0.9753874160107285	0.2721341765888248	T	T	T
0.0396865321910465	0.1690204448691611	0.2699786135525257	T	T	T
0.5393275375600441	0.1734729975038185	0.2701206684993663	T	T	T
0.3838225135762021	0.7651342623588477	0.2730053304298920	T	T	T
0.8910279287615015	0.7712077429911561	0.2785479972815461	T	T	T
0.4806706841911892	0.3703682715497866	0.2913869419951122	T	T	T
0.9959918117485739	0.3884921418932308	0.2868367285768958	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0654137978704914	0.0093592690908456	0.1839399938319296	T	T	T
0.5642736471533782	0.0099398634659965	0.1828963594402244	T	T	T
0.3956936133515224	0.4223605724502248	0.2017268002611781	T	T	T
0.8926501438448410	0.4211643497546496	0.1974357187970066	T	T	T
0.3084664038263170	0.8893899821047002	0.2299790902829560	T	T	T
0.8097033454748352	0.8930151004151782	0.2257159730184734	T	T	T
0.1269883368229775	0.3023121895135350	0.2462467025314801	T	T	T
0.6334436933046955	0.3072437783304230	0.2548678847530591	T	T	T
0.0475607543039098	0.6941748026146132	0.2811835318021020	T	T	T
0.5313892769661134	0.6871949137769815	0.2796923488559331	T	T	T
0.3711414336262237	0.1019806804751676	0.2861061030871603	T	T	T
0.8700051790382795	0.1019179803433807	0.2861307755671999	T	T	T
0.7927287266603298	0.5322243563800030	0.3375716997591471	T	T	T
0.7450927674124679	0.7456552331047572	0.3391632558077736	T	T	T
0.7883423673452831	0.5436890936039610	0.4000806837596617	T	T	T

COH formation and dissociation on Fe₃C₂(510)

Fe₃C₂(510)-CO+H (IS)

1.0000000000000000
10.1180000000000003 0.0000000000000000 0.0000000000000000
-0.7809265139842700 12.8064770233652006 0.0000000000000000
0.0000000000000000 -0.0000000000000600 17.4192900000000002
Fe C O H
60 25 1 1

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F

0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2150856145887532	0.9386801297179201	0.1340847903241666	T	T	T
0.7155254176313891	0.9386616033637099	0.1338135210395472	T	T	T
0.3389288245433145	0.5353154135009255	0.1394465023020557	T	T	T
0.8388633531405273	0.5361930768279345	0.1397469243335620	T	T	T
0.1359534237098683	0.1431639634946641	0.1455059503907692	T	T	T
0.6362481278279077	0.1437471305041619	0.1464305859980752	T	T	T
0.2239460786788372	0.3421373954206028	0.1422275092185437	T	T	T
0.7260776450470916	0.3426774916698668	0.1435177472071055	T	T	T
0.2855814480016725	0.7517032790311678	0.1489790870925167	T	T	T
0.7870028369351415	0.7499603454928019	0.1498664411163927	T	T	T
0.4639637219516492	0.8818924821110989	0.1533678290170739	T	T	T
0.9628438359401633	0.8829067169587840	0.1527837952379359	T	T	T
0.4711407390315907	0.2943620285579123	0.1626108931658830	T	T	T
0.9676146043025258	0.2917360756843970	0.1619617823792189	T	T	T
0.0766347006861886	0.4886854975911529	0.1612955534923949	T	T	T
0.5779140262428285	0.4879137174016258	0.1605540652036300	T	T	T
0.3937594196797992	0.0941308342503880	0.1635809506933376	T	T	T
0.8926973883879893	0.0953884609245019	0.1646951349984051	T	T	T
0.0383672045223661	0.6923242780877982	0.1663816376031966	T	T	T
0.5413854163029563	0.6915244992598831	0.1662953789082604	T	T	T
0.2065540073991352	0.6224395511933382	0.2511759583129562	T	T	T
0.7015781440642221	0.6193125321468467	0.2551301637302759	T	T	T
0.2900754532346463	0.2253385139232207	0.2542014019039912	T	T	T
0.7897971833069902	0.2275463275542202	0.2606909033901224	T	T	T
0.1352216630528934	0.8247647728172517	0.2551268697062070	T	T	T
0.6357732233371864	0.8241191029099281	0.2545469255195490	T	T	T
0.2136239555219253	0.0219917549494333	0.2593923218417485	T	T	T
0.7136819805621276	0.0219663975469523	0.2594015743567779	T	T	T
0.2392591736578014	0.4311532419332932	0.2666194189198202	T	T	T
0.7433431324150110	0.4285455890537305	0.2692523860304239	T	T	T
0.4421641496971928	0.5614552717050718	0.2673067579069955	T	T	T
0.9473844903945515	0.5608209751785334	0.2697290088889874	T	T	T
0.4563689554070141	0.9753496500382081	0.2716440712225481	T	T	T
0.9558418698428254	0.9735348033458834	0.2721865659956623	T	T	T
0.0392152591261314	0.1694761261362960	0.2713431510837546	T	T	T
0.5395511854959477	0.1723307519658071	0.2729341838768070	T	T	T
0.3917594267199209	0.7626121553133703	0.2732338973870567	T	T	T
0.8900093370434546	0.7607408024946165	0.2731833427360125	T	T	T
0.4781443058607970	0.3693939683928594	0.2919128628261052	T	T	T
0.9832430214101034	0.3710970826640264	0.2888002519467844	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0646591893908985	0.0096059336064239	0.1840262623011789	T	T	T
0.5653921959489087	0.0093131819394638	0.1832980705808934	T	T	T
0.3951352122275827	0.4232345579780947	0.2022225116899735	T	T	T
0.8941675612024294	0.4234073241189639	0.2001903907333372	T	T	T
0.3086123832134264	0.8870790177426020	0.2310967260508062	T	T	T
0.8086822653478689	0.8864954767384851	0.2304466945124987	T	T	T
0.1308274284814376	0.3027203444604438	0.2527230720014070	T	T	T
0.6255902778809599	0.3061159042024568	0.2445153916571074	T	T	T
0.0526624302633136	0.6904489813444853	0.2813198728659408	T	T	T
0.5500520962609429	0.6895127683680340	0.2814117320952094	T	T	T
0.3701018138061696	0.1009861682570389	0.2862657728415579	T	T	T
0.8696658836184095	0.1000413187137962	0.2872175040632686	T	T	T
0.7661410209742014	0.5680912616949881	0.3442948218192162	T	T	T

0.7809457248632984	0.5605939552561060	0.4120743906235563	T	T	T
0.8306036758871567	0.3354279049813458	0.3269047768360256	T	T	T

Fe₅C₂(510)-COH (TS)

1.000000000000000

10.1180000000000003	0.000000000000000	0.000000000000000
-0.7809265139842700	12.8064770233652006	0.000000000000000
0.000000000000000	-0.000000000000600	17.419290000000002

Fe C O H

60 25 1 1

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2155421686409970	0.9384399872163998	0.1339503712794755	T	T	T
0.7160379705280835	0.9384454115650496	0.1339522926972306	T	T	T
0.3389408483603055	0.5353381392215257	0.1396825921334854	T	T	T
0.8394740895504839	0.5362103285475351	0.1399623295841283	T	T	T
0.1365037400330731	0.1429468713984318	0.1450811863188965	T	T	T
0.6363397933117595	0.1423122930395497	0.1456364567207750	T	T	T
0.2245468959549720	0.3424514770496184	0.1425348156693162	T	T	T
0.7224108505391642	0.3415701848151256	0.1425166413390016	T	T	T
0.2855963289022519	0.7513053497526747	0.1489265485428141	T	T	T
0.7867231399175605	0.7500012497375593	0.1498925267011607	T	T	T
0.4635942158231935	0.8818753814548582	0.1532113527473063	T	T	T
0.9629929180001529	0.8824317967010853	0.1530111844493668	T	T	T
0.4704356477489987	0.2937373111204068	0.1629172143491493	T	T	T
0.9679107094758834	0.2927903050492914	0.1621803447430560	T	T	T
0.0779257050273753	0.4884051538242098	0.1603247393388892	T	T	T
0.5781994698504999	0.4886551648494245	0.1598313388472853	T	T	T
0.3940701221763654	0.0939141532697098	0.1635611721765095	T	T	T
0.8941989025967788	0.0944773174669323	0.1641291447797064	T	T	T
0.0375347198570306	0.6917415696610663	0.1665561968681464	T	T	T
0.5396791905610540	0.6913979187484075	0.1664642736130567	T	T	T
0.2059951742135506	0.6216328075437993	0.2509509397368160	T	T	T
0.6998975483245496	0.6216602241782992	0.2553768714849253	T	T	T
0.2901638662528077	0.2245932279198640	0.2549158965566877	T	T	T
0.7900502535860694	0.2250231383525661	0.2552902008766771	T	T	T
0.1350838370571660	0.8239387445955993	0.2554116667972845	T	T	T
0.6353350710522915	0.8241945810695280	0.2549222276499754	T	T	T
0.2138823970228350	0.0215186141222735	0.2592550222193176	T	T	T
0.7139335812578890	0.0212509612229889	0.2595621366830207	T	T	T
0.2415595995177370	0.4301949778023531	0.2669935673638908	T	T	T
0.7473768882879308	0.4285291454392008	0.2657832257753772	T	T	T
0.4410138810033280	0.5617267750138670	0.2676608567564560	T	T	T
0.9476770402590415	0.5594237132213147	0.2703798058582697	T	T	T
0.4563474962027286	0.9745061459778783	0.2720046516758015	T	T	T
0.9563369498964518	0.9731269138012015	0.2722322014030999	T	T	T
0.0394173616113681	0.1698663119240432	0.2702415642662844	T	T	T
0.5392392723994196	0.1713011550414065	0.2718133907818419	T	T	T
0.3903037489582915	0.7626015499724599	0.2734124931586862	T	T	T
0.8893417325088127	0.7598836562215494	0.2736176013299637	T	T	T

0.4795858720459203	0.3694586018808244	0.2915090126137937	T	T	T
0.9786794244539745	0.3669863310156965	0.2916905256520583	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0651490781469638	0.0091276379806998	0.1837904327759268	T	T	T
0.5654791916561495	0.0084961990708904	0.1838204049164504	T	T	T
0.3965730665314625	0.4239185701991367	0.2025615957496524	T	T	T
0.8990524289494430	0.4239020071079383	0.2007058886321429	T	T	T
0.3082214972392394	0.8868568684705662	0.2310907495701377	T	T	T
0.8086958987909940	0.8860435684629774	0.2312441927266821	T	T	T
0.1335214837689122	0.3025945548250880	0.2596322452223496	T	T	T
0.6306187705246586	0.3049300379444641	0.2512734025807117	T	T	T
0.0522462429179892	0.6895020156552902	0.2813217055384126	T	T	T
0.5483566347981981	0.6901584281580946	0.2822232214488517	T	T	T
0.3703342402220919	0.1002045265750917	0.2865112714697483	T	T	T
0.8704573106761988	0.1002143851941996	0.2866465412153469	T	T	T
0.7764674645779531	0.5553379910190404	0.3330512801538213	T	T	T
0.8007653037286565	0.5173625338611353	0.3997619065331942	T	T	T
0.8562189248421116	0.4383726543104340	0.3695972361971891	T	T	T

Fe₅C₂(510)-COH (FS)

1.0000000000000000

10.1180000000000003	0.0000000000000000	0.0000000000000000
-0.7809265139842700	12.8064770233652006	0.0000000000000000
0.0000000000000000	-0.0000000000000600	17.4192900000000002

Fe C O H
60 25 1 1

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2178710347956438	0.9389335636647089	0.1336681226508849	T	T	T
0.7181687323718420	0.9390737113767675	0.1336599609074755	T	T	T
0.3394787586100778	0.5362931505325420	0.1403357464175977	T	T	T
0.8405622388718788	0.5373206045927770	0.1400467053407670	T	T	T
0.1374137774116320	0.1435945194276359	0.1469483614745346	T	T	T
0.6373351096711508	0.1428446400949531	0.1463655403552030	T	T	T
0.2247507069407307	0.3440071533320119	0.1416803531514575	T	T	T
0.7243401560950937	0.3438297180118379	0.1423996860594130	T	T	T
0.2865259943155709	0.7509073143691942	0.1492989184257434	T	T	T
0.7876627737964073	0.7504873171229131	0.1492957037793765	T	T	T
0.4651981056181632	0.8821658128314395	0.1534708574238111	T	T	T
0.9647848654423712	0.8827362420971493	0.1534408954017404	T	T	T

0.4584937793373142	0.2928119168290550	0.1588210197998799	T	T	T
0.9592859087927511	0.2937502203424614	0.1589872846828175	T	T	T
0.0788159324633761	0.4874171461231753	0.1617299114461714	T	T	T
0.5791588990168874	0.4869797686946365	0.1606973734492254	T	T	T
0.3960551935870888	0.0953755215484816	0.1643213131843458	T	T	T
0.8965710814741499	0.0960137264998383	0.1647739282822809	T	T	T
0.0387724125411405	0.6909351597957282	0.1666945404206862	T	T	T
0.5396587000476982	0.6909694763474847	0.1663288292037544	T	T	T
0.2054915366985634	0.6199641716951048	0.2520672569485700	T	T	T
0.7020642563960510	0.6204878625043437	0.2541646232295694	T	T	T
0.2935873625190100	0.2257553449150788	0.2608528283345636	T	T	T
0.7955675749104026	0.2262234175475921	0.2598455132703207	T	T	T
0.1373432918160887	0.8229681113378177	0.2552943824238465	T	T	T
0.6375522469668359	0.8238749601579219	0.2543220805962952	T	T	T
0.2184660417072433	0.0219030724955064	0.2588118151709929	T	T	T
0.7187455350020097	0.0222441044965712	0.2589359533405211	T	T	T
0.2471996745885675	0.4262429328013232	0.2683647296692404	T	T	T
0.7492178715982313	0.4295522441705139	0.2706638883324652	T	T	T
0.4422726711701206	0.5616642542559132	0.2668849331048842	T	T	T
0.94352251182805893	0.5604990190889136	0.2708746685241802	T	T	T
0.4605845273279331	0.9756144566718982	0.2717652807974608	T	T	T
0.9610572915047613	0.9745590579333967	0.2721067926917850	T	T	T
0.0465139573820642	0.1778471707987779	0.2716606783334335	T	T	T
0.5460678996112533	0.1787194993459137	0.2710181440626227	T	T	T
0.3922219795940400	0.7616348288578987	0.2724030378956609	T	T	T
0.8897420434656046	0.7600422186725887	0.2728370069462391	T	T	T
0.4942888550456989	0.3681354863392141	0.2870509586518287	T	T	T
0.0005024775278058	0.3722320169886935	0.2861617416699593	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0683071888653240	0.0088540892897468	0.1831461102161638	T	T	T
0.5683845495067699	0.0083918019566315	0.1833086605069623	T	T	T
0.3988242668092417	0.4230474366281359	0.2013336578380683	T	T	T
0.8967290784067167	0.4240188778715870	0.2017934307999363	T	T	T
0.3104925287990654	0.8876360032343520	0.2325802875934406	T	T	T
0.8111230082004118	0.8873327802756691	0.2319443830214916	T	T	T
0.1529802643965603	0.2999562771536997	0.2987794130475370	T	T	T
0.6537749804907758	0.3037909063785760	0.2933826678868774	T	T	T
0.0511462325787945	0.6883514068490818	0.2815075795478205	T	T	T
0.5514505044657425	0.6896118519667290	0.2821206560024835	T	T	T
0.3767787958708207	0.1018663422810891	0.2853179653510811	T	T	T
0.8771861392869740	0.1017486655465134	0.2852882957004427	T	T	T
0.7814299566211488	0.5522976606636908	0.3339688929629660	T	T	T
0.7758995578120733	0.5603021746526229	0.4109646501770567	T	T	T
0.8157085580172960	0.5002136640767767	0.4344404668962566	T	T	T

Fe₅C₂(510)-C+OH (TS)

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1.000000000000000
 10.1180000000000003  0.0000000000000000  0.0000000000000000
-0.7809265139842700  12.8064770233652006  0.0000000000000000
 0.0000000000000000 -0.0000000000000600  17.4192900000000002
Fe  C  O  H
 60 25  1  1

```

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F

0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2166931000709039	0.9393180523885178	0.1336845501277362	T	T	T
0.7169218177797837	0.9387671939037687	0.1340271751378455	T	T	T
0.3395845985782138	0.5364141692175911	0.1406691570283074	T	T	T
0.8411120904678663	0.5371963532513213	0.1403689529715984	T	T	T
0.1371648055479011	0.1444427087324338	0.1471875367634977	T	T	T
0.6366582721985208	0.1416549783066470	0.1443324730412856	T	T	T
0.2288975739974968	0.3441291640401520	0.1407912992138667	T	T	T
0.7225381766810910	0.3434750313218928	0.1452766615915253	T	T	T
0.2860886389539301	0.7520562142047634	0.1483870746414599	T	T	T
0.7868292057313886	0.7503378672766022	0.1506817420510003	T	T	T
0.4644564654320207	0.8823066662348291	0.1535926683762032	T	T	T
0.9638438283012853	0.8826330483758883	0.1529131563706539	T	T	T
0.4647513107780519	0.2927032296610384	0.1610890697504017	T	T	T
0.9614081136235949	0.2932614380666911	0.1596955446734828	T	T	T
0.0808356352208675	0.4864075186872086	0.1611646155775636	T	T	T
0.5782542747059133	0.4883153222360445	0.1609111251774363	T	T	T
0.3944313222998374	0.0949449190974430	0.1640007055681191	T	T	T
0.8961827112793931	0.0940567804155081	0.1641163859628142	T	T	T
0.0404659282574963	0.6924969667712536	0.1655878301080884	T	T	T
0.5394619649457438	0.6917700126251256	0.1664262376956595	T	T	T
0.2091200020204854	0.6218538677028349	0.2504698483618635	T	T	T
0.6999935985233185	0.6213970409025995	0.2551451972839184	T	T	T
0.2898384725925792	0.2269932748069185	0.2607861724358303	T	T	T
0.7918029136607352	0.2230890716280868	0.2536869337772862	T	T	T
0.1372962840584970	0.8258783806199790	0.2549090153974922	T	T	T
0.6363767937680387	0.8246857422502581	0.2552073909470512	T	T	T
0.2159784803816208	0.0228603386445424	0.2585864586806729	T	T	T
0.7161940075182246	0.0215588394188869	0.2596397013907522	T	T	T
0.2403793116541830	0.4261264808284318	0.2684380016266864	T	T	T
0.7523252630499492	0.4298388447642855	0.2695287187175280	T	T	T
0.4415141248833896	0.5611642965961753	0.2671543820038795	T	T	T
0.9521872550502473	0.5648148699879151	0.2672448743153332	T	T	T
0.4581816650683109	0.9754910387253247	0.2723109734016311	T	T	T
0.9591699313485536	0.9740075818227749	0.2717821404085943	T	T	T
0.0428159716016778	0.1775040720990549	0.2716543043005643	T	T	T
0.5420691890542779	0.1727141334562827	0.2694839837911200	T	T	T
0.3902929864018154	0.7629013110490860	0.2730141807547352	T	T	T
0.8916248112282718	0.7595447076233487	0.2745589808497729	T	T	T
0.4823204390317324	0.3689114290105661	0.2889008921299918	T	T	T
0.9923472430977345	0.3724164182200604	0.2905401351545015	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0668761343365643	0.0092588979988094	0.1826912228161147	T	T	T
0.5666746821345887	0.0088715376916666	0.1840874211822632	T	T	T
0.3944805995941055	0.4218894307858509	0.2013663302288179	T	T	T
0.8993946396936143	0.4233957117368747	0.2002543512606988	T	T	T
0.3095019032454739	0.8887851787218533	0.2314695279759904	T	T	T
0.8106506757400708	0.8858313309365574	0.2319332926420380	T	T	T
0.1466040246230151	0.3004856951828715	0.2989576388866977	T	T	T
0.6384035953974224	0.3054381057935968	0.2605383112895847	T	T	T
0.0571783802654456	0.6916161145993059	0.2799425125984933	T	T	T

0.5477412709951769	0.6903155131609522	0.2815920716066168	T	T	T
0.3727414368495657	0.1017323684580281	0.2861163703333450	T	T	T
0.8749027936777775	0.1008882214772782	0.2851630146533821	T	T	T
0.8084521018202449	0.5678543886110998	0.3252602876474726	T	T	T
0.7889064709086369	0.4417632929597018	0.3815018826010932	T	T	T
0.8063356043578045	0.4180141166762483	0.4335690421621931	T	T	T

Fe₃C₂(510)-C+OH (FS)

1.000000000000000

10.1180000000000003	0.000000000000000	0.000000000000000
-0.7809265139842700	12.8064770233652006	0.000000000000000
0.000000000000000	-0.0000000000000600	17.4192900000000002

Fe	C	O	H
60	25	1	1

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2151951261478988	0.9395851661295402	0.1336941686700918	T	T	T
0.7161393997679890	0.9388025475606497	0.1337711941264401	T	T	T
0.3399815316914395	0.5370960217952566	0.1407723335450771	T	T	T
0.8414914068118042	0.5361106531117386	0.1400825208099006	T	T	T
0.1364777748062783	0.1444743434052476	0.1467418521987648	T	T	T
0.6362678108990507	0.1431736420061954	0.1450277108269273	T	T	T
0.2324282823511431	0.3443204968247809	0.1405327110911033	T	T	T
0.7260094168988707	0.3437333990267937	0.1464465833927343	T	T	T
0.2845825911787042	0.7528210825490982	0.1483613368186404	T	T	T
0.7866119817957268	0.7506187761004536	0.1502493493549384	T	T	T
0.4633483300771098	0.8829081202480900	0.1532588689555197	T	T	T
0.9633929706302788	0.8821618444770474	0.1527991290976349	T	T	T
0.4730291734021891	0.2952723898215605	0.1627328599773178	T	T	T
0.9614795401750714	0.2925265800365753	0.1608961857122181	T	T	T
0.0808503462994640	0.4839188120016781	0.1602641117093408	T	T	T
0.5777766719549282	0.4889120336585126	0.1603951960043011	T	T	T
0.3934524079824467	0.0951646393824127	0.1638686852106219	T	T	T
0.8931289075030989	0.0953895413205141	0.1648729942421661	T	T	T
0.0389230854520003	0.6902824631420184	0.1661782833676495	T	T	T
0.5366361013786417	0.6934034677071089	0.1658023589158753	T	T	T
0.2097360334412201	0.6223352163628886	0.2502866262774527	T	T	T
0.6960383937785910	0.6223566244810710	0.2511316612320512	T	T	T
0.2901685328218055	0.2279155299311648	0.2590774447436822	T	T	T
0.7872200017268769	0.2235672528536588	0.2602146911130325	T	T	T
0.1357222918111582	0.8249356174681993	0.2553098375803289	T	T	T
0.6346583309483300	0.8260856660474807	0.2546525894045760	T	T	T
0.2149277760508849	0.0230084063836808	0.2585906932907315	T	T	T
0.7146327517285193	0.0216323131433078	0.2593432755351706	T	T	T
0.2376243191527415	0.4283862623669261	0.2686418200506444	T	T	T
0.7471901667526942	0.4359297443946384	0.2714692045841747	T	T	T
0.4421209427246159	0.5631357723973559	0.2670225068450152	T	T	T
0.9544929116535030	0.5594942151542178	0.2703395276548418	T	T	T
0.4573386551224199	0.9757995284377540	0.2718401217979845	T	T	T
0.9572025431188695	0.9725080226800019	0.2715072319441956	T	T	T
0.0442815664442423	0.1729894841547073	0.2714025830264786	T	T	T

0.5402678327516137	0.1728615732806024	0.2716944680572952	T	T	T
0.3889253872425667	0.7644959963528024	0.2733381125250205	T	T	T
0.8901744877296522	0.7562710837267559	0.2747864021791525	T	T	T
0.4775065602671044	0.3710895466589963	0.2913214940857654	T	T	T
-0.0109411045154643	0.3667632929183043	0.2935873813893259	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0651482411829951	0.0097807040512253	0.1829255235649129	T	T	T
0.5660087969291833	0.0095029146084527	0.1834239038783364	T	T	T
0.3932116924327011	0.4228705650483106	0.2019826857664759	T	T	T
0.8992712762535379	0.4232811342945975	0.2015447435962286	T	T	T
0.3077810758016056	0.8890719426247137	0.2310232286625068	T	T	T
0.8099792203302567	0.8836447520382990	0.2314378902870202	T	T	T
0.1453112088636380	0.2997078768211361	0.2948363284855559	T	T	T
0.6231435120003148	0.3086934653433027	0.2431673972643408	T	T	T
0.0565865828577198	0.6901585404603455	0.2802136874657988	T	T	T
0.5469912714680264	0.6927017023612508	0.2814125014248157	T	T	T
0.3715874734424317	0.1016848546425902	0.2859403280886947	T	T	T
0.8736435454874991	0.0989494832988421	0.2851150678630424	T	T	T
0.8023270559037073	0.5683872595486587	0.3198002521190838	T	T	T
0.8245088497090287	0.3301155225888541	0.3515680955888914	T	T	T
0.8179169853477437	0.3202471342585994	0.4068108929614851	T	T	T

CO dissociation on K₂O-Fe₅C₂(510)

K₂O-Fe₅C₂(510)-CO (IS)

1.0000000000000000		
10.1180000000000003	0.0000000000000000	0.0000000000000000
-0.7809265139842700	12.8064770233652006	0.0000000000000000
0.0000000000000000	-0.0000000000000600	17.4192900000000002

Fe C O K
60 25 2 2

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2163268188888650	0.9385454137153917	0.1326029492716888	T	T	T
0.7173214964518685	0.9391814932141056	0.1340493114183845	T	T	T
0.3384963734555825	0.5350192443296837	0.1436255805638063	T	T	T
0.8383575169961384	0.5362561423066567	0.1413636868455538	T	T	T
0.1346714284085871	0.1447939973357119	0.1461604634146124	T	T	T
0.6354186022306166	0.1472358147369165	0.1524539809179725	T	T	T
0.2307263761674557	0.3453916185461237	0.1392837081057856	T	T	T
0.7255768515124615	0.3454498168039068	0.1390299017915861	T	T	T
0.2848585465520925	0.7506914235777603	0.1495066823040892	T	T	T

0.7848496025239678	0.7503578370689086	0.1507363272652050	T	T	T
0.4630012115399595	0.8819853695907852	0.1525641501833543	T	T	T
0.9636550668528291	0.8815676370287707	0.1533087092125383	T	T	T
0.4729482631360481	0.2969803766058750	0.1638875085375822	T	T	T
0.9625125106598013	0.2948381837880626	0.1597317131162911	T	T	T
0.0792149048604261	0.4857637246422183	0.1611673338654811	T	T	T
0.5765226607165521	0.4903666515970583	0.1579563619552470	T	T	T
0.3963932401535988	0.0956281957309477	0.1642741138765925	T	T	T
0.8950795608809350	0.0953363298335626	0.1639419659620205	T	T	T
0.0395651250761418	0.6905709419419931	0.1668190218735335	T	T	T
0.5391763272447470	0.6911571945353093	0.1668451051389881	T	T	T
0.2058862442506658	0.6169427313718218	0.2538794247041624	T	T	T
0.7014547716141576	0.6188009211053699	0.2589423395730216	T	T	T
0.2808867666279411	0.2258366284412688	0.2491063150394985	T	T	T
0.7956862807467476	0.2273068078773259	0.2529069565605938	T	T	T
0.1350213301478984	0.8216835788540899	0.2555392936624909	T	T	T
0.6362286480423317	0.8251753738562988	0.2553349018929283	T	T	T
0.2123742403564358	0.0190428065477139	0.2571645084984635	T	T	T
0.7123159090321877	0.0232399054747638	0.2598010652254498	T	T	T
0.2457891837474964	0.4239904046170258	0.2681034714307586	T	T	T
0.7363098732341832	0.4278481867520129	0.2635760732260858	T	T	T
0.4567217283987348	0.5587291888416006	0.2724722481333270	T	T	T
0.9440862742343064	0.5593591116325757	0.2683650887016797	T	T	T
0.4563608904557389	0.9755072068684253	0.2700421170650332	T	T	T
0.9564515379557621	0.9763245750970110	0.2710126237957037	T	T	T
0.0391219758627994	0.1796506918189181	0.2739076549715060	T	T	T
0.5295235032706458	0.1795588586746651	0.2877287875051724	T	T	T
0.3879977338883846	0.7611891878385515	0.2724298486157185	T	T	T
0.8903605115773880	0.7610328028964463	0.2733413398802150	T	T	T
0.4989205972273946	0.3684965018939202	0.2972093522815250	T	T	T
0.9943403794382554	0.3690986083368702	0.2881615046400455	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0648687004899576	0.0092401778479078	0.1810269479735631	T	T	T
0.5666412890187462	0.0086578646034979	0.1816086743001626	T	T	T
0.4024562653898408	0.4246942946309099	0.2068352585141110	T	T	T
0.8998290679265234	0.4248200733483015	0.2033104357260432	T	T	T
0.3075164519087925	0.8862838306184668	0.2311850095920288	T	T	T
0.8098623669513528	0.8872392622379327	0.2317454097133179	T	T	T
0.1505440603071291	0.3002438313396488	0.3024188971285977	T	T	T
0.6299932497630198	0.2957859515627928	0.2346341271024945	T	T	T
0.0499469685051062	0.6872782866687873	0.2821903584216613	T	T	T
0.5473471453827135	0.6940734558741787	0.2807895030241810	T	T	T
0.3662658406803083	0.0998484429087871	0.2826797683503935	T	T	T
0.8713950183555970	0.1029392002359641	0.2856336228865057	T	T	T
0.6114245923034728	0.4921138364612054	0.3374214231554884	T	T	T
0.6262152656734998	0.5131148339827870	0.4066952278308384	T	T	T
0.5129800966005026	0.2656788520700616	0.3738063716713482	T	T	T
0.7392295103776692	0.3274017604587104	0.4348437831896035	T	T	T
0.2902666281862368	0.1922777273097846	0.4283344038240403	T	T	T

K₂O-Fe₅C₂(510)-C+O (TS)

1.0000000000000000		
10.1180000000000003	0.0000000000000000	0.0000000000000000
-0.7809265139842700	12.8064770233652006	0.0000000000000000
0.0000000000000000	-0.0000000000000600	17.4192900000000002
Fe	C	O
60	25	2

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F

0.3524200000000022	0.8641300000000032	0.0267500000000003	F	F	F
0.8524200000000024	0.8641300000000032	0.0267500000000003	F	F	F
0.1786799999999996	0.46654000000000112	0.0302900000000008	F	F	F
0.6786800000000007	0.46654000000000112	0.0302900000000008	F	F	F
0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.48548000000000025	0.2084899999999976	0.0384200000000022	F	F	F
0.98548000000000028	0.2084899999999976	0.0384200000000022	F	F	F
0.01212000000000030	0.6209100000000025	0.0448999999999985	F	F	F
0.51212000000000029	0.6209100000000025	0.0448999999999985	F	F	F
0.09857000000000023	0.8142700000000005	0.0451300000000004	F	F	F
0.59857000000000024	0.8142700000000005	0.0451300000000004	F	F	F
0.42483000000000000	0.4166799999999997	0.0486700000000023	F	F	F
0.92483000000000000	0.4166799999999997	0.0486700000000023	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999985	F	F	F
0.5377799999999977	0.0205500000000001	0.0560899999999985	F	F	F
0.2152583280595790	0.9386856015935319	0.1326467777652549	T	T	T
0.7163924398264629	0.9401461482810877	0.1335606498035220	T	T	T
0.3409668527064354	0.5374015037131161	0.1474717642384614	T	T	T
0.8419248718138752	0.5395473625483194	0.1412708651438899	T	T	T
0.1355598421298889	0.1441117092066945	0.1451071109664964	T	T	T
0.6370480961589433	0.1466895362145777	0.1525740319709440	T	T	T
0.2317352678654375	0.3473306389143521	0.1395791763106090	T	T	T
0.7238897819233697	0.3439356743841348	0.1371700475330631	T	T	T
0.2850144268682068	0.7505255832497435	0.1496385719791027	T	T	T
0.7833889255213167	0.7527227290238160	0.1490908841376295	T	T	T
0.4622525571612456	0.8827548568756625	0.1521367275432553	T	T	T
0.9630593067487754	0.8822420808550617	0.1529566159152905	T	T	T
0.4726255420110085	0.2938885756627149	0.1615126567448867	T	T	T
0.9633906451637877	0.2929694117038381	0.1577324210387844	T	T	T
0.0811569647749024	0.4870336853856632	0.1630494521394110	T	T	T
0.5755235712741685	0.4888596698825557	0.1622899319019487	T	T	T
0.3968531904321674	0.0943823647364894	0.1635914337026575	T	T	T
0.895590829741717	0.0937840081093920	0.1634870936396398	T	T	T
0.0381183978516243	0.6897009477110887	0.1674828335665950	T	T	T
0.5383602417184539	0.6929943983710628	0.1666771041311795	T	T	T
0.2042034873408070	0.6193522066077257	0.2545292399089507	T	T	T
0.7008191044408202	0.6246392966672897	0.2550233348862950	T	T	T
0.2797865249846873	0.2261671641627459	0.2470306139672208	T	T	T
0.7972265300254505	0.2251474734644756	0.2517582954484789	T	T	T
0.1340830915043386	0.8231311367929578	0.2558151608603036	T	T	T
0.6342664435659359	0.8300263008842023	0.2536114611322768	T	T	T
0.2128620725573315	0.0213807301066173	0.2569915524804870	T	T	T
0.7129366097416788	0.0242907090848075	0.2599007810924420	T	T	T
0.2409730658277225	0.4277969642859135	0.2698572091829704	T	T	T
0.7546981060158808	0.4186152899900434	0.2614339207692015	T	T	T
0.4514789224762796	0.5677082334046959	0.2742608332742765	T	T	T
0.9383849902115529	0.5617025778420466	0.2741426841848881	T	T	T
0.4562924997518981	0.9763530976319462	0.2700334633512415	T	T	T
0.9579336317995841	0.9756522346341674	0.2717865955900244	T	T	T
0.0411835337932044	0.1775841219924555	0.2728694833132624	T	T	T
0.5299742098240183	0.1827390040513135	0.2891665428888187	T	T	T
0.3865012794967295	0.7655743921117677	0.2726091359863272	T	T	T
0.8900877442704245	0.7638349237597846	0.2710496679293193	T	T	T
0.5070674330295816	0.3734703483878651	0.2912931775299639	T	T	T
0.9987799577552043	0.3660323752745192	0.2837082354408923	T	T	T
0.3220200000000020	0.5286800000000015	0.0000000000000000	F	F	F
0.8220200000000022	0.5286800000000015	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999966	0.0082499999999968	F	F	F
0.7192900000000005	0.9343099999999966	0.0082499999999968	F	F	F
0.0579600000000014	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000004	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000012	F	F	F
0.7973500000000014	0.2090699999999970	0.1178400000000012	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0648018869526241	0.0098665839356898	0.1814240135318793	T	T	T
0.5662162702623207	0.0089781516401488	0.1819117277905609	T	T	T
0.3940679625240536	0.4176382042553673	0.2074620776514315	T	T	T
0.9051354871795881	0.4250689461686438	0.1968118960896773	T	T	T
0.3055170037084616	0.8891965252606177	0.2312676863109148	T	T	T

0.8087186818715376	0.8901953145596527	0.2319344093163012	T	T	T
0.1517584218773652	0.2986707070347968	0.3040757250004036	T	T	T
0.6309040895676886	0.2924568758849028	0.2318711171889306	T	T	T
0.0489690518786899	0.6895792808406037	0.2822339833499798	T	T	T
0.5471948594381696	0.7011163878705907	0.2810141908211380	T	T	T
0.3680987207774967	0.1014540343919288	0.2815217590686041	T	T	T
0.8732204448618450	0.1022222726406461	0.2857419122528017	T	T	T
0.6114021542269072	0.4979485023070903	0.2960290196712384	T	T	T
0.7625163348993985	0.5276959926312247	0.3411015137015107	T	T	T
0.5073215409432281	0.2734834489023473	0.3710658238325273	T	T	T
0.7317219864627068	0.3489473779779558	0.4299314772330780	T	T	T
0.2897619555560031	0.1927836058636140	0.4271408326044700	T	T	T

K₂O-Fe₅C₂(510)C+O (FS)

1.0000000000000000		
10.1180000000000003	0.0000000000000000	0.0000000000000000
-0.7809265139842700	12.8064770233652006	0.0000000000000000
0.0000000000000000	-0.0000000000000600	17.4192900000000002

Fe C O K
60 25 2 2

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2149764966722111	0.9390230843531284	0.1328737422374102	T	T	T
0.7149437887776476	0.9394545193407676	0.1340526094281676	T	T	T
0.3421835398605355	0.5388744254034015	0.1464346364998586	T	T	T
0.8457104048263223	0.5478399084582632	0.1493999763320091	T	T	T
0.1359427039685867	0.1436515254682563	0.1452998684116555	T	T	T
0.6355143634244840	0.1463878180414607	0.1508260214653690	T	T	T
0.2308985594779603	0.3474397275548847	0.1382962098491979	T	T	T
0.7241617668161864	0.3453104487654526	0.1387233061814218	T	T	T
0.2840003475360994	0.7520649756317651	0.1489833920830908	T	T	T
0.7843248480606583	0.7521464737767373	0.1499332462237277	T	T	T
0.4617440935562203	0.8830259903753931	0.1525044427735833	T	T	T
0.9627308618383115	0.8826835472980045	0.1530187327245190	T	T	T
0.4747352940113156	0.2964778643306369	0.1627864129154189	T	T	T
0.9640347159156779	0.2888822823470730	0.1573312475193663	T	T	T
0.0801038664926653	0.4884663907552652	0.1643716375618635	T	T	T
0.5773919155410182	0.4914367190234906	0.1662028701401835	T	T	T
0.3950843954518343	0.0958249601059421	0.1639746828431755	T	T	T
0.8952728383423471	0.0931173428124810	0.1627055253346880	T	T	T
0.0383906341486232	0.6914213601933565	0.1674723434937081	T	T	T
0.5391384817758703	0.6944242942606834	0.1670747139671572	T	T	T
0.2068891324668581	0.6243678571871309	0.2535732591741564	T	T	T
0.6978162881994755	0.6265600106941410	0.2589527494075973	T	T	T
0.2818054332259389	0.2293997873264172	0.2474074289088214	T	T	T
0.7942009153159753	0.2256857470944310	0.2496269255163431	T	T	T
0.1331496766740127	0.8282056146060165	0.2549261806595621	T	T	T
0.6346616163490734	0.8312917218733166	0.2550695086549841	T	T	T
0.2111178404224260	0.0244121454748387	0.2574047706426607	T	T	T
0.7109082899407617	0.0258265392937853	0.2595819854617805	T	T	T
0.2442259494090034	0.4309106813759509	0.2687249474219755	T	T	T
0.7564611820739182	0.4271132591798306	0.2640187592826422	T	T	T
0.4491755662732330	0.5701979114946981	0.2731885477065071	T	T	T
0.9450293135444404	0.5706014777646305	0.2772822672927757	T	T	T

0.4560857783346003	0.9775813798835600	0.2706706726914875	T	T	T
0.9567319523634017	0.9781640438859313	0.2719462966023568	T	T	T
0.0371531017975579	0.1811508227702060	0.2713662443757755	T	T	T
0.5312550008820801	0.1813026720334342	0.2865885290316025	T	T	T
0.3859866315321228	0.7692832360427616	0.2737173188769734	T	T	T
0.8889477299757401	0.7666653806622478	0.2727513247936641	T	T	T
0.4994270133056451	0.3716632991574098	0.2938231732781563	T	T	T
0.9916933510609484	0.3770509738329664	0.2822858531790531	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0639460694228121	0.0097793467316071	0.1814594478877481	T	T	T
0.5640561658352873	0.010115753553736	0.1813564293888375	T	T	T
0.3905678800297084	0.4165169883297495	0.2022915281646970	T	T	T
0.8943164403289744	0.4170370916687656	0.1835704417461359	T	T	T
0.3062525551310969	0.8917844493771271	0.2303326344377767	T	T	T
0.8089938588598055	0.8916958886992932	0.2306886766445302	T	T	T
0.1441782416884511	0.3051278272520699	0.2929228398150411	T	T	T
0.6320651872324032	0.2960579236627237	0.2331635263653820	T	T	T
0.0512367609054714	0.6959465306694361	0.2831609480024680	T	T	T
0.5442517374596234	0.7028619704848992	0.2822782768649740	T	T	T
0.3677940746391949	0.1033472550079639	0.2814742760082378	T	T	T
0.8713621616466005	0.1038813429384355	0.2859434295458769	T	T	T
0.6041904451296261	0.4974863883158278	0.2870619733211368	T	T	T
0.8860281877063996	0.4593706805632419	0.3430255798875831	T	T	T
0.5112600723568894	0.2710589597949499	0.3721655784210696	T	T	T
0.7485779524191528	0.3136530856855693	0.4248614166847910	T	T	T
0.2890540731762864	0.1942233869087039	0.4250724976601389	T	T	T

HCO formation and dissociation on $K_2O-Fe_5C_2(510)$

$K_2O-Fe_5C_2(510)-CO+H$ (IS)

1.0000000000000000		
10.1180000000000003	0.0000000000000000	0.0000000000000000
-0.7809265139842700	12.8064770233652006	0.0000000000000000
0.0000000000000000	-0.0000000000000600	17.4192900000000002

Fe C O K H
60 25 2 2 1

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2163716108596098	0.9383772564105402	0.1326618117970467	T	T	T
0.7169373236903589	0.9386607874410769	0.1342410043399938	T	T	T
0.3391293845954101	0.5352784273371586	0.1429350106285994	T	T	T
0.8388141410211826	0.5366098949905672	0.1413519416170137	T	T	T

0.1348584955257775	0.1444324347916594	0.1462443821666588	T	T	T
0.6358771951648235	0.1472457459661118	0.1525362997320555	T	T	T
0.2305386225776880	0.3457958652344263	0.1398407578107696	T	T	T
0.7248021835046891	0.3453338039610787	0.1382653546124698	T	T	T
0.2849542857140361	0.7507473825124064	0.1495277060458383	T	T	T
0.7849347569596423	0.7500643557669979	0.1507535836997918	T	T	T
0.4634987050355048	0.8814714902941040	0.1528244080631721	T	T	T
0.9637623565056535	0.8811781014009593	0.1535704743851339	T	T	T
0.4727167670209912	0.2969461763321416	0.1637374091957663	T	T	T
0.9620992833211202	0.2948826796513775	0.1595806224936117	T	T	T
0.0795433201056992	0.4856206775737741	0.1610782818347467	T	T	T
0.5761224402022226	0.4906763582862012	0.1589162247945572	T	T	T
0.3964748234501544	0.0949826403856336	0.1643214156649920	T	T	T
0.8950506485127248	0.0952110215060855	0.1638624362950544	T	T	T
0.0402448527341412	0.6903351385906208	0.1668672828330629	T	T	T
0.5384500365156597	0.6906751130188751	0.1670855330896314	T	T	T
0.2042119806060892	0.6173149898839270	0.2543607457876939	T	T	T
0.7000580807443162	0.6177922374735456	0.2588662367549613	T	T	T
0.2816260601136457	0.2254357177485652	0.2485652379932567	T	T	T
0.7958930016418519	0.2270429490470833	0.2527057869985792	T	T	T
0.1345728265104072	0.8217745716359989	0.2556325683035168	T	T	T
0.6355537206318205	0.8252077345116593	0.2550037336890572	T	T	T
0.2119668915974254	0.0191149869383881	0.2572370121929156	T	T	T
0.7115746246916083	0.0234412833720765	0.2596961170157225	T	T	T
0.2485220768414826	0.4243234535945117	0.2699934504320378	T	T	T
0.7381303816984268	0.4268159576261735	0.2630342882051105	T	T	T
0.4558528777158759	0.5595845493658951	0.2743309962540073	T	T	T
0.9421176653743643	0.5598677080091862	0.2676954127953614	T	T	T
0.4560861839257539	0.9744929879613451	0.2701640869378045	T	T	T
0.9559460444881600	0.9762254269524954	0.2712585720722694	T	T	T
0.0389977610936396	0.1797214131305722	0.2739956935714319	T	T	T
0.5297187934812038	0.1780093740943127	0.2860567309143106	T	T	T
0.3871546504193186	0.7612212033466629	0.2728446292525287	T	T	T
0.8897471009681592	0.7612457400047108	0.2732340743598797	T	T	T
0.5001427720868672	0.3678033004653721	0.2971082951991396	T	T	T
0.9944527834680781	0.3682574644483612	0.2877797296086101	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0647678593409856	0.0091169432349402	0.1810056564353856	T	T	T
0.5662297175438067	0.0087629966020059	0.1811043285018075	T	T	T
0.4024607019684386	0.4242730576997132	0.2062961239260778	T	T	T
0.9014645962371860	0.4253123254399099	0.2028712783632095	T	T	T
0.3072235200901728	0.8861282523810494	0.2307868901238243	T	T	T
0.8095559790487364	0.8871752510276202	0.2316500760693237	T	T	T
0.1513790552425980	0.3002018190026664	0.3010453728677133	T	T	T
0.6306220553927757	0.2958343085828559	0.2343224515102572	T	T	T
0.0487209500904186	0.6877116115518660	0.2820004211084686	T	T	T
0.5472729155681244	0.6944021108439159	0.2810456684895710	T	T	T
0.3662314687531261	0.0992773063898982	0.2825125050766455	T	T	T
0.8711036770915922	0.1028022338971767	0.2855489975990972	T	T	T
0.6141794881893122	0.4919672989578366	0.3366001814239653	T	T	T
0.6302322971521567	0.5102192468521796	0.4062014668215930	T	T	T
0.5137982038609715	0.2641550721777298	0.3727512020503677	T	T	T
0.7411059113132684	0.3211022848853597	0.4330258658942360	T	T	T
0.2915581085472787	0.1924394543004337	0.4279982550305289	T	T	T
0.2975188315135720	0.5416566211478882	0.3173121258681093	T	T	T

K₂O-Fe₅C₂(510)-HCO (TS)

1.000000000000000		
10.1180000000000003	0.0000000000000000	0.0000000000000000
-0.7809265139842700	12.8064770233652006	0.0000000000000000
0.0000000000000000	-0.0000000000000600	17.4192900000000002

Fe C O K H
60 25 2 2 1

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2163315952720922	0.9388534528454064	0.1328604269480617	T	T	T
0.7175831095172830	0.9391706497058472	0.1341250788457075	T	T	T
0.3393380836034308	0.5368452463422110	0.1441631433508535	T	T	T
0.8388500190790655	0.5372214109112878	0.1417433321159233	T	T	T
0.1350940079172601	0.1442759869578137	0.1461707383272350	T	T	T
0.6353160923443643	0.1470669495860188	0.1511779697433704	T	T	T
0.2317969955335889	0.3459387108769808	0.1385814557522855	T	T	T
0.7243684715270089	0.3453344918276504	0.1406502246764176	T	T	T
0.2854538822261702	0.7508494654950135	0.1494520217982431	T	T	T
0.7855063449904602	0.7505947976076829	0.1499543681996531	T	T	T
0.4637127338254076	0.8818638900295938	0.1525387370996588	T	T	T
0.9629509150218777	0.8824191913215037	0.1531464232094907	T	T	T
0.4720503993141092	0.2966260355291307	0.1628120436622791	T	T	T
0.9623148075944032	0.2933552601513828	0.1587005608970807	T	T	T
0.0791778535344549	0.4862993464799146	0.1612692446174316	T	T	T
0.5753522431829839	0.4898999833415121	0.1601940510804520	T	T	T
0.3957874526451990	0.0956383992996341	0.1641176712284998	T	T	T
0.8950645808795611	0.0942281345275034	0.1637098456253690	T	T	T
0.0398859171265712	0.6916924934842710	0.1665798091295972	T	T	T
0.5367607721073734	0.6894067587875999	0.1674626848874395	T	T	T
0.2072322543011710	0.6198178119965779	0.2532077958213567	T	T	T
0.7038753084340499	0.6207176759784088	0.2563183209212694	T	T	T
0.2802592951360694	0.2267972167220133	0.2490906071816378	T	T	T
0.7949759648284997	0.2257168104668856	0.2516925967980173	T	T	T
0.1346962442474987	0.8235991061446559	0.2554602277432152	T	T	T
0.6366474908872404	0.8265313911434410	0.2552119944394763	T	T	T
0.2118722021714328	0.0202228451109127	0.2576450433563405	T	T	T
0.7109107445833859	0.0240860957800882	0.2597733381675921	T	T	T
0.2374326281204772	0.4253981127031198	0.2667672476726525	T	T	T
0.7469749328748095	0.4263042292942462	0.2674505649557856	T	T	T
0.4509371054866877	0.5631564784229393	0.2733925053352365	T	T	T
0.9501467745493066	0.5583744534101900	0.2679168475903612	T	T	T
0.4565125081019095	0.9756326484124184	0.2700522988922785	T	T	T
0.9561089300542005	0.9759815605646341	0.2718262333540574	T	T	T
0.0386701339300657	0.1779338930964676	0.2742136890819618	T	T	T
0.5303718845650288	0.1797790066942624	0.2876087424373130	T	T	T
0.3884358784376856	0.7634977534168290	0.2727438906117668	T	T	T
0.8904911458529380	0.7609593610383846	0.2725629283531740	T	T	T
0.4959264999701594	0.3671954704586305	0.2952723701458843	T	T	T
0.9948420188074156	0.3665310744496911	0.2859193517056768	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0649531000151244	0.0092890200365175	0.1817758217624880	T	T	T

0.5660029933919082	0.0091191813791123	0.1808318667160352	T	T	T
0.3988765334244667	0.4240431324003662	0.2056116935547993	T	T	T
0.8992233184886437	0.4229944712460829	0.2005889657269558	T	T	T
0.3072194168784187	0.8871923649684144	0.2311999484451153	T	T	T
0.8098480375958340	0.8876785233015658	0.2312387004156419	T	T	T
0.1496003457063132	0.2981125379804113	0.3038377089623784	T	T	T
0.6283577308721203	0.2956303047473883	0.2346944704951352	T	T	T
0.0510348837273126	0.6891809172424789	0.2817041215191339	T	T	T
0.5472705334488009	0.6956211232505912	0.2796195073273903	T	T	T
0.3671242724155943	0.1008282988965614	0.2816876613284094	T	T	T
0.8706888470052210	0.1024050568398276	0.2862183153992914	T	T	T
0.5634413498262342	0.4941097070673469	0.3385872289787358	T	T	T
0.6858685046314653	0.5134262216569259	0.3632527713418487	T	T	T
0.5141054439305053	0.2663681092671169	0.3736539949549269	T	T	T
0.7476640834435331	0.3062972016018242	0.4282924353465533	T	T	T
0.2922781017317072	0.1871514020349692	0.4272829272627822	T	T	T
0.4805177010067723	0.5482544276288521	0.3691969191686854	T	T	T

K₂O-Fe₅C₂(510)-HCO (FS)

1.0000000000000000
10.1180000000000003 0.0000000000000000 0.0000000000000000
-0.7809265139842700 12.8064770233652006 0.0000000000000000
0.0000000000000000 -0.0000000000000600 17.4192900000000002

Fe C O K H
60 25 2 2 1

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2161672039320897	0.9387205683738375	0.1330092197674438	T	T	T
0.7174470548232926	0.9388768360263654	0.1342833518321675	T	T	T
0.3383359350238509	0.5351891229431466	0.1406924589783074	T	T	T
0.8381785697712738	0.5365141421768859	0.1419639465730946	T	T	T
0.1348290978368308	0.1443413677599164	0.1462761485705199	T	T	T
0.6351088943028711	0.1479400489506618	0.1524185269783457	T	T	T
0.2309375659637310	0.3453103522427630	0.1387416430320608	T	T	T
0.7247783718446013	0.3454010977944706	0.1398935952523938	T	T	T
0.2848346722635967	0.7514859201691130	0.1488361786354338	T	T	T
0.7849866347380863	0.7502141723112837	0.1506987611878882	T	T	T
0.4637990096479760	0.8815185187807114	0.1528907847249733	T	T	T
0.9630170990281182	0.8818127879797220	0.1534106570821294	T	T	T
0.4730693166638854	0.2976227785195633	0.1638443008626649	T	T	T
0.9624938517058005	0.2936269039154647	0.1589682106689236	T	T	T
0.0787184904402491	0.4859289716400126	0.1607722951780391	T	T	T
0.5757197462478361	0.4910225268745672	0.1604183165550692	T	T	T
0.3966219207665839	0.0961970154944752	0.1644909262897683	T	T	T
0.8944142260810238	0.0942602841846270	0.1637539978258235	T	T	T
0.0396127727186193	0.6914404644406884	0.1665857633996162	T	T	T
0.5403987683449947	0.6911239658912058	0.1671935387669270	T	T	T
0.2077325221308184	0.6196698121559515	0.2523272319611006	T	T	T
0.7032977235281619	0.6203556232721226	0.2606086816290689	T	T	T
0.2804399293788374	0.2261754045742755	0.2498580084923684	T	T	T
0.7954903252277257	0.2262896708819631	0.2523070564115272	T	T	T
0.1345430052875644	0.8230082679665541	0.2554888567626931	T	T	T
0.6359339473555029	0.8247889926974382	0.2561817147136131	T	T	T

0.2124784859482672	0.0196592885676599	0.2577914156264092	T	T	T
0.71113764220365048	0.0228696874509547	0.2595877139413889	T	T	T
0.2388761527243547	0.4239139068498868	0.2668735625204423	T	T	T
0.7435308930192812	0.4258314436086159	0.2661527803925242	T	T	T
0.4469742342106777	0.5615398821346386	0.2718684135491080	T	T	T
0.9511519428658146	0.5579696225264922	0.2679184272799551	T	T	T
0.4567932310404638	0.9757763788536616	0.2698075216959926	T	T	T
0.9557009288212329	0.9758642244568521	0.2716785360703513	T	T	T
0.0386380460938079	0.1771939380981258	0.2745156583452713	T	T	T
0.5286507185527517	0.1823138587987095	0.2879238006695243	T	T	T
0.3870956145911967	0.7631677941916304	0.2729158068034629	T	T	T
0.8904834611779276	0.7598650194409126	0.2725030682050604	T	T	T
0.4886308785582990	0.3691552680503886	0.2981087579556642	T	T	T
0.9948420823484962	0.3662008271398001	0.2865179393113518	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0648020263984676	0.0093225728114081	0.1820045303465989	T	T	T
0.5665472102819862	0.0091684428595343	0.1807847079691114	T	T	T
0.4003129243548454	0.4264585471278055	0.2059788457244242	T	T	T
0.8989728114902783	0.4231445480054914	0.2019464608152394	T	T	T
0.3070776790961365	0.8871533467513416	0.2311490359532025	T	T	T
0.8092223823400053	0.8871510053145282	0.2321703688504466	T	T	T
0.1487745251623364	0.2975579395751456	0.3042406238391043	T	T	T
0.6291580297980609	0.2971845088463146	0.2352708294559290	T	T	T
0.0515620129290863	0.6882997227723935	0.2821610958739985	T	T	T
0.5446709710820280	0.6937664098032803	0.2809369389553028	T	T	T
0.3670913129476303	0.1005797169593293	0.2825929067223030	T	T	T
0.8698555449465937	0.1022593251745867	0.2860886261125113	T	T	T
0.5468771024943884	0.4960226450349302	0.3532308338241359	T	T	T
0.6829165827710210	0.5183686541188928	0.3505669438244202	T	T	T
0.5125463703137951	0.2674722376544706	0.3751314020430506	T	T	T
0.7483019840489874	0.3090028045800330	0.4272999190460862	T	T	T
0.2916533518754604	0.1863783712776786	0.4281552304662588	T	T	T
0.5095523360946649	0.5066105899784291	0.4125532216509069	T	T	T

K₂O-Fe₅C₂(510)-CH+O (TS)

1.0000000000000000		
10.1180000000000003	0.0000000000000000	0.0000000000000000
-0.7809265139842700	12.8064770233652006	0.0000000000000000
0.0000000000000000	-0.0000000000000060	17.4192900000000002

Fe C O K H
60 25 2 2 1

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F

0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2160409829465791	0.9381396712315258	0.1327994503373170	T	T	T
0.7168123162644233	0.9389482070704549	0.1340702660006251	T	T	T
0.3387161074933762	0.5342790968369842	0.1442441057248523	T	T	T
0.8398695989301721	0.5382900780532480	0.1417200558306764	T	T	T
0.1354158400609330	0.1438583227843001	0.1460286531391873	T	T	T
0.6357679075646933	0.1459240481344105	0.1508435033986878	T	T	T
0.2309213209292040	0.3460787311694745	0.1395561961677521	T	T	T
0.7241368308895835	0.3444594213092320	0.1389233675522329	T	T	T
0.2855901762772295	0.7503685669180531	0.1495793702809110	T	T	T
0.7843177330628699	0.7512748444442299	0.1499225953421762	T	T	T
0.4630798983557145	0.8817568087361715	0.1527185733810061	T	T	T
0.9628722305205195	0.8820964663338268	0.1528414564938261	T	T	T
0.4734989401932208	0.2957413955968616	0.1630727090891136	T	T	T
0.9626719093114414	0.2931222748088309	0.1578628702221659	T	T	T
0.0788429604689803	0.4862864579041090	0.1611386711079198	T	T	T
0.5752637622301756	0.4891538188576743	0.1597470416459600	T	T	T
0.3964972629863419	0.0959821675028090	0.1639087024806794	T	T	T
0.8952649277607805	0.0933973863369194	0.1633987783151712	T	T	T
0.0386213044154037	0.6905423200900612	0.1673243998059711	T	T	T
0.5385563472255805	0.6899144658518803	0.1672689780493166	T	T	T
0.2065415999976866	0.6195321238687371	0.2528952318035602	T	T	T
0.7025007974900026	0.6222378477321504	0.2587205149816961	T	T	T
0.2806741193293357	0.2271452237468169	0.2478393478017205	T	T	T
0.7957321007499726	0.2244001470505543	0.2504307947799463	T	T	T
0.1339340406906282	0.8232884563023968	0.2553116645210305	T	T	T
0.6359138928525028	0.8263584651095877	0.2555848660995839	T	T	T
0.2127771787435818	0.0199257545662477	0.2573509105760679	T	T	T
0.7111350515897439	0.0237209196576058	0.2599221079919478	T	T	T
0.2369599964046414	0.4271774326286978	0.2673299245509007	T	T	T
0.7490954878549954	0.4226807731100280	0.2640223865041214	T	T	T
0.4529559974889231	0.5624573701250333	0.2744408999019797	T	T	T
0.9459282895127489	0.5587146464315954	0.2714233981241450	T	T	T
0.4569763074104424	0.9765341336460969	0.2701748734146429	T	T	T
0.9565643929355654	0.9751900319337480	0.2715438404125686	T	T	T
0.0391253814650950	0.1771875259160949	0.2734866802195559	T	T	T
0.5274644839559153	0.1844339331872055	0.2873039224205012	T	T	T
0.3876759779342584	0.7633911888349165	0.2730484647856551	T	T	T
0.8902915813972841	0.7617524081214534	0.2723611193158461	T	T	T
0.5094822516707451	0.3761298339349268	0.2952784728284623	T	T	T
0.9957439869451128	0.3650556293643564	0.2845692911552100	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0652799552044685	0.0090096039597220	0.1815627951534449	T	T	T
0.5660362890843589	0.0086982419196726	0.1812191097646538	T	T	T
0.4023095443815143	0.4233324463747621	0.2114525307724958	T	T	T
0.9002374820819148	0.4235325348535486	0.1992360760202606	T	T	T
0.3071495682425252	0.8870868269472527	0.2314564312099073	T	T	T
0.8093823461431917	0.8878827858759040	0.2309316263718969	T	T	T
0.1502268643897762	0.2980269606344889	0.3029368215939158	T	T	T
0.6329245505248791	0.2979817885389380	0.2346621197422085	T	T	T
0.0510733294090480	0.6888877484196732	0.2823500490418159	T	T	T
0.5460411262886028	0.6959724433093958	0.2814741610683760	T	T	T
0.3677607990657586	0.1011492390955843	0.2818352570168091	T	T	T
0.8714555118959525	0.1017674449951949	0.2857304839744231	T	T	T
0.5554483100499628	0.4965368053136883	0.3489894992542849	T	T	T
0.7392027908180063	0.5271501085971683	0.3392587472297087	T	T	T
0.5100843320755146	0.2708010243831214	0.3713087291999436	T	T	T
0.7477745782414458	0.3092304094260784	0.4245288777467501	T	T	T
0.2902187112685269	0.1919276735862446	0.4266590228668713	T	T	T
0.5602928785480720	0.5207031565018555	0.4096139776480237	T	T	T

K₂O-Fe₃C₂(510)-CH+O (FS)

1.00000000000000
 10.118000000000003 0.000000000000000 0.000000000000000
 -0.7809265139842700 12.8064770233652006 0.000000000000000
 0.000000000000000 -0.0000000000000600 17.419290000000002
 Fe C O K H
 60 25 2 2 1

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2158632484546447	0.9396489231263140	0.1328824938266732	T	T	T
0.7155222142914445	0.9393561557532966	0.1336886287712183	T	T	T
0.3394199163124377	0.5359577668761925	0.1449082238409995	T	T	T
0.8448896600403457	0.5465981045588958	0.1486597081372888	T	T	T
0.1362205700081129	0.1423670572072026	0.1444155407346639	T	T	T
0.6357268789363281	0.1459159913100844	0.1495180453144232	T	T	T
0.2310296352962547	0.3473339951248934	0.1386232364803275	T	T	T
0.7254259911522861	0.3452346154043529	0.1391645443951437	T	T	T
0.2836718690334423	0.7521684430376293	0.1489221375350468	T	T	T
0.7836636127846165	0.7517615489388434	0.1498288872920611	T	T	T
0.4623837481023561	0.8824141480595729	0.1527086310785880	T	T	T
0.9626723134929027	0.8821188233169883	0.1532073369987529	T	T	T
0.4740980407680920	0.2964613362336621	0.1634581823309631	T	T	T
0.9642571355411499	0.2888621391708781	0.1568560508486932	T	T	T
0.0781532302979131	0.4878467687155031	0.1624834336796529	T	T	T
0.5764934582232611	0.4896650939173894	0.1610117426876177	T	T	T
0.3964495349202420	0.0951998939471642	0.1634985873710045	T	T	T
0.8953691316167296	0.0924084065707829	0.1620083408623303	T	T	T
0.0379305404363741	0.6908847071334385	0.1673259737661545	T	T	T
0.5381765736994549	0.6919269440668917	0.1668940314394947	T	T	T
0.2077321696799888	0.6226057922308249	0.2521561422885050	T	T	T
0.7009192076675833	0.6228180739288297	0.2577744518807939	T	T	T
0.2800592978422672	0.2269726637558757	0.2454096548601264	T	T	T
0.7941628104067324	0.2250569450695580	0.2489435007813300	T	T	T
0.1342387844710458	0.8271572415127066	0.2553441461557144	T	T	T
0.6357008586953492	0.8286134283520163	0.2543514307889557	T	T	T
0.2122859193850270	0.0227805896384859	0.2575447110113391	T	T	T
0.7116285910785494	0.0250844775205045	0.2592977672327771	T	T	T
0.2400824846720493	0.4308797990151968	0.2669185152071205	T	T	T
0.7571059713766648	0.4293673557924649	0.2653798277747954	T	T	T
0.4554962999094574	0.5639754126875087	0.2731261987022582	T	T	T
0.9476770455551440	0.5688503188703102	0.2774584564119530	T	T	T
0.4570370378011799	0.9782685579138755	0.2701528253923237	T	T	T
0.9565518402234190	0.9777177463045938	0.2719861872039588	T	T	T
0.0374954676997378	0.1793030429896049	0.2701481832786261	T	T	T
0.5296605774902881	0.1845140832092987	0.2875644003242654	T	T	T
0.3875535700106157	0.7655914143081506	0.2725006639864546	T	T	T
0.8897979796318005	0.7651889189607554	0.2725638058274439	T	T	T
0.5150702938637833	0.3774448245201148	0.2939730279421076	T	T	T
0.9890206771795090	0.3739805634251582	0.2825498910727759	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F

0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0637730914779796	0.0091012090817012	0.1821761284697115	T	T	T
0.5653055648490519	0.0094451711041889	0.1813735668177911	T	T	T
0.4001937753471622	0.4227339660225033	0.2102762743007521	T	T	T
0.8943783945158795	0.4169550549910763	0.1850623265177952	T	T	T
0.3076388831531425	0.8898958032294679	0.2307041560346757	T	T	T
0.8095858019366059	0.8906699180348078	0.2310160717816746	T	T	T
0.1434454467567342	0.3036165893757459	0.2912338961142163	T	T	T
0.6348979078839916	0.3000988956322048	0.2339309745905222	T	T	T
0.0525859401117665	0.6944545612961915	0.2827904020203501	T	T	T
0.5469665776178999	0.6990315871632260	0.2805779140222869	T	T	T
0.36812522609201074	0.1030507142167413	0.2815738567275989	T	T	T
0.8711405132245686	0.1034402432901003	0.2859072767366636	T	T	T
0.6178033650461839	0.5024412603998366	0.3213522845906069	T	T	T
0.8891117656809642	0.4593109410407548	0.3441568631460069	T	T	T
0.5074222600937608	0.2741835141156665	0.3707075425828734	T	T	T
0.7527615923834459	0.3034771699769999	0.4225367771469308	T	T	T
0.2852122690917284	0.2007915496624277	0.4238284035277280	T	T	T
0.6377246115459372	0.5264689540492830	0.3818330119629663	T	T	T

COH formation and dissociation on $K_2O-Fe_5C_2(510)$

$K_2O-Fe_5C_2(510)-CO+H$ (IS)

1.000000000000000		
10.1180000000000003	0.0000000000000000	0.0000000000000000
-0.7809265139842700	12.8064770233652006	0.0000000000000000
0.0000000000000000	-0.0000000000000600	17.4192900000000002

Fe C O K H
60 25 2 2 1

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2164807321470250	0.9388285331061794	0.1326320519010620	T	T	T
0.7176129597928319	0.9396021350078868	0.1338552768160964	T	T	T
0.3391430605231659	0.5358426611605221	0.1414971295507233	T	T	T
0.8385984240745060	0.5351500671159870	0.1380454292455993	T	T	T
0.1342949138487444	0.1452624201718629	0.1459312324242595	T	T	T
0.6349486374455214	0.1471287752731982	0.1514519147412732	T	T	T
0.2320925246117823	0.3461796463427310	0.1390877740852229	T	T	T
0.7227542346463581	0.3439503914958245	0.1382507022808752	T	T	T
0.2844940262799547	0.7510849493264120	0.1494907317430255	T	T	T
0.7839275426910888	0.7525065893029844	0.1491968858842180	T	T	T
0.4636117928930599	0.8813316914901725	0.1528902491905721	T	T	T
0.9643393084447810	0.8814059579062574	0.1536609626555319	T	T	T
0.4719594005666637	0.2968154111658237	0.1632946582250492	T	T	T
0.9619599445743090	0.2950176467915278	0.1596640704620270	T	T	T
0.0793627391600279	0.4865099894670449	0.1627088861425097	T	T	T
0.5755947894812796	0.4892311323385786	0.1603272302701098	T	T	T
0.3970727275230742	0.0966203188134977	0.1645485868587015	T	T	T
0.8943465363760827	0.0953481585642188	0.1641067066252250	T	T	T
0.0389304147053889	0.6904773349258743	0.1669647560501381	T	T	T

0.5375911343743884	0.6900211736302078	0.1667064243192019	T	T	T
0.2065360228041357	0.6184228887792063	0.2529942581569676	T	T	T
0.7075203256061678	0.6219665051978769	0.2519526074445008	T	T	T
0.2797136364880466	0.2259135446623950	0.2496903236204328	T	T	T
0.7930067802577117	0.2272140149474444	0.2531234220362310	T	T	T
0.1355130220773571	0.8220244210292713	0.2553662970430081	T	T	T
0.6354039056796258	0.8241333233165502	0.2549815719895222	T	T	T
0.2130294818004642	0.0192502895687090	0.2571148467384376	T	T	T
0.7113822962734027	0.0233951364273823	0.2592647144853916	T	T	T
0.2396357660368992	0.4230620719176486	0.2674493867818306	T	T	T
0.7445340422742667	0.4280125284857271	0.2627701171940703	T	T	T
0.4485652588895307	0.5601722209075725	0.2732359209483819	T	T	T
0.9442628239705200	0.5601065445927191	0.2703838544501780	T	T	T
0.4572251054910741	0.9761376282109185	0.2699195151027045	T	T	T
0.9561419153272649	0.9759281560153157	0.2710752477546143	T	T	T
0.0378851303135795	0.1781471871600167	0.2732142027999834	T	T	T
0.5282558222033676	0.1850605317151522	0.2882340900474706	T	T	T
0.3905732343134233	0.7610627947201900	0.2728191525885231	T	T	T
0.8909277741154317	0.7608217964498928	0.2727714614374157	T	T	T
0.4870915246661704	0.3692339107258112	0.2979492388756148	T	T	T
0.9917018765970815	0.3660366623048330	0.2884994674175173	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0651070085054241	0.0099123491029737	0.1812545720731655	T	T	T
0.5660516562979498	0.0086252543302553	0.1806916848072694	T	T	T
0.4021488793736290	0.4269860800214742	0.2057607374924294	T	T	T
0.9027592681810900	0.4267145226723050	0.2022399849815896	T	T	T
0.3079053731649008	0.8862869621537411	0.2319383812166289	T	T	T
0.8089484390761248	0.8866812994341202	0.2321348785904005	T	T	T
0.1475817447565896	0.2975693080857244	0.3041967987995008	T	T	T
0.6294536013452905	0.3040651968475557	0.2370062544684421	T	T	T
0.0508148055987913	0.6880527360512643	0.2823192918125536	T	T	T
0.5507082299865211	0.6897756566126335	0.2811987504732746	T	T	T
0.3671500045985884	0.1007252358375116	0.2821133587926191	T	T	T
0.8700967246759534	0.1026007065119702	0.2851516109367634	T	T	T
0.4932778441962623	0.4838312665187021	0.3653555274067304	T	T	T
0.5177132341152746	0.5032185361417885	0.4320311367863796	T	T	T
0.5105428862190972	0.2655487574265896	0.3747817193590414	T	T	T
0.7193294176135127	0.3572021367712289	0.4367269047596706	T	T	T
0.2880629830400260	0.1917771799219972	0.4295056638451035	T	T	T
0.7890262198924278	0.5388529770237162	0.3170757694903431	T	T	T

K₂O-Fe₃C₂(510)-COH (TS)

1.000000000000000
10.118000000000003 0.000000000000000 0.000000000000000
-0.7809265139842700 12.8064770233652006 0.000000000000000
0.000000000000000 -0.0000000000000600 17.419290000000002

Fe C O K H
60 25 2 2 1

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F

0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2153831059582486	0.9387994616816779	0.1323344420341137	T	T	T
0.7172977304044674	0.9392973551607213	0.1338213980731333	T	T	T
0.3388495933081269	0.5351085308037706	0.1460051437893505	T	T	T
0.8387481352084780	0.5349134686877339	0.1398693639806576	T	T	T
0.1333811399888913	0.1457144952569097	0.1453775234796508	T	T	T
0.6360037063664913	0.1457211048642887	0.1521995850378960	T	T	T
0.2300354094709535	0.3462664693337451	0.1393268561321354	T	T	T
0.7175256462959205	0.3409595743215225	0.1364854077775377	T	T	T
0.2850454939336834	0.7503751328636590	0.1497148185739413	T	T	T
0.7850197696814569	0.7511827062582569	0.1499098268921645	T	T	T
0.4625697580319549	0.8818510115981604	0.1526069894234379	T	T	T
0.9641447541362441	0.8814008346724593	0.1535686328549410	T	T	T
0.4703701942260610	0.2947689038083878	0.1632062815696399	T	T	T
0.9614638966499621	0.2974873302995724	0.1602259710956329	T	T	T
0.0816550147048370	0.4875237117469276	0.1613210758099421	T	T	T
0.5745671703443644	0.4889964821865372	0.1584162260265831	T	T	T
0.3960641275500703	0.0949356974525468	0.1640241111656865	T	T	T
0.8951576914637553	0.0942768085291212	0.1633939900086942	T	T	T
0.0389297132319247	0.6907794207485695	0.1675781645055556	T	T	T
0.5384354651975698	0.6909251000081204	0.1665990126286473	T	T	T
0.2065590889323825	0.6186381031128037	0.2542662203047105	T	T	T
0.7038746847868911	0.6192142317014682	0.2548622415048476	T	T	T
0.2798624916543157	0.2262628182390814	0.2477904630147391	T	T	T
0.7966049674580824	0.2251377862052896	0.2520401541111628	T	T	T
0.1347628312167809	0.8235636004634319	0.2551287632066365	T	T	T
0.6353245878059188	0.8269516066691195	0.2538854147789254	T	T	T
0.2121019475861127	0.0200611492661744	0.2567740829788435	T	T	T
0.7120845122090064	0.0232085786228445	0.2602533403458006	T	T	T
0.2417472962953629	0.4262944460369838	0.2683101356335615	T	T	T
0.7479356141335676	0.4241424750598031	0.2585233834187336	T	T	T
0.4589681505275071	0.5618256587023773	0.2739139836159288	T	T	T
0.9427016255297641	0.5648472059357998	0.2723044162857445	T	T	T
0.4562146069531640	0.9763725487761005	0.2701332750571978	T	T	T
0.9572932504906180	0.9752152069118122	0.2711984906950605	T	T	T
0.0398978183213316	0.1781660807026069	0.2737997160306748	T	T	T
0.5266392859564386	0.1819944731430578	0.2893964856123273	T	T	T
0.3892431539138225	0.7627044920758037	0.2721479522145826	T	T	T
0.8896422410436673	0.7619151296766330	0.2747021309236908	T	T	T
0.5134021705757680	0.3735531746438300	0.2943237593761125	T	T	T
0.9962715524247823	0.3663839869600327	0.2886708631717966	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0647876407045221	0.0101953673962879	0.1807668579003555	T	T	T
0.5661886567839535	0.0079425649009433	0.1819854470022925	T	T	T
0.4022123005074383	0.4229540902939206	0.2115493959634357	T	T	T
0.9141441867132035	0.4359112468304860	0.2070509295615053	T	T	T
0.3073259303064502	0.8873224989248033	0.2309952038735511	T	T	T
0.8096227651033286	0.8871013674530019	0.2319335930971575	T	T	T
0.1519846478723909	0.2987015673779787	0.3036206399402979	T	T	T
0.6317521677056156	0.2929126635986093	0.2336842227551821	T	T	T
0.0513787344442369	0.6905622778960824	0.2832651437662195	T	T	T
0.5500745791895494	0.6962210820718094	0.2800505551082858	T	T	T
0.3662941053333348	0.1000846631185103	0.2827081165600068	T	T	T
0.8721164864081963	0.1016358170514157	0.2854285263232197	T	T	T
0.6207368099540749	0.4971870422153983	0.3230985318970574	T	T	T
0.6824347388110932	0.5296481297161403	0.3881181336485911	T	T	T
0.5063053065286425	0.2724406030773763	0.3716521514822271	T	T	T

0.7393383224037202	0.3272638272451405	0.4306758115175275	T	T	T
0.2873765595395934	0.1922552836003170	0.4278323164344932	T	T	T
0.7881546854913961	0.5736202019548587	0.3507688340728513	T	T	T

K₂O-Fe₅C₂(510)-COH (FS)

1.00000000000000		
10.118000000000003	0.000000000000000	0.000000000000000
-0.7809265139842700	12.8064770233652006	0.000000000000000
0.000000000000000	-0.0000000000000600	17.4192900000000002

Fe C O K H
60 25 2 2 1

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2154443379187169	0.9387258308285090	0.1324963251358701	T	T	T
0.7168898489324227	0.9391679534690781	0.1338978702271024	T	T	T
0.3390760236384849	0.5352335169335108	0.1462900044681868	T	T	T
0.8395757677953838	0.5368698438712829	0.1401031139938285	T	T	T
0.1339175463000497	0.1448098175486639	0.1456679613953324	T	T	T
0.6358484882924382	0.1469854726742373	0.1524879828932144	T	T	T
0.2306266520539452	0.3459407566223739	0.1388877980840741	T	T	T
0.7237519985441964	0.3442092544839953	0.1382319766621840	T	T	T
0.2854087008218410	0.7506096474558996	0.1497085576160849	T	T	T
0.7848341008002306	0.7506357863396669	0.1500373144970948	T	T	T
0.4625849436256825	0.8823331224682301	0.1525310952393654	T	T	T
0.9633248482941699	0.8812995213832144	0.1536341509703469	T	T	T
0.4725892681062049	0.2955784893989147	0.1630708090535121	T	T	T
0.9627931750318774	0.2951289010140877	0.1595430509287739	T	T	T
0.0803982664243749	0.4863595708605841	0.1606487386943472	T	T	T
0.5743478928007190	0.4888346192775512	0.1585860619313851	T	T	T
0.3961360267439385	0.0954694377518101	0.1639269699746692	T	T	T
0.8948970332769014	0.0947994587202410	0.1637721562313391	T	T	T
0.0398789550286836	0.6911929415904693	0.1671430488220285	T	T	T
0.5384765794373484	0.6909423318047117	0.1666712204062184	T	T	T
0.2066620594418564	0.6194239845764775	0.2543905808435575	T	T	T
0.7010228954908222	0.6175487578946212	0.2568826548244855	T	T	T
0.2792756223639377	0.2273752714009039	0.2473156461689819	T	T	T
0.7964822134084245	0.2261668484327759	0.2525277786005251	T	T	T
0.1342873065184746	0.8230279249458776	0.2555003799014719	T	T	T
0.6357789822074598	0.8265634478380590	0.2541741560757241	T	T	T
0.2120068043455723	0.0202289480139917	0.2567638006142688	T	T	T
0.7119073979070766	0.0232418031454933	0.2601393226635786	T	T	T
0.2389953162567929	0.4270984092345726	0.2676858018556927	T	T	T
0.7468074420790914	0.4268619169818224	0.2635943173889774	T	T	T
0.4582271435865710	0.5618155450980858	0.2746663465379271	T	T	T
0.9450888746411609	0.5612499892856818	0.2686989112940905	T	T	T
0.4560313630642974	0.9769165623383804	0.2699696599169831	T	T	T
0.9566239326884524	0.9759571008243634	0.2713525741189111	T	T	T
0.0387015854220231	0.1790491624449513	0.2736239826666706	T	T	T
0.5255683085693202	0.1830935284779268	0.2890401755782163	T	T	T
0.3888598098941270	0.7629468565976232	0.2721842078034930	T	T	T
0.8888005741378999	0.7605409101520477	0.2737678976614262	T	T	T
0.5133567580175753	0.3751118639938176	0.2940095217296629	T	T	T
0.9921525751907357	0.3670773561988482	0.2882693202963078	T	T	T

0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0643113855908789	0.0094959142406593	0.1809010838773271	T	T	T
0.5662967883140972	0.0089121748662135	0.1817108153093109	T	T	T
0.4008771086519426	0.4226982456197743	0.2119705370644230	T	T	T
0.9061628564006101	0.4285238442125485	0.2021869664311239	T	T	T
0.3070802581004974	0.8872401189756133	0.2311924878303491	T	T	T
0.8095925431060780	0.8873350462832735	0.2321278284936719	T	T	T
0.1491618137088225	0.3000878200025449	0.3026442002266838	T	T	T
0.6320889458495714	0.2946224730469091	0.2340488760124599	T	T	T
0.0499242440244092	0.6892981156019052	0.2828296033136788	T	T	T
0.5494969840789533	0.6965026628758065	0.2806030073788907	T	T	T
0.3657677786963412	0.1006611921204992	0.2826662083585396	T	T	T
0.8712404509745789	0.1023780945304896	0.2859339980894154	T	T	T
0.6188136857122565	0.4987599078704004	0.3268334842446567	T	T	T
0.6410545186180774	0.5185913499298026	0.4063212086891875	T	T	T
0.5036390097840818	0.2735062922093369	0.3711871884629827	T	T	T
0.7364594754658419	0.3196165737104290	0.4310227970534223	T	T	T
0.2851109832298921	0.1950013660382039	0.4271906035715153	T	T	T
0.7041608531966046	0.5799521041861498	0.4083770276706211	T	T	T

K₂O-Fe₅C₂(510)-C+OH (TS)

1.0000000000000000		
10.1180000000000003	0.0000000000000000	0.0000000000000000
-0.7809265139842700	12.8064770233652006	0.0000000000000000
0.0000000000000000	-0.0000000000000060	17.4192900000000002
Fe	C	O
60	25	2
2	2	1

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2154701710474519	0.9392246843402774	0.1323303987770410	T	T	T
0.7169148979196406	0.9389603392781936	0.1340555975525227	T	T	T
0.3394348637435612	0.5358021285916960	0.1430249271933643	T	T	T
0.8376576448687780	0.5334501399220857	0.1398545906833260	T	T	T
0.1338207074364977	0.1465742711244660	0.1467211102922698	T	T	T
0.6359392010575263	0.1446533990717065	0.1513458507545270	T	T	T
0.2318553725661083	0.3463972514266897	0.1391536570537039	T	T	T
0.7132669707579306	0.3388599097323928	0.1356545896104810	T	T	T
0.2841979283947764	0.7513707571770438	0.1491394649287999	T	T	T
0.7859027508201517	0.7504472458238322	0.1503354060129811	T	T	T
0.4629539227607927	0.8817048073973852	0.1524663768086118	T	T	T
0.9633326579321004	0.8822188455384909	0.1531898129181712	T	T	T
0.4701830819960274	0.2959754918550501	0.1644125427592582	T	T	T

0.9591673149579198	0.2989766739553924	0.1608961843843180	T	T	T
0.0831973519055211	0.4879724528796282	0.1615494404374193	T	T	T
0.5758699406062731	0.4896635878826834	0.1615188808545593	T	T	T
0.3956181722634127	0.0950348689134494	0.1645243012974280	T	T	T
0.8948383467399711	0.0954124556616499	0.1635702809901542	T	T	T
0.0398775509762033	0.6920928811478758	0.1670278876108982	T	T	T
0.5399968082772888	0.6923771317405142	0.1664995040954451	T	T	T
0.2070237062809784	0.6200139523147884	0.2535687259418009	T	T	T
0.7014795873464471	0.6206831782933419	0.2589792455739044	T	T	T
0.2823443011194612	0.2266024064445117	0.2499699465295575	T	T	T
0.7953477366052240	0.2245659131162268	0.2527849954713833	T	T	T
0.1348843353018200	0.8247517237490425	0.2545763555164690	T	T	T
0.6357963164352399	0.8273771611832207	0.2543825006624527	T	T	T
0.2112203882443466	0.0211949652642213	0.2572217014670185	T	T	T
0.7122711088160235	0.0232664392706706	0.2600816545922722	T	T	T
0.2454189650651266	0.4271916060342039	0.2693351053343774	T	T	T
0.7486289740043429	0.4207514649062427	0.2571833563314671	T	T	T
0.4532868944999033	0.5629931394165498	0.2698772352970162	T	T	T
0.9471509936893644	0.5655082600435423	0.2704694202433239	T	T	T
0.4556400588902640	0.9750260390263271	0.2706047175550257	T	T	T
0.9577067708979921	0.9761235395233464	0.2713309524323576	T	T	T
0.0408198802378678	0.1792722331895576	0.2744744973614882	T	T	T
0.5310375004112025	0.1765863136258549	0.2857601573197445	T	T	T
0.3875195412978226	0.7644649088784438	0.273061006925510	T	T	T
0.8904855649296746	0.7633580982122742	0.2732932206239055	T	T	T
0.5055669845770520	0.3704267013231938	0.3003853304732136	T	T	T
0.9979246647789644	0.3662607732649756	0.2896973246901607	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0649370576144718	0.0103406243637499	0.1805860385715227	T	T	T
0.5658207672229164	0.0076817966736146	0.1821675658335449	T	T	T
0.3973069558688045	0.4206266644739923	0.2058540666348243	T	T	T
0.9173059785023360	0.4375444123307402	0.2083966547411345	T	T	T
0.3068689801012103	0.8883097895194932	0.2303895585415760	T	T	T
0.8101523088071463	0.8881244235851357	0.2318165939041441	T	T	T
0.1544904316595479	0.2999363642580580	0.3038800299990637	T	T	T
0.6307246239083529	0.2931436845399483	0.2334454963591424	T	T	T
0.0524479272274699	0.6926160267933500	0.2834588380939319	T	T	T
0.5473579022859466	0.6980758415872494	0.2807977547534754	T	T	T
0.3659488671595488	0.0998509248096889	0.2828486607778887	T	T	T
0.8731796868272094	0.1019549394550635	0.2853818449624592	T	T	T
0.6146598282947370	0.4959156804956180	0.2994857731671348	T	T	T
0.5603116687635411	0.4778988716316539	0.4109699513617973	T	T	T
0.5199267187398476	0.2601601076628847	0.3717844264685524	T	T	T
0.7358494336430521	0.3494673613322771	0.4346334914861236	T	T	T
0.2976488692912147	0.1999520154327372	0.4305538103475204	T	T	T
0.5303543023960683	0.5485218697772911	0.4160591677643838	T	T	T

K₂O-Fe₃C₂(510)-C+OH(FS)

1.000000000000000		
10.1180000000000003	0.000000000000000	0.0000000000000000
-0.7809265139842700	12.8064770233652006	0.0000000000000000
0.0000000000000000	-0.0000000000000600	17.4192900000000002

Fe C O K H
60 25 2 2 1

Selective dynamics

Direct

0.2394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.7394699999999972	0.2602600000000024	0.0193299999999965	F	F	F
0.3524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.8524200000000022	0.8641300000000030	0.0267499999999998	F	F	F
0.1786799999999999	0.4665400000000020	0.0302900000000008	F	F	F
0.6786799999999999	0.4665400000000020	0.0302900000000008	F	F	F

0.2651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.7651299999999992	0.6599000000000004	0.0305200000000028	F	F	F
0.2917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.7917699999999996	0.0723199999999977	0.0369999999999990	F	F	F
0.4854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.9854800000000026	0.2084899999999976	0.0384200000000021	F	F	F
0.0121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.5121200000000030	0.6209100000000021	0.0448999999999984	F	F	F
0.0985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.5985700000000023	0.8142700000000005	0.0451300000000003	F	F	F
0.4248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.9248300000000000	0.4166799999999995	0.0486700000000013	F	F	F
0.0377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.5377799999999979	0.0205500000000001	0.0560899999999975	F	F	F
0.2146976419936135	0.9390808108532143	0.1325130383228348	T	T	T
0.7167902085207851	0.9391299287070443	0.1338988942489382	T	T	T
0.3408699088245991	0.5364318979420003	0.1446472523880825	T	T	T
0.8386640613737035	0.5342647632381081	0.1407818164211800	T	T	T
0.1339605142835232	0.1450395261942951	0.1444625443264097	T	T	T
0.6354200506070734	0.1441256076652769	0.1505607035762167	T	T	T
0.2313474912530110	0.3470574554845728	0.1411314052468828	T	T	T
0.7136865533231739	0.3396306315179140	0.1353651582572455	T	T	T
0.2834339527010672	0.7517389474686738	0.1487835137387771	T	T	T
0.7857408025621412	0.7509983131923472	0.1500615417858290	T	T	T
0.4624947935862925	0.8816140391538507	0.1525678186419545	T	T	T
0.9630096180301676	0.8825767872988758	0.1531051766100937	T	T	T
0.4696053350636473	0.2945263820167708	0.1639726966399023	T	T	T
0.9606373407847211	0.2984618088860241	0.1601991384503432	T	T	T
0.0844442640925903	0.4885368111910626	0.1626247985054027	T	T	T
0.5764605124526533	0.4903714969043564	0.1644777931419254	T	T	T
0.3950808749057159	0.0926751495284284	0.1638626626655238	T	T	T
0.8953762510643762	0.0943841318966231	0.1628771820820103	T	T	T
0.0393580296493061	0.6930476968475053	0.1672622771357260	T	T	T
0.5410567683714281	0.6938682767186318	0.1663648163641842	T	T	T
0.2067360650756781	0.6218801254219770	0.2529156112051041	T	T	T
0.7034603521040266	0.6227281437808215	0.2584003208408327	T	T	T
0.2803812701184715	0.2218882119109692	0.2464839569311458	T	T	T
0.7937580008275444	0.2229516653440714	0.2489982664500623	T	T	T
0.1343063938216240	0.8263866251070716	0.2547841978142011	T	T	T
0.6360286412775963	0.8296484799310776	0.2551219730378545	T	T	T
0.2111158810587775	0.0209345720137537	0.2578946633724880	T	T	T
0.7112588407470979	0.0241655636740855	0.2601529480813370	T	T	T
0.2517897912417063	0.4293889602965826	0.2773257392536110	T	T	T
0.7509463590953394	0.4189184269642987	0.2584199534747677	T	T	T
0.4541220240147769	0.5689482580557641	0.2699440263978992	T	T	T
0.9487215692184359	0.5664253705746438	0.2707005505666229	T	T	T
0.4556182226488575	0.9752387460344375	0.2711568110944939	T	T	T
0.9562036770575244	0.9753284295590249	0.2722077349144733	T	T	T
0.0392689362591732	0.1755662501822550	0.2720281388552820	T	T	T
0.5322201450757349	0.1759392921333179	0.2851790591903475	T	T	T
0.3874303418521537	0.7657083764033593	0.2727666496226526	T	T	T
0.8912100806148238	0.7646360558212603	0.2736180610920939	T	T	T
0.5030069799378651	0.3721855486644768	0.2969220431594545	T	T	T
0.9938194650880152	0.3637009686168232	0.2890229733238686	T	T	T
0.3220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.8220200000000020	0.5286800000000014	0.0000000000000000	F	F	F
0.2192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.7192900000000009	0.9343099999999964	0.0082499999999968	F	F	F
0.0579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.5579600000000013	0.3464999999999989	0.0671699999999973	F	F	F
0.4552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.9552300000000002	0.7521300000000011	0.0754200000000012	F	F	F
0.2973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.7973500000000016	0.2090699999999970	0.1178400000000011	F	F	F
0.1946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.6946200000000005	0.6146999999999991	0.1260899999999978	F	F	F
0.0646059282959715	0.0103270456579574	0.1819754829285198	T	T	T
0.5653689579323176	0.0074584903798119	0.1822731607312298	T	T	T
0.3911488120157273	0.4167775243727681	0.2030188949126094	T	T	T
0.9186052711770963	0.4383633608678585	0.2083768890771499	T	T	T
0.3068397413533052	0.8890068292742671	0.2302092642638646	T	T	T
0.8101042356658835	0.8881769054621698	0.2303557547061227	T	T	T
0.1493868261569024	0.2967231795609269	0.2941336785624759	T	T	T
0.6288407426233057	0.2924197680215020	0.2325109579679347	T	T	T
0.0525588920877949	0.6941551779318421	0.2838315156254001	T	T	T

0.5487346984123348	0.7008471195268722	0.2815436918309841	T	T	T
0.3667726908071511	0.1001188319079845	0.2835320195006449	T	T	T
0.8711973965803294	0.1018237368655890	0.2860188816240082	T	T	T
0.6119804163776361	0.4954236802620632	0.2889460975579198	T	T	T
0.3553122471289389	0.4231681476464744	0.3772274658807770	T	T	T
0.5294259476299369	0.2622166776364729	0.3698053565146144	T	T	T
0.7600568805412089	0.2841560017327091	0.4247935076677047	T	T	T
0.2974720037074670	0.2297459245234741	0.4285982943094493	T	T	T
0.3769591217777647	0.4934112984100445	0.3968067582310963	T	T	T

CO dissociation on Fe₅C₂(111)

Fe₅C₂(111)-CO (IS)

1.000000000000000		
12.3812999725000008	0.0000000000000000	0.0000000000000000
-2.0391083097000000	13.2888646689000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.8052997588999986

Fe C O
80 33 1

Selective dynamics

Direct

0.8393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.7309522256095946	0.2195612072779181	0.4674332898756805	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999985	F	F	F
0.5593680075937775	0.0979962407053436	0.4377813554131555	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000003	F	F	F
0.5945463482929393	0.2771774284843627	0.3883853056626268	T	T	T
0.8070399759999987	0.3298200070000021	0.3692500000000010	F	F	F
0.6866763857857341	0.0425890400190179	0.5101092308228502	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.2334556929547402	0.2209008737379382	0.4668188158968195	T	T	T
0.1632599980000009	0.3849500119999973	0.2899999919999985	F	F	F
0.0606653830141015	0.0974158247389419	0.4386810084472915	T	T	T
0.1955399960000008	0.0652299970000030	0.2403199970000003	F	F	F
0.0941697995666017	0.2779965511779365	0.3883987183363543	T	T	T
0.3070400060000011	0.3298200070000021	0.3692500000000010	F	F	F
0.1881986258434875	0.0428132358360472	0.5104503341082404	T	T	T
0.0044699999999978	0.4602699880000003	0.2462999970000013	F	F	F
0.9049996884551985	0.1720346347852332	0.3944833926130161	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.4035712381339834	0.1521713781837298	0.5053013911534302	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999982	F	F	F
0.4333414991366201	0.3268710721786398	0.4627388090069915	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F
0.8787717144152769	0.4907777746771160	0.4477025835408061	T	T	T
0.5044699910000006	0.4602699880000003	0.2462999970000013	F	F	F
0.4045622022689610	0.1734444604152026	0.3942218780806302	T	T	T
0.9981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.9007337777454688	0.1513623590021597	0.5059050084109060	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999982	F	F	F
0.9307643515017656	0.3252065614286189	0.4621048912676142	T	T	T
0.4722500150000002	0.2798599899999985	0.2958799900000031	F	F	F
0.3789160997922394	0.4912358847058604	0.4473610843551201	T	T	T
0.7199699880000026	0.1401900050000009	0.3529999849999967	F	F	F
0.6295293076759639	0.3602065585514306	0.4912305456536366	T	T	T
0.7826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.6900067194106039	0.4675164659658714	0.4029945680598278	T	T	T
0.2199700030000002	0.1401900050000009	0.3529999849999967	F	F	F
0.1277391799396302	0.3577682446101637	0.4954182094463576	T	T	T
0.2826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.1897055127366860	0.4660648058411863	0.4031890296983534	T	T	T
0.8393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.7324869991122431	0.7194948404385041	0.4665682475817497	T	T	T
0.6632599830000032	0.8849499820000020	0.2899999919999985	F	F	F
0.5599602080408994	0.5979390282429571	0.4368890537821376	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000003	F	F	F
0.5949377560441265	0.7773007349726130	0.3882395500500012	T	T	T
0.8070399759999987	0.8298199769999997	0.3692500000000010	F	F	F
0.6865424599590471	0.5432692008309629	0.5101443691579016	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.2316028907086094	0.7199239168863646	0.4678891798842739	T	T	T
0.1632599980000009	0.8849499820000020	0.2899999919999985	F	F	F
0.0631091409129657	0.5954797192922967	0.4403606903347432	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000003	F	F	F

0.0947806239835099	0.7766115086372837	0.3888045057934707	T	T	T
0.3070400060000011	0.8298199769999997	0.3692500000000010	F	F	F
0.2018870838549538	0.5351980682304931	0.5111879623627922	T	T	T
0.0044699999999978	0.9602699880000003	0.2462999970000013	F	F	F
0.9056426456824176	0.6714671878348658	0.3939945421637879	T	T	T
0.4981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.4038700919460751	0.6522942942490466	0.5054231538886588	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999982	F	F	F
0.4350179412407504	0.8256059211440769	0.4623749389673880	T	T	T
0.9722499849999977	0.7798600200000010	0.2958799900000031	F	F	F
0.8784661411509370	0.9896073837572185	0.4487399039273473	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000013	F	F	F
0.4047673141179897	0.6723075518675098	0.3939085864242497	T	T	T
0.9981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.9048926118519942	0.6525376434089307	0.5054361883580495	T	T	T
0.0303299999999993	0.6151900289999972	0.3136900069999982	F	F	F
0.9357970957900194	0.8246140038127692	0.4624813025722318	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3785587957039683	0.9902094640862459	0.4490050731394715	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999967	F	F	F
0.6312733824317834	0.8595176229577712	0.4911635489252509	T	T	T
0.7826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.6898684141753217	0.9674808454967975	0.4027192705704521	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999967	F	F	F
0.1318796816419475	0.8607022712417479	0.4916360704131384	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.1899355186950879	0.9674371900399209	0.4026358702553915	T	T	T
0.8641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.7771534728288972	0.3669096847626513	0.4614456258757128	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999986	F	F	F
0.5379244396620724	0.4554770792790872	0.4620534110703745	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999985	F	F	F
0.5464593873529446	0.2290632725391599	0.4786456821755145	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000016	F	F	F
0.7795014049380142	0.0928007531078513	0.4378392044731775	T	T	T
0.3641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.2758606637943378	0.3688669278087265	0.4614827758786051	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999986	F	F	F
0.0366275618259108	0.4514586514883933	0.4587865231015324	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999985	F	F	F
0.0417882881268655	0.2280401004209986	0.4756075051288678	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000016	F	F	F
0.2799898513039614	0.0931923973667622	0.4376565090426713	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.7798779758895287	0.8653120948490776	0.4621011997176553	T	T	T
0.6384199860000024	0.7358700039999988	0.3038099999999986	F	F	F
0.5385526248328351	0.9544201990504826	0.4620089469520041	T	T	T
0.6260200139999981	0.5126500129999982	0.3228900129999985	F	F	F
0.5487171565019107	0.7279615734830256	0.4781424930549144	T	T	T
0.8765599729999991	0.8823999760000021	0.2866800130000016	F	F	F
0.7807129307533960	0.5932656594441867	0.4382715740761122	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.2796529863654700	0.8661305344090492	0.4617706378056159	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999986	F	F	F
0.0383700947818535	0.9539812371180703	0.4613502257583396	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999985	F	F	F
0.0510155510430669	0.7278615188206651	0.4796237069640315	T	T	T
0.3765600030000016	0.8823999760000021	0.2866800130000016	F	F	F
0.2788094961599896	0.5943020131940470	0.4369490602234179	T	T	T
0.1500165450769702	0.3843938030557728	0.5779973694594541	T	T	T
0.1668386758061507	0.3995438418775447	0.6332652078406654	T	T	T

Fe₅C₂(111)-C+O (TS)

1.000000000000000		
12.3812999725000008	0.0000000000000000	0.0000000000000000
-2.0391083097000000	13.2888646689000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.8052997588999986

Fe C O

80 33 1

Selective dynamics

Direct

0.8393200040000143	0.0101000000000013	0.3195700050000025	F	F	F
0.7373923651700349	0.2178025930872733	0.4669183106611978	T	T	T

0.6632599830000033	0.3849500119999973	0.2899999919999982	F	F	F
0.5621927256189881	0.0968281004033828	0.4382411665123395	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000002	F	F	F
0.5963286578763488	0.2761020958869876	0.3887582714439650	T	T	T
0.8070399760000101	0.3298200070000021	0.3692499999999965	F	F	F
0.6885094677640266	0.0373199352784324	0.5096431004058799	T	T	T
0.3393200040000012	0.0101000000000013	0.3195700050000025	F	F	F
0.2425825709905453	0.2205244202734349	0.4681787402218694	T	T	T
0.1632599980000009	0.3849500119999973	0.2899999919999982	F	F	F
0.0634684686361929	0.0978782131111794	0.4381097586903925	T	T	T
0.1955399960000037	0.0652299970000030	0.2403199970000002	F	F	F
0.0999115444766482	0.2778968783252032	0.3892249251267075	T	T	T
0.3070400060000014	0.3298200070000021	0.3692499999999965	F	F	F
0.1902275516487205	0.0429651381351106	0.5104740284265791	T	T	T
0.0044699999999977	0.4602699880000002	0.2462999970000008	F	F	F
0.9063988352420501	0.1723376446052036	0.3945513160698222	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799979999985	F	F	F
0.4101149578360271	0.1504443189370770	0.5047011512250491	T	T	T
0.5303300019999996	0.1151899990000018	0.3136900069999981	F	F	F
0.4467797216382554	0.3241967019525424	0.4648888052128343	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F
0.8803406613910091	0.4890367320216245	0.4493008172774018	T	T	T
0.5044699910000008	0.4602699880000002	0.2462999970000008	F	F	F
0.4059274363069351	0.1729977368253792	0.3940089569701087	T	T	T
0.9981200100000009	0.4347699879999993	0.3632799979999985	F	F	F
0.9041294862467202	0.1493981926957093	0.5055594051011564	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999981	F	F	F
0.9408647031333016	0.3259492152883601	0.4625398690888078	T	T	T
0.4722500150000003	0.2798599899999985	0.2958799900000031	F	F	F
0.3739058350194268	0.4829945599126454	0.4487774098365609	T	T	T
0.7199699880000028	0.1401900050000009	0.3529999849999923	F	F	F
0.6427808822851673	0.3597307130662620	0.4910301732538384	T	T	T
0.7826200129999998	0.2548600140000019	0.2565700110000008	F	F	F
0.6905367026856605	0.4685061242119524	0.4012165048651995	T	T	T
0.2199700030000004	0.1401900050000009	0.3529999849999923	F	F	F
0.1358877655690311	0.3560238715396994	0.4938245416649456	T	T	T
0.2826200129999990	0.2548600140000019	0.2565700110000008	F	F	F
0.1844898272557151	0.4684478000952592	0.4009539257823528	T	T	T
0.8393200040000011	0.5101000069999984	0.3195700050000025	F	F	F
0.7382193734845255	0.7196337546690311	0.4653307840084652	T	T	T
0.6632599830000033	0.8849499820000017	0.2899999919999982	F	F	F
0.5587255560900158	0.5941327825578293	0.4373069004182876	T	T	T
0.6955400109999988	0.5652300120000007	0.2403199970000002	F	F	F
0.5951656052816233	0.7745001616385907	0.3887533979287292	T	T	T
0.8070399759999987	0.8298199769999995	0.3692499999999965	F	F	F
0.6887594094139748	0.5442276932804192	0.5095923393937498	T	T	T
0.3393200040000012	0.5101000069999984	0.3195700050000025	F	F	F
0.2300057672594634	0.7224679292088034	0.4654410209420145	T	T	T
0.1632599980000008	0.8849499820000017	0.2899999919999982	F	F	F
0.0617499081075014	0.5975427118430369	0.4380162846236010	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000002	F	F	F
0.0944751784935201	0.7767773773569794	0.3884931716511077	T	T	T
0.3070400060000011	0.8298199769999995	0.3692499999999965	F	F	F
0.2019246019999819	0.5397967703227838	0.5097746708814942	T	T	T
0.0044699999999976	0.9602699880000003	0.2462999970000008	F	F	F
0.9052063194828588	0.6710843110862068	0.3940236206024158	T	T	T
0.4981200100000011	0.9347699879999992	0.3632799979999985	F	F	F
0.3913116344597125	0.6409489886652611	0.5116685435026112	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999981	F	F	F
0.4293704355449035	0.8262280176985691	0.4634859003176928	T	T	T
0.9722499849999977	0.7798600200000010	0.2958799900000031	F	F	F
0.8800129725090060	0.9886869916609631	0.4478160567528117	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000008	F	F	F
0.4047254740795989	0.6720582562519655	0.3967301220975941	T	T	T
0.9981200100000009	0.9347699879999992	0.3632799979999985	F	F	F
0.9072488260085013	0.6508177126290042	0.5056314462663050	T	T	T
0.0303299999999992	0.6151900289999972	0.3136900069999981	F	F	F
0.9364308172541478	0.8239306381699257	0.4630646022069226	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3791422610123423	0.9914732099248232	0.4480315475921363	T	T	T
0.7199699880000032	0.6401900050000009	0.3529999849999923	F	F	F
0.6251857327387864	0.8540895714229990	0.4895293969817052	T	T	T
0.7826200130000003	0.7548599839999994	0.2565700110000008	F	F	F
0.6903181132554090	0.9658273108584685	0.4025627510679419	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999923	F	F	F

0.1317052544608032	0.8614600843202034	0.4919931048530929	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000008	F	F	F
0.1892406148285369	0.9671335782293744	0.4026765597319811	T	T	T
0.8641700150000153	0.1591799999999992	0.3057599959999987	F	F	F
0.7915426172519907	0.3614627202143532	0.4659999563077600	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999985	F	F	F
0.5486493509043325	0.4516966138434668	0.4601465315413246	T	T	T
0.6260200140000070	0.0126500000000007	0.3228900129999984	F	F	F
0.5593378264603573	0.2284450037531909	0.4802714315845618	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000015	F	F	F
0.7812399820932258	0.0908731353438599	0.4371813677653738	T	T	T
0.3641700149999991	0.1591799999999992	0.3057599959999987	F	F	F
0.3111585422010405	0.3520471254779266	0.5055564063330212	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999985	F	F	F
0.0482090356558526	0.4548993191530145	0.4616283306407944	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999984	F	F	F
0.0471501524554513	0.2274155931750279	0.4761661768671878	T	T	T
0.3765600030000018	0.3824000059999975	0.2866800130000015	F	F	F
0.2808178726162130	0.0923707595249217	0.4366350734009641	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999987	F	F	F
0.7783058427944107	0.8661532438335527	0.4612966110025236	T	T	T
0.6384199860000024	0.7358700039999988	0.3038099999999985	F	F	F
0.5352892746051574	0.9534528674178817	0.4621013753715045	T	T	T
0.6260200139999991	0.5126500129999982	0.3228900129999984	F	F	F
0.5237500611244249	0.7210102663744464	0.4720684938710653	T	T	T
0.8765599729999993	0.8823999760000019	0.2866800130000015	F	F	F
0.7820847208812630	0.5906441792981392	0.4378467498648432	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999987	F	F	F
0.2790118107024243	0.8695137471686714	0.4617222520591684	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999985	F	F	F
0.0387058180941022	0.9539464298537700	0.4602889836373912	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999984	F	F	F
0.0533789984702830	0.7274019849715502	0.4799189818039941	T	T	T
0.3765600030000016	0.8823999760000019	0.2866800130000015	F	F	F
0.2759983789122297	0.5921436033590909	0.4342117166214084	T	T	T
0.2698294246880322	0.4318357492825398	0.5304715114209780	T	T	T
0.3226569259367021	0.5511838051765189	0.5724506142154406	T	T	T

Fe₅C₂(111)C+O (FS)

1.0000000000000000
12.3812999725000008 0.0000000000000000 0.0000000000000000
-2.0391083097000000 13.2888646689000005 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.8052997588999986
Fe C O
80 33 1

Selective dynamics

Direct

0.8393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.7341855342297111	0.2200766065059571	0.4655340228934449	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999985	F	F	F
0.5615669253265116	0.0964624602974590	0.4369694194158361	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000003	F	F	F
0.5961021284657332	0.2776549917464113	0.3886354434693765	T	T	T
0.8070399759999987	0.3298200070000021	0.3692500000000010	F	F	F
0.6903992912459613	0.0442173240351952	0.5093462152440547	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.2445280859074777	0.2177887222901355	0.4672104479085771	T	T	T
0.1632599980000009	0.3849500119999973	0.2899999919999985	F	F	F
0.0617143755443671	0.0974012385456098	0.4386792813586256	T	T	T
0.1955399960000008	0.0652299970000030	0.2403199970000003	F	F	F
0.0998959734414713	0.2763270323096905	0.3894581429159437	T	T	T
0.3070400060000011	0.3298200070000021	0.3692500000000010	F	F	F
0.1892773003474754	0.0421416428457245	0.5093445325805716	T	T	T
0.0044699999999978	0.4602699880000003	0.2462999970000013	F	F	F
0.9062451779593317	0.1736042307069001	0.3951815152046269	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.4105633898158716	0.1499757403467774	0.5042646296335946	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999982	F	F	F
0.4422003957597412	0.3242802373356822	0.4624135275006160	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F
0.8789451257097044	0.4922962107856675	0.4486937865117545	T	T	T
0.5044699910000006	0.4602699880000003	0.2462999970000013	F	F	F
0.4061616789456450	0.1722071840597510	0.3936522543984454	T	T	T

0.9981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.8956984321033291	0.1482112619184105	0.5067721094165738	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999982	F	F	F
0.9355106399451980	0.3291411878498202	0.4630006855645666	T	T	T
0.4722500150000002	0.2798599899999985	0.2958799900000031	F	F	F
0.3740473080631532	0.4899516203018916	0.4574643407567133	T	T	T
0.7199699880000026	0.1401900050000009	0.3529999849999967	F	F	F
0.6385207302254450	0.3587013008531336	0.4934269212887464	T	T	T
0.7826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.6917336713029565	0.4683767268951630	0.4033209171104922	T	T	T
0.2199700030000002	0.1401900050000009	0.3529999849999967	F	F	F
0.1313634281754294	0.3525115075872153	0.4925867809083762	T	T	T
0.2826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.1859497167605245	0.4669378666206523	0.3997015533247971	T	T	T
0.8393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.7331818101779134	0.7205485732116209	0.4643257419028718	T	T	T
0.6632599830000032	0.8849499820000020	0.2899999919999985	F	F	F
0.5623116271597925	0.5916653505684710	0.4296893797593427	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000003	F	F	F
0.5964417110819843	0.7780181080214001	0.3865020198742140	T	T	T
0.8070399759999987	0.8298199769999997	0.3692500000000010	F	F	F
0.6679785260497788	0.5432549261857241	0.5148294473262160	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.2303171936916014	0.7186676058268689	0.4640993537152747	T	T	T
0.1632599800000009	0.8849499820000020	0.2899999919999985	F	F	F
0.0605114262584368	0.5968792754664548	0.4378890805601131	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000003	F	F	F
0.0941045570296996	0.7757063430564082	0.3885722902232310	T	T	T
0.3070400060000011	0.8298199769999997	0.3692500000000010	F	F	F
0.1943356594911570	0.5333154881360290	0.5078642273784788	T	T	T
0.0044699999999978	0.9602699880000003	0.2462999970000013	F	F	F
0.9022742540814666	0.6700595310219422	0.3946057359351322	T	T	T
0.4981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.4849330197199393	0.6315044597849780	0.5275651365692914	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999982	F	F	F
0.4366510914695211	0.8226520065715592	0.4632701548283005	T	T	T
0.9722499849999977	0.7798600200000010	0.2958799900000031	F	F	F
0.8793689382404135	0.9890257656873555	0.4490712381846724	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000013	F	F	F
0.4039646767999729	0.6708655985086229	0.4018064084036868	T	T	T
0.9981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.9085854082781737	0.6532523224651809	0.5054529174980472	T	T	T
0.0303299999999993	0.6151900289999972	0.3136900069999982	F	F	F
0.9381799410021914	0.8243200224781967	0.4626293317838974	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3793032225822097	0.9870163899594405	0.4499329205428655	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999967	F	F	F
0.6333731626115486	0.8618667405952027	0.4901242097276237	T	T	T
0.7826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.6906903571884851	0.9672566340173158	0.4018882180613659	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999967	F	F	F
0.1350971855339497	0.8603491141909446	0.4916764923035515	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.1900846433396403	0.9662784207044824	0.4020450368520370	T	T	T
0.8641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.7854213506238142	0.3653328446300717	0.4627905916304427	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999986	F	F	F
0.5472942796093199	0.4474541624347586	0.4548745348159516	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999985	F	F	F
0.5571474251855847	0.2268841659686403	0.4792423827692141	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000016	F	F	F
0.7803683712814032	0.0918761676081016	0.4353892784239276	T	T	T
0.3641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.3028125883220993	0.3477383760050760	0.5038237443804131	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999986	F	F	F
0.0427884646192173	0.4549793750404196	0.4623836240344654	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999985	F	F	F
0.0298253443931474	0.2251336390228378	0.4716338854420813	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000016	F	F	F
0.2828378755854838	0.0893787889425200	0.4363069999562031	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.7845681090838592	0.8641679709019938	0.4627683591329155	T	T	T
0.6384199860000024	0.7358700039999988	0.3038099999999986	F	F	F
0.5376538526548278	0.9543612767462879	0.4617645516769134	T	T	T
0.6260200139999981	0.5126500129999982	0.3228900129999985	F	F	F

0.5513976661913896	0.7300607269153105	0.4719013893929784	T	T	T
0.8765599729999991	0.8823999760000021	0.2866800130000016	F	F	F
0.7771523792623520	0.5912562821401358	0.4429963606198941	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.2845864759734986	0.8624600459065220	0.4643079542481348	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999986	F	F	F
0.0403923943886715	0.9531371044531034	0.4608084342840889	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999985	F	F	F
0.0572318562796618	0.7270778217873970	0.4805700070715434	T	T	T
0.3765600030000016	0.8823999760000021	0.2866800130000016	F	F	F
0.2746815458046712	0.5911082403338305	0.4347841986603049	T	T	T
0.2686582537604894	0.4288021948203165	0.5316574388495678	T	T	T
0.5829530959346672	0.5796792322209970	0.5776375425723941	T	T	T

HCO formation and dissociation on Fe₃C₂(111)

1.0000000000000000		
12.3812999725000008	0.0000000000000000	0.0000000000000000
-2.0391083097000000	13.2888646689000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.8052997588999986

Fe C O H

80 33 1 1

Selective dynamics

Direct

0.8393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.7303937380237228	0.2195646038538755	0.4673833730894122	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999985	F	F	F
0.5590861499098891	0.0979552485663975	0.4378603915049685	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000003	F	F	F
0.5942062500620905	0.2769944487449822	0.3883430962926301	T	T	T
0.8070399759999987	0.3298200070000021	0.3692500000000010	F	F	F
0.6862402072579011	0.0410420542296061	0.5101205268546446	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.2336850440312929	0.2222045658939648	0.4665184544213682	T	T	T
0.1632599800000009	0.3849500119999973	0.2899999919999985	F	F	F
0.0605474147234982	0.0975156819531758	0.4383436738975205	T	T	T
0.1955399960000008	0.0652299970000030	0.2403199970000003	F	F	F
0.0943228176704713	0.2785000462146188	0.3883663634239981	T	T	T
0.3070400060000011	0.3298200070000021	0.3692500000000010	F	F	F
0.1864842884096437	0.0427429903636141	0.5102525822850599	T	T	T
0.0044699999999978	0.4602699880000003	0.2462999970000013	F	F	F
0.9048847164238989	0.1721400582753699	0.3946237237921367	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.4034882972126319	0.1521721712015258	0.5053414290927829	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999982	F	F	F
0.4332488323021551	0.3268118818635189	0.4631186754727637	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F
0.8788007770825924	0.4910217801069459	0.4475478258220936	T	T	T
0.5044699910000006	0.4602699880000003	0.2462999970000013	F	F	F
0.4043583724767220	0.1734247981131869	0.3941917173991253	T	T	T
0.9981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.8998425107169007	0.1511780471864026	0.5060111698861309	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999982	F	F	F
0.9303640651163785	0.3257111580960179	0.4619985710521997	T	T	T
0.4722500150000002	0.2798599899999985	0.2958799900000031	F	F	F
0.3799607617602393	0.4901115306939454	0.4464518368370980	T	T	T
0.7199699880000026	0.1401900050000009	0.3529999849999967	F	F	F
0.6294354718902431	0.3603109967811741	0.4912825063948192	T	T	T
0.7826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.6899922657461561	0.4670568390822903	0.4029746424151768	T	T	T
0.2199700030000002	0.1401900050000009	0.3529999849999967	F	F	F
0.1261763516125670	0.3577117870954197	0.4957204809393518	T	T	T
0.2826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.1878409303364794	0.4657507788529949	0.4038434806907845	T	T	T
0.8393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.7343999781599484	0.7199553059981338	0.4664699013047834	T	T	T
0.6632599830000032	0.8849499820000020	0.2899999919999985	F	F	F
0.5606709184509774	0.5978978428093400	0.4373457078876937	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000003	F	F	F
0.5959918955594653	0.7778664113920167	0.3880101938217954	T	T	T
0.8070399759999987	0.8298199769999997	0.3692500000000010	F	F	F
0.6878685224455747	0.5434331773807997	0.5101622378287333	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.2350641977427979	0.7183395968917868	0.4693742121050807	T	T	T

0.1632599980000009	0.8849499820000020	0.2899999919999985	F	F	F
0.0633818011514824	0.5956470129282907	0.4402829501154564	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000003	F	F	F
0.0969843346914452	0.7760178167055600	0.3891476346977837	T	T	T
0.3070400060000011	0.8298199769999997	0.3692500000000010	F	F	F
0.2147192791114642	0.5324763313234123	0.5110269388951070	T	T	T
0.0044699999999978	0.9602699880000003	0.2462999970000013	F	F	F
0.9066183239840535	0.6717647292044460	0.3943644552726857	T	T	T
0.4981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.3990379490505096	0.6516292176327578	0.5075305607875815	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999982	F	F	F
0.4330390861410791	0.8278782353045150	0.4616051590338938	T	T	T
0.9722499849999977	0.7798600200000010	0.2958799900000031	F	F	F
0.8779618718493341	0.9903224897878746	0.4481576661163406	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000013	F	F	F
0.4071114892179643	0.6731538217727314	0.3947069685863397	T	T	T
0.9981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.9012195182047902	0.6513200433349995	0.5062065526768647	T	T	T
0.0303299999999993	0.6151900289999972	0.3136900069999982	F	F	F
0.9343182015172871	0.8262046382090881	0.4625686484123516	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3778982061822510	0.9915663042746878	0.4483296303856636	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999967	F	F	F
0.6285824063325274	0.8578365313150960	0.4908567019449185	T	T	T
0.7826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.6894799766543677	0.9671474917010874	0.4027829530235490	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999967	F	F	F
0.1300482472232444	0.8592788397234495	0.4913462882235076	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.1895979870657897	0.9672036182593496	0.4029396172924621	T	T	T
0.8641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.7768952216595411	0.3671578609029807	0.4613988174683447	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999986	F	F	F
0.5381129579711730	0.4557469566900943	0.4626016872814760	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999985	F	F	F
0.5467981966508429	0.2289948689411254	0.4788304116054921	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000016	F	F	F
0.7787253312912054	0.0930999501321792	0.4377809674545344	T	T	T
0.3641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.2747952809653620	0.3712448302064001	0.4624691237603438	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999986	F	F	F
0.0372173014089111	0.4520329421069987	0.4585458814493433	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999985	F	F	F
0.0400063738454651	0.2277022899927925	0.4747464750775301	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000016	F	F	F
0.2794484552398063	0.0939109802789642	0.4379507867466282	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.7777768813369723	0.8665969636009098	0.4616325009777845	T	T	T
0.6384199860000024	0.7358700039999988	0.3038099999999986	F	F	F
0.5373650630166498	0.9547482446225777	0.4623282839530860	T	T	T
0.6260200139999981	0.5126500129999982	0.3228900129999985	F	F	F
0.5386735204120470	0.7272286953716016	0.4751271695717147	T	T	T
0.8765599729999991	0.8823999760000021	0.2866800130000016	F	F	F
0.7804031463545514	0.5930208859807712	0.4374415220625246	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.2775318145509373	0.8668630247784285	0.4598359186533882	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999986	F	F	F
0.0369203412544874	0.9544036843508270	0.4618258386621205	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999985	F	F	F
0.0420825936970833	0.7277041104733284	0.4769333714492973	T	T	T
0.3765600030000016	0.8823999760000021	0.2866800130000016	F	F	F
0.2807522920764625	0.5921179440610100	0.4324810102181988	T	T	T
0.1415881409319431	0.3804387766590756	0.5790370596516500	T	T	T
0.1522073991595707	0.3943872607309828	0.6347623660718941	T	T	T
0.2663388051513700	0.6507078565368044	0.5450732559461030	T	T	T

Fe₅C₂(111)-HCO (TS)

1.0000000000000000		
12.3812999725000008	0.0000000000000000	0.0000000000000000
-2.0391083097000000	13.2888646689000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.8052997588999986
Fe	C	O
80	33	1

Selective dynamics

Direct

0.8393200040000012	0.0101000000000013	0.3195700050000025	F	F	F
0.7347235764369141	0.2192673657822793	0.4666727262328258	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999982	F	F	F
0.5584175946683163	0.0977738899055775	0.4382710250622022	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000002	F	F	F
0.5954066360226141	0.2762970930590334	0.3882972774291518	T	T	T
0.8070399759999989	0.3298200070000021	0.3692499999999903	F	F	F
0.6854703369382757	0.0425051181485273	0.5096346479509598	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000025	F	F	F
0.2294150873822757	0.2236840453245135	0.4671435602798904	T	T	T
0.1632599980000009	0.3849500119999973	0.2899999919999982	F	F	F
0.0622104974547814	0.0978064489022432	0.4382934291767158	T	T	T
0.1955399960000009	0.0652299970000030	0.2403199970000002	F	F	F
0.0957948237886892	0.2816406813579729	0.3888205398467443	T	T	T
0.3070400060000012	0.3298200070000021	0.3692499999999903	F	F	F
0.1864951165866349	0.0424449411346210	0.5113884414254978	T	T	T
0.0044699999999960	0.4602699880000002	0.2462999970000008	F	F	F
0.9057555526100286	0.1723772468531690	0.3942517573673225	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799979999960	F	F	F
0.3968274998439281	0.1529040382927674	0.5059411355999239	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999981	F	F	F
0.4292987032071666	0.3288881365212556	0.4629899037522377	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F
0.8794194975713109	0.4889458180768163	0.4479434469675372	T	T	T
0.5044699910000007	0.4602699880000002	0.2462999970000008	F	F	F
0.4044926041796461	0.1740697487791431	0.3948774786829004	T	T	T
0.9981200100000011	0.4347699879999993	0.3632799979999960	F	F	F
0.9034992881090884	0.1499766022905579	0.5055122038545489	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999981	F	F	F
0.9317022305963254	0.3244792918712882	0.4620431069945942	T	T	T
0.4722500150000004	0.2798599899999985	0.2958799900000031	F	F	F
0.3746655486665419	0.4944820631676196	0.4472051096874451	T	T	T
0.7199699880000028	0.1401900050000009	0.3529999849999921	F	F	F
0.6262251004761087	0.3585059487915260	0.4898596761767965	T	T	T
0.7826200129999992	0.2548600140000019	0.2565700110000008	F	F	F
0.6905300340626273	0.4672496225403580	0.4027666441962392	T	T	T
0.2199700030000003	0.1401900050000009	0.3529999849999921	F	F	F
0.1251342984897629	0.3584770708095569	0.5021842008489932	T	T	T
0.2826200129999990	0.2548600140000019	0.2565700110000008	F	F	F
0.1878002923819026	0.4664692880995976	0.4080075618201723	T	T	T
0.8393200040000013	0.5101000069999984	0.3195700050000025	F	F	F
0.7330447389515468	0.7184046644977926	0.4664281257801511	T	T	T
0.6632599830000033	0.8849499820000017	0.2899999919999982	F	F	F
0.5582441146273787	0.5979020606331157	0.4371746002851556	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000002	F	F	F
0.5952060366611611	0.7772345081332208	0.3880378320558607	T	T	T
0.8070399759999990	0.8298199769999995	0.3692499999999903	F	F	F
0.6857864433947667	0.5410500196757352	0.5096375891398516	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000025	F	F	F
0.2304738751394796	0.7206329455345004	0.4679512249926405	T	T	T
0.1632599980000008	0.8849499820000017	0.2899999919999982	F	F	F
0.0684242264248751	0.5945014152673380	0.4411952304727391	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000002	F	F	F
0.0950258865557601	0.7762912677016740	0.3888887136527890	T	T	T
0.3070400060000011	0.8298199769999995	0.3692499999999903	F	F	F
0.1642948530706636	0.5115516499738247	0.6143950358204096	T	T	T
0.0044699999999943	0.9602699880000003	0.2462999970000008	F	F	F
0.9058650119533612	0.6694845310186693	0.3939071074033075	T	T	T
0.4981200100000009	0.9347699879999992	0.3632799979999960	F	F	F
0.3959133763453752	0.6523991045718305	0.5057420820447031	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999981	F	F	F
0.4332092504125467	0.8265188911682406	0.4629738021373707	T	T	T
0.9722499849999982	0.7798600200000010	0.2958799900000031	F	F	F
0.8795058955512678	0.9882852851084054	0.4489267712059704	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000008	F	F	F
0.4030574653240819	0.6724560314177604	0.3945309107488514	T	T	T
0.9981200100000013	0.9347699879999992	0.3632799979999960	F	F	F
0.9083961021298038	0.6508737157996487	0.5047377504400414	T	T	T
0.0303299999999976	0.6151900289999972	0.3136900069999981	F	F	F
0.9363650509990620	0.8228290632357521	0.4618994284665529	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3771786439892186	0.9915574582433395	0.4484681590843138	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999921	F	F	F

0.6289732546902269	0.8582371814115208	0.4904905811217805	T	T	T
0.7826200129999993	0.7548599839999994	0.2565700110000008	F	F	F
0.6899721722647082	0.9668810652758674	0.4027335787594753	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999921	F	F	F
0.1320381812421249	0.8610496820169258	0.4923362388938660	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000008	F	F	F
0.1893752570610225	0.9677781227489293	0.4029122911083061	T	T	T
0.8641700149999993	0.1591799999999992	0.3057599959999987	F	F	F
0.7766514978731512	0.3670186144850042	0.4617508809848827	T	T	T
0.63841998600000030	0.2358700039999988	0.3038099999999985	F	F	F
0.5347616665240106	0.4560009376715042	0.4635222057917131	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999984	F	F	F
0.5359464043875142	0.2294145532460612	0.4760781918559432	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000015	F	F	F
0.7810353841088503	0.0915536751540386	0.4381438127062893	T	T	T
0.3641700149999992	0.1591799999999992	0.3057599959999987	F	F	F
0.2707010333319547	0.3715757214199690	0.4586273161316251	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999985	F	F	F
0.0364114245925869	0.4484939775175914	0.4560882562673301	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999984	F	F	F
0.0420700111387075	0.2300932999355861	0.4731009991154867	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000015	F	F	F
0.2771447723127249	0.0946572006131846	0.4384240202485754	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999987	F	F	F
0.7785955489689931	0.8646315209103349	0.4616838108423149	T	T	T
0.63841998600000025	0.7358700039999988	0.3038099999999985	F	F	F
0.5360968748118609	0.9547145420807104	0.4625813106855130	T	T	T
0.6260200139999982	0.5126500129999982	0.3228900129999984	F	F	F
0.5415647765369292	0.7275265122666882	0.4764250488429472	T	T	T
0.8765599729999991	0.8823999760000019	0.2866800130000015	F	F	F
0.7817738264768267	0.5925506120337884	0.4387423790883414	T	T	T
0.3641700149999997	0.6591799859999981	0.3057599959999987	F	F	F
0.2780500076693855	0.8671996508153781	0.4609818182669179	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999985	F	F	F
0.0393719916587906	0.9534619220469975	0.4605574614912446	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999984	F	F	F
0.0570014197341026	0.7265118002229107	0.4813860023453534	T	T	T
0.3765600030000016	0.8823999760000019	0.2866800130000015	F	F	F
0.2712600793252651	0.5941874457582084	0.4400103039075332	T	T	T
0.0856659356267751	0.3828975900931219	0.5989172348302499	T	T	T
0.1383603164233267	0.3078544783329318	0.5911868993723672	T	T	T
-0.0013467788564462	0.3604241810816660	0.6105896176730905	T	T	T

Fe₅C₂(111)-HCO (FS)

1.0000000000000000		
12.3812999725000008	0.0000000000000000	0.0000000000000000
-2.0391083097000000	13.2888646689000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.8052997588999986

Fe C O H

80 33 1 1

Selective dynamics

Direct

0.8393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.7315459177419915	0.2196691680380670	0.4672514542211576	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999985	F	F	F
0.5592986808835400	0.0975793463827076	0.4375724336566208	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000003	F	F	F
0.5946854904612446	0.2770796836675340	0.3883595464320912	T	T	T
0.8070399759999987	0.3298200070000021	0.3692500000000010	F	F	F
0.6864828993535979	0.0424628911080218	0.5099789359370923	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.2314941850980434	0.2205559751350485	0.4665866533773758	T	T	T
0.1632599980000009	0.3849500119999973	0.2899999919999985	F	F	F
0.0609726622494108	0.0980501089216587	0.4389004701737360	T	T	T
0.1955399960000008	0.0652299970000030	0.2403199970000003	F	F	F
0.0951801562261676	0.2794743021141156	0.3892488249234736	T	T	T
0.3070400060000011	0.3298200070000021	0.3692500000000010	F	F	F
0.1881647884403714	0.0418428143680007	0.5105545713479845	T	T	T
0.0044699999999978	0.4602699880000003	0.2462999970000013	F	F	F
0.9049908566287358	0.1720786408627610	0.3941627391121238	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.4032390995929225	0.1526307326369036	0.5052101014342861	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999982	F	F	F
0.4340593873773517	0.3264492331104687	0.4622123142546497	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F

0.8789082197058395	0.4903598932595582	0.4478364676334429	T	T	T
0.5044699910000006	0.4602699880000003	0.2462999970000013	F	F	F
0.4046468859514517	0.1731696444456255	0.3941955103416498	T	T	T
0.9981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.9018314111727914	0.1519992079856040	0.5054957816998867	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999982	F	F	F
0.9330897827470030	0.3253864017039053	0.4618427646123395	T	T	T
0.4722500150000002	0.2798599899999985	0.2958799900000031	F	F	F
0.3777333476740573	0.4908225960673452	0.4478494907995602	T	T	T
0.7199699880000026	0.1401900050000009	0.3529999849999967	F	F	F
0.6300664925611229	0.3599948808544384	0.4911369998936413	T	T	T
0.7826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.6901263461668592	0.4673372390732889	0.4028471369690005	T	T	T
0.2199700030000002	0.1401900050000009	0.3529999849999967	F	F	F
0.1301638114978572	0.3596460409947501	0.4978903223768376	T	T	T
0.2826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.1881950254918619	0.4654158720131039	0.4039402703950477	T	T	T
0.8393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.7322809710418010	0.7194548385577675	0.4664955547158008	T	T	T
0.6632599830000032	0.8849499820000020	0.2899999919999985	F	F	F
0.5594489623279223	0.5975921390617905	0.4366044686005635	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000003	F	F	F
0.5946850748503488	0.7773365059375588	0.3881992620985764	T	T	T
0.8070399759999987	0.8298199769999997	0.3692500000000010	F	F	F
0.6856717547065269	0.5427732848925203	0.5098030919042696	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.2316394325518809	0.7201935081492261	0.4677337338564385	T	T	T
0.1632599980000009	0.8849499820000020	0.2899999919999985	F	F	F
0.0608472428788601	0.5969419742927435	0.4379942298378230	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000003	F	F	F
0.0950098316023689	0.7764470620041847	0.3887772586183523	T	T	T
0.3070400060000011	0.8298199769999997	0.3692500000000010	F	F	F
0.1962366369410659	0.5396418228729432	0.5114103444165177	T	T	T
0.0044699999999978	0.9602699880000003	0.2462999970000013	F	F	F
0.9049080315499283	0.6719796768175086	0.3939002356773182	T	T	T
0.4981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.4041623575183274	0.6506994069943592	0.5058839094664347	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999982	F	F	F
0.4344604149950150	0.8250529016824427	0.4626509205879894	T	T	T
0.9722499849999977	0.7798600200000010	0.2958799900000031	F	F	F
0.8786794877971228	0.9896540577240702	0.4487181394557047	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000013	F	F	F
0.4042156799549431	0.6723713089001054	0.3942102204349940	T	T	T
0.9981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.9048677500485733	0.6523718398810281	0.5052414453683554	T	T	T
0.0303299999999993	0.6151900289999972	0.3136900069999982	F	F	F
0.9354347041804039	0.8244974281456472	0.4624138533680344	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3783377222543705	0.9900099745093174	0.4491180170130796	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999967	F	F	F
0.6308686607670914	0.8593691741005687	0.4910104747507636	T	T	T
0.7826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.6900307934900392	0.9674928148951270	0.4026573657836983	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999967	F	F	F
0.1315339913281015	0.8606733780163883	0.4916250880374369	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.1898552176291052	0.9676071329686859	0.4026300076565552	T	T	T
0.8641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.7783532780660075	0.3667805781547116	0.4616085469606734	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999986	F	F	F
0.5376650539933762	0.4551143885785210	0.4619208189639777	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999985	F	F	F
0.5467222545421644	0.2286267409846821	0.4784362322029302	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000016	F	F	F
0.7798394443687274	0.0928492220381794	0.4379534528572405	T	T	T
0.3641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.2754374648848595	0.3678102707956286	0.4593340436918506	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999986	F	F	F
0.0388588162087208	0.4518426708127419	0.4572417131409224	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999985	F	F	F
0.0446169037647076	0.2291844169915348	0.4765032976112503	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000016	F	F	F
0.2799083293824752	0.0935637546346915	0.4380353966920925	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.7794759545559231	0.8653932554136039	0.4618633242348610	T	T	T

0.6384199860000024	0.7358700039999988	0.3038099999999986	F	F	F
0.5376875903544185	0.9541727870887919	0.4621672780740940	T	T	T
0.6260200139999981	0.5126500129999982	0.3228900129999985	F	F	F
0.5479449242138792	0.7277674170600962	0.4779084060428359	T	T	T
0.8765599729999991	0.8823999760000021	0.2866800130000016	F	F	F
0.7811104379939251	0.5928645339851980	0.4386451007193274	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.2790672604612144	0.8661412107786364	0.4616893834910996	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999986	F	F	F
0.0383138716148151	0.9540773447798445	0.4611178493391864	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999985	F	F	F
0.0512057177235364	0.7276119353832994	0.4795313092548144	T	T	T
0.3765600030000016	0.8823999760000021	0.2866800130000016	F	F	F
0.2790517236999501	0.5940569359565202	0.4379002346847587	T	T	T
0.1647034667774537	0.4465132488847930	0.5799290096237147	T	T	T
0.1758921827519022	0.3557895875856351	0.5917496688584898	T	T	T
0.1199282433465481	0.4871026687203855	0.6164009185595120	T	T	T

Fe₅C₂(111)-CH+O (TS)

```

1.0000000000000000
12.3812999725000008  0.0000000000000000  0.0000000000000000
-2.0391083097000000  13.2888646689000005  0.0000000000000000
0.0000000000000000  0.0000000000000000  20.8052997588999986

```

Fe C O H

80 33 1 1

Selective dynamics

Direct

0.8393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.7280665727324105	0.2210556906832286	0.4673867727268514	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999985	F	F	F
0.5594946800703304	0.0980335614437835	0.4377492791865651	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000003	F	F	F
0.5934394472835842	0.2775641013561835	0.3880003760462235	T	T	T
0.8070399759999987	0.3298200070000021	0.3692500000000010	F	F	F
0.6881537292174220	0.0414371718380609	0.5103022349215560	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.2411538232512968	0.2275875704396796	0.4766779480574528	T	T	T
0.1632599800000009	0.3849500119999973	0.2899999919999985	F	F	F
0.0611269951406648	0.0995284542208703	0.4376863628467376	T	T	T
0.1955399960000008	0.0652299970000030	0.2403199970000003	F	F	F
0.0961885925725678	0.2764568056427489	0.3891672990067302	T	T	T
0.3070400060000011	0.3298200070000021	0.3692500000000010	F	F	F
0.1840841388603752	0.0441636947788218	0.5104225985546811	T	T	T
0.0044699999999978	0.4602699880000003	0.2462999970000013	F	F	F
0.9046753367130937	0.1724225901515071	0.3947842854506897	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.4082836513131697	0.1547668707634332	0.5060786190400526	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999982	F	F	F
0.4357978107816913	0.3282567662902397	0.4616300499742397	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F
0.8796508957857514	0.4932558467652192	0.4468050068130374	T	T	T
0.5044699910000006	0.4602699880000003	0.2462999970000013	F	F	F
0.4031054989227349	0.1732378485031746	0.3946144822173320	T	T	T
0.9981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.8889324900554767	0.1477412717350223	0.5073914660256119	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999982	F	F	F
0.9260888017365504	0.3286651427755410	0.4632319588941122	T	T	T
0.4722500150000002	0.2798599899999985	0.2958799900000031	F	F	F
0.3793368773611255	0.4923894102746828	0.4465171340865522	T	T	T
0.7199699880000026	0.1401900050000009	0.3529999849999967	F	F	F
0.6299322957250011	0.3623477970332467	0.4915693606833259	T	T	T
0.7826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.6897901638102105	0.4681439847870629	0.4031261108452284	T	T	T
0.2199700030000002	0.1401900050000009	0.3529999849999967	F	F	F
0.1196174583892695	0.3501247503684228	0.4980861819757430	T	T	T
0.2826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.1851182768759130	0.4663351212918533	0.4056370696343056	T	T	T
0.8393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.7344487637779743	0.7207273644348386	0.4659982003224249	T	T	T
0.6632599830000032	0.3849499820000020	0.2899999919999985	F	F	F
0.5592804935989132	0.5990415240511886	0.4364088220782772	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000003	F	F	F
0.5948050379630146	0.7773101024055245	0.3879388274934722	T	T	T

0.8070399759999987	0.8298199769999997	0.3692500000000010	F	F	F
0.6858805346148512	0.5451385073830577	0.5099707199361576	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.2314759546712492	0.7207404238470878	0.4690081393260723	T	T	T
0.1632599980000009	0.8849499820000020	0.2899999919999985	F	F	F
0.0672793665974555	0.5952486908695226	0.4422980233290967	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000003	F	F	F
0.0949379158631359	0.7765040749160578	0.3891358964741829	T	T	T
0.3070400060000011	0.8298199769999997	0.3692500000000010	F	F	F
0.2221221342020080	0.5123942630236830	0.5171787038175508	T	T	T
0.0044699999999978	0.9602699880000003	0.2462999970000013	F	F	F
0.9060726650265867	0.6716799966235936	0.3940693461813514	T	T	T
0.4981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.4001903394483161	0.6506286834698055	0.5061538165811346	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999982	F	F	F
0.4334852749919096	0.8267788034254460	0.4631735568856252	T	T	T
0.9722499849999977	0.7798600200000010	0.2958799900000031	F	F	F
0.8780453118593579	0.9893698228581381	0.4486345765384883	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000013	F	F	F
0.4031765911245885	0.6735197257780440	0.3946842242210697	T	T	T
0.9981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.9081064710961695	0.6539658889395481	0.5053225422588924	T	T	T
0.0303299999999993	0.6151900289999972	0.3136900069999982	F	F	F
0.9373060981263713	0.8254251187528817	0.4631847653885279	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3781032222939366	0.9921245071787851	0.4492305128942342	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999967	F	F	F
0.6293052489670614	0.8589970774985327	0.4907565178895658	T	T	T
0.7826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.6895749339682723	0.9671678144802295	0.4027023041539445	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999967	F	F	F
0.1321046006159183	0.8632504311035462	0.4922600245424919	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.1901475484539785	0.9687170878811350	0.4032148186481136	T	T	T
0.8641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.7763123971970532	0.3695298545972313	0.4612859544412265	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999986	F	F	F
0.5382678273170721	0.4577112549933329	0.4622866087056362	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999985	F	F	F
0.5504839804725438	0.2298230529512489	0.4787813731129131	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000016	F	F	F
0.7773517192637273	0.0930616898669233	0.4365443614444034	T	T	T
0.3641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.2692167631884779	0.3724967836235953	0.4535463410698458	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999986	F	F	F
0.0339809023466613	0.4500793235882906	0.4572367735315547	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999985	F	F	F
0.0179722631642324	0.2243018856501442	0.4685969775310316	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000016	F	F	F
0.2777473462847876	0.0983644125426704	0.4402439314501034	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.7792658215460349	0.8661106143385547	0.4620214137193375	T	T	T
0.6384199860000024	0.7358700039999988	0.3038099999999986	F	F	F
0.5374140673453520	0.9552840098313747	0.4625838010144164	T	T	T
0.6260200139999981	0.5126500129999982	0.3228900129999985	F	F	F
0.5442166063669909	0.7278013812919319	0.4769631793192245	T	T	T
0.8765599729999991	0.8823999760000021	0.2866800130000016	F	F	F
0.7812407631483375	0.5942498687498542	0.4384768709954378	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.2787960478858619	0.8673854122481393	0.4611545286089432	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999986	F	F	F
0.0383162220035114	0.9567721220964486	0.4624427549085968	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999985	F	F	F
0.0563570005031553	0.7282671297790803	0.4809375004872199	T	T	T
0.3765600030000016	0.8823999760000021	0.2866800130000016	F	F	F
0.2739680944377841	0.5947585102816907	0.4384035961161615	T	T	T
0.1791775075008920	0.4056199502631960	0.5740017678114196	T	T	T
0.1935662308294866	0.2669460253245661	0.5550585517820323	T	T	T
0.1623562847495734	0.3861304930027898	0.6246292067148054	T	T	T

Fe₅C₂(111)-CH+O (FS)

1.0000000000000000

12.3812999725000008 0.0000000000000000 0.0000000000000000

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-2.0391083097000000 13.2888646689000005 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.8052997588999986
Fe C O H
80 33 1 1
Selective dynamics
Direct
0.8393200040000011 0.0101000000000013 0.3195700050000028 F F F
0.7349753518156561 0.2199210718774439 0.4659611603556307 T T T
0.6632599830000032 0.3849500119999973 0.2899999919999985 F F F
0.5594968109421175 0.0972093058517736 0.4373976949642228 T T T
0.6955400109999985 0.0652299970000030 0.2403199970000003 F F F
0.5959814029229733 0.2772180000418393 0.3881201034269787 T T T
0.8070399759999987 0.3298200070000021 0.3692500000000010 F F F
0.6881193172756132 0.0441412026963354 0.5097593122901027 T T T
0.3393200040000011 0.0101000000000013 0.3195700050000028 F F F
0.2302803665714233 0.2207976114795161 0.4707247018247626 T T T
0.1632599800000009 0.3849500119999973 0.2899999919999985 F F F
0.0612104088613705 0.0990365328923217 0.4389728990948308 T T T
0.1955399960000008 0.0652299970000030 0.2403199970000003 F F F
0.0960265717675807 0.2773717387440463 0.3890361298024930 T T T
0.3070400060000011 0.3298200070000021 0.3692500000000010 F F F
0.1955591470778220 0.0438172705327404 0.5090198495081864 T T T
0.0044699999999978 0.4602699880000003 0.2462999970000013 F F F
0.9056775825069093 0.1721894567307616 0.3941609532307577 T T T
0.4981200100000009 0.4347699879999993 0.3632799980000030 F F F
0.3989576277350240 0.1557591634566863 0.5108567751011964 T T T
0.5303300019999995 0.1151899990000018 0.3136900069999982 F F F
0.4310219313780633 0.3285690848751357 0.4615805464800040 T T T
0.9722499849999977 0.2798599899999985 0.2958799900000031 F F F
0.8787338410705586 0.4906430925725895 0.4464265175293097 T T T
0.5044699910000006 0.4602699880000003 0.2462999970000013 F F F
0.4056049037306125 0.1725963780122289 0.3958150145020661 T T T
0.9981200100000009 0.4347699879999993 0.3632799980000030 F F F
0.9034493338661553 0.1515525481109199 0.5060106490793810 T T T
0.0303299999999993 0.1151899990000018 0.3136900069999982 F F F
0.9330871562523482 0.3254105632621091 0.4625430913976560 T T T
0.4722500150000002 0.2798599899999985 0.2958799900000031 F F F
0.3763810990351453 0.4929356211709824 0.4470946072842206 T T T
0.7199699880000026 0.1401900050000009 0.3529999849999967 F F F
0.6271417289239603 0.3571996048006381 0.4904963125884096 T T T
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0.6897259031290413 0.4670464436364453 0.4029986409718617 T T T
0.2199700030000002 0.1401900050000009 0.3529999849999967 F F F
0.1285489847353407 0.3641467690394832 0.4978885060468246 T T T
0.2826200129999989 0.2548600140000019 0.2565700110000009 F F F
0.1885119316961032 0.4673646092317438 0.4041624118029407 T T T
0.8393200040000011 0.5101000069999984 0.3195700050000028 F F F
0.7338338018108266 0.7189806522473762 0.4663744860883275 T T T
0.6632599830000032 0.8849499820000020 0.2899999919999985 F F F
0.5591087651979547 0.5975644073966114 0.4370101450006620 T T T
0.6955400109999985 0.5652300120000007 0.2403199970000003 F F F
0.5946826546566588 0.7766955437560085 0.3883043210859322 T T T
0.8070399759999987 0.8298199769999997 0.3692500000000010 F F F
0.6851336022315535 0.5411621539089421 0.5093453088968730 T T T
0.3393200040000011 0.5101000069999984 0.3195700050000028 F F F
0.2329739721259907 0.7213632164992917 0.4668428632414128 T T T
0.1632599800000009 0.8849499820000020 0.2899999919999985 F F F
0.0641039594877043 0.5959964817003577 0.4406310735599213 T T T
0.1955399960000008 0.5652300120000007 0.2403199970000003 F F F
0.0955033943950165 0.7765401598714351 0.3891297418328786 T T T
0.3070400060000011 0.8298199769999997 0.3692500000000010 F F F
0.1995620081942198 0.5365896424953237 0.5166730344544415 T T T
0.0044699999999978 0.9602699880000003 0.2462999970000013 F F F
0.9052528684819592 0.6717329163308013 0.3939384787875080 T T T
0.4981200100000009 0.9347699879999993 0.3632799980000030 F F F
0.4060874393942245 0.6523414238503481 0.5054435915372684 T T T
0.5303300019999995 0.6151900289999972 0.3136900069999982 F F F
0.4363289036529397 0.8258558512662867 0.4630674215461277 T T T
0.9722499849999977 0.7798600200000010 0.2958799900000031 F F F
0.8797275650392976 0.9889576385841443 0.4496177161218920 T T T
0.5044699910000006 0.9602699880000003 0.2462999970000013 F F F
0.4038385221261562 0.6730912344623934 0.3940300692946734 T T T
0.9981200100000009 0.9347699879999993 0.3632799980000030 F F F
0.9076853538354422 0.6526895260091962 0.5051061727994359 T T T
0.0303299999999993 0.6151900289999972 0.3136900069999982 F F F

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0.9380672686397578	0.8246532034847696	0.4623077229172451	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3792182976358512	0.9906865179497636	0.4502968366421261	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999967	F	F	F
0.6332910210787143	0.8598670155022576	0.4910289954439506	T	T	T
0.7826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.6905812790828261	0.9673344905779712	0.4025292190648163	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999967	F	F	F
0.1338608015782111	0.8613166939074921	0.4926558522275962	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.1882098914413405	0.9663686698641467	0.4024355247180409	T	T	T
0.8641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.7768758940107884	0.3676397646467411	0.4613618073708796	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999986	F	F	F
0.5358969623282162	0.4545698149626723	0.4618670172762991	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999985	F	F	F
0.5364994042676319	0.2271341745280208	0.4746891865071433	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000016	F	F	F
0.7816436978550552	0.0919595769246312	0.4377222457358809	T	T	T
0.3641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.2734411814511362	0.3692011096808467	0.4580097330837534	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999986	F	F	F
0.0349214383448291	0.4513973925281613	0.4554843664912173	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999985	F	F	F
0.0444731318890479	0.2315545576785835	0.4781981803918121	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000016	F	F	F
0.2788749832506748	0.0906154567443317	0.4321227901472563	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.7823452388242833	0.8641206108597200	0.4629226434123069	T	T	T
0.6384199860000024	0.7358700039999988	0.3038099999999986	F	F	F
0.5403717099384207	0.9549255057455384	0.4627083343517264	T	T	T
0.6260200139999981	0.5126500129999982	0.3228900129999985	F	F	F
0.5520655236343613	0.7281743935984785	0.4787325344229305	T	T	T
0.8765599729999991	0.8823999760000021	0.2866800130000016	F	F	F
0.7816214782622051	0.5926359000611112	0.4386357014531751	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.2819310672580807	0.8653013609212722	0.4631326694688075	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999986	F	F	F
0.0429608663637711	0.9553257816408731	0.4610964013530381	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999985	F	F	F
0.0561435571620640	0.7282137820705988	0.4805279636228952	T	T	T
0.3765600030000016	0.8823999760000021	0.2866800130000016	F	F	F
0.2771232068118964	0.5955848294446058	0.4383190939385796	T	T	T
0.1616337029607910	0.4260890247754172	0.5717846273772246	T	T	T
0.2659293223695718	0.1489369376397066	0.5564868132765273	T	T	T
0.1621716936682150	0.4061662482372044	0.6231780063266552	T	T	T

COH formation and dissociation on Fe₅C₂(111)

Fe₅C₂(111)-COH (TS)

1.0000000000000000		
12.3812999725000008	0.0000000000000000	0.0000000000000000
-2.0391083097000000	13.2888646689000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.8052997588999986

Fe C O H

80 33 1 1

Selective dynamics

Direct

0.8393200040000012	0.0101000000000013	0.3195700050000025	F	F	F
0.7309505340032844	0.2197620989399686	0.4676375312461137	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999982	F	F	F
0.5598130308105935	0.0979594498747573	0.4379547509410792	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000002	F	F	F
0.5944352123590986	0.2770294899532393	0.3884276365428103	T	T	T
0.8070399759999989	0.3298200070000021	0.3692499999999954	F	F	F
0.6868037163637496	0.0414401345060822	0.5104959336629202	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000025	F	F	F
0.2338075383311594	0.2211324626768963	0.4666443463149787	T	T	T
0.1632599980000009	0.3849500119999973	0.2899999919999982	F	F	F
0.0610388477807132	0.0976678065740823	0.4394456956218922	T	T	T
0.1955399960000009	0.0652299970000030	0.2403199970000002	F	F	F
0.0948211846365182	0.2787682151520656	0.3889679955234422	T	T	T
0.3070400060000012	0.3298200070000021	0.3692499999999954	F	F	F
0.1878300464994165	0.0419089568022868	0.5107982971925630	T	T	T

0.0044699999999969	0.4602699880000002	0.2462999970000008	F	F	F
0.9052691580902700	0.1720769262955559	0.3945460692371051	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799979999974	F	F	F
0.4033529124953155	0.1529541914581140	0.5054324536380725	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999981	F	F	F
0.4334770549082303	0.3268475360312856	0.4626984883556748	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F
0.8779328044889289	0.4912607090773847	0.4469878229440092	T	T	T
0.5044699910000007	0.4602699880000002	0.2462999970000008	F	F	F
0.4045564584994046	0.1727088921432210	0.3942279250428666	T	T	T
0.9981200100000011	0.4347699879999993	0.3632799979999974	F	F	F
0.8993680193202411	0.1516103111023220	0.5060097656847964	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999981	F	F	F
0.9300546235920069	0.3257186526076239	0.4620409150585743	T	T	T
0.4722500150000004	0.2798599899999985	0.2958799900000031	F	F	F
0.3772698192251311	0.4911431224258505	0.4472150214763124	T	T	T
0.7199699880000028	0.1401900050000009	0.3529999849999921	F	F	F
0.6293011053487628	0.3603998571477534	0.4912150418724656	T	T	T
0.7826200129999992	0.2548600140000019	0.2565700110000008	F	F	F
0.6895113972443152	0.4675780410544332	0.4029161789598850	T	T	T
0.2199700030000003	0.1401900050000009	0.3529999849999921	F	F	F
0.1274338487422599	0.3591352569431256	0.4973847330679946	T	T	T
0.2826200129999990	0.2548600140000019	0.2565700110000008	F	F	F
0.1885907268016423	0.4655895143950371	0.4036059573900076	T	T	T
0.8393200040000013	0.5101000069999984	0.3195700050000025	F	F	F
0.7328703305224290	0.7196144549053416	0.4667766073471106	T	T	T
0.6632599830000033	0.8849499820000017	0.2899999919999982	F	F	F
0.5592615435086019	0.5978664155732945	0.4369509053067152	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000002	F	F	F
0.5949174194732845	0.7772928555751863	0.3880727663200831	T	T	T
0.8070399759999990	0.8298199769999995	0.3692499999999954	F	F	F
0.6855009846140931	0.5431211990806804	0.5100180234739984	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000025	F	F	F
0.2333162170347593	0.7215528459944119	0.4671836623828416	T	T	T
0.1632599980000008	0.8849499820000017	0.2899999919999982	F	F	F
0.0616051824096944	0.5961531550722999	0.4401233767212715	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000002	F	F	F
0.0949621011782601	0.7769742434868167	0.3886743821328135	T	T	T
0.3070400060000011	0.8298199769999995	0.3692499999999954	F	F	F
0.1970604835366089	0.5394865641374798	0.5102094154517598	T	T	T
0.0044699999999960	0.9602699880000003	0.2462999970000008	F	F	F
0.9055735905617740	0.6719425448554174	0.3941031088103634	T	T	T
0.4981200100000009	0.9347699879999992	0.3632799979999974	F	F	F
0.3990954833755596	0.6502053093594532	0.5065328233830864	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999981	F	F	F
0.4333119934082720	0.8265024625366660	0.4626604867333170	T	T	T
0.9722499849999982	0.7798600200000010	0.2958799900000031	F	F	F
0.8779679059950022	0.9905527014173330	0.4485182193634757	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000008	F	F	F
0.4052583368780702	0.6726400769365997	0.3945350289747330	T	T	T
0.9981200100000013	0.9347699879999992	0.3632799979999974	F	F	F
0.9031326173107262	0.6526243368768549	0.5054530140750033	T	T	T
0.0303299999999984	0.6151900289999972	0.3136900069999981	F	F	F
0.9341938533757644	0.8254511268289507	0.4623117898871381	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3786032212882852	0.9912732849317177	0.4486928210925819	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999921	F	F	F
0.6293058120486005	0.8584957530991217	0.4909484908931581	T	T	T
0.7826200129999993	0.7548599839999994	0.2565700110000008	F	F	F
0.6896331537329400	0.9670994587523496	0.4028751901872972	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999921	F	F	F
0.1304913319809816	0.8606034693643769	0.4913608747716743	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000008	F	F	F
0.1898871098540334	0.9675941504170072	0.4025840733990149	T	T	T
0.8641700149999993	0.1591799999999992	0.3057599959999987	F	F	F
0.7768598542697351	0.3674162160211198	0.4612443916225925	T	T	T
0.6384199860000030	0.2358700039999988	0.3038099999999985	F	F	F
0.5366791968388472	0.4554193908216837	0.4622119237368804	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999984	F	F	F
0.5463749895046087	0.2290245988085474	0.4786679742783803	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000015	F	F	F
0.7784973563225041	0.0932003510175454	0.4376175367531219	T	T	T
0.3641700149999992	0.1591799999999992	0.3057599959999987	F	F	F
0.2746015953599820	0.3677615448430808	0.4599979496121902	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999985	F	F	F

0.0346805176689154	0.4513602116286581	0.4577915259800089	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999984	F	F	F
0.0399375713884801	0.2285905512021547	0.4747129615349865	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000015	F	F	F
0.2792482049500830	0.0936983550156322	0.4380400737709889	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999987	F	F	F
0.7782420779554953	0.8662915610800153	0.4618541905732676	T	T	T
0.6384199860000025	0.7358700039999988	0.3038099999999985	F	F	F
0.5376025034374653	0.9542919417584279	0.4620879046041577	T	T	T
0.6260200139999982	0.5126500129999982	0.3228900129999984	F	F	F
0.5417503296086342	0.7275109512928248	0.4768547615794451	T	T	T
0.8765599729999991	0.8823999760000019	0.2866800130000015	F	F	F
0.7800742711323418	0.5931057030699867	0.4380043869846206	T	T	T
0.3641700149999997	0.6591799859999981	0.3057599959999987	F	F	F
0.2787461612647763	0.8672705310772030	0.4619796578134256	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999985	F	F	F
0.0371921321158887	0.9540750470120581	0.4611579744869328	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999984	F	F	F
0.0478012230100561	0.7286852229650508	0.4786632034383170	T	T	T
0.3765600030000016	0.8823999760000019	0.2866800130000015	F	F	F
0.2789039981986584	0.5944106989699488	0.4366270247787796	T	T	T
0.1742845879675779	0.4075532946803413	0.5706058472880338	T	T	T
0.2358285363310015	0.4580617792294519	0.6125926789240327	T	T	T
0.2895017525375599	0.5203912745063469	0.5909254671321537	T	T	T

Fe₅C₂(111)-COH (FS)

1.0000000000000000		
12.3812999725000008	0.0000000000000000	0.0000000000000000
-2.0391083097000000	13.2888646689000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.8052997588999986

Fe C O H

80 33 1 1

Selective dynamics

Direct

0.8393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.7332187870027871	0.2195994958724490	0.4670458856099152	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999985	F	F	F
0.5589064979792520	0.0981737652835249	0.4380005754585024	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000003	F	F	F
0.5950783460436461	0.2768762962619756	0.3884738234204870	T	T	T
0.8070399759999987	0.3298200070000021	0.3692500000000010	F	F	F
0.6861359169853547	0.0428471240416903	0.5097667783593667	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.2288858480025340	0.2214941182587292	0.4676247947819981	T	T	T
0.1632599980000009	0.3849500119999973	0.2899999919999985	F	F	F
0.0604646833640541	0.0984712645473532	0.4386699649479208	T	T	T
0.1955399960000008	0.0652299970000030	0.2403199970000003	F	F	F
0.0938578841944866	0.2773418210953211	0.3883378643160139	T	T	T
0.3070400060000011	0.3298200070000021	0.3692500000000010	F	F	F
0.1885470522559067	0.0438715557969707	0.5106096924697257	T	T	T
0.0044699999999978	0.4602699880000003	0.2462999970000013	F	F	F
0.9045511939843639	0.1718545705813353	0.3940848939106238	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.4018400430590081	0.1526637722440218	0.5051453523397300	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999982	F	F	F
0.4335147107315137	0.3269172179222104	0.4625015061161241	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F
0.8791098967817658	0.4898949522054358	0.4473295894245845	T	T	T
0.5044699910000006	0.4602699880000003	0.2462999970000013	F	F	F
0.4044130378380724	0.1739189091741536	0.3942754675573069	T	T	T
0.9981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.9057597638575112	0.1527007408366426	0.5054336334500836	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999982	F	F	F
0.9348189945331568	0.3242765956941309	0.4625879378843056	T	T	T
0.4722500150000002	0.2798599899999985	0.2958799900000031	F	F	F
0.3773272094395251	0.4917233992766913	0.4474336257663720	T	T	T
0.7199699880000026	0.1401900050000009	0.3529999849999967	F	F	F
0.6302369391530636	0.3596328154295297	0.4909214495612750	T	T	T
0.7826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.6901294587335619	0.4677638858241037	0.4028036058633668	T	T	T
0.2199700030000002	0.1401900050000009	0.3529999849999967	F	F	F
0.1319366400941605	0.3630620277859697	0.4971523817284450	T	T	T
0.2826200129999989	0.2548600140000019	0.2565700110000009	F	F	F

0.1894072546709699	0.4673521276886893	0.4034519220547572	T	T	T
0.8393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.7329100743658695	0.7190013378839244	0.4665344474799750	T	T	T
0.6632599830000032	0.8849499820000020	0.2899999919999985	F	F	F
0.5589354187609958	0.5976824818933520	0.4368590767920049	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000003	F	F	F
0.5948979432418211	0.7768693404591934	0.3882747878571678	T	T	T
0.8070399759999987	0.8298199769999997	0.3692500000000010	F	F	F
0.6854467503753202	0.5430764107556495	0.5096727971266590	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.2318294695595995	0.7205636181749389	0.4679849460486884	T	T	T
0.1632599800000009	0.8849499820000020	0.2899999919999985	F	F	F
0.0643505724119739	0.5958898223787339	0.4400163049466701	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000003	F	F	F
0.0948568714199717	0.7764389490997285	0.3889151964636953	T	T	T
0.3070400060000011	0.8298199769999997	0.3692500000000010	F	F	F
0.1999062057770741	0.5356363942113733	0.5158891271627140	T	T	T
0.0044699999999978	0.9602699880000003	0.2462999970000013	F	F	F
0.9054735007321092	0.6715625332064793	0.3938984098782272	T	T	T
0.4981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.4033785164797034	0.6504884691844606	0.5052255867722645	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999982	F	F	F
0.4348915776021134	0.8255295870231296	0.4627753523457405	T	T	T
0.9722499849999977	0.7798600200000010	0.2958799900000031	F	F	F
0.8789043294462789	0.9893003751409172	0.4487040721529970	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000013	F	F	F
0.4036970923367476	0.6729088205888374	0.3940612221685326	T	T	T
0.9981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.9072679399931368	0.6525842199106600	0.5048981044657648	T	T	T
0.0303299999999993	0.6151900289999972	0.3136900069999982	F	F	F
0.9364060647164574	0.8243874297294369	0.4624731930651242	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3778734820247963	0.9904322127804528	0.4493342239791578	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999967	F	F	F
0.6314169198599809	0.8593354751556154	0.4909507848073164	T	T	T
0.7826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.6899819512829489	0.9676364679303049	0.4026472071433778	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999967	F	F	F
0.1324214722209660	0.8618722343078659	0.4917822488367903	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.1896915578730874	0.9679039198700122	0.4026714030022164	T	T	T
0.8641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.7791931353207275	0.3663343260547425	0.4619579858469209	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999986	F	F	F
0.5376253281867586	0.4547898656270223	0.4617537992532078	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999985	F	F	F
0.5453171751379856	0.2291821030226555	0.4783637639463339	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000016	F	F	F
0.7808826392952452	0.0925780416912674	0.4385062091427563	T	T	T
0.3641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.2777090797414762	0.3673265217123576	0.4600868671369088	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999986	F	F	F
0.0374237513472980	0.4512887716109683	0.4562021374031760	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999985	F	F	F
0.0514578909007995	0.2304744354217396	0.4800797926339773	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000016	F	F	F
0.2790998694945231	0.0945752334851213	0.4376766689529848	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.7801373366980924	0.8648264500696254	0.4620921733590863	T	T	T
0.6384199860000024	0.7358700039999988	0.3038099999999986	F	F	F
0.5384095201952374	0.9543275863584013	0.4621656630954024	T	T	T
0.6260200139999981	0.5126500129999982	0.3228900129999985	F	F	F
0.5479307123978684	0.7280699695106105	0.4781943686123930	T	T	T
0.8765599729999991	0.8823999760000021	0.2866800130000016	F	F	F
0.7818946718376121	0.5925341165489199	0.4387957055449784	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.2800413390569404	0.8659207859858614	0.4623779211530209	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999986	F	F	F
0.0387411872582842	0.9546463677502457	0.4611800369940126	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999985	F	F	F
0.0547741847034255	0.7281768617188896	0.4806633143900296	T	T	T
0.3765600030000016	0.8823999760000021	0.2866800130000016	F	F	F
0.2761058202999924	0.5947263763739480	0.4381012840493813	T	T	T
0.1737649409091464	0.4222185654562854	0.5723922405704238	T	T	T

0.1896219340628797	0.3945131365103421	0.6322612253531175	T	T	T
0.2229076775730338	0.4524777930718739	0.6579243931143346	T	T	T

Fe₅C₂(111)-C+OH (TS)

1.0000000000000000		
12.3812999725000008	0.0000000000000000	0.0000000000000000
-2.0391083097000000	13.2888646689000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.8052997588999986

Fe C O H

80 33 1 1

Selective dynamics

Direct

0.8393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.7347395353742874	0.2203842726582324	0.4665874110836228	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999985	F	F	F
0.5591827173936526	0.0986101796175566	0.4379756841711330	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000003	F	F	F
0.5948493459096568	0.2767810954976479	0.3885913496578703	T	T	T
0.8070399759999987	0.3298200070000021	0.3692500000000010	F	F	F
0.6871937219679392	0.0440273056403275	0.5101457416847154	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.2242526198395785	0.2234425318410338	0.4715495358534546	T	T	T
0.1632599980000009	0.3849500119999973	0.2899999919999985	F	F	F
0.0600034380898221	0.1007994756046095	0.4392643963895463	T	T	T
0.1955399960000008	0.0652299970000030	0.2403199970000003	F	F	F
0.0967143611859473	0.2819385544782828	0.3910490280013753	T	T	T
0.3070400060000011	0.3298200070000021	0.3692500000000010	F	F	F
0.1881183984809678	0.0437784516478423	0.5106108434614038	T	T	T
0.0044699999999978	0.4602699880000003	0.2462999970000013	F	F	F
0.9045554131324385	0.1734471267592721	0.3941564344313973	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.4009059260361927	0.1552233012739464	0.5056099796005247	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999982	F	F	F
0.4326394490099436	0.3266400060348380	0.4620165636568724	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F
0.8793802825817048	0.4874439021766990	0.4474366232240226	T	T	T
0.5044699910000006	0.4602699880000003	0.2462999970000013	F	F	F
0.4041276908401741	0.1735660428823314	0.3943010531660671	T	T	T
0.9981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.9073233381095333	0.1527013859565063	0.5054618726843103	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999982	F	F	F
0.9428455894807175	0.3246307669232952	0.4649153857501457	T	T	T
0.4722500150000002	0.2798599899999985	0.2958799900000031	F	F	F
0.3770182964243105	0.4919218149795362	0.4475387716954491	T	T	T
0.7199699880000026	0.1401900050000009	0.3529999849999967	F	F	F
0.6302408740986957	0.3591632004745752	0.4911396860688346	T	T	T
0.7826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.6898621234450139	0.4672713777487996	0.4028593068132812	T	T	T
0.2199700030000002	0.1401900050000009	0.3529999849999967	F	F	F
0.1426501766180973	0.3734423307452372	0.5083068914382121	T	T	T
0.2826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.1892661212623483	0.4696760112423089	0.4061724103490536	T	T	T
0.8393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.7331818542240779	0.7181669014713654	0.4666768212128559	T	T	T
0.6632599830000032	0.8849499820000020	0.2899999919999985	F	F	F
0.5577847054607897	0.5975227996034201	0.4377600379876210	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000003	F	F	F
0.5957120631431227	0.7770395853472597	0.3888216570319034	T	T	T
0.8070399759999987	0.8298199769999997	0.3692500000000010	F	F	F
0.6859150702372245	0.5432934853457643	0.5095363677637206	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.2347880028145961	0.7249655193278034	0.4647571798452572	T	T	T
0.1632599980000009	0.8849499820000020	0.2899999919999985	F	F	F
0.0582624061720008	0.5985667526026749	0.4365537994342751	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000003	F	F	F
0.0949952206265834	0.7772461070873813	0.3885479590148084	T	T	T
0.3070400060000011	0.8298199769999997	0.3692500000000010	F	F	F
0.1815336372284525	0.5539713281884800	0.5117559836300533	T	T	T
0.0044699999999978	0.9602699880000003	0.2462999970000013	F	F	F
0.9037965855196949	0.6718671260685811	0.3938016983019502	T	T	T
0.4981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.4083550059714744	0.6542071694241104	0.5035951318024025	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999982	F	F	F
0.4377218865921206	0.8276809802285037	0.4634742535388279	T	T	T
0.9722499849999977	0.7798600200000010	0.2958799900000031	F	F	F

0.8794778075165959	0.9889360276528664	0.4499049161506056	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000013	F	F	F
0.4046845663939431	0.6754588674168582	0.3934224369482084	T	T	T
0.9981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.9079354096939629	0.6517781726147923	0.5047923031156040	T	T	T
0.0303299999999993	0.6151900289999972	0.3136900069999982	F	F	F
0.9372890553435396	0.8237792154459722	0.4623469337471012	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3785755679849499	0.9928492087652574	0.4489419789165572	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999967	F	F	F
0.6349417696803646	0.8606918021217015	0.4917437298700280	T	T	T
0.7826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.6903099687613761	0.9681293949750731	0.4026558519665001	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999967	F	F	F
0.1330689705154356	0.8626774014816088	0.4913756486252952	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.1903205481435941	0.9689498408633300	0.4029738181718694	T	T	T
0.8641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.7804667449433583	0.3661112995733347	0.4629902481008507	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999986	F	F	F
0.5377507003720704	0.4540511008385349	0.4614874053781109	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999985	F	F	F
0.5458362138484234	0.2288071959370675	0.4782255924711368	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000016	F	F	F
0.7815753864099780	0.0927757739432551	0.4385754372697901	T	T	T
0.3641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.2742912012369980	0.3667941672205490	0.4573749896197538	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999986	F	F	F
0.0430586712687793	0.4535730591890553	0.4574299136376447	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999985	F	F	F
0.0575017257813435	0.2330753253176921	0.4829352997061087	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000016	F	F	F
0.2777287427712032	0.0987090776897299	0.4389427683179135	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.7817967026836804	0.8638359297605874	0.4620356050123120	T	T	T
0.6384199860000024	0.7358700039999988	0.3038099999999986	F	F	F
0.5417831281547932	0.9551333421058302	0.4613745684590595	T	T	T
0.6260200139999981	0.5126500129999982	0.3228900129999985	F	F	F
0.5533312935416614	0.7295743593479710	0.4802150197189291	T	T	T
0.8765599729999991	0.8823999760000021	0.2866800130000016	F	F	F
0.7828843652535049	0.5910448081507906	0.4388157562298156	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.2826160690993513	0.8676937093416619	0.4630835037770750	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999986	F	F	F
0.0395465390164971	0.9557180617640315	0.4613242198330176	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999985	F	F	F
0.0580103629683543	0.7283602687998693	0.4806148541312861	T	T	T
0.3765600030000016	0.8823999760000021	0.2866800130000016	F	F	F
0.2809909142669509	0.5960915666348919	0.4394378358502355	T	T	T
0.1984483111589852	0.4624878202830804	0.5753049158216107	T	T	T
0.2653936153261394	0.5397488047460118	0.6074883655889087	T	T	T
0.3442017658751743	0.5552097506446506	0.5926713013741979	T	T	T

Fe₅C₂(111)-C+OH (FS)

1.0000000000000000		
12.3812999725000008	0.0000000000000000	0.0000000000000000
-2.0391083097000000	13.2888646689000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.8052997588999986

Fe C O H

80 33 1 1

Selective dynamics

Direct

0.8393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.7311801591056499	0.2193643661613015	0.4668267388124633	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999985	F	F	F
0.5590885691336995	0.0980220819903219	0.4375274046367821	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000003	F	F	F
0.5943375291420316	0.2767634158505795	0.3882495252052450	T	T	T
0.8070399759999987	0.3298200070000021	0.3692500000000010	F	F	F
0.6871080006288869	0.0429681584545256	0.5098415965426842	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.2304371562515974	0.2225117224326943	0.4669364639208078	T	T	T
0.1632599800000009	0.3849500119999973	0.2899999919999985	F	F	F
0.0607088483309725	0.0981501722494754	0.4382290919791575	T	T	T
0.1955399960000008	0.0652299970000030	0.2403199970000003	F	F	F

0.0932213288479668	0.2772245551813322	0.3879970777127525	T	T	T
0.3070400060000011	0.3298200070000021	0.3692500000000010	F	F	F
0.1875268365252553	0.0442484132408069	0.5106277701252283	T	T	T
0.0044699999999978	0.4602699880000003	0.2462999970000013	F	F	F
0.9048155744677790	0.1711850686402214	0.3943598221410503	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.4034022579489798	0.1536479623939177	0.5053977270214908	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999982	F	F	F
0.4328085436682743	0.3274407818743598	0.4628883518198409	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F
0.8790000716471127	0.4889325493863928	0.4480345831538719	T	T	T
0.5044699910000006	0.4602699880000003	0.2462999970000013	F	F	F
0.4040557679024356	0.1737524992357142	0.3943375505168900	T	T	T
0.9981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.9010588103006150	0.1496944701075222	0.5060661214898163	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999982	F	F	F
0.9320065492955244	0.3227935172071508	0.4621740995156914	T	T	T
0.4722500150000002	0.2798599899999985	0.2958799900000031	F	F	F
0.3795581762216643	0.4928001280637792	0.4476239194950009	T	T	T
0.7199699880000026	0.1401900050000009	0.3529999849999967	F	F	F
0.6296009877382960	0.3599553424874441	0.4908907704396561	T	T	T
0.7826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.6902720009774497	0.4674725670734316	0.4027457864581072	T	T	T
0.2199700030000002	0.1401900050000009	0.3529999849999967	F	F	F
0.1274264757212693	0.3635143485709111	0.4975742188744598	T	T	T
0.2826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.1896762148369795	0.4683911142369259	0.4059305694721827	T	T	T
0.8393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.7339800477559367	0.7188389177033926	0.4659872722860267	T	T	T
0.6632599830000032	0.8849499820000020	0.2899999919999985	F	F	F
0.5603138825973206	0.5973287237439878	0.4357171323165762	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000003	F	F	F
0.5955051409377619	0.7777505129893840	0.3877572078171521	T	T	T
0.8070399759999987	0.8298199769999997	0.3692500000000010	F	F	F
0.6863344810729085	0.5429818887011948	0.5096693889884419	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.2314244755830642	0.7222036932565788	0.4666277721990099	T	T	T
0.1632599880000009	0.8849499820000020	0.2899999919999985	F	F	F
0.0691725327364876	0.5946922025036414	0.4434250594625325	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000003	F	F	F
0.0943209540651844	0.7760082871888233	0.3890224158256234	T	T	T
0.3070400060000011	0.8298199769999997	0.3692500000000010	F	F	F
0.2280011023693418	0.5298134765002582	0.5249881962835447	T	T	T
0.0044699999999978	0.9602699880000003	0.2462999970000013	F	F	F
0.9067171548595807	0.6702851891896587	0.3938838299395302	T	T	T
0.4981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.4118466338389676	0.6550950774694477	0.5104703243011497	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999982	F	F	F
0.4368761206874450	0.8261092013591933	0.4612801861253459	T	T	T
0.9722499849999977	0.7798600200000010	0.2958799900000031	F	F	F
0.8787945290624709	0.9884228452011304	0.4494070843862988	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000013	F	F	F
0.4033593087947747	0.6714698141823520	0.3954441073803716	T	T	T
0.9981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.9092012056497697	0.6512891936458283	0.5047960542319001	T	T	T
0.0303299999999993	0.6151900289999972	0.3136900069999982	F	F	F
0.9382762508684488	0.8235595652503533	0.4628657014355858	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3789446285196127	0.9915109527685320	0.4494475895009433	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999967	F	F	F
0.6336096805688229	0.8596611625249919	0.4908511372099376	T	T	T
0.7826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.6901484316549988	0.9677487885274388	0.4021721055800350	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999967	F	F	F
0.1339582279562936	0.8635955028709430	0.4916810749065646	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.1907074846187283	0.9683205122483609	0.4025359461942400	T	T	T
0.8641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.7786685720453514	0.3662476917578605	0.4624002261942903	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999986	F	F	F
0.5387400072813462	0.4560551578088057	0.4622894908725980	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999985	F	F	F
0.5474317739040773	0.2287495661589556	0.4785524419897045	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000016	F	F	F
0.7799294471519140	0.0918911345565753	0.4377480577511833	T	T	T

0.3641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.2745679348346719	0.3692833306145744	0.4590169168262760	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999986	F	F	F
0.0319680113913092	0.4482809605616956	0.4553714683684919	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999985	F	F	F
0.0432869028652252	0.2283727824498449	0.4766242338796045	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000016	F	F	F
0.2792769379307291	0.0946015002200068	0.4380864511966218	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.7830271713160243	0.8635543357567547	0.4634122249984651	T	T	T
0.6384199860000024	0.7358700039999988	0.3038099999999986	F	F	F
0.5405881566261859	0.9545209952157641	0.4615058907594887	T	T	T
0.6260200139999981	0.5126500129999982	0.3228900129999985	F	F	F
0.5508189462843339	0.7278711080167224	0.4766353985474783	T	T	T
0.8765599729999991	0.8823999760000021	0.2866800130000016	F	F	F
0.7825529250397397	0.5924073499863437	0.4387275242143339	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.2817644431530146	0.8668780735686865	0.4624427224700253	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999986	F	F	F
0.0387596363053929	0.9547025280362208	0.4621532537469643	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999985	F	F	F
0.0582546811490583	0.7296030837398422	0.4816364598875589	T	T	T
0.3765600030000016	0.8823999760000021	0.2866800130000016	F	F	F
0.2740800431782231	0.5949537679146292	0.4384184243671527	T	T	T
0.1580029690844445	0.4211331697865854	0.5684295685649184	T	T	T
0.3211803114780348	0.6139839147465571	0.5850509538798071	T	T	T
0.3445082442900112	0.5776801669059826	0.6217780099110097	T	T	T

CO dissociation on K₂O-Fe₅C₂(111)

K₂O-Fe₅C₂(111)-CO (IS)

1.0000000000000000		
12.3812999725000008	0.0000000000000000	0.0000000000000000
-2.0391083097000000	13.2888646689000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.8052997588999986

Fe C O K
80 33 2 2

Selective dynamics

Direct

0.8393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.7312370078883036	0.2194679228279514	0.4666038236554907	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999985	F	F	F
0.5603102569200654	0.0979227440136635	0.4384745884062596	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000003	F	F	F
0.5954354092553114	0.2771476532994367	0.3884056498216864	T	T	T
0.8070399759999987	0.3298200070000021	0.3692500000000010	F	F	F
0.6897874611949153	0.0416639590442256	0.5100214357690025	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.2345870630016673	0.2210713472488896	0.4671480090368805	T	T	T
0.1632599800000009	0.3849500119999973	0.2899999919999985	F	F	F
0.0600947950502025	0.0974334289963493	0.4392413196085013	T	T	T
0.1955399960000008	0.0652299970000030	0.2403199970000003	F	F	F
0.0947497444669806	0.2779315260416743	0.3889175107272894	T	T	T
0.3070400060000011	0.3298200070000021	0.3692500000000010	F	F	F
0.1879088978904040	0.0429919823838896	0.5102924275299123	T	T	T
0.0044699999999978	0.4602699880000003	0.2462999970000013	F	F	F
0.9055888929721519	0.1725304877808935	0.3942971420059149	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799980000003	F	F	F
0.4029813612556044	0.1537098380671762	0.5051494423087670	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999982	F	F	F
0.4340597408643676	0.3261624748635379	0.4615419883629639	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F
0.8783747107538561	0.4909065272129077	0.4475217635352310	T	T	T
0.5044699910000006	0.4602699880000003	0.2462999970000013	F	F	F
0.4048401595166068	0.1725477479421502	0.3940533541693160	T	T	T
0.9981200100000009	0.4347699879999993	0.3632799980000003	F	F	F
0.9003564083719905	0.1494856540761014	0.5051779208034823	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999982	F	F	F
0.9309954199190077	0.3256126441141780	0.4623367667531239	T	T	T
0.4722500150000002	0.2798599899999985	0.2958799900000031	F	F	F
0.3789145799443329	0.4918881184683122	0.4459350221665389	T	T	T
0.7199699800000026	0.1401900050000009	0.3529999849999967	F	F	F
0.6297647031660074	0.3592250417026024	0.4912462918395893	T	T	T
0.7826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.6894186131981330	0.4680270706916860	0.4038328734642002	T	T	T

0.2199700030000002	0.1401900050000009	0.3529999849999967	F	F	F
0.1285668226002583	0.3577020140128099	0.4963968710707818	T	T	T
0.2826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.1892347236308207	0.4660349381222103	0.4035853300987110	T	T	T
0.8393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.7339892791503649	0.7203855240780703	0.4655338880290006	T	T	T
0.6632599830000032	0.8849499820000020	0.2899999919999985	F	F	F
0.5622918693635987	0.5980113380940982	0.4392856063595106	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000003	F	F	F
0.5944039881798734	0.7760142479113139	0.3882360220613877	T	T	T
0.8070399759999987	0.8298199769999997	0.3692500000000010	F	F	F
0.6913679047282174	0.5384133660832614	0.5172771431820608	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.2330831867649295	0.7201794539921972	0.4677594455583918	T	T	T
0.1632599800000009	0.8849499820000020	0.2899999919999985	F	F	F
0.0629662990425979	0.5949974964688345	0.4404043233612168	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000003	F	F	F
0.0949157083976561	0.7762754453632982	0.3889525563237758	T	T	T
0.3070400060000011	0.8298199769999997	0.3692500000000010	F	F	F
0.2038694199267564	0.5352392129878394	0.5114692702285200	T	T	T
0.0044699999999978	0.9602699880000003	0.2462999970000013	F	F	F
0.9044140121684815	0.6707346965913282	0.3943067819613227	T	T	T
0.4981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.4041395089099069	0.6535926353378870	0.5046522596237634	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999982	F	F	F
0.4360458360307271	0.8258922287819570	0.4631906778454346	T	T	T
0.9722499849999977	0.7798600200000010	0.2958799900000031	F	F	F
0.8785013014649448	0.9887843685399641	0.4495186544202973	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000013	F	F	F
0.4057587570012914	0.6719055482362229	0.3936810779131417	T	T	T
0.9981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.9054768167427236	0.6503962204521896	0.5048113514963282	T	T	T
0.0303299999999993	0.6151900289999972	0.3136900069999982	F	F	F
0.9363942872805432	0.8239212888791653	0.4633915109160948	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3789406637416670	0.9905489551575115	0.4487194151148998	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999967	F	F	F
0.6330269658579968	0.8608088740300959	0.4898725020307306	T	T	T
0.7826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.6900397459086509	0.9685485448482991	0.4019363062874453	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999967	F	F	F
0.1323469172696324	0.8606217810712803	0.4916123376254479	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.1896826804717116	0.9675894824128987	0.4025890975048438	T	T	T
0.8641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.7784478697313284	0.3676658318234852	0.4619648828284340	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999986	F	F	F
0.5380754559001281	0.4531032978075921	0.4581112409508410	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999985	F	F	F
0.5457231789166872	0.2293088614338276	0.4781860451621634	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000016	F	F	F
0.7802846671112135	0.0921166439369544	0.4365547333570494	T	T	T
0.3641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.2762966235090978	0.3690259524479922	0.4604841962582211	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999986	F	F	F
0.0368274527693379	0.4515128350640032	0.4589423591414436	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999985	F	F	F
0.0409500531719595	0.2283774820041109	0.4760660448205732	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000016	F	F	F
0.2801732173516574	0.0931420870307313	0.4375842299806549	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.7828975906577311	0.8644388676029819	0.4645585448849341	T	T	T
0.6384199860000024	0.7358700039999988	0.3038099999999986	F	F	F
0.5391164947043070	0.9545310492480703	0.4613917644912410	T	T	T
0.6260200139999981	0.5126500129999982	0.3228900129999985	F	F	F
0.5508209417141966	0.7298398325104666	0.4798346037063173	T	T	T
0.8765599729999991	0.8823999760000021	0.2866800130000016	F	F	F
0.7772178438630377	0.5929175055014737	0.4386808546780881	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.2806131218523403	0.8657037602116002	0.4620262721079478	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999986	F	F	F
0.0383662108569445	0.9536102071882226	0.4616692059765278	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999985	F	F	F
0.0513368381624951	0.7275095504318414	0.4797329021947150	T	T	T
0.3765600030000016	0.8823999760000021	0.2866800130000016	F	F	F

0.2795497961681622	0.5945133700302313	0.4368925208967236	T	T	T
0.1657393539483552	0.3866044718211653	0.5762585205004087	T	T	T
0.2028515534175621	0.4019989041967448	0.6291299641192524	T	T	T
0.6497360599338909	0.5521679978249224	0.5947631991679642	T	T	T
0.6847251551086404	0.7381194540120581	0.6191868271664815	T	T	T
0.4521880317043294	0.4414567405666232	0.6042388089228071	T	T	T

K₂O-Fe₃C₂(111)-C+O (TS)

1.0000000000000000		
12.3812999725000008	0.0000000000000000	0.0000000000000000
-2.0391083097000000	13.2888646689000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.8052997588999986

Fe C O K
80 33 2 2

Selective dynamics

Direct

0.8393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.7391506875155709	0.2159929372360979	0.4670181254811642	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999985	F	F	F
0.5634541446383682	0.0964279820010137	0.4389221692134448	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000003	F	F	F
0.5978450827438572	0.2763674188108916	0.3889469766955164	T	T	T
0.8070399759999987	0.3298200070000021	0.3692500000000010	F	F	F
0.6922592325869474	0.0314837897407859	0.5088462868754550	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.2445506506358636	0.2203194754793006	0.4685490037818501	T	T	T
0.1632599800000009	0.3849500119999973	0.2899999919999985	F	F	F
0.0636451452329671	0.0978132437876213	0.4385389296034171	T	T	T
0.1955399960000008	0.0652299970000030	0.2403199970000003	F	F	F
0.1003427221195894	0.2774259964609239	0.3894112541573987	T	T	T
0.3070400060000011	0.3298200070000021	0.3692500000000010	F	F	F
0.1916847992640074	0.0425288029897186	0.5101312658959534	T	T	T
0.0044699999999978	0.4602699880000003	0.2462999970000013	F	F	F
0.9069662828813445	0.1724232714452666	0.3940943937885442	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.4105275959185288	0.1506714919306474	0.5042753329854703	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999982	F	F	F
0.4491809936256408	0.3241365788340726	0.4644687616768629	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F
0.8784165768805291	0.4870502250463697	0.4488806813778076	T	T	T
0.5044699910000006	0.4602699880000003	0.2462999970000013	F	F	F
0.4066168892213883	0.1733243300115865	0.3938977802516769	T	T	T
0.9981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.9056442444238932	0.1480097573593485	0.5047318630999463	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999982	F	F	F
0.9437723739667186	0.3255749240329371	0.4626751671090572	T	T	T
0.4722500150000002	0.2798599899999985	0.2958799900000031	F	F	F
0.3727955577626030	0.4830012010845920	0.4475181688683953	T	T	T
0.7199699880000026	0.1401900050000009	0.3529999849999967	F	F	F
0.6465581193618564	0.3584042791992513	0.4900692764354480	T	T	T
0.7826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.6891655994867599	0.4713046656409292	0.4014562430154662	T	T	T
0.2199700030000002	0.1401900050000009	0.3529999849999967	F	F	F
0.1389607673727755	0.3558792875400255	0.4936201633995575	T	T	T
0.2826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.1845633137445333	0.4685759679680241	0.4007468623143567	T	T	T
0.8393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.7394122353423398	0.7205625875850998	0.4640906501621671	T	T	T
0.6632599830000032	0.8849499820000020	0.2899999919999985	F	F	F
0.5599115947963585	0.5941783844800170	0.4390167036273255	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000003	F	F	F
0.5942476564600748	0.7731799429264693	0.3883263171580508	T	T	T
0.8070399759999987	0.8298199769999997	0.3692500000000010	F	F	F
0.6919416273632979	0.5393074510652900	0.5147332269067598	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.2295439505633984	0.7217799028500629	0.4657997751054890	T	T	T
0.1632599800000009	0.8849499820000020	0.2899999919999985	F	F	F
0.0607610931956164	0.5966240535919193	0.4377117785069529	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000003	F	F	F
0.0943228160764380	0.7769732429005081	0.3885776403101605	T	T	T
0.3070400060000011	0.8298199769999997	0.3692500000000010	F	F	F
0.2001721838011467	0.5387777691374046	0.5098163639359403	T	T	T
0.0044699999999978	0.9602699880000003	0.2462999970000013	F	F	F

0.9044962434225510	0.6700217618225061	0.3942165344664121	T	T	T
0.4981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.3917865682508177	0.6404095099819193	0.5115845756788011	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999982	F	F	F
0.4276728490951474	0.8259566982484507	0.4650980788021683	T	T	T
0.9722499849999977	0.7798600200000010	0.2958799900000031	F	F	F
0.8799553620922701	0.9884688077338605	0.4485590537581510	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000013	F	F	F
0.4050708966234430	0.6713124988148079	0.3970632080359864	T	T	T
0.9981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.9063434236346880	0.6488877446154210	0.5046404118090136	T	T	T
0.0303299999999993	0.6151900289999972	0.3136900069999982	F	F	F
0.9357315392060856	0.8237875861765643	0.4633872199257766	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3793256743255343	0.9912394906528470	0.4473139247552212	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999967	F	F	F
0.6242736671766547	0.8536076879221743	0.4865274194710620	T	T	T
0.7826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.6908596508159727	0.9665408166496503	0.4011395833022310	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999967	F	F	F
0.1305121487413204	0.8606777088069123	0.4923717120582192	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.1889818688350546	0.9667928680930853	0.4028811589499556	T	T	T
0.8641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.7967943225503824	0.3582079494597399	0.4682061516387600	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999986	F	F	F
0.5519533492423803	0.4504453007882202	0.4574035759332640	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999985	F	F	F
0.5607850442060185	0.2284533989479784	0.4802121411278018	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000016	F	F	F
0.7822587954673901	0.0898512838418893	0.4355472805747333	T	T	T
0.3641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.3149092415282163	0.3530132554400502	0.5057708620030843	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999986	F	F	F
0.0494658982518850	0.4544947661679299	0.4619324634392616	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999985	F	F	F
0.0495505597109939	0.2275646039975878	0.4766709031255311	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000016	F	F	F
0.2814927622973723	0.0923826986323646	0.4362142437524644	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.7801169865768932	0.8665795269766933	0.4638582446378587	T	T	T
0.6384199860000024	0.7358700039999988	0.3038099999999986	F	F	F
0.5343887081729943	0.9534750854188517	0.4624749721695421	T	T	T
0.6260200139999981	0.5126500129999982	0.3228900129999985	F	F	F
0.5236066376687685	0.7216474379072486	0.4733706225934274	T	T	T
0.8765599729999991	0.8823999760000021	0.2866800130000016	F	F	F
0.7796516048069653	0.5896422111752188	0.4376020545440155	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.2774811781553254	0.8697673179851264	0.4617874973168976	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999986	F	F	F
0.0385230717011870	0.9532828050044507	0.4602750547392174	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999985	F	F	F
0.0514315572761744	0.7267279031692145	0.4798687488837601	T	T	T
0.3765600030000016	0.8823999760000021	0.2866800130000016	F	F	F
0.2757576523859195	0.5921506345360659	0.4343945396675398	T	T	T
0.2718433032386184	0.4321549191803655	0.5314429185852326	T	T	T
0.3308223472003052	0.5459561135842032	0.5743312273792540	T	T	T
0.6645885729178709	0.5568676195878468	0.5938245834910122	T	T	T
0.6722157138966512	0.7411008927326341	0.6161068481621496	T	T	T
0.4800929891829815	0.4365930873722472	0.6111251071875710	T	T	T

K₂O-Fe₃C₂(111)C+O (FS)

1.0000000000000000		
12.381299725000008	0.0000000000000000	0.0000000000000000
-2.0391083097000000	13.2888646689000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.8052997588999986

Fe C O K
80 33 2 2

Selective dynamics

Direct

0.8393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.7364425174388685	0.2179010251039517	0.4668113198213954	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999985	F	F	F

0.5632523856631436	0.0968141091556978	0.4386031339135403	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000003	F	F	F
0.5969465062932943	0.2770502280488593	0.3887669627928216	T	T	T
0.8070399759999987	0.3298200070000021	0.3692500000000010	F	F	F
0.6916336726948663	0.0331824071149943	0.5088371118331714	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.2449006815593130	0.2176223102125426	0.4673433041020043	T	T	T
0.1632599980000009	0.3849500119999973	0.2899999919999985	F	F	F
0.0624408316724996	0.0972336028434879	0.4386785835409183	T	T	T
0.1955399960000008	0.0652299970000030	0.2403199970000003	F	F	F
0.0995413569505945	0.2764657335704754	0.3890973357774988	T	T	T
0.3070400060000011	0.3298200070000021	0.3692500000000010	F	F	F
0.1905456449299214	0.0424858036043627	0.5098515740094131	T	T	T
0.0044699999999978	0.4602699880000003	0.2462999970000013	F	F	F
0.9067746390446020	0.1734482566576489	0.3947594151000559	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.4101787403170462	0.1512857145103998	0.5044597641019292	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999982	F	F	F
0.4462141140416145	0.3240190392829490	0.4632101486858665	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F
0.8793172174671711	0.4900550016602341	0.4484969385799499	T	T	T
0.5044699910000006	0.4602699880000003	0.2462999970000013	F	F	F
0.4067547244443057	0.1724938548751067	0.3934919049690003	T	T	T
0.9981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.8986362402052226	0.1462371457103495	0.5056560517669915	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999982	F	F	F
0.9379267062028914	0.3279592743691064	0.4626362084376476	T	T	T
0.4722500150000002	0.2798599899999985	0.2958799900000031	F	F	F
0.3753950809934973	0.4854507356040901	0.4516099127689561	T	T	T
0.7199699880000026	0.1401900050000009	0.3529999849999967	F	F	F
0.6414539933914982	0.3592161527068317	0.4913623864118482	T	T	T
0.7826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.6893909477077531	0.4690173554111604	0.4018351527381419	T	T	T
0.2199700030000002	0.1401900050000009	0.3529999849999967	F	F	F
0.1342315526529086	0.3532073641143057	0.4913109433693177	T	T	T
0.2826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.1859731240211873	0.4682970898170426	0.4004050247096369	T	T	T
0.8393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.7391294818933891	0.7209510783354974	0.4643246891972060	T	T	T
0.6632599830000032	0.8849499820000020	0.2899999919999985	F	F	F
0.5603645909877530	0.5948949656536382	0.4388450154943414	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000003	F	F	F
0.5946183920466621	0.7736877118944487	0.3877262268477789	T	T	T
0.8070399759999987	0.8298199769999997	0.3692500000000010	F	F	F
0.6933974073497897	0.5388384090087851	0.5141273319137490	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.2300238015158121	0.7211533072218950	0.4662956949253555	T	T	T
0.1632599980000009	0.8849499820000020	0.2899999919999985	F	F	F
0.0617573060256673	0.5972583437768180	0.4391547866097326	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000003	F	F	F
0.0949128562726032	0.7767925127016985	0.3885518345625248	T	T	T
0.3070400060000011	0.8298199769999997	0.3692500000000010	F	F	F
0.2005772174220301	0.5343523484755753	0.5088848719938397	T	T	T
0.0044699999999978	0.9602699880000003	0.2462999970000013	F	F	F
0.9049497458816487	0.6707447297367561	0.3943671155059051	T	T	T
0.4981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.3940453448567540	0.6494012904211317	0.5152326975420444	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999982	F	F	F
0.4279252073949298	0.8269822454370250	0.4642648943793679	T	T	T
0.9722499849999977	0.7798600200000010	0.2958799900000031	F	F	F
0.8785858937995782	0.9886321640635990	0.4483288707975052	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000013	F	F	F
0.4054512797872472	0.6706008625342209	0.3969831330250752	T	T	T
0.9981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.9043900756295610	0.6494160533828788	0.5059498314295788	T	T	T
0.0303299999999993	0.6151900289999972	0.3136900069999982	F	F	F
0.9352541361541974	0.8245145473631221	0.4632863045561174	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3795603668772680	0.9914374465089506	0.4476066747651823	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999967	F	F	F
0.6250538296223779	0.8549264542055820	0.4860007145079042	T	T	T
0.7826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.6903466431116084	0.9666481044879051	0.4009022668385404	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999967	F	F	F
0.1296265173289964	0.8604941957057405	0.4920542179810367	T	T	T

0.2826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.1894531984403826	0.9661848429482662	0.4027650216522656	T	T	T
0.8641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.7897133867780085	0.3628261719464019	0.4651179889128775	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999986	F	F	F
0.5488463662764129	0.4514319190224574	0.4580376929868652	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999985	F	F	F
0.5583204914887391	0.2283506128263816	0.4798424444891995	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000016	F	F	F
0.7802871965334431	0.0909027468710594	0.4353257753044063	T	T	T
0.3641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.3074583368523684	0.3473963587964523	0.5044780885807832	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999986	F	F	F
0.0452551438772945	0.4545014775247000	0.4618242176232210	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999985	F	F	F
0.0348103829312649	0.2256774598289542	0.4731510824275611	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000016	F	F	F
0.2819541789133151	0.0911550684146587	0.4356880513349744	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.7806384943665562	0.8664135097406594	0.4633324435510504	T	T	T
0.6384199860000024	0.7358700039999988	0.3038099999999986	F	F	F
0.5339764322434517	0.9547039416438239	0.4628089796738302	T	T	T
0.6260200139999981	0.5126500129999982	0.3228900129999985	F	F	F
0.5213574488827672	0.7213229608127948	0.4707069271542677	T	T	T
0.8765599729999991	0.8823999760000021	0.2866800130000016	F	F	F
0.7788147947633182	0.5904402613099858	0.4370536151709886	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.2765110932894793	0.8692813572630365	0.4602623060574392	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999986	F	F	F
0.0367580857341416	0.9534762124462044	0.4607746559725998	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999985	F	F	F
0.0476771650690692	0.7275761404119362	0.4787039962662685	T	T	T
0.3765600030000016	0.8823999760000021	0.2866800130000016	F	F	F
0.2792279693514906	0.5936376731778621	0.4365639892735097	T	T	T
0.2682624061386238	0.4256763778992458	0.5326075960363982	T	T	T
0.4154995512832818	0.6396227280377667	0.5949414832559612	T	T	T
0.6742102521880303	0.5588239258710033	0.5929537828637890	T	T	T
0.6112552751386630	0.7294151926268675	0.6170351547587712	T	T	T
0.4680212552776153	0.4603183131723611	0.6119518234332451	T	T	T

HCO formation and dissociation on $K_2O-Fe_3C_2(111)$

$K_2O-Fe_3C_2(111)-CO+H$ (IS)

1.0000000000000000		
12.3812999725000008	0.0000000000000000	0.0000000000000000
-2.0391083097000000	13.2888646689000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.8052997588999986
Fe	C	O
80	33	2
2	2	1

Selective dynamics

Direct

0.8393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.7325648502244907	0.2192992666336360	0.4665922144037556	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999985	F	F	F
0.5605185295532473	0.0977564932142010	0.4387813465118445	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000003	F	F	F
0.5956362741450029	0.2769977070627300	0.3885768614848865	T	T	T
0.8070399759999987	0.3298200070000021	0.3692500000000010	F	F	F
0.6894639039636987	0.0384783023950777	0.5098807144860044	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.2353413992427127	0.2215464680532564	0.4666476120465902	T	T	T
0.1632599980000009	0.3849500119999973	0.2899999919999985	F	F	F
0.0605625130927158	0.0975728697429027	0.4389668496477105	T	T	T
0.1955399960000008	0.0652299970000030	0.2403199970000003	F	F	F
0.0952060081987453	0.2783617714596393	0.3886269383797759	T	T	T
0.3070400060000011	0.3298200070000021	0.3692500000000010	F	F	F
0.1883210719122559	0.0435724008025685	0.5103445002146930	T	T	T
0.0044699999999978	0.4602699880000003	0.2462999970000013	F	F	F
0.9056658186623883	0.1724302439793245	0.3943304634455078	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.4030704192364183	0.1533106186010875	0.5051205402664609	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999982	F	F	F
0.4342482911161968	0.3259050990611445	0.4616455566543621	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F
0.8787122576728262	0.4910516268421460	0.4474855026089237	T	T	T

0.5044699910000006	0.4602699880000003	0.2462999970000013	F	F	F
0.4050702045683848	0.1725591187248515	0.3940190437757167	T	T	T
0.9981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.9000107514092065	0.1495715076403756	0.5052560615686624	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999982	F	F	F
0.9319148926520966	0.3263491341383727	0.4622766204818796	T	T	T
0.4722500150000002	0.2798599899999985	0.2958799900000031	F	F	F
0.3804156696241149	0.4906814649760626	0.4449821863755405	T	T	T
0.7199699880000026	0.1401900050000009	0.3529999849999967	F	F	F
0.6303595892246199	0.3588598376684171	0.4911606439386211	T	T	T
0.7826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.6894561195162673	0.4681531235813865	0.4037672082011112	T	T	T
0.2199700030000002	0.1401900050000009	0.3529999849999967	F	F	F
0.1289115402890491	0.3573446287248678	0.4961741640406461	T	T	T
0.2826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.1888303554051409	0.4668595604340628	0.4039826853317079	T	T	T
0.8393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.7367563564777911	0.7208153858119347	0.4650306522797580	T	T	T
0.6632599830000032	0.8849499820000020	0.2899999919999985	F	F	F
0.5623571789140505	0.5976879715852120	0.4393258956823807	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000003	F	F	F
0.5952288250235196	0.7763346680327911	0.3879501596589350	T	T	T
0.8070399759999987	0.8298199769999997	0.3692500000000010	F	F	F
0.6912433950241007	0.5392952584266374	0.5168504953228165	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.2307238046039735	0.7208406592664597	0.4664939480859178	T	T	T
0.1632599980000009	0.8849499820000020	0.2899999919999985	F	F	F
0.0633602471922659	0.5951981995728070	0.4399738140584307	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000003	F	F	F
0.0947949180873091	0.7766418158750682	0.3885533225658279	T	T	T
0.3070400060000011	0.8298199769999997	0.3692500000000010	F	F	F
0.2136727638543438	0.5330820277669689	0.5122805128553433	T	T	T
0.0044699999999978	0.9602699880000003	0.2462999970000013	F	F	F
0.9048505226544347	0.6704717549939189	0.3943467031704531	T	T	T
0.4981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.3970064253994390	0.6502099732035959	0.5073208178038244	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999982	F	F	F
0.4312608196012953	0.8273837694740565	0.4631289989235440	T	T	T
0.9722499849999977	0.7798600200000010	0.2958799900000031	F	F	F
0.8781888053986904	0.9892493190547735	0.4489534918986545	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000013	F	F	F
0.4072679559676705	0.6733901407045808	0.3949674774227736	T	T	T
0.9981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.9044364846571994	0.6498286065504674	0.5051087565541277	T	T	T
0.0303299999999993	0.6151900289999972	0.3136900069999982	F	F	F
0.9349612237103290	0.8246869222595119	0.4632953166092954	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3787727784775761	0.9918058109868145	0.4481721417736231	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999967	F	F	F
0.6278782230246392	0.8577354551805724	0.4889492175743722	T	T	T
0.7826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.6899283606969598	0.9677618783509083	0.4020558816710028	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999967	F	F	F
0.1299101648479902	0.8606731100993369	0.4916252888485734	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.1894266141865061	0.9672106428844689	0.4029115899769353	T	T	T
0.8641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.7787958946547854	0.3674751568926107	0.4617911441620642	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999986	F	F	F
0.5393456293393349	0.4527652238642832	0.4579319759941347	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999985	F	F	F
0.5457666521070719	0.2292934245095853	0.4782365829089950	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000016	F	F	F
0.7799309390813705	0.0921890671721493	0.4365626217470976	T	T	T
0.3641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.2768197918386238	0.3697979444535157	0.4609231333961562	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999986	F	F	F
0.0388543865101116	0.4527881724839801	0.4595297774897117	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999985	F	F	F
0.0399429251763476	0.2283719594727747	0.4750969224095393	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000016	F	F	F
0.2799846083054682	0.0935752764866855	0.4372130813021324	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.7795567525892645	0.8661078386000353	0.4636578181305719	T	T	T
0.6384199860000024	0.7358700039999988	0.3038099999999986	F	F	F

0.5367970751333155	0.9544857683739848	0.4621646921542452	T	T	T
0.6260200139999981	0.5126500129999982	0.3228900129999985	F	F	F
0.5368595209491906	0.7277185728226347	0.4760882515755520	T	T	T
0.8765599729999991	0.8823999760000021	0.2866800130000016	F	F	F
0.7772745933687463	0.5924097332548299	0.4379205992843384	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.2776809494107613	0.8683126688523986	0.4608989829624745	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999986	F	F	F
0.0368070706311910	0.9541869840723222	0.4614343182991397	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999985	F	F	F
0.0477114832667055	0.7275905900216324	0.4788482328237224	T	T	T
0.3765600030000016	0.8823999760000021	0.2866800130000016	F	F	F
0.2797353417782052	0.5944341899144769	0.4348941006147564	T	T	T
0.1612546673773539	0.3763119130132048	0.5777520382150590	T	T	T
0.1919518488197402	0.3821214931897143	0.6320972172608791	T	T	T
0.6508055763310175	0.5532987723108364	0.5943223971826932	T	T	T
0.6830807326039919	0.7391885538340155	0.6186435038041245	T	T	T
0.4513498549968798	0.4446773477144892	0.6044669562127101	T	T	T
0.3100656539614089	0.5925717417270420	0.5649957850117011	T	T	T

K₂O-Fe₃C₂(111)-HCO (TS)

1.0000000000000000		
12.3812999725000008	0.0000000000000000	0.0000000000000000
-2.0391083097000000	13.2888646689000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.8052997588999986

Fe C O K H
80 33 2 2 1

Selective dynamics

Direct

0.8393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.7321860665994976	0.2193580529431213	0.4663755932915996	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999985	F	F	F
0.5603022650190327	0.0978755357315734	0.4382907725336034	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000003	F	F	F
0.5958019933403539	0.2765915216727275	0.3884422261743753	T	T	T
0.8070399759999987	0.3298200070000021	0.3692500000000010	F	F	F
0.6898982770338249	0.0410167821900865	0.5096789074311976	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.2317663268956321	0.2216641267285306	0.4664073969494603	T	T	T
0.1632599980000009	0.3849500119999973	0.2899999919999985	F	F	F
0.0604484802853386	0.0981483400428759	0.4387257946747320	T	T	T
0.1955399960000008	0.0652299970000030	0.2403199970000003	F	F	F
0.0937625687305012	0.2778446409016304	0.3884428872129488	T	T	T
0.3070400060000011	0.3298200070000021	0.3692500000000010	F	F	F
0.1880604095683865	0.0436566127075686	0.5103169483853274	T	T	T
0.0044699999999978	0.4602699880000003	0.2462999970000013	F	F	F
0.9052801076232784	0.1720720035823702	0.3941282767996248	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.4021304914149866	0.1542751593957136	0.5049805689494186	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999982	F	F	F
0.4346738794548856	0.3259296610212509	0.4611596166717862	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F
0.8781124224057529	0.4902007183324027	0.4473262998150202	T	T	T
0.5044699910000006	0.4602699880000003	0.2462999970000013	F	F	F
0.4048013695986947	0.1725774210790859	0.3939931648682650	T	T	T
0.9981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.9022096942027390	0.1508634116774863	0.5054939321339118	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999982	F	F	F
0.9325358495169500	0.3251692668288566	0.4623149038894078	T	T	T
0.4722500150000002	0.2798599899999985	0.2958799900000031	F	F	F
0.3776246247211698	0.4918774183209172	0.4454898123016618	T	T	T
0.7199699880000026	0.1401900050000009	0.3529999849999967	F	F	F
0.6309772531979639	0.3583681367349791	0.4914562829713389	T	T	T
0.7826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.6890606249855845	0.4679743599102655	0.4035964978324138	T	T	T
0.2199700030000002	0.1401900050000009	0.3529999849999967	F	F	F
0.1282648862609822	0.3613253768987704	0.4962475322416354	T	T	T
0.2826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.1888106227049895	0.4668527028700852	0.4040562876578665	T	T	T
0.8393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.7350184191922119	0.7203055531828345	0.4654545218341268	T	T	T
0.6632599830000032	0.8849499820000020	0.2899999919999985	F	F	F
0.5612998526994231	0.5975978092689839	0.4387474411657984	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000003	F	F	F
0.5949299852499298	0.7761383927760980	0.3882319984856060	T	T	T

0.8070399759999987	0.8298199769999997	0.3692500000000010	F	F	F
0.6868649762948310	0.5384867618954035	0.5168495115787650	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.2328639793612641	0.7217834572817565	0.4676202028460424	T	T	T
0.1632599980000009	0.8849499820000020	0.2899999919999985	F	F	F
0.0632012811463643	0.5956138868737397	0.4394937651288850	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000003	F	F	F
0.0945393767924645	0.7757580641702004	0.3889773359811042	T	T	T
0.3070400060000011	0.8298199769999997	0.3692500000000010	F	F	F
0.2037001915614750	0.5365853138962693	0.5142207921852444	T	T	T
0.0044699999999978	0.9602699880000003	0.2462999970000013	F	F	F
0.9037816794455387	0.6705775846470670	0.3943112201208481	T	T	T
0.4981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.4023474454733044	0.6540536658343888	0.5059003169675457	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999982	F	F	F
0.4351766145264524	0.8265764815112184	0.4631791331350215	T	T	T
0.9722499849999977	0.7798600200000010	0.2958799900000031	F	F	F
0.8789916642304573	0.9891879495366572	0.4497744640394970	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000013	F	F	F
0.4051103560938255	0.6718129642946037	0.3941994975196813	T	T	T
0.9981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.9060283577122615	0.6502393675841687	0.5044760683432113	T	T	T
0.0303299999999993	0.6151900289999972	0.3136900069999982	F	F	F
0.9359694281413533	0.8241606919058857	0.4631728857046060	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3790069899344382	0.9913371402813246	0.4482482028763358	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999967	F	F	F
0.6315640189265531	0.8598289184006116	0.4897424291583543	T	T	T
0.7826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.6904060517282030	0.9682070163998092	0.4019895937779002	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999967	F	F	F
0.1311015681955966	0.8612911273825407	0.4915418220635766	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.1898704049583488	0.9678542375583675	0.4028162292091281	T	T	T
0.8641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.7800851550796971	0.3670096839351395	0.4627305686926104	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999986	F	F	F
0.5390481941146946	0.4522291673323990	0.4578473897818829	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999985	F	F	F
0.5461998213370234	0.2288702010646513	0.4782432689232428	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000016	F	F	F
0.7811141228698353	0.0921678168241941	0.4369052816538307	T	T	T
0.3641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.2760779854688519	0.3679958487422025	0.4591201024633200	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999986	F	F	F
0.0365233899051995	0.4511625657884341	0.4565448027710372	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999985	F	F	F
0.0441046970051287	0.2296031801476663	0.4769141272584659	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000016	F	F	F
0.2800675550320410	0.0939662374187379	0.4377064846530669	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.7816437085296642	0.8649584178441075	0.4637778461999055	T	T	T
0.6384199860000024	0.7358700039999988	0.3038099999999986	F	F	F
0.5386802356597223	0.9548461329661097	0.4619354193061072	T	T	T
0.6260200139999981	0.5126500129999982	0.3228900129999985	F	F	F
0.5467639350396725	0.7292954504449244	0.4785107882875032	T	T	T
0.8765599729999991	0.8823999760000021	0.2866800130000016	F	F	F
0.7770786124497638	0.5917252632192860	0.4390326709265260	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.2791910053797931	0.8672574752638968	0.4614137365095094	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999986	F	F	F
0.0380082185846059	0.9544005547449367	0.4618671118759070	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999985	F	F	F
0.0517008770966602	0.7275376394222441	0.4798676016842288	T	T	T
0.3765600030000016	0.8823999760000021	0.2866800130000016	F	F	F
0.2776913567485340	0.5946915406444507	0.4381734627469440	T	T	T
0.1739372888197083	0.4305533041133335	0.5759947816104717	T	T	T
0.1923639408724983	0.3763842454485535	0.6209857641208593	T	T	T
0.6418112830330932	0.5510522592016032	0.5937270429923611	T	T	T
0.6821593437742347	0.7363252053107103	0.6190792300398661	T	T	T
0.4395180017441346	0.4382476920828818	0.6019785997976469	T	T	T
0.1805238383376836	0.5257485124051529	0.5926197162333914	T	T	T

K₂O-Fe₃C₂(111)-HCO (FS)

1.0000000000000000
12.3812999725000008 0.0000000000000000 0.0000000000000000
-2.0391083097000000 13.2888646689000005 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.8052997588999986

Fe C O K H
80 33 2 2 1

Selective dynamics

Direct

0.8393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.7325071867375117	0.2192763971746120	0.4664697697930558	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999985	F	F	F
0.5606190428645665	0.0973553591117944	0.4381907404669227	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000003	F	F	F
0.5957763476075011	0.2771236999399332	0.3883908914949687	T	T	T
0.8070399759999987	0.3298200070000021	0.3692500000000010	F	F	F
0.6901799760634429	0.0413061142155239	0.5098817176984853	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.2324087478391876	0.2213965702757996	0.4670112407979840	T	T	T
0.1632599980000009	0.3849500119999973	0.2899999919999985	F	F	F
0.0610057365502709	0.0987802582378658	0.4395280866116991	T	T	T
0.1955399960000008	0.0652299970000030	0.2403199970000003	F	F	F
0.0956777638665273	0.2796480926358040	0.3898405327121890	T	T	T
0.3070400060000011	0.3298200070000021	0.3692500000000010	F	F	F
0.188661523925606	0.0419878927735099	0.5103911521621319	T	T	T
0.0044699999999978	0.4602699880000003	0.2462999970000013	F	F	F
0.9057043070862084	0.1722802235277482	0.3939039178030430	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.4031760453561227	0.1543582335452177	0.5048797874443852	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999982	F	F	F
0.4354478489621801	0.3258209365541954	0.4606011296809193	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F
0.8782552339924892	0.4900708611609216	0.4476417564773553	T	T	T
0.5044699910000006	0.4602699880000003	0.2462999970000013	F	F	F
0.4050420936456666	0.1721712779135689	0.3939762767720794	T	T	T
0.9981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.9031457794896465	0.1510006546846661	0.5047740030446809	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999982	F	F	F
0.9345967950042902	0.3256494324312583	0.4623455052473255	T	T	T
0.4722500150000002	0.2798599899999985	0.2958799900000031	F	F	F
0.3781237609508079	0.4917893043940161	0.4449555372545415	T	T	T
0.7199699880000026	0.1401900050000009	0.3529999849999967	F	F	F
0.6310962878949776	0.3585154786515309	0.4912612329399553	T	T	T
0.7826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.6894776625623791	0.4679002443930919	0.4036600126185663	T	T	T
0.2199700030000002	0.1401900050000009	0.3529999849999967	F	F	F
0.1326668519572206	0.3611489307491839	0.4991698589247418	T	T	T
0.2826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.1877437201991453	0.4656452827742394	0.4043364234730860	T	T	T
0.8393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.7341816543099200	0.7205430767534633	0.4654983460313932	T	T	T
0.6632599830000032	0.8849499820000020	0.2899999919999985	F	F	F
0.5614750789680027	0.5980516220782878	0.4385954240227941	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000003	F	F	F
0.5942379176312720	0.7761532307826361	0.3882083235742246	T	T	T
0.8070399759999987	0.8298199769999997	0.3692500000000010	F	F	F
0.6841840787346232	0.5373972091411493	0.5169741515680047	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.2326550721776234	0.7207821195913366	0.4672277278932510	T	T	T
0.1632599980000009	0.8849499820000020	0.2899999919999985	F	F	F
0.0609903690415570	0.5959476637201665	0.4381197982684912	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000003	F	F	F
0.0948186000236765	0.7760856471475239	0.3889305067623725	T	T	T
0.3070400060000011	0.8298199769999997	0.3692500000000010	F	F	F
0.1995256929470847	0.5418691897968266	0.5118785752618061	T	T	T
0.0044699999999978	0.9602699880000003	0.2462999970000013	F	F	F
0.9031192781550552	0.6704762564360177	0.3943121366027578	T	T	T
0.4981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.4040623864161015	0.6520027179430876	0.5051609149071487	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999982	F	F	F
0.4351674418938171	0.8253506186619862	0.4636964390014927	T	T	T
0.9722499849999977	0.7798600200000010	0.2958799900000031	F	F	F
0.8795737627968205	0.9888974872383273	0.4497080673158632	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000013	F	F	F
0.4053636841122942	0.6722887662230032	0.3937928456300882	T	T	T
0.9981200100000009	0.9347699879999993	0.3632799980000030	F	F	F

0.9057587671081960	0.6506361740110761	0.5043552571241642	T	T	T
0.0303299999999993	0.6151900289999972	0.3136900069999982	F	F	F
0.9365292790720969	0.8237585490882476	0.4631633775109515	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3787758303713876	0.9904433385487399	0.4485446548767683	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999967	F	F	F
0.6324064852208625	0.8605333932247996	0.4897294915893217	T	T	T
0.7826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.6906727662035523	0.9685201044677937	0.4019368586754408	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999967	F	F	F
0.1320113098950708	0.8605659356829265	0.4917363099248643	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.1894146235608824	0.9678823522091090	0.4026663213618782	T	T	T
0.8641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.7805532844518227	0.3664977825884030	0.4622891478794942	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999986	F	F	F
0.5391115558775895	0.4528064300069916	0.4579568621870408	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999985	F	F	F
0.5467738962375958	0.2285756929959161	0.4778604162614175	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000016	F	F	F
0.7813292069027016	0.0922282647420413	0.4368309105678816	T	T	T
0.3641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.2769786681578418	0.3690622851347394	0.4587942332127390	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999986	F	F	F
0.0394970650486745	0.4520304014191606	0.4576331345095159	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999985	F	F	F
0.0469229229083222	0.2305143262198074	0.4779830723653555	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000016	F	F	F
0.2802854505495825	0.0939235245779344	0.4380781820833745	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.7825834632535612	0.8646650187947298	0.4643851342526230	T	T	T
0.6384199860000024	0.7358700039999988	0.3038099999999986	F	F	F
0.5382772798965689	0.9542804784074095	0.4615889324996929	T	T	T
0.6260200139999981	0.5126500129999982	0.3228900129999985	F	F	F
0.5497737504253279	0.7296798939255097	0.4796640996173003	T	T	T
0.8765599729999991	0.8823999760000021	0.2866800130000016	F	F	F
0.7769504280276177	0.5919947599378328	0.4401720628598146	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.2799640233336084	0.8664266818652984	0.4618546329196265	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999986	F	F	F
0.0392806712673564	0.9542182226434716	0.4615192627251586	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999985	F	F	F
0.0527133409869485	0.7267138537425857	0.4799437459611531	T	T	T
0.3765600030000016	0.8823999760000021	0.2866800130000016	F	F	F
0.2806408041975720	0.5945007034017834	0.4375331644866007	T	T	T
0.1667392435069100	0.4494368951830647	0.5805101680178634	T	T	T
0.1887670394691470	0.3607473075867444	0.5935685561450843	T	T	T
0.6386787550801902	0.5495182106851210	0.5938332505839301	T	T	T
0.6814126797173364	0.7349278048104364	0.6191372093652623	T	T	T
0.4321803302007873	0.4353085208851951	0.6001742764734970	T	T	T
0.1103801111684597	0.4816424963135194	0.6145959793608113	T	T	T

K₂O-Fe₅C₂(111)-CH+O (TS)

1.0000000000000000		
12.3812999725000008	0.0000000000000000	0.0000000000000000
-2.0391083097000000	13.2888646689000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.8052997588999986

Fe C O K H
80 33 2 2 1

Selective dynamics

Direct

0.8393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.7306414050622504	0.2206118151672305	0.4664770899571362	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999985	F	F	F
0.5611167046000941	0.0976048349576091	0.4382420287680687	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000003	F	F	F
0.5952307723846996	0.2777362230373902	0.3882585238032833	T	T	T
0.8070399759999987	0.3298200070000021	0.3692500000000010	F	F	F
0.6915683184535566	0.0405713231797488	0.5103865439429986	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.2370500053197900	0.2229329178736385	0.4686081352224919	T	T	T
0.1632599800000009	0.3849500119999973	0.2899999919999985	F	F	F
0.0605503317262058	0.0978552217354928	0.4384637816963022	T	T	T
0.1955399960000008	0.0652299970000030	0.2403199970000003	F	F	F
0.0978699924135017	0.2793893834597291	0.3898872972962781	T	T	T

0.3070400060000011	0.3298200070000021	0.3692500000000010	F	F	F
0.1851098034157037	0.0434330642411321	0.5106848548703995	T	T	T
0.0044699999999978	0.4602699880000003	0.2462999970000013	F	F	F
0.9060628898042691	0.1733021292292040	0.3945333172398631	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.4053770296175893	0.1551668411935885	0.5051711771908427	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999982	F	F	F
0.4358501309779897	0.3265411096748599	0.4603377739344860	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F
0.8788059944792961	0.4921550884442583	0.4472291321302843	T	T	T
0.5044699910000006	0.4602699880000003	0.2462999970000013	F	F	F
0.4045333304441452	0.1718368261078322	0.3941135648561611	T	T	T
0.9981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.8922717353038114	0.1464325964680685	0.5061067736033883	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999982	F	F	F
0.9294618176683189	0.3279899143746015	0.4622864970180814	T	T	T
0.4722500150000002	0.2798599899999985	0.2958799900000031	F	F	F
0.3796155603330925	0.4919753158354191	0.4438728170837726	T	T	T
0.7199699880000026	0.1401900050000009	0.3529999849999967	F	F	F
0.6301381543827946	0.3598055197496557	0.4917055371770735	T	T	T
0.7826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.6893215073276054	0.4681570768419182	0.4038536146195706	T	T	T
0.2199700030000002	0.1401900050000009	0.3529999849999967	F	F	F
0.1250212778609990	0.3550594791383896	0.5005455537843427	T	T	T
0.2826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.1858059604696915	0.4654673277697999	0.4056933284872801	T	T	T
0.8393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.7343530487957892	0.7208805489679928	0.4653909608557350	T	T	T
0.6632599830000032	0.8849499820000020	0.2899999919999985	F	F	F
0.5619021002141229	0.5985623552120057	0.4381896152308634	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000003	F	F	F
0.5943288493058143	0.7768169203492877	0.3879827327640346	T	T	T
0.8070399759999987	0.8298199769999997	0.3692500000000010	F	F	F
0.6861267552299033	0.5381170785900470	0.5167180134134708	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.2333873553947889	0.7205998784939497	0.4678865391142638	T	T	T
0.1632599800000009	0.8849499820000020	0.2899999919999985	F	F	F
0.0655545935652236	0.5949719280656983	0.4416461879910256	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000003	F	F	F
0.0953017143623198	0.7757499556473767	0.3891467113556809	T	T	T
0.3070400060000011	0.8298199769999997	0.3692500000000010	F	F	F
0.2185516041606422	0.5300856450943676	0.5141357586307236	T	T	T
0.0044699999999978	0.9602699880000003	0.2462999970000013	F	F	F
0.9049646884142735	0.6703695581144368	0.3944120522025386	T	T	T
0.4981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.4034172947442643	0.6520640040905470	0.5056015625701936	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999982	F	F	F
0.4357052736131647	0.8256399098496638	0.4635309524045220	T	T	T
0.9722499849999977	0.7798600200000010	0.2958799900000031	F	F	F
0.8778082748962438	0.9883678904828156	0.4490537983478342	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000013	F	F	F
0.4053289027639263	0.6720904129633488	0.3938337677922054	T	T	T
0.9981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.9061393700475392	0.6508519642234816	0.5049578706370772	T	T	T
0.0303299999999993	0.6151900289999972	0.3136900069999982	F	F	F
0.9369045028632212	0.8241824470274336	0.4638077851272145	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3794792803518172	0.9908643484254980	0.4488531248811257	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999967	F	F	F
0.6325029638145717	0.8603184076605593	0.4898034167814495	T	T	T
0.7826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.6897332630161859	0.9683466592188149	0.4018047360869874	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999967	F	F	F
0.1320975968221416	0.8616301539066124	0.4916446087860881	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.1903293469130921	0.9682564990699489	0.4029787830941960	T	T	T
0.8641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.7786472412696510	0.3691041009868571	0.4621979233130971	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999986	F	F	F
0.5394911770260502	0.4542198235645218	0.4580033188720107	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999985	F	F	F
0.5482809504950649	0.2291847730927604	0.4781070940209883	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000016	F	F	F
0.7791691024478670	0.0923849445881890	0.4354854341795095	T	T	T
0.3641700149999991	0.1591799999999992	0.3057599959999990	F	F	F

0.2704697503511599	0.3730441866869310	0.4573425710306402	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999986	F	F	F
0.0370746157084142	0.4494778508330776	0.4562174120891556	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999985	F	F	F
0.0250445917475867	0.2249894944654274	0.4698898142498977	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000016	F	F	F
0.2803240807099640	0.0943646902140700	0.4392018284104515	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.7829139727141914	0.8645141853057707	0.4647127945522957	T	T	T
0.6384199860000024	0.7358700039999988	0.3038099999999986	F	F	F
0.5387214869360262	0.9547099333166797	0.4617108556016564	T	T	T
0.6260200139999981	0.5126500129999982	0.3228900129999985	F	F	F
0.5498648229129216	0.7291259162445206	0.4789315067923186	T	T	T
0.8765599729999991	0.8823999760000021	0.2866800130000016	F	F	F
0.7771045530078501	0.5928365433159887	0.4392727551279526	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.2798841945010039	0.8667177372720279	0.4609001626836342	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999986	F	F	F
0.0374356716235793	0.9548112679906976	0.4623936265900111	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999985	F	F	F
0.0521540726568846	0.7275543460168722	0.4799993362653266	T	T	T
0.3765600030000016	0.8823999760000021	0.2866800130000016	F	F	F
0.2786114277298188	0.5955190811297897	0.4356003561248202	T	T	T
0.1709220364651589	0.4459090867558347	0.5841432639507436	T	T	T
0.1716932660946009	0.3322781494418534	0.5810441563709997	T	T	T
0.6429801310923025	0.5513762787543355	0.5936020015056227	T	T	T
0.6831392453070732	0.7366226630939228	0.6195969167523712	T	T	T
0.4264147001140509	0.4346216103140204	0.6011103756413870	T	T	T
0.1229022782387106	0.4535536514096498	0.6280727947241120	T	T	T

K₂O-Fe₅C₂(111)-CH+O (FS)

1.0000000000000000		
12.3812999725000008	0.0000000000000000	0.0000000000000000
-2.0391083097000000	13.2888646689000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.8052997588999986
Fe	C	O
80	33	2
2	2	1

Selective dynamics

Direct

0.8393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.7331044412867310	0.2201544737615972	0.4663654097934271	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999985	F	F	F
0.5597361606979292	0.0980554463267917	0.4380771095850452	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000003	F	F	F
0.5951489777519805	0.2770530427339059	0.3882688088458554	T	T	T
0.8070399759999987	0.3298200070000021	0.3692500000000010	F	F	F
0.6874442955078474	0.0412139370911360	0.5101681821122488	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.2352634948902089	0.2246427122228556	0.4718960655162243	T	T	T
0.1632599980000009	0.3849500119999973	0.2899999919999985	F	F	F
0.0572505102109469	0.0981608083354213	0.4372363522420515	T	T	T
0.1955399960000008	0.0652299970000030	0.2403199970000003	F	F	F
0.0930680054102530	0.2748197200481425	0.3928413833659732	T	T	T
0.3070400060000011	0.3298200070000021	0.3692500000000010	F	F	F
0.1849882606297706	0.0444302338239860	0.5093502625176473	T	T	T
0.0044699999999978	0.4602699880000003	0.2462999970000013	F	F	F
0.9036410215311423	0.1727262794460830	0.3937622917052713	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.4054719233963181	0.1557187673207669	0.5048032743428875	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999982	F	F	F
0.4369252966940752	0.3272974495233826	0.4608904227301241	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F
0.8795547419868688	0.4877422022592414	0.4475971222329537	T	T	T
0.5044699910000006	0.4602699880000003	0.2462999970000013	F	F	F
0.4038462191942541	0.1738465752211909	0.3942461497531880	T	T	T
0.9981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.8934592300373509	0.1442099292462733	0.5042976215093189	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999982	F	F	F
0.9385808183354428	0.3227594757935257	0.4646772902308136	T	T	T
0.4722500150000002	0.2798599899999985	0.2958799900000031	F	F	F
0.3793772782584632	0.4939032719266832	0.4448825351352773	T	T	T
0.7199699880000026	0.1401900050000009	0.3529999849999967	F	F	F
0.6339984751656762	0.3595298440606509	0.4908256422547591	T	T	T
0.7826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.6893443479501296	0.4697504894884869	0.4030206723388849	T	T	T

0.2199700030000002	0.1401900050000009	0.3529999849999967	F	F	F
0.1404388449069945	0.3740644792450558	0.5032819788356767	T	T	T
0.2826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.1894805839111073	0.4692270150243187	0.4050689655884239	T	T	T
0.8393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.7367179943650127	0.7191879709720205	0.4651805919271733	T	T	T
0.6632599830000032	0.8849499820000020	0.2899999919999985	F	F	F
0.5619825323215789	0.5981787918656242	0.4384322852492678	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000003	F	F	F
0.5951732398378103	0.7760463014826984	0.3882558777206603	T	T	T
0.8070399759999987	0.8298199769999997	0.3692500000000010	F	F	F
0.6912895987011806	0.5397588466569034	0.5162824459159092	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.2331219412962085	0.7227434187113286	0.4663923884478904	T	T	T
0.1632599800000009	0.8849499820000020	0.2899999919999985	F	F	F
0.0648344422842829	0.5946552617215679	0.4399756858049791	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000003	F	F	F
0.0947698288110028	0.7765529430323213	0.3890065401813669	T	T	T
0.3070400060000011	0.8298199769999997	0.3692500000000010	F	F	F
0.2101896920259482	0.5471585846917471	0.5181677086909809	T	T	T
0.0044699999999978	0.9602699880000003	0.2462999970000013	F	F	F
0.9045829118635953	0.6700176460624082	0.3940045934262699	T	T	T
0.4981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.4040840133824433	0.6522508582577190	0.5048301253919836	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999982	F	F	F
0.4361583894383726	0.8265864394769443	0.4637535370099810	T	T	T
0.9722499849999977	0.7798600200000010	0.2958799900000031	F	F	F
0.8776157724823863	0.9868260950793055	0.4488499974606270	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000013	F	F	F
0.4059703705274763	0.6739431927501242	0.3935616142899863	T	T	T
0.9981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.9103632566429429	0.6496189662955505	0.5039225114564200	T	T	T
0.0303299999999993	0.6151900289999972	0.3136900069999982	F	F	F
0.9384280543601367	0.8231051944819044	0.4634465792394135	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3785188698374685	0.9920720877175793	0.4485162900310216	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999967	F	F	F
0.6338668745790907	0.8595831407438222	0.4897186365442223	T	T	T
0.7826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.6897727035561703	0.9680160190691285	0.4017952253022858	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999967	F	F	F
0.1339316490605156	0.8631239042014833	0.4921712515704769	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.1895793009886680	0.9686765134493236	0.4028072446831106	T	T	T
0.8641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.7846788458043541	0.3651686776491380	0.4645865756117833	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999986	F	F	F
0.5418604527562002	0.4531778293028429	0.4569460952230345	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999985	F	F	F
0.5502760329284626	0.2299634629341408	0.4785430641884831	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000016	F	F	F
0.7784914300552022	0.0905169600291883	0.4362936460117129	T	T	T
0.3641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.2783105172575271	0.3717507817675426	0.4574852086089648	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999986	F	F	F
0.0399216348266280	0.4491222093715720	0.4547060649651003	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999985	F	F	F
0.0429419210927686	0.2208050149262178	0.4905806517006154	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000016	F	F	F
0.2795854146924039	0.0954190090607153	0.4389313403223411	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.7838680972866806	0.8627931682172437	0.4642336040693750	T	T	T
0.6384199860000024	0.7358700039999988	0.3038099999999986	F	F	F
0.5399321094752114	0.9540103002551023	0.4613236235662364	T	T	T
0.6260200139999981	0.5126500129999982	0.3228900129999985	F	F	F
0.5491021868717396	0.7296616278981476	0.4789287765377737	T	T	T
0.8765599729999991	0.8823999760000021	0.2866800130000016	F	F	F
0.7802212568082652	0.5903376699168005	0.4382588352016860	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.2828416604146461	0.8666835052985746	0.4625206299688177	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999986	F	F	F
0.0379814914540470	0.9546006152657559	0.4614984747612564	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999985	F	F	F
0.0577859586769623	0.7277162098456196	0.4803148621855960	T	T	T
0.3765600030000016	0.8823999760000021	0.2866800130000016	F	F	F

0.2793511328390225	0.5967905211597627	0.4362604598915668	T	T	T
0.1690865174964310	0.4464749022687176	0.5763141257943959	T	T	T
0.1142859164333330	0.2377474336334502	0.5415019864961635	T	T	T
0.6489067066190848	0.5527249875093464	0.5938465935867909	T	T	T
0.6870522950347089	0.7383283146730037	0.6185482716957013	T	T	T
0.4506910488588257	0.4450579502976327	0.6000812792566037	T	T	T
0.1518498918719815	0.4216616665775885	0.6264921308304343	T	T	T

COH formation and dissociation on K₂O-Fe₅C₂(111)

K₂O-Fe₅C₂(111)-COH (TS)

1.0000000000000000		
12.3812999725000008	0.0000000000000000	0.0000000000000000
-2.0391083097000000	13.2888646689000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.8052997588999986

Fe	C	O	K	H
80	33	2	2	1

Selective dynamics

Direct

0.8393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.7329566294512168	0.2193869225705334	0.4665987457055349	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999985	F	F	F
0.5608289574061605	0.0978998406959411	0.4387358343400017	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000003	F	F	F
0.5956678925594969	0.2768754448850163	0.3884110827065015	T	T	T
0.8070399759999987	0.3298200070000021	0.3692500000000010	F	F	F
0.6902360116551493	0.0406094484657183	0.5101587725651583	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.2353040999139264	0.2213630110301664	0.4672843236656170	T	T	T
0.1632599980000009	0.3849500119999973	0.2899999919999985	F	F	F
0.0607189466888097	0.0977865612666559	0.4398352405018767	T	T	T
0.1955399960000008	0.0652299970000030	0.2403199970000003	F	F	F
0.0960198024655469	0.2785718548780904	0.3896760290245286	T	T	T
0.3070400060000011	0.3298200070000021	0.3692500000000010	F	F	F
0.1884630628224320	0.0427030057852949	0.5104806868889665	T	T	T
0.0044699999999978	0.4602699880000003	0.2462999970000013	F	F	F
0.9059093124492633	0.1726646015264086	0.3941107485556118	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.4033271941498856	0.1538757017415834	0.5050923136520878	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999982	F	F	F
0.4350654848478315	0.3260513324340653	0.4613142958440750	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F
0.8779571168162860	0.4903582997761328	0.4470564331462602	T	T	T
0.5044699910000006	0.4602699880000003	0.2462999970000013	F	F	F
0.4050301181227274	0.1724179101768333	0.3940732044171827	T	T	T
0.9981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.9011406880623023	0.1492186296636126	0.5050314700573298	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999982	F	F	F
0.9323939229366137	0.3253632923916436	0.4624441012940463	T	T	T
0.4722500150000002	0.2798599899999985	0.2958799900000031	F	F	F
0.3781869074232743	0.4916629414286429	0.4460395146774564	T	T	T
0.7199699880000026	0.1401900050000009	0.3529999849999967	F	F	F
0.6314071395421265	0.3589658087214561	0.4905918545731844	T	T	T
0.7826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.6889202317259630	0.4687289311076668	0.4033358715439182	T	T	T
0.2199700030000002	0.1401900050000009	0.3529999849999967	F	F	F
0.1302177118423840	0.3597539331332964	0.4985641206190923	T	T	T
0.2826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.1884961396360272	0.4656942469457404	0.4037330948242832	T	T	T
0.8393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.7347595229147972	0.7203621298310132	0.4653795144692830	T	T	T
0.6632599830000032	0.8849499820000020	0.2899999919999985	F	F	F
0.5620131909924533	0.5977652562221093	0.4399170164216138	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000003	F	F	F
0.5946614306728646	0.7758705245898034	0.3882918204644085	T	T	T
0.8070399759999987	0.8298199769999997	0.3692500000000010	F	F	F
0.6944912472067644	0.5382450111205745	0.5169383065576089	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.2341300023367915	0.7216503607519075	0.4668968902066317	T	T	T
0.1632599980000009	0.8849499820000020	0.2899999919999985	F	F	F
0.0615701723907334	0.5955539672566673	0.4398794372445439	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000003	F	F	F
0.0951186311115687	0.7764880709321932	0.3888921253496166	T	T	T
0.3070400060000011	0.8298199769999997	0.3692500000000010	F	F	F
0.1988309450176103	0.5394684340429021	0.5102786792924846	T	T	T

0.004469999999978	0.9602699880000003	0.2462999970000013	F	F	F
0.9044430726243414	0.6714078016980458	0.3941574158211937	T	T	T
0.4981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.4004774825855956	0.6516523586434824	0.5064567448460453	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999982	F	F	F
0.4349881322743689	0.8264297036047936	0.4635658036380367	T	T	T
0.9722499849999977	0.7798600200000010	0.2958799900000031	F	F	F
0.8785401262062964	0.9892376362165832	0.4491690771297424	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000013	F	F	F
0.4063823926639646	0.6724547559552685	0.3942445558994724	T	T	T
0.9981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.9049207039737668	0.6495873157157257	0.5045379115999337	T	T	T
0.0303299999999993	0.6151900289999972	0.3136900069999982	F	F	F
0.9355483481932093	0.8243469949106622	0.4633653050075451	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3790820139859422	0.9913293720083372	0.4482501417011499	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999967	F	F	F
0.6317059773065115	0.8598785928616892	0.4896781573616971	T	T	T
0.7826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.6899606498794634	0.9682322217289473	0.4020215375987169	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999967	F	F	F
0.1314101727448359	0.8605892863484109	0.4915937575331045	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.1896183031771904	0.9675872004941087	0.4026808495716908	T	T	T
0.8641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.7805120494743361	0.3671577576621788	0.4627354739377335	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999986	F	F	F
0.5387314270252532	0.4525308087291196	0.4576830623559672	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999985	F	F	F
0.5466646006669365	0.2294376935533715	0.4782603955997505	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000016	F	F	F
0.7803191706122872	0.0919791439184331	0.4363949010020063	T	T	T
0.3641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.2775634779078373	0.3675363477903444	0.4601501371421330	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999986	F	F	F
0.0365523421926764	0.4509202265584764	0.4572634272386693	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999985	F	F	F
0.0423200263030785	0.2293364863983668	0.4764530052657013	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000016	F	F	F
0.2798378175616417	0.0936164227792005	0.4375254806099999	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.7820671569452494	0.8650834155537609	0.4642305657598733	T	T	T
0.6384199860000024	0.7358700039999988	0.3038099999999986	F	F	F
0.5386489443308924	0.9543256441126059	0.4614734245717528	T	T	T
0.6260200139999981	0.5126500129999982	0.3228900129999985	F	F	F
0.5455499896901725	0.7293476274025649	0.4791697292070133	T	T	T
0.8765599729999991	0.8823999760000021	0.2866800130000016	F	F	F
0.7777547004171068	0.5924064054676953	0.4378709297095183	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.2801126087494865	0.8666576186794974	0.4620612889791578	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999986	F	F	F
0.0376788866892981	0.9534815746536798	0.4614112766627874	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999985	F	F	F
0.0494083097468130	0.7281674322964204	0.4793111168018647	T	T	T
0.3765600030000016	0.8823999760000021	0.2866800130000016	F	F	F
0.2803028026856321	0.5945135099855738	0.4364526334239512	T	T	T
0.1744751627773140	0.4120553251152939	0.5710590245268163	T	T	T
0.2324537842103752	0.4600549960766976	0.6177663594517971	T	T	T
0.6568542717649458	0.5521366595905346	0.5951825355672791	T	T	T
0.6863439629980855	0.7384798233186844	0.6184411766820244	T	T	T
0.4694952676045258	0.4338320619737342	0.6043853897872469	T	T	T
0.2719593393459823	0.5320153162281862	0.5988977504465596	T	T	T

K₂O-Fe₅C₂(111)-COH (FS)

1.0000000000000000		
12.3812999725000008	0.0000000000000000	0.0000000000000000
-2.0391083097000000	13.2888646689000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.8052997588999986
Fe	C	O
80	33	2
2	2	1
Selective dynamics		
Direct		
0.8393200040000011	0.0101000000000013	0.3195700050000028

0.7337539495693225	0.2194035026713161	0.4662285724019714	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999985	F	F	F
0.5598792278795792	0.0980672391189972	0.4385768166959615	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000003	F	F	F
0.5959066639175394	0.2769282173071274	0.3884716015735981	T	T	T
0.8070399759999987	0.3298200070000021	0.3692500000000010	F	F	F
0.6894482123572566	0.0420239843981849	0.5094146157597859	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.2309995677078772	0.2224297768802249	0.4680858653090637	T	T	T
0.1632599980000009	0.3849500119999973	0.2899999919999985	F	F	F
0.0605073230476770	0.0987408575073765	0.4394550358583418	T	T	T
0.1955399960000008	0.0652299970000030	0.2403199970000003	F	F	F
0.0941836921180998	0.2772891807615134	0.3888934872816942	T	T	T
0.3070400060000011	0.3298200070000021	0.3692500000000010	F	F	F
0.1883771351634800	0.0436481113064099	0.5106925846635599	T	T	T
0.0044699999999978	0.4602699880000003	0.2462999970000013	F	F	F
0.9051882924325357	0.1720300610174963	0.3939634157883960	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.4022967193508346	0.1545152515699557	0.5049430681436593	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999982	F	F	F
0.4352498061423252	0.3263830012301234	0.4612738464505163	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F
0.8788034989693794	0.4893477482633860	0.4474604250564010	T	T	T
0.5044699910000006	0.4602699880000003	0.2462999970000013	F	F	F
0.4045449545476708	0.1731606262298599	0.3940987398875323	T	T	T
0.9981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.9058813416136557	0.1512639612222379	0.5048408281743568	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999982	F	F	F
0.9360245215638316	0.3243543713400076	0.4627500582120726	T	T	T
0.4722500150000002	0.2798599899999985	0.2958799900000031	F	F	F
0.3779432846194720	0.4923900021191426	0.4455996486064906	T	T	T
0.7199699880000026	0.1401900050000009	0.3529999849999967	F	F	F
0.6320702248024010	0.3585203836427925	0.4906629169440769	T	T	T
0.7826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.6894600587081368	0.4685888743528682	0.4033705844365434	T	T	T
0.2199700030000002	0.1401900050000009	0.3529999849999967	F	F	F
0.1330262647909245	0.3633115453517172	0.4986157601398636	T	T	T
0.2826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.1890813341649526	0.4671435705614852	0.4039606855618114	T	T	T
0.8393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.7345241597979583	0.7195996792033335	0.4654230303375982	T	T	T
0.6632599830000032	0.8849499820000020	0.2899999919999985	F	F	F
0.5619866740971468	0.5979485382843451	0.4389001599654999	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000003	F	F	F
0.5945282433628760	0.7759442483692237	0.3881017881976703	T	T	T
0.8070399759999987	0.8298199769999997	0.3692500000000010	F	F	F
0.6914289904427529	0.5375865992070566	0.5165961765265603	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.2329610227859898	0.7207495100073282	0.4680026968169850	T	T	T
0.1632599980000009	0.8849499820000020	0.2899999919999985	F	F	F
0.0646363451835747	0.5949284254078795	0.4400724607764691	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000003	F	F	F
0.0951183582365547	0.7762311846087535	0.3891148393536909	T	T	T
0.3070400060000011	0.8298199769999997	0.3692500000000010	F	F	F
0.2051967741820714	0.5362567309797073	0.5160274780873249	T	T	T
0.0044699999999978	0.9602699880000003	0.2462999970000013	F	F	F
0.9044937091373986	0.6705173272432237	0.3941837289331871	T	T	T
0.4981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.4037912517008012	0.6520147813065283	0.5049343423974725	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999982	F	F	F
0.4359694639918870	0.8259638913320428	0.4635472271723404	T	T	T
0.9722499849999977	0.7798600200000010	0.2958799900000031	F	F	F
0.8793354880163946	0.9883005328596469	0.4500463975906332	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000013	F	F	F
0.4051521535152941	0.6724866090930874	0.3938092050458918	T	T	T
0.9981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.9083397034677032	0.6497353262841037	0.5041598270360403	T	T	T
0.0303299999999993	0.6151900289999972	0.3136900069999982	F	F	F
0.9372562712263022	0.8233248918999057	0.4632907009519475	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3784003128035945	0.9910478367526531	0.4487043553605808	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999967	F	F	F
0.6333859524035249	0.8603936583095289	0.4895362361031660	T	T	T
0.7826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.6904512821829636	0.9686223875131055	0.4018183418239621	T	T	T

0.2199700030000002	0.6401900050000009	0.3529999849999967	F	F	F
0.1329303115643722	0.8615572615447289	0.4918491431555852	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.1894146760523966	0.9680486024890123	0.4027121025381428	T	T	T
0.8641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.7824845284936823	0.3662119469623317	0.4634104737320316	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999986	F	F	F
0.5400113357236429	0.4528979159770968	0.4576948294014942	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999985	F	F	F
0.5466024324980137	0.2294233819098369	0.4782768680707373	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000016	F	F	F
0.7819466719998618	0.0917710125842879	0.4371517153276023	T	T	T
0.3641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.2786744524719469	0.3684782952923474	0.4599662227879343	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999986	F	F	F
0.0381967230166402	0.4510377780540439	0.4561007583726330	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999985	F	F	F
0.0519023152609556	0.2311416048902512	0.4809673499060390	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000016	F	F	F
0.2793220947471118	0.0946662101921869	0.4378812625461617	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.7836813639284791	0.8634924905964277	0.4646927715799046	T	T	T
0.6384199860000024	0.7358700039999988	0.3038099999999986	F	F	F
0.5390764089731535	0.9543529852057384	0.4615110085425722	T	T	T
0.6260200139999981	0.5126500129999982	0.3228900129999985	F	F	F
0.5497236664972126	0.7297775842372288	0.4793815020284236	T	T	T
0.8765599729999991	0.8823999760000021	0.2866800130000016	F	F	F
0.7787089192056057	0.5918300096568391	0.4388464970350071	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.2808960665716749	0.8661122993053482	0.4623009195331433	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999986	F	F	F
0.0390055255383699	0.9541910725838418	0.4615902805608751	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999985	F	F	F
0.0550882268220211	0.7273843898969495	0.4807056766442003	T	T	T
0.3765600030000016	0.8823999760000021	0.2866800130000016	F	F	F
0.2777364963928806	0.5951651788481812	0.4374863361416528	T	T	T
0.1693791510437575	0.4262018901282359	0.5733875445932661	T	T	T
0.1740437474819199	0.4031781886011869	0.6362089931052820	T	T	T
0.6510370573330461	0.5519398816137924	0.5943595930025487	T	T	T
0.6875059775041613	0.7380276708164396	0.6180260196454483	T	T	T
0.4550043713283799	0.4403338867225612	0.6003900854633027	T	T	T
0.1893354378619743	0.4661715207321485	0.6607703794571765	T	T	T

K₂O-Fe₃C₂(111)-C+OH (TS)

1.0000000000000000		
12.381299725000008	0.0000000000000000	0.0000000000000000
-2.0391083097000000	13.2888646689000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.8052997588999986
Fe	C	O
80	33	2
2	2	1

Selective dynamics

Direct

0.8393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.7318198539671160	0.2197828572059960	0.4661896565649698	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999985	F	F	F
0.5592170766504734	0.0984153224409379	0.4384562939643048	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000003	F	F	F
0.5949270419320134	0.2768802068900626	0.3884240949738665	T	T	T
0.8070399759999987	0.3298200070000021	0.3692500000000010	F	F	F
0.6887147741400713	0.0429846811102824	0.5097005838668843	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.2304670914780281	0.2230914562807739	0.4681330124479890	T	T	T
0.1632599980000009	0.3849500119999973	0.2899999919999985	F	F	F
0.0600373276987236	0.0984755746658359	0.4392297179841271	T	T	T
0.1955399960000008	0.0652299970000030	0.2403199970000003	F	F	F
0.0931480981619598	0.2770122147505029	0.3888595496528144	T	T	T
0.3070400060000011	0.3298200070000021	0.3692500000000010	F	F	F
0.1877070443556073	0.0432332749593100	0.5105999098169255	T	T	T
0.0044699999999978	0.4602699880000003	0.2462999970000013	F	F	F
0.9048414177433797	0.1718448234351725	0.3940295628610804	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.4020058269033682	0.1545101281435630	0.5050454618358526	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999982	F	F	F
0.4337833508844472	0.3266654769940237	0.4615534028362716	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F

0.8784111405814086	0.4891685658018590	0.4477335205279346	T	T	T
0.5044699910000006	0.4602699880000003	0.2462999970000013	F	F	F
0.4039605393441458	0.1734467828897725	0.3942216348456712	T	T	T
0.9981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.9031522570839489	0.1501737107236475	0.5050056510093418	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999982	F	F	F
0.9329519976968951	0.3237748539896071	0.4619570627596991	T	T	T
0.4722500150000002	0.2798599899999985	0.2958799900000031	F	F	F
0.3800935582324250	0.4921423016802580	0.4452150183688139	T	T	T
0.7199699880000026	0.1401900050000009	0.3529999849999967	F	F	F
0.6308405760769656	0.3589139616611329	0.4909776456456557	T	T	T
0.7826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.6893022590946288	0.4682432975441385	0.4033785546095006	T	T	T
0.2199700030000002	0.1401900050000009	0.3529999849999967	F	F	F
0.1291619458722603	0.3644203964641890	0.4984896103884857	T	T	T
0.2826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.1888143944479842	0.4674933162401026	0.4054702956551182	T	T	T
0.8393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.7342499154769833	0.7202924449734756	0.4653240723632772	T	T	T
0.6632599830000032	0.8849499820000020	0.2899999919999985	F	F	F
0.5635429575998885	0.5979787633853508	0.4390428843966196	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000003	F	F	F
0.5940018880427521	0.7766550500960159	0.3881864569244363	T	T	T
0.8070399759999987	0.8298199769999997	0.3692500000000010	F	F	F
0.6951874053227062	0.5382095372039873	0.5172611872537995	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.2324549200607449	0.7206355960571096	0.4687976856991539	T	T	T
0.1632599980000009	0.8849499820000020	0.2899999919999985	F	F	F
0.0668689525076719	0.5949097040351802	0.4414014713166817	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000003	F	F	F
0.0950287081091521	0.7762085715878388	0.3891415231521937	T	T	T
0.3070400060000011	0.8298199769999997	0.3692500000000010	F	F	F
0.2319473232898394	0.5368375513024773	0.5196096461214582	T	T	T
0.0044699999999978	0.9602699880000003	0.2462999970000013	F	F	F
0.9050138617885980	0.6695230350968492	0.3942332952010755	T	T	T
0.4981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.4101761061268756	0.6561151965687494	0.5057524455510594	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999982	F	F	F
0.4369821171656759	0.8265041366922123	0.4626010584724449	T	T	T
0.9722499849999977	0.7798600200000010	0.2958799900000031	F	F	F
0.8791616615897194	0.9880414093616501	0.4500909878923341	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000013	F	F	F
0.4043548083965891	0.6712812370951330	0.3941346472958711	T	T	T
0.9981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.9077994925831256	0.6492095388764096	0.5044647539905416	T	T	T
0.0303299999999993	0.6151900289999972	0.3136900069999982	F	F	F
0.9380343588416316	0.8231003240068570	0.4634394369882610	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3788308312092900	0.9914081869277874	0.4485082781144258	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999967	F	F	F
0.6350390663670750	0.8616254104480949	0.4902391265274278	T	T	T
0.7826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.6903306493636746	0.9687973552465510	0.4018224736633678	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999967	F	F	F
0.1335916286294229	0.8615724951003202	0.4918891653783153	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.1899330771729170	0.9683126399220305	0.4028527013034274	T	T	T
0.8641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.7803663128132321	0.3673652652010685	0.4633185250578235	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999986	F	F	F
0.5402698676263903	0.4534248848904912	0.4578024438557871	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999985	F	F	F
0.5463576121339824	0.2296283276753913	0.4787956202574045	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000016	F	F	F
0.7813701166054781	0.0918316872333153	0.4373524881274481	T	T	T
0.3641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.2753995989608794	0.3709894554911138	0.4605618031804776	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999986	F	F	F
0.0333410273159472	0.4490268031700078	0.4549416662168128	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999985	F	F	F
0.0472225944881548	0.2301511900924919	0.4794397221436549	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000016	F	F	F
0.2791688881617935	0.0948872374942898	0.4382484499733157	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.7845974946665891	0.8634119142552485	0.4650248671727497	T	T	T

0.6384199860000024	0.7358700039999988	0.3038099999999986	F	F	F
0.5405464315060503	0.9549699232887834	0.4612304063959111	T	T	T
0.6260200139999981	0.5126500129999982	0.3228900129999985	F	F	F
0.5568630446885063	0.7300761529936538	0.4801293343566659	T	T	T
0.8765599729999991	0.8823999760000021	0.2866800130000016	F	F	F
0.7780650455852171	0.5924256008821638	0.4382793539168057	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.2812696371816876	0.8662596428574754	0.4618256668560597	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999986	F	F	F
0.0391631765725074	0.9537779581847049	0.4618976767114105	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999985	F	F	F
0.0546978091271965	0.7280332247913323	0.4810308391114425	T	T	T
0.3765600030000016	0.8823999760000021	0.2866800130000016	F	F	F
0.2767527052049502	0.5955315614554449	0.4376100817604276	T	T	T
0.1533062914165648	0.4322606222216350	0.5692822037531126	T	T	T
0.2739688832340375	0.4958096656207617	0.6108849567708761	T	T	T
0.6578429501785161	0.5537406743064028	0.5953567736128345	T	T	T
0.6920654707696131	0.7396239774341903	0.6189060730427398	T	T	T
0.4667889200141366	0.4349224211127091	0.6059454110988778	T	T	T
0.2338234812776218	0.5314860389061751	0.6413537935767974	T	T	T

K₂O-Fe₃C₂(111)-C+OH (FS)

1.0000000000000000		
12.3812999725000008	0.0000000000000000	0.0000000000000000
-2.0391083097000000	13.2888646689000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.8052997588999986

Fe C O K H
80 33 2 2 1

Selective dynamics

Direct

0.8393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.7292107070763995	0.2182675382416011	0.4666433987879464	T	T	T
0.6632599830000032	0.3849500119999973	0.2899999919999985	F	F	F
0.5626588811380655	0.0966175705244741	0.4374743701110941	T	T	T
0.6955400109999985	0.0652299970000030	0.2403199970000003	F	F	F
0.5978269672539206	0.2771948216648213	0.3884375642121928	T	T	T
0.8070399759999987	0.3298200070000021	0.3692500000000010	F	F	F
0.6920042810021999	0.0392688942350471	0.5105781184830431	T	T	T
0.3393200040000011	0.0101000000000013	0.3195700050000028	F	F	F
0.2409600264375162	0.2155188997963037	0.4651618316443426	T	T	T
0.1632599800000009	0.3849500119999973	0.2899999919999985	F	F	F
0.0604672789933350	0.0968143729021865	0.4395815688549064	T	T	T
0.1955399960000008	0.0652299970000030	0.2403199970000003	F	F	F
0.0975241499893947	0.2764371264224955	0.3904167911672564	T	T	T
0.3070400060000011	0.3298200070000021	0.3692500000000010	F	F	F
0.1908014919947353	0.0431589930958551	0.5098883542196991	T	T	T
0.0044699999999978	0.4602699880000003	0.2462999970000013	F	F	F
0.9062089851092825	0.1712356624710502	0.3948029675688816	T	T	T
0.4981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.4116274559878598	0.1506659076020957	0.5042313432851685	T	T	T
0.5303300019999995	0.1151899990000018	0.3136900069999982	F	F	F
0.4488170932513458	0.3227492470461607	0.4602896468782762	T	T	T
0.9722499849999977	0.2798599899999985	0.2958799900000031	F	F	F
0.8768158275945980	0.4917088267039436	0.4485718762221808	T	T	T
0.5044699910000006	0.4602699880000003	0.2462999970000013	F	F	F
0.4060705700077520	0.1717435398203033	0.3932159162810898	T	T	T
0.9981200100000009	0.4347699879999993	0.3632799980000030	F	F	F
0.8911837838510389	0.1446752792836518	0.5066830201111198	T	T	T
0.0303299999999993	0.1151899990000018	0.3136900069999982	F	F	F
0.9223851077846044	0.3234657773812997	0.4613325066996748	T	T	T
0.4722500150000002	0.2798599899999985	0.2958799900000031	F	F	F
0.3844744481369168	0.4941117629952638	0.4465606769807187	T	T	T
0.7199699880000026	0.1401900050000009	0.3529999849999967	F	F	F
0.6360899524560263	0.3604046086425025	0.4932659601515308	T	T	T
0.7826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.6889225013444019	0.4692541811470605	0.4033325370945186	T	T	T
0.2199700030000002	0.1401900050000009	0.3529999849999967	F	F	F
0.1072331199246049	0.3520059871214757	0.4955815031076818	T	T	T
0.2826200129999989	0.2548600140000019	0.2565700110000009	F	F	F
0.1832318620638319	0.4683201414619335	0.4093052534324845	T	T	T
0.8393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.7339988685946812	0.7211615301056519	0.4647105360619905	T	T	T
0.6632599830000032	0.8849499820000020	0.2899999919999985	F	F	F
0.5628116696230501	0.5981346865925675	0.4377210107761342	T	T	T
0.6955400109999985	0.5652300120000007	0.2403199970000003	F	F	F

0.5946688641831142	0.7775643166204038	0.3876399519821979	T	T	T
0.8070399759999987	0.8298199769999997	0.3692500000000010	F	F	F
0.6895100027945134	0.5395782918745036	0.5169355017357098	T	T	T
0.3393200040000011	0.5101000069999984	0.3195700050000028	F	F	F
0.2344165127013002	0.7246899773403286	0.4652313375769731	T	T	T
0.1632599800000009	0.8849499820000020	0.2899999919999985	F	F	F
0.0637282521320427	0.5954930008412761	0.4424481051144148	T	T	T
0.1955399960000008	0.5652300120000007	0.2403199970000003	F	F	F
0.0937486769941304	0.7758218253547767	0.3890781013218753	T	T	T
0.3070400060000011	0.8298199769999997	0.3692500000000010	F	F	F
0.2341205860914149	0.5561084616948698	0.5165779549194264	T	T	T
0.0044699999999978	0.9602699880000003	0.2462999970000013	F	F	F
0.9042357997329494	0.6702922691101231	0.3943676619740723	T	T	T
0.4981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.4167693524876573	0.6608152507135615	0.5123121900712676	T	T	T
0.5303300019999995	0.6151900289999972	0.3136900069999982	F	F	F
0.4375158087799130	0.8256946642503019	0.4627522788395406	T	T	T
0.9722499849999977	0.7798600200000010	0.2958799900000031	F	F	F
0.8783513617280780	0.9872540055450170	0.4493446438553801	T	T	T
0.5044699910000006	0.9602699880000003	0.2462999970000013	F	F	F
0.4057343351648541	0.6717059634966167	0.3949419127985487	T	T	T
0.9981200100000009	0.9347699879999993	0.3632799980000030	F	F	F
0.9066540987929784	0.6516277500607333	0.5048485226512736	T	T	T
0.0303299999999993	0.6151900289999972	0.3136900069999982	F	F	F
0.9383032115334579	0.8232971925125412	0.4640432422520138	T	T	T
0.4722500150000002	0.7798600200000010	0.2958799900000031	F	F	F
0.3811807297210744	0.9905896883772384	0.4486839372414275	T	T	T
0.7199699880000026	0.6401900050000009	0.3529999849999967	F	F	F
0.6349407517516508	0.8613033043193764	0.4903193172478284	T	T	T
0.7826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.6901435904307476	0.9683694899094378	0.4014432787677767	T	T	T
0.2199700030000002	0.6401900050000009	0.3529999849999967	F	F	F
0.1338828946354609	0.8613876851422627	0.4919138090685696	T	T	T
0.2826200129999989	0.7548599839999994	0.2565700110000009	F	F	F
0.1898149541028991	0.9676292910828878	0.4024924879121236	T	T	T
0.8641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.7790362597771879	0.3665200647088751	0.4620764652864813	T	T	T
0.6384199860000024	0.2358700039999988	0.3038099999999986	F	F	F
0.5481351744293007	0.4547663058749278	0.4583273995621158	T	T	T
0.6260200139999981	0.0126500000000007	0.3228900129999985	F	F	F
0.5593323906348723	0.2272242540326228	0.4802856839742641	T	T	T
0.8765599729999991	0.3824000059999975	0.2866800130000016	F	F	F
0.7797645972715239	0.0908883207265016	0.4354304074140116	T	T	T
0.3641700149999991	0.1591799999999992	0.3057599959999990	F	F	F
0.3063807438536066	0.3532156915324646	0.4737615384804874	T	T	T
0.1384200010000001	0.2358700039999988	0.3038099999999986	F	F	F
0.0258762215705820	0.4486958238678315	0.4565617631290485	T	T	T
0.1260199990000004	0.0126500000000007	0.3228900129999985	F	F	F
0.0249455459342227	0.2232255505035644	0.4738606705067884	T	T	T
0.3765600030000016	0.3824000059999975	0.2866800130000016	F	F	F
0.2835397947798926	0.0901040264836146	0.4358132087006421	T	T	T
0.8641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.7851633916747356	0.8635442962361823	0.4661961834757094	T	T	T
0.6384199860000024	0.7358700039999988	0.3038099999999986	F	F	F
0.5413761357269513	0.9543192269363331	0.4610419167250171	T	T	T
0.6260200139999981	0.5126500129999982	0.3228900129999985	F	F	F
0.5571188852162692	0.7298935028879572	0.4784443626753614	T	T	T
0.8765599729999991	0.8823999760000021	0.2866800130000016	F	F	F
0.7764106583696468	0.5935656633858416	0.4388297575013099	T	T	T
0.3641700149999991	0.6591799859999981	0.3057599959999990	F	F	F
0.2834758850060921	0.8682333158506580	0.4634118697840436	T	T	T
0.1384200010000001	0.7358700039999988	0.3038099999999986	F	F	F
0.0395588861358628	0.9529039404584985	0.4605540969867554	T	T	T
0.1260199990000004	0.5126500129999982	0.3228900129999985	F	F	F
0.0570702105520925	0.7280177369705395	0.4824204370120985	T	T	T
0.3765600030000016	0.8823999760000021	0.2866800130000016	F	F	F
0.2788973666511748	0.5981210880700121	0.4335925565512753	T	T	T
0.2510412154494672	0.4226935858475674	0.5036682806831783	T	T	T
0.3309399780024779	0.6113669355821811	0.5911691539289586	T	T	T
0.6545729333806546	0.5584621819649249	0.5950326520026599	T	T	T
0.6971509641059628	0.7448571878974550	0.6184544044946215	T	T	T
0.4547218011249520	0.4558967426578396	0.6045284691125434	T	T	T
0.3035150467682105	0.6687394770383179	0.6105451338233004	T	T	T

CO dissociation on Fe₃C₂(010)

Fe₅C₂(010)-CO (IS)

1.000000000000000
 9.9837999344000004 0.000000000000000 0.000000000000000
 -1.5315638797000000 11.4316603084999997 0.000000000000000
 0.000000000000000 0.000000000000000 18.9298000335999994

Fe C O

40 17 1

Selective dynamics

Direct

0.03714999999999969	0.25363000000000011	0.2882999999999996	F	F	F
0.09747999999999973	0.68397000000000022	0.2882999999999996	F	F	F
0.53714999999999969	0.25363000000000011	0.2882999999999996	F	F	F
0.59747999999999973	0.68397000000000022	0.2882999999999996	F	F	F
0.48413999999999965	0.87116000000000033	0.28837999999999965	F	F	F
0.15048999999999978	0.06642999999999969	0.28837999999999965	F	F	F
0.98413999999999965	0.87116000000000033	0.28837999999999965	F	F	F
0.65048999999999978	0.06642999999999969	0.28837999999999965	F	F	F
0.06730999999999991	0.46880000000000017	0.29153999999999977	F	F	F
0.56730999999999991	0.46880000000000017	0.29153999999999977	F	F	F
0.31730999999999991	0.46880000000000017	0.32540999999999980	F	F	F
0.81730999999999991	0.46880000000000017	0.32540999999999980	F	F	F
0.40048999999999978	0.06642999999999969	0.32858000000000023	F	F	F
0.23413999999999965	0.87116000000000033	0.32858000000000023	F	F	F
0.90048999999999978	0.06642999999999969	0.32858000000000023	F	F	F
0.73413999999999965	0.87116000000000033	0.32858000000000023	F	F	F
0.34747999999999973	0.68397000000000022	0.32865000000000032	F	F	F
0.28714999999999969	0.25363000000000011	0.32865000000000032	F	F	F
0.84747999999999973	0.68397000000000022	0.32865000000000032	F	F	F
0.78714999999999969	0.25363000000000011	0.32865000000000032	F	F	F
0.4762044730107608	0.3722816360571026	0.4027684561034486	T	T	T
0.9788356437759337	0.3720992036040934	0.4048091704311627	T	T	T
0.1546219377349346	0.5625679013689526	0.4051586857812285	T	T	T
0.6520218792452200	0.5640329840008947	0.4062685310276010	T	T	T
0.0388051019852389	0.7481311722710141	0.4090389527035305	T	T	T
0.5393433675644547	0.7483080532818444	0.4082604137697375	T	T	T
0.0957818815477808	0.1896741136677762	0.4085716385864329	T	T	T
0.5953320525986451	0.1896668308473412	0.4087438939972077	T	T	T
0.5675199130048708	0.9688861863340528	0.4124412507721120	T	T	T
0.0673554863785526	0.9688465423119053	0.4119882985072785	T	T	T
0.8178329991705966	0.9670983197851925	0.4352549372825679	T	T	T
0.3175182323728279	0.9686119093004423	0.4354771880826911	T	T	T
0.7819969625418367	0.7406765776781864	0.4464970853521638	T	T	T
0.3505081044486266	0.1939224746133026	0.4448933165800159	T	T	T
0.2835265150762146	0.7430757884730737	0.4439556084279158	T	T	T
0.8502475362916101	0.1941708427968825	0.4445517436747867	T	T	T
0.9010288809441912	0.5584084246338014	0.4439032269486787	T	T	T
0.3960658973650255	0.5600055986941747	0.4460213166105434	T	T	T
0.2356267476665810	0.3771790671724446	0.4461460918890606	T	T	T
0.7351393702562190	0.3781921753389023	0.4456639790636260	T	T	T
0.23203000000000017	0.5823099999999997	0.26413000000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.26413000000000015	F	F	F
0.73203000000000017	0.5823099999999997	0.26413000000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.26413000000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.35282000000000012	F	F	F
0.48203000000000017	0.5823099999999997	0.35282000000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.35282000000000012	F	F	F
0.98203000000000017	0.5823099999999997	0.35282000000000012	F	F	F
0.9056288024993390	0.8483870482082773	0.3840293145992139	T	T	T
0.2287885063275983	0.0866896413500354	0.3834085456052562	T	T	T
0.7281952011248413	0.0866150608955452	0.3833216675616727	T	T	T
0.4065286381385818	0.8513407419886913	0.3832174197129511	T	T	T
0.6662478047401946	0.8556260480930737	0.4529028195147528	T	T	T
0.4678328836471448	0.0822257356155867	0.4534290310098281	T	T	T
0.1670524256909389	0.8553073730647816	0.4529891418508145	T	T	T
0.9675115346087795	0.0819540741763255	0.4526264903319331	T	T	T
0.7262976006208822	0.5583922335506308	0.4984547984993974	T	T	T
0.7091301786351888	0.5517241298754791	0.5617869192755069	T	T	T

Fe₅C₂(010)-C+O (TS)

1.000000000000000
 9.9837999344000004 0.000000000000000 0.000000000000000
 -1.5315638797000000 11.4316603084999997 0.000000000000000
 0.000000000000000 0.000000000000000 18.9298000335999994

Fe C O

40 17 1
 Selective dynamics
 Direct

0.0371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4767343048655667	0.3733458191493576	0.4037540979222065	T	T	T
0.9793463335598381	0.3753677636787885	0.4056118961111351	T	T	T
0.1545505063018872	0.5633374007850874	0.4059962035426737	T	T	T
0.6546889887604613	0.5709288249991611	0.4031479760385009	T	T	T
0.0421818479996796	0.7498185494240729	0.4075719176553649	T	T	T
0.5409942343140872	0.7499897680282090	0.4081708691679732	T	T	T
0.0955425844315474	0.1907581671777571	0.4084313893985599	T	T	T
0.5955043290740378	0.1893561934013936	0.4089467639372462	T	T	T
0.5674597212088980	0.9694272941022233	0.4125387863051381	T	T	T
0.0677041298426035	0.9695680958454757	0.4116427913250129	T	T	T
0.8175358154208094	0.9686115938767259	0.4351005866925911	T	T	T
0.3175475679544377	0.9696610020001525	0.4353889169462055	T	T	T
0.7877933124788530	0.7500517790525902	0.4501163932652013	T	T	T
0.3503033592549633	0.1943728665525876	0.4453810331388501	T	T	T
0.2850917988724475	0.7442264564601030	0.4441621723679527	T	T	T
0.8503224120969024	0.1944731174066287	0.4447617405326887	T	T	T
0.8992952558726178	0.5644208791684833	0.4451035575689505	T	T	T
0.3972991067518278	0.5606840104971680	0.4464994413238469	T	T	T
0.2362434270725948	0.3775261523577622	0.4455679149064182	T	T	T
0.7345437864762411	0.3756838357804205	0.4444225821044419	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9056492733813870	0.8486520234670332	0.3843292372539683	T	T	T
0.2289265288781121	0.0875696566117234	0.3836098971672494	T	T	T
0.7279024399716784	0.0870483438200975	0.3832458003318940	T	T	T
0.4071806991120597	0.8524370690191579	0.3831871074919276	T	T	T
0.6662772107770153	0.8570988088430134	0.4549831367655860	T	T	T
0.4680270409762426	0.0827269539814964	0.4538997922014484	T	T	T
0.1682219815532988	0.8570672342423117	0.4533066902427824	T	T	T
0.9676028286570940	0.0821617072951145	0.4520745224663476	T	T	T
0.7109662471256913	0.5146733377135133	0.4846898419749708	T	T	T
0.8274713967895121	0.6520061576156055	0.5174417191743770	T	T	T

Fe₅C₂(010)C+O (FS)

1.000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O

40 17 1
 Selective dynamics
 Direct

0.0371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F

0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4773104199990418	0.3736082009331992	0.4038758252063042	T	T	T
0.9799110287450689	0.3753632992524011	0.4055163323347247	T	T	T
0.1571002521768622	0.5644371041915390	0.4043226908412414	T	T	T
0.6542747377004481	0.5701644631730823	0.4051098047758257	T	T	T
0.0375682795415846	0.7502235385852368	0.4151902143013800	T	T	T
0.5414630717959573	0.7503482120405329	0.4073474081834591	T	T	T
0.0948909857546144	0.1918645998167047	0.4086586978090513	T	T	T
0.5959348154483830	0.1889935924157265	0.4090589388867543	T	T	T
0.5678679755538222	0.9700778759003295	0.4130378019921166	T	T	T
0.0694801203181126	0.9719690671984577	0.4104396599824071	T	T	T
0.8187228669561754	0.9694088101652577	0.4353386526624247	T	T	T
0.3191822328236675	0.9720515939538996	0.4353451248216196	T	T	T
0.7864442962156200	0.7496024122291486	0.4492128119316062	T	T	T
0.3519448577162431	0.1954461980106172	0.4454545542075545	T	T	T
0.2875703285564770	0.7458663616613413	0.4434713313571071	T	T	T
0.8513711253780721	0.1937152282835916	0.4448385185239751	T	T	T
0.9001355246737832	0.5618881531719617	0.4471500947959696	T	T	T
0.3968069185413612	0.5617365637523073	0.4460205039810523	T	T	T
0.2371329548928256	0.3778495128668820	0.4457577342386804	T	T	T
0.7362145821480234	0.3728926219412471	0.4431177151219576	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9058378869262652	0.8554630515923913	0.3815063517645267	T	T	T
0.2302960743191183	0.0899209235765765	0.3834032371853082	T	T	T
0.7292632204770271	0.0875177857478543	0.3833665723554238	T	T	T
0.4079212933745510	0.8547249656669954	0.3826415807162263	T	T	T
0.6664404737612725	0.8580595483006831	0.4541355421660089	T	T	T
0.4695715766572914	0.0836457784324142	0.4555118857912924	T	T	T
0.1711932293413557	0.8599618242008770	0.4514094150360129	T	T	T
0.9689669646148164	0.0821477762846369	0.4536938145112103	T	T	T
0.7256729882013262	0.5117541988826744	0.4823991424789910	T	T	T
0.9324534773159749	0.7011791296055532	0.4974326455931590	T	T	T

HCO formation and dissociation on Fe₅C₂(010)

Fe₅C₂(010)-CO+H (IS)

1.00000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O H

40 17 1 1

Selective dynamics

Direct

0.0371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F

0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4761243536148401	0.3722226258476026	0.4028998213589929	T	T	T
0.9793538182713797	0.3730889730065189	0.4052731973467664	T	T	T
0.1542218816255057	0.5636727768880544	0.4051002245210292	T	T	T
0.6505593369639249	0.5641455838305615	0.4063942930065881	T	T	T
0.0377134114009545	0.7502264977858242	0.4115748055631734	T	T	T
0.5407737855909772	0.7487588399735520	0.4083190978233943	T	T	T
0.0957996229214240	0.1907041186505663	0.4088776828558450	T	T	T
0.5955638920195662	0.1897929646112059	0.4088112243406987	T	T	T
0.5680414286684224	0.9691278214432213	0.4127560493422757	T	T	T
0.0682908672025623	0.9707392142935756	0.4110407453572365	T	T	T
0.8184099102472079	0.9681258289805510	0.4353076475126800	T	T	T
0.3184704193479187	0.9699612087415732	0.4354815619917444	T	T	T
0.7843391689850727	0.7427749391602266	0.4467374095379346	T	T	T
0.3514160433386467	0.1944071459546803	0.4452810189902371	T	T	T
0.2847878480274089	0.7442079852643577	0.4433327271763836	T	T	T
0.8504405812084563	0.1945564247804569	0.4447084043980376	T	T	T
0.8973870850945285	0.5579356595347175	0.4431014887855779	T	T	T
0.3954914672594193	0.5605513924080350	0.4457837684422497	T	T	T
0.2356383836064691	0.3773668572883149	0.4459560477288109	T	T	T
0.7359628237093491	0.3768162302175326	0.4447517274360025	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9054220835876758	0.8510919753475450	0.3828707338684888	T	T	T
0.2297352163121285	0.0882475025421197	0.3835023794230886	T	T	T
0.7284059665555433	0.0865713964247559	0.3833399891161032	T	T	T
0.4075490091745277	0.8527673787324472	0.3829202891325078	T	T	T
0.6674240258973103	0.8562782554368563	0.4532656142513808	T	T	T
0.4689825921154654	0.0826216926247239	0.4543244108798299	T	T	T
0.1687829470438287	0.8576766167711749	0.4520766634895304	T	T	T
0.9679059801950132	0.0824466934052922	0.4530141176411687	T	T	T
0.7125080935268298	0.5509833918667794	0.4980511060921555	T	T	T
0.6994178784805906	0.5441217537514700	0.5613094826772816	T	T	T
0.9409999881779182	0.6943726468182595	0.4815239074658896	T	T	T

Fe₅C₂(010)-HCO (TS)

1.000000000000000
9.9837999344000004 0.0000000000000000 0.0000000000000000
-1.5315638797000000 11.4316603084999997 0.0000000000000000
0.0000000000000000 0.0000000000000000 18.9298000335999994

Fe C O H
40 17 1 1

Selective dynamics

Direct

0.0371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F

0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4751276684811084	0.3714620419903170	0.4020584493252456	T	T	T
0.9777388139098490	0.3751292926520428	0.4042745262609678	T	T	T
0.1527365232914498	0.5618976722398186	0.4062886198262302	T	T	T
0.6545934608377411	0.5659959594932507	0.4048271959706188	T	T	T
0.0380123298659367	0.7466228716852085	0.4089037988092624	T	T	T
0.5383898307329645	0.7477136582981797	0.4090927163628992	T	T	T
0.0957068829480624	0.1901762607352293	0.4083454811909872	T	T	T
0.5952221333346475	0.1890923857444654	0.4078368240200084	T	T	T
0.5666850219045131	0.9685123547925146	0.4123730888262575	T	T	T
0.0673602353566401	0.9684134736526124	0.4115759005715598	T	T	T
0.8175419584293896	0.9674410227730257	0.4355988957201081	T	T	T
0.3171684349715014	0.9685317231629290	0.4356018603318585	T	T	T
0.7825425087129475	0.7422485876746578	0.4464989832409038	T	T	T
0.3510852420094468	0.1943306908297925	0.4450695601894596	T	T	T
0.2827841220081873	0.7419009299162584	0.4442678266988725	T	T	T
0.8502828670786837	0.1946694167611833	0.4440638364806472	T	T	T
0.8960959605034137	0.5617971998006787	0.4468837841639076	T	T	T
0.3959694608032522	0.5583996070449486	0.4453404754237170	T	T	T
0.2344809261033088	0.3766516215331940	0.4459711886552907	T	T	T
0.7292385600079914	0.3745639717581340	0.4499855670072921	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9056747778512018	0.8493915518686863	0.3838480928597413	T	T	T
0.2291428094895650	0.0871986600138798	0.3834628434392792	T	T	T
0.7279252180560122	0.0856237776611583	0.3830236682568717	T	T	T
0.4060304083536173	0.8508583842435606	0.3832484827864595	T	T	T
0.6659426950675615	0.8556343188835086	0.4533505867925711	T	T	T
0.4679305668531865	0.0822525130776762	0.4534695313317706	T	T	T
0.1669337251968761	0.8548275089404376	0.4525923879858262	T	T	T
0.9674769886601293	0.0820977775776846	0.4520321244795923	T	T	T
0.7611458058744989	0.5473466449727443	0.5203234192050310	T	T	T
0.7127474278828205	0.4417715823181270	0.5416109088227926	T	T	T
0.7469129849124890	0.6160509418611241	0.5599819628216971	T	T	T

Fe₅C₂(010)-HCO (FS)

1.000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O H

40 17 1 1

Selective dynamics

Direct

0.0371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4754419765191428	0.3714472840309340	0.4026657087178206	T	T	T

0.9781541000170791	0.3744970014342188	0.4033385255738291	T	T	T
0.1533822665656656	0.5623392396251878	0.4058974438525813	T	T	T
0.6530084158878655	0.5617679272091354	0.4058918456681925	T	T	T
0.0379434142685341	0.7465109157800497	0.4089839334164286	T	T	T
0.5385227877613334	0.7468672424719043	0.4088630240322881	T	T	T
0.0957198316675783	0.1899218119242054	0.4082484801541633	T	T	T
0.5948550557518540	0.1888867072953564	0.4079831105982443	T	T	T
0.5665973504177531	0.9679133944754338	0.4122400234494431	T	T	T
0.0677706853803651	0.9683978788704404	0.4116796065088772	T	T	T
0.8173891359354277	0.9681556462582774	0.4355110446857638	T	T	T
0.3171743928428989	0.9679944742708124	0.4355569826183535	T	T	T
0.7837904785396728	0.7434746955138423	0.4437457031430905	T	T	T
0.3507341451392804	0.1939364941862786	0.4450621775065915	T	T	T
0.2826710074176409	0.7418140309914759	0.4446681289637173	T	T	T
0.8502659427494067	0.1941636845510354	0.4445353311534538	T	T	T
0.8948586673699391	0.5624463468663962	0.4483132427382562	T	T	T
0.3965073071673422	0.5582682448750469	0.4455727472064927	T	T	T
0.2344535270249538	0.3765213730481337	0.4461063261321366	T	T	T
0.7329463474578197	0.3740494273655571	0.4485709590923451	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9065935160286167	0.8506686918679499	0.3833135869147680	T	T	T
0.2290381902854725	0.0868708760008215	0.3833431721439393	T	T	T
0.7278896907135354	0.0858150644425363	0.3833750362095962	T	T	T
0.4058801915072650	0.8498770901598183	0.3834172887887676	T	T	T
0.6662142050055962	0.8550719365291612	0.4531516289828801	T	T	T
0.4675074953640167	0.0817140234596160	0.4532377209393260	T	T	T
0.1666319802575790	0.8545440507007187	0.4528979434427151	T	T	T
0.9677838939942786	0.0818686395571991	0.4522266736402600	T	T	T
0.7684032976870669	0.5150782924644838	0.5243595977519756	T	T	T
0.7564232103282627	0.4073345372884783	0.5475463978883345	T	T	T
0.7141603967159065	0.5742656026324215	0.5568156603653233	T	T	T

Fe₅C₂(010)-CH+O (TS)

1.000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O H

40 17 1 1

Selective dynamics

Direct

0.0371499999999996	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999996	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4753609392478251	0.3707685723036771	0.4026458620993129	T	T	T
0.9791055881599526	0.3717157130795771	0.4038962441086411	T	T	T
0.1535812005482469	0.5611112184997399	0.4054940528070935	T	T	T
0.6519776327390139	0.5594791294039971	0.4066760933076501	T	T	T
0.0384283303600949	0.7466879061589994	0.4092561607143917	T	T	T

0.5386783643596770	0.7463908336044388	0.4086444249772300	T	T	T
0.0952610852387258	0.1880929866779581	0.4082301107474790	T	T	T
0.5951506575486255	0.1882703614631189	0.4076171954562087	T	T	T
0.5671650431277115	0.9675649232800418	0.4122824425952737	T	T	T
0.0675479899415984	0.9675456495660298	0.4118837116115310	T	T	T
0.8177677979505436	0.9654079454150126	0.4353473664130208	T	T	T
0.3174294198800946	0.9670858138983750	0.4355976063144731	T	T	T
0.7821409187426134	0.7386797404593011	0.4455092301946507	T	T	T
0.3491314110915907	0.1924069396732669	0.4447674967836845	T	T	T
0.2825144435402663	0.7414029625747227	0.4442389481750547	T	T	T
0.8499665767288497	0.1918226430146520	0.4448132797879074	T	T	T
0.9020655384918489	0.5599392599649882	0.4467600791137140	T	T	T
0.3955771220177709	0.5582524685886388	0.4455356459685546	T	T	T
0.2350852962249618	0.3761094534182085	0.4456631012108415	T	T	T
0.7390688355323493	0.3748409682901072	0.4490156014594298	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9059089241558848	0.8478134013429249	0.3838835946164148	T	T	T
0.2287232400762368	0.0852434562521984	0.3830453185204674	T	T	T
0.7284943794870998	0.0846080810305306	0.3830646352504500	T	T	T
0.4059288687295335	0.8497433506449874	0.3834575169996540	T	T	T
0.6662633187883231	0.8539456116100836	0.4525482634653303	T	T	T
0.4674631906971087	0.0810160715601650	0.4527769625450616	T	T	T
0.1666564406969033	0.8541628497978722	0.4535189991306566	T	T	T
0.9678566283719630	0.0799670746672642	0.4526495816378932	T	T	T
0.7324093680426879	0.5534206312543178	0.4968029179320149	T	T	T
0.7260870945058640	0.4032086223824592	0.5363371343572136	T	T	T
0.7066626409293592	0.5806835581328756	0.5500791541833820	T	T	T

Fe₃C₂(010)-CH+O (FS)

1.000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O H

40 17 1 1

Selective dynamics

Direct

0.0371499999999999	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999997	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999999	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999997	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999996	0.8711600000000033	0.2883799999999996	F	F	F
0.1504899999999997	0.0664299999999996	0.2883799999999996	F	F	F
0.9841399999999996	0.8711600000000033	0.2883799999999996	F	F	F
0.6504899999999997	0.0664299999999996	0.2883799999999996	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999997	0.0664299999999996	0.3285800000000023	F	F	F
0.2341399999999996	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999997	0.0664299999999996	0.3285800000000023	F	F	F
0.7341399999999996	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999997	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999999	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999997	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999999	0.2536300000000011	0.3286500000000032	F	F	F
0.4775719733406060	0.3721533734446112	0.4028882063162100	T	T	T
0.9802624918479349	0.3715347859992463	0.4048168878496865	T	T	T
0.1543491792598189	0.5622124643796172	0.4062874660778997	T	T	T
0.6507274026823384	0.5667202335780193	0.4022915348713830	T	T	T
0.0383606941294682	0.7473442262129311	0.4093249372073721	T	T	T
0.5386200819616240	0.7492099208874929	0.4085135014176034	T	T	T
0.0932219022041927	0.1881806786137392	0.4087525126377110	T	T	T
0.5962215828520082	0.189188222763310	0.4104933965023541	T	T	T
0.5674184363341558	0.9686754915394463	0.4121780596637486	T	T	T
0.0670394349232708	0.9678353482417331	0.4125246875041746	T	T	T
0.8176345653330742	0.9649580485196465	0.4358277691688545	T	T	T

0.3172253128030683	0.9678224563822103	0.4354406254441271	T	T	T
0.7791695647380683	0.7373358911178771	0.4485786365432705	T	T	T
0.3499520277089998	0.1929731830044871	0.4440766366073681	T	T	T
0.2833913443209211	0.7425711940851438	0.4445723474934488	T	T	T
0.8449648211943490	0.1843258509850582	0.4468582146648801	T	T	T
0.9038946302085876	0.5594726671689403	0.4444277769149242	T	T	T
0.3960940022658982	0.5598929559500192	0.4454484896893624	T	T	T
0.2388398934405347	0.3766650840937995	0.4449246296036140	T	T	T
0.7388570024845017	0.3832636577031437	0.4464287599459587	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9056391591552568	0.8480380255443776	0.3846373450447215	T	T	T
0.2274489133189769	0.0853910480374653	0.3833924427050782	T	T	T
0.7295219140517669	0.0848565026605867	0.3836688726660638	T	T	T
0.4053849375786675	0.8511837572232362	0.3830073783830416	T	T	T
0.6661844726574473	0.8549450426455308	0.4537054850909664	T	T	T
0.4663236841813163	0.0800903655743048	0.4538757758355502	T	T	T
0.1667450682575490	0.8549114171852567	0.4537565154872616	T	T	T
0.9675889641345927	0.0799053280047690	0.4551260493854294	T	T	T
0.7360364031638912	0.5714817646771535	0.4902015978123757	T	T	T
0.7736597755522077	0.2726763664961994	0.5077579507323050	T	T	T
0.7046884110495167	0.5612990055154096	0.5458727396540991	T	T	T

COH formation and dissociation on Fe₅C₂(010)

Fe₅C₂(010)-COH (TS)

1.000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O H

40 17 1 1

Selective dynamics

Direct

0.0371499999999996	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4766732046621244	0.3730801785571089	0.4030005722285109	T	T	T
0.9794389261516903	0.3744699648483338	0.4057678320733050	T	T	T
0.1525099835625554	0.5620051502603990	0.4063799429281154	T	T	T
0.6576874197961103	0.5686211942614552	0.3991007210052915	T	T	T
0.0387035252690496	0.7478987306386894	0.4089409372788484	T	T	T
0.5388383893258744	0.7477512499115829	0.4100754376758231	T	T	T
0.0959054016612605	0.1899225981780522	0.4083733694325059	T	T	T
0.5959837042577500	0.1901799509398767	0.4087532219484361	T	T	T
0.5675127061282460	0.9686246422295925	0.4122318957146551	T	T	T
0.0677566987412259	0.9687925476883392	0.4118656515004068	T	T	T
0.8181052976392607	0.9678001083205982	0.4351339418274328	T	T	T
0.3175922396193456	0.9681907395044556	0.4354465795903435	T	T	T
0.7833177909130142	0.7421332525753124	0.4465167480179100	T	T	T
0.3509734040223063	0.1941705434172041	0.4448084664247151	T	T	T
0.2831602930297277	0.7418812386377950	0.4445645815052502	T	T	T

0.8505139346740611	0.1952297090367046	0.4444191580219369	T	T	T
0.8978551044494745	0.5598313102328151	0.4463627329498692	T	T	T
0.3973242646706078	0.5598360597525071	0.4454013391703032	T	T	T
0.2361137297026686	0.3779181052345515	0.4462374891189940	T	T	T
0.7338692578598719	0.3809793709874402	0.4460660091567933	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9055828427450858	0.8485987086650894	0.3839528688888711	T	T	T
0.2289206382640366	0.0868601966038015	0.3834791553204815	T	T	T
0.7280058451950625	0.0865823226471646	0.3833431736572271	T	T	T
0.4064151039946623	0.8503530003878262	0.3834860736587165	T	T	T
0.6668295690284937	0.8563027570541661	0.4531721337232971	T	T	T
0.4680501031593930	0.0821969644156286	0.4528600926295839	T	T	T
0.1669440671790163	0.8550052622473645	0.4528884086675712	T	T	T
0.9676640359241713	0.0823134305306964	0.4522822328388835	T	T	T
0.7268181013680879	0.5710891800556668	0.4929186313535770	T	T	T
0.6499704000595274	0.5701657376967655	0.5467380960780236	T	T	T
0.5317257562773556	0.5874741106972248	0.5134019772176663	T	T	T

Fe₃C₂(010)-COH (FS)

1.0000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O H

40 17 1 1

Selective dynamics

Direct

0.03714999999999969	0.25363000000000011	0.2882999999999996	F	F	F
0.09747999999999973	0.68397000000000022	0.2882999999999996	F	F	F
0.53714999999999969	0.25363000000000011	0.2882999999999996	F	F	F
0.59747999999999973	0.68397000000000022	0.2882999999999996	F	F	F
0.48413999999999965	0.87116000000000033	0.28837999999999965	F	F	F
0.15048999999999978	0.06642999999999969	0.28837999999999965	F	F	F
0.98413999999999965	0.87116000000000033	0.28837999999999965	F	F	F
0.65048999999999978	0.06642999999999969	0.28837999999999965	F	F	F
0.06730999999999991	0.46880000000000017	0.29153999999999977	F	F	F
0.56730999999999991	0.46880000000000017	0.29153999999999977	F	F	F
0.31730999999999991	0.46880000000000017	0.32540999999999980	F	F	F
0.81730999999999991	0.46880000000000017	0.32540999999999980	F	F	F
0.40048999999999978	0.06642999999999969	0.32858000000000023	F	F	F
0.23413999999999965	0.87116000000000033	0.32858000000000023	F	F	F
0.90048999999999978	0.06642999999999969	0.32858000000000023	F	F	F
0.73413999999999965	0.87116000000000033	0.32858000000000023	F	F	F
0.34747999999999973	0.68397000000000022	0.32865000000000032	F	F	F
0.28714999999999969	0.25363000000000011	0.32865000000000032	F	F	F
0.84747999999999973	0.68397000000000022	0.32865000000000032	F	F	F
0.78714999999999969	0.25363000000000011	0.32865000000000032	F	F	F
0.4759011738943913	0.3705715131287142	0.4021212898556248	T	T	T
0.9813770547986189	0.3726524022975796	0.4053460227632775	T	T	T
0.1556694025336272	0.5637143137479724	0.4045239976811388	T	T	T
0.6478384802423239	0.5636647310510925	0.4068198614398073	T	T	T
0.0386623788730451	0.7484058882402890	0.4096318230847548	T	T	T
0.538553545157686	0.7493015144558919	0.4084002791732144	T	T	T
0.0961773577917938	0.1883522624332166	0.4085187334184065	T	T	T
0.5962495246849064	0.1888318382729750	0.4095885663103566	T	T	T
0.5689326668794179	0.9689496795498560	0.4118966376247563	T	T	T
0.0672121318734408	0.9683965550931556	0.4114515358301502	T	T	T
0.8186659324812244	0.9657014286339723	0.4347097318726515	T	T	T
0.3181256979423094	0.9689193850019091	0.4354143587207741	T	T	T
0.7795002893328189	0.7375818023542680	0.4471749686401411	T	T	T
0.3532142411894058	0.1923657817396279	0.4439938409212751	T	T	T
0.2825749794143830	0.7445934189869843	0.4431874630090994	T	T	T
0.8518897866105988	0.1943686334039127	0.4437965707175265	T	T	T
0.9041674616302682	0.5570877018747926	0.4447804900025394	T	T	T
0.3942640655966520	0.5618178254640315	0.4451175055962452	T	T	T
0.2384794541849895	0.3749257019697720	0.4446277742139834	T	T	T
0.7368251333659223	0.3809723567841385	0.4455621374372362	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F

0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9051725767475004	0.8470230858450394	0.3836674753921708	T	T	T
0.2295915883672667	0.0868923253155612	0.3832773228769575	T	T	T
0.7289775878377952	0.0872023589132174	0.3828162673836970	T	T	T
0.4065150807818715	0.8519415582364591	0.3826321206096969	T	T	T
0.6666021989219906	0.8559569469090705	0.4525342763554118	T	T	T
0.4694494185990794	0.0802937834658455	0.4542951159351339	T	T	T
0.1669228794236573	0.8569460445516077	0.4529610739103213	T	T	T
0.9678421221181416	0.0805531069259157	0.4520250377613959	T	T	T
0.7394765209302270	0.5640077372306765	0.4939389065580425	T	T	T
0.6985504652507846	0.5627443101081597	0.5626680024055689	T	T	T
0.7748373523870030	0.5523294030398095	0.5935623314490800	T	T	T

Fe₅C₂(010)-C+OH (TS)

1.0000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O H
40 17 1 1

Selective dynamics

Direct

0.0371499999999996	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999996	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999996	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999996	0.2536300000000011	0.3286500000000032	F	F	F
0.4750870979287001	0.3701838656271154	0.4017386549364028	T	T	T
0.9783156025605606	0.3715150725323245	0.4038719898607816	T	T	T
0.1584693315644560	0.5630295973126641	0.4033070611291742	T	T	T
0.6493481853117903	0.5639229060672712	0.4046009528003056	T	T	T
0.0397817140800536	0.7496707325465098	0.4088408703429894	T	T	T
0.5391413243727843	0.7489631419997861	0.4081031271652847	T	T	T
0.0952655906102120	0.1889420567186979	0.4083829308010793	T	T	T
0.5957166312036064	0.1889884044148940	0.4087514845421799	T	T	T
0.5686926741515563	0.9684404033606305	0.4122131133885489	T	T	T
0.0675932285336043	0.9688850045253468	0.4111452965840983	T	T	T
0.8183498417687550	0.9647317375454358	0.4349712641686281	T	T	T
0.3179631012879338	0.9691664284855529	0.4353910507379690	T	T	T
0.7788662471170639	0.7349455613084338	0.4504455197280058	T	T	T
0.3530502280720999	0.1926103793483635	0.4446015103958456	T	T	T
0.2831203423549481	0.7445152860017009	0.4435505137762437	T	T	T
0.8510149322506756	0.1936217977258503	0.4442684490113163	T	T	T
0.9202996702913390	0.5626836659526790	0.4472702772150550	T	T	T
0.3960444730270271	0.5609262464170669	0.4451760007708669	T	T	T
0.2376743355207109	0.3749882081306395	0.4449117970156453	T	T	T
0.7310799293527648	0.3796959638087932	0.4517104295501823	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F

0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9037712298458325	0.8455844316545940	0.3839436848674991	T	T	T
0.2296916783619833	0.0880502572447392	0.3833137153399184	T	T	T
0.7288473901793989	0.0865758441772539	0.3828092295678554	T	T	T
0.4065635029483149	0.8512709928691512	0.3825156757838145	T	T	T
0.6667559216688540	0.8549208269604165	0.4530268280528161	T	T	T
0.4694265055877687	0.0803211538113883	0.4540386625792834	T	T	T
0.1672775621582091	0.8572146206946720	0.4526987020212239	T	T	T
0.9674116934469454	0.0803129562236463	0.4518316691078853	T	T	T
0.7531576003280116	0.5628157203307450	0.4835074512788201	T	T	T
0.7150018555293770	0.4249282547173842	0.5488896969529934	T	T	T
0.6190100495555902	0.4179614174238512	0.5614862304258825	T	T	T

Fe₅C₂(010)-C+OH (FS)

1.0000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O H

40 17 1 1

Selective dynamics

Direct

0.03714999999999969	0.25363000000000011	0.2882999999999996	F	F	F
0.09747999999999973	0.68397000000000022	0.2882999999999996	F	F	F
0.53714999999999969	0.25363000000000011	0.2882999999999996	F	F	F
0.59747999999999973	0.68397000000000022	0.2882999999999996	F	F	F
0.48413999999999965	0.87116000000000033	0.28837999999999965	F	F	F
0.15048999999999978	0.06642999999999969	0.28837999999999965	F	F	F
0.98413999999999965	0.87116000000000033	0.28837999999999965	F	F	F
0.65048999999999978	0.06642999999999969	0.28837999999999965	F	F	F
0.06730999999999991	0.46880000000000017	0.29153999999999977	F	F	F
0.56730999999999991	0.46880000000000017	0.29153999999999977	F	F	F
0.31730999999999991	0.46880000000000017	0.32540999999999980	F	F	F
0.81730999999999991	0.46880000000000017	0.32540999999999980	F	F	F
0.40048999999999978	0.06642999999999969	0.32858000000000023	F	F	F
0.23413999999999965	0.87116000000000033	0.32858000000000023	F	F	F
0.90048999999999978	0.06642999999999969	0.32858000000000023	F	F	F
0.73413999999999965	0.87116000000000033	0.32858000000000023	F	F	F
0.34747999999999973	0.68397000000000022	0.32865000000000032	F	F	F
0.28714999999999969	0.25363000000000011	0.32865000000000032	F	F	F
0.84747999999999973	0.68397000000000022	0.32865000000000032	F	F	F
0.78714999999999969	0.25363000000000011	0.32865000000000032	F	F	F
0.4750037705172516	0.3686387934350976	0.4025098374336855	T	T	T
0.9775158996580404	0.3685002001425698	0.4022017805966317	T	T	T
0.1598220372737806	0.5625763023283014	0.4025246163383191	T	T	T
0.6406510524599506	0.5564286265978475	0.4065888605074391	T	T	T
0.0407577687043194	0.7502904956796153	0.4091768497819580	T	T	T
0.5405098654701610	0.7485821490617672	0.4081781418216288	T	T	T
0.0951874245776749	0.1888523276711802	0.4080570554221438	T	T	T
0.5925502413304097	0.1877157227082941	0.4064555724505799	T	T	T
0.5692775349437548	0.9678954385200543	0.4127662215175380	T	T	T
0.0682964810155100	0.9693161000578220	0.4114245850722197	T	T	T
0.8190803221627945	0.9639257630867172	0.4348921746984709	T	T	T
0.3188518319583705	0.9676870870881400	0.4356054550303011	T	T	T
0.7804610536444760	0.7330083335913705	0.4483999753068791	T	T	T
0.3518582751290943	0.1906242164323339	0.4448071715769790	T	T	T
0.2832880499051094	0.7440222355494216	0.4436033687749546	T	T	T
0.8473195637486928	0.1914484471615143	0.4491446163616870	T	T	T
0.9321581597246492	0.5615433339218727	0.4496702202189753	T	T	T
0.3954137477727547	0.5604390154652460	0.4448742379401144	T	T	T
0.2373987047565515	0.3745058844789923	0.4452417666515660	T	T	T
0.7380308519832143	0.3845719023333058	0.4502754429924851	T	T	T
0.23203000000000017	0.5823099999999997	0.26413000000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.26413000000000015	F	F	F
0.73203000000000017	0.5823099999999997	0.26413000000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.26413000000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.35282000000000012	F	F	F
0.48203000000000017	0.5823099999999997	0.35282000000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.35282000000000012	F	F	F
0.98203000000000017	0.5823099999999997	0.35282000000000012	F	F	F
0.9044442774561410	0.8458511187759494	0.3841437412623254	T	T	T
0.2299837307633880	0.0870059930040413	0.3835972222767526	T	T	T
0.7293186367636872	0.0863486186896628	0.3825153378197522	T	T	T
0.4071546876671495	0.8510552113534665	0.3826242046108231	T	T	T
0.6675731885380625	0.8540170938047424	0.4533963046844946	T	T	T

0.4696179288569092	0.0789581216475890	0.4548487440022434	T	T	T
0.1676181422045675	0.8572321126885410	0.4537529879359797	T	T	T
0.9671882132250238	0.0806944977475160	0.4517968709474277	T	T	T
0.7606196302363659	0.5620808239052784	0.4771449447121650	T	T	T
0.7791484497412571	0.2801230785306806	0.5263993824162680	T	T	T
0.6974667110234036	0.2392743972878392	0.5483080247999441	T	T	T

CO dissociation on K₂O-Fe₃C₂(010)

K₂O-Fe₃C₂(010)-CO (IS)

1.00000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O K
40 17 2 2

Selective dynamics

Direct

0.0371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4778289264239226	0.3705097156508970	0.4007391504040221	T	T	T
0.9809261638236053	0.3718600422030376	0.4066477000973659	T	T	T
0.1531700789988132	0.5651253186961113	0.4022409960294318	T	T	T
0.6497454422260774	0.5645841455701250	0.4085182633309393	T	T	T
0.0380038675754789	0.7485049944064212	0.4116437235150805	T	T	T
0.5392042388118974	0.7488506814101407	0.4088645245387859	T	T	T
0.0957402138070746	0.1886013369280425	0.4092951980909157	T	T	T
0.5956593108183955	0.1892973801035544	0.4114635382852957	T	T	T
0.5683268866666195	0.9695949674580172	0.4134358881079271	T	T	T
0.0665976429227575	0.9678654286963806	0.4127513125745582	T	T	T
0.8175137348147760	0.9667404878667976	0.4355229277568978	T	T	T
0.3176481173240115	0.9687993864782591	0.4362151061207099	T	T	T
0.7820743057663486	0.7401797302307221	0.4484498750725775	T	T	T
0.3499798590531206	0.1910920353090098	0.4422689157899491	T	T	T
0.2844217843244575	0.7459995753012677	0.4414820049158185	T	T	T
0.8506032602086712	0.1934868906823848	0.4449984642043203	T	T	T
0.8978280686923078	0.5578040594515786	0.4424237884649933	T	T	T
0.3935621849011304	0.5602609516440048	0.4491002222066862	T	T	T
0.2358547201723098	0.3766137463398718	0.4491383402433184	T	T	T
0.7383977237132048	0.3799207451833783	0.4441222795202062	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9047937642919055	0.8482012547812999	0.3844172372675226	T	T	T
0.2273262935744849	0.0839961247927937	0.3832445467303131	T	T	T
0.7284747452935596	0.0864074554781146	0.3836832287123559	T	T	T
0.4079452943934014	0.8541229411304743	0.3829739375187173	T	T	T
0.6663738028374592	0.8556373065217168	0.4544316495085367	T	T	T
0.4677496112608919	0.0813689081683207	0.4565560978853377	T	T	T
0.1674016637191245	0.8562019104112415	0.4557180560666843	T	T	T
0.9673405928549974	0.0808780196701302	0.4539376733821693	T	T	T

0.7366805141811901	0.5573656207457292	0.5001093159440659	T	T	T
0.7109217893536682	0.5480568839802258	0.5644671463146540	T	T	T
0.3098639082841267	0.4712378509703249	0.5237833952701172	T	T	T
0.1068802856401581	0.5658934813525734	0.5755275936613813	T	T	T
0.5052580724150820	0.3738426815476650	0.5797746557234214	T	T	T

K₂O-Fe₅C₂(010)-C+O (TS)

1.000000000000000		
9.9837999344000004	0.000000000000000	0.000000000000000
-1.5315638797000000	11.4316603084999997	0.000000000000000
0.000000000000000	0.000000000000000	18.9298000335999994

Fe C O K

40 17 2 2

Selective dynamics

Direct

0.0371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4768816572124795	0.3703686231840963	0.4000437311064989	T	T	T
0.9800229878552795	0.3743597248064462	0.4060044764766631	T	T	T
0.1544929747916187	0.5652730283120198	0.4021467402202314	T	T	T
0.6526987109984450	0.5692815204436508	0.4053308138151808	T	T	T
0.0420242927109520	0.7502406785609179	0.4082042907041608	T	T	T
0.5409038315149917	0.7498612869646388	0.4083435760193846	T	T	T
0.0958178330853762	0.1900857297223051	0.4090513869190235	T	T	T
0.5956918136825106	0.1888226829028883	0.4108372156613853	T	T	T
0.5683794690925955	0.9695888722245746	0.4133851997025214	T	T	T
0.0672827242898841	0.9687584619518993	0.4122295345141460	T	T	T
0.8177990726372832	0.9677999363157471	0.4354267020413304	T	T	T
0.3176145330649147	0.9697341945896915	0.4361488154073895	T	T	T
0.7902737107858517	0.7474075661756335	0.4527551082469087	T	T	T
0.3499584766415956	0.1917160554408349	0.4424791424986095	T	T	T
0.2858941490887476	0.7472113230141533	0.4412990138032835	T	T	T
0.8509301442773317	0.1934330817136959	0.4447636540437088	T	T	T
0.8968492866396980	0.5631557788286400	0.4422337357470391	T	T	T
0.3941623378387750	0.5617375952612286	0.4486229003360293	T	T	T
0.2364214148245169	0.3772715118222504	0.4488534585201663	T	T	T
0.7392042063895710	0.3758613472922368	0.4428768500868336	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9046920891354736	0.8480810589135738	0.3843793017665879	T	T	T
0.2278845799504496	0.0853040250130169	0.3833784833579784	T	T	T
0.7283565415752101	0.0865994176165034	0.3834746208731756	T	T	T
0.4084906785275503	0.8548778916297740	0.3829834157389456	T	T	T
0.6672506835101246	0.8557292895001093	0.4550707372119483	T	T	T
0.4679254336010610	0.0819179468434224	0.4564259889045638	T	T	T
0.1681889981778630	0.8571582031960723	0.4554906281477590	T	T	T
0.9679643912263852	0.0813105203133414	0.4532520240433844	T	T	T
0.7157619504912326	0.5130652104645730	0.4867860915027861	T	T	T
0.8389273804556175	0.6452721053844729	0.5216744037343508	T	T	T
0.3110914767113131	0.4727240296360228	0.5230273452829894	T	T	T

0.0955066152452055	0.5783519201346008	0.5728519340888736	T	T	T
0.5141634389142553	0.3745830856570074	0.5755153653196970	T	T	T

K₂O-Fe₅C₂(010)C+O (FS)

1.00000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O K
40 17 2 2

Selective dynamics

Direct

0.0371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4763721296145486	0.3700617726224774	0.3997881317580475	T	T	T
0.9805218220854042	0.3746167989163845	0.4059568632777180	T	T	T
0.1559442233000132	0.5660525095580278	0.4006895547006839	T	T	T
0.6518041401890563	0.5691256323689954	0.4074605290348923	T	T	T
0.0374237060234852	0.7491193817605210	0.4157874971080026	T	T	T
0.5408336866808735	0.7509711030766365	0.4077813790554734	T	T	T
0.0953568206236356	0.1906732289156375	0.4092260109253854	T	T	T
0.5954376406948487	0.1889718804132791	0.4110570387137049	T	T	T
0.5685951348232320	0.9713204650909376	0.4136746048750706	T	T	T
0.0683331667647347	0.9703973294669189	0.4114595331934232	T	T	T
0.8184749212884929	0.9695394653909432	0.4354141634173032	T	T	T
0.3191625554052900	0.9719038845270098	0.4360060310123632	T	T	T
0.7863595697901516	0.7499226684875324	0.4506634533252404	T	T	T
0.3500109863836383	0.1923996247845900	0.4427451905534151	T	T	T
0.2881111081401368	0.7490852380788632	0.4402900317943423	T	T	T
0.8523584245024720	0.1929200918068615	0.4449504785193492	T	T	T
0.8944697113746450	0.5601238932190284	0.4447981134306624	T	T	T
0.3932750909600266	0.5628454172688112	0.4483191043637985	T	T	T
0.2366830305604753	0.3782145568055143	0.4487478860391518	T	T	T
0.7392193113756843	0.3720559611396899	0.4418174884173940	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9056169309945026	0.8547052174723201	0.3820908548897410	T	T	T
0.2286552164476880	0.0870839719739108	0.3829803844239036	T	T	T
0.7293727092869174	0.0880185911359557	0.3837231240219786	T	T	T
0.4093774848093162	0.8578319128912474	0.3823694687250926	T	T	T
0.6661566626418749	0.8586430161982400	0.4545785655993390	T	T	T
0.4686155441794070	0.0834764645803460	0.4579113395174376	T	T	T
0.1710542835957809	0.8602893735089957	0.4537945185002065	T	T	T
0.9693685736672606	0.0811569430644008	0.4548973789731686	T	T	T
0.7213569186152700	0.5053779165739466	0.4853518601814481	T	T	T
0.9302776837175191	0.6955625213925338	0.5012344401422205	T	T	T
0.3126412106967509	0.4736782728525027	0.5229854706131279	T	T	T
0.1107481994599022	0.5859932421831061	0.5728351409603779	T	T	T
0.5127204436183548	0.3727427077829654	0.5745939948965760	T	T	T

HCO formation and dissociation on K₂O-Fe₅C₂(010)

K₂O-Fe₅C₂(010)-CO+H (IS)

1.000000000000000
 9.9837999344000004 0.000000000000000 0.000000000000000
 -1.5315638797000000 11.4316603084999997 0.000000000000000
 0.0000000000000000 0.0000000000000000 18.9298000335999994

Fe C O K H
 40 17 2 2 1

Selective dynamics

Direct

0.0371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4768988318684770	0.3692578251350027	0.3997317299461018	T	T	T
0.9806466399910394	0.3729951471820377	0.4061264046814635	T	T	T
0.1532879633395925	0.5650385091561956	0.4019972244870499	T	T	T
0.6481351135809817	0.5629111171531401	0.4092401159249670	T	T	T
0.0366894684566377	0.7497379560863994	0.4132973722780449	T	T	T
0.5401358897535748	0.7485684443119042	0.4089278427488570	T	T	T
0.0961136861921521	0.1897992508893614	0.4094650588083293	T	T	T
0.5958405932159141	0.1888142102171532	0.4110870213883430	T	T	T
0.5685413342017501	0.9696696543150733	0.4133267112828211	T	T	T
0.0672556986330196	0.9693220694750602	0.4118013407191505	T	T	T
0.8180993814333130	0.9682395893042837	0.4355893173396623	T	T	T
0.3183534057960822	0.9694147340809326	0.4359531877635331	T	T	T
0.7832084209726495	0.7428525594998524	0.4475793661223134	T	T	T
0.3506128669800175	0.1909178678902650	0.4421930352447581	T	T	T
0.2852240643109917	0.7459689965711032	0.4412196539401709	T	T	T
0.8514426089651820	0.1940299326049660	0.4449365875126872	T	T	T
0.8948264742278857	0.5578112666428439	0.4417642427819891	T	T	T
0.3929721895744736	0.5601109061495241	0.4486528552596454	T	T	T
0.2365052286353417	0.3761095469564990	0.4482739980153638	T	T	T
0.7389146962353156	0.3770764557446583	0.4430623310262766	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9048443379226107	0.8510984180349072	0.3831062563610648	T	T	T
0.2283470052264046	0.0853345833116511	0.3830290411613978	T	T	T
0.7289097248248885	0.0867313861834133	0.3835566547861817	T	T	T
0.4084462084504773	0.8545496279792185	0.3826922806538341	T	T	T
0.6669447995291499	0.8565881891893734	0.4541530072243121	T	T	T
0.4685794618632544	0.0817594846151477	0.4569919136893212	T	T	T
0.1688160843590378	0.8577667446572007	0.4540051571249246	T	T	T
0.9681888767810765	0.0814208365707749	0.4541932606087616	T	T	T
0.7263640252649930	0.5387984648678753	0.4985495909272273	T	T	T
0.7082646606686340	0.5308254276297152	0.5635099938204732	T	T	T
0.3090418507413382	0.4705643179180292	0.5230258488438410	T	T	T
0.0883392962147995	0.5424816927807602	0.5740618490367354	T	T	T
0.4992619535648902	0.3612180647309846	0.5782989309937790	T	T	T
0.9388817189611911	0.6899647207947174	0.4829798477893330	T	T	T

K₂O-Fe₅C₂(010)-HCO (TS)

```

1.000000000000000
 9.9837999344000004  0.000000000000000  0.000000000000000
-1.5315638797000000  11.4316603084999997  0.0000000000000000
 0.000000000000000  0.000000000000000  18.9298000335999994
Fe C O K H
 40 17 2 2 1
Selective dynamics
Direct
0.03714999999999969 0.25363000000000011 0.2882999999999996 F F F
0.09747999999999973 0.68397000000000022 0.2882999999999996 F F F
0.53714999999999969 0.25363000000000011 0.2882999999999996 F F F
0.59747999999999973 0.68397000000000022 0.2882999999999996 F F F
0.48413999999999965 0.87116000000000033 0.28837999999999965 F F F
0.15048999999999978 0.06642999999999969 0.28837999999999965 F F F
0.98413999999999965 0.87116000000000033 0.28837999999999965 F F F
0.65048999999999978 0.06642999999999969 0.28837999999999965 F F F
0.06730999999999991 0.46880000000000017 0.29153999999999977 F F F
0.56730999999999991 0.46880000000000017 0.29153999999999977 F F F
0.31730999999999991 0.46880000000000017 0.32540999999999980 F F F
0.81730999999999991 0.46880000000000017 0.32540999999999980 F F F
0.40048999999999978 0.06642999999999969 0.32858000000000023 F F F
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0.34747999999999973 0.68397000000000022 0.32865000000000032 F F F
0.28714999999999969 0.25363000000000011 0.32865000000000032 F F F
0.84747999999999973 0.68397000000000022 0.32865000000000032 F F F
0.78714999999999969 0.25363000000000011 0.32865000000000032 F F F
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0.9795891584836608 0.3739894102456402 0.4051758552229597 T T T
0.1536946406510004 0.5654282598245021 0.4029071504642677 T T T
0.6502386877987572 0.5606269070406921 0.4097004675893171 T T T
0.0378356481526516 0.7485310065292916 0.4108206080493634 T T T
0.5380995011877422 0.7472317662406437 0.4088376635786363 T T T
0.0958457206461691 0.1891426912718953 0.4093537757443871 T T T
0.5952562876610145 0.1889547617864263 0.4100636064758230 T T T
0.5671382001256768 0.9691040515688100 0.4127237479570234 T T T
0.0665932448155938 0.9682728170872815 0.4130892382380620 T T T
0.8170819233769082 0.9686634632817424 0.4358014440502575 T T T
0.3173351765585856 0.9681051353794529 0.4361481599165130 T T T
0.7819440937908878 0.7449653182985772 0.4440131623824883 T T T
0.3500963411090390 0.1899905042725757 0.4408459794332690 T T T
0.2832242097120585 0.7446866890122938 0.4427774925274982 T T T
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0.3943352825600944 0.5584160880589475 0.4492761989383505 T T T
0.2369047964509764 0.3747829503940877 0.4475979346880328 T T T
0.7351808057585781 0.3770683570322911 0.4464965209953479 T T T
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0.40259999999999996 0.35528999999999966 0.26413000000000015 F F F
0.73203000000000017 0.58230999999999997 0.26413000000000015 F F F
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0.48203000000000017 0.58230999999999997 0.35282000000000012 F F F
0.65259999999999996 0.35528999999999966 0.35282000000000012 F F F
0.98203000000000017 0.58230999999999997 0.35282000000000012 F F F
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0.7181117235173170 0.4406413105603156 0.5569074228842747 T T T
0.3092703251499284 0.4675335401675769 0.5230550352420482 T T T
0.0761495146203949 0.5111299558576528 0.5748934185463849 T T T
0.4811734195572245 0.3366456914599310 0.5791893413919474 T T T
0.7686663055300735 0.6175352151802124 0.5310184939422881 T T T

```

K₂O-Fe₃C₂(010)-HCO (FS)

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1.000000000000000
 9.9837999344000004  0.000000000000000  0.000000000000000
-1.5315638797000000  11.4316603084999997  0.000000000000000

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0.0000000000000000 0.0000000000000000 18.9298000335999994
Fe C O K H
40 17 2 2 1
Selective dynamics
Direct
0.0371499999999969 0.2536300000000011 0.2882999999999996 F F F
0.0974799999999973 0.6839700000000022 0.2882999999999996 F F F
0.5371499999999969 0.2536300000000011 0.2882999999999996 F F F
0.5974799999999973 0.6839700000000022 0.2882999999999996 F F F
0.4841399999999965 0.8711600000000033 0.2883799999999965 F F F
0.1504899999999978 0.0664299999999969 0.2883799999999965 F F F
0.9841399999999965 0.8711600000000033 0.2883799999999965 F F F
0.6504899999999978 0.0664299999999969 0.2883799999999965 F F F
0.0673099999999991 0.4688000000000017 0.2915399999999977 F F F
0.5673099999999991 0.4688000000000017 0.2915399999999977 F F F
0.3173099999999991 0.4688000000000017 0.3254099999999980 F F F
0.8173099999999991 0.4688000000000017 0.3254099999999980 F F F
0.4004899999999978 0.0664299999999969 0.3285800000000023 F F F
0.2341399999999965 0.8711600000000033 0.3285800000000023 F F F
0.9004899999999978 0.0664299999999969 0.3285800000000023 F F F
0.7341399999999965 0.8711600000000033 0.3285800000000023 F F F
0.3474799999999973 0.6839700000000022 0.3286500000000032 F F F
0.2871499999999969 0.2536300000000011 0.3286500000000032 F F F
0.8474799999999973 0.6839700000000022 0.3286500000000032 F F F
0.7871499999999969 0.2536300000000011 0.3286500000000032 F F F
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0.9790803860245403 0.3747029773141220 0.4035740978036805 T T T
0.1535469327175377 0.5662863268338690 0.4027028776124159 T T T
0.6512132514807831 0.5620084500688504 0.4067537741072043 T T T
0.0389471931005578 0.7484175202195313 0.4104422717759457 T T T
0.5393600099316442 0.7477826369904137 0.4088534614105693 T T T
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0.5954257632811669 0.1892002895770460 0.4101145200416338 T T T
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0.0674093358167736 0.9686108689172148 0.4126973330581090 T T T
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0.3177222468662516 0.9681684198720560 0.4359470440731060 T T T
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0.3498017647012766 0.1906181088948384 0.4410369000608068 T T T
0.2845659425835216 0.7445139693550220 0.4430474492978976 T T T
0.8514482935876000 0.1943436314241548 0.4442644943345277 T T T
0.8916234225272245 0.5650603029670848 0.4439762759450026 T T T
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0.2362258194602401 0.3756113512576745 0.4475890708918460 T T T
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0.2320300000000017 0.5823099999999997 0.2641300000000015 F F F
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0.9025999999999996 0.3552899999999966 0.2641300000000015 F F F
0.1525999999999996 0.3552899999999966 0.3528200000000012 F F F
0.4820300000000017 0.5823099999999997 0.3528200000000012 F F F
0.6525999999999996 0.3552899999999966 0.3528200000000012 F F F
0.9820300000000017 0.5823099999999997 0.3528200000000012 F F F
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0.2271497452683244 0.0839454045642672 0.3828561406559615 T T T
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0.9679014424697308 0.0816706655805534 0.4538757133854949 T T T
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0.0685556735025882 0.5062007175387185 0.5736279235144295 T T T
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0.6895134319959260 0.5734608862485376 0.5423320354201194 T T T

K₂O-Fe₅C₂(010)-CH+O (TS)

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-1.5315638797000000 11.4316603084999997 0.0000000000000000
0.0000000000000000 0.0000000000000000 18.9298000335999994
Fe C O K H
40 17 2 2 1

Selective dynamics

Direct

0.0371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4758309300995395	0.3685894467025236	0.3992435660468371	T	T	T
0.979006917080837	0.3716970634475119	0.4033991941442397	T	T	T
0.1518975451670468	0.5631457026320650	0.4037914050373709	T	T	T
0.6496333581816741	0.5586580084175362	0.4081058426093153	T	T	T
0.0383188250894414	0.7478403670436372	0.4106472149368372	T	T	T
0.5385339200382633	0.7467613591316276	0.4091902123218069	T	T	T
0.0958400925265302	0.1881183594574127	0.4093726025200011	T	T	T
0.5954977438062203	0.1882298285473188	0.4092967950060859	T	T	T
0.5674094149330472	0.9681563691981158	0.4128415510390326	T	T	T
0.0670645502280164	0.9676012560811937	0.4121495037003943	T	T	T
0.8173044406712728	0.9657635270336095	0.4357267497875283	T	T	T
0.3176579379019487	0.9673175719164834	0.4359497297263712	T	T	T
0.7814541239303269	0.7405144616545446	0.4454053313797965	T	T	T
0.3494045129770241	0.1896080756476498	0.4413653753740476	T	T	T
0.2836099142089347	0.7432388668915416	0.4429616905477514	T	T	T
0.8506571426830828	0.1920872548200508	0.4442528896359731	T	T	T
0.8958837846294350	0.5631972758815135	0.4433603602913081	T	T	T
0.3938618789304294	0.5571121177400680	0.4491446235551866	T	T	T
0.2363967539495333	0.3743417488343395	0.4475340995392660	T	T	T
0.7372199853059660	0.3747095060717887	0.4511017752216038	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9053228786878179	0.8488940518780297	0.3840162698577111	T	T	T
0.2275618840739096	0.0833609009304678	0.3827836233474290	T	T	T
0.7283385398851864	0.0842764648039364	0.3831807568148464	T	T	T
0.4067410287721019	0.8509319777541908	0.3830234093217404	T	T	T
0.6655194301237272	0.8547021609400078	0.4542097562684649	T	T	T
0.4677080933025515	0.0809894481733263	0.4553520523458667	T	T	T
0.1671556421793053	0.8552270459959309	0.4546067776824922	T	T	T
0.9673104293721526	0.0797577042049828	0.4534586142535967	T	T	T
0.7348792347722485	0.5555383393427443	0.4998242318946733	T	T	T
0.7540607500699933	0.4148229013974362	0.5428849268753843	T	T	T
0.3087140472363827	0.4659561498265039	0.5227769926023959	T	T	T
0.0445436135985167	0.4722536399632180	0.5740227572956637	T	T	T
0.4986556563412272	0.3461180227952614	0.5772796412088523	T	T	T
0.6929466634213086	0.5870044515668585	0.5486943126559228	T	T	T

K₂O-Fe₅C₂(010)-CH+O (FS)

1.00000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O K H
40 17 2 2 1

Selective dynamics

Direct

0.0371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
--------------------	--------------------	--------------------	---	---	---

0.097479999999973	0.6839700000000022	0.288299999999996	F	F	F
0.537149999999969	0.2536300000000011	0.288299999999996	F	F	F
0.597479999999973	0.6839700000000022	0.288299999999996	F	F	F
0.484139999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.150489999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.984139999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.650489999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.067309999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.567309999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.317309999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.817309999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.400489999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.234139999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.900489999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.734139999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.347479999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.287149999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.847479999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.787149999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4791048339112023	0.3705734843637948	0.3997565240132544	T	T	T
0.9878476134958636	0.3721035015579940	0.4101552956291807	T	T	T
0.1542262362805454	0.5657019030017190	0.4021307837572524	T	T	T
0.6486801714194518	0.5656891109799429	0.4047179482455406	T	T	T
0.0369713637438609	0.7476053147708163	0.4116857022987768	T	T	T
0.5382284707575367	0.7500770782512793	0.4088159920873558	T	T	T
0.0957463405709868	0.1861336619066088	0.4086332747200205	T	T	T
0.5957599206932728	0.1901779784524636	0.4106513268514154	T	T	T
0.5684464867043449	0.9703181393023385	0.4132797915704858	T	T	T
0.0659065621179547	0.9661295139212576	0.4119524808297720	T	T	T
0.8172042714100418	0.9668901684445083	0.4359635900868397	T	T	T
0.3176912678747357	0.9680519180793270	0.4362970967004540	T	T	T
0.7775827785545563	0.7405577431121524	0.4483973931108734	T	T	T
0.3494411389911811	0.1900586850437888	0.4409130974442552	T	T	T
0.2839484589185148	0.7444203251475987	0.4429965070581687	T	T	T
0.8514477998455227	0.1905256336968642	0.4495433903128356	T	T	T
0.8993775326908283	0.5637286464742001	0.4432004725309860	T	T	T
0.3949058036605243	0.5595306311443655	0.4491697226343346	T	T	T
0.2421369594011115	0.3755258705199546	0.4470630581187678	T	T	T
0.7396836550873149	0.3826322928960527	0.4442607654419486	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9041846305146435	0.8484873917114328	0.3842037704812835	T	T	T
0.2273439080771443	0.0819888277320511	0.3825909506730380	T	T	T
0.7298683265575734	0.0871909507966309	0.3844782023187077	T	T	T
0.4067795073067401	0.8529965107869147	0.3829840487955525	T	T	T
0.6653303476527275	0.8566960163766523	0.4552448449875909	T	T	T
0.4673141082491795	0.0813365541724122	0.4561645753791695	T	T	T
0.1670328396409740	0.8555286015668605	0.4550814345238853	T	T	T
0.9682144677257848	0.0780513739157863	0.4541632081250028	T	T	T
0.7370163004795220	0.5803286556183685	0.4930617228106270	T	T	T
0.8843763340988974	0.3346766562183895	0.4977278046130554	T	T	T
0.3185803734627290	0.4643767471358092	0.5236016120119096	T	T	T
0.0742775412390099	0.4901403415195635	0.5720060163152891	T	T	T
0.5095583761131105	0.3521610278583298	0.5716530326341122	T	T	T
0.7015764885895680	0.5747329748414932	0.5484452953772302	T	T	T

COH formation and dissociation on K₂O-Fe₅C₂(010)

K₂O-Fe₅C₂(010)-COH (TS)

1.000000000000000		
9.9837999344000004	0.000000000000000	0.000000000000000
-1.5315638797000000	11.4316603084999997	0.000000000000000
0.000000000000000	0.000000000000000	18.9298000335999994

Fe C O K H
40 17 2 2 1

Selective dynamics

Direct

0.037149999999969	0.2536300000000011	0.288299999999996	F	F	F
0.097479999999973	0.6839700000000022	0.288299999999996	F	F	F

0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4779232015098414	0.3714445628393309	0.4000424368060685	T	T	T
0.9805619759757604	0.3734167255775413	0.4065503479906853	T	T	T
0.1523490643289303	0.5640671376224695	0.4032375712198671	T	T	T
0.6552483707629059	0.5686743064831278	0.4000065782002702	T	T	T
0.0381003054305866	0.7478132215915331	0.4110648891818458	T	T	T
0.5383258475698413	0.7482863891263107	0.4107196924723576	T	T	T
0.0956907255078243	0.1887653212382279	0.4090184888229041	T	T	T
0.5966148835032379	0.1898729933770189	0.4110791272090041	T	T	T
0.5682168229247141	0.9694294090403308	0.4128181860806400	T	T	T
0.0669337458822472	0.9677523296449738	0.4125134141148888	T	T	T
0.8180550889551046	0.9679200634601164	0.4354619598652148	T	T	T
0.3178046465475848	0.9683658462463467	0.4361483590546799	T	T	T
0.7823512405150238	0.7421612307631107	0.4467671654232795	T	T	T
0.3511122468739065	0.1911112021541570	0.4414255032849089	T	T	T
0.2843278006820161	0.7442975129849143	0.4421119093756850	T	T	T
0.8509805241392298	0.1945682994848031	0.4450175648425751	T	T	T
0.8944067258557081	0.5589607432748552	0.4438565527751427	T	T	T
0.3984674378434417	0.5602250565448024	0.4501938117044024	T	T	T
0.2370345715563605	0.3756145300749589	0.4479207272433223	T	T	T
0.7382449566244893	0.3813595396295916	0.4437873300747617	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9050546052709779	0.8489922498356273	0.3842135623534729	T	T	T
0.2277068861879483	0.0840289202915352	0.3832902196930377	T	T	T
0.7288880542251599	0.0869203880258241	0.3835092483069627	T	T	T
0.4073549263623144	0.8530480394197696	0.3831138206589019	T	T	T
0.6668657732623124	0.8570189387559871	0.4543250590443560	T	T	T
0.4682511412898791	0.0814930683556668	0.4559259909726978	T	T	T
0.1675179327750523	0.8555466741021528	0.4550057029175763	T	T	T
0.9677910371956839	0.0812810394282289	0.4538414774879382	T	T	T
0.7286953407113930	0.5697459146111026	0.4925408576562449	T	T	T
0.6496919537662903	0.5707235626076597	0.5478778690689770	T	T	T
0.3079793788456381	0.4689501919988125	0.5223042233535534	T	T	T
0.0991782407646747	0.5561523624361878	0.5741370703841400	T	T	T
0.4999383542273560	0.3590258591455265	0.5772976946104820	T	T	T
0.538548800882588	0.5982314076541584	0.5123022465446638	T	T	T

K₂O-Fe₃C₂(010)-COH (FS)

1.000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O K H
40 17 2 2 1

Selective dynamics

Direct

0.0371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F

0.150489999999978	0.066429999999969	0.288379999999965	F	F	F
0.984139999999965	0.871160000000033	0.288379999999965	F	F	F
0.650489999999978	0.066429999999969	0.288379999999965	F	F	F
0.067309999999991	0.468800000000017	0.291539999999977	F	F	F
0.567309999999991	0.468800000000017	0.291539999999977	F	F	F
0.317309999999991	0.468800000000017	0.325409999999980	F	F	F
0.817309999999991	0.468800000000017	0.325409999999980	F	F	F
0.400489999999978	0.066429999999969	0.328580000000023	F	F	F
0.234139999999965	0.871160000000033	0.328580000000023	F	F	F
0.900489999999978	0.066429999999969	0.328580000000023	F	F	F
0.734139999999965	0.871160000000033	0.328580000000023	F	F	F
0.347479999999973	0.683970000000022	0.328650000000032	F	F	F
0.287149999999969	0.253630000000011	0.328650000000032	F	F	F
0.847479999999973	0.683970000000022	0.328650000000032	F	F	F
0.787149999999969	0.253630000000011	0.328650000000032	F	F	F
0.477443238598987	0.3696141556372901	0.3993474031869718	T	T	T
0.9818210588012333	0.3727728340428523	0.4070442233008654	T	T	T
0.1539771523281171	0.5653093983127061	0.4019821200805778	T	T	T
0.6488351856192842	0.5664407719640533	0.4050761914305148	T	T	T
0.037643285989887	0.7479435817912173	0.4116279583465170	T	T	T
0.5388992041513911	0.7494533436902698	0.4094947909718141	T	T	T
0.0959109028034973	0.1892433186798652	0.4092896309363312	T	T	T
0.5970838585496760	0.1897278947322232	0.4117774383055150	T	T	T
0.568808572099706	0.9698584367837020	0.4133190937971848	T	T	T
0.0665960102935031	0.9677959025346303	0.4123505410340728	T	T	T
0.8179742756473320	0.9665217151992558	0.4356727587012588	T	T	T
0.3177492971192223	0.9685998510922752	0.4361656103894160	T	T	T
0.7812233964363579	0.7389987152764430	0.4478592321535266	T	T	T
0.3506770720935194	0.1904938011495494	0.4412487490844849	T	T	T
0.2844212593872091	0.7453010661659064	0.4417355946994848	T	T	T
0.8504747335398589	0.1945597044082261	0.4450711528799263	T	T	T
0.9006601550773552	0.5565636718758068	0.4436811034751930	T	T	T
0.3934578721038302	0.5593536210933067	0.4486853894923080	T	T	T
0.2377692321592383	0.3756759219471020	0.4486159175096907	T	T	T
0.7385810160798102	0.3843096141728349	0.4436785459672228	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9047641257477529	0.8483579103504453	0.3844055257442787	T	T	T
0.2275293970705364	0.0839181578175733	0.3831932611857940	T	T	T
0.7289809395220536	0.0865373072523167	0.3836010282861589	T	T	T
0.4076747354295018	0.8541124863145828	0.3829544191249944	T	T	T
0.6669534726140820	0.8556772459250793	0.4547790681292477	T	T	T
0.4682869424540864	0.0816342740636330	0.4565095071466327	T	T	T
0.1676216071821491	0.8559110201552896	0.4550812901912178	T	T	T
0.9672915188550566	0.0812431835504576	0.4535017515276465	T	T	T
0.7386865302983261	0.5691301715781601	0.4927289790102287	T	T	T
0.6907418262610050	0.5697517622514605	0.5627518560465843	T	T	T
0.3171404520069636	0.4671775174303050	0.5238837614004737	T	T	T
0.1030159322153773	0.5506826223865369	0.5740447382167103	T	T	T
0.5087783016436228	0.3522767245207307	0.5742744902922085	T	T	T
0.6205049651749353	0.6222669913336186	0.5614535237056858	T	T	T

K₂O-Fe₃C₂(010)-C+OH (TS)

1.000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O K H
40 17 2 2 1

Selective dynamics

Direct

0.03714999999999969	0.25363000000000011	0.2882999999999996	F	F	F
0.09747999999999973	0.68397000000000022	0.2882999999999996	F	F	F
0.53714999999999969	0.25363000000000011	0.2882999999999996	F	F	F
0.59747999999999973	0.68397000000000022	0.2882999999999996	F	F	F
0.48413999999999965	0.871160000000033	0.288379999999965	F	F	F
0.150489999999978	0.066429999999969	0.288379999999965	F	F	F
0.984139999999965	0.871160000000033	0.288379999999965	F	F	F
0.650489999999978	0.066429999999969	0.288379999999965	F	F	F

0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4760925707291059	0.3686709160006704	0.3991369239349045	T	T	T
0.9803561268160230	0.3723969500150277	0.4063189685593737	T	T	T
0.1558292876078780	0.5651097198455749	0.4017398640618164	T	T	T
0.6525241428887227	0.5676879379088997	0.4061399539135646	T	T	T
0.0399530278694587	0.7481583893660450	0.4098225100926192	T	T	T
0.5398615398827336	0.7491040255377311	0.4085613998956677	T	T	T
0.0954958469701845	0.1892312383890247	0.4088414171836471	T	T	T
0.5960971176159052	0.1884784190302949	0.4112851881266051	T	T	T
0.5679722439477091	0.9695019722166488	0.4127356227273923	T	T	T
0.0662512430275240	0.9673480822924676	0.4126541482584635	T	T	T
0.8171890116709996	0.9671789050121484	0.4354289427059641	T	T	T
0.3171674428483547	0.9685065312489464	0.4361889228961391	T	T	T
0.7865134689107374	0.7426988220361869	0.4522674374257460	T	T	T
0.3489236682906807	0.1901986027596924	0.4416902828700140	T	T	T
0.2850320448091309	0.7463269932256087	0.4417615349005718	T	T	T
0.8503619092470607	0.1929083170189433	0.4450748125416908	T	T	T
0.9009110621359753	0.5576116999961146	0.4419134303263968	T	T	T
0.3955759720239185	0.5604348626427963	0.4489130135745460	T	T	T
0.2373102290706734	0.3765986877517437	0.4488435791172662	T	T	T
0.7376619505803323	0.3755456869201101	0.4437184285924263	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9041881410380309	0.8472801187895046	0.3842320668399344	T	T	T
0.2268293376051746	0.0834674954120489	0.3830908997554426	T	T	T
0.7288234898957451	0.0866308814123929	0.3832795609844933	T	T	T
0.4075642332296454	0.8537781118107748	0.3829697369303985	T	T	T
0.6666074233359435	0.8558817094674795	0.4540688221599981	T	T	T
0.4673756915539845	0.0813956933381977	0.4561512631379608	T	T	T
0.1669966011208134	0.8557554421223528	0.4559184817603708	T	T	T
0.9676142450461760	0.0808340492657831	0.4534372383917049	T	T	T
0.7261408260350108	0.5171480058206127	0.4864881384023051	T	T	T
0.8063505038318451	0.6279309191897164	0.5517357787576372	T	T	T
0.3157880392913436	0.4692229282555793	0.5234598007735681	T	T	T
0.1021580389778788	0.5708541083153068	0.5741927161369671	T	T	T
0.5107581319138155	0.3550213900537209	0.5733726034869738	T	T	T
0.7221062618938577	0.6527615351374466	0.5688849883816596	T	T	T

K₂O-Fe₃C₂(010)-C+OH (FS)

1.000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O K H
40 17 2 2 1

Selective dynamics

Direct

0.0371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F

0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4776179823130206	0.3700359382306501	0.4008973771473842	T	T	T
0.9794939635636446	0.3751782365582759	0.4055736786323234	T	T	T
0.1542626840939092	0.5649476226505044	0.4021461792164651	T	T	T
0.6538174387643093	0.5693299066791364	0.4062049782952523	T	T	T
0.0429752167622278	0.7498648856032530	0.4065758101934879	T	T	T
0.5411589881594773	0.7500206318918597	0.4082104995433424	T	T	T
0.0954679999338485	0.1900594454544442	0.4091916161293663	T	T	T
0.5951446636285618	0.1879576300758414	0.4108576926491026	T	T	T
0.5681108426199599	0.9700641876593828	0.4123826799815718	T	T	T
0.0673065934886965	0.9686567749180500	0.4132316841454473	T	T	T
0.8177439779840969	0.9701059891495609	0.4351878824533114	T	T	T
0.3176678224211196	0.9694434931258118	0.4360057201534397	T	T	T
0.7909604553151610	0.7498763309315627	0.4516957959167374	T	T	T
0.3485250538811461	0.1912198784067548	0.4421052794253483	T	T	T
0.2864417011057126	0.7472915666385802	0.4408834877547688	T	T	T
0.8525766246921477	0.1931663097992420	0.4448676725447003	T	T	T
0.8934489982574907	0.5629068396547651	0.4459047967746853	T	T	T
0.3946999599348243	0.5610035396787215	0.4487991516318474	T	T	T
0.2358452982569853	0.3782186806758429	0.4489953447535948	T	T	T
0.7379393691943951	0.3702936334899146	0.4416481569949322	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9069093669359454	0.8510535470680528	0.3833138372345123	T	T	T
0.2267684261431016	0.0845894693817973	0.3830076716863005	T	T	T
0.7293240606136365	0.0880623242430182	0.3833754803887879	T	T	T
0.4084778501752058	0.8550089265829832	0.3827882268469688	T	T	T
0.6672602531348943	0.8576860475310433	0.4535379616057792	T	T	T
0.4673497514847501	0.0818621917138080	0.4562209793563282	T	T	T
0.1683180548205135	0.8566210486026452	0.4552165354053117	T	T	T
0.9691526425909230	0.0814358258254732	0.4547389246405181	T	T	T
0.7043586358631090	0.4968602286374158	0.4852799145494447	T	T	T
0.8804627932480745	0.6718811397923014	0.5328826439365529	T	T	T
0.3140586763543525	0.4714283952635718	0.5235209455928213	T	T	T
0.1182464479143168	0.5939919546519368	0.5737451473179506	T	T	T
0.5048524786121782	0.3582910243266497	0.5754723446449037	T	T	T
0.8001701426351301	0.6298837258988601	0.5559962997241809	T	T	T

CO dissociation on Fe₅C₂(010*)

Fe₅C₂(010*)-CO (IS)

1.000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O
40 16 1

Selective dynamics

Direct

0.0371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F

0.400489999999978	0.066429999999969	0.328580000000023	F	F	F
0.234139999999965	0.871160000000033	0.328580000000023	F	F	F
0.900489999999978	0.066429999999969	0.328580000000023	F	F	F
0.734139999999965	0.871160000000033	0.328580000000023	F	F	F
0.347479999999973	0.683970000000022	0.328650000000032	F	F	F
0.287149999999969	0.253630000000011	0.328650000000032	F	F	F
0.847479999999973	0.683970000000022	0.328650000000032	F	F	F
0.787149999999969	0.253630000000011	0.328650000000032	F	F	F
0.4779954053630740	0.3709935671078556	0.4039386956319794	T	T	T
0.9775638422827402	0.3709509988542534	0.4040734671658777	T	T	T
0.1560943201961845	0.5625669126365036	0.4053075021457779	T	T	T
0.6538452282436708	0.5625130955243892	0.4041436115566576	T	T	T
0.0370880568533506	0.7474107378337688	0.4098130592599142	T	T	T
0.5442518121312443	0.7524369717237164	0.4095982953377311	T	T	T
0.0941305374934045	0.1869860242285265	0.4087262137414153	T	T	T
0.5952035878461456	0.1880930332749604	0.4085983899367360	T	T	T
0.5677141971849942	0.9680763637253897	0.4109400371863962	T	T	T
0.0662898696100678	0.9664555642866186	0.4111178076110788	T	T	T
0.8136427291161548	0.9639213421776426	0.4371918377807698	T	T	T
0.3160966132428136	0.9678593977285956	0.4360796800478599	T	T	T
0.7724876045527200	0.7456419939298646	0.4423584313251893	T	T	T
0.3510274583672788	0.1926659995851162	0.4434938069407218	T	T	T
0.2813914928047096	0.7432295608996070	0.4428541496385526	T	T	T
0.8492825873427913	0.1917043984638844	0.4435166425421127	T	T	T
0.8987632589237672	0.5612322653915212	0.4454682242781385	T	T	T
0.4005503969780321	0.5605476619705271	0.4442753803854300	T	T	T
0.2356524916760432	0.3753819274489745	0.4447935724078878	T	T	T
0.7359604729913488	0.3760742667230906	0.4454602526658646	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9005431107823364	0.8480831608453836	0.3834506888715514	T	T	T
0.2272318308513276	0.0849673518877494	0.3830270437505399	T	T	T
0.7271281362707686	0.0823140900805799	0.3829021543847688	T	T	T
0.4059773904113185	0.8514948681595458	0.3837580594800278	T	T	T
0.6579104111419181	0.8618554601041081	0.4851023255086099	T	T	T
0.4674047314951004	0.0805194274141689	0.4524746519530747	T	T	T
0.1645122816537630	0.8557310437333421	0.4539722954731603	T	T	T
0.9638809710757825	0.0774288151047144	0.4506012090800097	T	T	T
0.6303281088443687	0.8660576323720088	0.5478251291232954	T	T	T

Fe₅C₂(010*)-C+O (TS)

1.000000000000000		
9.9837999344000004	0.000000000000000	0.000000000000000
-1.5315638797000000	11.4316603084999997	0.000000000000000
0.000000000000000	0.000000000000000	18.9298000335999994

Fe C O

40 16 1

Selective dynamics

Direct

0.037149999999969	0.253630000000011	0.288299999999996	F	F	F
0.097479999999973	0.683970000000022	0.288299999999996	F	F	F
0.537149999999969	0.253630000000011	0.288299999999996	F	F	F
0.597479999999973	0.683970000000022	0.288299999999996	F	F	F
0.484139999999965	0.871160000000033	0.288379999999965	F	F	F
0.150489999999978	0.066429999999969	0.288379999999965	F	F	F
0.984139999999965	0.871160000000033	0.288379999999965	F	F	F
0.650489999999978	0.066429999999969	0.288379999999965	F	F	F
0.067309999999991	0.468800000000017	0.291539999999977	F	F	F
0.567309999999991	0.468800000000017	0.291539999999977	F	F	F
0.317309999999991	0.468800000000017	0.325409999999980	F	F	F
0.817309999999991	0.468800000000017	0.325409999999980	F	F	F
0.400489999999978	0.066429999999969	0.328580000000023	F	F	F
0.234139999999965	0.871160000000033	0.328580000000023	F	F	F
0.900489999999978	0.066429999999969	0.328580000000023	F	F	F
0.734139999999965	0.871160000000033	0.328580000000023	F	F	F
0.347479999999973	0.683970000000022	0.328650000000032	F	F	F
0.287149999999969	0.253630000000011	0.328650000000032	F	F	F
0.847479999999973	0.683970000000022	0.328650000000032	F	F	F
0.787149999999969	0.253630000000011	0.328650000000032	F	F	F

0.4775862250121436	0.3714873900542854	0.4033372979221445	T	T	T
0.9785147763256195	0.3708605157329489	0.4041584658288330	T	T	T
0.1558943417386620	0.5638206609805947	0.4041988788361831	T	T	T
0.6553050241091766	0.5663846293428231	0.4063455585161110	T	T	T
0.0398954449499865	0.7496638011144000	0.4082339185338577	T	T	T
0.5350165733947263	0.7491534942901588	0.4089317747983036	T	T	T
0.0948180255288082	0.1882682275537601	0.4089866717467503	T	T	T
0.5954225845546707	0.1881948533292871	0.4093904812560559	T	T	T
0.5680106815363031	0.9689375451616117	0.4134540390048865	T	T	T
0.0677855771137683	0.9688625104431838	0.4112468368541886	T	T	T
0.8174608223638273	0.9675900477396538	0.4366433425110204	T	T	T
0.3169835217815933	0.9690612773683912	0.4355900682933263	T	T	T
0.7905830839047012	0.7431152807663082	0.4457988057536214	T	T	T
0.3516972281251822	0.1932230415286777	0.4446793010717902	T	T	T
0.2822673248407413	0.7438505565640730	0.4443045806325501	T	T	T
0.8510685647220404	0.1920546367170385	0.4440053614948443	T	T	T
0.9017404245733912	0.5573609179858768	0.4451255869827132	T	T	T
0.3944206419914703	0.5597894316374185	0.4453662098838260	T	T	T
0.2368808611888910	0.3760797404993519	0.4450461106622712	T	T	T
0.7360720053145273	0.3761396200179035	0.4447693261054569	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9056922144612481	0.8498610504258390	0.3827297021993949	T	T	T
0.2290617268087368	0.0876667960557308	0.3831538234299579	T	T	T
0.7283728898900987	0.0852539918620012	0.3833630046481419	T	T	T
0.4058405622121061	0.8515784315949708	0.3828478303570295	T	T	T
0.6661696498639804	0.8571145070726438	0.4560002202777258	T	T	T
0.4680886052161329	0.0805034562458487	0.4542166301341622	T	T	T
0.1665452173199106	0.8566083527666543	0.4529407546705498	T	T	T
0.9681112995805734	0.0798462045542256	0.4534297883335094	T	T	T
0.6257293556087461	0.7175412024021650	0.4963944454860235	T	T	T

Fe₅C₂(010*)C+O (FS)

1.000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O
40 16 1

Selective dynamics
Direct

0.0371499999999996	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999996	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4762483544099991	0.3695732733514197	0.4029989517999986	T	T	T
0.9803320532322669	0.3733935839445612	0.4050526583938796	T	T	T
0.1552317067069612	0.5634205949570297	0.4054140780053053	T	T	T
0.6515220203350786	0.5609903818302387	0.4083190950859800	T	T	T
0.0374963399581811	0.7481760473432898	0.4084224651535479	T	T	T
0.5371854413019527	0.7536431845689766	0.4177174910325086	T	T	T
0.0962549312173014	0.1888911461254290	0.4094024871962801	T	T	T
0.5957496724479981	0.1888102848117743	0.4093533807983455	T	T	T

0.5667881773327890	0.9703896656871073	0.4112555460428334	T	T	T
0.0679820132542198	0.9696428323770944	0.4115753062994374	T	T	T
0.8196696112280396	0.9708327004901594	0.4354681976696284	T	T	T
0.3173250623692880	0.9691227607566866	0.4351522627191499	T	T	T
0.7798707972099705	0.7464257814253630	0.4442481189906051	T	T	T
0.3519352846469336	0.1936599785733711	0.4448832869999359	T	T	T
0.2806274289593139	0.7438438002360408	0.4432922975555860	T	T	T
0.8534271990098307	0.1937068436109854	0.4446939939208583	T	T	T
0.8987416987654416	0.5598890779111981	0.4447192317610825	T	T	T
0.4038826841711467	0.5610021067468187	0.4447759669019727	T	T	T
0.2385849180276651	0.3772712549510675	0.4444137820423072	T	T	T
0.7372275836366005	0.3741547279307396	0.4447873091615312	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9047174814672214	0.8516512182961711	0.3836748989182137	T	T	T
0.2292344709298091	0.0884076107072944	0.3829777669559430	T	T	T
0.7307007740835079	0.0890335871094862	0.3828881918143059	T	T	T
0.4054324754149007	0.8511495304443558	0.3828682096595031	T	T	T
0.6680560633800420	0.8668792332059652	0.4549250580742626	T	T	T
0.4683271330050176	0.0815983835860600	0.4536433866208875	T	T	T
0.1653531000509024	0.8570155864810697	0.4523911182944286	T	T	T
0.9701710869448631	0.0817125046721445	0.4551163134574974	T	T	T
0.5679205952783311	0.6308610848899677	0.4847435304030094	T	T	T

HCO formation and dissociation on Fe₅C₂(010*)

Fe₅C₂(010*)-CO+H (IS)

1.000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O H
40 16 1 1

Selective dynamics

Direct

0.03714999999999969	0.25363000000000011	0.2882999999999996	F	F	F
0.09747999999999973	0.68397000000000022	0.2882999999999996	F	F	F
0.53714999999999969	0.25363000000000011	0.2882999999999996	F	F	F
0.59747999999999973	0.68397000000000022	0.2882999999999996	F	F	F
0.48413999999999965	0.87116000000000033	0.28837999999999965	F	F	F
0.15048999999999978	0.06642999999999969	0.28837999999999965	F	F	F
0.98413999999999965	0.87116000000000033	0.28837999999999965	F	F	F
0.65048999999999978	0.06642999999999969	0.28837999999999965	F	F	F
0.06730999999999991	0.46880000000000017	0.29153999999999977	F	F	F
0.56730999999999991	0.46880000000000017	0.29153999999999977	F	F	F
0.31730999999999991	0.46880000000000017	0.32540999999999980	F	F	F
0.81730999999999991	0.46880000000000017	0.32540999999999980	F	F	F
0.40048999999999978	0.06642999999999969	0.32858000000000023	F	F	F
0.23413999999999965	0.87116000000000033	0.32858000000000023	F	F	F
0.90048999999999978	0.06642999999999969	0.32858000000000023	F	F	F
0.73413999999999965	0.87116000000000033	0.32858000000000023	F	F	F
0.34747999999999973	0.68397000000000022	0.32865000000000032	F	F	F
0.28714999999999969	0.25363000000000011	0.32865000000000032	F	F	F
0.84747999999999973	0.68397000000000022	0.32865000000000032	F	F	F
0.78714999999999969	0.25363000000000011	0.32865000000000032	F	F	F
0.4766672794087378	0.3709230739354732	0.4028432622069616	T	T	T
0.9796037301779125	0.3713953189940847	0.4047149792706241	T	T	T
0.1534139886870557	0.5616676492303029	0.4061840923879688	T	T	T
0.6499677329485382	0.5626608258382864	0.4056781531768117	T	T	T
0.0375499255353887	0.7476520070758227	0.4091497214207926	T	T	T
0.5439599586687809	0.7523255882665969	0.4084782819867295	T	T	T
0.0948305477694721	0.1871593060080952	0.4082667432119948	T	T	T
0.5948747992894986	0.1879273418550133	0.4086378612627312	T	T	T
0.5677513127746758	0.9678156493734237	0.4107065599952515	T	T	T
0.0651178476328472	0.9665394974633881	0.4104210973860055	T	T	T
0.8140452458472314	0.9640084455949745	0.4363578651924082	T	T	T
0.3162095873301076	0.9677788857690279	0.4354988380582517	T	T	T
0.7727935755704968	0.7459160079965838	0.4432327326275139	T	T	T
0.3516620163674098	0.1915658011236502	0.4436827938084468	T	T	T

0.2806808279935433	0.7439760415566476	0.4420745360067222	T	T	T
0.8499808880728842	0.1921524467631899	0.4428909809131777	T	T	T
0.8955274720496814	0.5611154394999273	0.4440769549134402	T	T	T
0.3963120760554347	0.5617993557785362	0.4444959962456972	T	T	T
0.2377684277710299	0.3738750397879949	0.4441479110794492	T	T	T
0.7354587112116758	0.3744592467536624	0.4451025018206524	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.8995574798248128	0.8464266870826728	0.3841543075897441	T	T	T
0.2276680409090789	0.0854146020575432	0.3831886089568847	T	T	T
0.7265635659024600	0.0824007735829254	0.3825581929204622	T	T	T
0.4063742197541643	0.8513893022117455	0.3837748890927313	T	T	T
0.6568967453304616	0.8636229390591310	0.4838314557971761	T	T	T
0.4677682777860407	0.0797063877561419	0.4525433655011071	T	T	T
0.1647471113241500	0.8565382574934529	0.4530752709313339	T	T	T
0.9637856534965935	0.0776908820652529	0.4499712547530554	T	T	T
0.6305690274811455	0.8642747350155299	0.5468543849718486	T	T	T
0.7429967970707235	0.6006863335740955	0.4819261542607015	T	T	T

Fe₃C₂(010*)-HCO (TS)

1.000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O H

40 16 1 1

Selective dynamics

Direct

0.0371499999999996	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999997	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999996	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999997	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999996	0.8711600000000033	0.2883799999999996	F	F	F
0.1504899999999997	0.0664299999999996	0.2883799999999996	F	F	F
0.9841399999999996	0.8711600000000033	0.2883799999999996	F	F	F
0.6504899999999997	0.0664299999999996	0.2883799999999996	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999997	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999997	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999998	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999998	F	F	F
0.4004899999999997	0.0664299999999996	0.3285800000000023	F	F	F
0.2341399999999996	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999997	0.0664299999999996	0.3285800000000023	F	F	F
0.7341399999999996	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999997	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999996	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999997	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999996	0.2536300000000011	0.3286500000000032	F	F	F
0.4788323304978874	0.3731688375858937	0.4048815803756867	F	F	F
0.9790795360909215	0.3721085361049319	0.4044784123398202	F	F	F
0.1557061007199181	0.5643866953627850	0.4042450133619226	F	F	F
0.6548140002588099	0.5621894725536762	0.4024356278143983	F	F	F
0.0398957139212399	0.7482836883507957	0.4092811066792379	F	F	F
0.5429854637504050	0.7504215704131241	0.4091193663567481	F	F	F
0.0955177004477505	0.1881074042808137	0.4079713790462378	F	F	F
0.5946006056966695	0.1900148723856248	0.4083345465186241	F	F	F
0.5635200094134305	0.9716141968753078	0.4081105916450554	F	F	F
0.0663777099304994	0.9668517676953030	0.4091944025830188	F	F	F
0.8175766956549069	0.9625495465353495	0.4399815643606004	F	F	F
0.3151273740596139	0.9692124350880746	0.4355785018252902	F	F	F
0.7773353653214201	0.7409503778126947	0.4407224454773910	F	F	F
0.3503757683873943	0.1946792776484756	0.4441756908847694	F	F	F
0.2825125458392392	0.7442941468457178	0.4441118013947118	F	F	F
0.8511951533186846	0.1922754715106620	0.4425402220850430	F	F	F
0.8978996598807072	0.5617805781949343	0.4451254630695871	F	F	F
0.3977160290726331	0.5617261359096517	0.4441627946475109	F	F	F
0.236550758090862	0.3763013864327291	0.4444026019194709	F	F	F
0.7376609739150695	0.3755617411745220	0.4449825929227842	F	F	F
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F

0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9005229597662776	0.8444761950239723	0.3837846705804822	F	F	F
0.2285342596417195	0.0859139356449319	0.3826352725553619	F	F	F
0.7282150801568577	0.0859372559460070	0.3819835235862570	F	F	F
0.4055093610061959	0.8508617284574669	0.3843779870931314	F	F	F
0.6625725006591594	0.8273163776465182	0.4850496719608302	F	F	F
0.4656453721195959	0.0829941411059991	0.4523075675516495	F	F	F
0.1655112760785258	0.8569420514455288	0.4540662505494097	F	F	F
0.9657708579887725	0.0777962333154960	0.4488344562302302	T	T	T
0.6591562376135016	0.9340734390683920	0.5082644472640183	T	T	T
0.7185937671093044	0.7654105033938450	0.5250491191453803	T	T	T

Fe₃C₂(010*)-HCO (FS)

1.0000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O H
40 16 1 1

Selective dynamics

Direct

0.0371499999999996	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999997	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999996	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999997	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999997	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999997	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4780876223042038	0.3724904409694361	0.4041947007515972	T	T	T
0.978330969842838	0.3714924252503434	0.4041120084967125	T	T	T
0.1565950072730256	0.5635403362423764	0.4041870390576562	T	T	T
0.6550219339906433	0.5640374941580013	0.4022483234010894	T	T	T
0.0378678021768748	0.7470199177412585	0.4097248518518838	T	T	T
0.5436565954604793	0.7510719714362651	0.4107256597389880	T	T	T
0.0943088991824464	0.1875394420813381	0.4085150163734349	T	T	T
0.5954286820300209	0.1897878677233754	0.4082016604649971	T	T	T
0.5659844671765848	0.9700193526117405	0.4089836399517811	T	T	T
0.0662123154690261	0.9663268725047034	0.4097698397039917	T	T	T
0.8182964693696968	0.9625400303039926	0.4392788916955556	T	T	T
0.3154552551169131	0.9688619773543879	0.4356845486286508	T	T	T
0.7736973575952252	0.7414493202343875	0.4441291851506687	T	T	T
0.3503007516554264	0.1939391374380426	0.4441620575762518	T	T	T
0.2825980440583929	0.7436181865838115	0.4431039911959532	T	T	T
0.8503826328589177	0.1925937720290819	0.4436585686284648	T	T	T
0.8985715704171153	0.5598512374766800	0.4451505327070091	T	T	T
0.3986344668013082	0.5602483061370455	0.4444028708483454	T	T	T
0.2351365514233802	0.3758209556806715	0.4448616458804633	T	T	T
0.7363062673740118	0.3769801060904235	0.4454438456623789	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F

0.8994333829854375	0.8453060723273395	0.3846555065763601	T	T	T
0.2276232528621129	0.0856019087629206	0.3830027682243248	T	T	T
0.7300351479436578	0.0864354136618064	0.3820105048512940	T	T	T
0.4064770653927308	0.8505578509596594	0.3837664379427357	T	T	T
0.6445089087984371	0.8171196955573746	0.4979947044187119	T	T	T
0.4665242722324997	0.0826629072991577	0.4514013297436845	T	T	T
0.1654299865187779	0.8557745177477518	0.4533048065995737	T	T	T
0.9643854910549560	0.0765782392802563	0.4497365430999868	T	T	T
0.6622151792860176	0.9362109647367185	0.4997732405129037	T	T	T
0.6113855175235567	0.7799949185966139	0.5500622922984891	T	T	T

Fe₅C₂(010*)-CH+O (TS)

1.000000000000000		
9.9837999344000004	0.000000000000000	0.000000000000000
-1.5315638797000000	11.4316603084999997	0.000000000000000
0.000000000000000	0.000000000000000	18.9298000335999994

Fe C O H

40 16 1 1

Selective dynamics

Direct

0.0371499999999996	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999996	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4773797779011417	0.3720627687741711	0.4036844976207661	F	F	F
0.9776066860853315	0.3725439927914138	0.4045211321028503	F	F	F
0.1556066252756807	0.5622419019458675	0.4052721647353934	F	F	F
0.6560196301192320	0.5645657635981465	0.4027308341196516	F	F	F
0.0363560854757878	0.7471075803700415	0.4089516331228538	F	F	F
0.5392939486362067	0.7489336988391884	0.4076613870683374	F	F	F
0.0979960407000320	0.1898640255728239	0.4078278923801122	F	F	F
0.5941110717452744	0.1865883255673708	0.4069639905436446	F	F	F
0.5693022052130416	0.9649400914486392	0.4172750155747593	F	F	F
0.0679615038802908	0.9666804185317019	0.4095766366393363	F	F	F
0.8135470930786255	0.9664288402949381	0.4446032314616843	F	F	F
0.3157707376431986	0.9678418956415769	0.4360291846730462	F	F	F
0.7707179250902243	0.7472124771920789	0.4440052043471425	F	F	F
0.3528317388179616	0.1934934823568355	0.4445567792548175	F	F	F
0.2804048684185432	0.7427578822484406	0.4422515526388651	F	F	F
0.8476263993491671	0.1915541822789351	0.4442950485030366	F	F	F
0.8975539389751219	0.5620759353469751	0.4460106200189458	F	F	F
0.3994389299239742	0.5600600777880445	0.4454358314557538	F	F	F
0.2361477407364205	0.3755426164886870	0.4457908794944458	F	F	F
0.7336731217695558	0.3761871169309003	0.4453971857649393	F	F	F
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.8988008182769462	0.8457642485786891	0.3842360392269626	F	F	F
0.2300203852249041	0.0861915366983510	0.3829196265166743	F	F	F
0.7271015780252057	0.0825884770930969	0.3815912244076571	F	F	F
0.4065703709641539	0.8527537968800090	0.3833451614877674	F	F	F
0.6437231427292502	0.8428947787196677	0.4820563597988539	F	F	F
0.4683012934503665	0.0802477013901779	0.4534099793870467	F	F	F
0.1639875670350222	0.8560939782681913	0.4537679698789105	F	F	F

0.9671579235369734	0.0793997881392841	0.4442110233779815	T	T	T
0.7287685750588366	0.9860453534472100	0.5228084789252208	T	T	T
0.6043657468499219	0.8282237042731353	0.5353016176127253	T	T	T

Fe₅C₂(010*)-CH+O (FS)

1.000000000000000		
9.9837999344000004	0.000000000000000	0.000000000000000
-1.5315638797000000	11.4316603084999997	0.000000000000000
0.000000000000000	0.000000000000000	18.9298000335999994

Fe C O H

40 16 1 1

Selective dynamics

Direct

0.0371499999999996	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999996	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4783560126672207	0.3731919684717845	0.4046019384035122	T	T	T
0.9760328564642333	0.3712368414919633	0.4061121755114671	T	T	T
0.1539319153863021	0.5621149396580949	0.4057342639520406	T	T	T
0.6573786289630752	0.5651257454121056	0.4032579044160182	T	T	T
0.0351830681586577	0.7473924060782104	0.4093538604396109	T	T	T
0.5391445655356502	0.7485382010992195	0.4102792121783668	T	T	T
0.1008825167477966	0.1914889310006069	0.4058161455681466	T	T	T
0.5920355729139395	0.1881164506360057	0.4065925911614708	T	T	T
0.5617508956250747	0.9654911987213736	0.4110022138745894	T	T	T
0.0700040025268850	0.9664119314496219	0.4079888731142698	T	T	T
0.8023501222239210	0.9740463832122271	0.4486999122714542	T	T	T
0.3148495694284235	0.9668545280033111	0.4361913647778388	T	T	T
0.7727349115445955	0.7512784351413997	0.4428793990636693	T	T	T
0.3532503404817838	0.1932929604861667	0.4443542027839963	T	T	T
0.2780431744404135	0.7416062874196839	0.4433846586630688	T	T	T
0.8416497485041071	0.1826854201340115	0.4521666458755186	T	T	T
0.8968854827823164	0.5629140358991621	0.4462336103493952	T	T	T
0.3988575934737708	0.5600071708320539	0.4453774189411554	T	T	T
0.2365215004826511	0.3762015188259433	0.4461388801110407	T	T	T
0.7357148991424166	0.3733607987525978	0.4463559640354798	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.8988765002409397	0.8462749968580366	0.3835289058499705	T	T	T
0.2324048582651943	0.0873152047082413	0.3826265515212063	T	T	T
0.7249429160799581	0.0858100263026280	0.3807528896822443	T	T	T
0.4034452286884878	0.8475588523509622	0.3835867401111143	T	T	T
0.6475773648880206	0.8541451976799981	0.4762332978851468	T	T	T
0.4678522416903980	0.0785968974433085	0.4534988515597480	T	T	T
0.1628399635037682	0.8556647194966096	0.4548066972512997	T	T	T
0.9681061443739913	0.0801796916846437	0.4330080238303279	T	T	T
0.7908048881731208	0.0787403900181181	0.5205958243023839	T	T	T
0.6144040012759363	0.8615182110470845	0.5314963464203118	T	T	T

COH formation and dissociation on Fe₅C₂(010*)

Fe₅C₂(010*)-COH (TS)

```

1.000000000000000
 9.9837999344000004  0.0000000000000000  0.0000000000000000
-1.5315638797000000  11.4316603084999997  0.0000000000000000
 0.0000000000000000  0.0000000000000000  18.9298000335999994
Fe C O H
 40 16 1 1
Selective dynamics
Direct
0.0371499999999996 0.2536300000000011 0.2882999999999996 F F F
0.0974799999999973 0.6839700000000022 0.2882999999999996 F F F
0.5371499999999969 0.2536300000000011 0.2882999999999996 F F F
0.5974799999999973 0.6839700000000022 0.2882999999999996 F F F
0.4841399999999965 0.8711600000000033 0.2883799999999965 F F F
0.1504899999999978 0.0664299999999969 0.2883799999999965 F F F
0.9841399999999965 0.8711600000000033 0.2883799999999965 F F F
0.6504899999999978 0.0664299999999969 0.2883799999999965 F F F
0.0673099999999991 0.4688000000000017 0.2915399999999977 F F F
0.5673099999999991 0.4688000000000017 0.2915399999999977 F F F
0.3173099999999991 0.4688000000000017 0.3254099999999980 F F F
0.8173099999999991 0.4688000000000017 0.3254099999999980 F F F
0.4004899999999978 0.0664299999999969 0.3285800000000023 F F F
0.2341399999999965 0.8711600000000033 0.3285800000000023 F F F
0.9004899999999978 0.0664299999999969 0.3285800000000023 F F F
0.7341399999999965 0.8711600000000033 0.3285800000000023 F F F
0.3474799999999973 0.6839700000000022 0.3286500000000032 F F F
0.2871499999999969 0.2536300000000011 0.3286500000000032 F F F
0.8474799999999973 0.6839700000000022 0.3286500000000032 F F F
0.7871499999999969 0.2536300000000011 0.3286500000000032 F F F
0.4781800472612226 0.3724368323857944 0.4039380330485582 T T T
0.9769308041562046 0.3732941364084068 0.4043604810450598 T T T
0.1544614764473599 0.5630497796360047 0.4052135539629419 T T T
0.6539882819929307 0.5671479460396367 0.4034988468363120 T T T
0.0397638778375321 0.7480235032529777 0.4091251100216499 T T T
0.5414444138194703 0.7516412591804088 0.4072259130678525 T T T
0.0958512443414699 0.1882230480732507 0.4089613661819900 T T T
0.5962902307296964 0.1881916271678889 0.4097649926065720 T T T
0.5701962449509872 0.9683772428352441 0.4165373792782825 T T T
0.0662601082842639 0.9670989302907461 0.4109340155197447 T T T
0.8169971418425029 0.9646827091691904 0.4364065251030346 T T T
0.3171993709537212 0.9691954711643440 0.4363055211877324 T T T
0.7743108601864743 0.7467488776326592 0.4425117150781041 T T T
0.3532595155161592 0.1930390527760518 0.4439489498953619 T T T
0.2843504420321310 0.7436950268004787 0.4431633578752032 T T T
0.8495415524918674 0.1916087552315506 0.4432248689518477 T T T
0.8947335646010580 0.5661367572328441 0.4468581705092072 T T T
0.3977247020074498 0.5611908108131334 0.4444842845232949 T T T
0.2354097743123454 0.3758093408353986 0.4451433808548341 T T T
0.7345120770893963 0.3773177755415759 0.4460287565992965 T T T
0.2320300000000017 0.5823099999999997 0.2641300000000015 F F F
0.4025999999999996 0.3552899999999966 0.2641300000000015 F F F
0.7320300000000017 0.5823099999999997 0.2641300000000015 F F F
0.9025999999999996 0.3552899999999966 0.2641300000000015 F F F
0.1525999999999996 0.3552899999999966 0.3528200000000012 F F F
0.4820300000000017 0.5823099999999997 0.3528200000000012 F F F
0.6525999999999996 0.3552899999999966 0.3528200000000012 F F F
0.9820300000000017 0.5823099999999997 0.3528200000000012 F F F
0.9030357529607169 0.8470012685641674 0.3836608454464298 T T T
0.2290344201830770 0.0860289405600626 0.3835912277241846 T T T
0.7268356236251852 0.0814651020162931 0.3831467885765067 T T T
0.4084576976206846 0.8549100642037983 0.3836755688954061 T T T
0.6587272929054511 0.8589497943964912 0.4758124245841364 T T T
0.4691583440487838 0.0803419589234120 0.4555454146232358 T T T
0.1670075057994243 0.8564937000860325 0.4532458999244987 T T T
0.9664476349595069 0.0791786546318259 0.4512047702134271 T T T
0.6752905393212484 0.8199660962563026 0.5400955130259300 T T T
0.7432337815962500 0.7251193779312937 0.5299982458712877 T T T

```

Fe₃C₂(010*)-COH (FS)

```

1.000000000000000
 9.9837999344000004  0.0000000000000000  0.0000000000000000
-1.5315638797000000  11.4316603084999997  0.0000000000000000
 0.0000000000000000  0.0000000000000000  18.9298000335999994
Fe C O H
 40 16 1 1
Selective dynamics

```

Direct

0.0371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4779423725116211	0.3714094791977636	0.4038254048992911	T	T	T
0.9778967795610497	0.3708773381425214	0.4042640933628057	T	T	T
0.1560741283938664	0.5625240194840084	0.4050843609365388	T	T	T
0.6541740981456587	0.5647106390517465	0.4038429876757368	T	T	T
0.0380387061463002	0.7472364133662912	0.4096352374855636	T	T	T
0.5442400787162194	0.7523926740781156	0.4104919993783079	T	T	T
0.0933722137270354	0.1867963040086663	0.4087325961508016	T	T	T
0.5950285628208775	0.1881419948704659	0.4085848510673654	T	T	T
0.5690930883156105	0.9680986104474218	0.4121766326069553	T	T	T
0.0659100646549243	0.9665540393214008	0.4117612271084474	T	T	T
0.8132779769332853	0.9636075990258949	0.4368761707005103	T	T	T
0.3165851571700560	0.9672942822353235	0.4357448125231509	T	T	T
0.7752874249292643	0.7464243858168638	0.4424415304474464	T	T	T
0.3504054342802357	0.1921093796717868	0.4435599414156960	T	T	T
0.2824333151728888	0.7431279539258787	0.4426850110606308	T	T	T
0.8490447593297757	0.1912648995572180	0.4437185532709702	T	T	T
0.8980920738499181	0.5610929547041715	0.4452154655264816	T	T	T
0.3993603580415179	0.5607200549783254	0.4442263401079158	T	T	T
0.2362172364237492	0.3751701659460855	0.4447960618478995	T	T	T
0.7361613343796034	0.3767858573440923	0.4452638302438809	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9015702489069081	0.8480361267928984	0.3838680340589147	T	T	T
0.2269053068262168	0.0848490787947105	0.3832316694187259	T	T	T
0.7274982213890080	0.0826135603025214	0.3830561717284444	T	T	T
0.4071032233189011	0.8507596454827143	0.3835473817568692	T	T	T
0.6598238873041075	0.8597481505320184	0.4778920505812685	T	T	T
0.4672416620540208	0.0804533449063802	0.4524018035932521	T	T	T
0.1655799626617150	0.8552327358966241	0.4538407616254388	T	T	T
0.9634188466928985	0.0769098334747753	0.4516258653367168	T	T	T
0.6291586237033132	0.8645538221926736	0.5486185092506609	T	T	T
0.5584354665882206	0.7995642543516980	0.5596052569228360	T	T	T

Fe₅C₂(010*)-C+OH (TS)

1.00000000000000
 9.9837999344000004 0.0000000000000000 0.0000000000000000
 -1.5315638797000000 11.4316603084999997 0.0000000000000000
 0.0000000000000000 0.0000000000000000 18.9298000335999994
 Fe C O H
 40 16 1 1

Selective dynamics

Direct

0.0371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F

0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4791025129126968	0.3726893498958287	0.4046656865287952	T	T	T
0.9777628080374881	0.3707616539972081	0.4042725818946890	T	T	T
0.1558567309877825	0.5638494746755590	0.4049837841575432	T	T	T
0.6574359810623263	0.5663580088123534	0.4033275393128963	T	T	T
0.0394046767001345	0.7468492021621459	0.4092131628765309	T	T	T
0.5416538005970888	0.7506953895074474	0.4067805922106431	T	T	T
0.0955312485900695	0.1871403993873520	0.4093489130210983	T	T	T
0.5949318534112518	0.1870110954912814	0.4093564123082277	T	T	T
0.5673709652923173	0.9677638416692818	0.4135738783293574	T	T	T
0.0654725703385640	0.9664275026235805	0.4114415147288758	T	T	T
0.8172211641557053	0.9662445762493951	0.4354869889275592	T	T	T
0.3165302558656424	0.9689185377288957	0.4357457652520954	T	T	T
0.7885314770661103	0.7417468678857189	0.4530025235675597	T	T	T
0.3527578759439401	0.1925974059055870	0.4439305659825409	T	T	T
0.2850684901138894	0.7434537164985999	0.4437018518521876	T	T	T
0.8514348082568799	0.1909833860610965	0.4432057749667097	T	T	T
0.8985796382213468	0.5580572221863149	0.4446836439903668	T	T	T
0.3979487408523930	0.5600343932098460	0.4440179102126741	T	T	T
0.2364506867644429	0.3763063071601114	0.4444144991449616	T	T	T
0.7359246584954974	0.3748779468132175	0.4441202863073729	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9027051913429386	0.8454703015733669	0.3836065421511333	T	T	T
0.2289031426560433	0.0856335000722106	0.3831873012227098	T	T	T
0.7280447424021514	0.0842177821462019	0.3828270124087789	T	T	T
0.4070174936197622	0.8522777697025348	0.3827501748662527	T	T	T
0.6650007836833158	0.8568568637333887	0.4572566888827688	T	T	T
0.4684823619958827	0.0796885407696498	0.4548617186116988	T	T	T
0.1670624858586495	0.8555137837439303	0.4527448204049689	T	T	T
0.9684763216254794	0.0789412250862178	0.4531873484507095	T	T	T
0.7067346095311445	0.7818896870978144	0.5419893650811969	T	T	T
0.6234887771960465	0.7274625582069010	0.5491148785605305	T	T	T

Fe₅C₂(010*)-C+OH (FS)

1.00000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O H

40 16 1 1

Selective dynamics

Direct

0.0371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F

0.400489999999978	0.066429999999969	0.3285800000000023	F	F	F
0.234139999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.900489999999978	0.066429999999969	0.3285800000000023	F	F	F
0.734139999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.347479999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.287149999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.847479999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.787149999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4773059969332664	0.3707643074387298	0.4027989625761036	T	T	T
0.9807894751404986	0.3717813229364685	0.4045204967539631	T	T	T
0.1559129056219791	0.5630206941656779	0.4054027693288407	T	T	T
0.6455170008577035	0.5638986374318705	0.4086840877266855	T	T	T
0.0405112109799007	0.7485785752035028	0.4091502113570177	T	T	T
0.5388502618376162	0.7507995713781307	0.4082032654135695	T	T	T
0.0960277018171855	0.1880356838341537	0.4097636886525818	T	T	T
0.5960793046247879	0.1884335810017047	0.4099839966768700	T	T	T
0.5683771039021663	0.9697594799843829	0.4117293352043734	T	T	T
0.0674881459186816	0.9685242199230405	0.4119125285878784	T	T	T
0.8181895307601357	0.9672473212001064	0.4348727301557311	T	T	T
0.3182144743565014	0.9693553967512707	0.4356450115037267	T	T	T
0.7833756427321260	0.7468446974801443	0.4486503882208907	T	T	T
0.3526604212407236	0.1928890865951022	0.4446324512413434	T	T	T
0.2843585385631778	0.7449125717686587	0.4434621732004042	T	T	T
0.8525681881874583	0.1929178271043734	0.4443145530354202	T	T	T
0.9051346905031319	0.5596432159995584	0.4448759988323420	T	T	T
0.3934332515897578	0.5611438899528498	0.4446648156014183	T	T	T
0.2375178562227391	0.3750411227410305	0.4447613194917147	T	T	T
0.7381458173487860	0.3724437545444743	0.4442378142776818	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9053822433068592	0.8482195205959144	0.3840169912457812	T	T	T
0.2293253897755887	0.0874921280800260	0.3834909677260754	T	T	T
0.7294829473643314	0.0881592537914195	0.3827901499624207	T	T	T
0.4061508076296661	0.8525783629056479	0.3824638165357999	T	T	T
0.6653488785454662	0.8589970060066499	0.4535836057648307	T	T	T
0.4689267675822946	0.0807698126724380	0.45472132411105315	T	T	T
0.1679882123711884	0.8569763535939707	0.4531435506930551	T	T	T
0.9682807793371737	0.0800787413343474	0.4536130631382998	T	T	T
0.7509550326690303	0.5943355851840615	0.5025742554808682	T	T	T
0.7109930253778223	0.5815884138544977	0.5492879447163765	T	T	T

CO dissociation on $K_2O-Fe_5C_2(010^*)$

$K_2O-Fe_5C_2(010^*)-CO$ (IS)

1.000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O K

40 16 2 2

Selective dynamics

Direct

0.037149999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.097479999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.537149999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.597479999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.484139999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.150489999999978	0.066429999999969	0.2883799999999965	F	F	F
0.984139999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.650489999999978	0.066429999999969	0.2883799999999965	F	F	F
0.067309999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.567309999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.317309999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.817309999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.400489999999978	0.066429999999969	0.3285800000000023	F	F	F
0.234139999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.900489999999978	0.066429999999969	0.3285800000000023	F	F	F
0.734139999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.347479999999973	0.6839700000000022	0.3286500000000032	F	F	F

0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4812151238842897	0.3744832574597205	0.4053555381779768	T	T	T
0.9811305252068436	0.3758300496784025	0.4068299306670514	T	T	T
0.1551512467745146	0.5675766930478700	0.4036562333501438	T	T	T
0.6552741681350254	0.5655104647145035	0.4027217451424637	T	T	T
0.0371417156841666	0.7496319603097178	0.4088279598559950	T	T	T
0.5439227639296405	0.7526602296117565	0.4121801608184190	T	T	T
0.0964170418423548	0.1904617874420181	0.4095516975456269	T	T	T
0.5963192769419261	0.1881056380215777	0.4107731233380245	T	T	T
0.5693547254797929	0.9685043754894280	0.4124515786328241	T	T	T
0.0668116778622874	0.9696675667209904	0.4108825946894001	T	T	T
0.8159046930138326	0.9678381822536840	0.4369983892043645	T	T	T
0.3166404080498353	0.9707970720059569	0.4342199174293596	T	T	T
0.7758225573416372	0.7493587423281590	0.4396565684998837	T	T	T
0.3545016114722119	0.1933526990312837	0.4444906370044195	T	T	T
0.2832456544788623	0.7482992588020284	0.4468134386804509	T	T	T
0.8522211211566132	0.1943599595696557	0.4428219248620422	T	T	T
0.8923965567108505	0.5636651406279644	0.4446411177478780	T	T	T
0.3937616320133015	0.5625894403690680	0.4445301990130404	T	T	T
0.2398985106538097	0.3768517757316306	0.4438227008063537	T	T	T
0.7359386523458228	0.3768806095428618	0.4447528124975331	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9022604149723725	0.8522284897571907	0.3836013042725861	T	T	T
0.2295088933883307	0.0896022571155338	0.3836571090527053	T	T	T
0.7280985148059579	0.0831206569828634	0.3832011272685922	T	T	T
0.4059150893816906	0.8543602876207268	0.3824474908535359	T	T	T
0.4685563111403521	0.0795579585889529	0.4561522336293032	T	T	T
0.1656977693247476	0.8590704950381790	0.4534689023192697	T	T	T
0.9662031681204394	0.0802881459966852	0.4519056116935863	T	T	T
0.6669605927962028	0.8640697297894742	0.4841947627520353	T	T	T
0.6481634570200354	0.8588563462035220	0.5506789738040890	T	T	T
0.4041776946088440	0.686592853906941	0.5079132296884525	T	T	T
0.4095694954237780	0.9046412201579009	0.5818589241793054	T	T	T
0.6106542937566305	0.6072530117574610	0.5750094141182027	T	T	T

K₂O-Fe₃C₂(010*)-C+O (TS)

1.000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O K

40 16 2 2

Selective dynamics

Direct

0.0371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4831380022674593	0.3752740903867677	0.4071736506228842	T	T	T

0.9816496148564724	0.3740293025090222	0.4065754043227762	T	T	T
0.1552791992064876	0.5680605711566479	0.4035923708136567	T	T	T
0.6583258578478453	0.5632347287927560	0.4026488275777605	T	T	T
0.0382694658614603	0.7478135721563438	0.4092300382528189	T	T	T
0.5437764176671506	0.7497871707510150	0.4046226575140456	T	T	T
0.0967431523189543	0.1886693579517817	0.4100487144313840	T	T	T
0.5956776501464244	0.1882264059081658	0.4106038437409074	T	T	T
0.5665889839462128	0.9687234425787958	0.4122157879256439	T	T	T
0.0668077684014178	0.9680085436124857	0.4111597062515028	T	T	T
0.8179073101960274	0.9679788437796237	0.4358076588851220	T	T	T
0.3157795963825491	0.9705587688987605	0.4347842484803975	T	T	T
0.7845174757994380	0.7432224659671661	0.4548540741464781	T	T	T
0.3544507851114457	0.1939012719471537	0.4455686072162439	T	T	T
0.2897543864690527	0.7483321300152310	0.4504735568156878	T	T	T
0.8534635525753251	0.1921477981024651	0.4432657046268366	T	T	T
0.8952606116916659	0.5586430518468445	0.4441397008417086	T	T	T
0.3921767077010564	0.5628756756292309	0.4449324560861718	T	T	T
0.2405416051903381	0.3766147997386655	0.4436998302418052	T	T	T
0.7386442933216455	0.3727876103288061	0.4436418196795421	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9019011612304205	0.8470914130614092	0.3844983699747643	T	T	T
0.2300017310715733	0.0894504035587453	0.3836652602370564	T	T	T
0.7290976189401672	0.0853866858529223	0.3828485609234171	T	T	T
0.4057019401932018	0.8515913603271765	0.3823831398842378	T	T	T
0.4689868201741783	0.0793244039545075	0.4557816962622568	T	T	T
0.1677816204697946	0.8569089770484160	0.4530154455932593	T	T	T
0.9697496068755189	0.0802845266811113	0.4545961917871094	T	T	T
0.6652530209455388	0.8604463891849075	0.4548433411082470	T	T	T
0.7057546824493395	0.7732192926086127	0.5371647058126948	T	T	T
0.3762978372111375	0.6647147445037771	0.5177867071644265	T	T	T
0.4955916915491506	0.8810378641754579	0.5751349106763296	T	T	T
0.5913680373434140	0.5595342888884172	0.5743151039906075	T	T	T

K₂O-Fe₃C₂(010*)C+O (FS)

1.0000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O K

40 16 2 2

Selective dynamics

Direct

0.0371499999999996	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999996	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999996	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999996	0.2536300000000011	0.3286500000000032	F	F	F
0.4801282717000949	0.3728708796970435	0.4037752917782693	T	T	T
0.9838246577441160	0.3760589369076075	0.4067422313559563	T	T	T
0.1550381527147149	0.5663702367758582	0.4036502109349869	T	T	T
0.6498383185818403	0.5656887663134834	0.4062583182523801	T	T	T
0.0413945609719134	0.7499215744345870	0.4085597983193792	T	T	T
0.5416768228575963	0.7523065232050498	0.4062217980701981	T	T	T

0.0974250918906482	0.1901868404560434	0.4106494031279000	T	T	T
0.5971589822855432	0.1897742340924880	0.4127969743850521	T	T	T
0.5693790513108477	0.9719461632098587	0.4113834404286433	T	T	T
0.0690016075753820	0.9702545036186853	0.4121897351903158	T	T	T
0.8195847461433480	0.9695647186725858	0.4347468965874804	T	T	T
0.3177728038028919	0.9702161765291577	0.4352718173008294	T	T	T
0.7842708153050775	0.7477763088432919	0.4498925216766558	T	T	T
0.3554220228455261	0.1939767062087194	0.4457676102635164	T	T	T
0.2884638628327137	0.7480421742402296	0.4509739596800927	T	T	T
0.8539250446950369	0.1945429478961777	0.4445873704918273	T	T	T
0.8989653966346416	0.5625180612832069	0.4446382274716237	T	T	T
0.3915381074228017	0.5648999673568841	0.4450703532473505	T	T	T
0.2420636574313837	0.3764640033381788	0.4442991486121852	T	T	T
0.7409133842543916	0.3729303173225879	0.4433229610991548	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9055625549323765	0.8504638206956713	0.3845430343261021	T	T	T
0.2306382288624605	0.0897789240247253	0.3841317273818624	T	T	T
0.7296427613290473	0.0888294994558486	0.3829395285279175	T	T	T
0.4052478559860203	0.8528474049153156	0.3819681127444643	T	T	T
0.4694397328607883	0.0795740655545576	0.4573119553040332	T	T	T
0.1685249520221909	0.8580860456460175	0.4539435972313513	T	T	T
0.9693372770509949	0.0813042811071410	0.4549672465390908	T	T	T
0.6675751159872033	0.8614745122888551	0.4537073665873326	T	T	T
0.7492509564728030	0.5981764204592046	0.4968873900676957	T	T	T
0.3855078087481097	0.6666524331065656	0.5187841623534200	T	T	T
0.4878669473844571	0.8775675606104731	0.5709359437195533	T	T	T
0.5499387098674038	0.4987140578732324	0.5733640520636122	T	T	T

HCO formation and dissociation on K₂O-Fe₅C₂(010*)

K₂O-Fe₅C₂(010*)-CO+H (IS)

1.000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O K H
40 16 2 2 1

Selective dynamics

Direct

0.0371499999999996	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999996	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4805802881163711	0.3744778249333392	0.4049037727230476	T	T	T
0.9810816003290005	0.3759957177782943	0.4070535007533192	T	T	T
0.1545370568503829	0.5664719706712487	0.4033413320722510	T	T	T
0.6539350292769778	0.5652061536323199	0.4048773473815721	T	T	T
0.0385941002594901	0.7495562613564767	0.4091558200289831	T	T	T
0.5479140861691895	0.7524077317185076	0.4060706135586458	T	T	T
0.0968981117780009	0.1916947967897621	0.409457896208116	T	T	T
0.5959756894083110	0.1881938491306270	0.4099045673198040	T	T	T
0.5703549436777788	0.9677086887573862	0.4129250171082059	T	T	T

0.0706055573499033	0.9708287379043934	0.4091317023053543	T	T	T
0.8190245053199544	0.9619704962993997	0.4394237393572085	T	T	T
0.3183803496598082	0.9693629932049611	0.4334408871528743	T	T	T
0.7802349443076851	0.7527064861186429	0.4444751962750397	T	T	T
0.3546950468445847	0.1926771772775740	0.4458074360514537	T	T	T
0.2850629828505511	0.7467627228077584	0.4481163152343789	T	T	T
0.8505606305001716	0.1943431994898206	0.4428839786173451	T	T	T
0.8936330099001468	0.5645866402953628	0.4443091013297322	T	T	T
0.3929373808075055	0.5652129480568225	0.4457367422755484	T	T	T
0.2403963849392301	0.3759180898792948	0.4444379027886933	T	T	T
0.7362497477711122	0.3781966523441646	0.4449405912212480	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9014693627438246	0.8493407981803492	0.3821309777300503	T	T	T
0.2306950171684236	0.0906755745758884	0.3841156728944264	T	T	T
0.7274834172740764	0.0831566353537820	0.3827906553174180	T	T	T
0.4072888835427573	0.8508845187736245	0.3828765338149542	T	T	T
0.4697447057208440	0.0793282259278952	0.4557835482829822	T	T	T
0.1673099701117532	0.8587640583238266	0.4528386344604456	T	T	T
0.9649414591862282	0.0804130652584727	0.4490057703196624	T	T	T
0.6501416316364841	0.8609047510371791	0.4820499414419580	T	T	T
0.6198163540647837	0.8529000251707938	0.5472635983202744	T	T	T
0.3643159312480064	0.6650365118231549	0.5183764947550842	T	T	T
0.3859404855774930	0.8999355728857191	0.5839919320526479	T	T	T
0.5981648881104942	0.6121833213044306	0.5760665172540180	T	T	T
0.8598813926844585	0.8714956811130802	0.4989541099545460	T	T	T

K₂O-Fe₅C₂(010*)-HCO (TS)

1.000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O K H
40 16 2 2 1

Selective dynamics

Direct

0.03714999999999969	0.25363000000000011	0.2882999999999996	F	F	F
0.09747999999999973	0.68397000000000022	0.2882999999999996	F	F	F
0.53714999999999969	0.25363000000000011	0.2882999999999996	F	F	F
0.59747999999999973	0.68397000000000022	0.2882999999999996	F	F	F
0.48413999999999965	0.87116000000000033	0.28837999999999965	F	F	F
0.15048999999999978	0.06642999999999969	0.28837999999999965	F	F	F
0.98413999999999965	0.87116000000000033	0.28837999999999965	F	F	F
0.65048999999999978	0.06642999999999969	0.28837999999999965	F	F	F
0.06730999999999991	0.46880000000000017	0.29153999999999977	F	F	F
0.56730999999999991	0.46880000000000017	0.29153999999999977	F	F	F
0.31730999999999991	0.46880000000000017	0.32540999999999980	F	F	F
0.81730999999999991	0.46880000000000017	0.32540999999999980	F	F	F
0.40048999999999978	0.06642999999999969	0.32858000000000023	F	F	F
0.23413999999999965	0.87116000000000033	0.32858000000000023	F	F	F
0.90048999999999978	0.06642999999999969	0.32858000000000023	F	F	F
0.73413999999999965	0.87116000000000033	0.32858000000000023	F	F	F
0.34747999999999973	0.68397000000000022	0.32865000000000032	F	F	F
0.28714999999999969	0.25363000000000011	0.32865000000000032	F	F	F
0.84747999999999973	0.68397000000000022	0.32865000000000032	F	F	F
0.78714999999999969	0.25363000000000011	0.32865000000000032	F	F	F
0.4822757396090406	0.3715017677391332	0.4060064701022064	T	T	T
0.9819063733373635	0.3749489469280059	0.4072976694338222	T	T	T
0.1536755669749716	0.5656871122002254	0.4049651192420882	T	T	T
0.6571105206963195	0.5615925092764158	0.4024358531970122	T	T	T
0.0369100050328002	0.7490327613497469	0.4083352945174682	T	T	T
0.5452926320232605	0.7469013262817160	0.4081484874763822	T	T	T
0.0985529985018544	0.1923209317784726	0.4084548007856242	T	T	T
0.5967612233306734	0.1868209798082718	0.4101607841075617	T	T	T
0.5643638529007844	0.9697297415759399	0.4062367359277363	T	T	T
0.0725010151769705	0.9701761402759022	0.4082682077573493	T	T	T
0.8201710903303306	0.9632890197068658	0.4425568684502443	T	T	T
0.3178629771946521	0.9695930502518119	0.4355524593433424	T	T	T
0.7758081118450125	0.7509725994227693	0.4466694176205095	T	T	T

0.3571640983644792	0.1933518437468181	0.4455574230770473	T	T	T
0.2848476165436339	0.7464630609093875	0.4484875388891993	T	T	T
0.8509299316684372	0.1925467811017914	0.4412862686062420	T	T	T
0.8923958509167221	0.5617224671458888	0.4439124317033758	T	T	T
0.3942516185815726	0.5602875654019087	0.4432491025507426	T	T	T
0.2410153861938484	0.3763626423377229	0.4448111006877532	T	T	T
0.7381441079089762	0.3745301169276194	0.4446297946447523	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.8961987860136772	0.8457107236097453	0.3828604718108505	T	T	T
0.2329445807597062	0.0910130679405200	0.3841931941138365	T	T	T
0.7277077788260998	0.0773738249316201	0.3829361451007691	T	T	T
0.4047859328373482	0.8521803655303948	0.3828802635320405	T	T	T
0.4704698687172209	0.0779264059915935	0.4573255767609953	T	T	T
0.1662410175215134	0.8573676697298024	0.4527068073237658	T	T	T
0.9677176040600544	0.0809478926015020	0.4463211488073685	T	T	T
0.7806481628987165	0.8711631380897666	0.5246563435872106	T	T	T
0.7143640587348257	0.7968657034500837	0.5666538903816698	T	T	T
0.4262378374833917	0.6913183309379337	0.5023864129247180	T	T	T
0.4870241575332462	0.8966895614923173	0.5714175212386139	T	T	T
0.6033098053887311	0.5666439992778585	0.5743350311572208	T	T	T
0.8633508022424247	0.9362485082420916	0.5488450919512775	T	T	T

K₂O-Fe₅C₂(010*)-HCO (FS)

1.000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O K H
40 16 2 2 1

Selective dynamics

Direct

0.0371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4837333746064804	0.3738862737893180	0.4070494614718023	T	T	T
0.9818067029912210	0.3733321195904352	0.4070178999478031	T	T	T
0.1542153286159724	0.5659680494743937	0.4053534511302587	T	T	T
0.6594609803876990	0.5656574105187938	0.4014654735644059	T	T	T
0.0387005672167613	0.7472491433799213	0.4076990034650954	T	T	T
0.5466623370234281	0.7491259147374376	0.4079683772944575	T	T	T
0.0952410690462476	0.1899180317591651	0.4089821721649341	T	T	T
0.5966310564974284	0.1879827865088629	0.4100158658396810	T	T	T
0.5634416735443117	0.9710548369232258	0.4056455119305333	T	T	T
0.0709242584545910	0.9675048770586244	0.4091658440795129	T	T	T
0.8192283810964485	0.9614521722508121	0.4412582214061462	T	T	T
0.3165877294201788	0.9699577274711033	0.4353667786984460	T	T	T
0.7817689421485735	0.7475350873758069	0.4511479725937301	T	T	T
0.3560506270745483	0.1944265124938195	0.4443543561290008	T	T	T
0.2859563616863732	0.7458246672291540	0.4491224228345894	T	T	T
0.8501473307104694	0.1913825643249496	0.4423158418833174	T	T	T
0.8940701044948776	0.5608115951605506	0.4440314834281433	T	T	T

0.3952345986416092	0.5603468557153336	0.4434865816560178	T	T	T
0.2405303471365785	0.3761075665516249	0.4444002985528494	T	T	T
0.7391003810980324	0.3751762174670591	0.4440336114644043	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.8963067388414018	0.8436249244536828	0.3828533677277303	T	T	T
0.2306916639836256	0.0896314158234849	0.3842846381916689	T	T	T
0.7275866654045988	0.0796054176918943	0.3827826647888832	T	T	T
0.4052130744599741	0.8524559027334934	0.3832113900011091	T	T	T
0.4693971964766045	0.0791033473233030	0.4560137140663755	T	T	T
0.1668402961148521	0.8559704300336038	0.4533686371343695	T	T	T
0.9648073052971980	0.0770513516383002	0.4486996569028755	T	T	T
0.8019392090361711	0.8965953211447840	0.5307182216912992	T	T	T
0.7340708553024161	0.7950176295803278	0.5500334879176018	T	T	T
0.4280285971064490	0.6906945686462123	0.5036338625362353	T	T	T
0.5003145810439364	0.8977609350591428	0.5678660025500375	T	T	T
0.6062288695428382	0.5682616936648236	0.5733346025070600	T	T	T
0.8661767788438880	0.9399068395637235	0.5738402170199727	T	T	T

K₂O-Fe₅C₂(010*)-CH+O (TS)

1.000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994
Fe	C	O
40	16	2
2	2	1

Selective dynamics

Direct

0.0371499999999996	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999963	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000032	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000032	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999990	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999964	0.8711600000000032	0.3285800000000023	F	F	F
0.9004899999999977	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000032	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999972	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4740196013471429	0.3859007036450228	0.4071334591876566	T	T	T
0.9684417451808225	0.3512825222783719	0.4030341855534377	T	T	T
0.1559852244023874	0.5793235431405271	0.3994616131018751	T	T	T
0.6570685782814869	0.5665049580283709	0.4022919095865557	T	T	T
0.0360282923431420	0.7500505315640060	0.4111269264247338	T	T	T
0.5438968336134349	0.7594254345360375	0.4093005426218211	T	T	T
-0.0062368142249622	0.1558043474105954	0.4343409664875459	T	T	T
0.5403907990749411	0.1990931630331502	0.4099046669416544	T	T	T
0.5195224834829124	0.9786042628644092	0.4123833851871996	T	T	T
-0.0018932610645381	0.9451529249456280	0.4520113040194905	T	T	T
0.7488671751177685	0.9354262092277720	0.4539316971523495	T	T	T
0.2457830766149923	0.9662393998056579	0.4306084136775966	T	T	T
0.7861623253939927	0.7317430558210899	0.4573806294710614	T	T	T
0.2441369630141613	0.1741166584945014	0.4320930879118458	T	T	T
0.2723613780768120	0.7558780193448650	0.4558834932991180	T	T	T
0.7531298466154076	0.1585668274541301	0.4577876817366088	T	T	T
0.9015035984867665	0.5492676212190213	0.4444779216931153	T	T	T
0.3848927952606834	0.5683980125001280	0.4422028288362211	T	T	T
0.2045193834299554	0.3976534516438292	0.4450087205200491	T	T	T
0.7335221680453882	0.3711172560296636	0.4417972051004789	T	T	T

0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000018	0.5823099999999997	0.3528200000000012	F	F	F
0.8850710989695494	0.8395798607803950	0.3891182496352764	T	T	T
0.0977541239732369	0.0519458453882420	0.3888781607356577	T	T	T
0.6946493461805422	0.0587582863237010	0.3823169743512909	T	T	T
0.3888851413589776	0.8436809636821408	0.3842338443305718	T	T	T
0.3942507012401207	0.0872921072414847	0.4390559568365810	T	T	T
0.1312953788688279	0.8500641259274162	0.4788790607181513	T	T	T
0.8832947558589253	0.0531734809132312	0.4874308044250550	T	T	T
0.7498755652139433	0.8618417635432031	0.5425368105301773	T	T	T
0.7191875112037770	0.7480844736775831	0.5576402129281905	T	T	T
0.4178637967821285	0.6896544803014237	0.5050063591309446	T	T	T
0.4679628052697133	0.8807705418880253	0.5775460913738691	T	T	T
0.5741491964391279	0.5250166670576555	0.5690913872689571	T	T	T
0.7946922467562387	0.9147146950751868	0.5856801631899623	T	T	T

K₂O-Fe₃C₂(010*)-CH+O (FS)

1.000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O K H
40 16 2 2 1

Selective dynamics

Direct

0.03714999999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.09747999999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.53714999999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.59747999999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.48413999999999965	0.8711600000000033	0.28837999999999965	F	F	F
0.15048999999999978	0.0664299999999969	0.28837999999999965	F	F	F
0.98413999999999965	0.8711600000000033	0.28837999999999965	F	F	F
0.65048999999999978	0.0664299999999969	0.28837999999999965	F	F	F
0.06730999999999991	0.4688000000000017	0.29153999999999977	F	F	F
0.56730999999999991	0.4688000000000017	0.29153999999999977	F	F	F
0.31730999999999991	0.4688000000000017	0.32540999999999980	F	F	F
0.81730999999999991	0.4688000000000017	0.32540999999999980	F	F	F
0.40048999999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.23413999999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.90048999999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.73413999999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.34747999999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.28714999999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.84747999999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.78714999999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4811577025113352	0.3746015188444738	0.4047254437589598	T	T	T
0.9849139689179581	0.3774414426042120	0.4083196012987242	T	T	T
0.1544985985745151	0.5674804620289140	0.4030239007147716	T	T	T
0.6492473102273983	0.5676395865118837	0.4045787503299281	T	T	T
0.0406880251255039	0.7500037569531834	0.4080798065851440	T	T	T
0.5461318145158636	0.7564526820645427	0.4096728312644976	T	T	T
0.0968101727984919	0.1911046139121763	0.4099871089240587	T	T	T
0.5968894385318764	0.1911061039017730	0.4120184718677485	T	T	T
0.5699797703700010	0.9727154269090387	0.4126327813599999	T	T	T
0.0676230470369889	0.9704357987483260	0.4110755364996375	T	T	T
0.8167478637346511	0.9672202633877319	0.4354375198020161	T	T	T
0.3181369150049373	0.9731276138867245	0.4343956986804365	T	T	T
0.7781498548902238	0.7504047726056448	0.4466621852051883	T	T	T
0.3558505510646409	0.1948717837443787	0.4459047485628237	T	T	T
0.2892030943487510	0.7522197666732003	0.4460384078692474	T	T	T
0.8518349795151990	0.1950061491762327	0.4441633767799686	T	T	T
0.8977468235246313	0.5643884372498774	0.4439867764031533	T	T	T
0.3891485508118785	0.5675033906333642	0.4433878039581602	T	T	T
0.2425153147571212	0.3773480037964541	0.4437286849502884	T	T	T
0.7400326977193697	0.3739666490634473	0.4435574054200871	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F

0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9021081353075520	0.8496853095931629	0.3848796134465737	T	T	T
0.2305265904802117	0.0918118012842494	0.3843280264509933	T	T	T
0.7287767511668357	0.0860906489961082	0.3828646562988798	T	T	T
0.4066505021842267	0.8544329482728046	0.3829686479432656	T	T	T
0.4701041682972107	0.0809049850767822	0.4576355593105862	T	T	T
0.1689090416044858	0.8595429271957788	0.4527527898492943	T	T	T
0.9657366578541869	0.0805491255303382	0.4517205877746044	T	T	T
0.6635816144110560	0.8667743125576808	0.4750554509542508	T	T	T
0.7477789077722408	0.6002735925865751	0.4949853881186436	T	T	T
0.3793545679848516	0.6742604058593155	0.5143481792350334	T	T	T
0.4121613283322665	0.8888067277612427	0.5770763487979105	T	T	T
0.5495263892355974	0.5081284327487234	0.5720549099555157	T	T	T
0.6490427827016305	0.8688078145094323	0.5334949079880683	T	T	T

COH formation and dissociation on $K_2O-Fe_5C_2(010^*)$

$K_2O-Fe_5C_2(010^*)$ -COH (TS)

1.000000000000000					
9.9837999344000004	0.0000000000000000	0.0000000000000000			
-1.5315638797000000	11.4316603084999997	0.0000000000000000			
0.0000000000000000	0.0000000000000000	18.9298000335999994			
Fe	C	O	K	H	
40	16	2	2	1	

Selective dynamics

Direct

0.03714999999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.09747999999999966	0.68397000000000022	0.2882999999999996	F	F	F
0.53714999999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.59747999999999973	0.68397000000000022	0.2882999999999996	F	F	F
0.48413999999999965	0.87116000000000032	0.28837999999999965	F	F	F
0.15048999999999978	0.06642999999999969	0.28837999999999965	F	F	F
0.98413999999999965	0.87116000000000032	0.28837999999999965	F	F	F
0.65048999999999978	0.06642999999999969	0.28837999999999965	F	F	F
0.06730999999999991	0.46880000000000017	0.29153999999999977	F	F	F
0.56730999999999991	0.46880000000000017	0.29153999999999977	F	F	F
0.31730999999999991	0.46880000000000017	0.32540999999999980	F	F	F
0.81730999999999990	0.46880000000000017	0.32540999999999980	F	F	F
0.40048999999999978	0.06642999999999969	0.32858000000000023	F	F	F
0.23413999999999964	0.87116000000000032	0.32858000000000023	F	F	F
0.90048999999999977	0.06642999999999969	0.32858000000000023	F	F	F
0.73413999999999965	0.87116000000000032	0.32858000000000023	F	F	F
0.34747999999999973	0.68397000000000022	0.32865000000000032	F	F	F
0.28714999999999969	0.2536300000000011	0.32865000000000032	F	F	F
0.84747999999999972	0.68397000000000022	0.32865000000000032	F	F	F
0.78714999999999969	0.2536300000000011	0.32865000000000032	F	F	F
0.4809646987172785	0.3757592148834266	0.4051147670774781	T	T	T
0.9808939155465562	0.3770859002877848	0.4066961323572295	T	T	T
0.1550296273911460	0.5691947746959016	0.4027864431668473	T	T	T
0.6546477104375008	0.5652395869353080	0.4032943303168322	T	T	T
0.0378151968996856	0.7505419688197903	0.4088797224285674	T	T	T
0.5440584998885086	0.7524201067900406	0.4082793429820867	T	T	T
0.0968097089922164	0.1916827818923803	0.4090856273055643	T	T	T
0.5952252796468611	0.1883674010827329	0.4099319478843291	T	T	T
0.5687187099785049	0.9679485466179336	0.4153229276297516	T	T	T
0.0671550909105329	0.9705684397680430	0.4101763723024360	T	T	T
0.8162898606828790	0.9677669774104486	0.4362690201205718	T	T	T
0.3160055564840217	0.9716122601743247	0.4345353740697857	T	T	T
0.7761222022264189	0.7491324755646385	0.4403142039470897	T	T	T
0.3544416406339344	0.1934599444324401	0.4449939051038610	T	T	T
0.2835761170071134	0.7473117459985510	0.4476053778148535	T	T	T
0.8515981192474956	0.1956410823635655	0.4428528304367973	T	T	T
0.8917775929587400	0.5678374964498939	0.4454905825195696	T	T	T
0.3929192534810239	0.5643067737748865	0.4447247504830180	T	T	T
0.2399731245925152	0.3781134633293635	0.4442800311643719	T	T	T
0.7369306782694338	0.3769627798596800	0.4448672984802802	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F

0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000018	0.5823099999999997	0.3528200000000012	F	F	F
0.9012825301280567	0.8503253692858189	0.3844268050787183	T	T	T
0.2300438898690959	0.0907499871244715	0.3835430339202861	T	T	T
0.7261983005424217	0.0834886279096391	0.3833660520464300	T	T	T
0.4068670868058654	0.8546168694876444	0.3827456167684340	T	T	T
0.4692177770701175	0.0799873055587547	0.4567663611208657	T	T	T
0.1664187651035279	0.8596614021535929	0.4528369376307610	T	T	T
0.9661033087393757	0.0818802503099355	0.4506634472246647	T	T	T
0.6630800962089342	0.8609883170401579	0.4755840916079232	T	T	T
0.6703747924938777	0.8401368081656385	0.5466836548340677	T	T	T
0.3884297248639670	0.6763399491352542	0.5138969449010365	T	T	T
0.4269941152523803	0.8948081191360971	0.5797848349420702	T	T	T
0.5941624364346400	0.5804916858395934	0.5745811541651259	T	T	T
0.7703878379755200	0.7770609591288629	0.5325875928368043	T	T	T

K₂O-Fe₅C₂(010*)-COH (FS)

1.000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O K H
40 16 2 2 1

Selective dynamics

Direct

0.03714999999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.09747999999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.53714999999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.59747999999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.48413999999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.15048999999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.98413999999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.65048999999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.06730999999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.56730999999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.31730999999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.81730999999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.40048999999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.23413999999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.90048999999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.73413999999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.34747999999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.28714999999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.84747999999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.78714999999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4813302077164729	0.3737977905086978	0.4055046956048067	T	T	T
0.9809186762342244	0.3745664587181257	0.4062901253108874	T	T	T
0.1540663621692566	0.5667352991065366	0.4040571130061659	T	T	T
0.6552441823743594	0.5653505308397992	0.4029979769174025	T	T	T
0.0361017355711562	0.7497124124298402	0.4089890403142039	T	T	T
0.5421287790045477	0.7526684596115290	0.4152552124567910	T	T	T
0.0954733772900050	0.1910165230324969	0.4096048194094618	T	T	T
0.5954299395364860	0.1877018808588461	0.4100933276328814	T	T	T
0.5699381864219004	0.9687075141172447	0.4141771508241554	T	T	T
0.0673577239701038	0.9705226026805128	0.4114280158396760	T	T	T
0.8170624545567862	0.9685882220786913	0.4364106621372804	T	T	T
0.3163301877660885	0.9706758894689789	0.4341710668646617	T	T	T
0.7772911246985645	0.7500503547724477	0.4399887878032652	T	T	T
0.3544384648688452	0.1930025753802736	0.4453987728116458	T	T	T
0.2811735889130539	0.7458663942993482	0.4462101637388117	T	T	T
0.8513262370595739	0.1947192537450310	0.4435520034275138	T	T	T
0.8932797424172598	0.5634702269941776	0.4449785067049138	T	T	T
0.3948424005687696	0.5617545484555371	0.4446538708896077	T	T	T
0.2403232104396002	0.3766943884191604	0.4445528656572763	T	T	T
0.7364473189780009	0.3774011422445184	0.4449367934397237	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999996	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999996	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9028206927095714	0.8532331073399476	0.3834616130236788	T	T	T
0.2298880762788697	0.0909336984010379	0.3841496903064203	T	T	T

0.7275689000589577	0.0840396261692823	0.3833538369898944	T	T	T
0.4067382826216502	0.8553433189308279	0.3823277597525710	T	T	T
0.4690632422656052	0.0795567756721844	0.4567009564736628	T	T	T
0.1661477397477946	0.8584824550547565	0.4529355305033420	T	T	T
0.9656024707081924	0.0808108876332546	0.4535175234012602	T	T	T
0.6671676061815595	0.8641802426283801	0.4769278925719734	T	T	T
0.6508633613681173	0.8643859528954354	0.5544788355219328	T	T	T
0.4090416718066304	0.6893110327996931	0.5071783218197394	T	T	T
0.3964295179320853	0.8981687191725586	0.5801761852911044	T	T	T
0.6089818097416153	0.5985780081072556	0.5734111588105960	T	T	T
0.7287249253525907	0.9197405250634182	0.5696760182953686	T	T	T

K₂O-Fe₅C₂(010*)-C+OH (TS)

1.000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O K H
40 16 2 2 1

Selective dynamics

Direct

0.0371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999967	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999969	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999973	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000032	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000032	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999990	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999964	0.8711600000000032	0.3285800000000023	F	F	F
0.9004899999999977	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000032	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999972	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4821162476464784	0.3733097537914411	0.4062582676468595	T	T	T
0.9810798678009429	0.3746302169804148	0.4063739590351114	T	T	T
0.1541296611980182	0.5673367639265104	0.4043202863231252	T	T	T
0.6566145928945892	0.5648901621403932	0.4029131214242482	T	T	T
0.0380993991668077	0.7499221179335587	0.4089170151218396	T	T	T
0.5399891519850047	0.7503344490057996	0.4119336270697907	T	T	T
0.0964675080619252	0.1903607758294060	0.4094077053601709	T	T	T
0.5956954201526963	0.1882950509686678	0.4103674460111743	T	T	T
0.5695830104084616	0.9692274278414817	0.4146640743348651	T	T	T
0.0666508234484160	0.9696549393460498	0.4115956863557317	T	T	T
0.8180649161775199	0.9701479559241778	0.4356071547734382	T	T	T
0.3158897746402267	0.9704152886271268	0.4348155777277140	T	T	T
0.7804928912168723	0.7479715948331245	0.4407951680914982	T	T	T
0.3542035782703217	0.1932453769777859	0.4454191328866270	T	T	T
0.2830262617477517	0.7473711968418363	0.4472773602521458	T	T	T
0.8526463973080697	0.1945207837350368	0.4435951999261176	T	T	T
0.8945568738968379	0.5621091395374193	0.4441620732100386	T	T	T
0.3941995087511931	0.5605864033566363	0.4435257383947779	T	T	T
0.2396613782798069	0.3772641045143401	0.4440276990656446	T	T	T
0.7382517923722105	0.3754678003211486	0.4440480898482655	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.9820300000000018	0.5823099999999997	0.3528200000000012	F	F	F
0.9045158236255953	0.8524025073830176	0.3829380828646674	T	T	T
0.2294852949280262	0.0897260636186104	0.3838327529328326	T	T	T
0.7275162936746705	0.0856898866860725	0.3831088777528173	T	T	T
0.4062068661741950	0.8552845346984537	0.3821547235980898	T	T	T
0.4690785269135112	0.0797077455854021	0.4564699805034452	T	T	T
0.1660701759191768	0.8587546479909705	0.4535691123692951	T	T	T

0.9679178815352963	0.0816441844316077	0.4539688843305725	T	T	T
0.6682673822135983	0.8600599240136566	0.4638005868509849	T	T	T
0.6856956587675075	0.8156558377364157	0.5612792236964619	T	T	T
0.4095179663146851	0.6858408549042807	0.5064544003237068	T	T	T
0.4573648557279756	0.8928589015874462	0.5769506039978620	T	T	T
0.6077121795702727	0.5817401331048054	0.5739716632779133	T	T	T
0.7734349752487931	0.8636238719253995	0.5673760437720837	T	T	T

K₂O-Fe₃C₂(010*)-C+OH (FS)

1.000000000000000		
9.9837999344000004	0.0000000000000000	0.0000000000000000
-1.5315638797000000	11.4316603084999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.9298000335999994

Fe C O K H
40 16 2 2 1

Selective dynamics

Direct

0.0371499999999996	0.2536300000000011	0.2882999999999996	F	F	F
0.0974799999999997	0.6839700000000022	0.2882999999999996	F	F	F
0.5371499999999996	0.2536300000000011	0.2882999999999996	F	F	F
0.5974799999999997	0.6839700000000022	0.2882999999999996	F	F	F
0.4841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.1504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.9841399999999965	0.8711600000000033	0.2883799999999965	F	F	F
0.6504899999999978	0.0664299999999969	0.2883799999999965	F	F	F
0.0673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.5673099999999991	0.4688000000000017	0.2915399999999977	F	F	F
0.3173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.8173099999999991	0.4688000000000017	0.3254099999999980	F	F	F
0.4004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.2341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.9004899999999978	0.0664299999999969	0.3285800000000023	F	F	F
0.7341399999999965	0.8711600000000033	0.3285800000000023	F	F	F
0.3474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.2871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.8474799999999973	0.6839700000000022	0.3286500000000032	F	F	F
0.7871499999999969	0.2536300000000011	0.3286500000000032	F	F	F
0.4834458508842083	0.3753315130783859	0.4068122127399003	T	T	T
0.9822442325844463	0.3755588332801159	0.4054124171442631	T	T	T
0.1565268313440810	0.5687253882983991	0.4036338343212070	T	T	T
0.6581062076541117	0.5668974088380856	0.4005708366596968	T	T	T
0.0426806496940594	0.7519870426030264	0.4065468397904097	T	T	T
0.5411030785990245	0.7497150628031582	0.4098281205860450	T	T	T
0.0961801659549946	0.1900031263944441	0.4103652493567869	T	T	T
0.5952829461635102	0.1891451062341552	0.4110734292167256	T	T	T
0.5683612749969866	0.9704483698852305	0.4109737637862359	T	T	T
0.0680309792237653	0.9707087559884847	0.4126984781245538	T	T	T
0.8182460908197818	0.9719336733949467	0.4349719286836976	T	T	T
0.3169487121879319	0.9701247372847456	0.4350843660849256	T	T	T
0.7885021535633853	0.7484321295331606	0.4491126732904111	T	T	T
0.3537676642733759	0.1940974353148881	0.4447874644950303	T	T	T
0.2849075661262616	0.7471092475823031	0.4498436896872398	T	T	T
0.8538800625721434	0.1952361765387799	0.4443681537711905	T	T	T
0.8982803900768569	0.5641514307044869	0.4472681458202601	T	T	T
0.3950026311160842	0.5624619011726976	0.4445721547227813	T	T	T
0.2410261070018754	0.3776344214124831	0.4442211511976683	T	T	T
0.7421345543933595	0.3754298664709266	0.4422937874369041	T	T	T
0.2320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.4025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.7320300000000017	0.5823099999999997	0.2641300000000015	F	F	F
0.9025999999999996	0.3552899999999966	0.2641300000000015	F	F	F
0.1525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.4820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.6525999999999996	0.3552899999999966	0.3528200000000012	F	F	F
0.9820300000000017	0.5823099999999997	0.3528200000000012	F	F	F
0.9058598315153552	0.8530210225506945	0.3828086407181110	T	T	T
0.2296068274459780	0.0891914094709564	0.3834918594296896	T	T	T
0.7296862629411799	0.0894108651585294	0.3830675156970795	T	T	T
0.4052307459808732	0.8536343307494270	0.3821984577270409	T	T	T
0.4688295792848002	0.0796708376602108	0.4561109004492915	T	T	T
0.1668765495338428	0.8587266485251887	0.4548913568202657	T	T	T
0.9695164454929304	0.0821307150462035	0.4557360209285186	T	T	T
0.6698758356113418	0.8613578266319228	0.4538688314235825	T	T	T
0.8469241941138186	0.6501100057907162	0.5331277470952159	T	T	T
0.4084373423539938	0.6828718850891430	0.5109077449193709	T	T	T

0.4884771114301258	0.8939108853827062	0.5699888684461556	T	T	T
0.6029556025326926	0.5445417312717020	0.5706264135973783	T	T	T
0.9324270591311249	0.6924017731578717	0.5499823542887010	T	T	T