

*Supplementary Materials*

# Changes in CO<sub>2</sub> Adsorption Affinity Related to Ni Doping in FeS Surfaces: A DFT-D3 Study

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## Atomic coordinates of Ni-doped FeS surface with a random dopant distribution

### (001)-S terminated Ni-doped FeS surface

Fe S

1.0

+7.1658632048 +0.0000000000 +0.0000000000

+0.0000000000 +7.1658632048 +0.0000000000

+0.0000000000 +0.0000000000 +35.0572536156

Fe S Ni

25 32 7

Selective

Cartesian

+1.7914658012 +1.7914658012 +1.2114035143 F F F

+0.0000000000 +0.0000000000 +6.2257169182 F F F

+1.7914658012 +1.7914658012 +6.2257169182 F F F

+1.7914658012 +1.7914658012 +11.2819980319 T T T

+0.0000000000 +0.0000000000 +16.3442568180 T T T

+1.7914658012 +1.7914658012 +16.3442568180 T T T

+0.0000000000 +3.5829316024 +1.2114035143 F F F

+0.0000000000 +3.5829316024 +6.2257169182 F F F

+1.7914658012 +5.3743974036 +6.2257169182 F F F

+0.0000000000 +3.5829316024 +11.2819980319 T T T

+1.7914658012 +5.3743974036 +11.2819980319 T T T

+0.0000000000 +3.5829316024 +16.3442568180 T T T

+3.5829316024 +0.0000000000 +1.2114035143 F F F

+5.3743974036 +1.7914658012 +1.2114035143 F F F

+5.3743974036 +1.7914658012 +6.2257169182 F F F

+3.5829316024 +0.0000000000 +11.2819980319 T T T

+5.3743974036 +1.7914658012 +11.2819980319 T T T

+5.3743974036 +1.7914658012 +16.3442568180 T T T

+3.5829316024 +3.5829316024 +1.2114035143 F F F

+5.3743974036 +5.3743974036 +1.2114035143 F F F

+3.5829316024 +3.5829316024 +6.2257169182 F F F

+5.3743974036 +5.3743974036 +6.2257169182 F F F

+5.3743974036 +5.3743974036 +11.2819980319 T T T

+3.5829316024 +3.5829316024 +16.3442568180 T T T

+5.3743974036 +5.3743974036 +16.3442568180 T T T

+1.7914658012 +0.0000000000 +0.0000000000 F F F

+0.0000000000 +1.7914658012 +2.4228067929 F F F

+1.7914658012 +0.0000000000 +5.0143134039 F F F

+0.0000000000	+1.7914658012	+7.4371201968	F F F
+1.7914658012	+0.0000000000	+10.0694106083	T T T
+0.0000000000	+1.7914658012	+12.4937956164	T T T
+1.7914658012	+0.0000000000	+15.1315636117	T T T
+0.0000000000	+1.7914658012	+17.5637614384	T T T
+1.7914658012	+3.5829316024	+0.0000000000	F F F
+0.0000000000	+5.3743974036	+2.4228067929	F F F
+1.7914658012	+3.5829316024	+5.0143134039	F F F
+0.0000000000	+5.3743974036	+7.4371201968	F F F
+1.7914658012	+3.5829316024	+10.0694106083	T T T
+0.0000000000	+5.3743974036	+12.4937956164	T T T
+1.7914658012	+3.5829316024	+15.1315636117	T T T
+0.0000000000	+5.3743974036	+17.5637614384	T T T
+5.3743974036	+0.0000000000	+0.0000000000	F F F
+3.5829316024	+1.7914658012	+2.4228067929	F F F
+5.3743974036	+0.0000000000	+5.0143134039	F F F
+3.5829316024	+1.7914658012	+7.4371201968	F F F
+5.3743974036	+0.0000000000	+10.0694106083	T T T
+3.5829316024	+1.7914658012	+12.4937956164	T T T
+5.3743974036	+0.0000000000	+15.1315636117	T T T
+3.5829316024	+1.7914658012	+17.5637614384	T T T
+5.3743974036	+3.5829316024	+0.0000000000	F F F
+3.5829316024	+5.3743974036	+2.4228067929	F F F
+5.3743974036	+3.5829316024	+5.0143134039	F F F
+3.5829316024	+5.3743974036	+7.4371201968	F F F
+5.3743974036	+3.5829316024	+10.0694106083	T T T
+3.5829316024	+5.3743974036	+12.4937956164	T T T
+5.3743974036	+3.5829316024	+15.1315636117	T T T
+3.5829316024	+5.3743974036	+17.5637614384	T T T
+0.0000000000	+0.0000000000	+1.2114035143	F F F
+1.7914658012	+5.3743974036	+1.2114035143	F F F
+3.5829316024	+0.0000000000	+6.2257169182	F F F
+0.0000000000	+0.0000000000	+11.2819980319	T T T
+3.5829316024	+3.5829316024	+11.2819980319	T T T
+3.5829316024	+0.0000000000	+16.3442568180	T T T
+1.7914658012	+5.3743974036	+16.3442568180	T T T

**(001)-Fe terminated Ni-doped FeS surface**

Fe S

1.0

+7.1658632048 +0.0000000000 +0.0000000000  
 +0.0000000000 +7.1658632048 +0.0000000000  
 +0.0000000000 +0.0000000000 +35.0572536156

Fe S Ni

25 32 7

Selective

Cartesian

+1.7914658012 +1.7914658012 +0.0000000000 F F F  
 +0.0000000000 +0.0000000000 +5.0143134039 F F F  
 +1.7914658012 +1.7914658012 +5.0143134039 F F F  
 +0.0000000000 +0.0000000000 +10.0297436457 T T T  
 +0.0000000000 +0.0000000000 +15.0361906824 T T T  
 +0.0000000000 +0.0000000000 +20.0284491829 T T T  
 +1.7914658012 +5.3743974036 +0.0000000000 F F F  
 +1.7914658012 +5.3743974036 +5.0143134039 F F F  
 +0.0000000000 +3.5829316024 +10.0297436457 T T T  
 +1.7914658012 +5.3743974036 +10.0290723664 T T T  
 +0.0000000000 +3.5829316024 +15.0361906824 T T T  
 +1.7914658012 +5.3743974036 +15.0364779577 T T T  
 +5.3743974036 +1.7914658012 +0.0000000000 F F F  
 +3.5829316024 +0.0000000000 +5.0143134039 F F F  
 +3.5829316024 +0.0000000000 +10.0297436457 T T T  
 +5.3743974036 +1.7914658012 +10.0290723664 T T T  
 +3.5829316024 +0.0000000000 +15.0361906824 T T T  
 +3.5829316024 +0.0000000000 +20.0284491829 T T T  
 +5.3743974036 +5.3743974036 +0.0000000000 F F F  
 +3.5829316024 +3.5829316024 +5.0143134039 F F F  
 +5.3743974036 +5.3743974036 +5.0143134039 F F F  
 +3.5829316024 +3.5829316024 +10.0297436457 T T T  
 +3.5829316024 +3.5829316024 +15.0361906824 T T T  
 +5.3743974036 +5.3743974036 +15.0364779577 T T T  
 +3.5829316024 +3.5829316024 +20.0284491829 T T T  
 +0.0000000000 +1.7914658012 +1.2114032786 F F F  
 +1.7914658012 +0.0000000000 +3.8029098896 F F F  
 +0.0000000000 +1.7914658012 +6.2257166825 F F F  
 +1.7914658012 +0.0000000000 +8.8172232935 F F F  
 +0.0000000000 +1.7914658012 +11.2410174998 T T T  
 +1.7914658012 +0.0000000000 +13.8235488529 T T T  
 +0.0000000000 +1.7914658012 +16.2519570143 T T T

+1.7914658012	+0.0000000000	+18.9229433896	T T T
+0.0000000000	+5.3743974036	+1.2114032786	F F F
+1.7914658012	+3.5829316024	+3.8029098896	F F F
+0.0000000000	+5.3743974036	+6.2257166825	F F F
+1.7914658012	+3.5829316024	+8.8172232935	F F F
+0.0000000000	+5.3743974036	+11.2410174998	T T T
+1.7914658012	+3.5829316024	+13.8235488529	T T T
+0.0000000000	+5.3743974036	+16.2519570143	T T T
+1.7914658012	+3.5829316024	+18.9229433896	T T T
+3.5829316024	+1.7914658012	+1.2114032786	F F F
+5.3743974036	+0.0000000000	+3.8029098896	F F F
+3.5829316024	+1.7914658012	+6.2257166825	F F F
+5.3743974036	+0.0000000000	+8.8172232935	F F F
+3.5829316024	+1.7914658012	+11.2410174998	T T T
+5.3743974036	+0.0000000000	+13.8235488529	T T T
+3.5829316024	+1.7914658012	+16.2519570143	T T T
+5.3743974036	+0.0000000000	+18.9229433896	T T T
+3.5829316024	+5.3743974036	+1.2114032786	F F F
+5.3743974036	+3.5829316024	+3.8029098896	F F F
+3.5829316024	+5.3743974036	+6.2257166825	F F F
+5.3743974036	+3.5829316024	+8.8172232935	F F F
+3.5829316024	+5.3743974036	+11.2410174998	T T T
+5.3743974036	+3.5829316024	+13.8235488529	T T T
+3.5829316024	+5.3743974036	+16.2519570143	T T T
+5.3743974036	+3.5829316024	+18.9229433896	T T T
+0.0000000000	+3.5829316024	+5.0143134039	F F F
+5.3743974036	+1.7914658012	+5.0143134039	F F F
+1.7914658012	+1.7914658012	+10.0290723664	T T T
+5.3743974036	+5.3743974036	+10.0290723664	T T T
+1.7914658012	+1.7914658012	+15.0364779577	T T T
+5.3743974036	+1.7914658012	+15.0364779577	T T T
+0.0000000000	+3.5829316024	+20.0284491829	T T T

### (011)-S terminated Ni-doped FeS surface

Fe S

1.0

+7.1658632048	+0.0000000000	+0.0000000000
+0.0000000000	+12.3257028652	+0.0000000000
+0.0000000000	+19.0502286697	+26.6607983532

Fe S Ni

25 32 7

Selective

Cartesian

+1.7914658012	+3.1245436487	+2.1618802692	F F F
+0.0000000000	+4.1660581982	+3.6194800634	F F F
+1.7914658012	+5.2075727478	+5.0770798575	F F F
+0.0000000000	+6.2252714428	+6.5801036101	T T T
+0.0000000000	+8.3588395250	+9.4835546675	T T T
+0.0000000000	+8.2458805317	+0.7042804751	F F F
+1.7914658012	+9.2873950813	+2.1618802692	F F F
+1.7914658012	+11.3704241804	+5.0770798575	F F F
+1.7914658012	+13.4429664617	+8.0392029411	T T T
+3.5829316024	+8.3588395250	+9.4835546675	T T T
+1.7914658012	+15.6257748403	+10.8408899198	T T T
+3.5829316024	+2.0830290991	+0.7042804751	F F F
+5.3743974036	+3.1245436487	+2.1618802692	F F F
+3.5829316024	+4.1660581982	+3.6194800634	F F F
+3.5829316024	+6.2252714428	+6.5801036101	T T T
+5.3743974036	+7.2801150291	+8.0392029411	T T T
+5.3743974036	+13.4429664617	+8.0392029411	T T T
+5.3743974036	+9.4629234077	+10.8408899198	T T T
+3.5829316024	+8.2458805317	+0.7042804751	F F F
+5.3743974036	+9.2873950813	+2.1618802692	F F F
+3.5829316024	+10.3289096308	+3.6194800634	F F F
+5.3743974036	+11.3704241804	+5.0770798575	F F F
+3.5829316024	+12.3881228754	+6.5801036101	T T T
+3.5829316024	+14.5216909576	+9.4835546675	T T T
+5.3743974036	+15.6257748403	+10.8408899198	T T T
+1.7914658012	+3.0686697471	+0.0000000000	F F F
+0.0000000000	+2.1389031925	+2.8661606073	F F F
+1.7914658012	+5.1516988462	+2.9151995883	F F F
+0.0000000000	+4.2219322916	+5.7813601956	F F F
+1.7914658012	+7.2144391110	+5.8739246273	T T T
+0.0000000000	+6.3050423595	+8.7561786263	T T T
+1.7914658012	+9.3406079183	+8.6687592689	T T T
+0.0000000000	+8.5671767328	+11.6756966739	T T T
+1.7914658012	+9.2315211797	+0.0000000000	F F F
+0.0000000000	+8.3017546251	+2.8661606073	F F F
+1.7914658012	+11.3145502788	+2.9151995883	F F F

+0.0000000000	+10.3847837242	+5.7813601956	F F F
+1.7914658012	+13.3772905436	+5.8739246273	T T T
+0.0000000000	+12.4678937921	+8.7561786263	T T T
+1.7914658012	+15.5034593509	+8.6687592689	T T T
+0.0000000000	+14.7300281654	+11.6756966739	T T T
+5.3743974036	+3.0686697471	+0.0000000000	F F F
+3.5829316024	+2.1389031925	+2.8661606073	F F F
+5.3743974036	+5.1516988462	+2.9151995883	F F F
+3.5829316024	+4.2219322916	+5.7813601956	F F F
+5.3743974036	+7.2144391110	+5.8739246273	T T T
+3.5829316024	+6.3050423595	+8.7561786263	T T T
+5.3743974036	+9.3406079183	+8.6687592689	T T T
+3.5829316024	+8.5671767328	+11.6756966739	T T T
+5.3743974036	+9.2315211797	+0.0000000000	F F F
+3.5829316024	+8.3017546251	+2.8661606073	F F F
+5.3743974036	+11.3145502788	+2.9151995883	F F F
+3.5829316024	+10.3847837242	+5.7813601956	F F F
+5.3743974036	+13.3772905436	+5.8739246273	T T T
+3.5829316024	+12.4678937921	+8.7561786263	T T T
+5.3743974036	+15.5034593509	+8.6687592689	T T T
+3.5829316024	+14.7300281654	+11.6756966739	T T T
+0.0000000000	+2.0830290991	+0.7042804751	F F F
+1.7914658012	+9.4629234077	+10.8408899198	T T T
+1.7914658012	+7.2801150291	+8.0392029411	T T T
+0.0000000000	+10.3289096308	+3.6194800634	F F F
+5.3743974036	+5.2075727478	+5.0770798575	F F F
+0.0000000000	+12.3881228754	+6.5801036101	T T T
+0.0000000000	+14.5216909576	+9.4835546675	T T T

### (011)-Fe terminated Ni-doped FeS surface

Fe S

1.0

+7.1658632048	+0.0000000000	+0.0000000000
+0.0000000000	+12.3257028652	+0.0000000000
+0.0000000000	+19.0502286697	+26.6607983532

Fe S Ni

25 32 7

Selective

Cartesian

+0.0000000000	+4.1660581980	+1.4575997941	F F F
+1.7914658012	+5.2075727475	+2.9151995882	F F F
+0.0000000000	+6.2490872970	+4.3727993823	F F F
+1.7914658012	+7.3045521397	+5.8299537331	T T T
+1.7914658012	+9.3943051054	+8.7664058700	T T T
+0.0000000000	+10.3902539233	+10.1844928093	T T T
+1.7914658012	+9.2873950810	+0.0000000000	F F F
+0.0000000000	+10.3289096306	+1.4575997941	F F F
+0.0000000000	+12.4119387296	+4.3727993823	F F F
+1.7914658012	+13.4674035723	+5.8299537331	T T T
+0.0000000000	+14.5090557820	+7.3017388555	T T T
+1.7914658012	+15.5571565380	+8.7664058700	T T T
+5.3743974036	+3.1245436484	+0.0000000000	F F F
+3.5829316024	+4.1660581980	+1.4575997941	F F F
+5.3743974036	+5.2075727475	+2.9151995882	F F F
+5.3743974036	+7.3045521397	+5.8299537331	T T T
+3.5829316024	+8.3462043494	+7.3017388555	T T T
+5.3743974036	+9.3943051054	+8.7664058700	T T T
+3.5829316024	+10.3902539233	+10.1844928093	T T T
+5.3743974036	+9.2873950810	+0.0000000000	F F F
+3.5829316024	+10.3289096306	+1.4575997941	F F F
+5.3743974036	+11.3704241801	+2.9151995882	F F F
+3.5829316024	+12.4119387296	+4.3727993823	F F F
+3.5829316024	+14.5090557820	+7.3017388555	T T T
+3.5829316024	+16.5531053559	+10.1844928093	T T T
+0.0000000000	+2.1389031926	+0.7042803381	F F F
+1.7914658012	+5.1516988469	+0.7533193201	F F F
+0.0000000000	+4.2219322916	+3.6194799262	F F F
+1.7914658012	+7.2347279459	+3.6685189083	F F F
+0.0000000000	+6.3177139617	+6.5348307611	T T T
+1.7914658012	+9.3288380070	+6.5955562375	T T T
+0.0000000000	+8.3317631637	+9.4623337132	T T T
+1.7914658012	+11.4320926179	+9.6021171428	T T T
+0.0000000000	+8.3017546252	+0.7042803381	F F F
+1.7914658012	+11.3145502795	+0.7533193201	F F F
+0.0000000000	+10.3847837242	+3.6194799262	F F F
+1.7914658012	+13.3975793785	+3.6685189083	F F F
+0.0000000000	+12.4805653943	+6.5348307611	T T T
+1.7914658012	+15.4916894396	+6.5955562375	T T T
+0.0000000000	+14.4946145963	+9.4623337132	T T T



+1.7914658012	+17.5949440505	+9.6021171428	T T T
+3.5829316024	+2.1389031926	+0.7042803381	F F F
+5.3743974036	+5.1516988469	+0.7533193201	F F F
+3.5829316024	+4.2219322916	+3.6194799262	F F F
+5.3743974036	+7.2347279459	+3.6685189083	F F F
+3.5829316024	+6.3177139617	+6.5348307611	T T T
+5.3743974036	+9.3288380070	+6.5955562375	T T T
+3.5829316024	+8.3317631637	+9.4623337132	T T T
+5.3743974036	+11.4320926179	+9.6021171428	T T T
+3.5829316024	+8.3017546252	+0.7042803381	F F F
+5.3743974036	+11.3145502795	+0.7533193201	F F F
+3.5829316024	+10.3847837242	+3.6194799262	F F F
+5.3743974036	+13.3975793785	+3.6685189083	F F F
+3.5829316024	+12.4805653943	+6.5348307611	T T T
+5.3743974036	+15.4916894396	+6.5955562375	T T T
+3.5829316024	+14.4946145963	+9.4623337132	T T T
+5.3743974036	+17.5949440505	+9.6021171428	T T T
+1.7914658012	+3.1245436484	+0.0000000000	F F F
+0.0000000000	+8.3462043494	+7.3017388555	T T T
+1.7914658012	+11.3704241801	+2.9151995882	F F F
+0.0000000000	+16.5531053559	+10.1844928093	T T T
+3.5829316024	+6.2490872970	+4.3727993823	F F F
+5.3743974036	+13.4674035723	+5.8299537331	T T T
+5.3743974036	+15.5571565380	+8.7664058700	T T T

### (111)-S terminated Ni-doped FeS surface

Fe S

1.0

+10.1340609304 +0.0000000000 +0.0000000000

+5.0670304652 +11.2360203534 +0.0000000000

-26.9399814749 -12.1489373080 +24.0450810804

Fe S Ni

25 32 7

Selective

Cartesian

+2.5335152326 +4.4754883172 +0.5843369685 F F F

+2.5335152326 +3.3329664577 +2.8456072386 F F F

+0.0000000000 +3.3329664577 +2.8456072386 F F F

+0.0280547049 +2.2314424083 +5.1288775223 T T T

-2.4330387271	+1.0919791392	+7.3241531553	T T T
-5.0100635993	+1.0227827723	+7.3669998026	T T T
+7.6005456978	+10.0934984939	+0.5843369685	F F F
+5.0670304652	+10.0934984939	+0.5843369685	F F F
+2.5335152326	+8.9509766344	+2.8456072386	F F F
+2.5615699375	+7.8494525850	+5.1288775223	T T T
+0.0156850132	+7.8223728625	+5.0986146853	T T T
+0.1004765055	+6.7099893159	+7.3241531553	T T T
+10.1340609304	+4.4754883172	+0.5843369685	F F F
+7.6005456978	+4.4754883172	+0.5843369685	F F F
+7.6005456978	+3.3329664577	+2.8456072386	F F F
+5.0670304652	+3.3329664577	+2.8456072386	F F F
+5.0950851701	+2.2314424083	+5.1288775223	T T T
+2.5492002458	+2.2043626858	+5.0986146853	T T T
+2.6339917381	+1.0919791392	+7.3241531553	T T T
+10.1340609304	+10.0934984939	+0.5843369685	F F F
+10.1340609304	+8.9509766344	+2.8456072386	F F F
+7.6005456978	+8.9509766344	+2.8456072386	F F F
+5.0827154784	+7.8223728625	+5.0986146853	T T T
+5.1675069707	+6.7099893159	+7.3241531553	T T T
+2.5904820985	+6.6407929490	+7.3669998026	T T T
+1.2667576163	+0.5099681009	+0.0000000000	F F F
+3.8002728489	+2.8229981465	+1.1686738307	F F F
-1.2667576163	-0.6325537586	+2.2612702701	F F F
+1.2667576163	+1.6804762870	+3.4299441008	F F F
-3.7970229344	-1.7532153994	+4.5154211464	T T T
-1.2271671532	+0.5297653084	+5.6479847840	T T T
-6.2757213361	-2.8730267362	+6.8004720304	T T T
-3.6282129399	-0.3922364918	+8.1790020589	T T T
+3.8002728489	+6.1279782776	+0.0000000000	F F F
+6.3337880815	+8.4410083232	+1.1686738307	F F F
+1.2667576163	+4.9854564181	+2.2612702701	F F F
+3.8002728489	+7.2984864637	+3.4299441008	F F F
-1.2635077018	+3.8647947773	+4.5154211464	T T T
+1.3063480794	+6.1477754851	+5.6479847840	T T T
-3.7422061035	+2.7449834405	+6.8004720304	T T T
-1.0946977073	+5.2257736849	+8.1790020589	T T T
+6.3337880815	+0.5099681009	+0.0000000000	F F F
+8.8673033141	+2.8229981465	+1.1686738307	F F F
+3.8002728489	-0.6325537586	+2.2612702701	F F F

+6.3337880815	+1.6804762870	+3.4299441008	F F F
+1.2700075308	-1.7532153994	+4.5154211464	T T T
+3.8398633120	+0.5297653084	+5.6479847840	T T T
-1.2086908709	-2.8730267362	+6.8004720304	T T T
+1.4388175253	-0.3922364918	+8.1790020589	T T T
+8.8673033141	+6.1279782776	+0.0000000000	F F F
+11.4008185467	+8.4410083232	+1.1686738307	F F F
+6.3337880815	+4.9854564181	+2.2612702701	F F F
+8.8673033141	+7.2984864637	+3.4299441008	F F F
+3.8035227634	+3.8647947773	+4.5154211464	T T T
+6.3733785446	+6.1477754851	+5.6479847840	T T T
+1.3248243617	+2.7449834405	+6.8004720304	T T T
+3.9723327579	+5.2257736849	+8.1790020589	T T T
+5.0670304652	+4.4754883172	+0.5843369685	F F F
-2.5178302194	+2.2043626858	+5.0986146853	T T T
+5.0670304652	+8.9509766344	+2.8456072386	F F F
-2.4765483667	+6.6407929490	+7.3669998026	T T T
+0.0569668659	+1.0227827723	+7.3669998026	T T T
+12.6675761630	+10.0934984939	+0.5843369685	F F F
+7.6286004027	+7.8494525850	+5.1288775223	T T T

### (111)-Fe terminated Ni-doped FeS surface

Fe S

1.0

+10.1340609304	+0.0000000000	+0.0000000000
+5.0670304652	+11.2360203534	+0.0000000000
-26.9399814749	-12.1489373080	+24.0450810804

Fe S Ni

25 32 7

Selective

Cartesian

+2.5335152316	+3.3329664573	+2.2612702712	F F F
-0.0000000010	+3.3329664573	+2.2612702712	F F F
+0.0000000004	+2.1904445984	+4.5225405401	F F F
-2.5375343395	+2.2072062449	+4.5292235121	T T T
-5.0401828606	+0.8525435479	+6.7650048576	T T T
-6.6223384426	-1.0528325491	+7.4582337280	T T T
+5.0670304655	+10.0934984941	+0.0000000000	F F F
+5.0670304642	+8.9509766340	+2.2612702712	F F F

+2.5335152330	+7.8084547751	+4.5225405401	F F F
-0.0040191069	+7.8252164216	+4.5292235121	T T T
+0.0192331166	+6.5763123865	+6.7282631802	T T T
-2.5066676280	+6.4705537246	+6.7650048576	T T T
+7.6005456981	+4.4754883174	+0.0000000000	F F F
+7.6005456968	+3.3329664573	+2.2612702712	F F F
+5.0670304642	+3.3329664573	+2.2612702712	F F F
+2.5527483492	+0.9583022098	+6.7282631802	T T T
+0.0268476046	+0.8525435479	+6.7650048576	T T T
-1.5553079774	-1.0528325491	+7.4582337280	T T T
+10.1340609307	+10.0934984941	+0.0000000000	F F F
+10.1340609294	+8.9509766340	+2.2612702712	F F F
+7.6005456968	+8.9509766340	+2.2612702712	F F F
+7.6005456982	+7.8084547751	+4.5225405401	F F F
+5.0630113583	+7.8252164216	+4.5292235121	T T T
+2.5603628372	+6.4705537246	+6.7650048576	T T T
+0.9782072552	+4.5651776276	+7.4582337280	T T T
+3.8002728499	+2.8229981468	+0.5843368615	F F F
-1.2667576162	-0.6325537588	+1.6769333016	F F F
+1.2667576160	+1.6804762867	+2.8456071327	F F F
-3.8002728500	-1.7750756188	+3.9382035728	F F F
-1.2607741910	+0.5093742839	+4.9749295646	T T T
-6.3645016930	-2.9474733080	+6.2409270685	T T T
-3.7743500163	-0.8277336481	+7.2546803754	T T T
-6.3092025443	+0.9994903824	+8.5007149100	T T T
+6.3337880825	+8.4410083235	+0.5843368615	F F F
+1.2667576164	+4.9854564179	+1.6769333016	F F F
+3.8002728486	+7.2984864634	+2.8456071327	F F F
-1.2667576174	+3.8429345579	+3.9382035728	F F F
+1.2727410416	+6.1273844606	+4.9749295646	T T T
-3.8309864604	+2.6705368687	+6.2409270685	T T T
-1.2408347837	+4.7902765286	+7.2546803754	T T T
-3.7756873117	+6.6175005591	+8.5007149100	T T T
+8.8673033151	+2.8229981468	+0.5843368615	F F F
+3.8002728490	-0.6325537588	+1.6769333016	F F F
+6.3337880812	+1.6804762867	+2.8456071327	F F F
+1.2667576152	-1.7750756188	+3.9382035728	F F F
+3.8062562742	+0.5093742839	+4.9749295646	T T T
-1.2974712278	-2.9474733080	+6.2409270685	T T T
+1.2926804489	-0.8277336481	+7.2546803754	T T T

-1.2421720791	+0.9994903824	+8.5007149100	T T T
+11.4008185477	+8.4410083235	+0.5843368615	F F F
+6.3337880816	+4.9854564179	+1.6769333016	F F F
+8.8673033138	+7.2984864634	+2.8456071327	F F F
+3.8002728478	+3.8429345579	+3.9382035728	F F F
+6.3397715068	+6.1273844606	+4.9749295646	T T T
+1.2360440048	+2.6705368687	+6.2409270685	T T T
+3.8261956815	+4.7902765286	+7.2546803754	T T T
+1.2913431535	+6.6175005591	+8.5007149100	T T T
+2.5335152329	+4.4754883174	+0.0000000000	F F F
-2.5142821160	+0.9583022098	+6.7282631802	T T T
+2.5335152316	+8.9509766340	+2.2612702712	F F F
+5.0670304656	+2.1904445984	+4.5225405401	F F F
-4.0888232100	+4.5651776276	+7.4582337280	T T T
+5.0862635818	+6.5763123865	+6.7282631802	T T T
+2.5294961257	+2.2072062449	+4.5292235121	T T T