

Electronic Supplementary Information for

**Computational Screening of Single-Atom Doped In₂O₃ Catalysts for the Reverse
Water Gas Shift Reaction**

Yuchen Wang ^{a,b} and Shenggang Li ^{a,b,c*}

*^aSchool of Physical Science and Technology, ShanghaiTech University, Shanghai
201210, P. R. China*

*^bCAS Key Laboratory of Low-Carbon Conversion Science and Engineering, Shanghai
Advanced Research Institute, Chinese Academy of Sciences, Shanghai 201203, P. R.
China*

^cUniversity of Chinese Academy of Sciences, Beijing 100049, P. R. China

**Corresponding author. Tel: +86-021-20350994.*

E-mail: lisg@sari.ac.cn (S. Li)

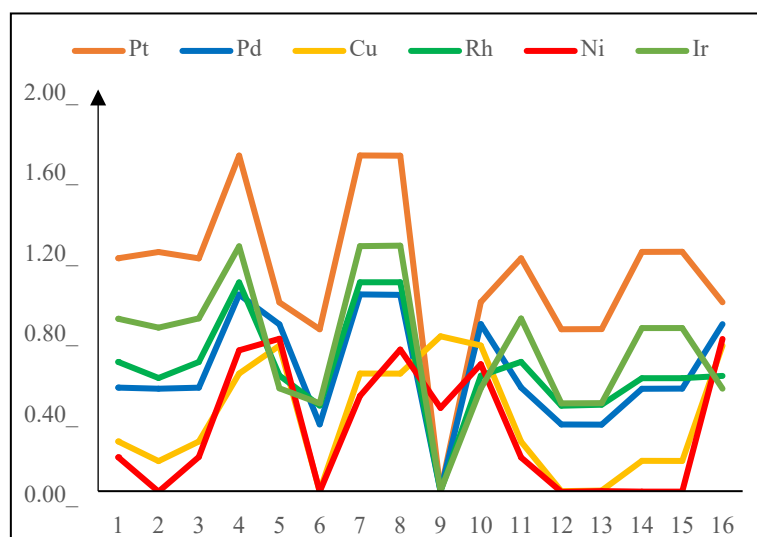


Figure S1. Relative energy maps of single-atom metals (Pt, Ir, Pd, Rh, Cu, Ni) doped at 16 sites on c-In₂O₃(111) surface.

Table S1. Classification of the metal sites (a-f) of M/In₂O₃(111).

Site	In site	Relative energy(eV)					
		Pt	Pd	Cu	Rh	Ni	Ir
a	1,3,11	1.16	0.52	0.25	0.64	0.17	0.86
b	2,14,15	1.19	0.51	0.15	0.56	0.47	0.81
c	4,7,8	1.67	0.98	0.59	1.04	0.70	1.22
d	5,10,16	0.94	0.83	0.72	0.58	0.76	0.51
e	6,12,13	0.81	0.30	0.00	0.43	0.00	0.44
f	9	0.00	0.00	0.77	0.00	0.41	0.00

Table S2. The O_V formation energy of $M/In_2O_3(111)$.

M- O_V	E_{f,O_V} /eV	M- O_V	E_{f,O_V} eV	M- O_V	E_{f,O_V} eV	M- O_V	E_{f,O_V} eV	M- O_V	E_{f,O_V} eV	M-O_V	E_{f,O_V} /eV
Pt ₉ - O _{V4}	2.71	Ir ₉ - O _{V4}	3.68	Pd ₉ - O _{V4}	1.99	Rh ₉ - O _{V4}	2.65	Cu ₁₂ - O _{V7}	1.42	Ni ₁₂ - O _{V7}	1.79
Pt ₉ - O _{V8}	2.70	Ir ₉ - O _{V8}	3.68	Pd ₉ - O _{V8}	1.99	Rh ₉ - O _{V8}	2.65	Cu ₁₂ - O _{V10}	0.66	Ni ₁₂ - O _{V10}	0.78
Pt ₇ - O _{V2}	2.16	Ir ₇ - O _{V2}	3.21	Pd ₇ - O _{V2}	2.05	Rh ₇ - O _{V2}	2.31	Cu ₇ - O _{V2}	1.63	Ni ₇ - O _{V2}	1.98
Pt ₇ - O _{V5}	1.92	Ir ₇ - O _{V5}	3.01	Pd ₇ - O _{V5}	1.58	Rh ₇ - O _{V5}	2.31	Cu ₇ - O _{V5}	0.72	Ni ₇ - O _{V5}	1.28
Pt ₇ - O _{V6}	3.52	Ir ₇ - O _{V6}	3.99	Pd ₇ - O _{V6}	2.77	Rh ₇ - O _{V6}	4.14	Cu ₇ - O _{V6}	2.18	Ni ₇ - O _{V6}	2.86
Pt ₈ - O _{V6}	2.73	Ir ₈ - O _{V6}	3.20	Pd ₈ - O _{V6}	2.62	Rh ₈ - O _{V6}	3.72	Cu ₈ - O _{V6}	2.19	Ni ₈ - O _{V6}	2.88
Pt ₁₁ - O _{V6}	2.86	Ir ₁₁ - O _{V6}	4.07	Pd ₁₁ - O _{V6}	2.57	Rh ₁₁ - O _{V6}	3.86	Cu ₁₁ - O _{V6}	2.00	Ni ₁₁ - O _{V6}	2.79

Table S3. The adsorption energy of CO_2 on $M_{7/8/11}-O_{V6}$ sites.

E_{ads}/eV	Pt	Ir	Pd	Cu	Rh	Ni
E _{ads} (M ₇ -O _{V6} -CO ₂)	-1.46	-1.10	-0.65	-0.50	-0.82	-0.35
E _{ads} (M ₈ -O _{V6} -CO ₂)	-0.66	-0.90	-0.28	-0.35	-0.81	-0.08
E _{ads} (M ₁₁ -O _{V6} -CO)	-0.85	/	-0.68	-0.48	-1.17	-0.43

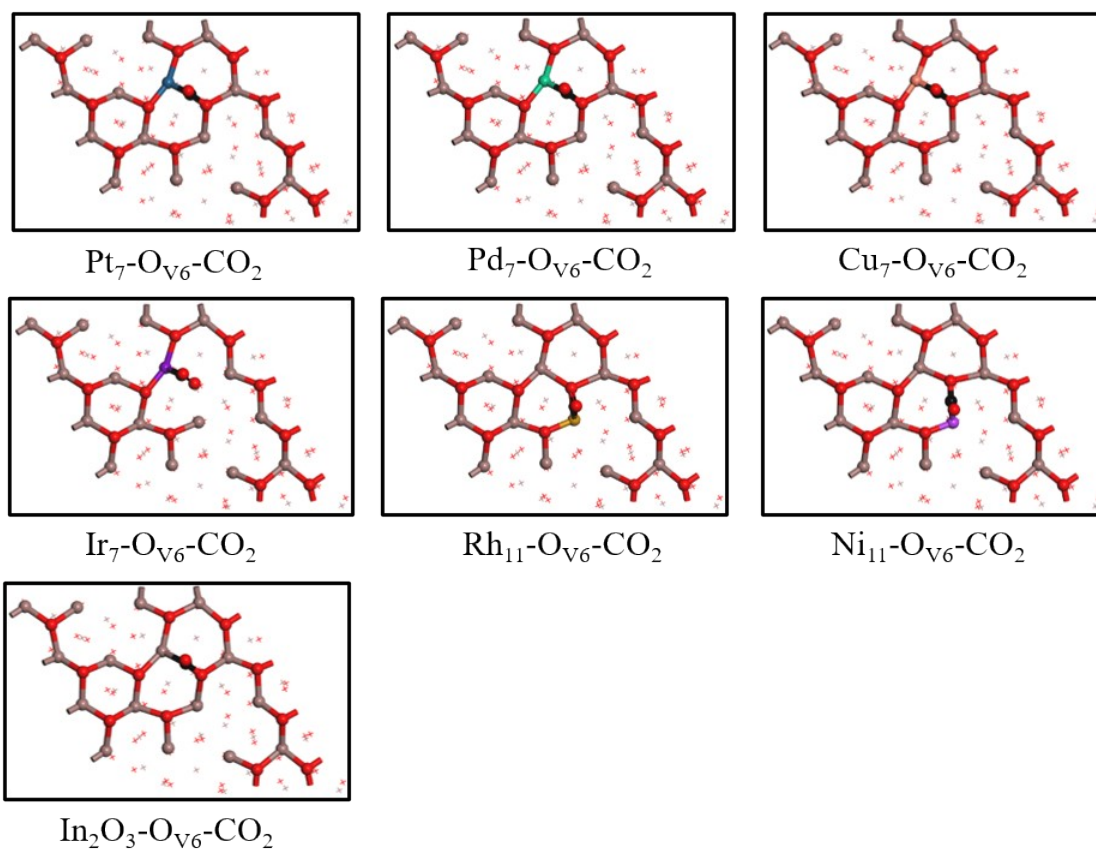


Figure S2. Optimized structure for the most stable CO₂ adsorption on M/In₂O₃(111) surfaces

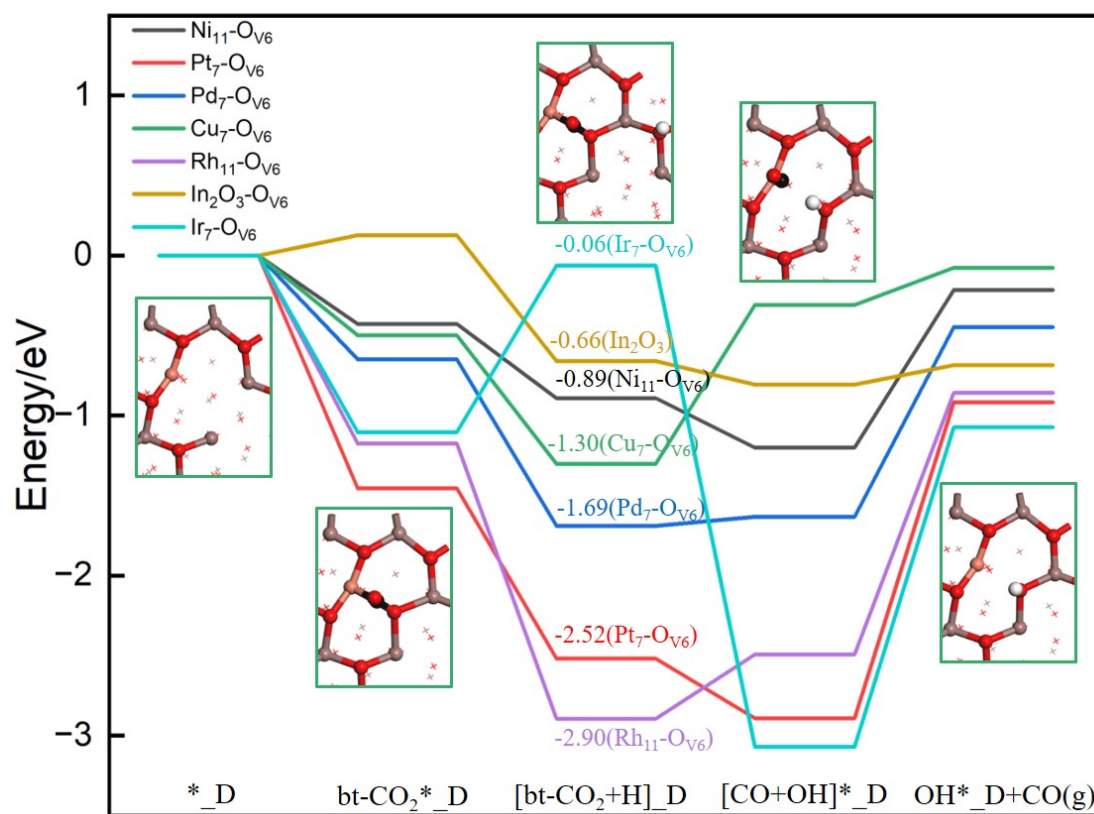


Figure S3. Energy profiles for CO₂ hydrogenation to form CO via the indirect dissociation pathway on the M/In₂O₃ (M = Ni, Pt, Pd, Cu, Rh, Ir.). The structures shown are for the Cu/In₂O₃ surface.

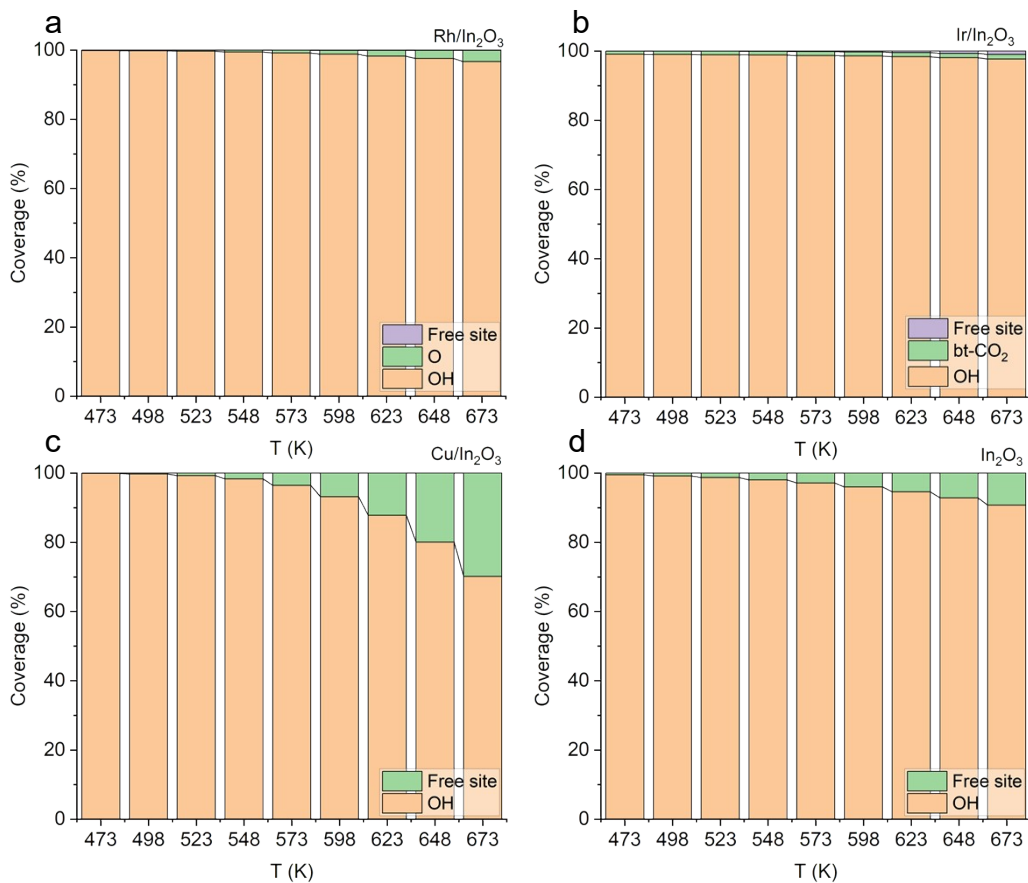


Figure S4. Calculated coverages of surface adsorbates. Coverages of the major surface species during the CO₂ hydrogenation reaction on the defective Rh/In₂O₃ model (a), on the defective Ir/In₂O₃ model (b), on the defective Cu/In₂O₃ model (c), and on the defective In₂O₃ model (d).

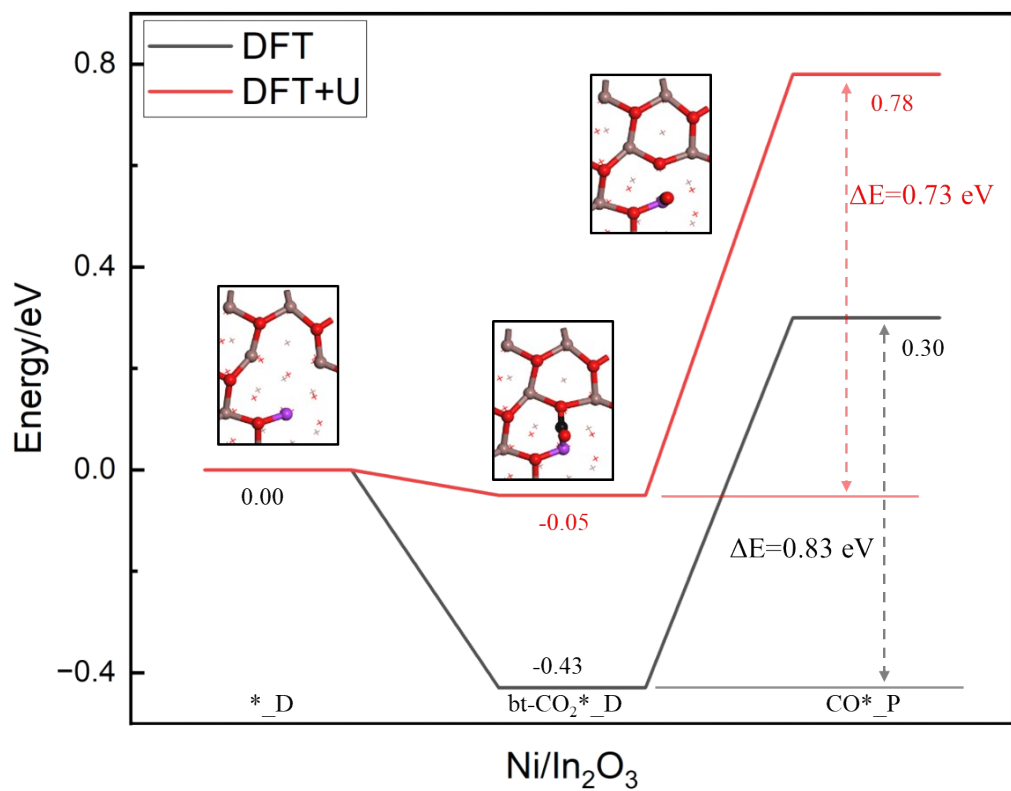


Figure S5. CO₂ direct dissociation energies on Ni/In₂O₃ in the presence or absence of Hubbard U correction ($U - J = 2.4$ eV for Ni).

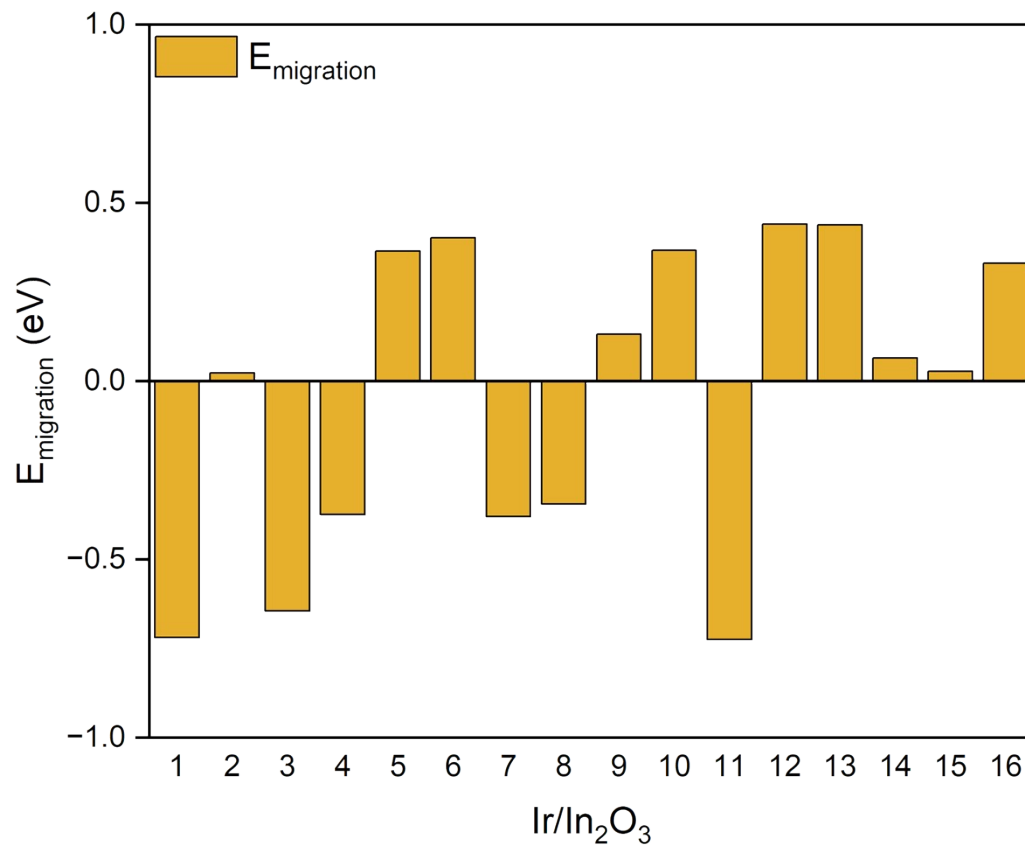


Figure S6. The migration energy of Ir atoms at 16 sites on the surface to the subsurface in the Ir/In₂O₃ model.

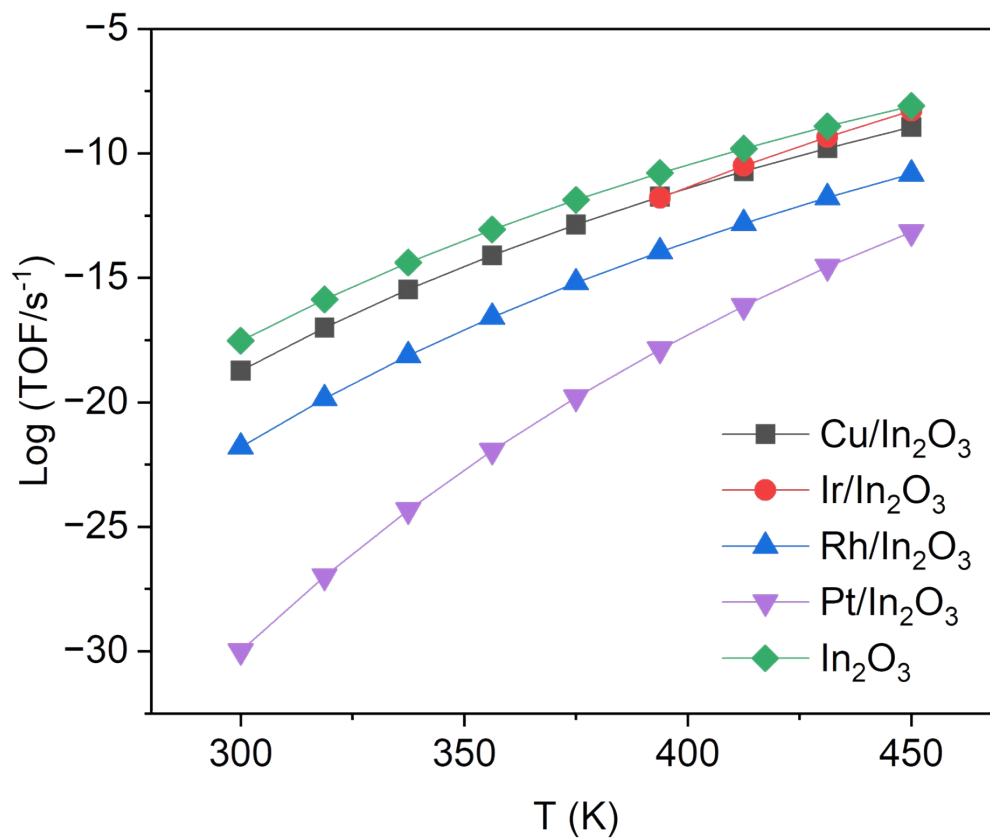


Figure S7. Plot of calculated turnover frequencies (TOFs) for CO₂ consumption over the Cu/In₂O₃, Ir/In₂O₃, Rh/In₂O₃, Pt/In₂O₃, and In₂O₃ models between 300-450 K.

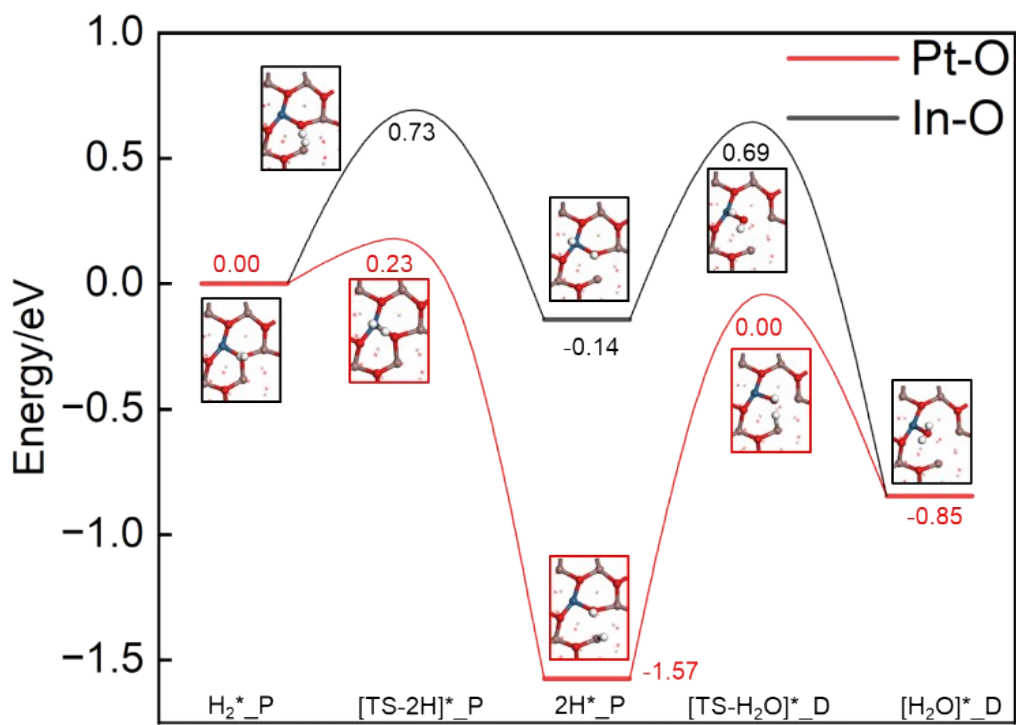


Figure S8. Energy profiles for O_V formation via H_2 reduction on the Pt/ In_2O_3 model. The structures with the red border show O_V formation at the Pt-O site, whereas those with the black border structure show O_V formation at the In-O site.

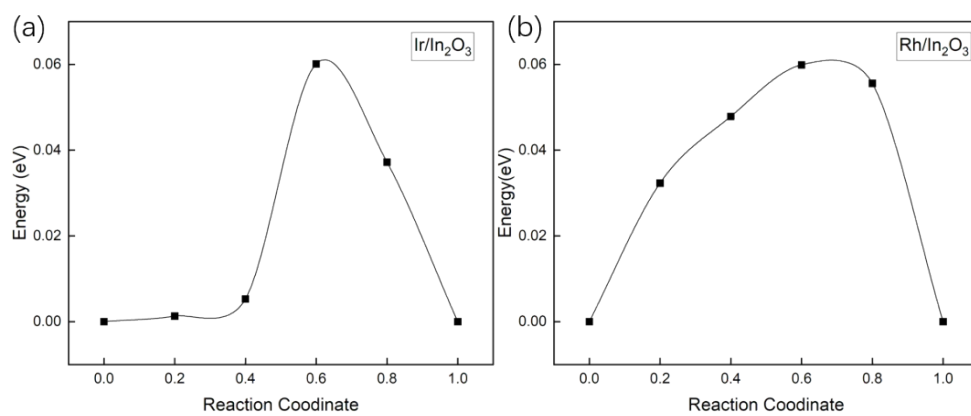


Figure S9. Potential energy profiles of the CI-NEB images for the Ir/In₂O₃ (a) and Rh/In₂O₃ (b)

models.

Table S4. The adsorption energy of CO₂ and CO on M₇-O_{V6} sites.

E _{ads} /eV	Pt	Ir	Pd	Cu	Rh	Ni	In ₂ O ₃
E _{ads} (M ₇ -O _{V6} -CO ₂)	-1.46	-1.10	-0.65	-0.50	-0.82	-0.35	0.13
E _{ads} (M ₇ -O _{V6} -CO)	-3.07	-2.29	-1.79	-0.71	-2.12	-0.79	-0.11

Table S5. Energy data for O_V formation via H₂ reduction of the M/In₂O₃ surfaces.

E/eV	Ni/In ₂ O ₃	Pt/In ₂ O ₃	Pd/In ₂ O	Cu/In ₂ O ₃	Rh/In ₂ O	In ₂ O	Ir/In ₂ O
			3		3	3	3
H ₂ _P	0.00	0.00	0.00	0.00	0.00	0.00	0.00
[TS-2H]*_P	0.94	0.73	0.70	0.66	1.05	1.08	0.75
2H*_P	0.46	-0.14	-0.21	-0.30	0.62	0.64	-0.13
[TS-H ₂ O]*_D	1.17	0.69	0.60	0.34	1.44	1.16	0.91
H ₂ O*_D	-0.88	-0.85	-1.13	-1.32	0.45	0.25	0.27

Table S6. Energy data for the direct dissociation of CO₂ on the M/In₂O₃ surfaces.

E/eV	Ni/In ₂ O	Pt/In ₂ O	Pd/In ₂ O	Cu/In ₂ O	Rh/In ₂ O	In ₂ O ₃	Ir/In ₂ O
	3	3	3	3	3		3
*_D	0.00	0.00	0.00	0.00	0.00	0.00	0.00
bt-CO ₂ _D	-0.43	-1.46	-0.65	-0.50	-1.17	0.13	-1.10
[TS-CO-O]*_D	0.32	-0.48	0.67	1.42	-1.16	0.45	-1.02
CO*_P	0.30	-1.11	0.35	1.31	-1.94	-0.20	-2.37
*_P+CO(g)	0.83	0.11	0.86	1.45	-0.23	-0.04	-0.35

Table S7. Energy data for the direct dissociation of CO₂ on the M/In₂O₃ surfaces.

E/eV	Ni/In ₂ O	Pt/In ₂ O	Pd/In ₂ O	Cu/In ₂ O	Rh/In ₂ O ₃	In ₂ O ₃	Ir/In ₂ O
	3	3	3	3			3
*_D	0.00	0.00	0.00	0.00	0.00	0.00	0.00
bt-CO ₂ _D	-0.43	-1.46	-0.65	-0.50	-1.17	0.13	-1.10
[bt-CO ₂ +H]*_D	-2.90	-2.52	-1.69	-1.30	-2.90	-0.66	-0.06
[CO+OH]*_D	-1.20	-2.89	-1.63	-0.31	-2.49	-0.81	-3.07
OH*_D+CO(g)	-0.22	-0.92	-0.45	-0.08	-0.86	-0.69	-1.07

Table S8. Elementary steps of the RWGS reaction on the M/In₂O₃ (M = Cu, Ir, Rh) models and the In₂O₃(111) surface, where “s” and “t” denote the O_V and “hydrogen reservoir” sites, respectively.

R1	CO _{2_g} + * _s -> CO _{2_s} #ln-CO2
R2	CO _{2_g} + * _s -> O ₂ C _s #bt-CO2
R3	H _{2_g} + 2* _t <-> H-H _t + * _t -> 2H _t
R4	H _{2_g} + O _s + * _t <-> OH-H _s + * _t -> OH _s + H _t
R5	OH _s + H _t <-> H-OH _s + * _t -> H ₂ O _s + * _t
R6	H ₂ O _s -> H ₂ O _g + * _s
R7	O _s + H _t -> OH _s + * _t
R8	CO _{2_s} + * _s <-> CO-O _s + * _s -> CO _s + O _s
R9	CO _s -> CO _g + * _s
R10	O ₂ C _s + H _t <-> O ₂ C-H _s + * _t -> COOH _s + * _t
R11	COOH _s + * _s <-> CO-OH _s + * _s -> CO _s + OH _s
R12	CO _s -> CO _g + * _s
R13	CO _g + * _s -> CO _s

Table S9. The absorption energies of the [InH-OH]* and [MH-OH]* structures.

E _{ads} /eV	Cu	Ni	Pt	Ir	Pd	Rh
[InH-OH]*	-0.30	0.46	-0.14	-0.13	-0.21	0.62
[MH-OH]*	-0.98	-0.79	-1.57	-1.03	-0.93	-0.98

Table S10. The C-O bond lengths for the Rh/In₂O₃ and Ir/In₂O₃ models during CO₂ direct dissociation.

C-O lengths/Å	IS	TS	FS
Rh/In ₂ O ₃	1.50	1.66	2.61
Ir/In ₂ O ₃	1.37	1.60	2.85

Table S11. Optimized fractional coordinates of the single-atom metal-doped (M=Pt, Cu, Pd, Ir, Ni, Rh) c-In₂O₃(111) surfaces.

The perfect Pt₇ doped c-In₂O₃(111) surface

O In Pt In

1.0000000000000000			
14.4442996979000000	0.0000000000000000	0.0000000000000000	
-7.2221498489000000	12.5091304781999995	0.0000000000000000	
0.0000000000000000	0.0000000000000000	17.9855003356999994	

O	In	Pt	In
72	27	1	20

Direct

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0.5156336877726424	0.9527096811292104	0.2893817490210620
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0.7934072485137235	0.9613388101064483	0.2975170440717287
0.4713901657165808	0.2945197591691818	0.6501578078287430
0.1330121164608386	0.6253287486900587	0.4697491316995526
0.3006612426001081	0.7316919696045410	0.3001114678592239
0.9785524110449739	0.0704500379294203	0.6354456649216317
0.6405996225561799	0.4065316345212386	0.4679538736304230
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0.2988933454787390	0.2425686258992032	0.6522652039268476
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0.9308700735156473	0.7891870743224815	0.4869714259724571
0.4749778867634379	0.3097477637276070	0.5071624155203018
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0.8049865950956336	0.9771094151413517	0.6763373583804513
0.5881204056698243	0.1188315366547897	0.3257739932658661
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0.0314320533597685	0.4653300717786492	0.6852663688218530

0.8570009801449080 0.6293008011696060 0.3358009177187191
0.5475290854561189 0.9729923030352614 0.6656248080501207

The perfect Pt₇-O_{V6} surface

O In Pt In

1.000000000000000
14.4442996979000000 0.0000000000000000 0.0000000000000000
-7.2221498489000000 12.5091304781999995 0.0000000000000000
0.0000000000000000 0.0000000000000000 17.9855003356999994

O In Pt In
71 27 1 20

Direct

0.8403715498000651 0.6136251742207847 0.4564917501744061
0.5160447169406837 0.9528957157892695 0.2898417389935328
0.1703833046008539 0.2782862620143632 0.6189951023902858
0.7925325614953863 0.9614584639706660 0.2988402465883944
0.4680140205016773 0.2907296139490607 0.6513890403469696
0.1334105309048932 0.6257477951262727 0.4693184855448344
0.3008781790168572 0.7311282986905446 0.3002652101280100
0.9775693288394462 0.0699144916167744 0.6357941356458799
0.6411578598228416 0.4078360214505930 0.4698955844618312
0.5297705075120382 0.2099772997200313 0.2684759365666500
0.1842173071762490 0.5391127658495156 0.6099762341793875
0.8574249611667751 0.8822855751928159 0.4414394916273599
0.8873790589828635 0.1306295616108584 0.4565889147314747
0.5477531576801490 0.4638950336018270 0.2898171986541628
0.2162515095010498 0.7890953224039771 0.6190517748414253
0.5388743155156397 0.7320430910013446 0.2989222819532963
0.2060934633039028 0.0749309595953506 0.6582337059096326
0.8744989852830679 0.4073362131513856 0.4692591536068944
0.7679625317726350 0.4686604040474076 0.2991545988615709
0.4221189417755936 0.8103838264010508 0.6338133810444189
0.0946955396787359 0.1338190621753212 0.4629132718310985
0.2913049849995367 0.2198862823955885 0.2690176498549621
0.9582899386710128 0.5422557427493836 0.6111500636215695
0.6163354736443271 0.8727923095344441 0.4431723791390780
0.3739711463957045 0.6589124774682285 0.4591264965719423
0.0368431062080352 0.9841460019262880 0.2879766016251569
0.7068971955449586 0.3329739872032660 0.6226858688983541
0.7669464670675582 0.7069549689213074 0.2993889689664261
0.4225713051756765 0.0286742263657979 0.6560190789251792
0.0916819361993300 0.3653753685588277 0.4689556022027332
0.0310021079139910 0.1990422770503693 0.2991842524409722
0.6848172949222309 0.5371381020640881 0.6564410061020719
0.3651040361385146 0.8602698245636017 0.4635901893421789

0.2814480630253807	0.9703745719168579	0.2680495808174808
0.9565518174999496	0.3156454144622748	0.6119929171495284
0.6246804566433750	0.6463775789173002	0.4444051799156220
0.2273702102745134	0.3177425633960184	0.3780013722463959
0.8897818149720006	0.6466392129496505	0.7106281451849715
0.5585857335823523	0.9886657072436718	0.5431756765235360
0.2678298751438388	0.9751527229504616	0.5309681798625741
0.9280848906923563	0.3063447343423794	0.3443751806783941
0.7594134624949384	0.1965976686090049	0.5370923280809240
0.4237020573073866	0.5291749280271113	0.3665354336264646
0.0987619024920070	0.8653157043811809	0.6996456835805731
0.5466897129367093	0.7213710051434491	0.5655435703915210
0.2161835221702839	0.0590846225643089	0.3861852476927899
0.8713093868757007	0.3889853252626906	0.7308577662810039
0.1817937740456727	0.8094910354605966	0.3780106739928870
0.8526890454681173	0.1367104691400216	0.7109207889236114
0.5136558645785255	0.4718712231607022	0.5455133440214247
0.5263311863142756	0.1920558479887326	0.5309526100178654
0.1951999602818490	0.5224497551872780	0.3501078325982328
0.8648666378361034	0.8701417998676266	0.7045736467562523
0.3043063433608983	0.4622482992800523	0.5346678449581744
0.9711448728605135	0.7937102084453292	0.3628959119575156
0.6331001139951199	0.1315241761717366	0.6996104901381416
0.7840564311755305	0.7253726974735413	0.5602608669124132
0.4399068151090644	0.0569858826419933	0.3875941596787417
0.1112364200275305	0.3801695827458438	0.7293597971871011
0.6893108199634067	0.2738694830446595	0.3800388152097498
0.3705361364476336	0.6098833379981953	0.7021203186702138
0.0301935514165406	0.9423592290969548	0.5432841014938952
0.3064094651896181	0.2305734250796937	0.5301293991500057
0.9771951695541687	0.5715274794206148	0.3476236048567387
0.6346846641464734	0.8888859592756809	0.6932759521275468
0.0349882813742283	0.7399658342125629	0.5334221335629107
0.7058702340137106	0.0776547196662104	0.3658470468288094
0.3622048523120304	0.3936785557875546	0.7034825496149901
0.7772581202698702	0.9592685586157248	0.5572004922484405
0.4457707854664129	0.2849457556102050	0.3884029372596043
0.1220938135624288	0.6277395386805343	0.7295691441798839
0.1404591993853945	0.1455718358962276	0.3303283337686416
0.8119676020408627	0.4813270586937061	0.6780074562464434
0.5984632365087287	0.6240793164876869	0.3226272231879254
0.2557565589102758	0.9526693266646878	0.6530563212968029
0.9255429466173877	0.2910984779860853	0.4961726035401252
0.4692871482942056	0.8126603681786985	0.5142050746119269

0.3544303347444346	0.8944423274950720	0.3317597551427405
0.0181372951846980	0.2293313868323354	0.6753132124222400
0.8764013640678224	0.8757166062971203	0.3208286086195668
0.5443902223724439	0.1993235501211992	0.6528099616276904
0.2088173097785891	0.5337515422752588	0.4933173488140807
0.6881160265367874	0.5619460785454823	0.5132246686864891
0.6053160573042747	0.3594963282412199	0.3306419858749082
0.2695652974309481	0.6868899959311564	0.6717137017749358
0.6243892830048547	0.9011007256745580	0.3225325436825616
0.2949639552678819	0.2395036611832228	0.6521488025404397
0.9647485755231187	0.5744293486804187	0.4947130895101058
0.9427121233642917	0.0314400281417770	0.5119764435950075
0.9321760195593223	0.7901098273936056	0.4853402503453738
0.4740566034094387	0.3079306889302066	0.5046549360763877
0.1446789675793134	0.6455305628413780	0.3475012488986831
0.8033327732653531	0.9773923955165523	0.6769689072871093
0.5883123967586344	0.1192389478007990	0.3254702260549648
0.2566890503208940	0.4488833975769773	0.6628429003969424
0.7112335412534951	0.0428806007763832	0.4875126188026266
0.1905959958029592	0.0633477565285437	0.5014775266007451
0.8539789888649744	0.3989930064110866	0.3472585074365822
0.5187246514674341	0.7249303393604217	0.6779386210533612
0.3817839871534213	0.3696509617327664	0.3254878367320712
0.0489157316323629	0.7043631480344245	0.6654073938941469
0.4580795361362925	0.5696004954928775	0.4891369796541502
0.4350838947672194	0.0259576450741799	0.5032356184648984
0.1000907510671938	0.3546913288594709	0.3469355865372031
0.7900894640504161	0.7071102819125554	0.6792764521319161
0.1307028097219445	0.9113526913731115	0.3227692860800896
0.7949563574604216	0.2403300645526786	0.6676313867192708
0.7006015450723472	0.3018538907833102	0.5010194592554917
0.7022639212650743	0.8032237286543652	0.5015754919873753
0.1991119525148294	0.2978710943742829	0.4981577040440644
0.2002952652996015	0.8004606950416157	0.4986398360338568
0.8703248111664612	0.1287599869933513	0.3350792493103861
0.5182369703189070	0.4614887271273028	0.6657044178207058
0.3729203450659319	0.6429228189334215	0.3365833298288932
0.0323120954265227	0.9595337422856078	0.6648721121989470
0.3670705419673462	0.1330642342686253	0.3123929648587135
0.0335110721912509	0.4654790172460364	0.6855658882973011
0.8570004014377263	0.6292893497268068	0.3348418441766502
0.5428237107477885	0.9703501811568760	0.6641624359379242

The perfect Pt₇-O_{V6}-bt-CO₂ surface

O In Pt In C O

1.000000000000000					
14.4443000000000001	0.000000000000000	0.000000000000000			
-7.22214999999999965	12.5091307398835685	0.000000000000000			
0.00000000000000011	0.00000000000000019	17.985499999999983			
O	In	Pt	In	C	O
71	27	1	20	1	2

Direct

0.8408735742006792	0.6133663102468976	0.4566343692593297
0.5151695304531070	0.9518224307745971	0.2906042738183337
0.1727653870871880	0.2797800136071363	0.6203793099387559
0.7923217269901232	0.9605068241502124	0.2991199469521336
0.4696344543104434	0.2892091636992317	0.6610824855320556
0.1334718478365275	0.6263462132968682	0.4692703771574824
0.3007459695422692	0.7308324379892378	0.3009057037090554
0.9776717283032823	0.0703392547393717	0.6363247996110236
0.6403003520681549	0.4056673421539510	0.4650414941778020
0.5295337114673362	0.2096967101489888	0.2686633109858889
0.1818316608277755	0.5384752661728367	0.6089295940551041
0.8554524355765599	0.8812883186647872	0.4429764093503405
0.8869220174672222	0.1285640516380136	0.4563868565462034
0.5478537278413322	0.4640079681137276	0.2906327121612068
0.2169197214052892	0.7910851549695531	0.6197062774476469
0.5389561988537590	0.7318857200707249	0.3001411171508415
0.2062305224309927	0.0771462267215152	0.6567940856868157
0.8741504952424533	0.4071290783742497	0.4691410880642830
0.7685354014781947	0.4687109776039098	0.2992747454113069
0.4252918077383733	0.8096711113818470	0.6351847516388677
0.0947647967503654	0.1345700951958992	0.4649341520225295
0.2901981571680288	0.2198978649171389	0.2688104059279227
0.9591889875752779	0.5428950993829256	0.6100915159936092
0.6166172153820521	0.8725688409101816	0.4440409901901349
0.3732065652137568	0.6587792853751367	0.4592276174477087
0.0359959558891336	0.9840955420095397	0.2896534672991551
0.7087773245312233	0.3276774669243766	0.6206090867997395
0.7664992273828560	0.7064482982504571	0.3003589039696550
0.4220713566357212	0.0292923745735383	0.6549046505160552
0.0914830360393004	0.3646826546322650	0.4693643265865403
0.0308313245960496	0.1989975156624212	0.2994550756355787
0.6957094724365589	0.5248075951280123	0.6366144107949255
0.3647235920786332	0.8598429457571231	0.4650909844266568
0.2805618371178844	0.9702985752211081	0.2689252888223749
0.9560796519902163	0.3139241280668014	0.6111937830507612

0.6247225933556575	0.6448806005561676	0.4460950931204397
0.2272456941215355	0.3173100419335184	0.3788203182127525
0.8884642864731026	0.6435933018619124	0.7135160152412828
0.5577583308440447	0.9892433562644410	0.5430493503609530
0.2672023002246650	0.9753889134536907	0.5309842078322443
0.9280161065435202	0.3056746721189751	0.3461754357561331
0.7591573256936099	0.1947826325294856	0.5351109754296945
0.4235006244932416	0.5289924788843767	0.3674892130800058
0.0982484456071283	0.8663120534695403	0.6996436288406204
0.5434367135453643	0.7193651981869983	0.5683582786538813
0.2159328790137581	0.0598343502897983	0.3873502250647769
0.8718385461356720	0.3881956298445586	0.7297151760274552
0.1816663488833027	0.8096903361674658	0.3785109511052115
0.8538295310562001	0.1370487542860349	0.7114249060500412
0.5131802945907611	0.4690658275574496	0.5456800637152868
0.5244570387467464	0.1930797086083252	0.5312946014953052
0.1946373629236106	0.5220194754963714	0.3507847089246849
0.8623466132327214	0.8676572511283441	0.7029468783214885
0.3039734623209589	0.4629883904543976	0.5346412873086149
0.9705964058260861	0.7934805119022956	0.3639924466073915
0.6333126164458559	0.1332804029973267	0.7013605677187840
0.7838724513816187	0.7259498047413860	0.5612959474203822
0.4396718510263881	0.0567854366084254	0.3878372132926034
0.1125940313582100	0.3813995901411611	0.7286106346631448
0.6899253697456554	0.2723997061047973	0.3790375928088996
0.3607178547045071	0.6147347302519592	0.7050621605442918
0.0298127926855747	0.9422241897709863	0.5437768348469051
0.3086141134610361	0.2319114723376403	0.5314894979974250
0.9774164708941087	0.5716028259523148	0.3480922523422199
0.6337926942880138	0.8996067158413560	0.6974819890273067
0.0346949462914130	0.7403022160255013	0.5340618080209742
0.7056911063289348	0.0765063837943599	0.3651953471707882
0.3707131206807959	0.4021039335140061	0.6986459324772626
0.7759875950291619	0.9586672861878082	0.5590923279605813
0.4437445668812131	0.2835065551241266	0.3867494568199403
0.1182894633079598	0.6273429707335602	0.7290451275666445
0.1403488421059854	0.1457166483783212	0.3312533587485259
0.8130420201254294	0.4790601886440656	0.6747145964054956
0.5981323631521509	0.6236101814082947	0.3246894314033901
0.2549893241559646	0.9545491885704943	0.6529387471276898
0.9249558945256323	0.2899685181041206	0.4952674164784872
0.4696923071110384	0.8118058253717514	0.5149057196391832
0.3538970361506332	0.8942543812823283	0.3325426886716973
0.0195593385958500	0.2302065607545004	0.6752505531533788

0.8755572322165600	0.8749573669365618	0.3225280640424425
0.5462122668526052	0.2005577333553497	0.6531445541566160
0.2083788086455708	0.5336019289962002	0.4929865308883463
0.6893132587330181	0.5587143086714818	0.5138845949011747
0.6056085187645839	0.3595656096844398	0.3310480957505585
0.2651678965276599	0.6865420010622708	0.6713808098801267
0.6242422403902161	0.9005906786904437	0.3232885707554413
0.2986685245104070	0.2434860726393332	0.6535450850710937
0.9650581917651422	0.5745450204939609	0.4941262485914025
0.9416679790459430	0.0303242925922883	0.5129825038245445
0.9305672777122499	0.7896128078366373	0.4866813113007533
0.4739109453431207	0.3085732190463572	0.5016351686774766
0.1447976891517807	0.6457223068816216	0.3477907779285858
0.8029401951546195	0.9770887577386584	0.6786806892629653
0.5877615574011469	0.1183562028717786	0.3251332396867086
0.2599993235540041	0.4527528643588750	0.6629681191949544
0.7108101705337524	0.0412864460321764	0.4874755428619750
0.1906085073987076	0.0645923815532182	0.5031133451102425
0.8540878679474933	0.3987938141901938	0.3474427132033970
0.5108737845680661	0.7401240550111142	0.6898999159335927
0.3813015126453539	0.3700481228703241	0.3250687856191551
0.0467444192737013	0.7044995052914195	0.6659477983337683
0.4591477837569169	0.5708817072646557	0.4920690971597030
0.4344891295625553	0.0262470408836689	0.5034436336361856
0.1001294946437205	0.3542096686378079	0.3477491805487199
0.7887101611267684	0.7010856695617215	0.6793200757910323
0.1302312487157652	0.9118383489939063	0.3242803472259452
0.7951699959130546	0.2390840107242881	0.6671438072997687
0.6997438422342214	0.3001171361198398	0.4998628013339705
0.6997390408599780	0.8008221377016973	0.5051924016776805
0.1997538897995930	0.2984648806676803	0.4995038243190063
0.1998153328780262	0.8007314435324364	0.4991028334728644
0.8701219493240008	0.1275792681881604	0.3352451890004003
0.5298985987138126	0.4607809615521683	0.6654587742941157
0.3730779710133156	0.6427388536822172	0.3375776870936919
0.0301898267174748	0.9589267384384493	0.6652350763766307
0.3665127113183097	0.1331761981968958	0.3122267282779952
0.0335518701215832	0.4650489268246649	0.6846409108301044
0.8566940766017946	0.6291763910485467	0.3353311709274735
0.5417826956262883	0.9746634299668807	0.6640360376775225
0.5785445131779677	0.6800501747683586	0.7531745164116802
0.5775498662735213	0.6967200411663811	0.8195400619339176
0.6213457181431040	0.6237479066488900	0.7234553098578385

The perfect Pt₇-O_{V6}-[CO₂+H]* surface

O In Pt In C O H

1.000000000000000

14.4443000000000001 0.000000000000000 0.000000000000000

-7.22214999999999965 12.5091307398835685 0.000000000000000

0.00000000000000011 0.0000000000000019 17.985499999999983

O In Pt In C O H

71 27 1 20 1 2 1

Direct

0.8428750299663466 0.6143677278451010 0.4553999433350231

0.5163852885098817 0.9522027441948524 0.2873905737175552

0.1722335422847517 0.2798326639072505 0.6206155960819724

0.7935501396086515 0.9607681932093428 0.2977011379499618

0.4714620799016335 0.2915828543187899 0.6587275947749086

0.1330803024298003 0.6250542482516548 0.4693159292570059

0.3016964120543388 0.7307021778517769 0.2994054604766782

0.9764359980628606 0.0692628693585107 0.6356099075499462

0.6409866575468354 0.4042353792898134 0.4656877067789563

0.5295444250780745 0.2095217385986727 0.2680208156369518

0.1819244881960486 0.5395463434255537 0.6103077831717681

0.8566153127274649 0.8812791986959924 0.4412916853203682

0.8870542962963168 0.1279594301524280 0.4558294049830688

0.5476883247973433 0.4623524381020909 0.2885483854606236

0.2212172903808303 0.7921311156207173 0.6189033251303678

0.5398932946673828 0.7310702626989499 0.2988600699774610

0.2060792041028713 0.0762636184352853 0.6598912144714703

0.8737615622861490 0.4067449513918995 0.4694129211011424

0.7690959555340440 0.4686519073297878 0.2991567586165894

0.4273927859381352 0.8062781377996789 0.6392765229794164

0.0954264506342069 0.1343107478607590 0.4648154502006528

0.2909174933715865 0.2195637792785129 0.2688935855571517

0.9517306325385193 0.5479374443899715 0.6100926645967338

0.6179992155369877 0.8757777372849064 0.4406378374641908

0.3693564568717919 0.6569324818920138 0.4572408845716197

0.0375616761639019 0.9842674971114294 0.2886717471683282

0.7060076792143194 0.3236968885263439 0.6188579135910195

0.7692983308241935 0.7071532024534419 0.2966216246902044

0.4214891281136393 0.0277892645518355 0.6589947122746811

0.0927664391075603 0.3656958126248218 0.4694179698291586

0.0314427040540660 0.1991309724051929 0.2991952016086834

0.7017725419309773 0.5295308217858987 0.6385483771867019

0.3677469540193872 0.8583264018781320 0.4659739880619356

0.2815084781178969 0.9701773159565515 0.2677994988413686

0.9552858597459584 0.3160187242327975 0.6104908115714189

0.6300472718018749	0.6407846800025050	0.4406605087452733
0.2277605277587918	0.3168179011987131	0.3790458952122427
0.8865991452625147	0.6495174000710995	0.7220709610314426
0.5582106857291338	0.9866328367237526	0.5454539687800771
0.2691781779858949	0.9758133424483407	0.5309222006957299
0.9288401419245449	0.3058983623808887	0.3474543563823732
0.7593477687317721	0.1935419916151588	0.5338267374444464
0.4244449168196920	0.5285831987467521	0.3665161700728003
0.0955018760923719	0.8627501604796761	0.6971311851533002
0.5464415219839829	0.7162443190377437	0.5554308509662857
0.2168794747598171	0.0591876092723693	0.3865493838751090
0.8700302809713488	0.3890950417881837	0.7287398561254022
0.1840231887796665	0.8096487929869323	0.3778311382150686
0.8533693337885190	0.1369548998718452	0.7093084620293925
0.5166055916287231	0.4704615908983101	0.5466669437226824
0.5232744464356962	0.1902519419891838	0.5309175053644510
0.1944409179192200	0.5213526709637651	0.3470491951617948
0.8620869111888382	0.8671968793062900	0.7033100679039063
0.3058516565145674	0.4632736779689785	0.5354646950056298
0.9724069168430209	0.7938042080889831	0.3633663972555674
0.6330189980303622	0.1329189562470062	0.7013495038205726
0.7851163093842227	0.7256115470906874	0.5597872072534030
0.4408019661808177	0.0550262785868419	0.3867740271118257
0.1102953816959096	0.3807584848352641	0.7286393270426751
0.6900738743718411	0.2721025674460267	0.3778292495276195
0.3548920710138654	0.6125897950123086	0.7145849855695877
0.0307908790333301	0.9420776484191706	0.5429402230492766
0.3084883915583874	0.2308816464858300	0.5321299276459096
0.9782456301374427	0.5717232837384958	0.3486135326551099
0.6335625335457367	0.8994990114806962	0.7043416353378837
0.0377624907591321	0.7415669876261179	0.5327286100781660
0.7068376197677962	0.0777816955057485	0.3631082794464108
0.3686567402373778	0.4001624684830105	0.6998842691506106
0.7751904968198896	0.9563637395408794	0.5580356257584770
0.4445962883762741	0.2836812069190117	0.3876150895915093
0.1136916080544474	0.6277255785961174	0.7272744995718636
0.1408955383761578	0.1456616645137170	0.3309885837221511
0.8064958102999370	0.4723412453916228	0.6723879279040413
0.5998175094618198	0.6226940622816532	0.3216365175789533
0.2556064591675422	0.9550224987424625	0.6527628773215339
0.9253690407708456	0.2896997940661133	0.4937976456295761
0.4718010702312884	0.8077815004465200	0.5172435750376578
0.3555478537803303	0.8937966090497875	0.3303332913011405
0.0188658309056862	0.2301456974936608	0.6740240964914929

0.8768083940892480	0.8752005338347789	0.3204940414851470
0.5434636086777124	0.1976229245396140	0.6531248290905634
0.2099874699904880	0.5339487181591011	0.4944454829700609
0.6906692408348578	0.5584278174038126	0.5119122188705193
0.6056941666132507	0.3592256725803971	0.3306142470690021
0.2665120050437715	0.6866573422692773	0.6748268087886768
0.6249265245818435	0.9006794678502830	0.3209486721271731
0.2981828005089158	0.2430467331930353	0.6539925867430838
0.9650110436387614	0.5746061106234162	0.4914103141631377
0.9413140847058448	0.0297688321927200	0.5123904188816184
0.9318226857878465	0.7901898405503225	0.4854562994762915
0.4746173002558810	0.3084756628469065	0.5031115723361225
0.1461903455307023	0.6448345010785066	0.3472795002069173
0.7996953647693201	0.9752828392671942	0.6778108462479291
0.5886465466305917	0.1180711336485582	0.3231904169544956
0.2607758304449696	0.4541223823741860	0.6651826933568386
0.7101166786241342	0.0395763749592145	0.4865797038037252
0.1917363342914310	0.0642841789289607	0.5018257886979718
0.8544482504175521	0.3986150531635586	0.3472975793218242
0.5064714985450615	0.7405952935076230	0.7058374430600628
0.3818726978350541	0.3696449505233541	0.3251068776408969
0.0521825715898410	0.7071604641598213	0.6577902144577361
0.4613318490879316	0.5712506922151350	0.4898891534921077
0.4366745274262500	0.0239211773480315	0.5024364644183680
0.1012328549763784	0.3543651803265013	0.3475062933860451
0.7750398390675083	0.7026648546831719	0.6775204987798578
0.1315072678379050	0.9114184318856718	0.3233103817344634
0.7934657690695218	0.2368923856293974	0.6652922873538630
0.6982977292910457	0.2969185200980633	0.4983411725469905
0.6987277651319949	0.7988411783684302	0.4995577310649072
0.2006370302417138	0.2988730185663742	0.4998938872811677
0.2036360805672967	0.8009647237400193	0.4977623391771615
0.8705951894848473	0.1274299941611678	0.3345836189992218
0.5291034133102911	0.4640000896611705	0.6667872108480345
0.3735621867701586	0.6421547658954186	0.3367132404104494
0.0298027150177246	0.9589046859606214	0.6640613122436020
0.3672332793313670	0.1328585679937393	0.3120339238626075
0.0327680692965495	0.4649394360832440	0.6846539879193055
0.8577391644058090	0.6297623314982663	0.3338583781492429
0.5414029837206683	0.9719290111377190	0.6670280463670805
0.5756461640637995	0.6803055566326802	0.7663712970821915
0.5923749656008152	0.6872940206186470	0.8325018860650882
0.6146436080089039	0.6223777206958635	0.7224999207018695
0.9056677428717544	0.6667391137084914	0.7740323371035617

The perfect Pt₇-O_{v6}-[CO+OH]* surface

O In Pt In C O H

1.00000000000000

14.444300000000001 0.000000000000000 0.000000000000000

-7.2221499999999965 12.5091307398835685 0.000000000000000

0.0000000000000011 0.0000000000000019 17.985499999999983

O In Pt In C O H

71 27 1 20 1 2 1

Direct

0.8432656533264291 0.6133233574550874 0.4546268340540557

0.5158258427420938 0.9517663936611738 0.2881053050252152

0.1736774171675044 0.2818089471259713 0.6204253124509953

0.7934201355231304 0.9604566503521537 0.2972547043539170

0.4694158556177130 0.2894661809127499 0.6663462142732598

0.1339287234906150 0.6249045441251027 0.4682251894165182

0.3022844908776126 0.7318633076165302 0.2993874526260766

0.9765558483597986 0.0695117056800966 0.6356433434678327

0.6396887715154602 0.4035436890304248 0.4602457313359522

0.5289018236584280 0.2083300962404231 0.2675019958040273

0.1863704609604578 0.5414508491252062 0.6107828430388232

0.8556921490187785 0.8811770581808014 0.4414972036002442

0.8870107668150173 0.1277472293271064 0.4556249783812384

0.5474750078022304 0.4622876063292946 0.2867817144034442

0.2189751510999329 0.7922486274676004 0.6208440662601569

0.5399093278980753 0.7312424143701937 0.2977927547416352

0.2061687997489743 0.0784782556682163 0.6550452482632443

0.8738538571992416 0.4067854108322452 0.4673571683476381

0.7695390679875024 0.4689159700270153 0.2976306205504720

0.4309339347099854 0.8052327087512698 0.6410595252770691

0.0951547331727203 0.1350622729263075 0.4656432353320626

0.2892230791912473 0.2186889252853083 0.2673062808913628

0.9605425140554810 0.5424151831506837 0.6078513962412715

0.6184998473169395 0.8756150029162079 0.4406515791343650

0.3696867258551448 0.6569362490182507 0.4557360965139371

0.0371900716619311 0.9840080261920829 0.2892833815093706

0.7085502049887595 0.3271172241546960 0.6174380445845367

0.7693010064878530 0.7068764212687279 0.2964159383958958

0.4218198956266238 0.0291457720700169 0.6538042572198459

0.0930430789569671 0.3670795224890119 0.4682603309018330

0.0313683370052280 0.1988017740668227 0.2990190325823823

0.6981761657284382 0.5229684154804336 0.6275030852364517

0.3667323419244803 0.8573120884928205 0.4689821728656154

0.2808497184723848 0.9699564550317485 0.2685112446619209

0.9564982200150228 0.3146722484113110 0.6092056930520794

0.6291093162988828	0.6405015361177185	0.4395660820118279
0.2277484178117298	0.3168686912210814	0.3783654181390115
0.8870825139329153	0.6428384827582319	0.7109414473689363
0.5581520399186447	0.9864814178870178	0.5445701137491088
0.2671270216831134	0.9746834761195526	0.5302355665916280
0.9288165123042320	0.3055794065942762	0.3459968088458896
0.7587905556701968	0.1940389211556642	0.5327393617004466
0.4241183936839436	0.5283088618017793	0.3644609582004381
0.0974050775146232	0.8669325358630690	0.6984319516894336
0.5451170385153261	0.7146439794850246	0.5550585409484878
0.2166341566598419	0.0600891717595594	0.3874589657154595
0.8704421723844892	0.3880475810832510	0.7274814604446770
0.1843403663201159	0.8098622223682749	0.3786827457968125
0.8527481470983054	0.1366388822706919	0.7083683605851120
0.5133167005729524	0.4668919512565454	0.5435065113397984
0.5228635017988679	0.1925841074268095	0.5301644924359873
0.1945616530768031	0.5214680849122225	0.3436182723332027
0.8591630966553711	0.8657681650598712	0.7019212616107495
0.3059398674776284	0.4641131470334814	0.5342346296640857
0.9719559305643863	0.7936479942388683	0.3637125637804745
0.6332654447932795	0.1365549261987023	0.7010592007934245
0.7840256002008729	0.7258654526998934	0.5590786946377321
0.4404907006184078	0.0546223401537137	0.3877876090621406
0.1116047885916863	0.3814650423065664	0.7281246284993502
0.6906813035167787	0.2717292727757435	0.3764953883219633
0.3511843297256084	0.6188577300802043	0.7210228910177751
0.0292339084865472	0.9415543067000326	0.5429692232792296
0.3096940652473558	0.2326188489974098	0.5311104831445321
0.9789682424833982	0.5719398173066038	0.3461382570088162
0.6319378983460746	0.9075499577449340	0.7079787703186128
0.0362304705631058	0.7402185597942254	0.5335350780290001
0.7068351898952220	0.0771110950946487	0.3628364556333828
0.3729794700753407	0.4061845948408109	0.6964199318640600
0.7736681795587137	0.9563840039697890	0.5587263025997550
0.4429560508191109	0.2826740235389029	0.3840439570794406
0.1126445785676921	0.6265574819770311	0.7291246169146547
0.1405949517048702	0.1454626418707308	0.3313466139607056
0.8132589834864256	0.4791383209068937	0.6704476299388221
0.5996439435687830	0.6225012556416678	0.3205378738721307
0.2544780258310290	0.9557379606200174	0.6520421285821234
0.9253129929857626	0.2900436837674454	0.4931348573894058
0.4728002395250874	0.8070020522309892	0.5164037735090150
0.3551435924381094	0.8940197598898108	0.3315105224334685
0.0194474810182150	0.2304856723776231	0.6733269636827818

0.8764937297494589	0.8748536176445270	0.3211322012169647
0.5460192083803529	0.2021528670448320	0.6519660790798361
0.2106893404264148	0.5347399473160580	0.4945692570586379
0.6900177290899581	0.5572096504171662	0.5091825945553154
0.6061604471703730	0.3592631813751772	0.3290762036616281
0.2627717903619418	0.6878335641395432	0.6757569296698728
0.6249751877589929	0.9004990932799130	0.3210296431951586
0.2995601101938349	0.2459249886527640	0.6528391591014203
0.9660862063367589	0.5742005073693668	0.4922670441452168
0.9406235956701158	0.0292440008068205	0.5126048292699585
0.9307784136092482	0.7890075868909100	0.4861958945042852
0.4736069202096244	0.3084997963024410	0.4982846433564143
0.1464786041403487	0.6451008030574792	0.3466177216778269
0.7990619308503659	0.9748494126548448	0.6779071996651940
0.5881725102126421	0.1176104681710450	0.3236527862948732
0.2629603551235983	0.4577284618369633	0.6657757661824197
0.7104200382224409	0.0400196958048555	0.4861682625270836
0.1909349436302332	0.0650038341812473	0.5034580108897286
0.8549593193604084	0.3989218635379063	0.3458913876814947
0.4991355957213403	0.7543793744891250	0.7204011058261749
0.3809317809677733	0.3695250651897183	0.3225407259273298
0.0451226249669669	0.7047616557436968	0.6641776223512379
0.4612317426282698	0.5707680774362999	0.4885142122112294
0.4351937968485739	0.0240708974648707	0.5038107804238487
0.1013404084290885	0.3547417126520391	0.3465842839615826
0.7851817376938072	0.6981875540958827	0.6769830612627276
0.1312848488783657	0.9116381570130612	0.3248833324041103
0.7946320846832404	0.2392460137952233	0.6647807766374729
0.6990343122759175	0.2989372436216449	0.4973056265912407
0.6982109898142608	0.7977882955005325	0.5008805280804005
0.2007384027484183	0.2998863437010723	0.4994772956285896
0.2015945819389423	0.7996590877373133	0.4992850669062139
0.8706484492051229	0.1272141757254661	0.3343132593141240
0.5334237953289120	0.4611248490933231	0.6639620660117280
0.3731627527707711	0.6418732241037390	0.3354396041426081
0.0282194715517057	0.9582749886211809	0.6642777465794513
0.3664004835166083	0.1325716511829527	0.3112985087316004
0.0328264632378455	0.4649874873091250	0.6841290569511492
0.8585563440063813	0.6296701028658509	0.3334897574868770
0.5420041179587942	0.9772701121959876	0.6648461391004609
0.5471354513013371	0.7216817823090654	0.8044868487482739
0.5744612433376166	0.7054017110917526	0.8613596795321014
0.6293915498792675	0.6046865375730887	0.7325034163174872
0.6261362225151871	0.5999055695770500	0.7861426681158058

The perfect Pt₇-O_{V6}-[TS-CO-O]* surface

O	In	Pt	In	C	O
1.000000000000000					
14.4443000000000001				0.000000000000000	0.000000000000000
-7.2221500000000001				12.5091307398836005	0.000000000000000
0.00000000000000011				0.00000000000000019	17.9855000000000018

O	In	Pt	In	C	O
71	27	1	20	1	2

Direct

0.8418772970123052	0.6125950609113229	0.4569261243221125
0.5157168898345188	0.9518924104399994	0.2889309028393499
0.1713329976887911	0.2789219911799654	0.6187701418725998
0.7932529493838917	0.9604614132737099	0.2977730781656652
0.4714588073870705	0.2941223074589825	0.6555134462716012
0.1325284420600582	0.6249740960766585	0.4688097731756056
0.3010756754924921	0.7308094055051473	0.2998069967658499
0.9784697424695690	0.0705253853066640	0.6348729056361944
0.6402603282072229	0.4052919766949606	0.4652584077520012
0.5290955266892524	0.2093161911229480	0.2695252262708567
0.1820783722113827	0.5384231728177109	0.6092883257894267
0.8557079326439770	0.8811291797169589	0.4422506910422108
0.8872495743846903	0.1284794717662159	0.4555076551638551
0.5477460769063582	0.4629678644351247	0.2900116816251394
0.2207549616361607	0.7909655542216316	0.6202345609573929
0.5393293527730575	0.7313532028140197	0.2988294238316358
0.2068092899670920	0.0769806575279892	0.6560258044279429
0.8747873282232039	0.4069952347619973	0.4684839016348348
0.7680922634785373	0.4685545233048567	0.2997703964564425
0.4323581061526122	0.8075187940687829	0.6450843572604396
0.0947286166743273	0.1336119499162305	0.4636720079692489
0.2905708030411588	0.2191744087838015	0.2693379702796634
0.9594000539620460	0.5428625074673701	0.6106324670260523
0.6185660549418215	0.8751594620099195	0.4411772155102962
0.3699233354703209	0.6576337245451269	0.4567822268843363
0.0366962949112301	0.9833326339690555	0.2895102759446538
0.7101478602439081	0.3274831078183733	0.6199214431442236
0.7678903070791566	0.7063533570761799	0.2991204373656812
0.4235999489667087	0.0293800899563031	0.6544735250040665
0.0911352861381673	0.3647631408514803	0.4684128096959816
0.0310829361809076	0.1983966265142321	0.2988028460332030
0.6940978259617264	0.5212208370623440	0.6350688747120121
0.3660431793671732	0.8585062554578400	0.4679151012857977
0.2808803421401327	0.9701031747703058	0.2689133236047592
0.9554282471357355	0.3146809107751867	0.6106206056083731

0.6265916234122700	0.6433833656099606	0.4435699718327384
0.2269813409089240	0.3171781390945115	0.3780862654559732
0.8858049731579193	0.6468799741741144	0.7106326949517636
0.5579868066748923	0.9859245725622613	0.5448043586064799
0.2675634907871458	0.9745006125826077	0.5309547693173254
0.9280662468247172	0.3055622933780370	0.3443328508711497
0.7585287728016139	0.1936045486549940	0.5340061611764333
0.4236776270682073	0.5289021915593346	0.3663407063839881
0.1003787962660223	0.8668480082727449	0.6995183644321636
0.5414935031041540	0.7204143964967512	0.5604413248256759
0.2164773961884197	0.0589729684473538	0.3875865814902716
0.8711344137013802	0.3896286490609670	0.7299246728319265
0.1838111688533476	0.8096854637848256	0.3789881992098699
0.8530972110754582	0.1367878430660971	0.7097719473855849
0.5123067462240057	0.4705967471616689	0.5447801551361231
0.5249072711982987	0.1921004101988756	0.5308598543177361
0.1939739629561587	0.5213540169847479	0.3479800483658932
0.8636643144309979	0.8686268807359898	0.7028313235611301
0.3037259173108369	0.4627781272898171	0.5336708581203818
0.9715299610007355	0.7931400338184159	0.3648368842873182
0.6334762247203907	0.1353598305472552	0.7022103465104411
0.7837398169492652	0.7261926538450256	0.5600893242916141
0.4401841248760018	0.0544842611422887	0.3882692226340075
0.1113696781072171	0.3807913860991795	0.7279286622530099
0.6903491548006631	0.2722831813357851	0.3788096081359659
0.3607976691470279	0.6123349189525383	0.7032820691786272
0.0300924583888383	0.9416876911392377	0.5433432278601668
0.3076164112050121	0.2313207091143280	0.5306263079914191
0.9780250157937680	0.5715398638494633	0.3457279034040976
0.6369862146477085	0.9002883573447645	0.6992871912226143
0.0360085796801380	0.7403089424703388	0.5348893388023467
0.7065317951818718	0.0771229537387686	0.3634644753941915
0.3664296181889669	0.3989962741767275	0.6996958509578824
0.7757495941258572	0.9578857580446679	0.5580747695850961
0.4438295384514024	0.2834191236943684	0.3883497803530552
0.1174336927313074	0.6275328557861385	0.7294449573634767
0.1403736588245707	0.1450076654339884	0.3313724770130610
0.8122749013300884	0.4809684260018535	0.6744951514993851
0.5988800204496594	0.6229766441781656	0.3236800581317885
0.2563170722410315	0.9545638436395422	0.6526868407163523
0.9246704834714713	0.2894254543970614	0.4947271152539113
0.4721248201091849	0.8102986920218856	0.5136611556717811
0.3546223044665652	0.8938965947558004	0.3313763114245268
0.0188625655394919	0.2299784830446653	0.6737924569814377

0.8761870377597626	0.8745599508701479	0.3223401539508999
0.5464103491150574	0.2029549574496720	0.6525851923506655
0.2084023514118555	0.5332491131568500	0.4928402435605914
0.6891643749277373	0.5585534708128588	0.5141301402644705
0.6054388539673833	0.3593519796457893	0.3324715005143156
0.2650749584581135	0.6849209940572824	0.6731440146476549
0.6250110964331889	0.9006101512575423	0.3212546342791971
0.2991115772154375	0.2435260556979653	0.6525942560110835
0.9650458575046968	0.5740163402260720	0.4948765416853733
0.9415731288964374	0.0294838114611588	0.5118133883958020
0.9299427180305598	0.7884807101387296	0.4875694441730476
0.4745580654242045	0.3099304043320495	0.5041614381473193
0.1451176885729257	0.6451807397401202	0.3472466008562040
0.8054329820869983	0.9771873711908251	0.6771646639835387
0.5882027166062367	0.1181938937787002	0.3248618552431730
0.2584799862781791	0.4504378549763116	0.6615294209164816
0.7111748153721810	0.0406233553677930	0.4864086434970241
0.1909320161679608	0.0640926036527548	0.5032384248635224
0.8545042495923043	0.3989274905320703	0.3468232361700120
0.5134141251202297	0.7401734756437508	0.7003696253342507
0.3817034210734748	0.3694824846076159	0.3255866499290495
0.0453077719373615	0.7048091947114571	0.6659950588434614
0.4599413603090094	0.5725283615411844	0.4907947371148537
0.4353463881211321	0.0251843713790363	0.5043221648785905
0.0998789448633310	0.3539285277867044	0.3467280207727815
0.7769494704359335	0.6988082165909757	0.6800735131297158
0.1307337140519224	0.9110280569165273	0.3248705535285641
0.7952441400648244	0.2405852726972803	0.6669437600683105
0.6998425936867978	0.2998919878457318	0.4993974626373380
0.6982860230155253	0.7990597995914868	0.5035189708183788
0.1996581654606146	0.2980837461821982	0.4984015557216138
0.2006204416865429	0.7995672646668373	0.4996342767945645
0.8704508309877059	0.1274974072881857	0.3342276510971289
0.5286596211030443	0.4712408827420635	0.6661916985721683
0.3727241756950354	0.6417644674996635	0.3361302731038766
0.0299011061028367	0.9574837838736349	0.6646854685057253
0.3667262203507685	0.1327893112780557	0.3134710619726214
0.0326513854972121	0.4651513492875424	0.6848153974066095
0.8574773299556557	0.6290666922427329	0.3355859612370687
0.5453852136462554	0.9769163874977153	0.6653228378992211
0.5441758668487972	0.7176027700295698	0.7958382294338017
0.5594067737626366	0.7084219694829966	0.8577468251437683
0.6112803002180580	0.6323196505007274	0.7077950152770361

The perfect Pt₇-CO* _P surface

O In Pt In O C

1.0000000000000000
14.4443000000000001 0.0000000000000000 0.0000000000000000
-7.2221499999999965 12.5091307398835685 0.0000000000000000
0.00000000000000011 0.00000000000000019 17.985499999999983

O In Pt In O C
71 27 1 20 2 1

Direct

0.8407251048125473 0.6134546582819006 0.4586731581123585
0.5159039972854985 0.9522710468945849 0.2904255730004789
0.1701250644375648 0.2765756064840109 0.6185425135945377
0.7925318248983885 0.9606514450681778 0.2989990731623327
0.4713917594164043 0.2956383964733323 0.6510408156971662
0.1329120561257003 0.6257705366917903 0.4699417582297448
0.3004064471532830 0.7306790546596225 0.3008347128070928
0.9801307288181889 0.0708925144112422 0.6358105165358436
0.6401501359457966 0.4070218602792477 0.4688912634877175
0.5295148808246649 0.2098557896327478 0.2711022629482744
0.1791773910158737 0.5356331962464075 0.6085881627383033
0.8572897362875960 0.8822075453895096 0.4425230927112930
0.8872909160633710 0.1292721595821842 0.4567454644707037
0.5481275438949936 0.4639365020846407 0.2926159667511234
0.2242220534463256 0.7909338424687806 0.6199033653491951
0.5388162931840341 0.7319512586944649 0.2997175046471321
0.2078104904252930 0.0758160869195095 0.6598221354243395
0.8747661390365034 0.4070916596223087 0.4699733049168671
0.7674458965895630 0.4683958088471474 0.3010959879016046
0.4362845298794621 0.8081575093939886 0.6540578361349734
0.0943835953082732 0.1322801291509473 0.4624942025297794
0.2913728044200973 0.2193271589773692 0.2696482573196267
0.9580657934478668 0.5432542839952894 0.6122502500246215
0.6174447659442599 0.8725377894353210 0.4438412844840007
0.3738194363006994 0.6588528071684132 0.4593762538163969
0.0365612050887090 0.9829388911032817 0.2886139675719036
0.7097947741420830 0.3305978327990656 0.6220251868403993
0.7665572956918127 0.7065109596004147 0.3016393143416154
0.4254612066223815 0.0293744901681840 0.6545047925998113
0.0898817606778001 0.3628565420285903 0.4688090060730440
0.0303957005868388 0.1981501308367235 0.2988767173762463
0.6894125751516684 0.5267428689501226 0.6423220107580009
0.3659228884741364 0.8592431741828873 0.4680800965565547
0.2812703938099119 0.9701876041499955 0.2688864395036680
0.9555272863315537 0.3151387598704042 0.6121947569576023

0.6225557764592421	0.6470415144312804	0.4472180452866988
0.2265013452499096	0.3169611957756193	0.3776502252428380
0.8847667437257072	0.6484773344092557	0.7109316337606283
0.5578633028153789	0.9849325003308754	0.5465710524077075
0.2676722501487307	0.9745276102176452	0.5321902954914833
0.9273284684901275	0.3053429019893233	0.3446818084021628
0.7582626228295727	0.1942150245227440	0.5369718835280920
0.4226945516941930	0.5288699067914584	0.3668062211903222
0.1020174546367463	0.8654411299664868	0.7003247861529281
0.5399484546896259	0.7255926750527119	0.5708728387657571
0.2162008340646897	0.0585050961612691	0.3869202486952852
0.8711363301377619	0.3909205151781928	0.7316057835389820
0.1836384363808282	0.8102089401562691	0.3796234728572311
0.8535695361962091	0.1373997179548732	0.7112888108887027
0.5112324754798289	0.4725337363211927	0.5454333861201327
0.5265770324586182	0.1921047336691308	0.5318283367781081
0.1943966633315748	0.5219848864010715	0.3518927659917090
0.8657961636773471	0.8694624697636749	0.7045196615121554
0.3012263535147190	0.4603117337187254	0.5326263772507354
0.9714939162739131	0.7931909101306357	0.3651225183668330
0.6345619511802053	0.1368753882310222	0.7039526999982960
0.7833707566968848	0.7274469850934800	0.5606611164034149
0.4394911985915204	0.0544837194772345	0.3894087693287032
0.1118933515290259	0.3808392760166732	0.7285887053663074
0.6899518921528541	0.2728003823328938	0.3810334853592371
0.3666262391854240	0.6078827261531161	0.6883164437917345
0.0310130130747590	0.9420966116571806	0.5443708684641915
0.3060087419791155	0.2297001342384674	0.5309929965281702
0.9771306624689483	0.5715898483830103	0.3483860434552311
0.6423342646102976	0.8984213880350768	0.6945779012340301
0.0362248198608333	0.7404449475893677	0.5362279980542165
0.7053423565376187	0.0760639372847994	0.3665977598582721
0.3642201263955711	0.3969611322821557	0.7014930756191157
0.7776926516675228	0.9589124328740014	0.5584695009921903
0.4440610072202409	0.2838282046824727	0.3904440751104307
0.1202058620372667	0.6276994195542899	0.7294905159407641
0.1400722372745714	0.1447661526543302	0.3302528669431096
0.8109674658224697	0.4826133810419449	0.6770722699339349
0.5981417168486085	0.6239674857855936	0.3249638696093640
0.2579753413651341	0.9539800304641312	0.6539759023035056
0.9243660690228710	0.2895707766086097	0.4962798215958571
0.4718390366313032	0.8129427941411919	0.5131840377088031
0.3544123484025617	0.8943947990965020	0.3316181906194804
0.0187029796782497	0.2298056866354724	0.6751433079494253

0.8764734787249346	0.8752030456233167	0.3223912364649464
0.5463821298473838	0.2036173461088400	0.6534820483071841
0.2067199440755677	0.5318504959468440	0.4917974230261704
0.6881354152443900	0.5602167842774335	0.5162597945324924
0.6050997146479314	0.3594449771444724	0.3343388893934912
0.2659030536649869	0.6825537171598842	0.6709092492192260
0.6247851651690233	0.9008078844957419	0.3227044256874366
0.2984250438791821	0.2415054739151866	0.6531137656727655
0.9646926137411872	0.5742035353307264	0.4959503198776056
0.9429949827550649	0.0304743930926437	0.5121547554917441
0.9314146386399190	0.7893918852162962	0.4877425913356707
0.4742010268122894	0.3091815880626239	0.5069574989308196
0.1442790346378789	0.6457542328460281	0.3482079451943547
0.8105048640437839	0.9797331646599798	0.6776269242600096
0.5880901236865270	0.1185693454367025	0.3268251541141802
0.2546393188309844	0.4451552243274403	0.6588600876536661
0.7118883400474700	0.0417650035218373	0.4883417641819338
0.1909720124098447	0.0630230607296314	0.5022543772028554
0.8539860696392082	0.3987678474537983	0.3478875783301646
0.5213921831556935	0.7345163478776945	0.6837641165210712
0.3816645782493795	0.3689713393139947	0.3264607201157575
0.0457330225005997	0.7042975804487586	0.6669071592499642
0.4561970880976393	0.5689631475883598	0.4897139516578192
0.4354197876977468	0.0258856392416852	0.5055801166053557
0.0991405131328731	0.3536066928083621	0.3469676085998981
0.7759203383346489	0.7017875718914858	0.6803168663493219
0.1305558152511858	0.9106882230302663	0.3241297116370891
0.7959258542902402	0.2422440880299619	0.6685853182786544
0.7005352157060806	0.3013162377108605	0.5013209665926847
0.7018032499902495	0.8024929403080544	0.5038394013359393
0.1981055238214181	0.2957292370224718	0.4975862782164310
0.2003853939153868	0.7999862721296145	0.5001115810248623
0.8699643242243109	0.1277459990866511	0.3352720031906237
0.5242231974756615	0.4745487007379050	0.6661314547820159
0.3726564204603537	0.6425742433471049	0.3367895083541244
0.0323746937249012	0.9574854946191196	0.6658864922755610
0.3669144353939990	0.1328250520458003	0.3141710004083912
0.0320304824648495	0.4649765063372252	0.6857448902590055
0.8565854188001097	0.6289073424926076	0.3367706820632573
0.5491161139149132	0.9787374750508527	0.6671407683190266
0.6027064218119684	0.6479376825546482	0.6981644813394629
0.5065519167368945	0.7418175058760293	0.8510607479549808
0.5109536764065505	0.7397823341639596	0.7874603073962139

The perfect Pt₇-H₂*_P surface

O In Pt In H

1.000000000000000				
14.4442996979000000	0.0000000000000000	0.0000000000000000		
-7.2221498489000000	12.5091304781999995	0.0000000000000000		
0.0000000000000000	0.0000000000000000	17.9855003356999994		

O	In	Pt	In	H
72	27	1	20	2

Direct

0.8413482606868008	0.6133044076672224	0.4570038970375884
0.5157580678809153	0.9528179226010014	0.2887275136538529
0.1706364687639015	0.2790346168261129	0.6187003037231246
0.7934195411327850	0.9615950159495359	0.2971811473786678
0.4712062978882336	0.2945316473803574	0.6488825629758859
0.1326263316880782	0.6253687136803817	0.4690854504887395
0.3006219631921027	0.7315601149962287	0.2994688329112389
0.9784245103408313	0.0706852545156580	0.6347031862214482
0.6405193547482583	0.4064111821348409	0.4676116704669935
0.5292435643238994	0.2103457341024373	0.2702219406040616
0.1828568049448499	0.5388059587459721	0.6098290820481495
0.8584272204186663	0.8832767522720096	0.4403895245903516
0.8879010099753583	0.1305826680187924	0.4550140962975074
0.5479203331869265	0.4633615408350659	0.2905174134287530
0.2213538374487271	0.7903392208888955	0.6200960146621277
0.5390735026655059	0.7320832372644432	0.2974582625367920
0.2067653166073871	0.0761971326807122	0.6566013770961419
0.8750384308643674	0.4073116006818047	0.4686867161815215
0.7675576925713087	0.468862224915882	0.3002424939177359
0.4327163424909982	0.8018529624232150	0.6441488889805971
0.0948771484863101	0.1341312858201325	0.4628048718694622
0.2910925804150614	0.2194998921184180	0.2695480747681053
0.9577193070885361	0.5432122818438627	0.6111383262855573
0.6181073372423648	0.8745510394788654	0.4401528023341061
0.3724415069275983	0.6586256816523034	0.4566810868682249
0.0374225456727261	0.9839976047407522	0.2881360627108387
0.7089472165013246	0.3289988137688053	0.6209522565873673
0.7680752234394115	0.7072670768782851	0.2984555697484690
0.4238303319801514	0.0266004120285144	0.6525748073422886
0.0909933137340163	0.3653884703684724	0.4683771141662801
0.0314617760608979	0.1991125951179740	0.2985166869187799
0.6890987851341623	0.5256835521459561	0.6393565606677141
0.3650087712072208	0.8590300598224526	0.4663951702454873
0.2812469783091552	0.9708528494480914	0.2685910156737390
0.9552439004108669	0.3158013187165130	0.6113351152035349

0.6252133970993359	0.6453672896151443	0.4424810991721841
0.2271482090074974	0.3181305373546962	0.3778697719369583
0.8826261189621193	0.6487226432008023	0.7086718206262458
0.5579001606707140	0.9848749097619465	0.5441591890309811
0.2670132304724157	0.9743245637038582	0.5308078075564006
0.9283406049588536	0.3066617138160825	0.3425307797437990
0.5988388357615826	0.6453828981891214	0.6998365799377998
0.7585965485286910	0.1943035275907528	0.5349815054283804
0.4229548680317053	0.5294183476946185	0.3643010133439623
0.1002600196802454	0.8663686889965584	0.6993535136460726
0.5452662394209288	0.7240278453042861	0.5600809669418271
0.2160676232305852	0.0589537599263426	0.3870747045093385
0.8697176344779191	0.3907318273285715	0.7302793254617973
0.1831728800895021	0.8098634858317261	0.3788085226286408
0.8520416542667734	0.1366126436127218	0.7093002878852761
0.5117535744694383	0.4728982317470539	0.5435058248748909
0.5262381452127589	0.1913170473474687	0.5302535072631929
0.1944070855907941	0.5224868569087544	0.3487243278914429
0.8631129232381296	0.8687729855285455	0.7019512235234640
0.3037498221208387	0.4633912426892535	0.5333963759570104
0.9716310050670461	0.7935179346021658	0.3639564961033080
0.6325007903013424	0.1330377364877869	0.7010500085172037
0.7830664173848838	0.7271999567373485	0.5585718548163542
0.4399518429269944	0.0548236800143512	0.3883913209701885
0.1098363361657843	0.3804685127824975	0.7285161244334825
0.6903688912408522	0.2730871515992550	0.3796019232601328
0.3669012211583551	0.6100262412459009	0.7035063203799182
0.0301387004961966	0.9422036904259278	0.5429742181822975
0.3061724963629630	0.2310219070994882	0.5299160433949290
0.9776112301983713	0.5719141544856590	0.3464731361030851
0.6364477217216264	0.8914835148551763	0.6930912513125606
0.0358333575363237	0.7404713993692885	0.5348942692163647
0.7064038876333526	0.0776122490404346	0.3636756247194163
0.3649327541552903	0.3970076243846504	0.7004079592629474
0.7772640656056478	0.9590967321661358	0.5557945003675959
0.4443777654461253	0.2844973224417940	0.3899737070726001
0.1176738481571345	0.6276802462438631	0.7294877203783752
0.1404255984026501	0.1455255173786670	0.3308413093517500
0.8098565763378200	0.4825308873786305	0.6753120018228372
0.5990078635699629	0.6240237229797007	0.3216698587484830
0.2563183970553341	0.9536120101838512	0.6525457363105893
0.9249024961309277	0.2902425644659834	0.4955331704847934
0.4717273399275682	0.8125446695805160	0.5108368814036320
0.3544410847944618	0.8946478183860387	0.3310203854972840

0.0177839636152101	0.2296691680704802	0.6741249853715512
0.8770351629858205	0.8757245324251604	0.3203751510019582
0.5450854216874804	0.2009613698448005	0.6519044469313562
0.2083656583669173	0.5338111297421606	0.4930053157670416
0.6884604828595816	0.5601331865860039	0.5142429951670684
0.6052540422625261	0.3598184947420015	0.3337252025596116
0.2661398033588009	0.6843445409569227	0.6739857007363983
0.6251546798433588	0.9015202091443013	0.3199456561787553
0.2984137557398570	0.2423857942615117	0.6518158487111535
0.9646054906688141	0.5742652877245479	0.4949652490386299
0.9426813675404982	0.0313195920055561	0.5111754296616581
0.9310465605541617	0.7893850531316577	0.4866614342744763
0.4746765018288030	0.3094861282910280	0.5068228193043939
0.1446961564686954	0.6457500029112258	0.3472917110045871
0.8048867873909281	0.9772021770825648	0.6758276309596698
0.5881484192937928	0.1190059162491872	0.3252443428156713
0.2561761995692857	0.4486025247875469	0.6623458604504979
0.7117031564963908	0.0419490291711851	0.4859959794218715
0.1907362014854617	0.0639777927256965	0.5025297259216325
0.8543114932472814	0.3992695917360882	0.3467742588324689
0.5150923401314230	0.7277477824664774	0.6768220573583512
0.3818693158193587	0.3692842973763747	0.3257442077197788
0.0441646391421091	0.7046565412821695	0.6660354347853596
0.4579387027781815	0.5698803324274395	0.4866858527602118
0.4349332461478966	0.0250853110147922	0.5045781496256717
0.0999433666702789	0.3547415427199959	0.3464852117093455
0.7711206657129775	0.7006184478554787	0.6789692624599838
0.1308555663214074	0.9112942104042295	0.3239880409538655
0.7944690193039610	0.2413115543115379	0.6675711652627955
0.7003246267922774	0.3006708115174072	0.5000894802077994
0.7026805291683075	0.8025535166284411	0.4993951768555014
0.1992993376272643	0.2983514565016349	0.4980314004246187
0.2001152686998225	0.7996605032897663	0.4996113198809923
0.8706799697918136	0.1289515558064358	0.3336078788183242
0.5247334818966325	0.4768413122341233	0.6647619839773404
0.3724866309087526	0.6427470604246155	0.3347480971845429
0.0295678951145508	0.9569230887687202	0.6643955621783200
0.3669948526055709	0.1333062039273847	0.3140390262924614
0.0313091644792813	0.4653361522407641	0.6851842899066831
0.8573034923781423	0.6294990634135568	0.3353836609117078
0.5471749379372811	0.9729949452148979	0.6651182218620401
0.6164215754840910	0.6489065162892702	0.8959419999897931
0.5923400658415785	0.6510953704483031	0.8602773437074392

The perfect Pt₇-[TS-2H]* surface

O	In	Pt	In	H
1.000000000000000				
14.4442996979000000		0.0000000000000000		0.0000000000000000
-7.2221498489000000		12.5091304781999995		0.0000000000000000
0.0000000000000000		0.0000000000000000		17.9855003356999994

O	In	Pt	In	H
72	27	1	20	2

Direct

0.8410252755138586	0.6134611821945457	0.4580996774027223
0.5161180224924058	0.9530359767679658	0.2893421400521849
0.1688239419680837	0.2784672842431062	0.6177126675981029
0.7934449897175959	0.9617232281093692	0.2978916150051015
0.4684115580428048	0.2898198542037762	0.6537542927082510
0.1329968199642410	0.6257248861329631	0.4694996911823974
0.3013241687817336	0.7315613709935824	0.3005409620685068
0.9786328916547359	0.0712247426418985	0.6348924239001299
0.6402021082365982	0.4067570807045540	0.4677046699284409
0.5295785662470902	0.2104704483842172	0.2701916876095171
0.1827490166293195	0.5390982645725170	0.6098507044621116
0.8577833845625207	0.8830174354960921	0.4412218430854771
0.8879393561572763	0.1308226478649437	0.4558201728703044
0.5479926857801842	0.4636448874716636	0.2907614828716716
0.2218941232731334	0.7904229469966262	0.6204249535203550
0.5393012944593932	0.7319665005998557	0.2990396389859785
0.2058895474092713	0.0753412148423723	0.6559365152260574
0.8748081897148945	0.4076918428577689	0.4693399501356294
0.7679759246266905	0.4692814072599104	0.3005688083263493
0.4335734476728783	0.8047555344225066	0.6446762844787554
0.0947174062371299	0.1335551790676913	0.4626051088033210
0.2910422296970085	0.2196518783989532	0.2696515422272401
0.9586399098278718	0.5439248431002889	0.6116687267891309
0.6181863946730055	0.8746813697581564	0.4413018021822113
0.3727214701467791	0.6584624481880789	0.4582209363471497
0.0372749440295612	0.9839123035015798	0.2887627637707308
0.7088544123836565	0.3300670219586398	0.6216113307042028
0.7675282306538850	0.7071918485615902	0.3000184469166937
0.4241244550575630	0.0271363859773920	0.6537189680577973
0.0907496841818655	0.3655232070122422	0.4684940515750366
0.0312466020889327	0.1991577447338719	0.2989720458895160
0.6911056005960513	0.5282030262596366	0.6402655231285900
0.3655955390516109	0.8594831269573545	0.4667004819064314
0.2814343022967779	0.9707337826073172	0.2689440710430242
0.9553220470834527	0.3166472582748020	0.6117392466491064

0.6247715296194976	0.6442093453046098	0.4446863371280138
0.2269945393457173	0.3180254591869365	0.3779010002109882
0.8847780081389343	0.6497110491220023	0.7097142098291788
0.5580884482025315	0.9858537231052922	0.5445755373490792
0.2675472507611578	0.9745298191561169	0.5312529578964547
0.9282402979254526	0.3068159202508121	0.3432328003808843
0.6040027426596171	0.6561729738201330	0.7048092625598521
0.7585017937153439	0.1949011870652657	0.5355840207866888
0.4234199067349403	0.5291358434098572	0.3663610934883626
0.1010192665873407	0.8667187327959458	0.6998698307707096
0.5449400183383016	0.7233341429154958	0.5617231632607225
0.2165425762218543	0.0591325360452813	0.3873151145870089
0.8706499515597373	0.3917578359509798	0.7308539916049137
0.1834766636559889	0.8101531112244658	0.3792022390696577
0.8530994909663340	0.1380442053855472	0.7101742285594151
0.5118548189784538	0.4710260803115458	0.5476710121075005
0.5256202270940925	0.1921893288538619	0.5311970090784324
0.1946591426142642	0.5225587251434733	0.3492639500378000
0.8650832567154709	0.8707053971136444	0.7031052824903323
0.3031511928864373	0.4625628987748514	0.5335400835649917
0.9716095211356529	0.7936668669745200	0.3646779778840861
0.6337152244397045	0.1344039176801484	0.7021044980201210
0.7835018051626748	0.7280971156949377	0.5599113729602930
0.4403082602945173	0.0554851049079657	0.3886205610690264
0.1111586117580280	0.3813926865634769	0.7285219690175363
0.6902723836558048	0.2734215824119636	0.3800644750621556
0.3682571978716711	0.6119591920435158	0.7022923780039532
0.0300713242150542	0.9422580488572311	0.5433078344388168
0.3063526959463042	0.2309052702320674	0.5302576769438694
0.9777693436704998	0.5722444695653048	0.3476504241509864
0.6379023727309545	0.8954655375453452	0.6952191231523749
0.0363597562440015	0.7410050203901932	0.5352383139016740
0.7064921974604060	0.0778060650253066	0.3644589429031962
0.3621074874526278	0.3945135272677862	0.6993459439166525
0.7770487738611314	0.9593176853406176	0.5568670065595004
0.4443540774590894	0.2844886141671008	0.3894532177222093
0.1189883658140980	0.6282985779529424	0.7301364443848820
0.1404001220085923	0.1455180312185765	0.3311446755035691
0.8110620435662459	0.4835472914008553	0.6759245736417028
0.5987132757492621	0.6236503175448943	0.3236393362936242
0.2567932110144087	0.9535922324697234	0.6529364178571545
0.9249033447194118	0.2907313903872081	0.4960844232470762
0.4718063293825511	0.8125981475255429	0.5120285751897568
0.3547512006508301	0.8947690307546050	0.3316773615392948

0.0182431511982751	0.2306387460945942	0.6742843461370471
0.8769175006210891	0.8757612906926763	0.3213098482802831
0.5456009103043999	0.2007173829442016	0.6528895584522284
0.2083889735939051	0.5338006753912209	0.4933143878270425
0.6881007952120435	0.5597323138930547	0.5162991815876514
0.6055052733222596	0.3600698084475972	0.3334355094318878
0.2672001699457824	0.6845698603550912	0.6742671290834928
0.6252252735655446	0.9015609494098418	0.3209537473947522
0.2953049997619528	0.2410517457032556	0.6519172588301848
0.9649936041438373	0.5748033464383265	0.4954946565028279
0.9426356198342513	0.0313730817821968	0.5118294361069649
0.9309020579364660	0.7893985721201079	0.4873699742732544
0.4741399660106501	0.3096882749623449	0.5057859261747467
0.1449923064557007	0.6459808786467813	0.3478360214890834
0.8061851268582718	0.9787549739228154	0.6767007243926768
0.5884402225523603	0.1192902282000668	0.3255920525429714
0.2575281399776952	0.4497461704325024	0.6618206408791057
0.7118608853912755	0.0423804811192696	0.4868171310603798
0.1907183261185683	0.0636365905344010	0.5027839624785629
0.8544133624389529	0.3996010232357168	0.3474260607454023
0.5179823236790480	0.7344569419181081	0.6796961631455379
0.3817762887790571	0.3696364842688581	0.3258264599290714
0.0457573793787533	0.7051934106139992	0.6666551701982971
0.4583201361254466	0.5691747063812403	0.4899126804075356
0.4353281551499718	0.0257897328803736	0.5046897426561331
0.0998089056330869	0.3548543630604607	0.3467528534847044
0.7755771217723569	0.7030392807227078	0.6797747832427679
0.1309776180450444	0.9113662560290084	0.3244840840701321
0.7953538133982797	0.2425081141973782	0.6683020529980623
0.7001397472949753	0.3012507697745500	0.5007474430715365
0.7023011299210153	0.8025114798207826	0.5007880164045797
0.1985720369242335	0.2978323381908378	0.4979171023532830
0.2005659848131778	0.7998181846193020	0.5000556824376269
0.8707147899385038	0.1290422131285933	0.3344244875894727
0.5251693343760250	0.4632444364048597	0.6704201858069233
0.3729357251010897	0.6425496140156919	0.3364607092078749
0.0302649180451691	0.9575304283316864	0.6647408052306825
0.3670497558371260	0.1333421510100866	0.3137771941302778
0.0323941941704298	0.4660931818278876	0.6856852198790124
0.8570605850616032	0.6295738189957270	0.3364371496475945
0.5474740622581857	0.9750582689202643	0.6655928933862479
0.5814173004484905	0.5869428007708944	0.7585536158417411
0.5674791244154257	0.5217948838799636	0.7808290649973607

The perfect Pt₇-2H* surface

O In Pt In H

1.000000000000000				
14.4442996979000000	0.0000000000000000	0.0000000000000000		
-7.2221498489000000	12.5091304781999995	0.0000000000000000		
0.0000000000000000	0.0000000000000000	17.9855003356999994		

O	In	Pt	In	H
72	27	1	20	2

Direct

0.8408535854746683	0.6131251801609975	0.4577923347029988
0.5157860481135039	0.9522129285277220	0.2879794987944301
0.1656929515270074	0.2767340445005181	0.6157611048588789
0.7923519695154949	0.9605548547302726	0.2969346867754940
0.4646869816919426	0.2848550656521294	0.6453942776717553
0.1323013812983747	0.6247100249677706	0.4686113618987507
0.3015655146686406	0.7299576058151463	0.3004524863507783
0.9773067652372366	0.0697979969319068	0.6340570097753058
0.6388141175735077	0.4059054303360828	0.4678406090590984
0.5287602137514029	0.2103758423720728	0.2707291628000796
0.1825359453499124	0.5379199653540818	0.6089818874401322
0.8573364667328555	0.8827269101311509	0.4400221294016600
0.8867955590052474	0.1300387126518251	0.4549176344972437
0.5468597534171087	0.4620783108035559	0.2916982671965420
0.2215202511901118	0.7895790685857520	0.6196199922779124
0.5386109363367453	0.7302449145537225	0.2994111916141196
0.2053294635590034	0.0746790671107990	0.6554879171080934
0.8744815415727927	0.4072708740046217	0.4684760618445656
0.7662294562092290	0.4682018164611517	0.3011725705734743
0.4322080376958692	0.8053222791863450	0.6439417772981357
0.0928800428026007	0.1317959157766630	0.4605098269148398
0.2909090834199829	0.2189662697677107	0.2696983341291264
0.9592115988298858	0.5438667720606535	0.6111736689940201
0.6178525659087196	0.8742797736149087	0.4404082160420445
0.3723236480789487	0.6569153477040494	0.4589911361934170
0.0363395632113287	0.9824520209004931	0.2870285905399851
0.7079611894469848	0.3300482889741716	0.6212017950802317
0.7664229193718755	0.7059712528146290	0.3001333220171941
0.4234626389244852	0.0260577159963732	0.6535872944743619
0.0892902011615092	0.3644120382895962	0.4671688667142570
0.0297146005416566	0.1977094912508210	0.2974820248614202
0.6998646401063244	0.5344404489508318	0.6367672481659399
0.3652515246976922	0.8582495712393836	0.4661840877305221
0.2809562351800606	0.9698211836810110	0.2675099674953357
0.9546129655170139	0.3161279813143885	0.6109031048080126

0.6244276649000031	0.6426200607884353	0.4455504291605047
0.2249428054233502	0.3167905568162596	0.3764816919273172
0.8893564409428972	0.6493881663264072	0.7130369270931572
0.5576422839167968	0.9848245711590253	0.5439586307156048
0.2673633196293991	0.9739864700024784	0.5301891395545266
0.9270525576718580	0.3058459410806471	0.3413783215015891
0.6093438375485718	0.6653204052460445	0.7094419841396356
0.7579247629127821	0.1943247164410383	0.5352121719731611
0.4232344189036081	0.5276931014644881	0.3683212381061949
0.1008945598863173	0.8663820704296785	0.6987778516496062
0.5458529621597981	0.7235166059542147	0.5613140064816863
0.2151493231954631	0.0572096515058255	0.3858240366480465
0.8707623527479833	0.3909487551310273	0.7300649839511274
0.1832747234429633	0.8091091916024709	0.3779441328595885
0.8522282198629999	0.1371478908605716	0.7089682639367320
0.5139681226839321	0.4720741644875627	0.5535374345714265
0.5264498769748036	0.1901305008228509	0.5294533694107013
0.1942139267944994	0.5213661472648397	0.3491156489129823
0.8652791760092856	0.8699252675344368	0.7031734274395749
0.3016790818459465	0.4604094275049670	0.5327356335916938
0.9712482423234489	0.7928908548628435	0.3635255151992368
0.6333907689499373	0.1348884960484246	0.7019351785817782
0.7859041003243695	0.7312630117667765	0.5590631449686623
0.4390605556678689	0.0533128886376953	0.3872128260298815
0.1109345623566952	0.3805309460151804	0.7276375687630078
0.6898243584849616	0.2722955735880084	0.3798937094480801
0.3676718824608345	0.6128282391807008	0.7020178256913064
0.0300486319761758	0.9420839415962786	0.5423001450655041
0.3033117731224930	0.2297239771947946	0.5283168495138660
0.9773719362367406	0.5713234541639807	0.3456277352327910
0.6372007577757079	0.8977611975395685	0.6955149626670811
0.0364083865162908	0.7407597374399492	0.5342356268067212
0.7055098093803339	0.0768536673940062	0.3636576448328095
0.3598297161884055	0.3919805207958115	0.6977116280423903
0.7763640509270118	0.9586808028684884	0.5561281290644733
0.4428204608084602	0.2832311469226445	0.3917590932362783
0.1191171258262759	0.6269971852173102	0.7299466956145054
0.1390998114130118	0.1441693073171570	0.3297334171920200
0.8120840259920639	0.4834612845299848	0.6758257731991006
0.5977001084181585	0.6217888809962659	0.3247202866358508
0.2564930446380795	0.9533054010013023	0.6518087280578884
0.9239294838519901	0.2899605605013242	0.4953662688666690
0.4717563519629885	0.8115048733003705	0.5112522035498264
0.3541637144773658	0.8934131041712734	0.3299516186938926

0.0172018046091383	0.2299267059680283	0.6734067539870482
0.8760978689063521	0.8747950060490032	0.3202469494155149
0.5449748967572204	0.1991988833783699	0.6512468455771649
0.2076841983155057	0.5324562679863885	0.4923529595785194
0.6881148857108432	0.5591156155595323	0.5169296142051583
0.6040139911044778	0.3589676676780744	0.3356936971618625
0.2661469347497937	0.6831739487393286	0.6734271888782327
0.6242256300715346	0.9002265847701492	0.3201468962840630
0.2921480273226565	0.2401455940306930	0.6497866714963040
0.9645577226537246	0.5742449047264033	0.4951312773952808
0.9417442257291782	0.0304784986313548	0.5106393501245987
0.9312781741175314	0.7893987881475503	0.4860087255738631
0.4735475914752894	0.3097733887708171	0.5092335721644007
0.1445873993180286	0.6447830313113421	0.3469608367624135
0.8054950013933138	0.9778595619432716	0.6755925495711792
0.5877895077910515	0.1185829597017221	0.3248444766854910
0.2577984553043327	0.4488358905739973	0.6608640661316496
0.7111566782350013	0.0418433439673792	0.4860445833111525
0.1900743183240963	0.0628376655223353	0.5009975055711317
0.8535181662330787	0.3988098308012496	0.3466184236963689
0.5160691742061174	0.7382126307930679	0.6809096587567142
0.3810752728825732	0.3681806734350373	0.3273045273935291
0.0474663173097632	0.7048088351715862	0.6665117023462533
0.4588321877840595	0.5674381982533315	0.4929508294894994
0.4349255167348575	0.0245898734648552	0.5031643233818310
0.0982804848531158	0.3536264313000019	0.3453822582831119
0.7850080470269901	0.7038853828136132	0.6770729877648348
0.1303145256570944	0.9099313940927601	0.3227029235991409
0.7947602503215409	0.2421997075503895	0.6673057807179358
0.6995541847462858	0.3008041661325556	0.5002195773915431
0.7018790751050685	0.8020087017413886	0.4999510139186307
0.1963520585695194	0.2961751605591764	0.4963527158805695
0.2003266755513723	0.7990487563777404	0.4988788502095709
0.8694748344992567	0.1279653202516772	0.3333702372804994
0.5289818087810891	0.4547525159138050	0.6797823369906895
0.3727874734873184	0.6408158210240111	0.3375030016526351
0.0309604917421921	0.9580659899304627	0.6637415638079606
0.3663273239972138	0.1324401960392071	0.3138507592647168
0.0323968936218823	0.4650879801455159	0.6849866001848607
0.8563053031984588	0.6285411308635842	0.3361312716290548
0.5471765481298105	0.9761477206838980	0.6648023461797782
0.6003022195230228	0.6524833302942343	0.7626750756163054
0.5775355312964887	0.4670858309913568	0.7718046364879080

The perfect Pt₇-[TS-H₂O]* surface

O In Pt In H

1.000000000000000				
14.4442996979000000	0.0000000000000000	0.0000000000000000		
-7.2221498489000000	12.5091304781999995	0.0000000000000000		
0.0000000000000000	0.0000000000000000	17.9855003356999994		

O	In	Pt	In	H
72	27	1	20	2

Direct

0.8463519168660258	0.6118051256152116	0.4527200771844986
0.5177644117080421	0.9515591212291604	0.2874650011699060
0.1724513060599240	0.2802181282775221	0.6191199436185654
0.7942835247264457	0.9590366100606371	0.2984648394761821
0.4621185638064557	0.2827578388389052	0.6613892129057616
0.1330833072553906	0.6223533398373424	0.4670882834823836
0.3032735845181972	0.7307038346867497	0.2983441491519877
0.9767179322530394	0.0673975003572067	0.6365003297148545
0.6408952028923773	0.4041099051539336	0.4601456309389280
0.5297456181865614	0.2064855313100102	0.2665482041220030
0.1871105715035719	0.5410959349720096	0.6097022031752063
0.8556501457346879	0.8766968666525164	0.4425258130709012
0.8868941172777625	0.1268944381998168	0.4573434808428138
0.5475676234771407	0.4606397633773394	0.2847157968608564
0.2227215236921733	0.7901226927130603	0.6204105959622305
0.5404535220719120	0.7300372152321649	0.2961187677954724
0.2050824809354997	0.0743825178330009	0.6522856556957799
0.8753221518958165	0.4067805067368575	0.4667371611261140
0.7696013871076798	0.4671855906897093	0.2964576290380952
0.4332231363233965	0.8050290374229997	0.6415382968621457
0.0952367964475936	0.1321635522821835	0.4654289815712499
0.2902556223957714	0.2168994559063261	0.2668937489189085
0.9575583671484748	0.5395624255236520	0.6106901977154482
0.6195202996449126	0.8753655272643120	0.4404284339451928
0.3702535495696780	0.6551745647730193	0.4548833011777718
0.0380203619399484	0.9823119891935680	0.2889818198729616
0.7044131503321005	0.3414463917571398	0.6177608457410556
0.7713169555582553	0.7053334115228757	0.2948501369758495
0.4245995556413260	0.0285024614299732	0.6554926209323375
0.0950447581467572	0.3663378013143934	0.4679663234664429
0.0316144848637597	0.1971249273119128	0.2990284713391937
0.6805993211504393	0.5373476545336123	0.6890266343202682
0.3691525990170658	0.8562733754779213	0.4684142761651844
0.2821027695838477	0.9686488254986398	0.2677077316293544
0.9581343151538704	0.3153986105181277	0.6089343826564280

0.6293860819256915	0.6411109266106363	0.4355252096737938
0.2282731780088935	0.3149567571854340	0.3775238640908066
0.8940862608069231	0.6474933602455384	0.7083983778420946
0.5600239864102908	0.9854279998870794	0.5458158113067372
0.2693808676975858	0.9731701723331088	0.5302007521410350
0.9294662200253895	0.3039736473149995	0.3482421866159240
0.5684290788960515	0.6900393257552592	0.7936873800955152
0.7596351453372551	0.1965275657611971	0.5357326610491282
0.4250278871675865	0.5266500157194014	0.3636817182585000
0.1003705491734949	0.8656983039635260	0.6987178949489513
0.5468251980025277	0.7125882622380432	0.5526956849321458
0.2179088760472513	0.0587136648842296	0.3871138170820737
0.8697938992402915	0.3863258073886730	0.7289393519661362
0.1859716309348502	0.8086352034931754	0.3783943461552176
0.8539177072371957	0.1374664710353346	0.7084403613614255
0.5238312157246526	0.4700151467783266	0.5458972849870996
0.5261417695585401	0.1920035330423222	0.5296072566671954
0.1956187259542426	0.5202030184320433	0.3427758207403987
0.8594623069873292	0.8660178404136563	0.7036724106179917
0.3087342905987774	0.4622445807939070	0.5344992404427928
0.9737041747140393	0.7925297527933135	0.3634151341952546
0.6367582559240047	0.1403509165547003	0.6991763539977216
0.7801535518145887	0.7121799154330938	0.5597549122120565
0.4415167996016767	0.0533971543636961	0.3873785094066668
0.1117014234673693	0.3807008275892865	0.7278420869276497
0.6913913905522805	0.2718414584939022	0.3769248698869712
0.3564053010085275	0.6147085300848019	0.7199172522183099
0.0285093376255102	0.9381901473617528	0.5432212653215825
0.3100228136475289	0.2322057289636175	0.5299488710310799
0.9801751594976134	0.5699814233106969	0.3396668326382720
0.6343269438086857	0.9058564594705343	0.7111927219349178
0.0384249687279292	0.7383803460640016	0.5342229507274169
0.7077877567089119	0.0768455356700992	0.3642269877486178
0.3668385546016154	0.4000551738830027	0.7008142310798067
0.7742045164755810	0.9538828273353488	0.5584922411589499
0.4452710491311238	0.2824467282175884	0.3838038447351858
0.1155059402774367	0.6251913088647953	0.7296663000015932
0.1412509843857399	0.1436658320580479	0.3306024118379259
0.8114928107771435	0.4812302415602153	0.6801424050392656
0.6005342861401133	0.6215829091524825	0.3164241702691350
0.2573109946711849	0.9535793274836823	0.6519917885384361
0.9269113928683531	0.2902014784833027	0.4925188291914973
0.4744172092158752	0.8057782089198080	0.5155682296352980
0.3565985027773761	0.8928524662783306	0.3303487051726570

0.0196599963651733	0.2295787404450348	0.6734837111941894
0.8774534043458503	0.8730074384791483	0.3208878972009446
0.5462936170481859	0.2022228255153649	0.6512888184181526
0.2120477994006730	0.5337697936479227	0.4936475744715237
0.6902920470858899	0.5591058809201922	0.5000299929256622
0.6067208202422776	0.3576626719824202	0.3264652698330973
0.2661517924020523	0.6853013652573900	0.6773699294554748
0.6256573110539843	0.8993870009979271	0.3209521393002609
0.2938780921878078	0.2405163745294718	0.6519254888523969
0.9668872599857903	0.5717785389678733	0.4953442236820135
0.9413123985510795	0.0274100036182142	0.5128694339015034
0.9333283700423660	0.7865575998549015	0.4853316946623329
0.4744103497838876	0.3061896949150343	0.4985497215210238
0.1469011293709630	0.6436744002564875	0.3450310077854580
0.7995298517275192	0.9760947119936054	0.6772369210309184
0.5896965270188471	0.1171651314772120	0.3239251198874750
0.2615643218033332	0.4559892950889077	0.6643719052986918
0.7112214447726352	0.0406080687453626	0.4870032439957726
0.1917370760660883	0.0624939755078876	0.5031113956981860
0.8560004462410986	0.3980641112744123	0.3447484882235181
0.5025469998898864	0.7508861973415044	0.7115844217571727
0.3815799799824131	0.3678544574043550	0.3218458991838002
0.0504732138392605	0.7044488357255748	0.6629987642172365
0.4618599538228988	0.5694052790615765	0.4868237800455569
0.4374813935070906	0.0229606990367749	0.5032891050971229
0.1022910041458640	0.3535740056684198	0.3457902169248634
0.7920137740225079	0.7039248219273722	0.6789376759940663
0.1328510142448966	0.9103697695699867	0.3243041970883996
0.7972391511433627	0.2407909956564026	0.6643505846150849
0.7016785054363212	0.3015079260564412	0.4979154434224936
0.6988936273959542	0.7968933570086695	0.4992713128792538
0.2010610867536709	0.2980510667615646	0.4979984052122887
0.2039213144131743	0.7977489365475373	0.4985444544080866
0.8713443568101451	0.1258929596860494	0.3352447558497453
0.5214312894471094	0.4511608283107104	0.6655231131305366
0.3736392230156634	0.6401625380135331	0.3341734994137662
0.0307458031346952	0.9571546502667875	0.6643355398283812
0.3674375907004216	0.1310743001384637	0.3107928724079447
0.0328486582550469	0.4642661128778069	0.6838234981600065
0.8624069328100434	0.6287673793974479	0.3304442673083461
0.5459791436129200	0.9777958574519171	0.6666781331473092
0.5048261225245930	0.6361294771661724	0.8194725820339300
0.6074476296902369	0.7475372182637410	0.8291316554052965

The perfect Pt₇-H₂O* surface

O In Pt In H

1.000000000000000				
14.4442996979000000	0.0000000000000000	0.0000000000000000		
-7.2221498489000000	12.5091304781999995	0.0000000000000000		
0.0000000000000000	0.0000000000000000	17.9855003356999994		

O	In	Pt	In	H
72	27	1	20	2

Direct

0.8463519168660258	0.6118051256152116	0.4527200771844986
0.5177644117080421	0.9515591212291604	0.2874650011699060
0.1724513060599240	0.2802181282775221	0.6191199436185654
0.7942835247264457	0.9590366100606371	0.2984648394761821
0.4621185638064557	0.2827578388389052	0.6613892129057616
0.1330833072553906	0.6223533398373424	0.4670882834823836
0.3032735845181972	0.7307038346867497	0.2983441491519877
0.9767179322530394	0.0673975003572067	0.6365003297148545
0.6408952028923773	0.4041099051539336	0.4601456309389280
0.5297456181865614	0.2064855313100102	0.2665482041220030
0.1871105715035719	0.5410959349720096	0.6097022031752063
0.8556501457346879	0.8766968666525164	0.4425258130709012
0.8868941172777625	0.1268944381998168	0.4573434808428138
0.5475676234771407	0.4606397633773394	0.2847157968608564
0.2227215236921733	0.7901226927130603	0.6204105959622305
0.5404535220719120	0.7300372152321649	0.2961187677954724
0.2050824809354997	0.0743825178330009	0.6522856556957799
0.8753221518958165	0.4067805067368575	0.4667371611261140
0.7696013871076798	0.4671855906897093	0.2964576290380952
0.4332231363233965	0.8050290374229997	0.6415382968621457
0.0952367964475936	0.1321635522821835	0.4654289815712499
0.2902556223957714	0.2168994559063261	0.2668937489189085
0.9575583671484748	0.5395624255236520	0.6106901977154482
0.6195202996449126	0.8753655272643120	0.4404284339451928
0.3702535495696780	0.6551745647730193	0.4548833011777718
0.0380203619399484	0.9823119891935680	0.2889818198729616
0.7044131503321005	0.3414463917571398	0.6177608457410556
0.7713169555582553	0.7053334115228757	0.2948501369758495
0.4245995556413260	0.0285024614299732	0.6554926209323375
0.0950447581467572	0.3663378013143934	0.4679663234664429
0.0316144848637597	0.1971249273119128	0.2990284713391937
0.6805993211504393	0.5373476545336123	0.6890266343202682
0.3691525990170658	0.8562733754779213	0.4684142761651844
0.2821027695838477	0.9686488254986398	0.2677077316293544
0.9581343151538704	0.3153986105181277	0.6089343826564280

0.6293860819256915	0.6411109266106363	0.4355252096737938
0.2282731780088935	0.3149567571854340	0.3775238640908066
0.8940862608069231	0.6474933602455384	0.7083983778420946
0.5600239864102908	0.9854279998870794	0.5458158113067372
0.2693808676975858	0.9731701723331088	0.5302007521410350
0.9294662200253895	0.3039736473149995	0.3482421866159240
0.5684290788960515	0.6900393257552592	0.7936873800955152
0.7596351453372551	0.1965275657611971	0.5357326610491282
0.4250278871675865	0.5266500157194014	0.3636817182585000
0.1003705491734949	0.8656983039635260	0.6987178949489513
0.5468251980025277	0.7125882622380432	0.5526956849321458
0.2179088760472513	0.0587136648842296	0.3871138170820737
0.8697938992402915	0.3863258073886730	0.7289393519661362
0.1859716309348502	0.8086352034931754	0.3783943461552176
0.8539177072371957	0.1374664710353346	0.7084403613614255
0.5238312157246526	0.4700151467783266	0.5458972849870996
0.5261417695585401	0.1920035330423222	0.5296072566671954
0.1956187259542426	0.5202030184320433	0.3427758207403987
0.8594623069873292	0.8660178404136563	0.7036724106179917
0.3087342905987774	0.4622445807939070	0.5344992404427928
0.9737041747140393	0.7925297527933135	0.3634151341952546
0.6367582559240047	0.1403509165547003	0.6991763539977216
0.7801535518145887	0.7121799154330938	0.5597549122120565
0.4415167996016767	0.0533971543636961	0.3873785094066668
0.1117014234673693	0.3807008275892865	0.7278420869276497
0.6913913905522805	0.2718414584939022	0.3769248698869712
0.3564053010085275	0.6147085300848019	0.7199172522183099
0.0285093376255102	0.9381901473617528	0.5432212653215825
0.3100228136475289	0.2322057289636175	0.5299488710310799
0.9801751594976134	0.5699814233106969	0.3396668326382720
0.6343269438086857	0.9058564594705343	0.7111927219349178
0.0384249687279292	0.7383803460640016	0.5342229507274169
0.7077877567089119	0.0768455356700992	0.3642269877486178
0.3668385546016154	0.4000551738830027	0.7008142310798067
0.7742045164755810	0.9538828273353488	0.5584922411589499
0.4452710491311238	0.2824467282175884	0.3838038447351858
0.1155059402774367	0.6251913088647953	0.7296663000015932
0.1412509843857399	0.1436658320580479	0.3306024118379259
0.8114928107771435	0.4812302415602153	0.6801424050392656
0.6005342861401133	0.6215829091524825	0.3164241702691350
0.2573109946711849	0.9535793274836823	0.6519917885384361
0.9269113928683531	0.2902014784833027	0.4925188291914973
0.4744172092158752	0.8057782089198080	0.5155682296352980
0.3565985027773761	0.8928524662783306	0.3303487051726570

0.0196599963651733	0.2295787404450348	0.6734837111941894
0.8774534043458503	0.8730074384791483	0.3208878972009446
0.5462936170481859	0.2022228255153649	0.6512888184181526
0.2120477994006730	0.5337697936479227	0.4936475744715237
0.6902920470858899	0.5591058809201922	0.5000299929256622
0.6067208202422776	0.3576626719824202	0.3264652698330973
0.2661517924020523	0.6853013652573900	0.6773699294554748
0.6256573110539843	0.8993870009979271	0.3209521393002609
0.2938780921878078	0.2405163745294718	0.6519254888523969
0.9668872599857903	0.5717785389678733	0.4953442236820135
0.9413123985510795	0.0274100036182142	0.5128694339015034
0.9333283700423660	0.7865575998549015	0.4853316946623329
0.4744103497838876	0.3061896949150343	0.4985497215210238
0.1469011293709630	0.6436744002564875	0.3450310077854580
0.7995298517275192	0.9760947119936054	0.6772369210309184
0.5896965270188471	0.1171651314772120	0.3239251198874750
0.2615643218033332	0.4559892950889077	0.6643719052986918
0.7112214447726352	0.0406080687453626	0.4870032439957726
0.1917370760660883	0.0624939755078876	0.5031113956981860
0.8560004462410986	0.3980641112744123	0.3447484882235181
0.5025469998898864	0.7508861973415044	0.7115844217571727
0.3815799799824131	0.3678544574043550	0.3218458991838002
0.0504732138392605	0.7044488357255748	0.6629987642172365
0.4618599538228988	0.5694052790615765	0.4868237800455569
0.4374813935070906	0.0229606990367749	0.5032891050971229
0.1022910041458640	0.3535740056684198	0.3457902169248634
0.7920137740225079	0.7039248219273722	0.6789376759940663
0.1328510142448966	0.9103697695699867	0.3243041970883996
0.7972391511433627	0.2407909956564026	0.6643505846150849
0.7016785054363212	0.3015079260564412	0.4979154434224936
0.6988936273959542	0.7968933570086695	0.4992713128792538
0.2010610867536709	0.2980510667615646	0.4979984052122887
0.2039213144131743	0.7977489365475373	0.4985444544080866
0.8713443568101451	0.1258929596860494	0.3352447558497453
0.5214312894471094	0.4511608283107104	0.6655231131305366
0.3736392230156634	0.6401625380135331	0.3341734994137662
0.0307458031346952	0.9571546502667875	0.6643355398283812
0.3674375907004216	0.1310743001384637	0.3107928724079447
0.0328486582550469	0.4642661128778069	0.6838234981600065
0.8624069328100434	0.6287673793974479	0.3304442673083461
0.5459791436129200	0.9777958574519171	0.6666781331473092
0.5048261225245930	0.6361294771661724	0.8194725820339300
0.6074476296902369	0.7475372182637410	0.8291316554052965

The perfect Cu₇ doped c-In₂O₃(111) surface

O In Cu In

1.000000000000000			
14.4442996979000000	0.0000000000000000	0.0000000000000000	
-7.2221498489000000	12.5091304781999995	0.0000000000000000	
0.0000000000000000	0.0000000000000000	17.9855003356999994	

O	In	Cu	In
72	27	1	20

Direct

0.8421793646059229	0.6129181692896872	0.4578895833828244
0.5160360171215115	0.9531378514408553	0.2884653295662430
0.1717280317138216	0.2802236796346986	0.6198623117496618
0.7937723747134544	0.9616072152029207	0.2972691019512579
0.4705819539734584	0.2943519718521002	0.6481037770354345
0.1320777615617709	0.6240816018158429	0.4692688480324100
0.3007549573091083	0.7320369442655703	0.2992285954632518
0.9776041821064732	0.0697811279647835	0.6358894285260071
0.6406843529467752	0.4060408972452060	0.4692740724722327
0.5284787656487069	0.2096500520155341	0.2710154586477116
0.1834951814911298	0.5395573615618589	0.6111250177773733
0.8568919051211425	0.8821075019687710	0.4413739114045383
0.8872957039310743	0.1292649700041084	0.4561231141812545
0.5472207832826208	0.4622086495374259	0.2893671378748863
0.2240169777620167	0.7903914220902254	0.6214088281230329
0.5393236798949443	0.7318628019315374	0.2972597863530880
0.2067121068447162	0.0763751004151936	0.6555174265617189
0.8748968771204143	0.4076362630273208	0.4695020268227721
0.7673241956374562	0.4690221796696550	0.3011950925457720
0.4375117228480697	0.8012258978877708	0.6465081512873280
0.0942765502927678	0.1335992228104704	0.4648628135640299
0.2906418078928726	0.2187038391053180	0.2712711132571028
0.9582544527384209	0.5430526610946957	0.6120615673365303
0.6195138242921737	0.8773702058084299	0.4391045197466951
0.3676427021274145	0.6568853184103665	0.4545784536435197
0.0375577837755225	0.9839293786890642	0.2899408103427695
0.7089465573605582	0.3301283882791707	0.6216368164278725
0.7693772123971805	0.7074553038676121	0.2971734648660703
0.4240993554013254	0.0259366668533085	0.6546394087592903
0.0918257754556842	0.3666484169784917	0.4687964402797938
0.0312858429408286	0.1989678959107176	0.2996146144723288
0.6865284849497800	0.5272118509011056	0.6424677974380794
0.3666121706825763	0.8578324382763308	0.4686823403309868
0.2811636510364298	0.9708833452398800	0.2702726656775060
0.9553541373270270	0.3155151101363406	0.6113656889034981

0.6283067563468845	0.6423254019351122	0.4395431466020158
0.2268986344350452	0.3177456580286901	0.3788719658966822
0.8828499592049422	0.6500432434045214	0.7069628965688658
0.5585355194523887	0.9834795770530036	0.5461244404592110
0.2678140600413302	0.9738243762322576	0.5317669909502071
0.9280571921436244	0.3062824887271595	0.3456725739855431
0.5967047348703185	0.6529804088419400	0.6962914053199778
0.7586241188090668	0.1944426155842610	0.5350199781062280
0.4230697858063683	0.5294314258128319	0.3636984158190457
0.1009654466665320	0.8666334034520149	0.6999368767231448
0.5432110277423365	0.7186410120417970	0.5525583105020967
0.2160859571876359	0.0587449790536112	0.3891653060903766
0.8701087589721140	0.3911045797308672	0.7305079043792574
0.1841002150674544	0.8095748727921389	0.3800911211792008
0.8505960790220116	0.1353410338556988	0.7085948641048264
0.5116221607182694	0.4734241918014460	0.5435212234418820
0.5264150123860936	0.1903020758599577	0.5310133814200366
0.1931746060522987	0.5216994610648217	0.3440729239234614
0.8623641747028031	0.8686243059680226	0.7029505388456676
0.3046134084398676	0.4636033090334075	0.5339086919672301
0.9717533178419708	0.7935199909886661	0.3655235601773504
0.6328328062626571	0.1333460460522352	0.7010960262835831
0.7823786983796499	0.7262194698341859	0.5585556075955380
0.4405822144511550	0.0539192664679765	0.3895915228305568
0.1106532080568445	0.3808603458058534	0.7286040003955017
0.6900992501400296	0.2734722377053646	0.3799882554017225
0.3725216627954409	0.6164076657005796	0.7016809869913041
0.0291985454419339	0.9409536297858242	0.5440114845155891
0.3061531593713511	0.2314217482079609	0.5303358684270192
0.9777480116744515	0.5720492907929303	0.3460044094757576
0.6314076840167675	0.8870398348655293	0.6990684025489866
0.0371492826791173	0.7406483785194198	0.5360679381550315
0.7070853652648684	0.0787675650600781	0.3634217820706191
0.3653801656876056	0.3982933430204701	0.7015962659636853
0.7751897246117808	0.9570481071125390	0.5572820516233892
0.4451845433943510	0.2851757419094807	0.3911951030687225
0.1195404950632540	0.6284567419476561	0.7300867414736568
0.1401137014636241	0.1451267527088463	0.3329474074197886
0.8098279618735318	0.4833759563797018	0.6759185191802501
0.5994951678403913	0.6233199947414179	0.3205243905500020
0.2569545219003956	0.9536313078117065	0.6532057050482674
0.9250228644323737	0.2901817463590913	0.4951435364354702
0.4730443777074897	0.8093022706447315	0.5122400640587303
0.3550164186581851	0.8944021895124952	0.3317553376648357

0.0178219190408656	0.2294032255587257	0.6740692142559166
0.8768036554390227	0.8754069646658589	0.3215081048117130
0.5446588170876350	0.2008489595347710	0.6524847798145096
0.2091349876676460	0.5341622550206305	0.4945676208577482
0.6879969785575965	0.5600865353951180	0.5139849443689429
0.6048892852626019	0.3596235199396048	0.3340004066218746
0.2700470916140736	0.6852628064024430	0.6758186596211770
0.6252690063424804	0.9016391829761250	0.3198018301956670
0.2991733311987116	0.2434080635764358	0.6520792468482057
0.9650427367443158	0.5742447637234080	0.4960018372560113
0.9410199010524930	0.0294594366134869	0.5125462630281198
0.9305274892068005	0.7885054103951700	0.4878717830706807
0.4749875637822579	0.3097007768205555	0.5085795625011396
0.1449499984672358	0.6452046897110514	0.3473503883067215
0.8007588399893263	0.9743725904266465	0.6769527728441196
0.5883700864458181	0.1190118744428568	0.3256594249141742
0.2590029949643581	0.4520643226584952	0.6628149839677406
0.7112305962888194	0.0413052838176298	0.4866161823259117
0.1907133521823467	0.0637253086903092	0.5047689490599683
0.8543118082545674	0.3995968165063502	0.3477113467418949
0.5162161473130574	0.7326828973644569	0.6803207842977479
0.3817666042307705	0.3690453512199995	0.3266132596323162
0.0454102911051029	0.7046939640930127	0.6666151286359823
0.4592748698824842	0.5721696886184695	0.4861130788124083
0.4361029200829735	0.0236692269484097	0.5058455271028051
0.1002263904896956	0.3549358625391161	0.3468007576428816
0.7694543489367901	0.7015645816912642	0.6786474851933415
0.1311020700674948	0.9112068547703001	0.3260183378436681
0.7946305785214048	0.2417860630498084	0.6674405465085202
0.7001854352559977	0.3004228103272867	0.5006487666935813
0.6988715632995451	0.7993946164866038	0.4989386645221326
0.1995194316071726	0.2986575372015726	0.4989677466477075
0.2014691772913833	0.7988375975821385	0.5006482040442128
0.8706358462599650	0.1283809026706650	0.3346773269838918
0.5233906478709085	0.4837327962336560	0.6642769692352557
0.3716076664751650	0.6418581510824901	0.3338410777345149
0.0290930854227982	0.9565659431759537	0.6651692935542139
0.3668949461569330	0.1330318707859055	0.3159889709291611
0.0321632992487529	0.4658124650494477	0.6857654478922677
0.8576300725157906	0.6297562709964892	0.3360651908963205
0.5474463809950872	0.9719320428466497	0.6671456823396489

The perfect Cu₇-O_{V6} surface

O In Cu In

1.000000000000000			
14.4442996979000000	0.0000000000000000	0.0000000000000000	
-7.2221498489000000	12.5091304781999995	0.0000000000000000	
0.0000000000000000	0.0000000000000000	17.9855003356999994	

O	In	Cu	In
71	27	1	20

Direct

0.8433797059630973	0.6132783986454262	0.4539271393907727
0.5161448411673965	0.9532490515280085	0.2892221349588117
0.1712234054064916	0.2802769044681611	0.6190781419772307
0.7927126020174151	0.9607945702705813	0.3001583711523952
0.4631147919980025	0.2838011819509994	0.6580143285642506
0.1324713028997323	0.6248941284657911	0.4676554801709008
0.3012912926833439	0.7312946064868915	0.2993422743385464
0.9756988015636082	0.0683499691140033	0.6371518051701676
0.6404876905614750	0.4061549404665450	0.4641977496870719
0.5294434662242127	0.2098797817401136	0.2673209653018401
0.1835849326302297	0.5396266854151933	0.6083940117987792
0.8540213051318956	0.8780557566836618	0.4441537440882550
0.8860783793337657	0.1290897137692823	0.4575053000647147
0.5469819383924296	0.4633420598921169	0.2878078436513551
0.2184556698440983	0.7902929324911238	0.6187025807703257
0.5388562832089566	0.7321572193330040	0.2978171326524840
0.2046193874265066	0.0750827978976493	0.6556945401641421
0.8748448592346312	0.4078229782605652	0.4679132277364112
0.7679277870011104	0.4688148216347527	0.2981796400409816
0.4247959897069739	0.8113357788393956	0.6325642795426790
0.0937015242645881	0.1332771585234362	0.4650805558670869
0.2903612442713461	0.2200171070234353	0.2682656487178077
0.9572831425881753	0.5405519307486062	0.6111706820831733
0.6173677362888460	0.8750432294367478	0.4423242230623320
0.3710535048017510	0.6580422592336750	0.4572130825266067
0.0360359835650664	0.9839611298914044	0.2891811550347638
0.7048258063528627	0.3392667365393251	0.6212371722160486
0.7683677843455644	0.7068457202767299	0.2978287599562386
0.4226470136823525	0.0290528283349618	0.6576221792643611
0.0921585718096040	0.3658167324462649	0.4685304198510583
0.0302520993961194	0.1985301142460295	0.2994135009682382
0.6807916678950089	0.5380852138313531	0.6889695104210680
0.3667191136908984	0.8603072002536207	0.4632702623009796
0.2810671569967554	0.9706026321948386	0.2680851216931183
0.9567986662932266	0.3150255221176033	0.6112569770948517

0.6259563252624707	0.6445307090710191	0.4397423810615746
0.2265647975044501	0.3166856677585569	0.3781248486321901
0.8947593686844827	0.6474444126739369	0.7099845541188748
0.5589126367405378	0.9899934142942802	0.5432847624950755
0.2687983610732964	0.9758017426960129	0.5304806419689775
0.9278653629370061	0.3057933745280424	0.3455411931453009
0.7595735677227758	0.1981261245277272	0.5370510745521861
0.4239018748953879	0.5290518245790341	0.3661674505028230
0.0985444808116581	0.8657578765277583	0.6986505570489825
0.5453467066427482	0.7165992657874788	0.5606507342764026
0.2162747870024005	0.0601645282054868	0.3867041190192405
0.8716716383705837	0.3876574687295323	0.7305794198290165
0.1822554932761993	0.8095547892386133	0.3777747334479626
0.8530044790024615	0.1368400526504871	0.7107116704973224
0.5222621073360532	0.4725873206124835	0.5486245861439513
0.5261629431320781	0.1934465169343914	0.5308263998931992
0.1945073370211767	0.5217004070496783	0.3477155013292004
0.8601706163135178	0.8672810633292716	0.7032993995060798
0.3065925211184774	0.4626393321704291	0.5341449733172219
0.9716180270934095	0.7942426707696589	0.3637063600075350
0.6347870431655044	0.1349999470143665	0.6987244339040264
0.7790568972676526	0.7143725765918295	0.5617607208300819
0.4401459214398002	0.0577417469598787	0.3869956284499831
0.1131166422868763	0.3816520116393501	0.7283347774690453
0.6897785310973903	0.2736746764122991	0.3788757994886434
0.3703957960239075	0.6190624396613940	0.7034251205832881
0.0285723460986931	0.9405320057198283	0.5434956228768729
0.3080217527506873	0.2322041741363641	0.5303535073006259
0.9781058945268805	0.5712981745244700	0.3422505138029205
0.6279552242414598	0.8916359563786120	0.7003160608885446
0.0358642307398747	0.7394335420210566	0.5335607812982162
0.7060847231484104	0.0783631283402777	0.3652517311246391
0.3648038154287291	0.3971138293872882	0.7013636787333897
0.7746354740591722	0.9574018496685813	0.5588508169094382
0.4448150766407450	0.2849503484503416	0.3866408020085274
0.1217566018513977	0.6276955477025478	0.7285171698488857
0.1401509193421927	0.1455710036988030	0.3306643166722029
0.8123405852797486	0.4814143920593122	0.6814739686000388
0.5982882331502835	0.6237926578415423	0.3196311980751351
0.2560280302942617	0.9536717523553354	0.6524673052579976
0.9257593212920473	0.2911586746564869	0.4952409540392300
0.4705297544410296	0.8103065659324697	0.5146565327060608
0.3546947149183535	0.8943937604342437	0.3316363762090834
0.0192562857605353	0.2298467083393296	0.6750730342044876

0.8757659759949170	0.8747710826679296	0.3225688346810598
0.5447776168440125	0.1994813941815706	0.6526726645668027
0.2098323664607968	0.5341806199531672	0.4927118323558144
0.6883332440459677	0.5613906485803596	0.5026591450536056
0.6053008248587629	0.3595784460439081	0.3289880251758087
0.2713269272226710	0.6872002742732045	0.6725598212083874
0.6240859746911338	0.9011330343708502	0.3225999555064329
0.2927344999368815	0.2402785159968374	0.6522681665527381
0.9656800154122649	0.5735503714607344	0.4955806136455437
0.9405926820206612	0.0295224018466829	0.5137213994620198
0.9315626862283685	0.7882805502553950	0.4860782931338414
0.4738338011934194	0.3078199321051196	0.5021045889659290
0.1450603914610761	0.6453592038799706	0.3459642700144338
0.7962317157314773	0.9750843563377376	0.6787331432305882
0.5883279195954048	0.1194164820254365	0.3246259251748353
0.2624982775631726	0.4572836286194412	0.6637371628427153
0.7103959606381446	0.0426859555777498	0.4875381654362997
0.1903704942321492	0.0635965430795569	0.5024259223039994
0.8541694551789962	0.3992162869996956	0.3460141828234453
0.5095444252497104	0.7417164086911620	0.6803700419243218
0.3810372177293521	0.3702145793030639	0.3245745580254827
0.0515831283255910	0.7047602181626120	0.6637315648427663
0.4607017178753074	0.5725066654810289	0.4909594648923047
0.4361204305048678	0.0259119789728218	0.5023574562976202
0.0999884627017215	0.3545228742166820	0.3465879782491431
0.7935604768097220	0.7050568906755528	0.6808645893788914
0.1309756871406011	0.9120251138708226	0.3236667368536640
0.7961300429875477	0.2405029820256527	0.6669222707452528
0.7010721106809469	0.3027152972209208	0.5001561552541234
0.6975726348923632	0.7996569039271600	0.5030502156603844
0.1992585761551691	0.2985282166340242	0.4985019365878435
0.2019274077944516	0.8001911494187249	0.4980891534729302
0.8699156823768153	0.1280993381847875	0.3356445884152002
0.5205923703291365	0.4515594323953044	0.6685533064207345
0.3727224726104884	0.6422811907291249	0.3361415854123339
0.0305770830485685	0.9588046616070669	0.6648599861005136
0.3666830642057016	0.1334231738211349	0.3113969546545840
0.0347143141654353	0.4658232939100231	0.6842497702256368
0.8599489652141735	0.6302393245593410	0.3320550374785062
0.5424103670677088	0.9720747764264906	0.6649383426191293

The perfect Cu₇-O_{v6}-bt-CO₂ surface

O In Cu In C O

1.000000000000000					
14.4443000000000001	0.000000000000000	0.000000000000000			
-7.22214999999999965	12.5091307398835685	0.000000000000000			
0.00000000000000011	0.00000000000000019	17.985499999999983			
O	In	Cu	In	C	O
71	27	1	20	1	2

Direct

0.8416822988820093	0.6124695341441280	0.4563736302175781
0.5153178472823495	0.9519124112986005	0.2892817540977769
0.1730160365760656	0.2812112293820013	0.6205864654772490
0.7928734735154740	0.9606229137855492	0.2983871185349438
0.4675632425757070	0.2874387594807195	0.6593603285090900
0.1318544236098676	0.6243134608287665	0.4686144548952110
0.3009214965069697	0.7311316104871727	0.2998072017693164
0.9761016664181419	0.0693889848851530	0.6365447380935383
0.6404362812354540	0.4051304169640280	0.4659518859886219
0.5287628352847997	0.2087269880577669	0.2684067229785905
0.1832692563005587	0.5399475375599017	0.6102723091462326
0.8547246171865415	0.8805551152626991	0.4425883982847455
0.8864548426429445	0.1283473598007543	0.4564368275844003
0.5469957418768193	0.4625855091141166	0.2885152299081382
0.2172887119409996	0.7902779705188019	0.6205791361016255
0.5392007082016355	0.7312562410315280	0.2987508824105118
0.2050151506774684	0.0764582788033035	0.6544083075321891
0.8743208767143076	0.4073910185227105	0.4686639096657088
0.7679460506029686	0.4686733996599614	0.2992461253541031
0.4273095698996284	0.8077825725505695	0.6376923834900922
0.0942934005534240	0.1343814569266443	0.4658878236394678
0.2897571023058061	0.2189002371982204	0.2693457734439577
0.9583800274078252	0.5424677256469136	0.6108039600358875
0.6176170779640323	0.8755894131695438	0.4413180620595347
0.3688330579129115	0.6573223579326696	0.4566372867033558
0.0364830024388536	0.9837978460900589	0.2902743312634203
0.7077389041371464	0.3291576501312456	0.6205506106314459
0.7684130058587578	0.7066836147555121	0.2977353505358684
0.4214772933496664	0.0279631994420729	0.6553760593237474
0.0921627125578483	0.3662000618987614	0.4689366315407391
0.0308506831414396	0.1986144062781285	0.2997432597851542
0.6919077706164027	0.5276693526086103	0.6417957625641140
0.3655169968495454	0.8580805752861113	0.4665857789304980
0.2805443308831904	0.9698520513494809	0.2694704026672102
0.9559266634477397	0.3144820132054791	0.6108155839497386

0.6279295614400960	0.6415856795055747	0.4414284248948294
0.2271023172760759	0.3170298610740412	0.3789320037035941
0.8876220306395788	0.6444135363585043	0.7124230520563390
0.5581691845846189	0.9876152601510543	0.5441480594184299
0.2671113536642428	0.9744424162213660	0.5307447685860105
0.9280610318470504	0.3057472635753875	0.3462206767270783
0.7590085320014484	0.1951361546208760	0.5345471706992069
0.4236379924412041	0.5287675456068116	0.3659845418245099
0.0975152196776623	0.8665770336818388	0.6994653570786546
0.5438262307577663	0.7164350949946160	0.5574252088696062
0.2160563394350996	0.0595618466561444	0.3882499775643437
0.8711106277282655	0.3879501525236994	0.7296892557768091
0.1824106684665220	0.8090000319329637	0.3789881276766313
0.8516559963224809	0.1355772297823129	0.7096621476535183
0.5132931770807382	0.4686685585560559	0.5444428437012755
0.5242520850287995	0.1917313566587203	0.5307572878056737
0.1937914550646301	0.5213202889263763	0.3459444323401649
0.8600534540736806	0.8669749590538108	0.7025990220461757
0.3052986991604189	0.4637091748146965	0.5348166205230980
0.9710191126395407	0.7933664721842182	0.3646208666293756
0.6329301664076236	0.1327386784346423	0.7003152749020277
0.7830137494631977	0.7240543112779103	0.5599404571960589
0.4400505341036396	0.0555129212909101	0.3881842107792870
0.1122531381052158	0.3811368535201265	0.7285426713871100
0.6897308238968746	0.2727418583350034	0.3785019538798801
0.3648348658047253	0.6187650156118755	0.7076055628292143
0.0283195284229517	0.9411002862194808	0.5436326904001986
0.3083866147962193	0.2322156383283476	0.5309621146012572
0.9776768797712699	0.5715164959656120	0.3447520806834385
0.6274447028790739	0.8922218952587216	0.7014280722970637
0.0351599244085179	0.7400350494309338	0.5344650368967273
0.7064936274630154	0.0778916432498405	0.3637017025185446
0.3699935133908852	0.4014188299504179	0.6998217182292451
0.7740743368692071	0.9570290669224866	0.5587536581593545
0.4444319067566159	0.2837327771935394	0.3865343995777177
0.1180828819969485	0.6274113221984254	0.7296947483821974
0.1401589138731506	0.1452871590561965	0.3322828616436371
0.8120861698122656	0.4793257357200539	0.6755274281341301
0.5990507175532698	0.6228659913823444	0.3219881052685695
0.2545601564429365	0.9538050039991995	0.6524677227332722
0.9251765962406160	0.2902039031624793	0.4946525947133111
0.4706389580139884	0.8085033798337123	0.5162534892594237
0.3543919062816489	0.8935662294207114	0.3326109601994640
0.0187578290326979	0.2297575635983039	0.6746137978562775

0.8757070853358426	0.8747154218740517	0.3221821188315844
0.5448446611346073	0.1988179584905254	0.6524547372421251
0.2092381736233498	0.5342777272189957	0.4943739743218576
0.6886984518954868	0.5587061032332712	0.5123424439317912
0.6053072764757956	0.3590952151075497	0.3301241088639836
0.2680060757320440	0.6874731275669153	0.6743083753397809
0.6243456945625370	0.9006078017516999	0.3217869049354929
0.2968019992512607	0.2429244134793064	0.6527546986765645
0.9648928369235306	0.5741293774655379	0.4949808205135782
0.9401412390777378	0.0294143114389596	0.5133695448701606
0.9303467021224174	0.7888401530823185	0.4865590062576105
0.4736369264738037	0.3075210275785769	0.5015337901395590
0.1448706487818550	0.6447884015131291	0.3469177180828067
0.7962845020426282	0.9736438210373589	0.6785708073056461
0.5878322497142128	0.1181044429892624	0.3247228906152003
0.2626684342776150	0.4569198730751771	0.6646033163911657
0.7099554386898819	0.0408006459425065	0.4867991370713429
0.1901176814972651	0.0640846404374577	0.5040715146008042
0.8543239377255631	0.3991678353790379	0.3469504858621431
0.5044859676731531	0.7437995421591209	0.6924693395212214
0.3810481723434222	0.3696447447533390	0.3247789510826946
0.0473200566586292	0.7046377761194533	0.6660007865948674
0.4603005760938930	0.5723251216897659	0.4896924035358952
0.4349526423715763	0.0240235108424852	0.5039786917046317
0.1003169521317369	0.3544810237086253	0.3471108775724626
0.7876338677344170	0.7021284197517492	0.6778548963822174
0.1306582208144280	0.9114108116585643	0.3252661688527106
0.7945115755721276	0.2392078130624639	0.6662946293789895
0.6996322512180276	0.2998568174796824	0.4994273294645479
0.6970869169904315	0.7987023390055188	0.5018029756856391
0.2000160822591369	0.2993932809332411	0.4996028611881728
0.2005274795422592	0.7992725100193085	0.4995376650890137
0.8701707936437527	0.1275631518219918	0.3350547914248771
0.5262173313746346	0.4587976738537539	0.6636313142652701
0.3724154495504830	0.6419729766427660	0.3361433207062334
0.0286834529371061	0.9584842334338799	0.6648437300329865
0.3663050944173862	0.1324345034268674	0.3128209811470909
0.0336969353735724	0.4653391522295436	0.6850987156936607
0.8577103863694767	0.6293498758055518	0.3347559417815838
0.5418275732572601	0.9719180733570136	0.6653999778139875
0.5702898943993182	0.6838178465335119	0.7564369987323978
0.5679522679367488	0.6973695431417641	0.8221481026770554
0.6111893755277664	0.6373061596103590	0.7167645106020524

The perfect Cu₇-O_{v6}-[CO₂+H]* surface

O In Cu In C O H

1.000000000000000
 14.4443000000000001 0.0000000000000000 0.0000000000000000
 -7.2221499999999965 12.5091307398835685 0.0000000000000000
 0.00000000000000011 0.00000000000000019 17.985499999999983

O In Cu In C O H
 71 27 1 20 1 2 1

Direct

0.8422812349806891 0.6144361154855315 0.4552854506768138
 0.5157760098459261 0.9521981083351453 0.2875368627984239
 0.1724279036559723 0.2800727190547205 0.6210309493171331
 0.7927978293619423 0.9606851223529828 0.2978854648149061
 0.4684495363379179 0.2876529544333585 0.6606023968874832
 0.1318175709928711 0.6246621872924027 0.4693285201923580
 0.3007369870741231 0.7302884695811561 0.2992466620242246
 0.9751419633858113 0.0685225750359205 0.6364193076722047
 0.6409680439464507 0.4048864771231428 0.4666423682478133
 0.5291554159880647 0.2091980353914116 0.2672527767274153
 0.1812514589652083 0.5391431756426103 0.6099967848314241
 0.8550689747260607 0.8803133301826794 0.4421527940630772
 0.8861894098777310 0.1275602615457487 0.4563061343895943
 0.5469930290675716 0.4626899080632714 0.2880122642695496
 0.2210221635864558 0.7917405716669188 0.6185751659188712
 0.5390328625588349 0.7310752163622468 0.2984036867438307
 0.2050086645458960 0.0753690024559119 0.6591113785251428
 0.8733970875968644 0.4070476090843732 0.4697898914124122
 0.7683670871570861 0.4685048447226322 0.2988195758094717
 0.4277758621525973 0.8068023682954136 0.6375122653100272
 0.0947057529639545 0.1340759546321847 0.4655561367283439
 0.2902918896107005 0.2196174462534448 0.2687219071476284
 0.9493809165165201 0.5480556870487335 0.6114370941700460
 0.6173765805283721 0.8753103922484964 0.4406772937426767
 0.3691240290641873 0.6571521241884075 0.4572161857813976
 0.0367284126912014 0.9842399109334330 0.2890427887504908
 0.7048726050687173 0.3252844451332912 0.6198895621676137
 0.7684272156924395 0.7070475503995426 0.2970433569524973
 0.4211669320489819 0.0266952201559917 0.6588534479112194
 0.0924595248600222 0.3653233383634051 0.4698001223401220
 0.0309270619516506 0.1991597476956649 0.2993459215888984
 0.6978728230767711 0.5309369574825427 0.6475343663553479
 0.3670980571038523 0.8586256515355677 0.4648503691810828
 0.2807598989756482 0.9700487876159539 0.2676906459514532
 0.9552624048874839 0.3158099539092972 0.6110373082669653

0.6283543587856327	0.6415948640415909	0.4409915701235795
0.2273925197658391	0.3166754998004946	0.3792506914443516
0.8880424726035645	0.6509314207373207	0.7240946928509652
0.5578869941896606	0.9873765183863653	0.5443137434200077
0.2685174912146234	0.9754826098325786	0.5308140961942670
0.9280731569192991	0.3055417319792582	0.3486586911190415
0.7592030198360751	0.1943022183023942	0.5346673957099162
0.4240866390530666	0.5287089608800074	0.3668181804022537
0.0951029457397471	0.8624955201975276	0.6976206230298332
0.5450636502051486	0.7165904675568169	0.5573989477371295
0.2165038304588382	0.0595375783691972	0.3867685644235282
0.8703171235118747	0.3883933356883519	0.7297621074044105
0.1829764373530252	0.8093311291372441	0.3776623353520049
0.8523212432380891	0.1361574000505822	0.7099692997503748
0.5171320394461080	0.4704585230323017	0.5467439098502787
0.5230920849540476	0.1904844134526685	0.5309990799806806
0.1940249136023118	0.5212628418584855	0.3481644736900688
0.8601340342154601	0.8668575080471814	0.7045126656845464
0.3056899952032353	0.4634731124643263	0.5357387418895949
0.9717600252353932	0.7938234711663932	0.3634394228445657
0.6330512726233933	0.1318965941072712	0.7008451043222371
0.7832862116705913	0.7230025915456979	0.5602643184266695
0.4400619434658547	0.0555157629765710	0.3863981252627321
0.1115805999998288	0.3813793638545502	0.7286971155108360
0.6891711314712311	0.2724543142389377	0.3781401521219008
0.3634826554010717	0.6178973987763636	0.7074423487271652
0.0294531575399624	0.9413239379736860	0.5434595883989841
0.3085637828809543	0.2312762575837160	0.5321166132268890
0.9773856157071813	0.5714248346772597	0.3473761381836181
0.6272718917763018	0.8913947075010868	0.7014984327515903
0.0370806849038672	0.7412164457497463	0.5331099529475142
0.7061359131607232	0.0777501607442766	0.3635222725353665
0.3692021935092523	0.4005506182417825	0.7004125231476828
0.7739699406108450	0.9561710897898448	0.5586532430536340
0.4449882462741679	0.2840130078388716	0.3865911027366420
0.1155777913153670	0.6279757178868148	0.7271354467385486
0.1403956119535417	0.1456195750113005	0.3311015397500920
0.8056197270217460	0.4719965684348463	0.6753618014639408
0.5989726423260626	0.6229374080847656	0.3213813793349886
0.2552718737090211	0.9545643484465571	0.6526653892850056
0.9251556333161730	0.2898150868131243	0.4940019524828036
0.4712183476760732	0.8084439713589012	0.5159957794720943
0.3547539033939685	0.8935772361213535	0.3302306032375085
0.0187611575133058	0.2298366105885455	0.6745712543493503

0.8759982155762691	0.8751813281563205	0.3210763303564182
0.5427675144785213	0.1961807506412581	0.6531710141367021
0.2092391023102137	0.5337962589027202	0.4938764355759522
0.6895525684191575	0.5591625723653675	0.5105576618530389
0.6051708286503132	0.3590610818346707	0.3290314310383599
0.2681545605499702	0.6867729419579606	0.6734360804271147
0.6242190618502099	0.9005734270956600	0.3209026334645737
0.2966476833978633	0.2419849356863032	0.6540811184045849
0.9639737155378837	0.5743586052544316	0.4924743542800856
0.9404406528150289	0.0294231866513895	0.5130467946683684
0.9315893198285131	0.7900900043957010	0.4852365939090100
0.4739222843945533	0.3075499266846372	0.5018095156604168
0.1451152035299499	0.6446101733429571	0.3470258878829898
0.7961521793302078	0.9742436416519710	0.6784567190620058
0.5881501608262827	0.1181849976022617	0.3233077975895670
0.2620753083525199	0.4558314205589784	0.6646520790871872
0.7097370234160328	0.0401413165120834	0.4864815433221729
0.1908982963920645	0.0640235442957784	0.5022012546403102
0.8538266457346688	0.3986120753640215	0.3474029746996002
0.5034913341622683	0.7433554552437496	0.6930681878145765
0.3812445459833949	0.3698560742942228	0.3248411919167647
0.0528740145111321	0.7071313989592412	0.6582767747682143
0.4607466465728702	0.5721182029001081	0.4904709811591460
0.4358660407318730	0.0241380406344839	0.5018827260884600
0.1006581518621068	0.3541657338550639	0.3477586711068280
0.7783520956886657	0.7041305443684555	0.6774968497128271
0.1309600869981198	0.9116415382431904	0.3234597213757678
0.7934347469263542	0.2369289077625046	0.6653777108486493
0.6983463848040572	0.2976754497338610	0.4988716592386221
0.6971359929658194	0.7988680767704980	0.5005881033508168
0.2002852438372893	0.2988355032696212	0.5000498612100026
0.2029184544598346	0.8007145348072194	0.4974401971703314
0.8700558843402948	0.1272590193900796	0.3348721844538302
0.5266485449027688	0.4581885731381941	0.6656756346598190
0.3728642314797366	0.6419683538191253	0.3365118675891383
0.0293237630390773	0.9589268371701481	0.6645095295835095
0.3666297024300123	0.1327456860361903	0.3114207323818087
0.0330558491970450	0.4648295391492698	0.6852402145897712
0.8576188206130460	0.6297960369811638	0.3333201089032828
0.5414520642658135	0.9711473803331354	0.6657604040514788
0.5664864791677662	0.6825327787387030	0.7574301794620938
0.5651780069111055	0.6944455268576893	0.8234340373699003
0.6076905229618164	0.6343043005205827	0.7181593780730895
0.9088605291423905	0.6707905335762774	0.7755610121911470

The perfect Cu₇-O_{v6}-[COOH]* surface

O In Cu In C O H

1.000000000000000

14.4443000000000001 0.000000000000000 0.000000000000000

-7.2221499999999965 12.5091307398835685 0.000000000000000

0.00000000000000011 0.00000000000000019 17.985499999999983

O In Cu In C O H

71 27 1 20 1 2 1

Direct

0.8421064932575490 0.6124961697654913 0.4553590473351025

0.5158123223918182 0.9518427569281624 0.2879725403659750

0.1725410958911205 0.2802437102589132 0.6194187870032420

0.7928924046183907 0.9604463365235110 0.2975564655493380

0.4640039908855652 0.2838199037318523 0.6629338550745416

0.1324338591362837 0.6243419011739252 0.4677379158118117

0.3013267548083794 0.7307014614642021 0.2989012312796315

0.9758629324468274 0.0689241609668360 0.6358374862033638

0.6406513653933243 0.4055467558472082 0.4646775715760420

0.5290940976716949 0.2078949917306441 0.2661160088204571

0.1836433677446641 0.5398346801790325 0.6088220781303223

0.8552401204807172 0.8802625801329934 0.4416042590181345

0.8861475797617200 0.1280321369877590 0.4559952414159955

0.5470719003538942 0.4624698524465191 0.2863537312831148

0.2193129747306970 0.7904419822171636 0.6195233630058795

0.5395796050549926 0.7310850135419410 0.2978355643885825

0.2047483910644309 0.0751639946279280 0.6557527097972170

0.8742175271486941 0.4069412292594131 0.4675662572513625

0.7686434505141623 0.4684986765737424 0.2974455538656613

0.4298993175824957 0.8069491002886066 0.6382468240682636

0.0944942122342327 0.1337400380751706 0.4646047480385627

0.2897101494349957 0.2186376190457449 0.2670705249983434

0.9574911463124343 0.5419044759071531 0.6097399974377997

0.6178243785625627 0.8751516872016628 0.4407170320716654

0.3702308921044746 0.6571682335559833 0.4561359121657501

0.0366826854494304 0.9832211354215278 0.2885622295611798

0.7059662246544717 0.3328021397389871 0.6193061027914009

0.7687119776645147 0.7064307521964990 0.2969301793326795

0.4219381236734965 0.0275422151490483 0.6546835045145906

0.0925413095253199 0.3653804750155307 0.4681336148140028

0.0308734099273606 0.1982445193254924 0.2988050306830067

0.6877136623550819 0.5338830180417269 0.6491563758546093

0.3665843733053567 0.8577214618978479 0.4664645739338006

0.2807393633762069 0.9692831784572303 0.2674392419330052

0.9563336132273307 0.3146346962464255 0.6097717196599705

0.6278914155034299	0.6414140379146983	0.4403838537650991
0.2275667913693401	0.3163380005414326	0.3776976549215726
0.8888273302663655	0.6440239134680048	0.7121243762539438
0.5584066208633525	0.9873884460150173	0.5436266281793508
0.2674636568299066	0.9742749072396696	0.5299880931068529
0.9282145018060333	0.3052317054391331	0.3459808036009295
0.7587296293662208	0.1957245220266065	0.5346282993693025
0.4240682658076369	0.5282135306790343	0.3650435902515489
0.0971539130532949	0.8650052042080469	0.6979579029271675
0.5453099810454787	0.7154354362160591	0.5577562995349677
0.2166254570435932	0.0595022151844358	0.3862691291318726
0.8706170148901443	0.3874805236895534	0.7286302012797206
0.1835788704752624	0.8093694987493503	0.3778733935264668
0.8518706124208154	0.1362678737259858	0.7089182330438529
0.5136056834349055	0.4668328320209981	0.5434257227889264
0.5240460795145151	0.1918908539867969	0.5299092673035392
0.1944644703784822	0.5211575681276052	0.3465096455336912
0.8601772758400338	0.8674463810882154	0.7032460525052976
0.3055971426296799	0.4630612273793808	0.5340976868646982
0.9717798664914663	0.7931719447682666	0.3634159833644227
0.6338160356965900	0.1352716470527318	0.6995724537465735
0.7839243372529329	0.7232634584909770	0.5588937111245573
0.4399745512487550	0.0551068606565742	0.3867622823190165
0.1124231321960917	0.3812866777346970	0.7274198187472785
0.6894054370964446	0.2727992450419122	0.3772576379754574
0.3646847205453179	0.6197682183147222	0.7063022517393142
0.0288339085194282	0.9409455410027492	0.5429160280244670
0.3086653151279978	0.2310792540050698	0.5303897023709609
0.9780011563752994	0.5712218853087855	0.3443228893144634
0.6276563794885642	0.8950321056888356	0.7009746692006480
0.0361105024070615	0.7397386054989769	0.5336460272728041
0.7062933170452576	0.0775337449393287	0.3635310111654793
0.3683316847295598	0.4012060543138198	0.6994833969697877
0.7740979058802036	0.9564105098613629	0.5580889799989044
0.4448674395877430	0.2832043484592487	0.3835913224790223
0.1175834049073902	0.6266111877144034	0.7284886999143922
0.1403374187334907	0.1448272325510928	0.3303367938734542
0.8117785319440558	0.4796118850428157	0.6756147385752564
0.5992491265121563	0.6225423400745753	0.3206048804822196
0.2547911493963720	0.9534281490321919	0.6518254031729454
0.9253721081884280	0.2901101313211548	0.4935180973392037
0.4721278722562446	0.8081007457537435	0.5154335097959070
0.3548345555011769	0.8934396156259861	0.3307888485397283
0.0187658596125707	0.2296582415735885	0.6739066439191489

0.8760144257478794	0.8746115100625168	0.3208640153153402
0.5444207788634068	0.1993995793642276	0.6517132537818781
0.2096019468266275	0.5337935997859526	0.4925801198152288
0.6885087631373752	0.5589712823459148	0.5104177800501690
0.6056478352815863	0.3587582739197625	0.3268431300728925
0.2671014060116056	0.6868111043606107	0.6731580234817314
0.6244813279725832	0.9003535853907263	0.3208864467624639
0.2946492016336839	0.2409208723088717	0.6524967940112950
0.9651837193279424	0.5737020374805535	0.4936100276419332
0.9405167771140565	0.0291626393470011	0.5123193743847855
0.9318314316084815	0.7890504140349633	0.4850937273161417
0.4730624819446121	0.3063156985832712	0.4981036175529984
0.1453091529059871	0.6447226090102250	0.3459946803355068
0.7975540859163531	0.9751021542515144	0.6774288233563284
0.5881252520600257	0.1179194338903466	0.3236102899785704
0.2615691179691312	0.4560655489939527	0.6627128925028976
0.7102419532994728	0.0410360538342336	0.4862915400194262
0.1902775305777869	0.0632427108160733	0.5019546427701949
0.8544411378608732	0.3987064239683980	0.3458072107604191
0.5037956691742558	0.7476325235081348	0.6952050923404884
0.3809826995245720	0.3694138166068046	0.3226004893188401
0.0479430300556823	0.7040010971693946	0.6642660010348382
0.4606091763412509	0.5717778875747049	0.4889544289834774
0.4352811625493815	0.0239115338208033	0.5025751492668975
0.1006505143255637	0.3539764750835834	0.3463054203145419
0.7930694799944054	0.7053742000207429	0.6762409894239241
0.1310552843857153	0.9109992482336314	0.3235797892833706
0.7948763695859542	0.2397439880265676	0.6649936988347129
0.6998615677013605	0.3005372347851334	0.4983093935242873
0.6977064452759191	0.7986518256226320	0.5005547820814273
0.2003083732713060	0.2986312444068212	0.4983544755112955
0.2014399873779431	0.7991582776312298	0.4983424106184232
0.8701292475644404	0.1271801668714017	0.3343084876735014
0.5220668521499533	0.4524797097232227	0.6622884123769995
0.3730727035730805	0.6417919290439095	0.3353666908566099
0.0299330126608587	0.9591208772220831	0.6642327932191935
0.3663878267557331	0.1319864045871178	0.3099961193329863
0.0331958854754187	0.4647755452684243	0.6839241129038954
0.8581556659079379	0.6291047089268327	0.3334904441641180
0.5425922658269609	0.9745573320081479	0.6644376077181507
0.5580172304787943	0.7002732881644570	0.7747977801455500
0.5492745380588780	0.7146627477178567	0.8393056527483893
0.6113883980433481	0.6407785167214098	0.7552928977799985
0.6266944941800913	0.6197553894102217	0.8037353534507505

The perfect Cu₇-O_{v6}-[TS-COOH]* surface

O In Cu In C O H

1.000000000000000

14.4443000000000001 0.000000000000000 0.000000000000000

-7.2221500000000001 12.5091307398836005 0.000000000000000

0.00000000000000011 0.0000000000000019 17.9855000000000018

O In Cu In C O H

71 27 1 20 1 2 1

Direct

0.8451813923663164 0.6127004919854102 0.4526059875410088

0.5175219854329902 0.9524090830182483 0.2877632514716657

0.1719600801476255 0.2789379588078289 0.6181492170148863

0.7942366697525770 0.9604544771907862 0.2977654418944655

0.4654670107194714 0.2854288944821983 0.6591441584068702

0.1338068955325068 0.6243797443012699 0.4671195844553812

0.3029953355131577 0.7308063485812308 0.2988087076799691

0.9762640348062726 0.0676004302263798 0.6362245739986484

0.6417708391062766 0.4055705630458157 0.4630738266278497

0.5306054454624962 0.2085638943257497 0.2664599546006153

0.1860147814407938 0.5394677190244739 0.6076234556078427

0.8561951671898660 0.8791232929211126 0.4418685981531896

0.8870389855932015 0.1277226620282087 0.4562750052143182

0.5484898420286255 0.4625304681365489 0.2865408064032347

0.2216002128405248 0.7912124603503261 0.6182583994211887

0.5407689261053930 0.7314393166075098 0.2969924636923282

0.2068133716984545 0.0757726211128830 0.6574899808363558

0.8756114973096742 0.4070484290937845 0.4668669863845241

0.7696001847651798 0.4679917682895102 0.2966605611630199

0.4309101952838850 0.8080735189484134 0.6364473652414637

0.0950035396879416 0.1327793340874371 0.4637311842880611

0.2918997956693671 0.2193196835478624 0.2669929596153732

0.9583488037375461 0.5404901551985920 0.6095969162664043

0.6193377578453177 0.8755378772283158 0.4405712297994923

0.3722726782354059 0.6574711641971711 0.4562125047309773

0.0378837394069838 0.9835570905086224 0.2876187017808647

0.7067614884996684 0.3367664956654193 0.6193508609699355

0.7703118604837887 0.7065362461404738 0.2960390347476907

0.4238299282150150 0.0285272795580241 0.6548114375355969

0.0936287074256285 0.3651017633715624 0.4677475193029558

0.0318900584103713 0.1983431639114511 0.2981632399757470

0.6871965461049798 0.5386593392615375 0.6743116279750863

0.3686241673327740 0.8585383355134822 0.4656460920404889

0.2828946693572038 0.9699315761958366 0.2668055335377031

0.9575621641447932 0.3142525203887116 0.6095635358565688

0.6289634607559756	0.6431439675405034	0.4382139905446879
0.2282298318168356	0.3161114974422645	0.3770626401644476
0.8978175559476278	0.6458935497455934	0.7117626334906345
0.5604082245880276	0.9881115172750149	0.5436337881398803
0.2692750090253302	0.9751538044275104	0.5296209716297067
0.9294207222220822	0.3051364099382606	0.3458245051770375
0.7601045277818733	0.1966030788429095	0.5350986940677529
0.4256161614146475	0.5284504696760295	0.3651515184681198
0.0990062190890281	0.8650123957252133	0.6965034349226780
0.5477184168240228	0.7157299053741026	0.5574213197495416
0.2177851665403402	0.0594907169779722	0.3850968697695918
0.8722644079887993	0.3866074685708102	0.7289160509625556
0.1848971452841379	0.8097668051298169	0.3771025192460668
0.8521022624075146	0.1351006966722615	0.7082577923204884
0.5222769158615824	0.4715968826496920	0.5467255586580619
0.5264054530768731	0.1927239143194925	0.5298285332437592
0.1961713291974398	0.5213437431562077	0.3475366002056974
0.8605104789345660	0.8661200388875075	0.7032215256872688
0.3077407095369235	0.4620843199651527	0.5332773936817664
0.9735993191858093	0.7937695110219479	0.3620239091260726
0.6354351873847340	0.1359625400850963	0.6987078131075912
0.7845288715984693	0.7175107014181390	0.5577833102041848
0.4414881139479772	0.0555616237234692	0.3865529205696749
0.1133481469267760	0.3806840023292193	0.7268179556012649
0.6910429205702302	0.2729042901020801	0.3774418550299092
0.3656224416715194	0.6188912787461125	0.7054820235511855
0.0302486441906763	0.9407046317767656	0.5426349287451132
0.3092711158387569	0.2311690058211141	0.5297143892635043
0.9797768627421101	0.5709827448062818	0.3415165165120876
0.6270888513166495	0.8931846889330822	0.7042507466104923
0.0377245091408642	0.7393633028171945	0.5328001334812278
0.7078096751974745	0.0778422420644595	0.3635499243900943
0.3666292506408544	0.3991250265534483	0.6990808957997674
0.7749149488017681	0.9557766906356043	0.5584576909170219
0.4461115071525272	0.2839411297935241	0.3851305628164834
0.1210297577024826	0.6263654652908509	0.7273202685690736
0.1416932150759824	0.1451522756642747	0.3291165233740817
0.8132679968988596	0.4800733111764817	0.6791512928365553
0.6002964660183853	0.6230052623825328	0.3185662697535239
0.2569604487782189	0.9543961712598501	0.6515236185081518
0.9266388907107944	0.2902657571089278	0.4932861681943685
0.4737147001463707	0.8084224518339513	0.5154397906451195
0.3565193164692588	0.8938176992422824	0.3304455764665525
0.0192603508758041	0.2287161097872680	0.6737068464082190

0.8773673957372431	0.8746522580180356	0.3203338979415369
0.5460903481921492	0.2005673735815870	0.6516591301203073
0.2114469478564910	0.5335759303790519	0.4911104353348386
0.6903145141059640	0.5604173519625005	0.5031157258452532
0.6068500560132938	0.3588453632378441	0.3274454755070715
0.2694709621286866	0.6870788025091028	0.6712169259265425
0.6258104466071481	0.9006180082074611	0.3207598736343779
0.2952260289747095	0.2408926931623198	0.6516847260630243
0.9667609599320869	0.5730703966765707	0.4938727122930717
0.9416652992532994	0.0287772969153114	0.5124887281437763
0.9345889765918662	0.7891277494802965	0.4835037500427611
0.4749478686067707	0.3077414739301719	0.5003488576139015
0.1467250679222310	0.6450513620544071	0.3452855133059176
0.7967767817255932	0.9735311376663982	0.6778245550907663
0.5897098229463126	0.1183813278674999	0.3235501867807448
0.2615335125405059	0.4543809861870894	0.6615446358734177
0.7115194019782022	0.0415452113908112	0.4861888940420167
0.1916628401230641	0.0631987843961456	0.5004793101261658
0.8557023661342358	0.3986832266980483	0.3449877376540719
0.5016086551156895	0.7483287499550754	0.6993801161371079
0.3825326288696215	0.3695832628556782	0.3232278337955636
0.0527908977886380	0.7042391747803922	0.6625720437611489
0.4626556935674129	0.5720498276957694	0.4894882893254975
0.4373162801076454	0.0246719490566719	0.5023099971167424
0.1016999504926925	0.3540437943645513	0.3457915900913445
0.8043810028640028	0.7070987886162804	0.6741160721420811
0.1327602351147061	0.9114792865990836	0.3219524928196315
0.7963570987965407	0.2398943389916725	0.6646523704126902
0.7016358797637947	0.3014162552063552	0.4984425314591058
0.6989984749326487	0.7989306818336943	0.5003395906305966
0.2005581720930792	0.2977566610185977	0.4974941433255166
0.2034637999782778	0.7997215831857142	0.4972586509733652
0.8714640386450893	0.1272509226109074	0.3342485454794305
0.5230237333303666	0.4541098821122960	0.6672064728811817
0.3747857335176855	0.6420708860042699	0.3353792810083179
0.0329732444069095	0.9604160591292420	0.6642089317937019
0.3681652410786029	0.1325955299072383	0.3102546517700289
0.0347280047347077	0.4645203676514945	0.6831997439497293
0.8609825063330819	0.6294266115442668	0.3307911852756154
0.5437466882071093	0.9743892323392841	0.6645630518166203
0.5239823112090284	0.6883203616491217	0.7880858389747994
0.4949201596660643	0.7022810427320603	0.8468711719550333
0.5659988147919668	0.6193680272372244	0.7785557898639891
0.6419380814134388	0.6644353335925723	0.7687042552805802

The perfect Cu₇-O_{v6}-[TS-CO-OH]* surface

O In Cu In C O H

1.00000000000000

14.4443000000000001 0.0000000000000000 0.0000000000000000

-7.2221500000000001 12.5091307398836005 0.0000000000000000

0.00000000000000011 0.00000000000000019 17.9855000000000018

O In Cu In C O H

71 27 1 20 1 2 1

Selective dynamics

Direct

0.8413896694033220	0.6128279716191148	0.4561480421251156	T	T	T
0.5154339421514923	0.9518435635697905	0.2883242386420106	T	T	T
0.1727331904803648	0.2811144259753374	0.6198480048719024	T	T	T
0.7927206804699251	0.9605496457127359	0.2978363892996984	T	T	T
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0.3009717527506277	0.7308270178288985	0.2990703148092013	T	T	T
0.9759195895757541	0.0699931733882689	0.6354929425422960	T	T	T
0.6400516242464104	0.4056310535129412	0.4645883315887003	T	T	T
0.5289678183150449	0.2083566920483355	0.2666274197981108	T	T	T
0.1824823677282582	0.5397599974525111	0.6087562612603932	T	T	T
0.8547763091880817	0.8804074130824535	0.4419948473098147	T	T	T
0.8860784315219685	0.1283803726735149	0.4558507515979933	T	T	T
0.5469818105711675	0.4626881892443099	0.2869723163196673	T	T	T
0.2188890468569301	0.7910628587870242	0.6196933619420891	T	T	T
0.5393614105590155	0.7312264903442495	0.2982035263901487	T	T	T
0.2046433709820339	0.0761064135267686	0.6561424431904203	T	T	T
0.8738930767705817	0.4069960749594486	0.4677298295638094	T	T	T
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0.4293698114947538	0.8071363617768105	0.6383668838011757	T	T	T
0.0943065203976854	0.1341925846926165	0.4646933549356003	T	T	T
0.2895264171737821	0.2189213517270981	0.2672845622328766	T	T	T
0.9573017782478600	0.5425431586779653	0.6094277591995811	T	T	T
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0.3700149676546450	0.6575019558300171	0.4562625566567802	T	T	T
0.0362986019337791	0.9833755098907684	0.2889587591943391	T	T	T
0.7063237385860118	0.3315410123804904	0.6191871450825244	T	T	T
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0.6893937556485233	0.5308875972423328	0.6435085803074334	T	T	T
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0.2803222243051892	0.9694694642596353	0.2677105017843613	T	T	T

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0.1831524212100378	0.8095637499053535	0.3780327853937585	T	T	T
0.8519951395960620	0.1371211858166159	0.7093203992458448	T	T	T
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0.1941323532962657	0.5213235439870449	0.3466981293133694	T	T	T
0.8603664397357492	0.8685382797080292	0.7030563297756035	T	T	T
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0.9712412102335459	0.7933121201452532	0.3639782044881879	T	T	T
0.6332678204652157	0.1355015469347611	0.6998906816819542	T	T	T
0.7831187873583698	0.7244680605068133	0.5598742073942767	T	T	T
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0.3083285523359463	0.2314201168487189	0.5307823699351999	T	T	T
0.9776130672080281	0.5715471955247595	0.3456398557724116	T	T	T
0.6280221308424048	0.8968837153306742	0.7006721617343113	T	T	T
0.0357636338298441	0.7401597592124178	0.5337034557327072	T	T	T
0.7060918620498471	0.0776193111212733	0.3634703999706679	T	T	T
0.3691055113876741	0.4024788902287881	0.6994366091758055	T	T	T
0.7739175716081071	0.9570929912574868	0.5581280184653129	T	T	T
0.4441997616116543	0.2832418350330265	0.3841001843991350	T	T	T
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0.1401537290374837	0.1451336454299832	0.3305825917767525	T	T	T
0.8115387043460912	0.4799536846087114	0.6746430353542135	T	T	T
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0.2544091841417661	0.9540831710925103	0.6520010516904061	T	T	T
0.9249201572499044	0.2901753394080806	0.4938320702414206	T	T	T
0.4716419518310435	0.8084533299203952	0.5154262282713593	T	T	T
0.3544224177587904	0.8936171433525459	0.3310676416781968	T	T	T

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0.6882416926638132	0.5586589215710024	0.5120441337510977	T	T	T
0.6054069243509205	0.3590665594348131	0.3279165943589866	T	T	T
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0.6242962535340452	0.9004878123832399	0.3211951302680416	T	T	T
0.2954243382786053	0.2422185691071205	0.6528453322812480	T	T	T
0.9650354985974475	0.5740971521052206	0.4933484908129592	T	T	T
0.9402387523437136	0.0295781130650127	0.5124420696104375	T	T	T
0.9308708344174935	0.7891736169460173	0.4859259296881706	T	T	T
0.4727409367576055	0.3071134817511543	0.4986303170008938	T	T	T
0.1450693042644327	0.6449884058781771	0.3463541318356319	T	T	T
0.797622239453113	0.9759452496175905	0.6776151083341566	T	T	T
0.5877868699195459	0.1180114074984884	0.3238241801945139	T	T	T
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0.7099340604111315	0.0410672769265099	0.4863330003397712	T	T	T
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0.8541133286979193	0.3987722537678618	0.3460738827027320	T	T	T
0.5037570330969929	0.7472737164774799	0.6940955291759946	T	T	T
0.3807919624062114	0.3696352067108387	0.3229569517700274	T	T	T
0.0466272357973207	0.7045012930811961	0.6643179514161737	T	T	T
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0.1305965097989777	0.9111881567578805	0.3239912097711676	T	T	T
0.7944270699896753	0.2400877235137542	0.6653004561813515	T	T	T
0.6992873810956426	0.3004606252587427	0.4984412515255077	T	T	T
0.6972672586446247	0.7987345962284775	0.5013606935631955	T	T	T
0.1999767469492089	0.2989695819141769	0.4986769617996096	T	T	T
0.2010280270635844	0.7995586597304204	0.4985843104609761	T	T	T
0.8699604075678505	0.1274245385910185	0.3343431007933020	T	T	T
0.5238937309252883	0.4548152448949980	0.6632251360404989	T	T	T
0.3728383096994837	0.6420256283198720	0.3356139857013553	T	T	T
0.0292288573482300	0.9594639552316252	0.6643861230071311	T	T	T
0.3661563144220063	0.1322497969307822	0.3103299767416590	T	T	T
0.0326870089647864	0.4652667395305592	0.6838861814581925	T	T	T
0.8573488853304441	0.6292189356829899	0.3344009630777099	T	T	T
0.5424218766764723	0.9750744128617437	0.6643927438678182	T	T	T
0.5602790614571503	0.7005024113038241	0.7726293211284562	T	T	T
0.5566474776010395	0.7079072171610241	0.8378634590147475	T	T	T
0.6212977624556817	0.6361309631844765	0.7473117881357410	T	T	T

0.6357249277023620 0.6153096427642312 0.7959427550757561 T T T

The perfect Cu₇-O_{v6}-[CO-OH]* surface

O In Cu In C O H

1.000000000000000

14.4443000000000001 0.000000000000000 0.000000000000000

-7.22214999999999965 12.5091307398835685 0.000000000000000

0.00000000000000011 0.00000000000000019 17.985499999999983

O In Cu In C O H

71 27 1 20 1 2 1

Direct

0.8418392215215736 0.6129833103237905 0.4557235683104807

0.5152451819865785 0.9518067446381472 0.2893119503092559

0.1728487077293446 0.2808097694473794 0.6201484525757103

0.7928297433051054 0.9606303614911520 0.2979911730301225

0.4694923434395707 0.2892659646929315 0.6641621096174923

0.1329626117857084 0.6253272370754931 0.4684122724375243

0.3012319319206807 0.7311857523025962 0.3000188873250906

0.9763788385949876 0.0696206735697800 0.6360128005480016

0.6397322814547152 0.4045591958043651 0.4623740322152918

0.5288855914533365 0.2090077593309794 0.2680998101935237

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0.8547533366303197 0.8807234697649956 0.4424313909205405

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0.5473110055039666 0.4631633360240157 0.2884036247828578

0.2178865817788326 0.7910357410174617 0.6202526088849908

0.5393722129366163 0.7316484293949385 0.2989121530639938

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0.6970441827027605 0.5225237832827936 0.6313337543437086

0.3657331284890126 0.8586001612642026 0.4667694789581037

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0.9557117838509538 0.3139294859649328 0.6104776376256387

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0.2668035196167962	0.9745929679629465	0.5304674206987555
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0.8711990975329931	0.3885335241266722	0.7288004863249283
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0.5128752097447906	0.4679157035079577	0.5449111600440221
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0.1942959773859632	0.5216152750776343	0.3477979328913039
0.8599654938006550	0.8666589040669848	0.7025483051788350
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0.2548513048891984	0.9548376591131607	0.6522899004364781
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0.6245255424174506	0.9006450130829670	0.3220987830963958
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0.9298706244929126	0.7888717582505809	0.4867506209219616
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0.7991594491332190	0.9753465249308888	0.6779363809441113
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0.8544603801637781	0.3990929378682352	0.3463605948520313
0.5044193613941147	0.7468265046383932	0.6921642563150502
0.3809056169960121	0.3700263536456195	0.3239451074486380
0.0461249351749112	0.7045568555526520	0.6652678355388222
0.4606748762284473	0.5722233111738422	0.4914761684012257
0.4347839326269876	0.0249570585509056	0.5039982350088210
0.1002376329849696	0.3542304938152358	0.3471782929774673
0.7850353839692655	0.6990114564526257	0.6785888378493803
0.1304627291691973	0.9116161033303055	0.3248234163336039
0.7946893420963613	0.2393540782325342	0.6662663917241850
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0.0284093605002956	0.9580487402269017	0.6647099515618847
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0.5433543674115779	0.9756713007064108	0.6643363531538158
0.5253090927823367	0.7350042435718682	0.8005167077453785
0.5060824251716449	0.7552935732544769	0.8582043943098767
0.6258589976596076	0.6098236805248377	0.7277365445124784
0.5931007205492976	0.6406859381144633	0.7583172217728499

The perfect Cu₇-O_{v6}-[TS-CO-O]* surface

O	In	Cu	In	C	O
1.000000000000000					
14.4443000000000001				0.000000000000000	0.000000000000000
-7.2221500000000001				12.5091307398836005	0.000000000000000
0.00000000000000011				0.0000000000000019	17.9855000000000018

O	In	Cu	In	C	O
71	27	1	20	1	2

Direct

0.8401977219606953	0.6139176852867856	0.4586240085449730
0.5142589107358621	0.9536134594991106	0.2889725965749597
0.1694313653193737	0.2810699303133055	0.6195022646933347
0.7920138436381898	0.9622127382548490	0.2982349442876253
0.4687239067983606	0.2955113245090739	0.6486167279619232
0.1306535717751151	0.6253925051828914	0.4691170296343588
0.2989185380167484	0.7325893928848867	0.2992195225216790
0.9753936888673452	0.0715907955735100	0.6350292255188759
0.6391265294135450	0.4070881636315596	0.4701700565302836
0.5272226792484190	0.2108131287767231	0.2709374712697736
0.1801064513071747	0.5392933212568651	0.6104168402660823
0.8546518331282061	0.8822907182840440	0.4426185350080011
0.8852335374609714	0.1302984808373184	0.4562240231559290
0.5459477587765955	0.4634296614238320	0.2905356331675008
0.2207805918541162	0.7912019041550502	0.6210041512493273
0.5377465432517615	0.7325270114649026	0.2980383928105005
0.2049909150512919	0.0778339052601800	0.6572379056308436
0.8731018086113763	0.4076656124872151	0.4693637613562311
0.7657039822029292	0.4700003342129264	0.3016209314710545
0.4319739633352970	0.8011114958267203	0.6433177470615523
0.0922834586275589	0.1345413574640930	0.4640305165783908
0.2893572840713401	0.2200906241831781	0.2710224532247045
0.9558903681125661	0.5423631868632248	0.6113116765325147
0.6172698422479551	0.8774188839357669	0.4399366589767638
0.3663043251845005	0.6580855457512939	0.4550298741602294
0.0354290155280093	0.9846025073522239	0.2900616545818034
0.7062040196101326	0.3304409454955339	0.6220078711425023
0.7675697855801920	0.7082818350602886	0.2980965794052264
0.4213236269946594	0.0267380255310559	0.6551047919486019
0.0893921078899801	0.3669488657990466	0.4684949429921132
0.0294259023732032	0.1996053690741330	0.2994540743676546
0.6857466725907714	0.5307007807463024	0.6448414507323078
0.3640885234433839	0.8589880167456595	0.4676286239723493
0.2793056512815789	0.9715429722688111	0.2698176854704504
0.9527776401281627	0.3151966975754552	0.6118528442734011

0.6271416579283565	0.6438084053337381	0.4412794695462954
0.2252064456113162	0.3188396459741941	0.3786872169639934
0.8853332401661991	0.6477971773402311	0.7093372123176123
0.5557790856569070	0.9846893390584471	0.5456850265353845
0.2656618237513879	0.9750958303435414	0.5317183803997938
0.9261771206859013	0.3071233307795450	0.3439055990314696
0.7564938137365635	0.1949515482572292	0.5355699021543003
0.4218030310666325	0.5304620009814134	0.3647394866809030
0.0979933767330655	0.8673253075787507	0.6990491359433416
0.5408459590524660	0.7192036771564537	0.5540742072537180
0.2146303760518171	0.0598521643271472	0.3883847929112407
0.8678650323657192	0.3901887651455854	0.7307621496471043
0.1817513893211148	0.8103528233971634	0.3795755217077069
0.8485572810480112	0.1354992588095166	0.7098321986138273
0.5101007104075336	0.4739119494939368	0.5439572053600579
0.5241408038683967	0.1910623676917580	0.5312809573859736
0.1916720161058102	0.5225416836979985	0.3450459072954963
0.8626550204366735	0.8715515925152343	0.7028924522476933
0.3026820815180837	0.4644155814516996	0.5339452448715232
0.9699978566432816	0.7945503780678813	0.3661408042420513
0.6300432708563107	0.1332898600573975	0.7009819961107053
0.7814877572178202	0.7270091243602058	0.5614003174059434
0.4384927673725397	0.0551298941484168	0.3891960765892750
0.1082456565380494	0.3809901897445194	0.7288642177280754
0.6881204281556828	0.2741255683431764	0.3803705775858586
0.3650528866761977	0.6159546398897965	0.7033866400819332
0.0282461609915502	0.9428897869289621	0.5439713719898992
0.3041609905575090	0.2319514826597637	0.5304068366110628
0.9758522204965202	0.5728405235347974	0.3469243797952694
0.6274781136634127	0.8877909301925733	0.6984233712836628
0.0350316290527019	0.7410583123963845	0.5359177393416774
0.7051215083803736	0.0793926059534180	0.3637544524266510
0.3625710399721875	0.3985302330293177	0.7018340603121251
0.7730690937529677	0.9582009927844672	0.5576436812889911
0.4434039518078509	0.2856595417583451	0.3911398810365780
0.1166653169064944	0.6281515710064661	0.7299648770799632
0.1385334049427470	0.1462318689792075	0.3324322589979601
0.8083082972618532	0.4822803294845798	0.6760408122364169
0.5981295251107611	0.6243845618469710	0.3219563371801605
0.2543323905198107	0.9545964770260291	0.6532583763654315
0.9230623415127703	0.2906466189088860	0.4958947223649902
0.4703146805030472	0.8104274371865534	0.5123224966069285
0.3529999869909623	0.8951139351895986	0.3317214327806070
0.0155191090573913	0.2297184142782631	0.6745974119485251

0.8750050448528809	0.8761372267054602	0.3225488983611814
0.5421252140042717	0.2009303495895886	0.6527244172359357
0.2070434853849610	0.5347073421899250	0.4941383942554765
0.6868518184538775	0.5611937947098068	0.5154917067194731
0.6033308716571005	0.3603940663759898	0.3343460186126328
0.2658841293270208	0.6855374078435449	0.6750784010507952
0.6234898749851295	0.9022079521710007	0.3205477818205852
0.2961847162298004	0.2440759916129787	0.6521355129533215
0.9633113265669504	0.5746418471808136	0.4955961006222129
0.9393443310069388	0.0309454232384448	0.5127780060114152
0.9289218689100839	0.7897061815682144	0.4885907416731028
0.4729664901038443	0.3100205904758369	0.5081715122674919
0.1431503956250580	0.6460654441108448	0.3473756167201292
0.7970491873991052	0.9744632868314738	0.6774802857530240
0.5865402189359011	0.1197205730871838	0.3257501653351229
0.2560688016662361	0.4524722786656136	0.6630572518950731
0.7088838145381674	0.0419233642417145	0.4868427971695643
0.1887778754945781	0.0647599183446605	0.5036621273193488
0.8524191899618926	0.4000640570094003	0.3476950899022187
0.5063404819463492	0.7292107756899976	0.6777241039124848
0.3802758617040884	0.3701228387529356	0.3269567714250850
0.0449188402471823	0.7052666558244144	0.6658334056506662
0.4574486678773885	0.5730155090010366	0.4868812586550590
0.4337959818651773	0.0247266761544393	0.5053930423322095
0.0980899039431573	0.3556097779545622	0.3465463085033196
0.7777896253562596	0.7030467801320217	0.6820393022394928
0.1291415632224715	0.9120402911180949	0.3255607177070045
0.7919499926582886	0.2409012241259954	0.6680225958510786
0.6983604572911386	0.3010896758186724	0.5010015724695400
0.6971422817035843	0.8002834899851796	0.5010418196705845
0.1973334959890526	0.2994776645818799	0.4988129586465513
0.1992752014724191	0.8000697241029382	0.5001793766230342
0.8688180011035569	0.1293712881404740	0.3347530289780699
0.5204295099843078	0.4793977994329913	0.6639765652058982
0.3701736594417563	0.6428549965525410	0.3344005520477181
0.0285031305503593	0.9599412177202991	0.6651750581079302
0.3652632538377996	0.1338568810902460	0.3152501887722732
0.0296540706778679	0.4656589060911103	0.6855447199582275
0.8557944567673308	0.6306346404762143	0.3368089393488387
0.5441355243132162	0.9715655972866811	0.6668434693144827
0.6634688132140576	0.6712978664185317	0.7892022586181676
0.6274321858658978	0.6826231148824164	0.8435582902597070
0.5816825729278926	0.6524734105491788	0.6984192410636166

The perfect Cu₇-CO*_P surface

O In Cu In C O

1.000000000000000					
14.444300000000001	0.000000000000000	0.000000000000000			
-7.2221499999999965	12.5091307398835685	0.000000000000000			
0.0000000000000011	0.0000000000000019	17.985499999999983			
O	In	Cu	In	C	O
71	27	1	20	1	2

Direct

0.8420158554320208	0.6125112808382543	0.4574413485560843
0.5157929122347319	0.9526870117358043	0.2880778515058146
0.1711773313645467	0.2798442891346799	0.6192171816464939
0.7934582238080122	0.9612366590510492	0.2969729245713741
0.4697903313586171	0.2933113282314961	0.6470134379232135
0.1317198246103674	0.6237207927893443	0.4686177122981214
0.3002831940589856	0.7314851459671716	0.2983088038637246
0.9772017177916130	0.0696505155517386	0.6353052638473321
0.6403656702667111	0.4055278957273797	0.4688474645910383
0.5282938827951879	0.2094784990133966	0.2708439882883517
0.1832907036620533	0.5394262252151201	0.6105325400883626
0.8569274131445754	0.8819366686551693	0.4408953070539369
0.8869792053952730	0.1291776704513001	0.4557590796433039
0.5469812101897870	0.4616283492905229	0.2895002832322403
0.2237284415843822	0.7900982742825983	0.6208220533138071
0.5390648241103787	0.7314073480020219	0.2968480890904067
0.2063239290752023	0.0759870825488391	0.6556961926829873
0.8749822311565695	0.4072497001253364	0.4689455838300704
0.7668311283521815	0.4685299724788854	0.3011101941829490
0.4370068047218882	0.8003479598731350	0.6448312905287963
0.0937999744967523	0.1332429510288557	0.4639769901165508
0.2903862685915020	0.2182668783734679	0.2707333117787370
0.9577219602969411	0.5427414172713000	0.6116427164367726
0.6192625272905693	0.8770093575939136	0.4386935726142578
0.3673013375328887	0.6565216609138045	0.4538853615696000
0.0372175006759030	0.9833874445707275	0.2890285289847596
0.7084319466032228	0.3298785091684637	0.6213839010178070
0.7692391525214469	0.7071795408894156	0.2966313983888595
0.4237302990866711	0.0253807720928541	0.6545268404589689
0.0913943907881200	0.3662490882624059	0.4681436732969946
0.0308109251899244	0.1983737001351872	0.2989952075425287
0.6860982877737594	0.5269364121089867	0.6420879385136544
0.3661992758981924	0.8574124235252465	0.4675735518044180
0.2807818188364311	0.9703046833509974	0.2695161793095772
0.9552571216693867	0.3155161583229322	0.6111263677169149

0.6283196639889286	0.6421890933648976	0.4390318516394819
0.2264413758200686	0.3173996828951375	0.3782212897856875
0.8825989036165222	0.6498395557410970	0.7065553545272051
0.5578875588980289	0.9829327118433214	0.5455159565164740
0.2675772679571938	0.9735929123942122	0.5311797553910436
0.9277281634601199	0.3058485399437975	0.3445697718471227
0.7584686608597448	0.1941884688889101	0.5349404784729967
0.4227699313206210	0.5290503528860920	0.3631949136823433
0.1004006305853062	0.8662582111571816	0.6993255472392204
0.5429384655951609	0.7182309881141489	0.5518025747914866
0.2155300190659551	0.0580891424427740	0.3883498500648615
0.8698836292874232	0.3909061948712013	0.7300519110838942
0.1836659254458993	0.8090901581356628	0.3793641059642653
0.8504099146232696	0.1351081337625440	0.7081773906509800
0.5113166049823585	0.4728199925636800	0.5427387450432883
0.5263292139619475	0.1895849288491090	0.5303808632748745
0.1928282602660756	0.5212708554610594	0.3436709312312238
0.8619395921446119	0.8685378379949482	0.7025015067902525
0.3042061957624329	0.4632491523884034	0.5332724029719909
0.9715140982349540	0.7931546870561534	0.3650336590173772
0.6324682911032450	0.1326485505924050	0.7005075988160812
0.7823421903856942	0.7259972075830073	0.5580032318412229
0.4399981090253079	0.0533783457179829	0.3889008005833726
0.1105193398396900	0.3806796784821969	0.7281293414742633
0.6899930246286815	0.2729655003259037	0.3797938365987845
0.3720496966033270	0.6159072898470842	0.7015426834371232
0.0290908978883125	0.9408384259224788	0.5435260823462863
0.3054336649035294	0.2307272518497147	0.5297454901521537
0.9774035738201372	0.5715718726329081	0.3450200934456114
0.6309303917908251	0.8866930490133899	0.6981890751912150
0.0370210662223233	0.7403980384196119	0.5354994028738721
0.7066739764183637	0.0783657880172220	0.3631505230797991
0.3649473827117197	0.3977754308730368	0.7007248931549138
0.7749298368377898	0.9567879092126220	0.5567172483094498
0.4444474378018385	0.2843521029399400	0.3909704149414351
0.1192967389282668	0.6282703462707790	0.7295277703614993
0.1397209169281566	0.1446959740141375	0.3321009829170191
0.8094586542365689	0.4831141985826770	0.6756581198288045
0.5993194239510941	0.6229188599817459	0.3200804862999982
0.2564424624492687	0.9532979163838887	0.6527175338258532
0.9247946817086362	0.2898853125348403	0.4949917071991199
0.4726412844119853	0.8089213111818735	0.5112536605957856
0.3545818485859157	0.8938273003762288	0.3311216165437274
0.0175954034435082	0.2291724056543142	0.6737987300913507

0.8765989301610114	0.8751200276238179	0.3209698535926293
0.5441567573435974	0.1999862040050980	0.6519914608846031
0.2087101552029302	0.5338047380995883	0.4938923457958749
0.6877906844712486	0.5596797981751426	0.5134583570500940
0.6045771587720981	0.3591451271660242	0.3342685382736960
0.2698339176247100	0.6849905511062085	0.6753816268527114
0.6250023763934275	0.9012179849336970	0.3193944329419015
0.2984844004099230	0.2427639010595428	0.6514697715792898
0.9648124474812386	0.5739566153887474	0.4956461261747999
0.9408356233150609	0.0293726675253483	0.5120804822791444
0.9304134820958585	0.7884013511397922	0.4873166416988870
0.4745976291170405	0.3088963531452768	0.5083441263579329
0.1445489087849069	0.6447613908414085	0.3466468995597848
0.8003582149252713	0.9742601292056770	0.6764089864078878
0.5880929812939867	0.1186608127729197	0.3252522356427752
0.2587106800935366	0.4518502815824531	0.6621651983217421
0.7108760787775669	0.0410336233535621	0.4862063613413021
0.1902314964966303	0.0632980619866720	0.5038067060533610
0.8541637166119579	0.3992076138719483	0.3471417757551533
0.5157371838629177	0.7318461968092761	0.6781656280382050
0.3814546789521494	0.3685266172964902	0.3264249161544056
0.0451369435416297	0.7044613934790364	0.6659875509574565
0.4589232030929742	0.5716345271819294	0.4854353119840091
0.4357096268180747	0.0231928241967010	0.5050577001242328
0.0996985867852787	0.3544910578802357	0.3461236452574736
0.7693620345495303	0.7014574736887119	0.6781053550635058
0.1307144285610411	0.9107266970295413	0.3252317539842031
0.7943041295815501	0.2414605904866752	0.6670088635008820
0.7001421334041539	0.3001654721154186	0.5003804803691909
0.6987896072114320	0.7991114839004863	0.4983743333499183
0.1990615229185314	0.2983170905336571	0.4983068754627204
0.2012640635689135	0.7986706145836170	0.5000049756350101
0.8702217417802902	0.1280714025920796	0.3342522704010865
0.5230428713981763	0.4832726581436005	0.6635553730861696
0.3711915558395032	0.6413569733074582	0.3331673821749441
0.0287595036123554	0.9564358328556830	0.6647455684784435
0.3665196597517890	0.1324920277880508	0.3153673176510375
0.0319404715911627	0.4656703456645165	0.6852793152278071
0.8574426014305017	0.6293488505099006	0.3355593574531825
0.5468241753159823	0.9712210395885924	0.6665530846725922
0.5450102421275584	0.7447506488181865	0.8847988383740999
0.4954904568670596	0.7843861550628026	0.8714072227585440
0.5962507511009786	0.6527326716067672	0.6951331906490760

The perfect Cu₇-H₂*_P surface

O In Cu In H

1.000000000000000				
14.4442996979000000	0.0000000000000000	0.0000000000000000		
-7.2221498489000000	12.5091304781999995	0.0000000000000000		
0.0000000000000000	0.0000000000000000	17.9855003356999994		

O	In	Cu	In	H
72	27	1	20	2

Direct

0.8424327700685662	0.6128961494335826	0.4574553503984468
0.5161202177147428	0.9531297091234396	0.2882273703936684
0.1718006472841768	0.2803968577790722	0.6192532042143106
0.7938853501465767	0.9616611445796260	0.2970105534964011
0.4705341116192406	0.2942802025208177	0.6472872213587086
0.1319794374763078	0.6242491992318001	0.4686145271860232
0.3007836803992857	0.7319804580112946	0.2986231070195249
0.9775602850426187	0.0701076850673314	0.6352799086944155
0.6408060420530850	0.4059050817843795	0.4689840320451744
0.5287523694485883	0.2099078307245329	0.2708900345798377
0.1838130838241978	0.5399653916839651	0.6103846738532007
0.8570503618914025	0.8822604972867707	0.4409543743283031
0.8873213895977592	0.1296038852590721	0.4556607764914427
0.5473750160929034	0.4621368478149541	0.2895018012745992
0.2241237781399827	0.7906784172053730	0.6208770016080188
0.5395334482294079	0.7318318084132245	0.2970723354067984
0.2067821163069079	0.0765440032140363	0.6558000707985986
0.8752390736977950	0.4075596297981302	0.4689667754148052
0.7671912098754977	0.4689294906788919	0.3010341508692974
0.4374163300431057	0.8012434251410561	0.6458536130152869
0.0942669126174069	0.1336882126695133	0.4639765475415281
0.2909854726600644	0.2189127284416350	0.2707552720452460
0.9581606370760676	0.5431779162952149	0.6116369636810103
0.6195108224496237	0.8772953633873554	0.4388151264083280
0.3677950775226936	0.6571454087182032	0.4541800669499276
0.0375612100402267	0.9838006304056205	0.2892257332156085
0.7088743386824731	0.3302012543322802	0.6214026746999497
0.7695942197695693	0.7074972032180845	0.2967533307558635
0.4240010138404411	0.0260546743401486	0.6546951069105690
0.0916609036219708	0.3664938818965532	0.4681780264835468
0.0312635336913030	0.1987982044158595	0.2990297943585001
0.6865349717911303	0.5274466855080814	0.6422244452148008
0.3665487223228144	0.8578960702494829	0.4680637621208300
0.2811899137788882	0.9708388128425935	0.2695124207144673
0.9556349298006681	0.3157670819459977	0.6111903011506835

0.6287572618166333	0.6424622789047659	0.4392679622798227
0.2268544547537021	0.3178084863189825	0.3782140035290830
0.8828663617512291	0.6500842407968970	0.7066921742398332
0.5583630331460760	0.9834100891824469	0.5456676856879393
0.2678465713684457	0.9741182106710118	0.5312861182376164
0.9281117579661479	0.3063266819926382	0.3442291898312735
0.5968111798467163	0.6533877296922137	0.6957948261338567
0.7588500188368826	0.1944345154156010	0.5349666434618666
0.4232119177130907	0.5294892889890177	0.3635138207626061
0.1006815662720310	0.8666930468182483	0.6992086387103645
0.5431830946881355	0.7186078291838863	0.5521331721360720
0.2160684152064239	0.0586616631619294	0.3883230241697970
0.8703373376189164	0.391305599995236	0.7300943001825217
0.1842480180069885	0.8097521531009527	0.3795173432889133
0.8509830424690332	0.1356029204676306	0.7084266293387229
0.5117968170572715	0.4734817206101865	0.5430455408499406
0.5266130889991345	0.1901283489481091	0.5306528688137117
0.1933374954340752	0.5217615091015427	0.3441711187637563
0.8624125478101391	0.8689942762513928	0.7025168309339026
0.3045385940701970	0.4636595879287910	0.5332386138025308
0.9718752412881945	0.7935072014642024	0.3650896378520136
0.6329774078958349	0.1333277688562283	0.7006067943952315
0.7827811986819120	0.7263426522479444	0.5581688134943540
0.4403999132182332	0.0538169872393695	0.3889855949002499
0.1110912607083814	0.3812928829811547	0.7280524195257737
0.6903818665756072	0.2733783110818722	0.3798483498051352
0.3725977981839166	0.6165423723306075	0.7013440934751717
0.0294719614540535	0.9414083353958322	0.5434519797844417
0.3059790928360350	0.2312779987869653	0.5297774296907964
0.9778586028608681	0.5720141688001361	0.3449030834564786
0.6312851572846098	0.8870527932316082	0.6985570582004625
0.0372131634029122	0.7407793545501393	0.5355489235062093
0.7071750310713010	0.0787255576362320	0.3631292390226004
0.3653300984863250	0.3983735870459215	0.7009213199886530
0.7753029732225499	0.9572271836739349	0.5568717681885788
0.4450105203498563	0.2849386062965762	0.3911034517592686
0.1196451313068520	0.6287115921229648	0.7294269706138901
0.1402021152891653	0.1451758859778227	0.3321044939381730
0.8097843203408246	0.4834472767331102	0.6756958637539231
0.5997593847545812	0.6233068910548684	0.3203047403531720
0.2568640870060628	0.9538196378723222	0.6527587083588652
0.9251621150110317	0.2902363093105721	0.4950347053334829
0.4730201461857126	0.8093628714048825	0.5116917787553344
0.3550023751620718	0.8943767626934456	0.3311518917433670

0.0181932365610049	0.2296698197177605	0.6737860244828277
0.8769049339568002	0.8754125154025275	0.3210641063610745
0.5445644259558206	0.2007200820567762	0.6521390298133182
0.2090452167361175	0.5341673338312201	0.4937048922067064
0.6882220916323778	0.5600357158135364	0.5136838187393538
0.6049874028666551	0.3595696153940726	0.3342192581730445
0.2701450759923691	0.6854459858469815	0.6753098676977631
0.6254154161861333	0.9016515845931040	0.3195257587896241
0.2990779312662527	0.2433893666593894	0.6515752708119280
0.9651140489193435	0.5742682220572368	0.4956426483469257
0.9411679990044122	0.0297619535244233	0.5120123945433075
0.9307741079908782	0.7887713283245728	0.4873598939403863
0.4750683296681763	0.3095677434730814	0.5084497145516824
0.1449496695414462	0.6453100402576770	0.3467897342425422
0.8007485529275795	0.9746593591383086	0.6765606912427712
0.5884445951425450	0.1190390594880273	0.3254011553103726
0.2591666639869827	0.4523915482735112	0.6620603958747093
0.7112634186556233	0.0413814189959820	0.4862440716569385
0.1907333861958246	0.0638262137501547	0.5038151527721211
0.8544918808103791	0.3996084563872668	0.3471845151544163
0.5162727290312656	0.7328337890293548	0.6795937491816738
0.3819337246219920	0.3690507263349180	0.3264740045015934
0.0454064065513269	0.7048927731055025	0.6659458036385079
0.4593832374709356	0.5721918642010516	0.4856998506451393
0.4360703391469462	0.0236922327360799	0.5052489293908443
0.1000631356938161	0.3548476574652119	0.3461666488919735
0.7697109852024772	0.7018610979911549	0.6782500214114474
0.1310993011387139	0.9111161059439202	0.3252191394862252
0.7947807068931938	0.2419316980594421	0.6671778981077949
0.7003728740229572	0.3003988925207056	0.5004014818147374
0.6989646187824328	0.7993898392484068	0.4986891405543477
0.1995456747994851	0.2986807825732790	0.4983493107785939
0.2015366673501689	0.7990598705294270	0.5001092599240199
0.8706952542754062	0.1285552899705006	0.3341786782962402
0.5234360057618271	0.4841284316571531	0.6638093369973871
0.3718110135050099	0.6419900306309478	0.3335322984218900
0.0292416623759186	0.9569506431330596	0.6646399865697907
0.3669580378837707	0.1330142509583901	0.3153715440886587
0.0323761688636916	0.4660837277115379	0.6851568602279693
0.8578038833181456	0.6297150982893295	0.3356503011211571
0.5474058243963301	0.9719567162435104	0.6666484028268147
0.5897276912817807	0.6535901804680645	0.8588057790921251
0.5813281981460795	0.6315399964543766	0.8968336133130468

The perfect Cu₇-[TS-2H]* surface

O	In	Cu	In	H
1.000000000000000				
14.4442996979000000		0.0000000000000000		0.0000000000000000
-7.2221498489000000		12.5091304781999995		0.0000000000000000
0.0000000000000000		0.0000000000000000		17.9855003356999994

O	In	Cu	In	H
72	27	1	20	2

Direct

0.8419927928757152	0.6137865863218090	0.4582011238054740
0.5160462871786478	0.9538739145376901	0.2886770296300694
0.1698748042216418	0.2805574585742698	0.6183843640805560
0.7934722638931193	0.9624506534208133	0.2977054069732121
0.4686829879671344	0.2919832181152953	0.6514502548681393
0.1321843591081051	0.6253209399257811	0.4693124462347606
0.3011366245570256	0.7326017607959310	0.2997609434680625
0.9773394814542796	0.0711444900434487	0.6357189331553081
0.6399472271188918	0.4064379717638555	0.4681096871843484
0.5287030392609787	0.2105799326792715	0.2707293575132743
0.1843367242435706	0.5413770626704416	0.6108965236243434
0.8566142684699881	0.8830934912740653	0.4416211867080204
0.8871586958843731	0.1307335736215751	0.4563836323672893
0.5471265503581594	0.4630772671049940	0.2898929447834904
0.2239211991408742	0.7915918818920482	0.6214975693828609
0.5393283477070372	0.7324276576542451	0.2984597501469899
0.2056715776396805	0.0764724865716741	0.6565310593473497
0.8747230785497596	0.4086560066119015	0.4695618964112907
0.7674342890303082	0.4699732866286850	0.3011213111266022
0.4375513466006626	0.8039029731683285	0.6461317883395524
0.0938185004023516	0.1339982868348210	0.4637698601823267
0.2904049366367227	0.2198164009339122	0.2705061000011827
0.9589901343251122	0.5445710272140388	0.6120400608319044
0.6190982220475266	0.8779266213267554	0.4399030111842893
0.3685189542773265	0.6579251011534222	0.4560174343435892
0.0370886278820920	0.9843481876372963	0.2894579002174592
0.7083402962088111	0.3313116589166686	0.6218166221662728
0.7688208009081734	0.7081065799407965	0.2981190943492371
0.4239088990298881	0.0273403388197589	0.6555844861887624
0.0912641557680149	0.3673676797620429	0.4685908364072013
0.0307289007678155	0.1996877396249722	0.2993778318678975
0.6891963017644522	0.5300752201361003	0.6406824726639090
0.3666578225361105	0.8587761231644585	0.4687663250635581
0.2809458313843554	0.9712657689748287	0.2695656238269883
0.9554774402314868	0.3172802203378009	0.6116150848814784

0.6276294494508766	0.6422542943866321	0.4412037244862361
0.2264230785862406	0.3183702942460227	0.3784001491616542
0.8837717305330802	0.6511330900910184	0.7077559582256937
0.5583304585469419	0.9853184736990928	0.5461651933031667
0.2678281878980462	0.9751242137317901	0.5318030861207725
0.9278797590593920	0.3073203023497499	0.3449101998959239
0.5981319593861746	0.6613429679620711	0.7020360359813519
0.7584955367466987	0.1957513010709475	0.5354862565099614
0.4232440335829302	0.5298343841130830	0.3654086867470613
0.1006189685483281	0.8675132263992901	0.6998018283212807
0.5440034707330247	0.7196670902125927	0.5544407436253351
0.2160222262562097	0.0595195871672079	0.3881184857196110
0.8707549978801536	0.3927255519142324	0.7304788009081719
0.1842611566155535	0.8107679577484619	0.3799814232001976
0.8514038873433479	0.1372956932722094	0.7091616616635595
0.5113425893163259	0.4715202079754415	0.5457949017002093
0.5254760879149578	0.1915240319880601	0.5313333704599266
0.1934625543405785	0.5226771046944031	0.3453654864311801
0.8630666392726812	0.8705856575396551	0.7033124945431942
0.3040893938971524	0.4637969415103072	0.5337961995385515
0.9717228374975831	0.7943974412012714	0.3656154244307706
0.6334934326840884	0.1346538879284597	0.7015973380366167
0.7829050667715094	0.7279591624010149	0.5590193840570251
0.4401292009710187	0.0548849086387056	0.3891786265914760
0.1119561244456206	0.3826317182733808	0.7282400909589289
0.6900965370286393	0.2741150532227751	0.3800248614433152
0.3729184314913166	0.6188569591677362	0.7026057931172422
0.0293320165413683	0.9423962709904304	0.5439154010635993
0.3056815964545522	0.2311913350929452	0.5303787388078824
0.9778760169300841	0.5731280422859427	0.3461628713383921
0.6317292755001247	0.8900903274663324	0.6996637413886445
0.0372506175086062	0.7419471070867469	0.5358678329973251
0.7067366818110150	0.0794208507615300	0.3639286557597326
0.3628215538674944	0.3963629491967844	0.7002181857131350
0.7750869140461346	0.9584391417509999	0.5576868121629275
0.4440886795121958	0.2849163623568589	0.3900983552160229
0.1201207213791046	0.6297920346615036	0.7302699849521890
0.1397470113328337	0.1458776714697491	0.3320702950729527
0.8107974298428489	0.4848196524472689	0.6757534062986396
0.5991243396493602	0.6237449667441338	0.3220071712866874
0.2566826369367297	0.9546261093688071	0.6532975497992254
0.9248789022801814	0.2914291729215836	0.4955736732950973
0.4729918317372486	0.8102424053204842	0.5132424386297861
0.3548858623003604	0.8951423270168241	0.3316467700047116

0.0182672876933354	0.2311841514284221	0.6740032169760567
0.8765109676614740	0.8762241388178077	0.3217403508109933
0.5448674270522407	0.2008950379846166	0.6528211361009323
0.2090291472441597	0.5349947890914912	0.4944218760509736
0.6878701156416877	0.5601931654046821	0.5146956651221343
0.6049628877775842	0.3604174380688895	0.3338516377988829
0.2706114947857080	0.6867110404772255	0.6760861739029399
0.6250506075132896	0.9022974735084682	0.3204847623549357
0.2951510599331268	0.2422825893787735	0.6518603568600236
0.9652231537057824	0.5755189527947010	0.4959533659862129
0.9410290654720713	0.0308646203000492	0.5126310128464017
0.9305598774740580	0.7897503477830470	0.4879000964971105
0.4737882492400591	0.3095157202980865	0.5066363922663552
0.1450882816601182	0.6462919086151953	0.3475429590180803
0.8014066401614374	0.9763740018700930	0.6772991456680197
0.5882380723605609	0.1197948621406792	0.3256709473347558
0.2607167197204461	0.4543947037242174	0.6624478651698108
0.7110852788142444	0.0424577017583193	0.4869652039521078
0.1901302720712083	0.0639783479048171	0.5035321977471906
0.8543358662555700	0.4006302148152212	0.3476983646955937
0.5177851388930674	0.7380224046868116	0.6814223831796582
0.3814407903521354	0.3700417668726237	0.3263495149478552
0.0461915754220772	0.7060290740580010	0.6667490548667319
0.4596789495924473	0.5722711981562222	0.4887318061998576
0.4358482792958034	0.0247277385437259	0.5053335920784187
0.0997378456962486	0.3557385955081353	0.3466641988495046
0.7725195522689222	0.7037686105415043	0.6784479846040531
0.1308202196015288	0.9117434448621768	0.3254308082781918
0.7950461266712405	0.2433437660590093	0.6677842168826502
0.6999381920626968	0.3015401947871376	0.5006936729280119
0.6988819156802156	0.8004823651019133	0.4996764857856454
0.1986990469910838	0.2990782400434917	0.4983870914944952
0.2015907581657409	0.7999266511234289	0.5007242652007494
0.8703094531270374	0.1293873895461976	0.3348820261497038
0.5237537625680724	0.4675563562732609	0.6675142974360314
0.3720879989703746	0.6426440644467144	0.3354440892974150
0.0292186097606699	0.9580105332457522	0.6652283452582375
0.3665621775659881	0.1336949446943615	0.3147036874862640
0.0331975502769932	0.4674471236243175	0.6857540654114086
0.8574487718092307	0.6305507027429522	0.3363894711287623
0.5471098883017559	0.9738272937044370	0.6671988679395338
0.5806459972420740	0.5939126856862457	0.7574494845605817
0.5729868113402190	0.5329260739444037	0.7802128099039691

The perfect Cu₇-2H* surface

O In Cu In H

1.000000000000000				
14.4442996979000000	0.0000000000000000	0.0000000000000000		
-7.2221498489000000	12.5091304781999995	0.0000000000000000		
0.0000000000000000	0.0000000000000000	17.9855003356999994		

O	In	Cu	In	H
72	27	1	20	2

Direct

0.8418416828428583	0.6137790938753539	0.4581237605032105
0.5158645526850958	0.9532060772298026	0.2875904599946147
0.1657578412056986	0.2783112841967070	0.6158358794853986
0.7926611585205113	0.9613942080399700	0.2967293205341133
0.4646182891682238	0.2868346141711658	0.6476051864964987
0.1321631549707065	0.6249034116218608	0.4687341350084034
0.3014696829018259	0.7311576974395922	0.2997334134688451
0.9756419233461284	0.0693915784785446	0.6348733691551908
0.6387887598479591	0.4063152954088249	0.4678077438937476
0.5282624672437821	0.2106910000021844	0.2707035592221668
0.1852214489918519	0.5409431849736830	0.6102665158519911
0.8560362061507335	0.8828306353847949	0.4404959042738608
0.8863180985069136	0.1301052945744502	0.4554481888516818
0.5463133858976030	0.4620225954474496	0.2901406056948119
0.2238455552128694	0.7912831916299270	0.6205693330085591
0.5388903660383223	0.7309156132757645	0.2988595531125318
0.2045891511744102	0.0757508858034811	0.6544380645117180
0.8741602713492008	0.4084163649228068	0.4689235706618590
0.7664166079371932	0.4692268381303811	0.3012938315450103
0.4355940818984332	0.8058351140514414	0.6448596567249998
0.0923926034456192	0.1324574702992164	0.4616685415195958
0.2902457632370973	0.2191819393150140	0.2702961031670508
0.9601191202883023	0.5449464691539545	0.6114261789169618
0.6189422638491932	0.8775411558968097	0.4390638913534469
0.3687535373020809	0.6568796805141454	0.4566900071192470
0.0363933202206161	0.9832244085176434	0.2881805400936358
0.7077638729302544	0.3315699589863911	0.6212709636942232
0.7675573982313422	0.7069051266019304	0.2987843702919096
0.4232896438653413	0.0270513735256829	0.6555729957472186
0.0901963485000870	0.3667314471351497	0.4673733818587782
0.0296233672076663	0.1985817588828760	0.2979802402499149
0.6985848250500658	0.5357010158505523	0.6372621816437920
0.3664098963922253	0.8584798031228175	0.4674017309178505
0.2806380304165577	0.9704688354033337	0.2684118921004690
0.9546946961455712	0.3169996191270773	0.6105302688040278

0.6267957944357018	0.6405537789764346	0.4429033630247273
0.2248218761090812	0.3173961717692157	0.3769643466651525
0.8889412841378833	0.6513207517934443	0.7115689108971828
0.5576988229385371	0.9851534849485285	0.5449113998441918
0.2679709960530359	0.9748688533797905	0.5305966927903141
0.9269692133615417	0.3064637317642261	0.3438997593271485
0.6036828459579254	0.6758985097578345	0.7046658022160974
0.7578224015244710	0.1953761840354522	0.5348254374488268
0.4234299485941538	0.5285355603972481	0.3674839437465297
0.1009426334611589	0.8676988409368385	0.6988251491722243
0.5443136518374934	0.7208259814925518	0.5551040986699856
0.2152488509522769	0.0581268743134658	0.3870414643866967
0.8710889065244594	0.3921271654425295	0.7296850512492646
0.1838142044203230	0.8097044015150628	0.3786845344558052
0.8498833682532775	0.1361662948341256	0.7075250535359572
0.5134628482812729	0.4721954148673719	0.5530725373461072
0.5256122158474459	0.1908258465165130	0.5302876712967372
0.1933612557067521	0.5217011319536790	0.3456048373895211
0.8631316927059928	0.8699578985053498	0.7034403423270309
0.3029037630988137	0.4620508320811199	0.5330357923554175
0.9713940877813441	0.7936973563793711	0.3646403968153164
0.6334873195099712	0.1358501613550616	0.7014842537200496
0.7853134343530013	0.7314268485649780	0.5586339176763609
0.4395015975452351	0.0538807797163484	0.3876548598381510
0.1114479564402321	0.3817632560386404	0.7270984780630173
0.6895642462218132	0.2732912177024396	0.3797643543816612
0.3751685306752486	0.6225226471590918	0.7019257650801308
0.0293067202786440	0.9422859412832733	0.5428105304034505
0.3036657433612406	0.2309223058442497	0.5286880119281930
0.9775567709765806	0.5722034035008970	0.3455600292480275
0.6297633269832332	0.8928728692485728	0.6988623700096486
0.0375365170460241	0.7420212601054937	0.5350078382441571
0.7061541381054427	0.0787450381443166	0.3629153072712393
0.3586145825096324	0.3935197072499125	0.6983363759747259
0.7742206996753541	0.9580311555008409	0.5568248730049220
0.4431217129819131	0.2842942851295949	0.3915596684240664
0.1204542663967935	0.6289953590286159	0.7300301569701454
0.1388111720350217	0.1447232223467677	0.3308144869262586
0.8124627527461720	0.4851973980273984	0.6755471837332977
0.5981228860444786	0.6219997454232081	0.3234905761529723
0.2565087425793289	0.9547377186491872	0.6520323536581808
0.9240536592119015	0.2909528834145840	0.4944890087001026
0.4729715714998902	0.8100018365856158	0.5114785213432577
0.3544684697320362	0.8940187755817978	0.3302114718032947

0.0166613754734317	0.2302592729747782	0.6727652558632576
0.8758298839905578	0.8753016384680926	0.3208151526931097
0.5444563932972197	0.2004464709994558	0.6518570558015788
0.2087659315994846	0.5340841644282444	0.4932149630074326
0.6881090410330608	0.5597237699164271	0.5162417882289635
0.6039018361031703	0.3597636808666409	0.3350960857929703
0.2696091699081604	0.6861348807375544	0.6753689078213866
0.6243956198135018	0.9011816424152904	0.3195682971795501
0.2917208976868625	0.2416985760083942	0.6499707525780218
0.9651336984796831	0.5752973531589566	0.4953201190819814
0.9403168563439438	0.0300886092524282	0.5113564559515370
0.9308456476605479	0.7898215917156294	0.4866337472220905
0.4734214026076051	0.3108368187556937	0.5089098354338224
0.1449172113484873	0.6452943530074264	0.3468135814423304
0.8005401570776378	0.9754444336036279	0.6758612078634454
0.5879311389398312	0.1194170900858668	0.3246063988990567
0.2602906886447240	0.4531034908025109	0.6607255384719185
0.7106167529680116	0.0423599055845226	0.4859411565336604
0.1897948688004757	0.0636651340660034	0.5022319494278323
0.8535276212063931	0.3998618336371516	0.3470989354009644
0.5155535754727196	0.7439057106315529	0.6809831477606157
0.3809301861024200	0.3690407308486247	0.3270946572869355
0.0479877562455728	0.7061260290986181	0.6663861382268947
0.4604167635994282	0.5705648813597207	0.4923112108003231
0.4356697600992191	0.0248607605497744	0.5034272539015073
0.0985466293178912	0.3547016448645586	0.3454192756779086
0.7821390965062792	0.7045780839892657	0.6765616144993455
0.1304401752879020	0.9107330262207231	0.3241129147907034
0.7945244161086685	0.2434128763802421	0.6663880224354973
0.6991136448736395	0.3014809157359509	0.5001752228704133
0.6986004792198900	0.8001634628268185	0.4992538743423690
0.1966285956828602	0.2976247674289409	0.4966538104729694
0.2014621057285032	0.7995846866336406	0.4994082433395532
0.8695182867811113	0.1283590299627373	0.3337920694214177
0.5274593203629460	0.4579457702499924	0.6782618071598144
0.3722110919169791	0.6410411695882726	0.3363588552452937
0.0296370857463269	0.9583524414623027	0.6640073234263899
0.3661088769063018	0.1330363235893350	0.3144444274702669
0.0332486762422438	0.4666868958708311	0.6850776781975485
0.8567011034756723	0.6295867789939896	0.3363515331187224
0.5462690576524614	0.9763089466624866	0.6656958092610554
0.5912136676999079	0.6590621071845654	0.7573504859850114
0.5757681804847771	0.4811996267632131	0.7707743547307970

The perfect Pt₇-[TS-H₂O]* surface

O In Cu In H

1.000000000000000				
14.4442996979000000	0.0000000000000000	0.0000000000000000		
-7.2221498489000000	12.5091304781999995	0.0000000000000000		
0.0000000000000000	0.0000000000000000	17.9855003356999994		

O	In	Cu	In	H
72	27	1	20	2

Direct

0.8413806474620340	0.6125932851533947	0.4574832186560920
0.5155240059486882	0.9520153462886651	0.2880222084792754
0.1670055507328588	0.2778554271957606	0.6165990060561115
0.7923808840796992	0.9603469391667372	0.2973506885774322
0.4645491661871581	0.2852662495842507	0.6566078059230696
0.1327002992682742	0.6239775371090409	0.4685501830571325
0.3014238971291454	0.7305935669713587	0.2998839110087475
0.9755434306422028	0.0685349111445496	0.6350565475694525
0.6390580084936645	0.4049993326629387	0.4659025191242544
0.5283133326830255	0.2089879456860737	0.2689647713593333
0.1846238411435820	0.5398814681516650	0.6105173554262509
0.8552269824092157	0.8810701884806179	0.4412183388695136
0.8862056725300371	0.1286939957398301	0.4558531291263924
0.5462900627376311	0.4616182430883693	0.2888636083779518
0.2219827836475438	0.7899953627101263	0.6204089540369934
0.5388083874451475	0.7302664488270579	0.2990328814683257
0.2035778152202345	0.0736223287744926	0.6543371448521815
0.8737321966637819	0.4072517591538188	0.4687184354387900
0.7672576057855840	0.4684013530776676	0.2997665661457160
0.4338916417382511	0.8072865175567802	0.6415378518577503
0.0930504542467665	0.1321560615979801	0.4626960026543629
0.2893560957795728	0.2182727294714975	0.2691965457003675
0.9605926410588339	0.5437792680442397	0.6105981231009616
0.6179488421971979	0.8755980803970366	0.4403090640928315
0.3691307784400097	0.6561109147034376	0.4571098978882186
0.0360773167344392	0.9826171615836919	0.2887598655294242
0.7075944208111875	0.3302519766384422	0.6203802613862273
0.7672500543880858	0.7059648327237124	0.2985262319535116
0.4225933943796561	0.0275613473807695	0.6556723099851390
0.0910507590478455	0.3661950757801805	0.4677623868353494
0.0298570772691522	0.1979830600910916	0.2986291936980340
0.6975071155304016	0.5326506812049465	0.6385883905459232
0.3664051467148910	0.8577094673527051	0.4669756068147217
0.2803238194068212	0.9693380437741389	0.2683399560199232
0.9551975419027443	0.3157463121858667	0.6103253938983116

0.6267490652023266	0.6394000712248791	0.4429379695350560
0.2256782917401443	0.3164617754508373	0.3776941506431608
0.8895648394773245	0.6485766947385065	0.7117375447242491
0.5578322231749090	0.9863492505368703	0.5442818086186146
0.2675643540530468	0.9737874918784531	0.5304971375024319
0.9271655865030102	0.3054299930771122	0.3449917925511735
0.6074135810711608	0.6911550348006068	0.7223772514148957
0.7580685681618384	0.1947896411039755	0.5344882649796689
0.4233622170958765	0.5276706442593433	0.3669547359965737
0.0996099844198616	0.8659600134919405	0.6989307047319597
0.5445511436444143	0.7178041771526197	0.5570445171137328
0.2155621834046901	0.0579092266017043	0.3870055878299078
0.8713706503839554	0.3904630465669982	0.7291978943242785
0.1832411761896122	0.8087979153314018	0.3785865879783115
0.8513924240955675	0.1363558148609317	0.7085283123525239
0.5120998171688481	0.4673484814404529	0.5495374499196005
0.5238411933710808	0.1911476467270029	0.5306319076347848
0.1935505433268752	0.5208597263339905	0.3447861647283965
0.8627488482111555	0.8689483438836335	0.7039364629604301
0.3039969489063178	0.4616767807870464	0.5342466412157819
0.9709125334267052	0.7927302767968061	0.3642484358400239
0.6337231532602744	0.1351720231290233	0.7011776133956571
0.7845556091074030	0.7283121577798601	0.5592653619035405
0.4395447932915412	0.0541012217116807	0.3874881784605169
0.1118506492320852	0.3810160344119102	0.7278017564576997
0.6892626209650393	0.2722903129758589	0.3787680435134300
0.3723560706028278	0.6217318455950276	0.7044132541226656
0.0287142064155823	0.9408659948761379	0.5428793102407632
0.3054208553068259	0.2297516768857939	0.5299046150021708
0.9774568407853109	0.5713451393204332	0.3464302820127361
0.6304472455564257	0.8965070519197237	0.7015091628569061
0.0369270796226529	0.7406194693246614	0.5342161308972558
0.7059174961673685	0.0774476363815896	0.3633424347005141
0.3566069927285105	0.3894511774486614	0.7013846312798035
0.7737623884413568	0.9567949488852570	0.5575387759502588
0.4430818586072370	0.2828974023625201	0.3880973309420846
0.1203580633398061	0.6279265378560833	0.7299839312997251
0.1389874598401186	0.1441362264110654	0.3312402952206189
0.8134012361613306	0.4828715549242616	0.6743968246186548
0.5980322428346828	0.6213950581991713	0.3233269629459621
0.2556780969976123	0.9530635219213860	0.6520870321017530
0.9243943268745064	0.2901900965989300	0.4942995219049677
0.4720327763758544	0.8085386372345299	0.5139805740034863
0.3542858935354209	0.8932105642870702	0.3309964969540540

0.0177834004422989	0.2299410797835044	0.6730437724620874
0.8754702197542620	0.8743455324255109	0.3212467983792793
0.5449273812484428	0.1998900849761198	0.6521552636783216
0.2091875488003016	0.5333726891903806	0.4943858797425292
0.6881258786770169	0.5577133326830533	0.5152947772879883
0.6044001568702170	0.3588226114336738	0.3319741300248589
0.2702353772096419	0.6860783543006761	0.6752360271346323
0.6239930909202924	0.9001088814134903	0.3206800868605527
0.2905140185616783	0.2389199190946484	0.6512922548431550
0.9653876395616350	0.5743754067403780	0.4944273375810616
0.9402390591450616	0.0290901627075374	0.5118731983512153
0.9306532005965703	0.7886244919170367	0.4863715751716553
0.4726381213603879	0.3085093814390962	0.5039287976401067
0.1449829571952835	0.6443098783080444	0.3468829063784022
0.8002193282912541	0.9755729949355482	0.6764247294530339
0.5876963743493880	0.1181349524416108	0.3243161358578153
0.2622528750261092	0.4550074302704326	0.6636312103268911
0.7101543456765445	0.0410849826628805	0.4862473552671190
0.1896038114441607	0.0625176178001257	0.5024502785597078
0.8536266339737841	0.3988503080982207	0.3470120998737903
0.5161759527647981	0.7487236922719694	0.6851024923589981
0.3804773098410957	0.3685964699506816	0.3253351531211155
0.0488051463792126	0.7048132857382824	0.6660262134794698
0.4602651600317998	0.5699109260842857	0.4917484445206236
0.4351748449653312	0.0241294962629043	0.5032328335422088
0.0992304560249359	0.3540453625845409	0.3460309728757109
0.7858469995664721	0.7038473383017818	0.6768197044590515
0.1302381522232028	0.9101381870799882	0.3242593540135029
0.7948337714385689	0.2416793664596121	0.6660222494737583
0.6988798530787954	0.3001873698030131	0.4994820041734335
0.6978347120645838	0.7985805303646228	0.5003949908100880
0.1977219879942013	0.2974600486317545	0.4977277854422550
0.2014244679314043	0.7986449073870873	0.4993167097166186
0.8695239013994553	0.1272943033367163	0.3343434086447697
0.5228044859749842	0.4531644557218532	0.6725031959528432
0.3721440092259492	0.6406161110501104	0.3365654521493207
0.0292336141698276	0.9573106482704731	0.6641843838739877
0.3658070023353583	0.1320200818725996	0.3129101626745981
0.0340268637926377	0.4658834462434466	0.6848660360812276
0.8564324790181743	0.6286218417543427	0.3358396087985442
0.5442654592531118	0.9756589061477375	0.6651827172825120
0.6250800618507293	0.7181485469802340	0.7732968772775044
0.5748519091911725	0.5700698121599534	0.7347819203898543

The perfect Cu₇-H₂O* surface

O In Cu In H

1.000000000000000				
14.4442996979000000	0.0000000000000000	0.0000000000000000		
-7.2221498489000000	12.5091304781999995	0.0000000000000000		
0.0000000000000000	0.0000000000000000	17.9855003356999994		

O	In	Cu	In	H
72	27	1	20	2

Direct

0.8402645459596637	0.6121674034952533	0.4554677132833677
0.5148999128604910	0.9515089773220440	0.2884454354838392
0.1725528652770516	0.2803794962930897	0.6189983781180989
0.7920003000780977	0.9598099706561209	0.2982725539961686
0.4611706944827871	0.2784958004167338	0.6616016926536398
0.1318357557340497	0.6239673895191847	0.4676909975836163
0.2997185309171763	0.7299037500041737	0.2986930150763254
0.9766621644881134	0.0705890520150494	0.6336156116243057
0.6403868738498155	0.4055000303529128	0.4663076310572873
0.5285852640957034	0.2077797124965710	0.2657939991841047
0.1821421738746385	0.5383688308543534	0.6080252791189540
0.8533229042315285	0.8781250143945942	0.4426741879937347
0.8855630416161837	0.1280339509644521	0.4556813975000290
0.5462665124141003	0.4621706275034005	0.2864081259306277
0.2160354293694292	0.7880555969079367	0.6185070715710451
0.5380956889759021	0.7305567882305891	0.2973693522961290
0.2036144712991273	0.0734872195294623	0.6551941418108305
0.8732737680743088	0.4063256033790673	0.4680155890125661
0.7676384556486070	0.4680794669227155	0.2975504740168771
0.4232844055820550	0.8094040486094617	0.6315168369173983
0.0941046928432007	0.1331441932273010	0.4636188454694385
0.2891780160918863	0.2182155562041815	0.2671500361052608
0.9555357894934129	0.5406000268604069	0.6100672513914012
0.6164381013628742	0.8734699266426562	0.4408803063066303
0.3698366797380977	0.6565775506158392	0.4559635083157390
0.0353740402889839	0.9828143242457927	0.2889071367212976
0.7038860842479105	0.3320506667395710	0.6214227405810381
0.7669213151236012	0.7056648163110896	0.2974350689018567
0.4212384239710747	0.0251491070029307	0.6561003227360214
0.0914943935988766	0.3643716310407458	0.4679443038955545
0.0299622209524433	0.1978423419206576	0.2984968638190039
0.6834062662849814	0.5337866803652263	0.6631889301856848
0.3651061899141246	0.8585818457926720	0.4626464181211977
0.2796731074794247	0.9685648982884643	0.2674239733066066
0.9556832197138800	0.3142021335383594	0.6100754874110735

0.6255603439492297	0.6415755810005076	0.4409102269409893
0.2267034822529334	0.3160412224529132	0.3773285584572493
0.8898481432278266	0.6446891846772032	0.7118558955175089
0.5582407045977563	0.9875558931123811	0.5427020957382463
0.2674542794948512	0.9739603491330302	0.5300140756299042
0.9271272262592648	0.3049528639277416	0.3453081347947130
0.6653229072284470	0.7088246071131028	0.7695732506875569
0.7585488732805024	0.1958496815597929	0.5351749524641072
0.4231106246239970	0.5277631311766970	0.3648727521437645
0.0969571196495562	0.8644455761046161	0.6978267813790472
0.5435006876029153	0.7148497891596339	0.5594955215498217
0.2160326449385070	0.0589222757879850	0.3859542041234896
0.8704464168144032	0.3868672132626556	0.7292183154904280
0.1810617852641232	0.8082436113849927	0.3775407712373906
0.8529368474481115	0.1365510019928736	0.7100717366961821
0.5146926412856292	0.4668017566382894	0.5450548918021425
0.5239865542094631	0.1910336557768852	0.5301469529837352
0.1933270708497080	0.5205598664122524	0.3468127614064001
0.8643562671773323	0.8710298122050695	0.7013320035124593
0.3051200786121578	0.4620927052035859	0.5334943774009772
0.9700170807473611	0.7927131124555648	0.3635303329755298
0.6335793235831501	0.1298069195107788	0.6981741195063443
0.7798890581075737	0.7190481494599821	0.5620631951216267
0.4393470752513460	0.0561729465721185	0.3865008176459702
0.1122158228599061	0.3808019100809142	0.7275324026148130
0.6881027627845742	0.2726320705451344	0.3779962229979972
0.3674494618428172	0.6168223921499049	0.7038749161621590
0.0283977946327969	0.9405354824027596	0.5420231201193726
0.3077916680129156	0.2303911168969384	0.5299835484331806
0.9763626726374689	0.5705355783443771	0.3457808635480553
0.6295280753831007	0.8853870309884243	0.7011148435957834
0.0344117375741911	0.7386696548635551	0.5329699573239584
0.7054701597317231	0.0772006160376068	0.3636154805378041
0.3666804128800632	0.3973377298420394	0.7007691960610661
0.7734851991506267	0.9568276222203995	0.5572014945731658
0.4447427413906438	0.2834429790922341	0.3840169962187944
0.1191316834580885	0.6261757699110386	0.7281209492096096
0.1395255109243571	0.1444475055968611	0.3303643721280911
0.8106099556198070	0.4794382998033222	0.6780941021998390
0.5976340470315028	0.6221809484364088	0.3205497987291573
0.2545900968281583	0.9514175596363262	0.6520300253071007
0.9247442782730892	0.2898275313699387	0.4939963922977036
0.4693760395329297	0.8088878549352078	0.5129696449206621
0.3535954517389394	0.8929122925370243	0.3312512184504863

0.0190250664808052	0.2298670866632403	0.6736742856510256
0.8748333309821306	0.8737193745014570	0.3215926452796377
0.5430265929309380	0.1945966473174955	0.6520883908226829
0.2085356563941560	0.5329443148439436	0.4923651176503349
0.6870957083778580	0.5595608368810753	0.5095497084129926
0.6046735453970807	0.3582024413196223	0.3265632853039460
0.2688478429891453	0.6857435801594211	0.6720749561441766
0.6233697248310442	0.8997130617512151	0.3211232747941558
0.2924714954284174	0.2385467590396170	0.6522059989886536
0.9642264208633665	0.5731117377157618	0.4939025550203271
0.9403028903825815	0.0292219325268668	0.5116571322958533
0.9297463238263733	0.7875932133564555	0.4860873679581011
0.4725584760822437	0.3051488844353986	0.4987684400052129
0.1438934338757901	0.6441904797405210	0.3461718639267111
0.7989111895756367	0.9766611153134686	0.6760459774440145
0.5872735502194787	0.1177868653696840	0.3238621801820311
0.2616956837862231	0.4558193173548143	0.6630318430545805
0.7094848557399376	0.0411019590788354	0.4859350897160531
0.1898303041063436	0.0623422004631773	0.5015583045173001
0.8529906050978605	0.3979976024407614	0.3463131462741357
0.5054869553232346	0.7358574008025806	0.6750657600695373
0.3802451836007750	0.3689254491558399	0.3227311078310009
0.0479552101900994	0.7032083749096578	0.6641650126730039
0.4592548479733320	0.5706363696042489	0.4892063367768735
0.4347598291580309	0.0236286609685909	0.5021930765193402
0.0994718257439460	0.3534065999677256	0.3461321784935689
0.7911427556786071	0.7056783966133876	0.6819119525392571
0.1296963211274975	0.9103536173700721	0.3234601969314266
0.7945996718912344	0.2390275654892063	0.6657621624762343
0.6993812222686486	0.3004218219860860	0.4996039305226671
0.6967783257433602	0.7983043566002972	0.5020261812833844
0.1995048151762092	0.2978364348772253	0.4979671906662655
0.2001995608246539	0.7987230499208136	0.4980331380277133
0.8693249211675025	0.1270556815441686	0.3341288786367420
0.5193569741492745	0.4458302868439126	0.6635201339932943
0.3716807801461218	0.6411608317045974	0.3350579746862472
0.0302324960707572	0.9590274902464677	0.6633112054505463
0.3656894669668189	0.1314402342438489	0.3099506344805205
0.0331865853370398	0.4647006833607960	0.6834396201639683
0.8568728765662080	0.6286689670537053	0.3337419763486639
0.5425108163201647	0.9677431429306171	0.6644817989846056
0.6543074756419677	0.7700053102728039	0.7615930170398936
0.5979268981847954	0.6515249723280963	0.7883213246782067

The perfect Pd₇ doped c-In₂O₃(111) surface

O In Pd In

1.000000000000000			
14.4442996979000000	0.0000000000000000	0.0000000000000000	
-7.2221498489000000	12.5091304781999995	0.0000000000000000	
0.0000000000000000	0.0000000000000000	17.9855003356999994	

O	In	Pd	In
72	27	1	20

Direct

0.8414496840590873	0.6131472363712041	0.4571065592595657
0.5153198917402106	0.9524954601784594	0.2893502256114996
0.1714568606888001	0.2797771785224225	0.6197908097901589
0.7931230016350016	0.9610678079259036	0.2974206160171586
0.4715561202749758	0.2945242358594947	0.6502220458335954
0.1325581323348055	0.6250003898321436	0.4692060591724548
0.3007454752717000	0.7320709930644462	0.2999087513378489
0.9783920922956295	0.0706016628741591	0.6357564206947554
0.6406582951578041	0.4061968335957773	0.4673667963276326
0.5284948863008202	0.2095669005723362	0.2709258714228017
0.1820875357981748	0.5389620573590455	0.6101532269378515
0.8574652396135698	0.8825149378959364	0.4409433729697823
0.8875286098829963	0.1292887139941218	0.4557227705421759
0.5476744021749367	0.4628949075525385	0.2901896260245431
0.2214721299374002	0.7899642893304444	0.6208693689312590
0.5390307834452365	0.7319486509725033	0.2975789594129067
0.2067330027965862	0.0762801666514730	0.6537490691945637
0.8746889799556745	0.4077412576085633	0.4691757033777401
0.7677073305439664	0.4687405089259907	0.3002988717822117
0.4339685161668693	0.8030607071841958	0.6448467784169549
0.0948603247448810	0.1344544021398895	0.4647938314791429
0.2903942775792296	0.2189415080227836	0.2707671691298708
0.9581236430154595	0.5436574135595545	0.6111607142961958
0.6179919941493602	0.8746850943260960	0.4406160739634160
0.3708937486011245	0.6581170946907086	0.4563256942115484
0.0372690599400331	0.9844013140066858	0.2897657836083568
0.7093944108683017	0.3291049061612832	0.6207602575712615
0.7681110485247682	0.7069696051204485	0.2980179444787331
0.4242309404038303	0.0270604204005749	0.6526158927628039
0.0916789914122363	0.3661072880686372	0.4689652281121713
0.0313503254293006	0.1992812138200663	0.2995115543235707
0.6895607306049764	0.5248166709063200	0.6389343213198974
0.3657212885842114	0.8585880736000048	0.4677067724681159
0.2810309274039954	0.9710092975313829	0.2703612854005742
0.9553896069290737	0.3156667371647141	0.6107162291624841

0.6261258070207288	0.6441224138846549	0.4417565834139598
0.2272849768899824	0.3180921085549295	0.3789512834200188
0.8833173118123232	0.6494784308203646	0.7083047634091070
0.5584929028604722	0.9845733728259026	0.5451856288031032
0.2671656930273477	0.9737644009926667	0.5312063625190554
0.9281457983831161	0.3061434927594707	0.3459267810829057
0.6008451562902586	0.6448458652301097	0.7006522167762879
0.7587389511871813	0.1942431093524113	0.5344727587278405
0.4230034549419185	0.5294199951718320	0.3643292816812975
0.1011117218350960	0.8672026101236592	0.7000009732649778
0.5436742158758766	0.7202369995170729	0.5577086344514814
0.2157843553664917	0.0591832863586431	0.3891083647494924
0.8700694702135271	0.3912501888914030	0.7298890684834306
0.1831619665076580	0.8097253592656607	0.3798024601472179
0.8529731661645105	0.1378564689087657	0.7098895415768499
0.5119043295743734	0.4725004239748074	0.5438377105968724
0.5261948759252371	0.1914533958522141	0.5306542694774735
0.1940229047226954	0.5222610678980645	0.3468109973860364
0.8630496314248290	0.8688438009841680	0.7025703577403990
0.3042951694834822	0.4637927700861780	0.5340517612980650
0.9712400248302210	0.7931506700880760	0.3642776780830458
0.6330334377137129	0.1338846945085075	0.7012834982629530
0.7827391350106127	0.7266092476049825	0.5588089166871356
0.4402584880478769	0.0546368576985829	0.3897559782346277
0.1096098855514422	0.3807702254251154	0.7287893746039159
0.6904021004705065	0.2729992663641219	0.3795790583574065
0.3648102874343614	0.6102093394114982	0.7038523282263706
0.0291477740611932	0.9413607099048439	0.5435700815595402
0.3071221251739516	0.2321730312533589	0.5304536592168244
0.9777067918244700	0.5719044499991233	0.3465896207693776
0.6373906163619552	0.8946374961031255	0.6971145169409847
0.0361340305462505	0.7407566856635804	0.5350196719102470
0.7064148276213508	0.0772793601545581	0.3638949957836969
0.3656585099143046	0.3973381576487968	0.7011274905996870
0.7765665920520100	0.9579884470630294	0.5570206381018383
0.4446307878258267	0.2847490211261628	0.3902107503765049
0.1179499756857681	0.6278860033229237	0.7298980534411010
0.1402338344791539	0.1455468418182551	0.3329459906279131
0.8102303405948583	0.4829034272517335	0.6749927767037162
0.5989452387646089	0.6236161311156403	0.3215664255215296
0.2567554166634798	0.9534094443770902	0.6526754169012821
0.9248322898433912	0.2901968515229911	0.4947348280903364
0.4716188721611377	0.8109607692919258	0.5129670385783095
0.3544391851001699	0.8946548435334640	0.3326960639008269

0.0180971140065188	0.2302351926104197	0.6743254717339658
0.8766288782536532	0.8752822433342130	0.3210823359170326
0.5458211459966053	0.2016033932685445	0.6523016997003224
0.2087656962648582	0.5341605537556873	0.4942154346856180
0.6884566441463216	0.5596509934968810	0.5144175542847771
0.6052462852768310	0.3596117108076459	0.3337728883195450
0.2674635636937073	0.6843853089987609	0.6750532125949854
0.6247762850580286	0.9012319231397511	0.3206244470970658
0.2992461352238168	0.2430735573505220	0.6522364243576760
0.9649274403752887	0.5746586237432446	0.4951397792507010
0.9419872743611519	0.0304385046356847	0.5123256788683775
0.9304602629715051	0.7889508954508891	0.4871074403277121
0.4750683562834502	0.3097229986321133	0.5069852508006591
0.1448856427302692	0.6457232725372093	0.3476127381061184
0.8044879071602745	0.9775876815894973	0.6772826701112573
0.5877968002957666	0.1185401339606709	0.3259486525087552
0.2571275662847218	0.4499335438712635	0.6636212444760196
0.7113997031640567	0.0410855632412339	0.4866974689887724
0.1908343582472193	0.0643263241353164	0.5050404724582592
0.8543449689597701	0.3993804735821646	0.3475244060210597
0.5167508738798279	0.7292519878045234	0.6786823179670500
0.3817262153030632	0.3692026972237599	0.3261304956194194
0.0448401366413861	0.7048461744127531	0.6664835824159316
0.4584919860244515	0.5703673533644910	0.4871240915194762
0.4355473097665226	0.0245830243023342	0.5061660557280496
0.1004515778165919	0.3549892282093251	0.3472868033392123
0.7708650827250368	0.7004558614993935	0.6793325447892790
0.1308033672235836	0.9117151617590045	0.3257329535610060
0.7950158665775682	0.2417320480274095	0.6671767787599864
0.7001857739495435	0.3004364967856838	0.5001768470658335
0.7010635220263377	0.8010457577134020	0.5001444174761792
0.1997622876173175	0.2990156573427787	0.4991679456992457
0.2005836148577295	0.7993815875075476	0.5003642354135062
0.8705724917462093	0.1280740004009554	0.3346211702901023
0.5254745187679331	0.4776493791129298	0.6653077195969143
0.3721710543750835	0.6426548872353151	0.3349330396400157
0.0288942875445949	0.9561794641270742	0.6648638240426621
0.3666499782824368	0.1331614841324435	0.3156660171240032
0.0316405170090939	0.4658111020349946	0.6847930479080605
0.8571267687292962	0.6292986427553335	0.3355828019522579
0.5481361988778339	0.9732076676120961	0.6663827206524839

The perfect Pd₇-O_{V6} surface

O In Pd In

1.000000000000000			
14.4442996979000000	0.0000000000000000	0.0000000000000000	
-7.2221498489000000	12.5091304781999995	0.0000000000000000	
0.0000000000000000	0.0000000000000000	17.9855003356999994	

O	In	Pd	In
71	27	1	20

Direct

0.8443920444693436	0.6132218810735329	0.4537082665313295
0.5165044612600344	0.9529523409607829	0.2882046890772406
0.1710597854597324	0.2808156436460987	0.6191047227891339
0.7930846360119497	0.9609901799542456	0.2992877637273895
0.4623188105716035	0.2842179357795486	0.6584371778025704
0.1328615430405683	0.6246881861065289	0.4679037015370818
0.3017174254822422	0.7314807780193376	0.2988420360130019
0.9760924496216750	0.0693601590068568	0.6363594922038096
0.6402997615411482	0.4053719571823184	0.4632029490237568
0.5289951504868465	0.2086292863797967	0.2672553204170762
0.1842284223399401	0.5406118320384266	0.6091084478076495
0.8552903650874093	0.8789879144459237	0.4430079009774073
0.8859828367285316	0.1287007931469469	0.4572421951057719
0.5470320569386113	0.4626792536354171	0.2866475949476988
0.2214863052644255	0.7912800016935371	0.6202174036654868
0.5395459033723971	0.7319711648549917	0.2971067556290130
0.2049877495167817	0.0757651307604354	0.6589197705773723
0.8745551382763428	0.4069794523614577	0.4673810915709040
0.7684126268227738	0.4687848472362953	0.2978380205821809
0.4287473533956928	0.8074460935000958	0.6407355058146647
0.0941482636279556	0.1334203505134710	0.4645699856486224
0.2899906136538822	0.2192987635634064	0.2672614927208375
0.9564218597506295	0.5404490953049869	0.6102334029312917
0.6181886046627422	0.8759463319155276	0.4415219889305657
0.3702856072190389	0.6573462563430792	0.4561183136806894
0.0366411378106760	0.9834752852531465	0.2885315575289226
0.7048274203373549	0.3392004161808119	0.6196238208598993
0.7697255490412966	0.7071151444899766	0.2964510437305194
0.4232750954841999	0.0287999042431637	0.6568650141548824
0.0926378046595933	0.3661916255152919	0.4683460195549944
0.0304359652051346	0.1984728800725403	0.2991660019404823
0.6809654397042026	0.5391819020397948	0.6821067402297808
0.3678680156506757	0.8580614238213807	0.4678836529402087
0.2812382855039857	0.9700512445358100	0.2673605950992664
0.9563112101889852	0.3157741588113794	0.6104769381592421

0.6280390494583296	0.6434904383311661	0.4377979676715490
0.2270846740155251	0.3165942687599755	0.3777160555803128
0.8935238560829786	0.6472085247049649	0.7099054464818045
0.5585378911535624	0.9865781123490859	0.5461976370545643
0.2686274990581948	0.9755317759110678	0.5310821939433930
0.9281481668430158	0.3055903067703116	0.3452582545452170
0.7584696341480215	0.1967215771737748	0.5366313152739690
0.4242082428429438	0.5287846180661445	0.3647554188203396
0.0980988227281831	0.8654899488660306	0.6976677653770417
0.5458074380337278	0.7146575028756770	0.5560913006464739
0.2167739138495231	0.0599485270311470	0.3858246657293368
0.8699482367259878	0.3878815937436785	0.7301197730887768
0.1848007285940337	0.8104361206129838	0.3784860704219758
0.8529290243219575	0.1380802823584561	0.7098789978166098
0.5208137308489137	0.4710444189710318	0.5458342027921534
0.5256310604533234	0.1924390007369769	0.5303057403475060
0.1948551775480914	0.5217131978426551	0.3464565019186821
0.8605530469561119	0.8684196346556449	0.7034055429060759
0.3067966775386672	0.4630346590221716	0.5343457529208477
0.9727802157135549	0.7941123749380478	0.3636534226585872
0.6350761469365545	0.1393811211301887	0.7005938206983392
0.7811832811273643	0.7159360716489245	0.5600351023540626
0.4398277545372616	0.0550537035256148	0.3874507025883432
0.1112278016544929	0.3816968478007609	0.7282077045591692
0.6897926118859228	0.2732034985932556	0.3779758342563116
0.3576266636577405	0.6153895242866309	0.7149980761788141
0.0293789103097314	0.9410925708262231	0.5433963813413627
0.3075729318356217	0.2312158584422578	0.5305520451118138
0.9786900343105233	0.5714032012031935	0.3430642238737516
0.6326188351249686	0.9031121951305854	0.7070949903800628
0.0372375364116635	0.7396649490865944	0.5340650168709178
0.7061120500910221	0.0781570516549007	0.3651885854376657
0.3652268540589174	0.3995273359287820	0.7004872303838428
0.7741625460048681	0.9561583098380418	0.5588377638667856
0.4442832403622296	0.2839440662047981	0.3852984609411528
0.1152556948625255	0.6261898467130839	0.7294203099315608
0.1400739892307934	0.1452662239490783	0.3298683395165990
0.8113009774943517	0.4815915888624800	0.6799792831838163
0.5993719441159131	0.6235580670763318	0.3182892741295718
0.2560536545722035	0.9546404064725028	0.6529518152590368
0.9256066867348448	0.2906740802672242	0.4944856855550829
0.4728072603270627	0.8075985792380180	0.5163516917339714
0.3552427424041750	0.8942146183114659	0.3305510442844243
0.0186524642126176	0.2305208037866830	0.6744772598430296

0.8763588366528910	0.8749827931283398	0.3214357466992041
0.5448925062570866	0.2014370101740139	0.6521426160871320
0.2103381809776251	0.5343435060055902	0.4929956512238747
0.6890189969810822	0.5608215901777281	0.5024230836226691
0.6054692614738213	0.3592135875066098	0.3281506702914260
0.2648489518066592	0.6852517019325387	0.6761927667835462
0.6245384544937339	0.9010879212489800	0.3219523932382632
0.2923909054342978	0.2406513344221516	0.6525930935826647
0.9658279743273693	0.5731189352346159	0.4945289669078556
0.9407743773428824	0.0294403996043052	0.5129083159582412
0.9329649003357753	0.7888720030210359	0.4855761862538646
0.4731396802209269	0.3066654143203937	0.5004465192204393
0.1458499169042953	0.6453680398475777	0.3461216611540788
0.7989717757692150	0.9772648364938025	0.6780305668506450
0.5882889902424417	0.1186081979609265	0.3245078565045917
0.2600527976699281	0.4559963114375315	0.6638278443858696
0.7101822048971181	0.0416639478485157	0.4876376306397538
0.1906552820617702	0.0632936871069172	0.5012310303691222
0.8544302428036217	0.3989960976274759	0.3454908707787790
0.5031860993884537	0.7474999891592048	0.7046482517072301
0.3808856443492021	0.3696907138958046	0.3231946775037979
0.0494753909549574	0.7049132275119022	0.6627701873025705
0.4607462918766337	0.5714178509802724	0.4883322165497487
0.4363258358594960	0.0242364680319690	0.5033176108737314
0.1004816118276921	0.3546296873204342	0.3462511717568877
0.7947740494026088	0.7065585603826876	0.6787870743411538
0.1315086769071755	0.9113883181716218	0.3233530457272150
0.7956674567743846	0.2414570098939158	0.6662313214414096
0.7008259860236659	0.3019868121853865	0.4990579790247090
0.6982113677407349	0.7988836271985674	0.5010046574574283
0.1997102136318237	0.2987288423013630	0.4981607087922454
0.2028778591034352	0.7996443721030276	0.4988991464665670
0.8699383294446500	0.1280575733411974	0.3352455751558247
0.5198325706913014	0.4520523133324751	0.6654456509705031
0.3731644136843773	0.6422868286470395	0.3352662803043301
0.0312017105874998	0.9600123983236123	0.6648513234909145
0.3665151838100139	0.1327294667191651	0.3105656265270780
0.0322072354669529	0.4651015804874267	0.6841889106920306
0.8604507985123845	0.6302440226943433	0.3317952309035799
0.5448238029435954	0.9773860271346120	0.6671778002735709

The perfect Pd₇-O_{V6}-bt-CO₂ surface

O In Pd In C O

1.000000000000000

14.4443000000000001 0.000000000000000 0.000000000000000

-7.22214999999999965 12.5091307398835685 0.000000000000000

0.00000000000000011 0.00000000000000019 17.9854999999999983

O In Pd In C O

71 27 1 20 1 2

Direct

0.8405070674839791 0.6129598909181095 0.4563900594564816

0.5145429238776309 0.9516204232449341 0.2903107519484127

0.1725512312905751 0.2804985353675243 0.6206411356666142

0.7917960311039446 0.9603163488177953 0.2988054400984573

0.4684311832638623 0.2883624926258793 0.6609682300823817

0.1323441135873473 0.6255983837574515 0.4688712566345813

0.3002342678929428 0.7307840526497444 0.3005798534814174

0.9766634454308351 0.0703458257996802 0.6364499894638679

0.6398426629687299 0.4053740294611419 0.4650588415423022

0.5286287764774549 0.2090824584655072 0.2684914474298409

0.1812803203550791 0.5390677347618725 0.6089715204177929

0.8545544262410268 0.8808262307074463 0.4427146560746263

0.8861314261435931 0.1282350704663647 0.4563826503000295

0.5468962008380480 0.4633742330834699 0.2896153797167959

0.2159578404174486 0.7905834923185291 0.6199793706100553

0.5384629883687425 0.7315537115343143 0.2996924229538122

0.2053136765294236 0.0770228182357887 0.6556528233518454

0.8737604572664726 0.4071552608744390 0.4688376715731390

0.7677660475388632 0.4684734081540471 0.2990211886612134

0.4242859609433344 0.8101325219810992 0.6357143386562956

0.0941284210170934 0.1345874247580074 0.4655381210808999

0.2893985895933928 0.2193485833764088 0.2689365303746952

0.9582225554904138 0.5429476132415447 0.6101584351301642

0.6161782204099605 0.8732359159712041 0.4433559483388259

0.3713510072712612 0.6583926433588756 0.4584479336439451

0.0355253870069089 0.9838549574857425 0.2898563549384277

0.7080464991726013 0.3284544091150532 0.6203428999247410

0.7663747242352944 0.7062277744044710 0.2993367696875856

0.4213932194909716 0.0291897077072207 0.6546712161315341

0.0911027043295488 0.3649566737462268 0.4692126668911055

0.0302128504902102 0.1986311542051768 0.2995911619322739

0.6940925821054432 0.5260269957648431 0.6379199976001846

0.3645575830123506 0.8591770107138863 0.4655644366815674

0.2800561811074556 0.9700265221579092 0.2693100328628480

0.9555247780087526 0.3143550500550945 0.6109890170810541

0.6253922746660660	0.6435080661960206	0.4444047197976154
0.2266354682981447	0.3170333170305032	0.3788502376351828
0.8878231884724950	0.6438304141016385	0.7133450843676118
0.5575820384682063	0.9887175913424974	0.5434774287154296
0.2665610620012648	0.9749874659075137	0.5308093612138707
0.9274212478572817	0.3054820993456427	0.3460086768068295
0.7586176252117488	0.1948345838477103	0.5348562496198792
0.4230223157584384	0.5288290917839664	0.3669833153091008
0.0974734599484726	0.8665668757285611	0.6995829436612014
0.5432320272327111	0.7173305709958995	0.5643895254215890
0.2152276500124446	0.0596542766010924	0.3877583845006969
0.8711465640887848	0.3884883459088525	0.7296830679142970
0.1812433727123029	0.8092973862329237	0.3786706328903214
0.8538569709341017	0.1380937991842909	0.7115172808837632
0.5126919316420246	0.4686089309840436	0.5450887835362351
0.5239134589295151	0.1927076001475928	0.5309749324610510
0.1938108754382686	0.5216131949406674	0.3493703340451968
0.8613003333719539	0.8677580570225836	0.7028145432979359
0.3039183822861629	0.4632734380111317	0.5346659461887249
0.9700240546818905	0.7931987052717471	0.3639098010443189
0.6327887059615502	0.1336440830144826	0.7010389751060827
0.7832293798170763	0.7253456417650611	0.5607271875904406
0.4393083711013523	0.0563987424830093	0.3881604435725179
0.1116952628967141	0.3815021816475904	0.7287291635599803
0.6893257627618901	0.2723842882860547	0.3786978729586091
0.3585742822656457	0.6138588688259203	0.7075366169105115
0.0285527026072674	0.9417725741400490	0.5437079204140922
0.3082201086421351	0.2321186953867175	0.5313177171523095
0.9768813766266483	0.5713861133523177	0.3468441750678359
0.6340164139467495	0.9018846343287681	0.7005538430619396
0.0342282280915103	0.7402031821303273	0.5338788078093827
0.7053111066321003	0.0766843932738698	0.3647627799487523
0.3703537150603967	0.4020456310153733	0.6988985195016996
0.7749127840276012	0.9579630750365669	0.5590505032632448
0.4434378630991503	0.2835345516966524	0.3864110602672543
0.1175920184954233	0.6274013672641514	0.7292215388066194
0.1396908999828836	0.1454268410620821	0.3316342352645750
0.8121943059092969	0.4792156146832778	0.6748144012692652
0.5977310656433760	0.6231089769454814	0.3238116636556551
0.2543549327966662	0.9542125241254057	0.6526733045989775
0.9244487402090299	0.2899006258607535	0.4951312846700501
0.4693002270201659	0.8102841659555009	0.5162906076605074
0.3535094934833641	0.8938496724203853	0.3329886334032207
0.0190965125838169	0.2306029662241808	0.6751481605046566

0.8749032169788785	0.8746275393129642	0.3222657052806335
0.5454202824836778	0.2001345332470230	0.6527942181685170
0.2081358091621481	0.5337747070897417	0.4933346560475474
0.6886144372042909	0.5585433738110480	0.5132650455880939
0.6049487089664025	0.3592624787796674	0.3304512538396795
0.2658495432659558	0.6868292612230986	0.6724728351793504
0.6235820594432915	0.9003749904596434	0.3230455533311994
0.2977302543452215	0.2434212232383771	0.6533033750291877
0.9645084055038406	0.5743971804120946	0.4942417699640052
0.9404826673842017	0.0298145032341544	0.5130774401233087
0.9299717607004543	0.7893424853167003	0.4864094885769993
0.4733187906729859	0.3080604837476231	0.5012230126781509
0.1442098515494239	0.6452672853403542	0.3474448421490863
0.8011936158000847	0.9775054113725261	0.6788609562984553
0.5871346322971525	0.1180368159429852	0.3250628211490605
0.2600105227569832	0.4541491937234560	0.6637365425099645
0.7099128721634074	0.0408577877406744	0.4873739390060989
0.1898927967847562	0.0644362701010735	0.5036044795555644
0.8536073508736558	0.3987268560811980	0.3471859964715210
0.5102434597573866	0.7408768392274810	0.6919355120707200
0.3805610414930936	0.3698479743256989	0.3248012175959764
0.0465842926763164	0.7046294125430969	0.6659630093785303
0.4592212720451982	0.5715934280609921	0.4915239238034690
0.4341688795060415	0.0252906716504227	0.5038822508242637
0.0995607696553832	0.3540705302020769	0.3476116857851483
0.7889861037608179	0.7020078780480468	0.6785284796534535
0.1297642535147128	0.9115680814480435	0.3246354022161272
0.7945883927587857	0.2393853130525822	0.6671519234528591
0.6992371702516401	0.2999336569337003	0.4995873610702999
0.6980577557912849	0.7998195258703582	0.5041845955730305
0.1994667929716578	0.2988904814933247	0.4996316151955276
0.1995964510746509	0.8001210534217694	0.4992608409968879
0.8694829197508601	0.1273323720262472	0.3351915317251791
0.5282311412758680	0.4595819572046466	0.6645482360919471
0.3723684134228337	0.6424897474617325	0.3372517437981043
0.0292545764658423	0.9590037564266914	0.6650879373062397
0.3658311388444614	0.1327515127770610	0.3124664613542506
0.0331547749523566	0.4654448172123569	0.6846399283182648
0.8563059724800357	0.6289598678402869	0.3350069696738503
0.5414442790416253	0.9738997848775977	0.6646539087595745
0.5788186337061901	0.6816132992418311	0.7558123405755254
0.5788922317180895	0.7012194818385293	0.8212845309366630
0.6190267923129509	0.6271435958453371	0.7228734471488323

The perfect Pd₇-O_{V6}-[CO₂+H]* surface

O In Pd In C O H

1.000000000000000

14.4443000000000001 0.000000000000000 0.000000000000000

-7.22214999999999965 12.5091307398835685 0.000000000000000

0.00000000000000011 0.00000000000000019 17.985499999999983

O In Pd In C O H

71 27 1 20 1 2 1

Direct

0.8417824627857632 0.6146437140838655 0.4555388908288135

0.5150358791033571 0.9521968561879379 0.2878461960056523

0.1718278772547234 0.2802303277495399 0.6210498019561840

0.7922977644134896 0.9607806168632054 0.2978421147210859

0.4700653199033450 0.2903251645255287 0.6607073217687853

0.1317126479464415 0.6251263651291205 0.4691317339093878

0.3002494012104379 0.7306062526995240 0.2995447873513011

0.9755462500843058 0.0694369561374444 0.6362884106371252

0.6403318909090868 0.4048647802284306 0.4661738938060070

0.5285379448094946 0.2095553850453897 0.2677872321826880

0.1800753110312650 0.5391169389299965 0.6095356928006544

0.8551555098698740 0.8808695110707985 0.4418174648214706

0.8860024094118850 0.1280151243603745 0.4558196898658713

0.5464986460147632 0.4627437936343927 0.2882812465964922

0.2201266818237806 0.7918966342995645 0.6185785781142540

0.5387433047998241 0.7313174890478840 0.2987640640056538

0.2052104380570620 0.0762283459418735 0.6595586739458305

0.8731447671470695 0.4071691952671597 0.4694264326911750

0.7678268978157448 0.4688217177639155 0.2990547675072432

0.4259841207794651 0.8072536479491805 0.6374888150649943

0.0942691652717888 0.1345515140650906 0.4656940157334798

0.2897441774107574 0.2197222787423380 0.2688230532577458

0.9500484798072806 0.5481719231259046 0.6106039803225074

0.6170650390766595 0.8754147099582935 0.4410006283526229

0.3688263756305984 0.6573855856356532 0.4573041396618501

0.0361735478692315 0.9843609009990404 0.2889202302469346

0.7053547765548041 0.3243636983126530 0.6193577004675336

0.7677411668539348 0.7071642011755259 0.2969045228246710

0.4208006847804445 0.0276482165260462 0.6575031799041158

0.0914828655248436 0.3653890878730811 0.4695145871750231

0.0303707241070619 0.1990650048709465 0.2994009199176021

0.7002036301210511 0.5297035343574112 0.6407505301594315

0.3666039777847309 0.8588279949289557 0.4651947753615808

0.2803070133677137 0.9703820102359572 0.2681108788029205

0.9544338555762133 0.3160952326126958 0.6108841725598465

0.6283058205408557	0.6412078340912353	0.4413334181062285
0.2266593057375431	0.3167646860760231	0.3792400320168558
0.8861145119829031	0.6488599106275240	0.7234675891225717
0.5575872223171958	0.9874053821151988	0.5443916759198048
0.2677663768843732	0.9757450410828500	0.5307239253850533
0.9275348527840725	0.3059294881591982	0.3468588509275532
0.7586398119893613	0.1941276301770115	0.5338758343486451
0.4234295028472446	0.5288385713387065	0.3665778937747550
0.0948476954284312	0.8628132599190866	0.6973182907998933
0.5450766730543951	0.7163233571007417	0.5572867092692698
0.2155023402158370	0.0596160104053251	0.3868167603003190
0.8697231948297625	0.3891804798956524	0.7295261249925787
0.1822636113132341	0.8095227854475295	0.3777371265859457
0.8536653095489644	0.1382181307705841	0.7104367925860254
0.5159217372562717	0.4704001135244999	0.5469806983150750
0.5225993303231012	0.1910441188600472	0.5308879397736715
0.1934232811041190	0.5213222962737758	0.3477380703609501
0.8614446181130263	0.8674228807566241	0.7036840959271096
0.3048634097969648	0.4635420578283893	0.5352196340095694
0.9709826733685983	0.7938496239184364	0.3633498001187224
0.6320972763863162	0.1327073509063784	0.7007977462024425
0.7839181591384202	0.7249517455688073	0.5603895782438597
0.4396382108130727	0.0557812412522727	0.3869108932700526
0.1095827731558216	0.3808629137417105	0.7290673931126123
0.6888748588482213	0.2725505993671879	0.3780205601488658
0.3526789295568878	0.6112885276585911	0.7143281202712876
0.0293278724591418	0.9418930863947121	0.5433151515553467
0.3080744844984830	0.2313089351123344	0.5323663631287073
0.9768250082854407	0.5717593944981432	0.3479235136921383
0.6342488374794725	0.9022510115752849	0.7047383709048892
0.0366506364106388	0.7416518676544391	0.5328897961524244
0.7056594728842346	0.0778246019674992	0.3631278757540132
0.3683185462388117	0.4004050873739655	0.6998985751013462
0.7744652462386683	0.9568440564189845	0.5584338372389008
0.4438954455148696	0.2842128778554665	0.3870920134069085
0.1138150078856835	0.6278967705859895	0.7271242224061559
0.1398055044634106	0.1457717677707814	0.3311585566663450
0.8056489043476228	0.4722395140684106	0.6736865271232193
0.5984752616448666	0.6229375635286981	0.3219491790321040
0.2548231580610065	0.9547946386154271	0.6525111236439401
0.9244659590458713	0.2898424138596386	0.4942702813903256
0.4704376773699160	0.8081944750369047	0.5171322510838996
0.3542485425083298	0.8938591076502470	0.3308376405955151
0.0184037046815232	0.2305099131313798	0.6745151392365000

0.8754111765909923	0.8751931732519623	0.3209155649496828
0.5426653386625333	0.1973757753519902	0.6530144410136421
0.2088047933031335	0.5339756721930564	0.4940378884938765
0.6895334718139263	0.5587398942369244	0.5121727025526115
0.6045785594910718	0.3594122258919373	0.3299700744845786
0.2668391725158166	0.6864371539961120	0.6740081182264726
0.6237256366103335	0.9007358009528756	0.3212329985179407
0.2973622342201837	0.2430606476565683	0.6542265031752956
0.9638322543004645	0.5747705382222567	0.4919975228547339
0.9400867270210349	0.0297563771884568	0.5128581424197879
0.9308591575667007	0.7902486084373320	0.4855140421918529
0.4736669100114030	0.3085537201231543	0.5024253416262059
0.1446229897108441	0.6447175194154604	0.3471624066767691
0.7988892081399851	0.9764670829620935	0.6785310955474361
0.5874481814310045	0.1183037232544886	0.3234820740221865
0.2599505362021707	0.4546925669007816	0.6655725157850727
0.7093817657236493	0.0399528266368929	0.4864685861304156
0.1904777700051614	0.0644536672679154	0.5023086516084004
0.8533358805140883	0.3988337021159333	0.3472852481751998
0.5066331093356160	0.7403054234151466	0.7018663359310187
0.3806454928967051	0.3699738441385586	0.3248932304655024
0.0519040184825279	0.7070561138179723	0.6581281140694853
0.4603067331006246	0.5717525116585063	0.4904816653877953
0.4355846590416626	0.0243760439805342	0.5025833376756883
0.0999141212991826	0.3542299670294980	0.3476952028775896
0.7763509103477391	0.7032161397807337	0.6778892000490981
0.1302469848283542	0.9117376914321699	0.3235819705359991
0.7929166002263635	0.2371199283273266	0.6658942809052102
0.6978237919257608	0.2976979259292231	0.4987006446113662
0.6974194284192610	0.7990841282412179	0.5007015943852791
0.1997846606155228	0.2991231239509818	0.5002394965350535
0.2025307336495663	0.8009686793661978	0.4976136110758504
0.8694182582518131	0.1274983081471735	0.3345266571429784
0.5279500483223497	0.4620041375431839	0.6667293875270576
0.3725275304686705	0.6424213500741808	0.3367345090064043
0.0290464369316183	0.9590528696490673	0.6643640632773181
0.3660993633334190	0.1330204881099795	0.3119913127444753
0.0323819426682140	0.4652002094629446	0.6849734444310603
0.8564467274913439	0.6298266750296304	0.3338586041969787
0.5412921488085728	0.9715621850297720	0.6660325014640918
0.5759817672201651	0.6812083557361104	0.7635795449992838
0.5907070213397561	0.6938809023795385	0.8296987542933344
0.6134074974168052	0.6247358955920020	0.7217915409638118
0.9043979761276583	0.6652356037715520	0.7756527388306546

The perfect Pd₇-O_{V6}-[CO+OH]* surface

O In Pd In C O H

1.000000000000000

14.4443000000000001 0.000000000000000 0.000000000000000

-7.2221499999999965 12.5091307398835685 0.000000000000000

0.00000000000000011 0.0000000000000019 17.985499999999983

O In Pd In C O H

71 27 1 20 1 2 1

Direct

0.8425330836311256 0.6132291903322060 0.4545459684571424

0.5151576985410673 0.9516983147266878 0.2880792779494032

0.1732503940140559 0.2817748553901777 0.6203416642855865

0.7927338436631285 0.9603704603689893 0.2971551479217118

0.4690704859314443 0.2893671103638158 0.6662611013149278

0.1332500769870697 0.6249084387904652 0.4680270982576767

0.3016276440770716 0.7317378201646894 0.2993136513492217

0.9759581112567367 0.0695042381850830 0.6355408784279332

0.6392565795426498 0.4036648158490102 0.4604223778279893

0.5283584712741090 0.2083203042215417 0.2672591551869192

0.1852450553162300 0.5411819713306748 0.6103655994211186

0.8550043414350246 0.8810271663454708 0.4413961947734164

0.8863892626862667 0.1277422306645916 0.4554392000772871

0.5468797903140561 0.4623639322589955 0.2867550408928726

0.2182684612215228 0.7919709583898270 0.6205470878363573

0.5392662021099601 0.7312199296290658 0.2977252048847355

0.2056121060767936 0.0783101797078729 0.6547703701402183

0.8734123442164223 0.4067711460724954 0.4672075911364514

0.7688671814408045 0.4688597115950615 0.2974711968130574

0.4293729772593250 0.8059547636374221 0.6400743889737054

0.0945822844793692 0.1350682818979829 0.4655912336304969

0.2887042934529482 0.2187344904294160 0.2672783293513475

0.9598910125736408 0.5425020552169688 0.6078078412186675

0.6177321895078256 0.8753574687128636 0.4407083161605621

0.3692392923765568 0.6570337594409942 0.4558579365109083

0.0365546844188843 0.9839712651973128 0.2891902517471932

0.7080590081688803 0.3271142069340231 0.6174886217487732

0.7685489512544309 0.7067659452916696 0.2963548835353028

0.4214026497387226 0.0289140678934461 0.6535879300607875

0.0923570641773062 0.3668576862766380 0.4681230926908406

0.0307845167701994 0.1986979697389408 0.2989064760577060

0.6974437790494626 0.5230816074629477 0.6281333535507234

0.3661420717121299 0.8574822411110397 0.4682850908375373

0.2802642804678446 0.9698899373826589 0.2684199474849915

0.9559431616678506 0.3145839448281450 0.6091385567787089

0.6283584268408026	0.6405580938195251	0.4397436882278907
0.2271722592662376	0.3168553218951487	0.3782956734988014
0.8864886463020666	0.6428045980079740	0.7110701829713111
0.5577512938572390	0.9867364339383904	0.5442556566474248
0.2665847325223399	0.9746242266245015	0.5300276369007584
0.9281975940590463	0.3055570352493835	0.3455546038339494
0.7583264375401016	0.1941010120926248	0.5326918582921847
0.4235916704996055	0.5283790017317732	0.3645808425315428
0.0969271392165341	0.8668375578595162	0.6982424746658683
0.5445424813445464	0.7146781349083372	0.5557650611208435
0.2160062219146662	0.0600650312228644	0.3873542304140862
0.8701768561017733	0.3881446481191860	0.7274459619799919
0.1834817233148932	0.8097200180469148	0.3785107996539154
0.8526794861314644	0.1370462186600057	0.7086649366057439
0.5128459990921843	0.4669865151901743	0.5435396066592284
0.5224218978469886	0.1925856596774968	0.5300458731464570
0.1939949349321344	0.5214229080924200	0.3439222425291210
0.8586892816820347	0.8657986520628780	0.7018647488795137
0.3053106415629987	0.4640677155336942	0.5341655509025667
0.9712530746886584	0.7935659988267063	0.3635235596287659
0.6328022581651253	0.1361243086649282	0.7008327288824276
0.7833681517646465	0.7257238848696409	0.5590184014680168
0.4399422699407858	0.0548541686748866	0.3876770235257012
0.1110974705272699	0.3814224947581474	0.7280208026978680
0.6900298408122199	0.2718045132523511	0.3764125061655481
0.3509245707527854	0.6176894950199513	0.7198313372431699
0.0286321763559016	0.9415108510492739	0.5427907457140246
0.3092700703927214	0.2326436896528426	0.5309644247759131
0.9782789430694876	0.5718523177414937	0.3458635392084083
0.6321526222846391	0.9072878174427953	0.7075538459389535
0.0355712056682458	0.7401773664865405	0.5333572774770844
0.7061850548967644	0.0770716511638381	0.3627627252319664
0.3724323465424269	0.4058264493720071	0.6964616267227740
0.7732969029717928	0.9565068085443880	0.5585273805844903
0.4425730623516902	0.2827180530460069	0.3839536151459512
0.1127923751237532	0.6266954513422761	0.7289106156352939
0.1400279542832675	0.1454447048795650	0.3313169878224711
0.8127999320129212	0.4790273937216253	0.6704953156213050
0.5989883044236380	0.6225340650230036	0.3206682475335629
0.2540700513454420	0.9555185126869888	0.6518124714253908
0.9247381730791520	0.2899513907581736	0.4931211912758897
0.4718927329909777	0.8070602151981747	0.5165970501042187
0.3545082942823547	0.8939607493839128	0.3316498563562064
0.0190614609417418	0.2305131160725902	0.6733348952383664

0.8758178855616420	0.8747834043997479	0.3210441584766569
0.5453920719350757	0.2016938034794155	0.6518411241333888
0.2099357235814699	0.5346009599771044	0.4942903373780907
0.6894312978497589	0.5572513201025254	0.5093212964737482
0.6055234201862730	0.3592245142228548	0.3288776524284445
0.2630757417078578	0.6877194914538521	0.6753026538502254
0.6242796754302551	0.9004471749160056	0.3211088072020306
0.2990841909152260	0.2457363126530695	0.6527132814025361
0.9654581422549363	0.5742184476463088	0.4921754298487008
0.9400102117442193	0.0292192346582939	0.5124536729599387
0.9301972373815861	0.7890105062646855	0.4860095767021551
0.4731717555111524	0.308478333359897	0.4982168620228811
0.1457786616221542	0.6450773125164574	0.3464707950726457
0.7985578178765922	0.9751936240925601	0.6778404705468245
0.5875321139363695	0.1176134469271368	0.3235557743103029
0.2624409530832588	0.4576964420355266	0.6656137576094316
0.7098161077728413	0.0400045451957250	0.4860588067661328
0.1903886585377226	0.0649564078662194	0.5033793721192484
0.8543285722624996	0.3988544330226790	0.3457308279291694
0.4992463692417630	0.7529450208903856	0.7162702999640165
0.3803672618680176	0.3695716197826588	0.3226189559676306
0.0448693527544346	0.7046741529433350	0.6641360015738849
0.4606747590972421	0.5709834975861836	0.4887390798328772
0.4346902661165004	0.0240681631473583	0.5037178890516600
0.1006512322427082	0.3546073060747821	0.3464851573559702
0.7848120857994116	0.6983716567195516	0.6767702686640336
0.1306541193765778	0.9116298058657764	0.3247333718128331
0.7941906516056078	0.2391894028383679	0.6648372675767087
0.6985378247496766	0.2989312596081172	0.4972979150249917
0.6974691335900696	0.7978377020022884	0.5009582632469749
0.2002036121215080	0.2998742705500528	0.4994012818007488
0.2010201211550563	0.7996262459041754	0.4991095322440453
0.8700105105464288	0.1271777629257078	0.3341286260562757
0.5326388829457596	0.4610674388941389	0.6638265230932647
0.3726389326008062	0.6419583779347712	0.3355664614757450
0.0276681191324760	0.9581816914596210	0.6641120608790250
0.3658185871423024	0.1325438093121313	0.3111750432401788
0.0325683583982907	0.4650937020112319	0.6838566062473972
0.8578376597856265	0.6295875599071002	0.3333791960833503
0.5419404217841421	0.9765544597747524	0.6646682730110880
0.5469496372395038	0.7204175751650046	0.8030058124465836
0.5720927113137768	0.7073636962586920	0.8612351890224211
0.6274939326162178	0.6070352536749570	0.7326529147682366
0.6296118293120005	0.5963466639686242	0.7856282857879440

The perfect Pd₇-O_{V6}-[TS-CO-O]* surface

O	In	Pd	In	C	O
1.000000000000000					
14.4443000000000001				0.000000000000000	0.000000000000000
-7.2221500000000001				12.5091307398836005	0.000000000000000
0.00000000000000011				0.00000000000000019	17.9855000000000018

O	In	Pd	In	C	O
71	27	1	20	1	2

Direct

0.8413467421324962	0.6129166921172574	0.4570583660196961
0.5148058498706750	0.9523297704216184	0.2888984159852278
0.1708952376263783	0.2794733420925110	0.6189299805243600
0.7924870941932598	0.9608561621508344	0.2976150665582435
0.4708099498426344	0.2936231537084631	0.6548092340219310
0.1314502178695513	0.6250159087898634	0.4686074005533536
0.3000861587617426	0.7312021967540324	0.2996282075646919
0.9775079775700872	0.0705339785245278	0.6349638295762509
0.6396616189472767	0.4054839961092905	0.4659842769204650
0.5282551747258524	0.2099005286525761	0.2698650423440130
0.1812614788989068	0.5386817806221345	0.6092000055501534
0.8550917295571597	0.8813345825426493	0.4421187162987716
0.8865112649992651	0.1289508242070204	0.4552968921423751
0.5467286868594632	0.4631218058211335	0.2900873159736485
0.2199663049467154	0.7908385771698192	0.6201797374592303
0.5383712609027483	0.7315999804532963	0.2985080698264359
0.2060466402811250	0.0770612488644088	0.6557781549745458
0.8741979258677662	0.4073317123706285	0.4685859536901550
0.7668648724450468	0.4688822655840093	0.3001846848867787
0.4307378803906149	0.8073217624784959	0.6432762826255621
0.0939520307195204	0.1339770746297132	0.4638940185262274
0.2898396732158844	0.2194086548854095	0.2696882647052509
0.9588147599396906	0.5429493540705373	0.6109438667668291
0.6178378014894237	0.8756944550991432	0.4407270182014326
0.3686355207698842	0.6578200128277991	0.4565892403208264
0.0359800266786457	0.9837101027689166	0.2895272859190935
0.7094491062437089	0.3276616262890192	0.6204985414523652
0.7672678603766786	0.7067997948483402	0.2987828746192841
0.4228748101774099	0.0288563547993642	0.6544040295536915
0.0903099380480984	0.3651775409362568	0.4682689864336781
0.0303129532302778	0.1986841704517683	0.2987495337743118
0.6934304140541342	0.5221361777518334	0.6359652734868916
0.3651899530580364	0.8587617908562895	0.4673194808509230
0.2801121077764109	0.9704825945807497	0.2691869161572972
0.9547559480099617	0.3147927391792857	0.6108616831704630

0.6263679411386516	0.6432467312310193	0.4429175700249656
0.2260370994283083	0.3175282483705923	0.3781010734577562
0.8856298377818927	0.6467599007259121	0.7110326980049869
0.5573399257338640	0.9861123880663831	0.5445702512995639
0.2668026901060493	0.9746177192491270	0.5309415988649167
0.9272104230000420	0.3060511602495169	0.3437490180345917
0.7579493895912214	0.1938977040980218	0.5341320626963503
0.4228259544265939	0.5293456746755550	0.3662111097843059
0.0996626771367265	0.8669905494029317	0.6994939773148107
0.5413933407349039	0.7201045770860383	0.5584205577351682
0.2155059985117438	0.0592226969454494	0.3878115088707296
0.8708654600119395	0.3896932512035923	0.7303207015262086
0.1825973544700865	0.8097171493564974	0.3790077352536321
0.8528119373799402	0.1370677142611371	0.7101528015455881
0.5120831280420589	0.4713426026283182	0.5451580262128509
0.5244539970923323	0.1920720612988762	0.5309440748072426
0.1930299816442085	0.5216344964586467	0.3474336415836621
0.8628502990887024	0.8686197471052159	0.7027067986599563
0.3031690225836229	0.4630430046635353	0.5335549743458357
0.9706646794114384	0.7935066824464323	0.3649111213005284
0.6327075380175693	0.1344607110246889	0.7019175462366727
0.7826751356614745	0.7261597349614717	0.5602388828108766
0.4394248355229136	0.0549814471443954	0.3884054243779604
0.1109489125031780	0.3808989608895921	0.7281165228309864
0.6895403472880026	0.2726715239693671	0.3791185908518653
0.3599468698475057	0.6118887239629486	0.7038591744792508
0.0291873393927850	0.9418902793080935	0.5433204178924707
0.3068340085227895	0.2316528517900725	0.5306778944811593
0.9770425897264148	0.5718200617576508	0.3451524209743789
0.6362919583440427	0.8998953221270114	0.6996002479313163
0.0352514758255609	0.7405120735304600	0.5351193891277516
0.7058311028564962	0.0776797143169072	0.3631734812238877
0.3662867180391525	0.3990046301484260	0.6998284809524686
0.7750530369778222	0.9581052300184529	0.5577188714299541
0.4431439882104963	0.2840209115763833	0.3889139859662464
0.1176539220354633	0.6278720695476073	0.7295224599673107
0.1395141765731915	0.1453308726377686	0.3315568105701536
0.8118503505520193	0.4809043157338643	0.6749421140988365
0.5981186119823060	0.6233348701509764	0.3232056845832317
0.2556638984839074	0.9544650875993896	0.6526133109886392
0.9240181810636989	0.2897304154587368	0.4949920081943240
0.4710479319507725	0.8103843297838287	0.5137044693252101
0.3537815217995231	0.8941635226281708	0.3316332160018995
0.0182887267435523	0.2300958973633824	0.6739991792349466

0.8754208230428898	0.8749378725194182	0.3221156232653287
0.5455846998121118	0.2019310872266677	0.6525799545076840
0.2076258882944572	0.5335872909545956	0.4929263920017997
0.6885083827493808	0.5590329062962811	0.5140023918810713
0.6044884750874525	0.3596973912246738	0.3329850667162961
0.2656694770355096	0.6853657896180740	0.6733085528100338
0.6241312824605880	0.9009973893964114	0.3209578582490182
0.2982187668332814	0.2434752765182605	0.6524885155347193
0.9643448789352469	0.5742457242698480	0.4952065047972409
0.9406766038524521	0.0298326866389673	0.5118065786083471
0.9293640291406753	0.7887492989491772	0.4875561609961685
0.4739485279839716	0.3099538771069378	0.5048232612776994
0.1440487994333117	0.6453157180139621	0.3470201116635752
0.8038959980252217	0.9771626922530745	0.6770808619346864
0.5873794590228517	0.1186549857920538	0.3249229121240994
0.2582200578609067	0.4510667458749817	0.6617980905853837
0.7103129491357139	0.0409135940660471	0.4861755741081163
0.1901594824208142	0.0643336012244984	0.5034514281233663
0.8536062153204795	0.3992932758819638	0.3468672481296444
0.5136482703132447	0.7380123007155210	0.6943591639973966
0.3808520885052094	0.3697605582242213	0.3258293883726595
0.0453505230536001	0.7049356858511515	0.6662041034443174
0.4591318170961488	0.5724876827968179	0.4901276850230461
0.4346832660355512	0.0251449783278565	0.5044090513849219
0.0989269325540784	0.3543245538411759	0.3465221306783921
0.7775822391236995	0.6992395171994953	0.6801044736675288
0.1299193078068156	0.9113578663882165	0.3249625413399052
0.7946271859238063	0.2404454304133724	0.6674490966072109
0.6992962918146204	0.3000562898855526	0.4997165544586916
0.6978038293416425	0.7994819072258285	0.5025822619571965
0.1988951511804457	0.2985240842299102	0.4984084467234232
0.1998789357857473	0.7996530672293991	0.4995683568031412
0.8696142396905300	0.1280300816299807	0.3339795862055936
0.5280661717052695	0.4704058267910006	0.6662846942872169
0.3716945067457329	0.6421431900956455	0.3359795494876963
0.0291199814203111	0.9576407255230952	0.6646213219655208
0.3659309302053670	0.1331106573380583	0.3138633466998075
0.0324772873519798	0.4654386396890587	0.6850051702327880
0.8567569129690634	0.6294868665077974	0.3355766318031555
0.5447479843328888	0.9753241879221392	0.6654526883390076
0.5496826825467099	0.7055771232795044	0.7887849378299816
0.5637546745746400	0.6949587768866414	0.8504464063903793
0.6114451491393631	0.6317085505835340	0.7108715502896567

The perfect Pd₇-CO*__P surface

O In Pd In C O

1.000000000000000					
14.4443000000000001	0.000000000000000	0.000000000000000			
-7.22214999999999965	12.5091307398835685	0.000000000000000			
0.00000000000000011	0.00000000000000019	17.985499999999983			

O	In	Pd	In	C	O
71	27	1	20	1	2

Direct

0.8416815294673986	0.6128177706341962	0.4570049869398242
0.5150039704291691	0.9516345760687757	0.2904942403167435
0.1709025368219585	0.2804214020884780	0.6201057631522955
0.7920455644064456	0.9603735301152105	0.2989664900778817
0.4709098220344835	0.2941984700876101	0.6505121098020578
0.1314936562602615	0.6251738441979198	0.4687482446763072
0.3003225354821068	0.7308535843743055	0.3004394738566925
0.9782014879020186	0.0718053510870806	0.6356564434583299
0.6398940037337415	0.4053682563101999	0.4662123252041319
0.5285246657000825	0.2093428783452078	0.2708416297935303
0.1795562675585373	0.5386989613117622	0.6085528604847094
0.8568988441568477	0.8823203569573222	0.4419501476087779
0.8866586832058653	0.1290737804662350	0.4565643979425847
0.5471024915423219	0.4629662156844668	0.2912995387116590
0.2222889227568858	0.7911955978991894	0.6209466565853600
0.5387064415691044	0.7317052460980016	0.2992166249937880
0.2066338028746451	0.0772725683977066	0.6571166547851089
0.8750896418300091	0.4075247589508750	0.4683542490788888
0.7667426263133127	0.4683128750645537	0.3004925496976719
0.4358293987680332	0.8024002388603468	0.6423722717119551
0.0940604733252883	0.1339211158569938	0.4642707059538754
0.2899418859885038	0.2188262873498835	0.2699809624963485
0.9572486880997768	0.5436730122167276	0.6115029132218471
0.6162902114225750	0.8721460678520836	0.4436914633407720
0.3724631741578501	0.6585322102904679	0.4583239145167906
0.0363229894788146	0.9833334037560757	0.2891603463976997
0.7097996319083784	0.3293767028432626	0.6203030827440879
0.7672326226412346	0.7065272796446970	0.2995622431367826
0.4234766565177367	0.0275232526412708	0.6537691377942187
0.0897694517811779	0.3640908339250715	0.4687921739264857
0.0299928528351507	0.1977889978322622	0.2997104389104522
0.6914568075209107	0.5237060498167567	0.6372857229630863
0.3649184016914848	0.8581933121690991	0.4676519151017596
0.2807112127265697	0.9702302650985141	0.2695335280322492
0.9546134456577273	0.3165700870978815	0.6116878548471183

0.6246648055470725	0.6448638516347883	0.4439337029790253
0.2262361976645869	0.3173126818238790	0.3784857659642236
0.8836493873943539	0.6484509081671190	0.7105369241017272
0.5572602118488554	0.9856633837701583	0.5452936741456742
0.2666801079199121	0.9744352957597903	0.5314783924376620
0.9271477983059045	0.3054316233418004	0.3428452988147830
0.7580944549996668	0.1939917904679843	0.5351839041436394
0.4223913218560952	0.5288320717416830	0.3656339315071871
0.1000534352657436	0.8671590160485969	0.6996786867960275
0.5424758877414162	0.7175680265253918	0.5638491257472669
0.2151815544472779	0.0586453025144006	0.3878985981662492
0.8698745673872855	0.3917157079429250	0.7313257364719120
0.1827053297478829	0.8096257137113737	0.3794594269772767
0.8554049311914522	0.1413513905278529	0.7120693533412134
0.5118339861975153	0.4707951949982202	0.5431879915380250
0.5255587674876683	0.1914777074106568	0.5306821016282914
0.1938765251626515	0.5217430179865065	0.3502297715070103
0.8631914489864640	0.8698770437340302	0.7025306073380191
0.3027388790689427	0.4628870471274478	0.5339836565758804
0.9710048247558898	0.7931106291580566	0.3646242991380131
0.6324412358085806	0.1362181299921881	0.7024055119161945
0.7837290828461114	0.7263271451129665	0.5588260946723470
0.4391655143912711	0.0544998049969394	0.3893581013556605
0.1080308354135901	0.3806670392904791	0.7298832195209395
0.6902653863191920	0.2722427471613802	0.3795238774795341
0.3472753953487545	0.6040390995523855	0.7130145948264984
0.0295320430850237	0.9420382586215026	0.5439332212299375
0.3059048498173981	0.2311590444077816	0.5307219468916627
0.9773515477806248	0.5714111627078656	0.3437510712241903
0.6434430912869153	0.9114175917649714	0.7027020492135863
0.0359158679350905	0.7407502819537846	0.5355041599621565
0.7049253924045304	0.0756546993916853	0.3658471554391436
0.3668321515616270	0.3992282858406319	0.6997492566023723
0.7757561593479636	0.9575277517302495	0.5584951416820196
0.4430534985333603	0.2834025987291119	0.3896548867260567
0.1163521986449260	0.6286424314721778	0.7296844043971977
0.1395273925577599	0.1449311139395179	0.3318190104703727
0.8104483442978749	0.4821417615877164	0.6755307586337000
0.5982666775481564	0.6233808237914548	0.3233962311027831
0.2561889386194964	0.9542837192903425	0.6531283638513636
0.9239986478787174	0.2897124167779615	0.4964189187275392
0.4701775028513799	0.8105868900225105	0.5156204854603754
0.3538029508925379	0.8939409346682098	0.3326830454862479
0.0182100450397766	0.2315370100010428	0.6749628755033652

0.8759992213088258	0.8750231529132034	0.3220364055281816
0.5459524920529826	0.2022656632663661	0.6523336917395274
0.2072162368449135	0.5330994966665379	0.4932069586865109
0.6885934960062126	0.5588941310109002	0.5139067148001281
0.6046761063489674	0.3591626293109166	0.3339578257580543
0.2662823427330602	0.6843088725105944	0.6743454894953724
0.6240068607641350	0.9003456324958530	0.3231981564558907
0.2981743346445079	0.2436596284631954	0.6525199028118568
0.9644273161939296	0.5740274968559884	0.4960055518822717
0.9414145972686002	0.0303000943092390	0.5126859084294478
0.9309549973689812	0.7892716253836158	0.4871474017469054
0.4737970313890226	0.3083482767887494	0.5058741868949679
0.1440410594688149	0.6453462056936919	0.3474120042165374
0.8064386867930292	0.9813994065437291	0.6787615231528393
0.5872998583037090	0.1179554923193360	0.3263621516571667
0.2550283524366634	0.4501727000713222	0.6646213691667934
0.7105345326658244	0.0406014511807560	0.4882538562292602
0.1901948059723905	0.0640171954124473	0.5034826413914935
0.8540554387118768	0.3990074026134294	0.3466997838257492
0.5248130213837472	0.7261683585688600	0.6769475770783311
0.3807947657577827	0.3688368271454696	0.3261546736307307
0.0447195867802213	0.7051780877586314	0.6669932469167805
0.4573137806418964	0.5690374956919709	0.4886655235479582
0.4346760390044545	0.0246158470858048	0.5055128415677478
0.0987927967660025	0.3537444170930126	0.3472749076657511
0.7758899334044431	0.7013522057620762	0.6786918697158281
0.1302752219245421	0.9110078461976497	0.3247865266361709
0.7946640969084396	0.2421451295862224	0.6692215462458341
0.7001835313056843	0.3003422289201408	0.5000907063181322
0.7007889419972207	0.8006841946232088	0.5024699702860693
0.1985570829662374	0.2982890398369971	0.4990774836977988
0.2001474614850764	0.7993383133085604	0.5003617987726476
0.8693668266064930	0.1276095596431699	0.3353843555020629
0.5266239392664019	0.4727253256302196	0.6640369876539831
0.3722357789142210	0.6426130775913643	0.3367871313619275
0.0295676973941769	0.9581410606320429	0.6652072424617551
0.3661451816424205	0.1326836543520344	0.3144131759960624
0.0315724278078766	0.4665611614384766	0.6857476310831282
0.8571705956261740	0.6289763385652866	0.3354792957625169
0.5465478769164293	0.9748719931549136	0.6666422418424935
0.5113267822951203	0.7341973960690563	0.7809439366507180
0.5072587643619367	0.7405015782928230	0.8442625585653414
0.6060728539382962	0.6408732689410345	0.6981561289927393

The perfect Pd₇-H₂*_P surface

O In Pd In H

1.000000000000000				
14.4442996979000000	0.000000000000000	0.000000000000000		
-7.2221498489000000	12.5091304781999995	0.000000000000000		
0.000000000000000	0.000000000000000	17.9855003356999994		

O	In	Pd	In	H
72	27	1	20	2

Direct

0.8418355296563490	0.6130268573910553	0.4569417145581388
0.5156539590447528	0.9525606381402861	0.2889772078599699
0.1710795340070884	0.2798140964220704	0.6189028876636872
0.7934077740509137	0.9614116154770009	0.2973143133413897
0.4713755687638280	0.2946567835799773	0.6484459507274040
0.1318472196895554	0.6248948703021752	0.4686789378270252
0.3005602126403961	0.7313945426024878	0.2992763060117296
0.9782366927233342	0.0709693110066788	0.6347977040137393
0.6405292035285146	0.4059451627899891	0.4673621587146909
0.5289911369648740	0.2101062032297092	0.2708538024505365
0.1815720735742024	0.5386924606421548	0.6092188560868624
0.8577932818619737	0.8826971472539297	0.4406915354694787
0.8875309316239216	0.1299405551503944	0.4552492717993501
0.5476161246424281	0.4628660693355767	0.2904191660462647
0.2216420596326293	0.7902906568599238	0.6204403989716775
0.5391548950300963	0.7319554626122158	0.2976072926226576
0.2068267667516388	0.0765610594566146	0.6560730680522487
0.8754190390334674	0.4075259221379268	0.4684651652259739
0.7671636030269533	0.4687549081184249	0.3005138679884736
0.4339342937032774	0.8031453925909462	0.6440544443910767
0.0946127467667621	0.1340196871163436	0.4631427784117031
0.2909578459356193	0.2191903550142140	0.2700175592278410
0.9577146577706637	0.5434200840707221	0.6114229405643142
0.6181163132226279	0.8748341165944771	0.4403089433687042
0.3707789357917665	0.6583029036608355	0.4562164975913184
0.0373467668186270	0.9838859321536271	0.2886068383123406
0.7094542316794834	0.3289535457068144	0.6207612386614458
0.7683477920263877	0.7071341631227871	0.2980274610313475
0.4239563884166663	0.0270157980152653	0.6521571249258146
0.0906460886222841	0.3650988327684760	0.4682107693307717
0.0311782513502319	0.1987662561057556	0.2987275433536201
0.6894677936601029	0.5249290320601292	0.6386507514342470
0.3653870202290844	0.8585503583402245	0.4671110354895698
0.2812614272280062	0.9707059471069180	0.2690902603307370
0.9551541081890211	0.3160833008490504	0.6113411178870674

0.6263172370212090	0.6442068542901844	0.4416103312792886
0.2268531455495664	0.3179041622404722	0.3779279023437598
0.8829302312013503	0.6491745621655622	0.7088080179998316
0.5582811394941651	0.9847035186781040	0.5447127941321515
0.2668674478266110	0.9741088161957160	0.5308269419695185
0.9280936764994919	0.3064003829091369	0.3423534873849117
0.6009576302339268	0.6454633132275830	0.6996673980265578
0.7586868014213950	0.1941535708754074	0.5347234222068755
0.4229944093973508	0.5295057901227945	0.3643205000135337
0.1005384811737623	0.8669351297106032	0.6994209711532930
0.5438435787332617	0.7205237858449912	0.5571272712811359
0.2159294026703223	0.0588322734508131	0.3875639748892377
0.8700672298190815	0.3913647916598537	0.7304996902186456
0.1834173760129391	0.8097421328208779	0.3790469491343405
0.8528540318524235	0.1377046402927117	0.7096453435182556
0.5119245385784831	0.4727028518516714	0.5432485104860824
0.5265213864920337	0.1911849055752497	0.5301419953587564
0.1939306972866147	0.5220986132962518	0.3481434778892815
0.8633075389948622	0.8692512882673901	0.7020716781043715
0.3036264798022196	0.4633226433372680	0.5330674735408990
0.9716220084408093	0.7934056374077261	0.3641971981916856
0.6325431689269423	0.1338139906276520	0.7014425149538585
0.7831475781679264	0.7267915877547679	0.5584836794028630
0.4399797633879816	0.0543784356791680	0.3890164899562092
0.1100841322343927	0.3808309130457896	0.7285829020114403
0.6906623338783282	0.2729972274670244	0.3795312657518657
0.3647329816152585	0.6101934933973383	0.7028754817632601
0.0297846440111193	0.9420489991112906	0.5431129636091412
0.3060628532403911	0.2311418564206842	0.5298850530975345
0.9777033780755715	0.5717968684672797	0.3446075098489024
0.6372398243322397	0.8948331277773688	0.6967073071309861
0.0360868432747944	0.7406330279928027	0.5351087544195345
0.7064193783128876	0.0774688699008363	0.3636654812080324
0.3656361729528857	0.3975202666959529	0.7002479306046620
0.7765670350584736	0.9581700436331442	0.5564216441871849
0.4441647812387454	0.2844206915716633	0.3904475092239709
0.1183528664605767	0.6281977501253402	0.7294869044823739
0.1402730858523352	0.1453521515016707	0.3314205033898265
0.8099510425956309	0.4827222981825938	0.6753587169692433
0.5991039649877599	0.6236391245274380	0.3215460517144316
0.2564437730597093	0.9537216364032113	0.6524977537011617
0.9247184195390805	0.2899659273736763	0.4956555444009708
0.4715551851898787	0.8112551751570780	0.5124516616118642
0.3544991363337808	0.8943747731419113	0.3316679931641953

0.0181449213792320	0.2302782100910516	0.6741098026757373
0.8768806152266017	0.8754738055780835	0.3208155610620211
0.5454303958580299	0.2012886231720137	0.6517752065342157
0.2080426475476902	0.5336354064158529	0.4929630624027761
0.6886119844091562	0.5596997877963161	0.5140583975115129
0.6051168467511683	0.3596936276510208	0.3344251400364040
0.2673963583376163	0.6843500687350722	0.6740341335268517
0.6250891926463058	0.9013486176007074	0.3203536547995278
0.2986853662022030	0.2430064312660017	0.6517660093938179
0.9646429178135202	0.5742299587623386	0.4955811329077943
0.9420882485930051	0.0307161045440564	0.5115743396503939
0.9308323153793161	0.7890978214334430	0.4869405089519206
0.4747788720177160	0.3094149834892795	0.5073371782108442
0.1445745589798568	0.6455960006023419	0.3470498925104384
0.8042854917049648	0.9775705149134223	0.6766328312649911
0.5879867946881279	0.1187297432389474	0.3256476440369225
0.2569932991693233	0.4500532795378819	0.6625193608643816
0.7113879443208277	0.0412960432586219	0.4863494767352702
0.1906704301196721	0.0640269123512495	0.5030878065030522
0.8544598800717110	0.3994327320977247	0.3466463599709062
0.5168134778458691	0.7296181832967024	0.6778949113434903
0.3817389941135588	0.3691400737747992	0.3261409539780881
0.0446795037617837	0.7048996614772426	0.6665239656915906
0.4582723958872635	0.5704457676262444	0.4868150919749159
0.4351989958886093	0.0245032191639348	0.5053936023640042
0.0996690179261667	0.3545548417953192	0.3464695534477605
0.7713138391888682	0.7007666882376581	0.6790582516551401
0.1309142676601680	0.9112226127101578	0.3244561732596550
0.7947192364599213	0.2417519435804082	0.6679691123787694
0.7004868362323509	0.3004682510124905	0.5000136648478442
0.7012902095831167	0.8011640618261551	0.4996971246951735
0.1992632362470377	0.2984713224298455	0.4982045884341822
0.2003801567086226	0.7993347160385724	0.4999182237152819
0.8705030448097308	0.1286349884274448	0.3339386797565819
0.5254737765134335	0.4781847980657842	0.6645536615866101
0.3723133081418951	0.6427015484805680	0.3349416681507688
0.0293914585576302	0.9571968252386545	0.6644998367942062
0.3668865037499616	0.1330712753750522	0.3147359147549467
0.0318285490121088	0.4659131250946945	0.6851655988132257
0.8575092583239905	0.6294199742716289	0.3353464129486292
0.5477327489801014	0.9732770439506742	0.6659245203166794
0.6165040411006639	0.6493687246179526	0.8982083067002300
0.5875638167192270	0.6529019817539667	0.8654993998514678

The perfect Pd₇-[TS-2H]* surface

O	In	Pd	In	H
1.000000000000000				
14.4442996979000000		0.0000000000000000		0.0000000000000000
-7.2221498489000000		12.5091304781999995		0.0000000000000000
0.0000000000000000		0.0000000000000000		17.9855003356999994

O	In	Pd	In	H
72	27	1	20	2

Direct

0.8414023715542516	0.6139662452752095	0.4578150741984702
0.5157840347319683	0.9534856826866489	0.2893615335224048
0.1691508220854187	0.2798148898423534	0.6180161329100489
0.7929582320234632	0.9621350440337942	0.2980558616072156
0.4690039224882429	0.2913679456839864	0.6507051214040547
0.1320316361003197	0.6258701211998708	0.4691140839300697
0.3011135093504269	0.7321882907140778	0.3004211862104748
0.9782425970485612	0.0721255895553349	0.6350018566552083
0.6399702885156375	0.4067622994028151	0.4674701768945109
0.5290109852281726	0.2109298164789663	0.2708652832258158
0.1819855359115286	0.5399474556520875	0.6097605565472362
0.8572187398099326	0.8834815976096710	0.4414592991442581
0.8873101066366869	0.1308673659992840	0.4560790486483962
0.5474017386170080	0.4638536357012342	0.2912784016933052
0.2220407761315937	0.7910185913409604	0.6207444650098753
0.5389971854690476	0.7324597695091134	0.2991980829876686
0.2059595028155412	0.0764105482354632	0.6560116360323306
0.8750130140412746	0.4086776176464119	0.4690673572435915
0.7672098783615175	0.4697994352207804	0.3009055673788055
0.4343970104719208	0.8058744208113787	0.6448594041952862
0.0940927375923901	0.1341063066014650	0.4628963549598813
0.2906181799414441	0.2201133737700493	0.2702263609129693
0.9585979994232844	0.5448522831614362	0.6119010464908635
0.6179515224286591	0.8755357751735471	0.4414740607490934
0.3711187013237473	0.6588575694052385	0.4579838830730545
0.0368368894546883	0.9844119698587976	0.2889515414458841
0.7091130476118935	0.3305760247455509	0.6214145654748799
0.7675827542834534	0.7077921689337142	0.2995875328732479
0.4239899499031967	0.0278997214589411	0.6540138282897664
0.0903394627374512	0.3661103769001005	0.4684091427590368
0.0305836975709799	0.1994890291367181	0.2991191890951718
0.6917958178874642	0.5283852948835681	0.6388591386648733
0.3657119702248252	0.8594267962296724	0.4675850809426378
0.2810934618987732	0.9712935123080253	0.2692074908455120
0.9551809265669364	0.3175181397860415	0.6116519486316788

0.6255921970146836	0.6443559991535240	0.4438656958471322
0.2263239284293279	0.3185733722833127	0.3780155045138142
0.8847578164142339	0.6506170398228210	0.7097310327277138
0.5582314593956934	0.9861753430353806	0.5453878273903865
0.2674061126884218	0.9751507105866213	0.5313882730262585
0.9276693185688626	0.3071754264883660	0.3432835337636048
0.6048258554354731	0.6547518295977034	0.7044699682745323
0.7584734459547526	0.1954494204786006	0.5354363823222461
0.4230743959727651	0.5298189842203572	0.3664904800420656
0.1009551841691003	0.8677772313069598	0.6998487014800868
0.5440287313821797	0.7213698613575971	0.5594037821314892
0.2159015534305790	0.0594552257127770	0.3875717645647899
0.8707828916328847	0.3928910437299397	0.7308859613688544
0.1834969688066881	0.8107079726757975	0.3794206947187372
0.8535048447085473	0.1394980167458684	0.7104362337074084
0.5118803062641810	0.4718123084403978	0.5467688257150677
0.5259864598642334	0.1921025763033353	0.5308280577925147
0.1940645197152106	0.5229384201194924	0.3485612591952389
0.8649420911268091	0.8716072776357806	0.7031490169012222
0.3029273835379553	0.4632099749102481	0.5335095068459128
0.9714299442798935	0.7942995348592520	0.3647875141499785
0.6335282189863517	0.1355013835734321	0.7023399909311729
0.7836845745911886	0.7285958771545533	0.5595694820823602
0.4398350926681138	0.0553465227450624	0.3890289276146230
0.1111423692665317	0.3823009254042415	0.7285823022444163
0.6904263477500041	0.2738687752795222	0.3799792917320987
0.3663197505403346	0.6124539434383710	0.7026133987367554
0.0297911343175424	0.9429037895539855	0.5435041728676394
0.3056219042506547	0.2313581309291610	0.5300426046593780
0.9777082382813246	0.5729041830242491	0.3454809176421601
0.6380478399264018	0.8979536809874464	0.6985853731836130
0.0363804148832377	0.7418326748466139	0.5353273239334896
0.7060249485722726	0.0781766006831930	0.3647155703776799
0.3631374651487911	0.3957106174848137	0.6991681942232741
0.7762220137292702	0.9592128014837201	0.5575405472801188
0.4437038332119667	0.2846541524532396	0.3902647473699321
0.1193168077092121	0.6293536877929686	0.7302507608730695
0.1397954797677180	0.1459596102953420	0.3315617855593275
0.8109806323777227	0.4842962879316882	0.6758122012929971
0.5985676691479054	0.6241477636586898	0.3235848000792652
0.2566738871793394	0.9543355899783698	0.6529638956890612
0.9245351774241258	0.2911875977254024	0.4960452821630482
0.4715676032830176	0.8119876310753030	0.5137431157612632
0.3545010707217455	0.8951724304296544	0.3319379710159269

0.0183447173760644	0.2317633990694291	0.6742461167851277
0.8764552101576079	0.8762582918676830	0.3216173628012994
0.5456951705904876	0.2013620563103227	0.6524554402281776
0.2079340134070010	0.5343504159140335	0.4936371138392295
0.6882937337747898	0.5601465783978362	0.5155573870593746
0.6050223814611005	0.3604587855825881	0.3344732557428181
0.2681972302072427	0.6853957100899254	0.6746805330493519
0.6247423844853596	0.9019717886156747	0.3214356004236230
0.2954346255380156	0.2422676970389490	0.6516333192909686
0.9648061113560809	0.5754669888224171	0.4960092119308201
0.9419035542684058	0.0315925640383273	0.5122209569747148
0.9307068563721762	0.7900598730410969	0.4874518619231684
0.4739777939291835	0.3097286671472621	0.5067990034628724
0.1447215231842473	0.6464620782744279	0.3475756185855577
0.8052764681558495	0.9794588413704062	0.6775395860239950
0.5880227885477657	0.1196475230384205	0.3259640992491406
0.2582204621709596	0.4515221028491181	0.6624152560310512
0.7112833302567383	0.0424042591238246	0.4872675741502597
0.1903613507330623	0.0642653774917334	0.5030362632161269
0.8543180159374243	0.4004647243030515	0.3472447553836798
0.5189379632512029	0.7354648089119882	0.6804715494810255
0.3814173100938373	0.3700289710709374	0.3265835747329786
0.0459946060518375	0.7060478999376137	0.6671479398235606
0.4584162150706129	0.5704347413889164	0.4899513307532816
0.4353184632169256	0.0255211130512791	0.5052255068224601
0.0992968700303432	0.3553855876573362	0.3467219666847312
0.7755481664753788	0.7036773410576922	0.6793861957759744
0.1306531785527680	0.9118553529199286	0.3247173035027651
0.7952886690958788	0.2434278340340683	0.6685159142059078
0.7002513785672834	0.3017092509948048	0.5006066301547177
0.7010482014126209	0.8021720746733932	0.5010660795588073
0.1982254615659400	0.2986224090270413	0.4981055201656316
0.2006378953403070	0.8001789537318744	0.5003089523083978
0.8700809034188368	0.1293217728132379	0.3347592239878417
0.5258472495649517	0.4658356297959073	0.6690461972168725
0.3725026667708808	0.6431345739372616	0.3367267538674677
0.0300752697949862	0.9585346957115830	0.6648863307082904
0.3666211355930893	0.1337911434635682	0.3144516975929768
0.0326857500564675	0.4672200773273689	0.6856829664275164
0.8571592488886487	0.6302761073664360	0.3361962084263951
0.5476576380810875	0.9753732614692575	0.6666962423087338
0.5727862995363617	0.5217215489082661	0.7807138066956073
0.5856075892231888	0.5865973766628774	0.7587308822639670

The perfect Pd₇-2H* surface

O In Pd In H

1.000000000000000				
14.4442996979000000	0.0000000000000000	0.0000000000000000		
-7.2221498489000000	12.5091304781999995	0.0000000000000000		
0.0000000000000000	0.0000000000000000	17.9855003356999994		

O	In	Pd	In	H
72	27	1	20	2

Direct

0.8410226998491716	0.6139608333427317	0.4577559497204612
0.5154765491147865	0.9528440250690631	0.2880543467259313
0.1659469703499030	0.2782479198677020	0.6160483404675787
0.7919753897135300	0.9611058668397111	0.2969923522621902
0.4647481020889892	0.2858341506072365	0.6448253911936054
0.1317581385882557	0.6252520740130405	0.4685037482942793
0.3012231491988802	0.7306685479885177	0.3003724787924450
0.9769371058652903	0.0709017494881349	0.6340020358558107
0.6389110411079384	0.4066832849528491	0.4676703613882823
0.5283506084350619	0.2109763118268649	0.2708257002754413
0.1821103880616607	0.5391002185971876	0.6090521933892359
0.8566668539837622	0.8832118747625337	0.4402119775186423
0.8864353189116035	0.1305226761138712	0.4550167395147546
0.5464125293146518	0.4626633643773151	0.2915375562668140
0.2218892747517382	0.7906900621578856	0.6197713598464364
0.5382516829581936	0.7308713374772339	0.2993218966815824
0.2051115291098549	0.0759103677351308	0.6541534416362225
0.8745283199926027	0.4083774130068121	0.4684249148461340
0.7658863368680046	0.4689821788027066	0.3012250471598094
0.4326024930709668	0.8065442899759059	0.6431735667411533
0.0925715694429844	0.1327052187828364	0.4608924012199588
0.2904411996246605	0.2195129773799546	0.2700600045640391
0.9592024688021473	0.5450182945014075	0.6114387631602490
0.6176174377314441	0.8750860873831259	0.4404560729157884
0.3713226538172214	0.6576074093579030	0.4586988285685610
0.0359955798435746	0.9832324073638675	0.2874369417555930
0.7082209665743012	0.3309671504864202	0.6211155857563326
0.7662700142986446	0.7066423520420904	0.2998879814051156
0.4234524235014932	0.0270609196978141	0.6538258738980612
0.0890704537640532	0.3653424583733637	0.4672563900203029
0.0293500204603427	0.1983274399746363	0.2977007369704101
0.6996714356917075	0.5347715945502290	0.6365423883598758
0.3653356240478542	0.8588525528840407	0.4663300461870373
0.2805090475254678	0.9704234788935701	0.2678684953211168
0.9544926162728695	0.3172638176683441	0.6109143967996691

0.6247491923165889	0.6429915045096660	0.4450760721208351
0.2245824491439705	0.3175864788843594	0.3766329342529773
0.8891647403005372	0.6508879281423440	0.7128290748388064
0.5576370291491392	0.9856473030867889	0.5440644955745938
0.2674258290923258	0.9748427663632915	0.5300510483427520
0.9266479657055469	0.3063973670365723	0.3417027335044671
0.6114003290088543	0.6661010987875933	0.7089792896680078
0.7578913492832416	0.1951561732808477	0.5350204005285504
0.4230510854228137	0.5284645971152410	0.3683246365023358
0.1011255102707442	0.8679080323451667	0.6987628995664822
0.5447746963960183	0.7223297057951272	0.5597759808275992
0.2147971563782352	0.0579454261446107	0.3862978102227627
0.8709516790731099	0.3923215941031007	0.7302871892567356
0.1829453588728470	0.8096595326649871	0.3780666897361838
0.8524225224198918	0.1385406774941673	0.7091940455170640
0.5139317437885618	0.4728925069365013	0.5532622751443207
0.5264694076811933	0.1908748761672663	0.5293641534041710
0.1937222782089937	0.5219106399548793	0.3486316414647667
0.8651684312500980	0.8712603595622163	0.7030982818003860
0.3016509570156178	0.4615347514274570	0.5328685324823366
0.9708979559951915	0.7935783739040031	0.3637025296327402
0.6333724180325033	0.1359577201590457	0.7018193061202304
0.7854241636118079	0.7317577302253159	0.5590820296871929
0.4388384004458227	0.0539919141825022	0.3873095803741203
0.1108320591847882	0.3816636612026061	0.7277668147767717
0.6897464025146325	0.2730219278321743	0.3797504946815546
0.3668417019885149	0.6142744966964071	0.7022867765799281
0.0296304940269259	0.9427582597061294	0.5423015578962134
0.3032501643234160	0.2310456860296669	0.5281115784872259
0.9771733194277488	0.5719898158821106	0.3446825026675573
0.6367597299163580	0.8997045874261473	0.6974131252444833
0.0364700593111056	0.7418018037656263	0.5343819071972712
0.7052369610869160	0.0774884409131903	0.3636387681993044
0.3603021922998834	0.3934423049185480	0.6976933442098595
0.7755761619577849	0.9590731449794347	0.5564656132112538
0.4428078733311690	0.2840713581371634	0.3918385433235613
0.1194986024815312	0.6285867945974309	0.7299627310741825
0.1387057879162245	0.1448195078015176	0.3302432205021765
0.8119887321910388	0.4845881242690100	0.6759265609527012
0.5974362229963737	0.6224279838723462	0.3245646645724273
0.2565114342828956	0.9544380088806909	0.6516233234761881
0.9237183435127799	0.2907108020555934	0.4953516408625498
0.4714776138945572	0.8115889758212742	0.5120508627702596
0.3538793898935839	0.8939809523699523	0.3302452846093101

0.0172134277519423	0.2310939711510464	0.6733439813532761
0.8756762591559011	0.8753449794731203	0.3204968907395917
0.5450242305703157	0.2001697552775392	0.6511556524773281
0.2075080659609828	0.5333591866002136	0.4926645126697490
0.6880414278245852	0.5598460703071602	0.5168363505342769
0.6037788833240196	0.3597045163074922	0.3357405987735030
0.2669519762534834	0.6844358577840957	0.6736509752379520
0.6238716543629259	0.9008193031174830	0.3203327669431231
0.2924132406869052	0.2417221408106465	0.6495867939302229
0.9644288403319775	0.5751305079710175	0.4955391049089924
0.9412183202363159	0.0309924528967424	0.5108404528291157
0.9308706745516722	0.7900822620571027	0.4862140851887930
0.4735868550166527	0.3106755022679728	0.5093508374039847
0.1442412803405021	0.6453328548686887	0.3468688357816922
0.8046961269805190	0.9788604925327202	0.6759819187935474
0.5875093583740940	0.1192486515459848	0.3248789790776180
0.2583042208373416	0.4507931521581964	0.6614663653036066
0.7107847337412551	0.0424406796671953	0.4861377427764152
0.1899378448079996	0.0639452119164814	0.5016285366689289
0.8533872777877254	0.3996974978777614	0.3466013183961654
0.5167328554061582	0.7398294143767014	0.6803919334475942
0.3807613169308314	0.3688936271759083	0.3275178166466830
0.0475472152350705	0.7060736714693294	0.6667739156330175
0.4588194018886118	0.5684181612008843	0.4929869140818255
0.4350285155348730	0.0252319008502642	0.5032435547968978
0.0979106876587651	0.3543080816004645	0.3455108257175430
0.7840067745221317	0.7047577479496924	0.6772974978517599
0.1300194519004566	0.9107298943011451	0.3232337944032326
0.7947823341532386	0.2434285336977206	0.6675409536526079
0.6995401928453311	0.3016366434461681	0.5001697962440879
0.7009183595620631	0.8021370681383175	0.5001808338048185
0.1962005733823245	0.2973074809752285	0.4965824725776175
0.2003601783452283	0.7997628110748554	0.4989914535999462
0.8691356237912701	0.1284561658135616	0.3335524431168035
0.5294182426346324	0.4562532962358088	0.6796955317008129
0.3723148658860205	0.6414076349428232	0.3375807400104727
0.0305591568383687	0.9590478359806957	0.6636473750145150
0.3659474604917513	0.1330597248725611	0.3141653329338531
0.0326084546024781	0.4664982761893873	0.6851264009881480
0.8562223193750036	0.6292945102988333	0.3361365902147678
0.5470553564440767	0.9768562990840048	0.6650641176479526
0.5767501567086923	0.4650641860067235	0.7717796069347255
0.6026046125707598	0.6547752425542614	0.7623854486943579

The perfect Pd₇-[TS-H₂O]* surface

O In Pd In H

1.000000000000000				
14.4442996979000000	0.0000000000000000	0.0000000000000000		
-7.2221498489000000	12.5091304781999995	0.0000000000000000		
0.0000000000000000	0.0000000000000000	17.9855003356999994		

O	In	Pd	In	H
72	27	1	20	2

Direct

0.8407869403414945	0.6124859262650746	0.4575696096000471
0.5153559528943483	0.9515675517777608	0.2880282464779580
0.1656597158001602	0.2772021294098108	0.6156552132733301
0.7918786627479297	0.9598667054367515	0.2974096363798192
0.4642895884214659	0.2856703839697035	0.6529708140678728
0.1319832491651618	0.6236598064682729	0.4682721570360885
0.3012076017676179	0.7299755687408811	0.3000754725746401
0.9768075019869016	0.0699870693957445	0.6338428944070050
0.6387033938705172	0.4051691135714760	0.4662399450669802
0.5280977436325589	0.2087551129775316	0.2693444296774815
0.1822163684300925	0.5381911202168065	0.6096855917643775
0.8556787954415799	0.8810389653229047	0.4407574654234444
0.8860878786427756	0.1288224308455878	0.4555432119491744
0.5460605087102592	0.4614928831852739	0.2895037917248394
0.2215650846673927	0.7888325033320965	0.6199642858476391
0.5384254441197408	0.7299142860380032	0.2993269012383040
0.2038856907658440	0.0728393568973168	0.6540684994515854
0.8737669121237317	0.4071249183427422	0.4682113179586169
0.7664979383859867	0.4679711851290954	0.2999127895818452
0.4324181062084715	0.8071937881668795	0.6441810163364564
0.0929229491520758	0.1315181653588344	0.4614083775173052
0.2893886322484426	0.2178935161494896	0.2690692658004928
0.9595955956518414	0.5438705453607557	0.6108410203612902
0.6171922839778828	0.8741826229627890	0.4409920353526397
0.3701056802231481	0.6561159013066272	0.4580989134200182
0.0358130458196423	0.9820247832920859	0.2880637358993936
0.7076847533742544	0.3307225466005084	0.6199435738016851
0.7664885940910469	0.7054619371103696	0.2991039040338866
0.4231471216022893	0.0275090045565261	0.6546811976298995
0.0898775959256205	0.3649737800877709	0.4672240708272291
0.0293007883282214	0.1973190894578959	0.2981893350754334
0.6975865602900997	0.5334750795641382	0.6389674491020402
0.3659942196541742	0.8572384493691461	0.4671546337023209
0.2802629144177399	0.9688991135358024	0.2678588805937511
0.9543426615355500	0.3164294566462112	0.6102058477871133

0.6257454442803627	0.6404048444734759	0.4441603203981510
0.2251583291985705	0.3162946443089305	0.3768738984878368
0.8898560546666768	0.6488652887005356	0.7128507985281423
0.5575381138957058	0.9851923405848380	0.5448390367923764
0.2673229753112372	0.9731739672926056	0.5302642014092591
0.9265744158783762	0.3050241571342907	0.3434316753033354
0.6277063289441646	0.6922441721210789	0.7293385943933609
0.7574188826384598	0.1942419490484350	0.5345523069761948
0.4230627665677348	0.5273234391369021	0.3673426202670170
0.1004111454956901	0.8657979155416085	0.6988089016245296
0.5444736598661808	0.7181517373261660	0.5589260994012009
0.2152820196581600	0.0571429570006533	0.3863297769580881
0.8703169746955280	0.3909517778327353	0.7297029562604245
0.1831837576386849	0.8085682750724789	0.3783098946619732
0.8527205904804255	0.1384147633383249	0.7090696202675979
0.5114736971052631	0.4675806676066027	0.5495677955750377
0.5242611734469895	0.1906032054234882	0.5300278618308709
0.1935266220225001	0.5206745382330746	0.3463110200788129
0.8664113220254567	0.8715631962424506	0.7039831952591998
0.3025091347090699	0.4605436237540873	0.5335555105798983
0.9707478687289993	0.7922575324545460	0.3637955691541858
0.6336265788373694	0.1368883151894523	0.7020369968030141
0.7849234846448299	0.7290806788128702	0.5596835322247835
0.4390759884400767	0.0532131816485990	0.3875172567850742
0.1101572804347123	0.3803732118635290	0.7278474705759246
0.6891650240703842	0.2719759934493039	0.3788038021072129
0.3673462608074611	0.6141411262023280	0.7029914049476733
0.0291029095615491	0.9410067609196315	0.5423998815033803
0.3042308393129113	0.2289982200821103	0.5292129568400715
0.9770872331017868	0.5709626103287215	0.3453543497760113
0.6376610143827200	0.9039161286967807	0.7013239467777372
0.0365474967093889	0.7403915637014292	0.5340297871115309
0.7051820239694887	0.0764172515002302	0.3638412885551349
0.3536646805836583	0.3865361066038605	0.7017472239093160
0.7747197574279098	0.9570158403233365	0.5571005897357070
0.4426447999286578	0.2824168864744480	0.3887187051113222
0.1192588336280017	0.6270914607996768	0.7303058575466170
0.1386164161569935	0.1436135066704600	0.3305764354632023
0.8124304124981312	0.4832066239467044	0.6747084277425751
0.5975829384566759	0.6211840722853490	0.3239269300958312
0.2560914557700013	0.9521130251082961	0.6518609351616304
0.9237379625962070	0.2898155804984645	0.4945412341174426
0.4714958803017589	0.8089658675434741	0.5143306526280880
0.3540081684102135	0.8928599998291172	0.3306395629672284

0.0171012976299826	0.2303936423006467	0.6728398425239743
0.8753623866406749	0.8740303106807619	0.3208658147667418
0.5450110223076398	0.2004388662063239	0.6515672997922203
0.2079923019932264	0.5324558703066617	0.4936595793612870
0.6878407529537678	0.5577623183258017	0.5162988730546539
0.6039371939187029	0.3584504759815171	0.3327604035028611
0.2677588510817839	0.6835173608097597	0.6748620681771385
0.6236451718126300	0.8996157297201016	0.3209850199298846
0.2892809863451928	0.2376625016849666	0.6506078070005124
0.9647172951689771	0.5739910023381398	0.4947931409309027
0.9407663731119279	0.0293464174754829	0.5111223599273818
0.9307046057260084	0.7885561502249273	0.4861387625141138
0.4723533938402792	0.3081628669479117	0.5049524256351535
0.1444247640091831	0.6440423766777347	0.3467139024404785
0.8044672349206270	0.9786702238407418	0.6761639814466800
0.5873665918514958	0.1177254520250696	0.3245585547161033
0.2583933283442474	0.4508137709654598	0.6625199186760304
0.7101746356354698	0.0407632542140775	0.4865582722113500
0.1895862694342529	0.0618892055442365	0.5016643739416098
0.8533647653958629	0.3985821900089821	0.3465025679654498
0.5180986828691122	0.7450298626135218	0.6880468649004686
0.3802564884957259	0.3679930717840131	0.3255633806323550
0.0484250238537904	0.7045816124664382	0.6663763080269464
0.4589549419681208	0.5682190446662473	0.4918590916121134
0.4349735710271776	0.0237316855307138	0.5034290718687774
0.0983990042691968	0.3534557900111577	0.3455712569935238
0.7880027856005243	0.7056291737560393	0.6775807813021251
0.1299836533474492	0.9095316753909120	0.3235799274252356
0.7946650838917068	0.2423826100075804	0.6666647960321356
0.6989130062144761	0.3002855369739176	0.4993324811708821
0.6992345058904197	0.7994766921307265	0.5006450924160852
0.1968002933626158	0.2965063891156309	0.4967763891638286
0.2008332262087107	0.7981544606827465	0.4991104516625718
0.8690283413279818	0.1270017223555721	0.3341009201791435
0.5209509525192790	0.4527198715460199	0.6732966393024933
0.3720661035289163	0.6404366418874570	0.3370800176008399
0.0305971179759098	0.9579772356926919	0.6637576429686541
0.3656037635109096	0.1315685338432006	0.3129398721451319
0.0325306516483113	0.4653728711532518	0.6851040299101229
0.8560467392720963	0.6281237206201152	0.3358380093863156
0.5462836997627574	0.9773641176931965	0.6658696869652438
0.5723921814633482	0.5713032315561685	0.7347139844624464
0.6437891842707318	0.7185337616085246	0.7804034755397594

The perfect Pd₇-H₂O* surface

O In Pd In H

1.000000000000000				
14.4442996979000000	0.0000000000000000	0.0000000000000000		
-7.2221498489000000	12.5091304781999995	0.0000000000000000		
0.0000000000000000	0.0000000000000000	17.9855003356999994		

O	In	Pd	In	H
72	27	1	20	2

Direct

0.8462022803346535	0.6119794206326056	0.4517360180086172
0.5177644409186249	0.9517574978474886	0.2866049297227136
0.1728331223520172	0.2803719218358455	0.6179440200164265
0.7943512279663756	0.9593385468914054	0.2973838074315892
0.4623606644797157	0.2823574870837933	0.6605284007963805
0.1331919040753284	0.6228084976763946	0.4657969532911034
0.3033693093398745	0.7309156014272317	0.2973283416514630
0.9769839765769835	0.0677560273523797	0.6352125009714059
0.6412984739032577	0.4045485634961524	0.4594475173958782
0.5299699816795034	0.2069345543665336	0.2653748677062183
0.1864222065139112	0.5407924511979771	0.6078524034846400
0.8556935248241728	0.8770189577366383	0.4413639347749940
0.8872601536016663	0.1273701177691757	0.4558620118797866
0.5477352470258430	0.4611288356816656	0.2837658634030025
0.2223598661928153	0.7901363300012278	0.6187590848640566
0.5406101643198560	0.7304541628503167	0.2951763348526183
0.2054250136290892	0.0746713313764842	0.6507277691257791
0.8756337772279112	0.4069582168141936	0.4654800261145355
0.7696730292233475	0.4675745001406351	0.2954524112095007
0.4315293832015821	0.8061951478841688	0.6391643562051398
0.0956111788325326	0.1326279872913452	0.4641538465209992
0.2904710737931178	0.2173128217578038	0.2658702173140385
0.9575725967383292	0.5398445068657648	0.6093991572259341
0.6194415807901431	0.8753047410966126	0.4395323478070552
0.3707155664910555	0.6557140846259324	0.4540684025646347
0.0380766689182837	0.9826262428133108	0.2879256492214159
0.7050468556238433	0.3405094726276238	0.6169335274955442
0.7712032794473199	0.7056136582926972	0.2941278729610534
0.4247360430427972	0.0284259124295161	0.6538473166747008
0.0949331906398536	0.3661643350374350	0.4666952078878103
0.0318934480226225	0.1973824118964767	0.2978151266175175
0.6819079938162045	0.5369901974185127	0.6845822811317596
0.3691317481370578	0.8568233678773123	0.4664210427731775
0.2823169915168149	0.9689483526696833	0.2666809866680606
0.9582108989043119	0.3155550857430378	0.6078456353857009

0.6292622401370267	0.6416156890451428	0.4349873142614394
0.2284918952928197	0.3154641078132618	0.3763054661297677
0.8947176787833722	0.6475840356367044	0.7078894183274620
0.5601844435743881	0.9861122739642860	0.5439992646448921
0.2694897017135815	0.9734081648600950	0.5287544896009605
0.9296167190880609	0.3043225139310956	0.3463019670604138
0.5650452278630873	0.6800788767395126	0.7864408938362211
0.7599387551710544	0.1966554209690178	0.5344719891162449
0.4252330688303824	0.5271262247918935	0.3628577010502889
0.1005512381648477	0.8659396599768929	0.6971881727511924
0.5468950791406292	0.7132201164486225	0.5527921827571397
0.2180518045239571	0.0590606484757281	0.3859427088772683
0.8703808134002816	0.3866943357567106	0.7278976072657459
0.1856842315071572	0.8088059577238325	0.3770615488299491
0.8542805930495833	0.1378155987856996	0.7073496800982254
0.5235380028626411	0.4700939337846048	0.5447025366367459
0.5263731158467804	0.1923850033977136	0.5284076642439250
0.1958533882753684	0.5205752324427443	0.3425163473751258
0.8598649571732835	0.8663995537791256	0.7024375427791082
0.3087043363771823	0.4624938703958600	0.5332992252007017
0.9737547884631482	0.7928189685530815	0.3623532224446798
0.6366428627461210	0.1395286948427025	0.6979599362181205
0.7806929146829045	0.7130997993898085	0.5585562584446732
0.4417409938901562	0.0541781402942393	0.3861597685281623
0.1120218969831291	0.3808762620431335	0.7265306801325937
0.6915707490621030	0.2722011783032336	0.3757440486132825
0.3569588835957178	0.6141840640622946	0.7162993526863244
0.0287805517225998	0.9386716113747602	0.5418786229959563
0.3103757293628718	0.2326301048775875	0.5287557390796441
0.9801811686250329	0.5702654273502021	0.3386300214862185
0.6344109098626615	0.9049158959628976	0.7070502802225661
0.0383139495839649	0.7386040111564880	0.5329626367490689
0.7079107857746708	0.0770659761124624	0.3630341815738315
0.3674114815545911	0.4003492414184964	0.6996714917531255
0.7749165965348809	0.9546259093402949	0.5570712134203889
0.4455480755014644	0.2829047090704009	0.3826190357908664
0.1166145877465829	0.6256120755825841	0.7280808100420794
0.1414443656509800	0.1439969911804141	0.3295947253739332
0.8118358412575614	0.4812257274705176	0.6788974510738773
0.6005228695418389	0.6219566284070049	0.3157030067624025
0.2574736782503732	0.9535684156116213	0.6504871155134115
0.9270458310416111	0.2903632653167785	0.4915483681735577
0.4740745003901382	0.8063355998053873	0.5145862679147668
0.3566948374035352	0.8931296719711976	0.3296516770694812

0.0198644526827996	0.2297897781316710	0.6722632438396011
0.8774925507769327	0.8733218161004215	0.3198915271249465
0.5464679090306255	0.2017483975116638	0.6500555061656991
0.2118804982559883	0.5338049311426774	0.4919129821861514
0.6903645175495302	0.5594642773097783	0.4994368171342357
0.6068442764075801	0.3580068863643228	0.3253872348634694
0.2668402768356392	0.6853975426854186	0.6750008649403937
0.6257580182939022	0.8997016824248497	0.3200315107544309
0.2942750558071696	0.2407198108603632	0.6507375559763221
0.9669627424120811	0.5720729094606977	0.4940032831171478
0.9415842586649200	0.0277900452341019	0.5114348002749800
0.9334131326981878	0.7869374668592647	0.4841315892590578
0.4747057876047711	0.3065018576800435	0.4973244617888443
0.1468992823390356	0.6440429573731944	0.3437585652528002
0.7997380787953871	0.9765268896199467	0.6759567887245728
0.5898004859459207	0.1174875951207190	0.3227610153310954
0.2614882170286862	0.4558313473610148	0.6627003584630466
0.7115419527539709	0.0408955262328991	0.4857305217936214
0.1919864348462577	0.0628699953192019	0.5019839193159442
0.8561135712169294	0.3983106112760191	0.3434426555069972
0.5032532881699617	0.7489873464891951	0.7056974118821107
0.3817680620811297	0.3683242417997923	0.3207944003669679
0.0507730458267620	0.7045506563631306	0.6618287803237368
0.4620715741693230	0.5700789669026445	0.4862179143346187
0.4375652446832012	0.0233818549371686	0.5020038071983355
0.1022938202686136	0.3537667825006431	0.3445138511269781
0.7932627032737973	0.7043622132813029	0.6775609313404900
0.1329134949316872	0.9107271868854181	0.3230919060733005
0.7972014611184552	0.2409276475959306	0.6634307227062273
0.7019753759518905	0.3016544441869590	0.4968176311227761
0.6989050528435147	0.7973424671258217	0.4985469728415515
0.2013449657553719	0.2983706182962598	0.4967651733977763
0.2038146156858656	0.7980340358722843	0.4971588338572044
0.8714821147814678	0.1262832070552617	0.3338203746279912
0.5218107519676229	0.4506083052227891	0.6642290473567249
0.3739655250657337	0.6406940439793881	0.3332885245415999
0.0310310229891771	0.9575743172954325	0.6630422413605712
0.3675865074268628	0.1313996578994034	0.3095977366126896
0.0332684247253566	0.4645636868217725	0.6823749770000832
0.8623218882654790	0.6290623760972088	0.3295603634487475
0.5461202376028549	0.9771433296487575	0.6647714595480841
0.4971084521089927	0.6253720934712512	0.8071296258677548
0.6004096873100804	0.7327171667066851	0.8253816767721532

The perfect Ir₇ doped c-In₂O₃(111) surface

O In Ir In

1.000000000000000			
12.5091307398835667	-7.2221499999999965	0.0000000000000000	
0.0000000000000000	14.4442999999999984	0.0000000000000000	
0.0000000000000000	0.0000000000000000	17.9854999999999947	

O	In	Ir	In
72	27	1	20

Direct

0.8412183493326871	0.6134256089854724	0.4572607516087472
0.5155383221612666	0.9526556765873172	0.2896663718169518
0.1710293724076490	0.2794829879938180	0.6199361326671938
0.7931605262595287	0.9614772730635558	0.2978463313945106
0.4709862818547187	0.2947098051164862	0.6526104469456790
0.1340836050902652	0.6255787213521072	0.4706080861061782
0.3005879575931430	0.7314559412019827	0.3002802948996090
0.9779069291723251	0.0702682449664077	0.6359251152920923
0.6404593834754743	0.4065011512921829	0.4671159993198591
0.5293813227024012	0.2100706235989122	0.2699680158271793
0.1879237281975580	0.5405331272198650	0.6126053993869029
0.8591633206024968	0.8845332104650536	0.4409617900057108
0.8878716615648533	0.1302040560766328	0.4564349005540534
0.5481549336612485	0.4634672392805547	0.2904356432071252
0.2204147039418573	0.7908590318528950	0.6204493020346005
0.5387953956092273	0.7318414940413710	0.2979084117024299
0.2065396118325982	0.0765049963995085	0.6556577179048663
0.8746554644516147	0.4076034490796816	0.4698415697196276
0.7683165490156920	0.4687866869028101	0.3001094690769771
0.4316691907053891	0.7999176154293433	0.6387557429026837
0.0951027279919223	0.1344620810362385	0.4641048797605590
0.2903432078153259	0.2190080173042014	0.2695373892047543
0.9592981944637068	0.5433680550202182	0.6117520847702058
0.6180710033401111	0.8735461377022266	0.4412587768984671
0.3751857613143478	0.6583736101099824	0.4576146245252248
0.0372894796898410	0.9842102110621740	0.2887268319634302
0.7087660815532343	0.3284367414654216	0.6217351407836381
0.7674914139656080	0.7069908702144094	0.2996901341922464
0.4232080031777057	0.0265831901518256	0.6534916157303886
0.0923925539027806	0.3664608083403180	0.4700530763318179
0.0316123498919595	0.1995392612707124	0.2995903274821922
0.6904598238549463	0.5246837572903542	0.6384276396018467
0.3642739986300234	0.8596764196617154	0.4651097148902542
0.2808971429906627	0.9705240440088394	0.2692206501003682
0.9562017338192268	0.3160475132647966	0.6121421892453666

0.6232528076469998	0.6460834925001584	0.4438609175205597
0.2277652625857257	0.3181333444500042	0.3789539638180726
0.8827497954181590	0.6481923100978417	0.7090511161560061
0.5574855161746477	0.9862824847608154	0.5434306258456038
0.2671665327100641	0.9745561163595269	0.5311973503574501
0.9287546088984312	0.3065308991988129	0.3459846161012022
0.5990797708633172	0.6443166594044627	0.6952897759360883
0.7591735694282978	0.1950364010059015	0.5357297894435782
0.4224763843059430	0.5284820609062416	0.3638092520317219
0.1003182654924849	0.8666299802269498	0.7005777803403567
0.5463847346781920	0.7271319735470980	0.5646055347044561
0.2160150081383413	0.0591620250896050	0.3879246256935295
0.8700071855011040	0.3901392665451990	0.7307905611751131
0.1820402460199453	0.8092044120658662	0.3792654886387600
0.8508457291236285	0.1353117196082222	0.7098569767766345
0.5117347171071132	0.4718424845821698	0.5433899016613772
0.5255711929165252	0.1922832668162822	0.5313540307580512
0.1951071523695827	0.5227416196380734	0.3497303622109317
0.8622793071870483	0.8677940794478669	0.7028075559395354
0.3047928727219339	0.4638185781597528	0.5348689191562220
0.9711676258639614	0.7934735435266966	0.3642114224174626
0.6320855470075922	0.1314635332059574	0.7009087517461728
0.7833042646437560	0.7273177483162376	0.5583799660334982
0.4400615745255967	0.0559434597022312	0.3885192578812889
0.1103295054277887	0.3806292999222556	0.7299542183935700
0.6902584848777660	0.2730099967721832	0.3800745641037208
0.3757020091044598	0.6181582886471756	0.7070659608956483
0.0299304559422306	0.9419035078075459	0.5439054113424764
0.3071410996024196	0.2318810796971520	0.5306631117529016
0.9777956584688151	0.5716923641008638	0.3485247545410781
0.6290378913521498	0.8809326681174657	0.6940479926388841
0.0355880784899955	0.7402444796544607	0.5351755749848699
0.7062501601315654	0.0772384995197656	0.3647947429828801
0.3656887387794033	0.3990616607090422	0.7008256555159759
0.7757120070392097	0.9585427718177878	0.5577015698451232
0.4444086739099325	0.2842476848631580	0.3891465281693501
0.1180493456817178	0.6280886797306876	0.7303560049843130
0.1402796613102048	0.1454441068618610	0.3318033868990949
0.8107713255961889	0.4821155033976671	0.6755464998809321
0.5987922131043929	0.6239250823064090	0.3218731822792200
0.2559774837138306	0.9541305562869822	0.6531535032215344
0.9253909542003341	0.2907928939326375	0.4959948593594412
0.4709826247767994	0.8139394666552269	0.5097633317509681
0.3540748899503574	0.8946301987163788	0.3318285438785035

0.0176204996290534	0.2291976109267900	0.6750654771379805
0.8769768492996093	0.8759057091164546	0.3208558757663230
0.5450212223831581	0.2010351555743267	0.6531128461552499
0.2097086076406448	0.5345216927484271	0.4947962090830143
0.6888506196128135	0.5599926207042075	0.5145000353332652
0.6056246796444640	0.3596413277800263	0.3329605324845383
0.2669285525970866	0.6874424148202511	0.6751099321112045
0.6250054085027692	0.9014623192153183	0.3206707918976668
0.2988619033455963	0.2429727710323002	0.6526426570166316
0.9649415879125013	0.5744319480361808	0.4954168329474973
0.9429282365424130	0.0317493950025495	0.5129689547917087
0.9314578778392856	0.7897457062092037	0.4868575427501157
0.4745334737336149	0.3093158384614663	0.5054710032841551
0.1448569300525292	0.6455459006427055	0.3483607821294007
0.8032130158348388	0.9754820584280800	0.6776156955616681
0.5882724506417543	0.1190242092920130	0.3255855462542861
0.2565991071748456	0.4487248272518076	0.6644759299875417
0.7118966257210824	0.0425233361199172	0.4869022462087469
0.1906988284124137	0.0642456942675029	0.5036354825225221
0.8543517141732948	0.3991081817795246	0.3478294999136360
0.5146112683047281	0.7251468771500127	0.6708526940612434
0.3815369909567319	0.3686447128228679	0.3250809647986235
0.0442427967851124	0.7050262015804671	0.6668133357547391
0.4568029861711754	0.5664087454187412	0.4853802043989759
0.4345963313393612	0.0262381053304512	0.5043875830200102
0.1006526333350241	0.3549596468027754	0.3479082210352851
0.7715214660855155	0.6998341898648296	0.6787358702168051
0.1306066488722120	0.9114428412718212	0.3245784864015419
0.7942500598139817	0.2406320397930747	0.6677456940126252
0.7001781523654426	0.3009227002525851	0.5008181339679222
0.7043926086873109	0.8036279455683986	0.4995240285049582
0.1995003615532012	0.2983906234438338	0.4992467629906504
0.1998538174062449	0.8002453459621367	0.4999829863176574
0.8708647349993861	0.1285692338428858	0.3350237678709641
0.5258972732506422	0.4749262293007253	0.6647508062951294
0.3724232389131988	0.6425936962036146	0.3349033294118984
0.0291199110199382	0.9566422556030156	0.6654367770999796
0.3668152188040076	0.1331110438442268	0.3139558623053827
0.0317694118686651	0.4654355281295062	0.6864106217741943
0.8573839918450347	0.6292669459201240	0.3358247391635502
0.5443208881079922	0.9715584669967675	0.6642447496427573

The perfect Ir₇-O_{V6} surface

O In Ir In

1.000000000000000			
12.5091307398835667	-7.222149999999965	0.000000000000000	
0.000000000000000	14.444299999999984	0.000000000000000	
0.000000000000000	0.000000000000000	17.985499999999947	

O	In	Ir	In
71	27	1	20

Direct

0.8413089264868142	0.6137307428281972	0.4573935621371188
0.5158038325338794	0.9526458488090517	0.2894446237706886
0.1691391396896500	0.2786377045912877	0.6190883844009843
0.7935491095381850	0.9618132086483038	0.2975256766381208
0.4696059120292094	0.2942585675889927	0.6514447609705455
0.1346187538765644	0.6257933979773590	0.4704324409737465
0.3010829480575546	0.7314721786652836	0.3003968810539289
0.9772592658145641	0.0699630124080367	0.6356068771690239
0.6404482592474515	0.4068002182580527	0.4677142201701359
0.5295743464035089	0.2103984663122908	0.2699858721386709
0.1856367094148347	0.5389285293008340	0.6122723411957212
0.8594701394622688	0.8842968651294832	0.4407852133773882
0.8882798286577217	0.1312928324987319	0.4557165477955627
0.5484797175312984	0.4637909460650531	0.2908689194297958
0.2204324008098219	0.7903220787166130	0.6206881590397140
0.5391618402984467	0.7319127894089713	0.2978822083374157
0.2066895803703322	0.0760352973239673	0.6568385205247510
0.8746804637836297	0.4071589095967467	0.4694208378986648
0.7684212160495013	0.4689540937884404	0.3002436542633816
0.4287014308195389	0.7983531206600210	0.6379089689822777
0.0952388542868075	0.1343225460854630	0.4630413380813858
0.2907201986528771	0.2194216594677521	0.2696314804003189
0.9593060355761587	0.5426012300058489	0.6109411919833996
0.6188319327300321	0.8742703494799863	0.4406610555229620
0.3749570665472127	0.6583639236356911	0.4579007180881912
0.0375703837741515	0.9841380194993463	0.2884776920573128
0.7074596653941009	0.3301379109771115	0.6213797897177298
0.7676633332762015	0.7071834622602337	0.2995420501951374
0.4235048093595501	0.0261809572436674	0.6536256673975420
0.0919370661276694	0.3664084765218443	0.4696750907843337
0.0319626751273829	0.1997373071977159	0.2991524025568748
0.6904574534197715	0.5327299145032123	0.6430742392453006
0.3649588862471377	0.8594780456672726	0.4651770570017897
0.2814146738529853	0.9706428983148100	0.2689602853306163
0.9550075810180383	0.3150526279217556	0.6124004673196379

0.6246623021081387	0.6464722909351935	0.4443715105713072
0.2278506870754494	0.3186022487986720	0.3787075295557292
0.8878743253941137	0.6476062012932465	0.7096409992836836
0.5578413606804860	0.9861052780478885	0.5433818880429095
0.2674747418066828	0.9743929921332226	0.5314122011896691
0.9289397676308059	0.3069574917308692	0.3441292512568155
0.7587531582766973	0.1951497367146479	0.5359087622319917
0.4235134259292145	0.5291094076244832	0.3650273157452116
0.1002113963140729	0.8665549747659245	0.6998516456919399
0.5497868222096622	0.7279268202663386	0.5642932497757380
0.2163365628609805	0.0589466260091069	0.3873998251121419
0.8689715552488635	0.3893155471564947	0.7306548762019189
0.1825557205253755	0.8094560456679388	0.3790957850938006
0.8500385401643022	0.1346494616898651	0.7101760452931019
0.5121226821382659	0.4716628781526628	0.5442401319935548
0.5254500010675826	0.1918394504490254	0.5311996062293906
0.1954913083887768	0.5228318050740314	0.3497051546492563
0.8642463822283183	0.8698308845653521	0.7037549091847819
0.3046239972523420	0.4635753703668385	0.5352522468731439
0.9716425697144671	0.7934947212652746	0.3637854825158316
0.6319627614071416	0.1324292453727376	0.7007321316939312
0.7855502230552353	0.7283549369049355	0.5589785771706069
0.4402148584702425	0.0557444733515265	0.3883845441810094
0.1083341935877899	0.3790535256938886	0.7302573028226643
0.6901956227952057	0.2730730083452061	0.3799400104212506
0.3683400574301794	0.6157866202550066	0.7099890230350160
0.0307822633102625	0.9426663597551541	0.5437260494950327
0.3060896240230221	0.2310712594646219	0.5306239349366896
0.9780232185344068	0.5719419863513492	0.3490797905829625
0.6298892821437745	0.8836824794536257	0.6908863254569305
0.0362570511447360	0.7403103629535258	0.5346976654165626
0.7065896664135811	0.0776687858155600	0.3642109419974813
0.3607225025811101	0.3956189563647008	0.7026257208812879
0.7776768898835971	0.9602058687156521	0.5563563690787753
0.4444277677971021	0.2841328537569078	0.3893136927917880
0.1160243093983871	0.6263269711789639	0.7310522302223299
0.1404458373979046	0.1455589778553352	0.3314703320028802
0.8110998824320158	0.4817406725443391	0.6751853721234468
0.5990059915090035	0.6241541721937864	0.3226146099027229
0.2563888968194740	0.9539225054274572	0.6533742713317746
0.9253433667031047	0.2908577456820218	0.4963933834299732
0.4724266434501964	0.8136232283248142	0.5096424474096249
0.3544935176249394	0.8946363338596902	0.3318331578048328
0.0162580087849366	0.2281348185266486	0.6753024525202378

0.8771396563744727	0.8760401596775444	0.3207231904166696
0.5442073168463077	0.2007053262926431	0.6529254749617254
0.2097821386006580	0.5342959537653036	0.4947500567088644
0.6887306591619340	0.5606017845770914	0.5146553650275676
0.6056805411822520	0.3598215707744795	0.3332985467099799
0.2639889934016010	0.6850569429508615	0.6760459420052308
0.6253615008300580	0.9015309828587246	0.3203962373760099
0.2962179612460460	0.2417034522540074	0.6525769829650688
0.9652056367841000	0.5742768007590607	0.4948029931164270
0.9434285678780904	0.0323064462279712	0.5121067078882598
0.9326694416156165	0.7904322723110445	0.4863135544640011
0.4740126581699982	0.3088289253567160	0.5057637611877823
0.1453354530037336	0.6456714216554402	0.3483498178026955
0.8012238254126379	0.9749224812819512	0.6764110298160498
0.5883193742208177	0.1190419568464165	0.3253691245262978
0.2542823831733368	0.4476759005107901	0.6646543422373702
0.7121300552959690	0.0429760203212070	0.4863824660491189
0.1909398633863899	0.0639243287016630	0.5028665245129332
0.8544551532198373	0.3991136536184798	0.3475987910474436
0.5060529791161672	0.7212240947632143	0.6715157358079966
0.3819372991383129	0.3691749452057407	0.3255792742178177
0.0465676483448620	0.7050466834192108	0.6659032415009712
0.4579993300411757	0.5683805291547677	0.4874427940494864
0.4350356996491617	0.0257592855017099	0.5043450661068892
0.1005208116694510	0.3550809173301897	0.3476137911609047
0.7838955426228649	0.7041166296752284	0.6786538722674638
0.1309980833902826	0.9113949002424488	0.3241407431859887
0.7935764948160274	0.2401947135773982	0.6678795209454269
0.7000104993292220	0.3009162927248915	0.5005717646585786
0.7047587450111351	0.8042693484519025	0.5004291360373780
0.1993193581548369	0.2984379613184149	0.4988048478949051
0.2006470161684152	0.8001694133517193	0.4998142344505330
0.8710974718759176	0.1291884854884413	0.3343642080522395
0.5217828289161391	0.4706607778040098	0.6662608039303106
0.3729046193184994	0.6425512638121317	0.3353636115054028
0.0313658497162232	0.9591313362987257	0.6652970692472066
0.3670689682021647	0.1332811092783239	0.3137947414412543
0.0305373815220764	0.4642029775859073	0.6865072052058880
0.8571337632557290	0.6292986922009077	0.3359817127258758
0.5462544790973849	0.9718320844569075	0.6644679916999232

The perfect Ir₇-O_{V6}-bt-CO₂ surface

O In Ir In C O

1.000000000000000					
12.5091307398835667				-7.222149999999965	0.000000000000000
0.000000000000000				14.444299999999984	0.000000000000000
0.000000000000000				0.000000000000000	17.985499999999947

O	In	Ir	In	C	O
71	27	1	20	1	2

Direct

0.8403017446047655	0.6139259442007029	0.4582251097072935
0.5155960140142613	0.9528557150388602	0.2889388479333861
0.1708711879184197	0.2780375825370421	0.6188906098246504
0.7931678079617651	0.9616427817264301	0.2979977536593329
0.4668189676847504	0.2873346509160147	0.6566568597122516
0.1324160219793689	0.6256962225627770	0.4688501232550250
0.3001713423730004	0.7310536656705036	0.2997510526317858
0.9785816153934239	0.0702289524158562	0.6355490989589588
0.6402736430954632	0.4075390288224732	0.4693406787791269
0.5290669064200385	0.2095206347214681	0.2685224139057941
0.1794968203360799	0.5369418179169335	0.6087627003875424
0.8564273866562767	0.8811852505644664	0.4422258565523778
0.8871197388798883	0.1302967887259165	0.4556069201955149
0.5475728592976290	0.4638591589261656	0.2898647493553909
0.2225783335202452	0.7895718019401360	0.6197395957714544
0.5385143169128029	0.7316775378289561	0.2989405917510351
0.2065849778420241	0.0745973861164502	0.6594872037994872
0.8740091490392418	0.4065058613327349	0.4688984205691918
0.7678157356202155	0.4692197383846467	0.2997827611960676
0.4328446143105794	0.8059727118508184	0.6572090101164205
0.0947240792076923	0.1334130012533614	0.4631419911705999
0.2908142031485931	0.2196719872698691	0.2686676089095886
0.9565823520273928	0.5417959255033202	0.6105546661531264
0.6190648274808841	0.8755567658692910	0.4402708839621232
0.3709095783105513	0.6577427594795773	0.4570764437825318
0.0364597889782972	0.9835645157246019	0.2887665225235013
0.7074153144629977	0.3318678910271468	0.6216032589499003
0.7669189531692168	0.7069463536434127	0.3003093591284290
0.4243967602156671	0.0270858605285447	0.6536182558521981
0.0905928143851318	0.3643437701049007	0.4682751185419753
0.0307795923618175	0.1987982022776910	0.2986516722802778
0.6874212017622967	0.5321520196029501	0.6493402067959402
0.3652137640947333	0.8595575318666094	0.4660016904131447
0.2805777494382603	0.9703115350970506	0.2678466128919507
0.9552353427192241	0.3144435516230783	0.6113326737631789

0.6241673361891409	0.6451453526262402	0.4453183151051996
0.2268182252226592	0.3172558274903508	0.3777075429764564
0.8878857230211029	0.6458416077189284	0.7117588862264681
0.5566035953590714	0.9840192198720010	0.5451618417138120
0.2671470051807860	0.9742601929622799	0.5314854572732619
0.9276064225607795	0.3063733190901923	0.3429909739875419
0.7575180253130777	0.1947803716139194	0.5362815869101273
0.4232432964205992	0.5288387371934289	0.3665063386801197
0.0997778641525742	0.8644142078578019	0.6985110375428950
0.5414877353637222	0.7252220123259826	0.5634363872665303
0.2164959537580748	0.0593461432539028	0.3863392249498275
0.8705917418555565	0.3890009223429231	0.7306973339569058
0.1830243952903292	0.8102319451555204	0.3786966331435486
0.8535039595228490	0.1374300533894821	0.7107061583707787
0.5122428100946688	0.4711333300634717	0.5469664927431821
0.5253586781083989	0.1922117850892190	0.5310506220611465
0.1936884305864232	0.5219000033336431	0.3490622378354067
0.8651237892790216	0.8696964095846241	0.7040437379145779
0.3028968752722297	0.4620639392604493	0.5337483705451200
0.9712937398974689	0.7935834543992630	0.3646595051082996
0.6344581764835631	0.1358489083731752	0.7024830421000712
0.7816973796672374	0.7256753436927069	0.5619521228559788
0.4394697488954759	0.0553943400322023	0.3880769661470408
0.1111723410851239	0.3803155455168108	0.7282456936046109
0.6886858579895712	0.2738017129756767	0.3797621486535807
0.3631711002194251	0.6093174314679771	0.6997606608141612
0.0302871412694448	0.9421630280255012	0.5434563194133631
0.3069006467154356	0.2301476807217287	0.5309685698949148
0.9766134339132232	0.5719406379803372	0.3487482953022453
0.6387557581441209	0.8974812781418088	0.6927509782303446
0.0357206897785490	0.7400388824620472	0.5352967455248853
0.7059402991265433	0.0782279258515453	0.3643736051229727
0.3651670600594356	0.3965411774972422	0.7013592400211367
0.7775387885296561	0.9596233564309670	0.5567464008652347
0.4448431904221710	0.2844679360293048	0.3876722385585237
0.1165248460247643	0.6258344756680910	0.7297764912776685
0.1402175261558941	0.1454657264558151	0.3300665317963626
0.8112263977248795	0.4809168867850937	0.6772071745636393
0.5980919614124983	0.6237376207534172	0.3235714210317422
0.2569406662591284	0.9526783273380213	0.6532713931298540
0.9245552043628885	0.2900289169249636	0.4956126690223391
0.4725851000694516	0.8130862391369444	0.5084689548483152
0.3540697635139801	0.8944823965471747	0.3304619835029017
0.0184847147637197	0.2294953973603712	0.6750355743998637

0.8760889091519506	0.8754332720457180	0.3216561420217510
0.5452720236843211	0.1998334348848458	0.6527587452704008
0.2071791357915140	0.5330592168333891	0.4925753439581135
0.6874101377018699	0.5608575696185200	0.5150855816021429
0.6049682012756239	0.3596035481878820	0.3303897763358616
0.2642965634666881	0.6818113574651927	0.6747053408500679
0.6249064384829521	0.9014799845570020	0.3199639850295188
0.2949891058817183	0.2396603003821621	0.6530768718501737
0.9642936180513605	0.5739130320207072	0.4942941180471720
0.9422893147042567	0.0309489336014682	0.5115820334119826
0.9312059299755500	0.7895147912793216	0.4869930368826383
0.4734562412449194	0.3082866872038816	0.5032078456174206
0.1442610702289258	0.6456995937372132	0.3472048815618771
0.8057915687042148	0.9785739686749042	0.6766334375020601
0.5878878353458776	0.1190633286316193	0.3251975238130015
0.2567514945696136	0.4490800475846426	0.6610117673895717
0.7112824118501825	0.0424718600013917	0.4866659134467003
0.1906570114856556	0.0630816055820605	0.5015666380273288
0.8535116368562071	0.3988394023516650	0.3469324131615231
0.5138911144438667	0.7350679534623057	0.6842403095002418
0.3813291344827558	0.3698035925046060	0.3248652545509884
0.0471444816916918	0.7036560921871418	0.6647538326472580
0.4575845773787862	0.5709085921983057	0.4901082566829370
0.4350068511006523	0.0255241673359537	0.5042880410659762
0.0994148999051564	0.3542903230179530	0.3463104165819750
0.7868834434628396	0.7047653439868949	0.6808431742081048
0.1303630559288183	0.9110873335027043	0.3237085966597618
0.7954418769206099	0.2408599723412232	0.6677785392122425
0.7000847468026795	0.3016587076677853	0.5005047414646564
0.7004021899595695	0.8024643925304334	0.5021804660944256
0.1989170528592356	0.2975672538559487	0.4978197249566195
0.2002115899073453	0.7994453836481308	0.4993500409114612
0.8700343112160455	0.1289123305524363	0.3339397675395908
0.5217150043313200	0.4575512667909502	0.6667433361056763
0.3717898571390055	0.6416583758515398	0.3353164353770408
0.0321667422187273	0.9585983276104162	0.6649572811034755
0.3665809703424250	0.1328895561680123	0.3121641639227801
0.0316674114080037	0.4640554308795271	0.6847445660444091
0.8564525810852593	0.6295123911627232	0.3360826639643258
0.5486552741912765	0.9763338892862701	0.6667746211476964
0.5674853779568859	0.6981931918471542	0.7735720307647316
0.5753668997522059	0.7029334200467113	0.8399032815407371
0.6027359052164155	0.6550668603213760	0.7202819459076747

The perfect Ir₇-O_{V6}-[CO₂+H]* surface

O In Ir In C O H

1.000000000000000

12.5091307398835667 -7.222149999999965 0.000000000000000

0.000000000000000 14.444299999999984 0.000000000000000

0.000000000000000 0.000000000000000 17.985499999999947

O In Ir In C O H

71 27 1 20 1 2 1

Direct

0.8400325694476951 0.6148066022486329 0.4611744219467852

0.5167124194089175 0.9524274461298414 0.2894999263633424

0.1722160741108684 0.2802651609212622 0.6187242443748425

0.7945299132697123 0.9615467572474335 0.2994209298464240

0.4643670216973468 0.2833402420773341 0.6627665633883346

0.1366860920047339 0.6277386361800754 0.4692949986115926

0.3018942920032560 0.7309782275866260 0.3003581441784101

0.9814089946774830 0.0762302940399739 0.6312890769489253

0.6419767261310140 0.4095937118459030 0.4701880275103735

0.5304804637355213 0.2101410027201570 0.2672091714173077

0.1827826462845716 0.5373601519381018 0.6094299104906510

0.8574667353826544 0.8813262425402150 0.4449532552080437

0.8887251872905865 0.1316044719773955 0.4546482543170028

0.5491139569960048 0.4654126703406957 0.2904774738185021

0.2213521404663030 0.7915780390939223 0.6179609352749549

0.5400434671886574 0.7319103136849475 0.3004267618674939

0.2078479554753263 0.0771008799554888 0.6603122345041046

0.8741240470050692 0.4049621003522308 0.4679113818578559

0.7698903999051609 0.4709859912959478 0.3004869722971426

0.4256523263214923 0.8057634081962365 0.6462470334922914

0.0968022751176048 0.1352477784563723 0.4614776992345638

0.2915519470638341 0.2205207107955394 0.2677215438349630

0.9590622091011871 0.5379380132704145 0.6072227299243682

0.6210925190444309 0.8740579196138735 0.4423514393960951

0.3770224341155843 0.6596435168565435 0.4597542852721972

0.0366792028516004 0.9835895306545209 0.2892255179177020

0.7071306699241877 0.3289019696565814 0.6211453295670021

0.7670205500511309 0.7072487639393964 0.3040233970873700

0.4241823504939336 0.0264931652315171 0.6522511209466855

0.0916315410726901 0.3650160659937457 0.4684758140911914

0.0325899336308320 0.1997333629217661 0.2982901693685478

0.6876354586512530 0.5263357898786439 0.6480361996901934

0.3659672671402390 0.8608218922752227 0.4640045230820771

0.2807954820639822 0.9701222326738730 0.2669137267211835

0.9553440724977618 0.3135396178927086 0.6116082639520051

0.6251148211571094	0.6468431498185313	0.4506711281517302
0.2289253584611763	0.3189869373587497	0.3776381693250130
0.8941339434275455	0.6437317212149878	0.7058419903820908
0.5574146586448987	0.9864743805050611	0.5429450627021266
0.2681857227187486	0.9757995982797899	0.5305531484029049
0.9292808827934179	0.3074008733067446	0.3401081895774569
0.7580639203404201	0.1946024136535564	0.5358565375046785
0.4251652421062559	0.5291775154688224	0.3681482202160756
0.1003751954988658	0.8662368800031072	0.6964246575494745
0.5472425550453455	0.7308419552916474	0.5701024100530522
0.2183320400715976	0.0602213945337552	0.3851328214788879
0.8697954878405030	0.3876668228661797	0.7299145108076945
0.1835483935557715	0.8103101786972577	0.3773539988518105
0.8516318263245829	0.1353230574537152	0.7110830152304275
0.5112666732474661	0.4689622641471049	0.5483276334863998
0.5247408909938369	0.1932775635813291	0.5309220023959372
0.1965712274262780	0.5229642937500695	0.3513336894046749
0.8738820450166319	0.8809463745109783	0.7033862347063315
0.3043706962282186	0.4636007391700227	0.5348285002183457
0.9719684315400440	0.7943740976801135	0.3669920219661545
0.6336072191818690	0.1338231356271534	0.7023693429038667
0.7841370307873408	0.7272070003117139	0.5708589484043008
0.4401558154029034	0.0565996208206198	0.3867482676154742
0.1100003139967983	0.3798294815819575	0.7289416348752726
0.6887515576963873	0.2739017952831523	0.3791930169094162
0.3575723202695998	0.6149184276439875	0.7067022553014024
0.0335580179183167	0.9449387027072970	0.5429424656470248
0.3086318383738860	0.2315040584121818	0.5307928046539323
0.9778120515766286	0.5724545629523868	0.3528019577068624
0.6317603671190551	0.8906297050951169	0.6877107062050011
0.0372427246498079	0.7395554400802399	0.5338895737168290
0.7068413710891399	0.0781957759666167	0.3642352061170872
0.3659913968550474	0.3992125156908001	0.7005203649908525
0.7791460913085192	0.9626553917268573	0.5572034698935907
0.4460354209342339	0.2846726315557959	0.3861705275237013
0.1134688277376908	0.6252994345047330	0.7289823126088943
0.1412846216202374	0.1460076698249896	0.3297993678282368
0.8127970799471357	0.4803241058743650	0.6742539768676197
0.5995569383450242	0.6244109873556075	0.3269589293938129
0.2569455872800662	0.9548564047161994	0.6527474740219151
0.9253352832753127	0.2901610200238897	0.4961495855024551
0.4742201949093622	0.8162055114794218	0.5077662388545204
0.3548086786537430	0.8949335181496431	0.3297479900767705
0.0178964240130580	0.2291371603696185	0.6748549492958218

0.8772833731491366	0.8755865504392022	0.3244466732786538
0.5452187219920637	0.1991015391725518	0.6528266216098438
0.2092705708040577	0.5338310620169936	0.4926129282308740
0.6903517822623197	0.5617382410273178	0.5226799650442542
0.6063467398210990	0.3603255524096809	0.3296024940677347
0.2582760217170106	0.6837021399795707	0.6731582289756273
0.6263845481857052	0.9014937670836926	0.3215415621716886
0.2954941558626616	0.2414161795323210	0.6530560126855589
0.9658914172039639	0.5734147682956704	0.4923065862608169
0.9448253023026186	0.0337431276523443	0.5114959128983141
0.9305433083972574	0.7893558259703366	0.4915622944405535
0.4747909210439769	0.3097179013762615	0.5011555953881724
0.1458678741503525	0.6460028294834931	0.3476997970888695
0.8049991885922003	0.9776538882733865	0.6765987714602318
0.5886968031001841	0.1192223511905181	0.3245095574277101
0.2551405740306036	0.4481912892401080	0.6625158696761774
0.7129807836745448	0.0430135844271362	0.4862397988652654
0.1921366449666571	0.0645989167870707	0.5000955679557140
0.8540132131735629	0.3984328903527855	0.3465544051881658
0.4989395940169917	0.7291100378098387	0.6766469648530750
0.3824948100742616	0.3703018883417016	0.3241720044159311
0.0476250568427986	0.7049424399113757	0.6609640870054083
0.4588500079912236	0.5682878632691288	0.4905355636232387
0.4352150880075302	0.0271721682509450	0.5028505117922718
0.1006664676733091	0.3548584390166560	0.3464479605822423
0.7914713390055573	0.7068785753302718	0.6977095170837532
0.1303448057332970	0.9110532889946684	0.3235051462911617
0.7945920297290527	0.2395297437229733	0.6675623570977236
0.7003385719606389	0.3018434033588707	0.5001744765990666
0.7053074834790921	0.8036444380807620	0.5076014691170599
0.2002665482626712	0.2985963942041996	0.4978460562799257
0.2012293817090991	0.8014767290460291	0.4977576495544030
0.8714635886854977	0.1297043406566508	0.3331416845934203
0.5233509831579569	0.4527384185915345	0.6678421100820651
0.3742076195622647	0.6427917748437842	0.3367692327200553
0.0347033575065893	0.9637006579767290	0.6644855879608166
0.3673845696405221	0.1331517303758314	0.3101490864510139
0.0303111340976391	0.4633249545984709	0.6844467214588283
0.8565666644950723	0.6302749982016810	0.3395141094670609
0.5479202084865978	0.9760282908322355	0.6642309738349915
0.5535490446031411	0.6831786258172494	0.7657014349022748
0.5616988340292676	0.6945800460983028	0.8314264605652449
0.5694176410486531	0.6338541364708810	0.7114389734260939
0.7363870144061658	0.6786275405897130	0.7868834028919224

The perfect Ir₇-O_{V6}-[CO+OH]* surface

O In Ir In C O H

1.000000000000000
12.5091307398835667 -7.2221499999999965 0.000000000000000
0.0000000000000000 14.4442999999999984 0.0000000000000000
0.0000000000000000 0.0000000000000000 17.9854999999999947

O In Ir In C O H
71 27 1 20 1 2 1

Direct

0.8414545971458038 0.6127554000518093 0.4576891816202415
0.5167126616900576 0.9513529535683930 0.2895246812637373
0.1722706732500434 0.2762658366406911 0.6182810366010021
0.7929998178985282 0.9599167963057603 0.2991103473438243
0.4697486571360571 0.2890939171620458 0.6533022396033906
0.1337152153677257 0.6250581093063993 0.4687537731177378
0.3015399488569671 0.7295199607165047 0.3003862234677687
0.9810534973932573 0.0699889519730676 0.6353887414525249
0.640828833806804 0.4057651654506367 0.4679196898030495
0.5301987235114500 0.2084199668274637 0.2687895277064956
0.1777705101079547 0.5333216630041959 0.6070030592359721
0.8573452518363752 0.8800316479258160 0.4425980859901820
0.8881132179395096 0.1288600672377267 0.4559146826409539
0.5485269966667768 0.4632195957159259 0.2907845681309096
0.2239315644748340 0.7891928813824837 0.6191322153664910
0.5396204589854805 0.7310404281906825 0.2999653884872329
0.2089937201394656 0.0743855638927770 0.6627719607269668
0.8756347846278012 0.4055545906455280 0.4685353062518076
0.7684547033225607 0.4678046976138455 0.2996876136544518
0.4362935757644901 0.8082037742075673 0.6500798824212447
0.0955353661878645 0.1315695137563180 0.4618547020856172
0.2919739116480442 0.2189945721147961 0.2679494058256848
0.9583532840999143 0.5415786498429950 0.6105661590264854
0.6179180664777335 0.8718030557296278 0.4439531736715507
0.3742486446909985 0.6580158657220838 0.4597416337723868
0.0367443285746254 0.9819007230131148 0.2878906832852075
0.7098232551984514 0.3305195059707340 0.6209663016864756
0.7670560246779160 0.7055250850176678 0.3011624823117624
0.4261956191493324 0.0279103300238802 0.6542699028787545
0.0906322091875679 0.3615212112366167 0.4678936912862416
0.0309823213955521 0.1971608060425949 0.2982250670390396
0.6906539701169353 0.5290584007995793 0.6448115551650430
0.3670826866875380 0.8578434676814107 0.4677434912126139
0.2817307071762982 0.9688636840866290 0.2670363544153347
0.9568733860638867 0.3135262879606476 0.6118100366225300

0.6241490103563755	0.6454781859346969	0.4470686515922144
0.2272878267486887	0.3158564201506989	0.3768592276080962
0.8884565481147402	0.6450242271685239	0.7121882227683045
0.5591132342711305	0.9855789888098844	0.5452973521249749
0.2686519973818240	0.9739760402270000	0.5316232251666012
0.9281946880217239	0.3048274824570694	0.3417470065037632
0.7593639128930718	0.1938459679968086	0.5367616077670394
0.4242862969899173	0.5281409232978833	0.3676209834386890
0.1015380476069505	0.8633027141773133	0.6986062521588811
0.5426537736373703	0.7222505976258152	0.5713947814970419
0.2172468922464816	0.0579146667452584	0.3848822135271194
0.8726867401569931	0.3889941405804280	0.7307825414894723
0.1848133161134921	0.8098780704432333	0.3785264432277256
0.8561196633248098	0.1373465682219803	0.7116047355482770
0.5128586754989000	0.4698848965885756	0.5453271862023709
0.5271477449623411	0.1909783918836436	0.5305211344493892
0.1953114162277919	0.5209886658365425	0.3517249715463853
0.8673125927284072	0.8688043080414812	0.7041885470469272
0.3026182668366180	0.4592570977886747	0.5323140132716512
0.9724424674073249	0.7924095268035456	0.3640777401561395
0.6364218690280675	0.1368491743330321	0.7035539443792586
0.7839088440483740	0.7253330227888101	0.5609346413805469
0.4396057718509804	0.0536362906728224	0.3879060756586630
0.1141212913907506	0.3800303240196742	0.7280757307277010
0.6901253861261144	0.2721505313762906	0.3795292394344986
0.3653913263672933	0.6080369878576097	0.6881416082599267
0.0324847133044554	0.9416996928484656	0.5435207448235305
0.3072004237792629	0.2278138345566107	0.5305178295603655
0.9778716821881425	0.5708048566650100	0.3476605518561487
0.6432961965774552	0.9010453546672070	0.6917279573059233
0.0368987590885139	0.7392544394493875	0.5348523251577966
0.7058628231293966	0.0756110767351981	0.3661848139717949
0.3674222867462797	0.3963883662277368	0.7009115632245690
0.7796350907334445	0.9588609372752763	0.5576265368877091
0.4448888915881473	0.2825607397594730	0.3876907986306627
0.1203370368208147	0.6256189154237878	0.7286322484542332
0.1407906093683541	0.1441054572040436	0.3288267617299366
0.8129022226491859	0.4801251140188586	0.6763239652543536
0.5986283145724911	0.6228446158612851	0.3249962022809600
0.2587401533600798	0.9525175053125982	0.6535420764360099
0.9255534120745396	0.2886613735876641	0.4962389700143364
0.4727852811924538	0.8111571904341928	0.5152206373888715
0.3551484730466211	0.8933223077587362	0.3304996238704903
0.0207178135264264	0.2290988064269490	0.6752026024427140

0.8766745503206458	0.8742893014641099	0.3221816310737027
0.5474963204094621	0.2005785637183500	0.6523129554608927
0.2075110764236340	0.5308157141411446	0.4911638795649453
0.6888995008899380	0.5591444428298626	0.5143514963123430
0.6057738446575734	0.3583929128542119	0.3311760572416876
0.2662871086498040	0.6803645222277280	0.6700785121153205
0.6251291708810349	0.8997750352609528	0.3230378279276543
0.2972678216600581	0.2390179492867352	0.6528161922848219
0.9656148383400501	0.5730257593310615	0.4943264631679980
0.9438031539602579	0.0296446386833568	0.5113467256005451
0.9328649699721441	0.7889331469295362	0.4865452288826761
0.4742115208513913	0.3063116195081854	0.5033650298344945
0.1452910687661650	0.6449443236298287	0.3473486182885158
0.8102119311066005	0.9792244759394547	0.6771253897746854
0.5885417202926683	0.1174914470093159	0.3256898674763425
0.2576175975458636	0.4466348299696439	0.6587064689642332
0.7125376236114837	0.0409576211881148	0.4877934388758804
0.1918525132647138	0.0615512296988131	0.4999426581571890
0.8546345120056896	0.3977042823674496	0.3465307992109634
0.5184160322591129	0.7386025659831755	0.6878882905229347
0.3821807006823729	0.3687991456447897	0.3252301176540821
0.0486124867200836	0.7027462514045086	0.6651878239201691
0.4584272931883568	0.5703583596021842	0.4918985425008335
0.4362499514485479	0.0242864935201615	0.5040077678277816
0.0997128072062931	0.3526841807762293	0.3461542239048558
0.7877194671473227	0.7034938678739526	0.6786422190462694
0.1311655203248624	0.9096525344873866	0.3224757431877107
0.7974292996258423	0.2404879309881783	0.6682083347185219
0.7015085898939400	0.3002963475944220	0.5000855542846181
0.7008961389763322	0.8011193287830591	0.5047629302311486
0.1993720026471334	0.2951377228567390	0.4969968306419518
0.2016472370923978	0.7990022099886892	0.4991492420053240
0.8703926272636285	0.1273098060336251	0.3344420208777546
0.5243908910968539	0.4604366042062679	0.6642590382012042
0.3738365984340707	0.6416970233461706	0.3374760602000630
0.0347073931272696	0.9582658835130503	0.6652082133761014
0.3673715945994743	0.1317432210102910	0.3114333173076506
0.0336954417792434	0.4634227306048080	0.6848424535378325
0.8573625275919928	0.6282114398356782	0.3357175978005353
0.5507014804024392	0.9784926042494341	0.6661800494883398
0.5030429303564454	0.7528773962126585	0.7875036037623593
0.4959101937153410	0.7615890460496124	0.8513134385911793
0.6060530938710637	0.6515218940492010	0.7114845332495996
0.6012713070120717	0.6436299442563139	0.7652145850988173

The perfect Ir₇-O_{V6}-[TS-CO-O]* surface

O	In	Ir	In	C	O
1.000000000000000					
12.5091307398836005				-7.2221500000000001	0.0000000000000000
0.0000000000000000				14.4443000000000001	0.0000000000000000
0.0000000000000000				0.0000000000000000	17.9855000000000018

O	In	Ir	In	C	O
71	27	1	20	1	2

Direct

0.8401309569240076	0.6139163090204961	0.4589439792555868
0.5153634283313705	0.9529272011956513	0.2890852151133019
0.1705827598221397	0.2777010865778162	0.6184201323359811
0.7929895420796234	0.9613839131484841	0.2981021070745546
0.4694561016726891	0.2916659902814479	0.6527410530628835
0.1314913231698015	0.6252771786083489	0.4685911216413437
0.2996554376329763	0.7309986410392139	0.2993922737972535
0.9789665032866981	0.0705026911459407	0.6354878142385199
0.6402613394143226	0.4079689683738077	0.4708571249442968
0.5288367651772272	0.2100149145181382	0.2695732686162982
0.1789474138890805	0.5365402231441797	0.6082331262851363
0.8557436407764331	0.8807917695144998	0.4425360429506855
0.8869966444492581	0.1302315513698400	0.4554124414144008
0.5472792107435109	0.4636354290429043	0.2904850684906216
0.2234465103574142	0.7899660423873934	0.6191972939559302
0.5382788213853978	0.7316940210232132	0.2987237895600426
0.2069186765122959	0.0751105308958993	0.6586756366149874
0.8743910877848365	0.4070675002057278	0.4690504322123423
0.7669449259278213	0.4692651138287871	0.3008512241839841
0.4363983314252964	0.8055898826116077	0.6547454420970514
0.0941438157304813	0.1329996594495584	0.4630527947992949
0.2911491080647398	0.2196350155058952	0.2696191529005522
0.9568950559193588	0.5424980041164860	0.6113288444416570
0.6188808551468060	0.8766034205341677	0.4399847277459158
0.3686016709693494	0.6575196680216033	0.4560719624772552
0.0361636469682604	0.9832834925690526	0.2890077754617039
0.7085773478974053	0.3312695548601794	0.6222847362450741
0.7668630412237168	0.7068552772383324	0.3001228244724846
0.4244530106379830	0.0276730792227718	0.6538171359294629
0.0898585405807684	0.3640863697165607	0.4677765276588227
0.0303875249587053	0.1984073530148048	0.2984972184237230
0.6876859647438970	0.5301486819198705	0.6478237005670611
0.3650633793197803	0.8598901771851781	0.4658518082021309
0.2804652758341002	0.9704370191680290	0.2685212552177911
0.9551613492510486	0.3149406197397662	0.6115371976380660

0.6246222887441873	0.6449046300956136	0.4447298192120518
0.2260873637558745	0.3171051463544332	0.3774280334439669
0.8869051930609425	0.6475038778910623	0.7112045939284849
0.5567354508534261	0.9848267470707596	0.5449142122984735
0.2671619661069085	0.9744388400073406	0.5313288050019457
0.9271701032096684	0.3064285862582121	0.3420861325485746
0.7578061517040080	0.1948534148571012	0.5358873999900965
0.4229172427222390	0.5291992787661128	0.3663172890614160
0.1009142199347397	0.8650938925129283	0.6989326721026075
0.5394079830920520	0.7247734854178304	0.5597665209911921
0.2159959247521841	0.0590362229718236	0.3868543011611962
0.8713643052833175	0.3903339205520561	0.7311455598666984
0.1826110622544196	0.8098529134650789	0.3787573894782607
0.8537784990783565	0.1378361476349196	0.7107531390282231
0.5119409869817527	0.4738197158530723	0.5478662102188439
0.5258843394807153	0.1922550987692477	0.5312080251295747
0.1927791040728764	0.5215119363763948	0.3479587237562990
0.8657163953052719	0.8699032086480585	0.7042404736446254
0.3021873955312607	0.4614776880791627	0.5325298848513130
0.9709441030046235	0.7935413568050572	0.3653404118567685
0.6340124640682810	0.1346745519664738	0.7019155066039142
0.7804913481627578	0.7261283170084680	0.5626085664582038
0.4394858183670522	0.0554190170971020	0.3883317795818416
0.1115893603940129	0.3806780090805745	0.7280153649093022
0.6886956753636854	0.2740511009877863	0.3804111495745269
0.3664405562987606	0.6081702783588442	0.6924538040785838
0.0299558091235366	0.9420158243040594	0.5436533931660988
0.3063774016222950	0.2303224486352784	0.5307074555082254
0.9763103760818297	0.5719682709700347	0.3475237853414196
0.6402995222447723	0.8958518936408281	0.6924030879864107
0.0357442195307422	0.7404434233878489	0.5356388626084104
0.7061279885460959	0.0787780544857631	0.3637823534305142
0.3639860456824309	0.3954847990998839	0.7022652437334618
0.7772847974271097	0.9596994662826418	0.5568144251177357
0.4449515626597779	0.2851644280255801	0.3897998975902883
0.1198689573998071	0.6274700474425418	0.7289435317044008
0.1399200737693147	0.1452150802856922	0.3303510329812216
0.8111832069807384	0.4820119922717117	0.6775826281980680
0.5979298952922010	0.6236900809815145	0.3237557180465188
0.2573085419673526	0.9528567687314153	0.6530502705577310
0.9243193264606162	0.2899427203174918	0.4959240056519396
0.4714243331513925	0.8128716340956983	0.5092300751573801
0.3539153101735519	0.8943323025841614	0.3308129361560084
0.0185797264215949	0.2298534295362637	0.6748902922522293

0.8758040712406919	0.8751388690919418	0.3221889772078825
0.5454114834847616	0.2005249596149276	0.6527535189121045
0.2065856190132121	0.5327109992652390	0.4921411552518556
0.6871013709283956	0.5612767551076685	0.5164096893204315
0.6044155994588580	0.3596668334936213	0.3321674089695837
0.2678438254833824	0.6829003753987234	0.6726557725325141
0.6246613159460639	0.9014922514514294	0.3201047450400151
0.2963952751378820	0.2405068825088248	0.6527173983885654
0.9640985281127384	0.5741959341864835	0.4952139870720524
0.9417176311542940	0.0305548106159829	0.5116183663616434
0.9300068368276195	0.7890437663385080	0.4880183142441752
0.4741651992847957	0.3098985802664605	0.5062372845399916
0.1437418157203716	0.6454342114240943	0.3470233070158900
0.8071723814474375	0.9789443234805237	0.6768509964561199
0.5878325015786897	0.1193056308715472	0.3254729556365946
0.2562498152774292	0.4478846547491573	0.6597857865957223
0.7110553028489502	0.0424152090782248	0.4865262392048545
0.1904415184543654	0.0632077731481725	0.5021377724631222
0.8533454212569189	0.3990693623717353	0.3471473468038035
0.5193456962219958	0.7332407908157677	0.6844734149251132
0.3814057623430106	0.3696769479019782	0.3260559388094817
0.0473339447379452	0.7040709218351061	0.6655396439746964
0.4574312006277579	0.5723876805883898	0.4899728345682624
0.4351614890038437	0.0258869450084595	0.5045386563237503
0.0986949596148333	0.3540614605628927	0.3458915965979656
0.7808959754608867	0.7033317925088293	0.6825532939388059
0.1300478358887389	0.9109024385494305	0.3241862011185105
0.7955826426215779	0.2415514594652089	0.6683821695499900
0.7001884940226768	0.3018197068180120	0.5010505270034673
0.6988307361134348	0.8019537511010758	0.5022556542242714
0.1984599588115333	0.2972397609359552	0.4974446085685805
0.1999709162737917	0.7994516197295092	0.4992963663382911
0.8698036010765681	0.1288229608117015	0.3338420698757842
0.5224353636160212	0.4655762150414783	0.6684171185874590
0.3712311877370081	0.6416185521224544	0.3350680097105169
0.0318512200679314	0.9579433713221097	0.6650765385818590
0.3665203933955924	0.1329472259145616	0.3135385862074363
0.0325844729164637	0.4651548526138667	0.6848803758189319
0.8562527891399323	0.6295903848970956	0.3367063730556282
0.5484175473549906	0.9748369216615015	0.6664562838227202
0.5590940395497022	0.7008207952317189	0.7778922155215664
0.5705773367898551	0.6993799038323028	0.8429567920368817
0.6027506895113972	0.6498734411151772	0.7188337285685847

The perfect Ir₇-CO*₂-P surface

O In Ir In C O

1.0000000000000000
12.5091307398835667 -7.2221499999999965 0.0000000000000000
0.0000000000000000 14.4442999999999984 0.0000000000000000
0.0000000000000000 0.0000000000000000 17.9854999999999947

O In Ir In C O
71 27 1 20 1 2

Direct

0.8412139758652558 0.6125579636204639 0.4576483029084137
0.5156061915124217 0.9519356135550034 0.2903188618320549
0.1705729638667598 0.2768843218997243 0.6182262790920615
0.7924797276288581 0.9605372370322215 0.2988336999261195
0.4722624305625506 0.2947632721658615 0.6477514623010289
0.1313046232802760 0.6246222471861307 0.4686068642830669
0.3005890572968790 0.7304611978043184 0.3006447585935917
0.9802958140622449 0.0709568444280560 0.6353300101377826
0.6405147400809816 0.4061042339350614 0.4686082498199226
0.5289925981235887 0.2096060455950612 0.2718384766764587
0.1766405184353586 0.5344785691970003 0.6075192931518479
0.8568224542105298 0.8812156851206756 0.4420815854514794
0.8877046990488234 0.1297305847026803 0.4556919675974229
0.5478042565088956 0.4633398531693587 0.2932410064388773
0.2225938604995670 0.7896054097308751 0.6195948215575849
0.5388229924967327 0.7318354212434279 0.2998589042571550
0.2080627799382195 0.0757475082470302 0.6585610836636567
0.8759451709218574 0.4070995503078749 0.4686403552327814
0.7664777565184252 0.4680360121328839 0.3013716497376441
0.4369443641879066 0.8076708098815367 0.6523115684647003
0.0943168785077892 0.1323188921340707 0.4623262365134956
0.2916592540233794 0.2193817245815876 0.2705107447486359
0.9578970627541319 0.5430456881665751 0.6119434203133407
0.6174849862203596 0.8731975641346346 0.4433588574110359
0.3718069341077370 0.6586748001209302 0.4591021594060136
0.0362912356538994 0.9827039271864174 0.2887411017695575
0.7107532711131520 0.3289998691781850 0.6214393226043708
0.7667038659088116 0.7061927773773740 0.3004883343881138
0.4251644404602767 0.0285802930533317 0.6524440622067516
0.0890309224664083 0.3624618542451460 0.4677966318543963
0.0302013897904566 0.1974890911783870 0.2986457301637256
0.6906346603079785 0.5244209107617921 0.6396852560968479
0.3657889628079072 0.8581614842657340 0.4689450736137508
0.2811308054806663 0.9701076978105541 0.2690432005500124

0.9553044468742249	0.3148809277507092	0.6122068020261914
0.6241412413542269	0.6460287261100921	0.4459836477972729
0.2257875577206254	0.3168180294967630	0.3772832075481301
0.8847932792161805	0.6482710457121633	0.7105765854144569
0.5587121858858005	0.9853707842453689	0.5460724297247487
0.2671062099830314	0.9738429310603653	0.5314128320420710
0.9273243210601857	0.3056683844580708	0.3405310256605714
0.7588256490420907	0.1937918260225688	0.5358503819605344
0.4229006269249049	0.5293504122405350	0.3671936370599649
0.1021111529453282	0.8657221001283221	0.6997499776277013
0.5413171018303536	0.7234567180520947	0.5673554722538694
0.2156203964609978	0.0578786302439503	0.3870497538354091
0.8715669779951222	0.3913601840242397	0.7313919340414105
0.1837091923426689	0.8097694122055870	0.3792544590042813
0.8547109438466155	0.1380573924778981	0.7112927038010088
0.5115891711956188	0.4727126064772353	0.5447734776653743
0.5274989999886739	0.1912242654633170	0.5304881795753938
0.1938062032872043	0.5214309369753164	0.3507601575485054
0.8664552637535905	0.8691715576393991	0.7031662192535233
0.3010533020632618	0.4600200786906191	0.5314646491744716
0.9713755859480309	0.7926651310526821	0.3644524745116580
0.6339679861741178	0.1355012012691452	0.7033223749273518
0.7839813528189928	0.7267686046674201	0.5599632335250396
0.4391087225306743	0.0534313967915719	0.3897180754556401
0.1120870510919051	0.3805417512695289	0.7283201252637074
0.6905977477398698	0.2725768083410978	0.3804668142406982
0.3667934710256193	0.6070155315205189	0.6835718661531156
0.0308773741603475	0.9418974153386201	0.5435707088641909
0.3056915659490830	0.2294483909571226	0.5302441411680520
0.9773533981626435	0.5713412790717479	0.3439152815136834
0.6436055993167858	0.8987918392283247	0.6915517999879225
0.0359190131856089	0.7402343583017387	0.5353570426818274
0.7055814628438352	0.0763449961438374	0.3656473706961887
0.3655122117378234	0.3958291009342113	0.7008268371828569
0.7790679640325566	0.9593896623830044	0.5572447415619542
0.4437608764406442	0.2835664701715564	0.3915581719515920
0.1211095500900358	0.6276683628816903	0.7290124427308370
0.1399131394888554	0.1445670727440007	0.3305758250446631
0.8109535044197362	0.4822647162276202	0.6762239684127311
0.5980692889208117	0.6236118948056751	0.3252060201481086
0.2577716391689452	0.9531119461406945	0.6530438129772167
0.9245092228942946	0.2891274050480837	0.4968113337463592
0.4718157000557993	0.8118087990531800	0.5154964619757644
0.3542768346000192	0.8939488649288072	0.3318936443216685

0.0191820099421845	0.2298312854548792	0.6749499085652604
0.8759902557859829	0.8747028053548477	0.3223145644208094
0.5467379958550653	0.2020669750743574	0.6520561731646566
0.2063160131026494	0.5315602425604168	0.4918025980708963
0.6883929975036428	0.5597090060199583	0.5155404328833584
0.6047121125918403	0.3590918434147454	0.3356092241981696
0.2678384186554859	0.6820238901289475	0.6702956528773910
0.6245510677878698	0.9005643273792115	0.3230773218225939
0.2991003218945410	0.2416165964869150	0.6522622257685564
0.9644105338400818	0.5738250237448584	0.4962687562169712
0.9426208528935618	0.0299775842634115	0.5114768452833213
0.9306904744007820	0.7887299317098366	0.4874229372907760
0.4748354991900232	0.3091292954312458	0.5083326326675135
0.1440477479080058	0.6451845592516591	0.3473485270414866
0.8097646790562314	0.9792113875232220	0.6774362764074121
0.5876433394887987	0.1180804735283523	0.3269740667725919
0.2557172045621007	0.4459210856949138	0.6590408242747304
0.7117998923675417	0.0409203293711277	0.4878493633188717
0.1909000268140816	0.0629462175464595	0.5024310908899492
0.8543215589615990	0.3989240855874576	0.3467573363232352
0.5213379314443082	0.7337624413003400	0.6859012564116997
0.3817351339991556	0.3691468993938558	0.3277806970029633
0.0462771669018847	0.7039911434390194	0.6672200968237280
0.4576614410998453	0.5719777105488255	0.4914572110306650
0.4354551913318326	0.0244652510454859	0.5062412480221503
0.0984688839208099	0.3533322492501972	0.3462582470318316
0.7746648098684730	0.7005864927266732	0.6801157607387320
0.1303803341743440	0.9103818302174257	0.3241362054302368
0.7961008542555789	0.2417687989134799	0.6692543658399625
0.7010698849682897	0.3005591339668001	0.5007192341024881
0.7000811575208546	0.8010724154150353	0.5044904628387342
0.1982091143916732	0.2960250022982091	0.4973681745684384
0.2001730247472231	0.7990464320805712	0.4999087947635775
0.8697622210922513	0.1279736768633261	0.3345642792367309
0.5258838908507414	0.4771802625493473	0.6655889050136790
0.3726205240362260	0.6424594702080312	0.3374497639540998
0.0319082842480613	0.9570892859097123	0.6650237417228294
0.3666879913246577	0.1325602174871972	0.3150973684046143
0.0328114779731049	0.4652024311833842	0.6853911025377845
0.8567874443670122	0.6286991534747643	0.3359751981968579
0.5499760090922829	0.9762591817645505	0.6672314178981029
0.5116949092818113	0.7409331004188574	0.7866593576933865
0.5082328623774126	0.7452442494566969	0.8511500826563012
0.6046959369905603	0.6465534254150433	0.6966930847968884

The perfect Ir₇-H₂*_P surface

O In Ir In H

1.000000000000000
12.5091307398835667 -7.2221499999999965 0.000000000000000
0.0000000000000000 14.4442999999999984 0.000000000000000
0.0000000000000000 0.0000000000000000 17.9854999999999947

O In Ir In H
72 27 1 20 2

Direct

0.8411828274701004 0.6133592538029149 0.4567670314817712
0.5157449647939158 0.9527146761269804 0.2892160093702201
0.1709708050401216 0.2793907610155547 0.6196804188093419
0.7936035779187300 0.9618291035147132 0.2973807647967727
0.4708960237465235 0.2944868795703893 0.6512441618736022
0.1345583184695195 0.6260483696094078 0.4705102718537219
0.3005137484281383 0.7315415282608452 0.2997756787132284
0.9775220426388199 0.0703305779180850 0.6351934072089404
0.6402707652532340 0.4058185694009705 0.4668894915852981
0.5298852363721180 0.2105608238753761 0.2697635216472081
0.1878540236292569 0.5401069330278307 0.6119035123978394
0.8595681007309620 0.8847976392631430 0.4404050264729036
0.8879647644364660 0.1305757903343335 0.4557753060919577
0.5487306692612589 0.4636790911982305 0.2906083985584088
0.2203230205341866 0.7912056365770658 0.6201697081189089
0.5391987600238374 0.7322605877767885 0.2970534679695744
0.2064250841592278 0.0766491116034932 0.6590240564048123
0.8749366554704647 0.4068782341386867 0.4695777780474466
0.7686297237961129 0.4687808344910467 0.3000769548655766
0.4313806688794304 0.7994412183553814 0.6376924831395049
0.0948963389220300 0.1344623097034624 0.4631464419275573
0.2908316930946683 0.2193804615674065 0.2688170693701486
0.9588680699752770 0.5428887438115458 0.6111353565157748
0.6181330928734207 0.8737714780804866 0.4405235007807053
0.3752653127029315 0.6585716973907582 0.4568608303887301
0.0377036853264949 0.9842473923058428 0.2877786913752463
0.7085226972696280 0.3278046768855950 0.6216263221807865
0.7679734116783552 0.7073963965870463 0.2987869925614811
0.4226596946863352 0.0263462876669177 0.6534407274160569
0.0919220862453285 0.3659638080954986 0.4696316551950079
0.0321100583781456 0.1996865968835659 0.2990550820947063
0.6903676916171645 0.5245899154485659 0.6375744638097141
0.3639971404879006 0.8598388028254914 0.4645790449759827
0.2812704073029133 0.9708131169906187 0.2682675051362896

0.9559359966410712	0.3155500167714171	0.6126164303205147
0.6235591303922347	0.6459759451198999	0.4429699961645298
0.2280942283291478	0.3183298850921449	0.3785770498172192
0.8823508673966489	0.6477596539458302	0.7085522518103022
0.5571731510479572	0.9861548494124832	0.5429073515208884
0.2669336861765776	0.9749999695501407	0.5312008694590307
0.9291568142302914	0.3068533548829966	0.3434886722105026
0.5988861622543004	0.6439905409129422	0.6935831981100344
0.7592435622584817	0.1946645016082583	0.5357648923046997
0.4226744900623655	0.5289361854279016	0.3628858334037318
0.0993110746786383	0.8659107002651205	0.6997099051753997
0.5465163718042950	0.7271693311744197	0.5635915341863866
0.2162296572259101	0.0592684574425479	0.3867311892211015
0.8698501897849955	0.3900702187732552	0.7306004255842460
0.1822408261515044	0.8096196652199460	0.3787084810990287
0.8507146337209047	0.1348083322616062	0.7102296196347991
0.5116402234212704	0.4717169041124722	0.5423664775588365
0.5257999743948095	0.1918742486783715	0.5309688876645172
0.1954536867011815	0.5229679116240114	0.3502018230460636
0.8620504015237342	0.8677165923622783	0.7021544219942945
0.3048321595642079	0.4635273911950532	0.5340515025912668
0.9714019889427761	0.7936724345319481	0.3636013704879015
0.6315769931639712	0.1307079704132349	0.7006135526667132
0.7833170997675878	0.7273545555745686	0.5576285610445729
0.4399788997057247	0.0558429891240875	0.3878093679314983
0.1104585482352771	0.3806075258575422	0.7298181938892943
0.6904973070471480	0.2727774947357741	0.3799644590179250
0.3754580203154954	0.6179082168022155	0.7063589526153533
0.0304493806111550	0.9424654839057571	0.5435664420011764
0.3063151159843264	0.2307523590176870	0.5306693363205895
0.9779124045854668	0.5718683977557174	0.3493709331524933
0.6285942584742025	0.8805166807359924	0.6934334429035759
0.0353635477826406	0.7400204531664188	0.5345765165086691
0.7065271706008843	0.0775004768702590	0.3641373100245276
0.3657365215766618	0.3989366705771347	0.7003628582727297
0.7756858658186665	0.9586266682416149	0.5569468265674169
0.4442960467743286	0.2841951698376557	0.3890290383996232
0.1178506115255805	0.6278365525642595	0.7296563732167802
0.1406345288687982	0.1456858681492130	0.3308114049124814
0.8103849098001393	0.4817480400443356	0.6749777474815790
0.5992349924262983	0.6244208131770596	0.3210198384860456
0.2554244832828286	0.9542856365573962	0.6532954868103370
0.9255247457263649	0.2904539321761585	0.4966697082013460
0.4709504624690196	0.8139953691825617	0.5088800118869812

0.3541892185783122	0.8948390643732329	0.3311145107759328
0.0174882965890476	0.2288326552004098	0.6753111051524153
0.8774273455049727	0.8761793071863633	0.3201979937556819
0.5446432249087253	0.2004377657029435	0.6528220055586079
0.2097870630191926	0.5343132297038165	0.4939933184095122
0.6888100873800923	0.5597705946829885	0.5137127816499180
0.6059831744007009	0.3597995965285984	0.3333826032453948
0.2667246897070342	0.6872893289910591	0.6742437934568370
0.6254635035648397	0.9017227249600737	0.3199515652466723
0.2984856594477371	0.2425322301437935	0.6526962229611848
0.9649771000966114	0.5741817029312691	0.4946632070859510
0.9428964569532803	0.0319882582862307	0.5123065860743847
0.9316570555656881	0.7899427592638424	0.4864401785117560
0.4741620191151700	0.3087017142960426	0.5055268048404696
0.1451563401479769	0.6458294480129340	0.3483859282580198
0.8028089737385904	0.9751797651439672	0.6768965246778396
0.5884736274172354	0.1191131954204473	0.3251757279174550
0.2564469868616095	0.4484918534560965	0.6640048367170593
0.7116979249091392	0.0425649389352988	0.4862947857297142
0.1903011110239810	0.0639380572533469	0.5021787312742394
0.8545645020226942	0.3988965521002209	0.3476052644625704
0.5142621743590667	0.7245542882576343	0.6697901080064882
0.3819712984957597	0.3688762446261721	0.3247946410975668
0.0437491109917586	0.7045695552891040	0.6661013435717834
0.4568704456485136	0.5664845127076862	0.4844197145461293
0.4342541257235465	0.0261495828580453	0.5037885194243454
0.1007304113093798	0.3550160368783787	0.3475040769456567
0.7713594838645567	0.6997195746263978	0.6778764270856493
0.1308292427769318	0.9114383116388163	0.3235976032234291
0.7938578230279011	0.2400951408535901	0.6681810600684265
0.7002309385206847	0.3004019590354752	0.5006296333028998
0.7045326868890326	0.8037043378744646	0.4987288444842183
0.1993922000181005	0.2981076698240740	0.4988853997286548
0.1997692962857517	0.8005066475333007	0.4997155612438838
0.8711976235085837	0.1292144116230727	0.3343032847743961
0.5257314158660413	0.4748629760657266	0.6635877413972854
0.3727416964513491	0.6430150130453588	0.3341691216792780
0.0291710283476917	0.9571249646735909	0.6652757752875386
0.3672142801253721	0.1334011066976851	0.3131631929954364
0.0316165119640304	0.4651553720794083	0.6863510461146393
0.8574605919938809	0.6294094528709452	0.3354834751107866
0.5437155348804947	0.9708898050918566	0.6636885513151771
0.5791120245910721	0.6247727539563951	0.8694026733398533
0.6122332687456477	0.6834096922453782	0.8677684612911077

The perfect Ir₇-[TS-2H]* surface

O In Ir In H

1.0000000000000000
12.5091307398836005 -7.2221500000000001 0.0000000000000000
0.0000000000000000 14.4443000000000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 17.9855000000000018

O In Ir In H
72 27 1 20 2

Direct

0.8407902198846923 0.6144689302907195 0.4575717072257133
0.5157982110190639 0.9535979415841755 0.2892106703917411
0.1688070329803678 0.2795431445257277 0.6184903703632332
0.7931191969831152 0.9626192633653200 0.2977483471067126
0.4679647532102282 0.2902950911604550 0.6530928326694924
0.1346033732378803 0.6268430019559965 0.4707082517100025
0.3010802260703859 0.7318643980284240 0.3007176491173140
0.9775632418951560 0.0716856405788763 0.6351173558780997
0.6398525233978444 0.4070873920059095 0.4673618493392416
0.5296661816908799 0.2116297836909848 0.2700488422027322
0.1884820836835782 0.5413570723343100 0.6121798634217673
0.8588982085152054 0.8853551009329977 0.4409640939304421
0.8877382062405482 0.1318018564927608 0.4559153018301751
0.5482239770373853 0.4644445021107131 0.2914642104444001
0.2204511757203952 0.7918425138598397 0.6202030519362612
0.5388891574001250 0.7324795391960069 0.2987120233238090
0.2058186109806622 0.0768458785803874 0.6581875964506310
0.8745327676935017 0.4079919793411613 0.4697304849643973
0.7682484725275222 0.4699184455130725 0.3005196699339347
0.4310359547275937 0.8009887489730911 0.6382926656539580
0.0944380973515581 0.1346766329552914 0.4624802541960407
0.2907260080102592 0.2203552895509033 0.2691341034401475
0.9594526309397780 0.5442541401034932 0.6112560549299419
0.6180353518404729 0.8743976946407035 0.4414123648232958
0.3760672914528060 0.6590352301859875 0.4589891355761425
0.0371053601372927 0.9847846790724235 0.2878169089058045
0.7078709070181032 0.3292499736474854 0.6221531509653270
0.7669896224894045 0.7080024181041563 0.3004629195286376
0.4227104152598945 0.0265690512732191 0.6541765423375385
0.0913153942660413 0.3668963527051967 0.4694798005100129
0.0313786158295361 0.2003431218669350 0.2989553904598686
0.6927838200175174 0.5280630699016433 0.6381949976732149
0.3644919433969971 0.8604111152199740 0.4648618225339849
0.2810325495049187 0.9712429865554888 0.2682019008872035

0.9558240322194750	0.3171948005880353	0.6125500737450650
0.6230317489325851	0.6462092998525298	0.4455459461943875
0.2271473172672563	0.3188791321194785	0.3782563512751512
0.8847446978987110	0.6492307397206744	0.7098577990098506
0.5572391245162368	0.9873633158766449	0.5432867230772523
0.2673680917592144	0.9760033479614191	0.5311596785095489
0.9286405218342644	0.3078906854765735	0.3432423829553447
0.6031581370906260	0.6535069652382510	0.6996655174103732
0.7588001077671687	0.1958263627969344	0.5361743580370504
0.4229523071089373	0.5291696575713990	0.3656377421473011
0.0997616711554614	0.8671440445286579	0.6997527605532607
0.5484261754380472	0.7292289575531418	0.5663799875833030
0.2159364846793431	0.0596926334520960	0.3865253734222400
0.8703356315170471	0.3913983691733733	0.7308253392570383
0.1824204856688610	0.8104489569738808	0.3787163834289509
0.8512208748546035	0.1367977341025288	0.7104758972848847
0.5121153586587964	0.4715430793361623	0.5468516341697491
0.5252657267195180	0.1926193698015448	0.5312035230851994
0.1956065267573454	0.5237221742838443	0.3509776618186926
0.8639118174006210	0.8705382014750369	0.7031399063050219
0.3039198484465527	0.4634243021187229	0.5343839331372729
0.9712298161432928	0.7946043589775318	0.3639177709405341
0.6322419977813827	0.1320069136563254	0.7012957543811236
0.7844079940609440	0.7293559016791464	0.5589881622531436
0.4396623958579117	0.0564831870700927	0.3877302546289563
0.1109726012342417	0.3818349972239519	0.7296069820252270
0.6900867525265284	0.2737615839896297	0.3803018432358650
0.3758107439338093	0.6204629889983587	0.7084937888699726
0.0304814905411558	0.9436180114844549	0.5435279184740421
0.3057280016626499	0.2313863201554312	0.5304393662674184
0.9778493177808234	0.5728306021517333	0.3497211795189243
0.6295283783365394	0.8848176722494142	0.6942906721385032
0.0358363548704665	0.7413277071355089	0.5345491734145279
0.7059804109516279	0.0781842517247171	0.3646745831128507
0.3634315405683168	0.3976049949983514	0.6988035550810268
0.7759776391972866	0.9603903275069479	0.5575251592301871
0.4436792195782062	0.2846113123215095	0.3894986091567015
0.1181685033683875	0.6288128658533533	0.7300670196255336
0.1400327109484681	0.1462343917020670	0.3306095036055531
0.8113979269472089	0.4832567513717089	0.6755075016770568
0.5985781135095321	0.6246326040934012	0.3233522187506756
0.2556028369892905	0.9549805369748986	0.6531553249902624
0.9250387336132604	0.2915371144707096	0.4967184650802310
0.4712613397667731	0.8146387300732877	0.5102640040279446

0.3542236664903768	0.8953696937058050	0.3310497188138021
0.0172932436228929	0.2302639201061688	0.6751219841826392
0.8769089313005576	0.8770223424788662	0.3207948618082165
0.5446758199712523	0.1998337003306298	0.6529917810938698
0.2096741885773490	0.5350155764015386	0.4941865377885502
0.6887216436184024	0.5605839438043997	0.5156247798299398
0.6055472731314477	0.3606795487162183	0.3339477039006796
0.2668635325085425	0.6881721580636775	0.6749104819524443
0.6249911692129143	0.9022288690832420	0.3208092481641767
0.2951863669273457	0.2421905909837659	0.6520868631554403
0.9650281815939407	0.5753906874665202	0.4947631407285590
0.9428156111681208	0.0330787285448898	0.5124053609772907
0.9316933726156400	0.7910305201982705	0.4867381657914389
0.4736702812109225	0.3095898798742169	0.5057465034368431
0.1451857734690253	0.6465623576105090	0.3485730777154508
0.8034847962787383	0.9771715830486930	0.6774099241459403
0.5882851632854852	0.1200497928194506	0.3252335763507494
0.2568975619983958	0.4495736858235058	0.6635988613332482
0.7116323080714565	0.0436087856734647	0.4867123315675687
0.1901737236387359	0.0644644768762433	0.5018608644361310
0.8541467860679243	0.3999336819399089	0.3477228142199777
0.5148338474225531	0.7287254088928514	0.6727212885283467
0.3815423144130786	0.3696770993196764	0.3255265556490761
0.0450464253640106	0.7059537862372219	0.6661974287545630
0.4574279273871671	0.5666332358017780	0.4878940654913057
0.4344324407815558	0.0268456166613627	0.5034985088207057
0.0999861256723484	0.3557567452404389	0.3473676383745767
0.7767838749614693	0.7031103533692755	0.6786054492596744
0.1305076260274985	0.9119465997039543	0.3234576046163112
0.7941411631565736	0.2416822023484965	0.6683430873947983
0.6999708153666033	0.3017462481606641	0.5010234914796052
0.7045488621431443	0.8049377396585600	0.5003457435530847
0.1982089210576554	0.2984065497200273	0.4983060290833949
0.2001815841221502	0.8013427949890551	0.4996752320808514
0.8706089460095183	0.1299961015371178	0.3343917869099876
0.5268730747761718	0.4636879990398596	0.6693041807277947
0.3730720799911457	0.6433465113303890	0.3362729435604271
0.0298879289115006	0.9588753640694830	0.6652805993716706
0.3668167897698594	0.1339943147408530	0.3131613359916531
0.0321349902859166	0.4664150513807681	0.6864104067473942
0.8568833515650801	0.6302877533925572	0.3362315780281586
0.5439779790909192	0.9725481471903032	0.6640640713782457
0.5733271970990723	0.5238520423601426	0.7782937631698224
0.5848947754908495	0.5884105458411282	0.7549204637485476

The perfect Ir₇-2H* surface

O In Ir In H

1.000000000000000
12.5091307398835667 -7.2221499999999965 0.000000000000000
0.0000000000000000 14.4442999999999984 0.000000000000000
0.0000000000000000 0.0000000000000000 17.9854999999999947

O In Ir In H
72 27 1 20 2

Direct

0.8405394395252963 0.6146298205643975 0.4573673851737889
0.5156207517099473 0.9532762011625062 0.2882982822810543
0.1658837492036687 0.2782474686887109 0.6170848635885321
0.7925133779811351 0.9621345404719992 0.2968568801631616
0.4647168327057649 0.2859772817569227 0.6452706322638398
0.1344701960345667 0.6265845809999726 0.4704540921120486
0.3014696122348107 0.7308729682772288 0.3010077578230672
0.9764446131485692 0.0705106967447512 0.6347599380298400
0.6390245256116325 0.4069759860999093 0.4675522023268320
0.5290967966466524 0.2119781550006866 0.2704927739454226
0.1876758536926519 0.5403072403455338 0.6118733934738991
0.8589505644607766 0.8856539902339107 0.4398495407853416
0.8873579207618532 0.1320061903763018 0.4550661794738390
0.5476130669104545 0.4636215574123835 0.2922330535620115
0.2198209119392078 0.7915220229351367 0.6197945087742509
0.5383221909798647 0.7313060750843070 0.2990133438804375
0.2053696177336860 0.0767319341656037 0.6566452869507280
0.8743932916258554 0.4078715097890951 0.4691706419145516
0.7672489341246826 0.4694254607808087 0.3008853482080696
0.4288805867139043 0.8012880299970062 0.6367365062903456
0.0932735606488723 0.1337365213166721 0.4609502713474668
0.2908219125983754 0.2201601809758710 0.2695312906259379
0.9596343435538405 0.5444307787214890 0.6108416467612142
0.6182358707668868 0.8746797781484467 0.4403439106357025
0.3763612584674381 0.6580306085314430 0.4599621256624510
0.0366186658674363 0.9841364694342293 0.2866947428032713
0.7071712824731964 0.3296937218923783 0.6218499868236030
0.7661414792498850 0.7073979274124627 0.3007898693461585
0.4222081286991837 0.0258322617433164 0.6541495779453642
0.0902869402086502 0.3665415891971366 0.4686609123744473
0.0305177223343323 0.1996363209600559 0.2979760315961289
0.7002950426330274 0.5344080515107813 0.6353198775276060
0.3642072284851540 0.8599205940245834 0.4640534509588851
0.2807724814613711 0.9707809595280026 0.2674969057138236

0.9551286454217598	0.3168949467494335	0.6121724585688673
0.6226293132765142	0.6455967226521142	0.4464895836629193
0.2257232540903581	0.3183566391150979	0.3773276514647457
0.8884821370717815	0.6493442225271846	0.7127392372061500
0.5570271381264904	0.9869702028910140	0.5423953679917216
0.2674922772836921	0.9759022205721621	0.5303423930328179
0.9280829750432529	0.3076242160742116	0.3417561729867749
0.6056269489841533	0.6586177110784424	0.7042082117187157
0.7585104443452738	0.1957411418429363	0.5359897099486716
0.4231397206151726	0.5282469595243202	0.3676666425320538
0.0997128131117698	0.8675022233436334	0.6991296196315643
0.5508454460417036	0.7319139736699507	0.5667218058523223
0.2149965721326043	0.0584968438482199	0.3857577775505578
0.8700718531186609	0.3909621258878500	0.7303863405858398
0.1820418792939486	0.8097526129379080	0.3779017801636976
0.8503458125924037	0.1361246149291299	0.7097241305545752
0.5143423418105378	0.4734781504349002	0.5528430042775457
0.5263993634861932	0.1913465806784828	0.5297508201957265
0.1954611111804333	0.5231190840406620	0.3510992930743368
0.8634472784338026	0.8696183279197339	0.7029333679004814
0.3025972848745248	0.4620693576674202	0.5340442086895603
0.9710136990869186	0.7942022631664569	0.3630278798748135
0.6319774213022641	0.1325602724069272	0.7010120688612058
0.7861617742436793	0.7325217914949256	0.5581207141075349
0.4389819408728696	0.0553926063572901	0.3866087898439314
0.1100656937136790	0.3809621283255140	0.7293816761815023
0.6899712663664386	0.2732997655739498	0.3801232096100738
0.3739900547995513	0.6217234658734404	0.7088531951706302
0.0305268849345267	0.9437666734239636	0.5426885215679884
0.3034732137304489	0.2313160101388013	0.5286958635407737
0.9776766982641500	0.5723529800702689	0.3491631417446548
0.6290201158869808	0.8872205002905930	0.6931834982553695
0.0358019512425339	0.7414870304743478	0.5338603160583149
0.7055694287917255	0.0780360595238919	0.3637995979776922
0.3615014285435998	0.3959483438982948	0.6974751366843600
0.7762341722807767	0.9609934878722498	0.5563569499080706
0.4429992346687697	0.2842608465007663	0.3917239110103906
0.1175340739886984	0.6280114079119220	0.7301406649037432
0.1392502464498579	0.1455868093133648	0.3298529973340160
0.8118862760983528	0.4834420101120843	0.6754239416264002
0.5977633962541756	0.6234832785596999	0.3243697633284421
0.2554131322306969	0.9552021917674048	0.6522927868007959
0.9245139066787820	0.2913197966272018	0.4964596422019223
0.4716000432722814	0.8144930319636072	0.5089752793299719

0.3538428373355046	0.8945736034464663	0.3300978116523437
0.0162032377668305	0.2296425708511968	0.6747825524381833
0.8764650568111614	0.8766400546127395	0.3198828536459527
0.5441607085743793	0.1987913227276985	0.6516103316703731
0.2093884049648680	0.5344657549732901	0.4938380577084642
0.6883599507933280	0.5605099545649964	0.5161085299258740
0.6046305614119137	0.3602010784301570	0.3357306294470245
0.2651677422115699	0.6870481234313812	0.6745444305988716
0.6244323190976752	0.9015830370712141	0.3198589964679904
0.2931255671558473	0.2423119770637604	0.6501853763348090
0.9646861171910901	0.5753020569785209	0.4943627676146060
0.9425677644925190	0.0329342119871962	0.5113440313551982
0.9319899714486586	0.7913849728314659	0.4855835185574683
0.4737788964058685	0.3105819539843903	0.5091846110881763
0.1450785803454185	0.6459083388184010	0.3482902555366132
0.8027507196843630	0.9766983878013672	0.6759801356558640
0.5879011269457727	0.1199193436588914	0.3245454544941892
0.2562236996192395	0.4484008155840761	0.6632696930323660
0.7114006653009007	0.0439213255789182	0.4858428165328252
0.1900890115409831	0.0644985122591418	0.5009535865301210
0.8536822154080003	0.3995746187257514	0.3471511720186994
0.5114913718249748	0.7314951774408177	0.6723486813881510
0.3813017806430049	0.3688895542854629	0.3270497653159577
0.0461812725239430	0.7060112844974376	0.6660102956890810
0.4579349671146505	0.5652133154038440	0.4909615248342726
0.4343020768176112	0.0264808227550696	0.5022322804016118
0.0990056817082887	0.3551602355524685	0.3466024570397955
0.7847510024387363	0.7039978225146812	0.6759102061123119
0.1301450418016342	0.9112835635286071	0.3223892195839643
0.7936078558370695	0.2416294027076992	0.6677960744825316
0.6997365749404053	0.3018358983935004	0.5006840327316086
0.7046934808922076	0.8054901246156384	0.4994307028362813
0.1966142626070023	0.2976196078532404	0.4972291545255682
0.1999592982461417	0.8011459428891239	0.4989194249193596
0.8699611507346682	0.1296663421599584	0.3335147606004992
0.5311287490331932	0.4566384774734378	0.6798609420992160
0.3730141141818985	0.6419759894519202	0.3373810248720381
0.0303103649929188	0.9594121325473588	0.6643782716000193
0.3663794709049507	0.1336544877015621	0.3135366158475529
0.0316603750742317	0.4656760621636393	0.6861170041865202
0.8562389731892497	0.6297115119758983	0.3361421487966137
0.5437707606381259	0.9735189811349892	0.6631070983817238
0.5773785332852313	0.4633794583194163	0.7720685885371520
0.5985973960715943	0.6513522553098421	0.7579191202266397

The perfect Ir₇-[TS-H₂O]* surface

O In Ir In H

1.0000000000000000
12.5091307398836005 -7.2221500000000001 0.0000000000000000
0.0000000000000000 14.4443000000000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 17.9855000000000018

O In Ir In H
72 27 1 20 2

Direct

0.8401696450581656 0.6141937295987396 0.4579108449606070
0.5159299912259946 0.9529850540121205 0.2887886225158438
0.1634613343901562 0.2768046358628578 0.6162590554233842
0.7927846324911523 0.9620416885288787 0.2975328622779784
0.4624522678998375 0.2843665401734249 0.6554607499486917
0.1350479288265627 0.6259693565072658 0.4707752539539795
0.3020264243829986 0.7308656217289782 0.3017633155664153
0.9761291001735909 0.0699596113317353 0.6350783236643149
0.6388449033341864 0.4066720504504893 0.4666645010355821
0.5295098013529806 0.2112811843267355 0.2697401561602433
0.1867028331443425 0.5387345364005707 0.6126166664817665
0.8582438660882791 0.8846815998663796 0.4407912055899446
0.8875957760681433 0.1319989493054665 0.4555558862811173
0.5479825031892227 0.4639858033165531 0.2918510731302162
0.2198689217174349 0.7899171805384013 0.6202219527215667
0.5387469087092823 0.7313294127711035 0.2999790893523825
0.2035188277945782 0.0733918620320747 0.6567380663030011
0.8738018656562038 0.4074417860818997 0.4694392283557279
0.7680874924382313 0.4694298016431157 0.3003282097465587
0.4282825684200031 0.8005790283635424 0.6369047795322051
0.0936541414325587 0.1329965858866060 0.4610470141803132
0.2904283909083473 0.2198176722252325 0.2689276523102943
0.9603500926305496 0.5440280938630394 0.6108755275966357
0.6180548513586139 0.8740673309506661 0.4416650769138959
0.3769030576158235 0.6574322196236652 0.4610539756108388
0.0366996866922580 0.9838031515849796 0.2874725123242060
0.7061957770817435 0.3295123105517837 0.6214768898122021
0.7659498538950302 0.7071143300048431 0.3018227356507855
0.4218824626544066 0.0254530992387247 0.6547543869695128
0.0903976964979610 0.3664099903477626 0.4687923068227614
0.0308949347824167 0.1995746499871638 0.2984923036156611
0.7014370731392557 0.5354135031389752 0.6376412334261492
0.3649201716481010 0.8595383601705279 0.4646179200711646
0.2810235349089067 0.9702856845457193 0.2676909228455788

0.9540680311541865	0.3165223561069134	0.6122277208309661
0.6224847095148319	0.6452473285073781	0.4484743659491411
0.2263846764756472	0.3180763039832315	0.3777934909326904
0.8908735047102518	0.6482945721091925	0.7148386266523528
0.5569121245830642	0.9876752770718634	0.5429626849634133
0.2672285815165119	0.9746340191758904	0.5307999052258150
0.9282580964904891	0.3074878429937656	0.3419700624890919
0.6223519313849689	0.6886496971752958	0.7244184123018612
0.7577246086688358	0.1954897081265115	0.5358703335664733
0.4234810511022380	0.5279402232671658	0.3680656093353892
0.0991989440303524	0.8656885557700724	0.6993977559840036
0.5527552457391783	0.7331926671034873	0.5709307631587350
0.2158572489057570	0.0585306216215482	0.3859470628266894
0.8689962694490988	0.3903071970021461	0.7306776057367016
0.1824389077914445	0.8095334978181198	0.3782806526101778
0.8501889361280388	0.1365877126889987	0.7103529767245887
0.5120201764756905	0.4688564004401489	0.5512688438017157
0.5235876224466613	0.1921547023640253	0.5311347948420434
0.1959236910690931	0.5228891767069229	0.3508551465336640
0.8650954634277438	0.8705364392860551	0.7044423694179694
0.3026945638452387	0.4611540940710132	0.5352754140354671
0.9711143268018034	0.7938508425618134	0.3633697043800555
0.6316923423316506	0.1336690181220252	0.7019419232907921
0.7870867771495730	0.7322580646333894	0.5594964824053636
0.4394951708496757	0.0557363060050992	0.3870764329946120
0.1077535423147166	0.3793143179885828	0.7302293430314077
0.6896529739906029	0.2730529854048436	0.3800093818367551
0.3740054932581563	0.6216755213337187	0.7102333852730176
0.0303401751951524	0.9430994040679346	0.5429705345878627
0.3038379378670932	0.2297556165622829	0.5304686693417121
0.9778986153127961	0.5722651553972591	0.3503366172517620
0.6314356443706670	0.8939792996652588	0.6948767910748407
0.0361278782924810	0.7409075772181896	0.5338498024229242
0.7057338520482555	0.0776617723536907	0.3644175724153654
0.3513156876360448	0.3870831357801374	0.7029332651942847
0.7767470644641605	0.9614395530841042	0.5569034105162765
0.4427518958649546	0.2833830484581868	0.3895319320352066
0.1175939542371338	0.6266569171090661	0.7312165764661798
0.1395523837153535	0.1453163493257634	0.3302504311271028
0.8124499759028446	0.4830508598427089	0.6748714824081116
0.5979663658522930	0.6234376170794190	0.3256975444855295
0.2549384764981354	0.9531217238468298	0.6527179007647984
0.9243566008243185	0.2912872043733294	0.4965909097037350
0.4719021692130084	0.8137560022061294	0.5108794383003924

0.3542899264526523	0.8944398025360339	0.3308799762378878
0.0150633525883224	0.2290263860671328	0.6747662572634661
0.8764841777571108	0.8764199202873408	0.3209334867420239
0.5435312142838500	0.1992283204635593	0.6528475169765318
0.2095353718747757	0.5337188490573130	0.4949478507095924
0.6882309683405994	0.5592593881517198	0.5176567042175398
0.6051363355507829	0.3601426517760165	0.3342748485897682
0.2650191716383794	0.6852854553086308	0.6754348368283226
0.6247285516069397	0.9013924709727680	0.3210701194919039
0.2882647498404027	0.2379582312896723	0.6520293484738731
0.9649474748081239	0.5749871670744936	0.4943489387727164
0.9426802351166871	0.0326313872368777	0.5116698091101286
0.9320578810851964	0.7908138252109752	0.4859325473838115
0.4722907317672406	0.3097446416308146	0.5059160740741941
0.1454628730439409	0.6455542362240935	0.3487315402869638
0.8033850633940803	0.9776501514470340	0.6763012665478922
0.5881453795904947	0.1195257275683010	0.3247085168320211
0.2541597612615107	0.4468421551408403	0.6647567503501763
0.7113348670653937	0.0435513069322699	0.4864171225670113
0.1898923807800649	0.0631924250388345	0.5011827031896541
0.8537869637792695	0.3993439933863194	0.3475296548127015
0.5125202782862780	0.7360488581388385	0.6772304411357308
0.3812371787982544	0.3690323010790088	0.3259020849753776
0.0473220980559124	0.7048108518104621	0.6666999614584994
0.4576662685061175	0.5644528280055084	0.4917812142459264
0.4341936697012677	0.0263516586683860	0.5026793489507844
0.0994143930132519	0.3550650446990011	0.3469427792640527
0.7910481455915467	0.7055149566659716	0.6767762494609716
0.1304259151123851	0.9109777490928923	0.3228835620938605
0.7929252879950166	0.2413180835520433	0.6678478443053062
0.6987458165911908	0.3013887390589418	0.5006789841242232
0.7042554744731140	0.8049803186679538	0.5018289259396140
0.1965614707177711	0.2969140386164442	0.4975826003111607
0.2004806955387654	0.8002381093670696	0.4993012775722885
0.8703124780047187	0.1295753818565946	0.3340810594355997
0.5215523138861256	0.4508934033307641	0.6789255401212833
0.3734557697032261	0.6419817906616837	0.3382454322419540
0.0302862145889836	0.9586063292245259	0.6647236642518186
0.3665587660404485	0.1333115980614808	0.3126769274291476
0.0308522398877905	0.4646957490968022	0.6868314033121393
0.8560995558979242	0.6293580955270839	0.3367353052339272
0.5439446032053972	0.9749113933838012	0.6635665107921608
0.5751961431677933	0.5787828285498408	0.7324169469249106
0.6364323126422841	0.7185049939283890	0.7746147715154108

The perfect Ir₇-H₂O* surface

O In Ir In H

1.000000000000000
12.5091307398835667 -7.2221499999999965 0.000000000000000
0.0000000000000000 14.4442999999999984 0.0000000000000000
0.0000000000000000 0.0000000000000000 17.9854999999999947

O In Ir In H
72 27 1 20 2

Direct

0.8412351658066555 0.6146253285557384 0.4569946587345056
0.5164335305717310 0.9533109340720622 0.2889877163586851
0.1714586263354866 0.2796705609547042 0.6207377768733626
0.7936748196499708 0.9629874840907261 0.2977284918896639
0.4618091836544351 0.2810318370217298 0.6663052613258376
0.1356844527707569 0.6273533087324443 0.4706090377495522
0.3015881831269805 0.7313938761531174 0.3005133429998179
0.9770817927273940 0.0705629191134926 0.6359110424875214
0.6405944960185728 0.4076665129830470 0.4661823053824639
0.5306915665199620 0.2104106578713698 0.2666605963870006
0.1854458382728044 0.5391567673493136 0.6115134784506114
0.8586619915546355 0.8844658079261813 0.4416946645417553
0.8881001769604805 0.1322431361568762 0.4558852426215571
0.5487588013202352 0.4651217898172994 0.2893964515019776
0.2197084364365147 0.7913223447539913 0.6202726932192018
0.5394893869147770 0.7324927580444701 0.2990326115508645
0.2052844871063780 0.0752061799216608 0.6631116069988359
0.8743566158881366 0.4067448005710146 0.4691866262528938
0.7700245314435841 0.4698517520707767 0.2983472253069085
0.4251939543386005 0.7990497356996548 0.6331416233880693
0.0961041097237956 0.1354153926231028 0.4631297213137454
0.2906634011156142 0.2206662519787944 0.2668622647833925
0.9576861940461922 0.5417781964952813 0.6100357204244449
0.6191491649295650 0.8747736561532027 0.4416547284292828
0.3764870883348411 0.6586736925993161 0.4594166842125092
0.0372491876743456 0.9846447588929007 0.2876301421309020
0.7042374436240415 0.3329776764999359 0.6215507617823078
0.7672374206181172 0.7079203762841005 0.3009682728164371
0.4222913383511599 0.0245633764986205 0.6561041225052240
0.0928512931877321 0.3660905752566828 0.4699873784451932
0.0322741828328498 0.2003875988457789 0.2988915925068159
0.6886255618711378 0.5384853474476664 0.6502626942820647
0.3656615462707939 0.8607418561461271 0.4640055980867474
0.2812067309753796 0.9703233768009389 0.2666794225208536

0.9567219924800596	0.3152069197766902	0.6124059492622436
0.6238911901190848	0.6473318521607638	0.4474137437421439
0.2288894893273805	0.3184384698923307	0.3786490645848710
0.8905075108100113	0.6438741212265473	0.7137425299717477
0.5576400754415400	0.9884435568010823	0.5428105535727586
0.2680383898012570	0.9760810935497000	0.5318357912819844
0.9295943299850580	0.3075873283746901	0.3437038807818082
0.5952843422377919	0.6777743777451014	0.7501953328105370
0.7589746881745500	0.1969239779809517	0.5373316503305511
0.4246145563137804	0.5291005270156407	0.3670384793335215
0.0963392172335388	0.8640211218271551	0.6983687481719554
0.5529956142036235	0.7324403261331409	0.5718133430207301
0.2172419185401657	0.0603821313086140	0.3851452414819347
0.8695920247522178	0.3875399956251193	0.7304701768925014
0.1830033481646142	0.8108126706299232	0.3782366105100852
0.8527503864317043	0.1372267237452787	0.7120750399412887
0.5126511028445772	0.4671370770126116	0.5450195714037689
0.5238628729167063	0.1929976333286345	0.5317559046238401
0.1964237488777238	0.5233251359179447	0.3517127475302679
0.8611797827392275	0.8695205964501116	0.7059793272804914
0.3052675030907619	0.4637427246468231	0.5366235680793561
0.9721286456413243	0.7946756877663752	0.3633748669007834
0.6338147067612805	0.1336533588393587	0.7008602534317954
0.7873294993123641	0.7284568840473209	0.5597354480699556
0.4398577764715026	0.0572782885241394	0.3864824475604618
0.1110434290611388	0.3809796590479076	0.7306081157920326
0.6894158274393987	0.2738098245598286	0.3792910351931960
0.3653119649574953	0.6207784284689075	0.7140369782706537
0.0315296472793682	0.9441662959572052	0.5436848032202145
0.3076642100166087	0.2304423462640237	0.5325088504863784
0.9781657529518221	0.5724574857325075	0.3509606512486353
0.6309231070225083	0.8924782841306316	0.6946994044350459
0.0362686442503501	0.7404506854860201	0.5342003844424543
0.7064422299758080	0.0785921198249972	0.3649084839843383
0.3675849134965578	0.4023734484272389	0.7017482991890079
0.7781484723597548	0.9625047554193630	0.5568736002350556
0.4445318322723924	0.2834399452606911	0.3844003913286668
0.1147819817165407	0.6256371411196567	0.7305583919998335
0.1410872541489466	0.1464305733784790	0.3295872129838877
0.8114931930950671	0.4799673133962321	0.6767031959481857
0.5989158706331195	0.6246678189435803	0.3241166158037398
0.2550282136614322	0.9543307458210678	0.6540437241270192
0.9260749103955443	0.2917189563078912	0.4964385678256129
0.4727997875961037	0.8142140446318812	0.5099092539437268

0.3547394485506404	0.8950431873062351	0.3306341848873691
0.0184050033421393	0.2296693528973531	0.6764184057136119
0.8769815975332164	0.8769994607334904	0.3211027649634369
0.5435515587079166	0.1978325225678030	0.6537951243987130
0.2100605548542639	0.5346043128159332	0.4939794589644558
0.6890861798158660	0.5612361817614115	0.5137686730809123
0.6066948956087979	0.3604893626633854	0.3288505155697699
0.2618259457353794	0.6853022341557178	0.6746798606254711
0.6255569721994610	0.9020873307334321	0.3210464609267586
0.2935713666750289	0.2400362104223465	0.6551832575837528
0.9654017225182872	0.5745863990195142	0.4933621859752544
0.9438018275656667	0.0333624903342115	0.5116502717109183
0.9341083049118729	0.7919460779598539	0.4852931010839980
0.4724376025308935	0.3066211235203560	0.4988323682687270
0.1458992944707679	0.6464212836329313	0.3484224177887483
0.8022510184378052	0.9790298448339927	0.6757981993230993
0.5886476378716713	0.1197459260182608	0.3243837584982139
0.2570086352138499	0.4509693607869024	0.6646113828189193
0.7118959457615245	0.0445611666974461	0.4864468787556768
0.1912121323116938	0.0641149967264211	0.5004176398347684
0.8544606943381954	0.3991376864713311	0.3471530853175931
0.5034156631822724	0.7336288749516690	0.6786794003967894
0.3818239037396461	0.3705219964265519	0.3233876497998292
0.0472553963597053	0.7040693411814027	0.6641126411556777
0.4586267343996564	0.5687324164039201	0.4903206230628082
0.4348429213870842	0.0268460232397182	0.5021738013185324
0.1012561799433886	0.3553262840186074	0.3477486192911290
0.7989645906677398	0.7084937015808315	0.6765455573033992
0.1310804758830751	0.9119376970062986	0.3224362683628134
0.7944929062838400	0.2397665838208636	0.6673800519955648
0.7000896162433677	0.3023898773519543	0.5004416497607631
0.7042253229602291	0.8055851342369633	0.5028657543983027
0.2005943293881497	0.2988596757233207	0.4992147887662980
0.2012921512401844	0.8014585185513606	0.4990057977582830
0.8712132771004614	0.1301993194948828	0.3342172009792808
0.5217723131476816	0.4487652354088652	0.6638933557593465
0.3737535667029863	0.6428431273287596	0.3366246833948567
0.0318859328728243	0.9610755348331225	0.6656416939018897
0.3671857614888239	0.1335688442578714	0.3092323369039974
0.0312172789603878	0.4639028887082934	0.6860656501153910
0.8573614584866364	0.6300326829599571	0.3355027125182712
0.5440236911707699	0.9738247862471113	0.6635989832517190
0.5428150472729504	0.6251954038977948	0.7843657592075078
0.6374447355682654	0.7425688574328434	0.7794454045202478

The perfect Ni₁₁ doped c-In₂O₃(111) surface

O In Ni In

1.000000000000000			
14.4442996979000000	0.0000000000000000	0.0000000000000000	
-7.2221498489000000	12.5091304781999995	0.0000000000000000	
0.0000000000000000	0.0000000000000000	17.9855003356999994	

O	In	Ni	In
72	41	1	6

Direct

0.8412123696573135	0.6128329367759331	0.4569779742656003
0.5150191787912732	0.9521890456180000	0.2897533045605028
0.1773464715786582	0.2842740691798327	0.6232106973948059
0.7927626193553109	0.9608033618575906	0.2977225907489726
0.4807819038149944	0.3065117579996947	0.6459976006362593
0.1328606180364544	0.6258530784446487	0.4698080818946268
0.3005643990339326	0.7318480872967034	0.3003601231035479
0.9774867149310102	0.0702842369019785	0.6373799405296177
0.6418991498429175	0.4058069720904932	0.4655611474743002
0.5287848306709850	0.2099930941458193	0.2704380817044187
0.1855200115228407	0.5413768601523491	0.6108039283503791
0.8562551524746447	0.8826864931453894	0.4418024215477971
0.8867276375092507	0.1282694823485332	0.4563931301746762
0.5474754033408956	0.4630033188367659	0.2898511724677459
0.2178601219317378	0.7922473577297379	0.6215520400406264
0.5387593915333847	0.7319147808984479	0.2978776066699876
0.2092525836458886	0.0815132780521565	0.6529215214847025
0.8750313185161599	0.4072277370453068	0.4691325255082570
0.7680940207254574	0.4687070310341081	0.2999447388188828
0.4283219142505320	0.8057796290571470	0.6361054960037879
0.0943808206268759	0.1358558357772748	0.4674542490103997
0.2900733305973558	0.2190354427950864	0.2709568062308103
0.9579115008717255	0.5426184632668454	0.6107408797692987
0.6173367968178287	0.8741781380689407	0.4415560603231492
0.3716471783200245	0.6586815560123030	0.4568229267063388
0.0368272467001942	0.9845575457665188	0.2902011808694174
0.7100936145477664	0.3277029657062646	0.6202645908408391
0.7676965139159483	0.7069651223840837	0.2980488938396949
0.4226493529842415	0.0310786650875894	0.6555793795036954
0.0921967853795361	0.3664714930855721	0.4698994342511141
0.0312543383086043	0.1988844676617398	0.3002956217936851
0.6828960098695880	0.5184771747547873	0.6374755187971015
0.3645421298565364	0.8595607198835237	0.4660502422996358
0.2807940914911412	0.9712282533400077	0.2709822288346733

0.9568326354655097	0.3144106567582121	0.6115680473206204
0.6256311614846860	0.6431709948498602	0.4417055110121473
0.2270318761319127	0.3177506690443985	0.3796345140310682
0.8796150806265693	0.6449684419717940	0.7060337557127939
0.5580668526966515	0.9867771735759361	0.5442488156648846
0.2672990063716408	0.9751453960820760	0.5311499947751389
0.9284650736661706	0.3059428124064776	0.3459220131432048
0.5944217228963010	0.6208363891328180	0.6953414257250858
0.7595700429251984	0.1945408656550517	0.5346218436107689
0.4229443952530111	0.5291991252691465	0.3649305372075708
0.0980550157281579	0.8681301631701051	0.7001883909595696
0.5432997689597875	0.7181461471000976	0.5583299359706597
0.2149016054836164	0.0596861153546320	0.3900278429979255
0.8709370349170277	0.3895963452275897	0.7293569461066568
0.1816857530929813	0.8093991362967830	0.3798350145357309
0.8531004840136067	0.1363136717485420	0.7110227454291543
0.5150917118082768	0.4726675164586316	0.5458437362196935
0.5261671995564993	0.1919417146335339	0.5309327770717863
0.1939358159750395	0.5222204794623397	0.3479259980062426
0.8565510560970432	0.8639100387110927	0.7017496539967922
0.3049851137464029	0.4650829298810190	0.5338029419855792
0.9702903003926791	0.7934321816424080	0.3646596690563402
0.6324095017650010	0.1312428471907202	0.6994066326674495
0.7815720142461484	0.7252054257948698	0.5585944467975408
0.4405508409660118	0.0560359466709185	0.3891573715305731
0.1132672214961436	0.3828679714883656	0.7292267626807447
0.6910629899217060	0.2724761395521083	0.3788874438530064
0.3607154219562321	0.6157218892919050	0.7124492588624183
0.0281054075357303	0.9413481217020044	0.5442526658917451
0.3086301110833822	0.2341555672092801	0.5296149065294249
0.9776984397144731	0.5718961760636374	0.3470121125658667
0.6299811907792228	0.8885350703093871	0.7022663085732850
0.0348536759872592	0.7405743441677614	0.5349473156677825
0.7062500575261087	0.0769438104369646	0.3640378395801316
0.3882463210622354	0.4143714717301472	0.6886015089015552
0.7739631184006889	0.9568054053183431	0.5591077564142269
0.4449290088164434	0.2850351009359080	0.3900709314572178
0.1168892242582988	0.6290112564237688	0.7291181163731165
0.1402832826360053	0.1457295279173924	0.3335946581623216
0.8091188923536246	0.4792953371877836	0.6741914065805782
0.5984093289755318	0.6233676446435222	0.3216253364279074
0.2550900466974783	0.9562089718456016	0.6529603225868147
0.9254490654641695	0.2900057776988298	0.4954867158720579
0.4696040651621593	0.8111157712101698	0.5134804749623223

0.3539858756731479	0.8944646059641308	0.3334321030445291
0.0208917998754070	0.2311737192556317	0.6757171846366937
0.8761510507055105	0.8751467184022031	0.3215162900411841
0.5469826317991713	0.2029465852149785	0.6520788706379380
0.2093532318927343	0.5352807879014554	0.4945805277876663
0.6879516247507892	0.5585907970337597	0.5140439863584817
0.6055131707673274	0.3598357588415811	0.3334028816698929
0.2680897261812059	0.6886037683013484	0.6749356090843760
0.6245321687382728	0.9010922982201370	0.3212804729296516
0.3067260430330797	0.2508980257475546	0.6506667577106309
0.9646145057620754	0.5743549886621568	0.4949511034441058
0.9405715806180865	0.0298657723759146	0.5137662214784707
0.9294720242215221	0.7888066625849310	0.4872628149715671
0.4769275993255603	0.3116936228265339	0.5067670579577496
0.1448502938910315	0.6458400106574529	0.3480498847853757
0.7997545091676864	0.9750249734403391	0.6795211263534555
0.5878172306534999	0.1185348408225064	0.3252875680836298
0.2647636787812265	0.4570443013842370	0.6652924286355357
0.7106905365942867	0.0408900481082378	0.4869839272285176
0.1908102292120949	0.0660525961290437	0.5063800815762182
0.8547537000716804	0.3993028753842411	0.3473782675689427
0.5204360360931717	0.7190539151035230	0.6778411319353811
0.3815834976779632	0.3692329293451866	0.3264643117213696
0.0438437750528147	0.7051764178687775	0.6655138721811376
0.4595539350005471	0.5698026625545761	0.4884235809719069
0.4349985655556085	0.0256226216795424	0.5050101265983850
0.1005551095325930	0.3547879944099397	0.3479895786430351
0.7669136361704276	0.6936345608381038	0.6780238571746696
0.1304813738754025	0.9122299624297014	0.3262751193801858
0.7953242596762515	0.2395028818018381	0.6672106756073668
0.7004368197862325	0.2997127893802153	0.4993454488885380
0.6998109802773212	0.8001011502235925	0.5000367259098859
0.2005582879843044	0.3002966180409993	0.5005116338088860
0.1999296822828343	0.8005204622888108	0.5006288805105910
0.8704040513566351	0.1276484851641735	0.3351093885519531
0.5337444271604568	0.4696195505156473	0.6587266085446927
0.3722659970577015	0.6426992712794064	0.3358327644605763
0.0261779247311682	0.9561347812936241	0.6653021441661592
0.3667094631331144	0.1336256810829571	0.3157372256039562
0.0338152365919187	0.4665665500566427	0.6847742716845980
0.8567602758302193	0.6292444350604677	0.3356144037290570
0.5421401719141310	0.969665559008147	0.6654585310161988

The perfect Ni₁₁-O_{V6} surface

O In Ni

1.000000000000000		
12.5091304782646002	-7.2221498489373399	0.0000000000000000
0.0000000000000000	14.4442996978254001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.9855003356999994

O	In	Ni
71	47	1

Direct

0.8398520697606283	0.6123427472403568	0.4573119489842810
0.5148782877433682	0.9518008952479304	0.2880470790892501
0.1703784760316667	0.2795498989924403	0.6192340843377896
0.7914262188720657	0.9605082517899296	0.2974282915592346
0.4686084034862673	0.2917414566199615	0.6434583465271159
0.1333150316931558	0.6253441811780526	0.4692634581354823
0.3000428171242679	0.7300548661377519	0.2996435973679180
0.9749880597796475	0.0686999845188678	0.6358514842788255
0.6406188830955902	0.4054102156893046	0.4666326077396402
0.5286725869267836	0.2097539907869205	0.2683556057624557
0.1863626757604672	0.5400675302211444	0.6106511784501008
0.8559803174791160	0.8828351910677005	0.4407434245522006
0.8851273248650430	0.1286078905432721	0.4560976091323863
0.5466656874025126	0.4623186218328557	0.2900558180449717
0.2180500319142078	0.7906449067515440	0.6195195971954758
0.5380242095279385	0.7308625765173592	0.2985553219833229
0.2053498000636081	0.0766369047038823	0.6544718324258111
0.8743717518615182	0.4060196746431404	0.4682008620764508
0.7670396563021653	0.4680271200535656	0.2994220221761887
0.4253662147173489	0.8086892131988495	0.6329996505382063
0.0923463272488728	0.1333455131563803	0.4631969233557408
0.2895241156819776	0.2186859766048380	0.2690494635741865
0.9576618466651617	0.5420810114638878	0.6100404861624549
0.6160757772068238	0.8725037590888998	0.4417735961910835
0.3735468062980952	0.6579157077047701	0.4580827414958260
0.0356051127496402	0.9830634473555807	0.2878832454314667
0.7073293070153089	0.3327871546261660	0.6201656528715173
0.7663994145742959	0.7062794371613133	0.2986639566160982
0.4214319695875454	0.0297492849511693	0.6570747168322361
0.0906812166240465	0.3652332430278312	0.4685320010393807
0.0296980422400612	0.1977394996408725	0.2988872825431718
0.6821277678062742	0.5348169128665626	0.6469479670407225
0.3640400508722048	0.8593318665175417	0.4630241521465748
0.2796489300261749	0.9697979924132628	0.2674646950397884
0.9565857789755869	0.3156251789045941	0.6116674882942221

0.6252071967771116	0.6432788701630977	0.4434370376697652
0.2258520948585197	0.3168768920801843	0.3777499747661306
0.8892967445073291	0.6444990532540233	0.7115884870775719
0.5568628579015952	0.9867026028940354	0.5427392271908200
0.2673569440328499	0.9747929182327799	0.5301267320871381
0.9272671776277845	0.3052740576590132	0.3428082265194130
0.7588692973424521	0.1952816110977501	0.5365763484843298
0.4227128044866518	0.5280179846203384	0.3660432114652977
0.0970065591097478	0.8656046168775543	0.6983197984642374
0.5462820535547064	0.7156154042289675	0.5630166290221057
0.2144465435259730	0.0579680382818767	0.3865715952305098
0.8707184785257891	0.3896370843356431	0.7295357780014009
0.1809039294433241	0.8085709224827370	0.3775397423490540
0.8525313002899357	0.1373317347011578	0.7105085282340659
0.5142899205592015	0.4692406654877788	0.5450605190427501
0.5268858221203969	0.1899024996915579	0.5293925441729972
0.1939953320797518	0.5215335983332768	0.3490722443939851
0.8588137663646623	0.8662644986194609	0.7030940726050111
0.3035928866208923	0.4625121187152262	0.5336348540564353
0.9698324866603282	0.7927821751146306	0.3634063905464053
0.6330770240732291	0.1349148696562518	0.6993581530461981
0.7857346174640631	0.7279432530152984	0.5582226203291887
0.4386596215389558	0.0550580842167327	0.3858837279392026
0.1131328192266862	0.3817082823011380	0.7288372476125551
0.6895726105589266	0.2717390287799670	0.3784437760191089
0.3640503158111494	0.6165595129138142	0.7115738826889233
0.0284331705237728	0.9415832996691001	0.5428080376124688
0.3046159573621869	0.2304174339905540	0.5281762344552484
0.9765910449616232	0.5709688061030231	0.3479814411559081
0.6298930556585579	0.8953891694927661	0.7030800225635710
0.0350713613211448	0.7399138945886379	0.5335951963844725
0.7044044554227245	0.0759727280536838	0.3646261082162888
0.3764643881781332	0.4026783661196969	0.6924193596252500
0.7725395681102661	0.9563284402738085	0.5585437952861734
0.4437630414697012	0.2828198062646300	0.3887155069654624
0.1183199755346332	0.6275049948984833	0.7293154204790732
0.1389820683647553	0.1445836025930372	0.3309001023761542
0.8096724584128328	0.4806073883643614	0.6754741843140675
0.5976559707158059	0.6224346993921358	0.3226825142167019
0.2545284890109666	0.9543453038056426	0.6520649360248767
0.9249080205698641	0.2899628920040928	0.4959146658722427
0.4692493825583782	0.8118158808268376	0.5103238957819467
0.3529602475446174	0.8934282459982397	0.3298502357646692
0.0192260487494704	0.2304311700895289	0.6749941359832866

0.8752058601000982	0.8749259053019520	0.3202493238983428
0.5451000212656784	0.2018127799666310	0.6513684017140687
0.2088152332162014	0.5335641145822945	0.4936950414212700
0.6869658584228127	0.5580747742589602	0.5157953140253018
0.6044479950766272	0.3587444255060954	0.3323037685358557
0.2664731376334607	0.6867477209376325	0.6734499610737007
0.6233550009071686	0.9001521650547188	0.3207414512771668
0.2972430950651959	0.2438152956865448	0.6503890935165687
0.9641554419731402	0.5734580060886647	0.4937006057298847
0.9401693020477949	0.0299464925095733	0.5120568730262306
0.9315246786613695	0.7896253379164309	0.4848378486010401
0.4736514776217066	0.3069707089023700	0.5054455583969739
0.1440006205032796	0.6445299173265640	0.3472789549373597
0.8006199700557396	0.9774571181733869	0.6778577636314413
0.5872641110592804	0.1182337222101304	0.3237174704911290
0.2627163351506118	0.4528088737601206	0.6644615309944814
0.7099976365420618	0.0418730063528577	0.4867088622064949
0.1893685570504835	0.0637848988243219	0.5020750590719830
0.8534329894397352	0.3981416918215077	0.3462902303829323
0.5140141433154202	0.7350241647300709	0.6757351547341588
0.3806912615648868	0.3681629505157798	0.3258355851853307
0.0479609432206222	0.7042057075063904	0.6641415576411523
0.4585524190167130	0.5669216825950872	0.4890899618272435
0.4340408520241774	0.0252626642765839	0.5012565636027696
0.0990582831592264	0.3537525214580585	0.3465781482831044
0.7926683991200056	0.7035727607167248	0.6749135082241623
0.1294988347716703	0.9107108263196385	0.3230543021323257
0.7951166682816698	0.2412808343406861	0.6669632034594789
0.7002387262147096	0.3004742701988768	0.4991074228670946
0.7005409336429687	0.8004570941190375	0.4995480549593648
0.1981337547802409	0.2978177785305610	0.4982511495503529
0.1996925397518669	0.8000595352968249	0.4982948832631606
0.8690474713604910	0.1276308913143455	0.3341991214465639
0.3718705273655809	0.6413231403522247	0.3361149406957102
0.0302358220005597	0.9594802965543592	0.6640333793923772
0.3658655919082639	0.1326125322295871	0.3122509864977597
0.0333978564863537	0.4652945164441780	0.6852112720651684
0.8552330120559226	0.6280909978437925	0.3356084790866546
0.5404684020005159	0.9749529519875608	0.6637845412173092
0.5189654941828666	0.4482253902689715	0.6546499313494268

The perfect Ni₁₁-O_{V6}-bt-CO₂ surface

O In Ni C

1.0000000000000000

12.5091304782646002 -7.2221498489373399 0.0000000000000000

0.0000000000000000 14.4442996978254001 0.0000000000000000

0.0000000000000000 0.0000000000000000 17.9855003356999994

O In Ni C

73 47 1 1

Selective dynamics

Direct

0.8390161750870864	0.6123903495689423	0.4579124210713761	T	T	T
0.5149724321977137	0.9517980450270604	0.2880887686110786	T	T	T
0.1715128072381343	0.2803618221963088	0.6193418988244879	T	T	T
0.7918363937374594	0.9604135604227603	0.2974567907896352	T	T	T
0.4690297877077537	0.2896134198200617	0.6398548976134301	T	T	T
0.1325179882841848	0.6249843217748092	0.4690529673127783	T	T	T
0.3000816603527013	0.7299387590565041	0.2997053267508524	T	T	T
0.9762537211297805	0.0708695951501895	0.6344892198352154	T	T	T
0.6402185191233107	0.4055057497591080	0.4674337842107649	T	T	T
0.5284405296332186	0.2102968042376712	0.2696483823151120	T	T	T
0.1850248181794444	0.5397897078019396	0.6099866108344922	T	T	T
0.8553207423300083	0.8816832537997219	0.4408389611945238	T	T	T
0.8854480397235224	0.1282852784559300	0.4555162631003350	T	T	T
0.5467501547687997	0.4623006618286953	0.2908355126407070	T	T	T
0.2172060019373041	0.7899597400661797	0.6194197670875429	T	T	T
0.5381916325249039	0.7309121797993453	0.2985529281658647	T	T	T
0.2053907183029861	0.0768004161835506	0.6524771087173659	T	T	T
0.8743842687167684	0.4063761259908750	0.4682474929588586	T	T	T
0.7666438434212711	0.4682143978032011	0.3003244607499680	T	T	T
0.4259068706995536	0.8085089590091717	0.6340972870906231	T	T	T
0.0921147956742600	0.1330768505984293	0.4628226538532155	T	T	T
0.2899027051813299	0.2188365253482235	0.2701014382024063	T	T	T
0.9569940558396568	0.5426205402272475	0.6103182480744899	T	T	T
0.6166593844007425	0.8733578397726747	0.4408757117859369	T	T	T
0.3725511050094036	0.6578343189586149	0.4577133633457862	T	T	T
0.0354498358576473	0.9829848425020529	0.2883141668404274	T	T	T
0.7085251998941597	0.3294980347695309	0.6198462197466476	T	T	T
0.7662325692690192	0.7062026942193064	0.2987007091219822	T	T	T
0.4210398785345240	0.0278587552670671	0.6555181793874235	T	T	T
0.0900743407888128	0.3649298541726029	0.4683278065013706	T	T	T
0.0297286025817515	0.1978255482965159	0.2987168541525033	T	T	T
0.6862803744159083	0.5277930701820048	0.6434654851352893	T	T	T
0.3638717764588131	0.8586621986118880	0.4635546291269576	T	T	T
0.2795263376460646	0.9698231364450887	0.2678567000767545	T	T	T

0.9559729690579795	0.3157891984916967	0.6113139886108315	T	T	T
0.6253356928700802	0.6431632195684069	0.4433881340543032	T	T	T
0.2254302196380086	0.3171543883414044	0.3776892044450170	T	T	T
0.8875993219940986	0.6460096854654084	0.7111457681017347	T	T	T
0.5571510972349960	0.9861186371537027	0.5423918915492310	T	T	T
0.2668207578939710	0.9742019898171610	0.5295577805494694	T	T	T
0.9273539115875775	0.3055739081342894	0.3428509614364796	T	T	T
0.7591004640313843	0.1943184796323354	0.5352404960644509	T	T	T
0.4226510400354895	0.5282818387148287	0.3662849295548811	T	T	T
0.0975403665046493	0.8665893571850820	0.6981177583035266	T	T	T
0.5447111938566094	0.7184061895704806	0.5608154459252663	T	T	T
0.2141663991656071	0.0575587887442591	0.3869006435323585	T	T	T
0.8706083870109238	0.3902346165428409	0.7294188244355824	T	T	T
0.1810431209092070	0.8083714238484666	0.3775971360420238	T	T	T
0.8530572498735044	0.1378442062137500	0.7102148037930703	T	T	T
0.5145001811031806	0.4730354180884370	0.5486809985798118	T	T	T
0.5275177969602307	0.1888869592565226	0.5278611359134022	T	T	T
0.1936482842131293	0.5214654971261595	0.3487094820489461	T	T	T
0.8623637454522309	0.8696726392634611	0.7018410247613214	T	T	T
0.3028909759334362	0.4626342415509582	0.5329980620463517	T	T	T
0.9695932111781497	0.7925027260606510	0.3636914227808251	T	T	T
0.6322013964539780	0.1333745943425933	0.6991185967948542	T	T	T
0.7831909287082125	0.7272123202567943	0.5594647629733093	T	T	T
0.4384244989982761	0.0541148107907525	0.3859557317641090	T	T	T
0.1132658276584718	0.3823483756965952	0.7282900151944375	T	T	T
0.6900398038556873	0.2720367647629729	0.3785447406771451	T	T	T
0.3639780296855830	0.6162400904014451	0.7093392618755415	T	T	T
0.0278835979275190	0.9412417765868412	0.5424195413344870	T	T	T
0.3039599807813709	0.2309521639412983	0.5268900027297891	T	T	T
0.9765134169558024	0.5712021832532909	0.3476575749988014	T	T	T
0.6310302534123230	0.8966661178541659	0.7010793458195890	T	T	T
0.0346854959557893	0.7400492499384115	0.5333952963690067	T	T	T
0.7049418776476118	0.0764746019417324	0.3636911498546665	T	T	T
0.3764588817198995	0.4016993216437257	0.6907058228058474	T	T	T
0.7730470750283868	0.9563028555954886	0.5580207968185048	T	T	T
0.4438513894186814	0.2835967916897953	0.3907425620752060	T	T	T
0.1183708073420035	0.6279935526100516	0.7289670253561997	T	T	T
0.6192312175474664	0.6655952886178701	0.7205121149927883	T	T	T
0.5622834780242890	0.5201265218703673	0.7966295959141980	T	T	T
0.1389676687184425	0.1445864122226543	0.3314024601197039	T	T	T
0.8084166498319140	0.4801540044605577	0.6752154169877328	T	T	T
0.5975218018417986	0.6223154562755266	0.3231349933692629	T	T	T
0.2543087908590806	0.9538175179355715	0.6514273147928381	T	T	T
0.9244843977197980	0.2896651696063423	0.4956299442038355	T	T	T

0.4694030597044246	0.8113111844507417	0.5110575934908334	T	T	T
0.3529584453334701	0.8932596976893614	0.3300478089056231	T	T	T
0.0196639274993469	0.2313852111797612	0.6743280600314693	T	T	T
0.8751714678403355	0.8744896960011334	0.3205315256329387	T	T	T
0.5445727075329536	0.1999618377845212	0.6499745982867590	T	T	T
0.2084022420620567	0.5335312598970958	0.4934886077867428	T	T	T
0.6858412887139381	0.5573926803522951	0.5175268935893481	T	T	T
0.6041450654996164	0.3589977123743115	0.3344492338235540	T	T	T
0.2670506668808776	0.6863495157964911	0.6731341049159763	T	T	T
0.6236711889388961	0.9003160317287003	0.3204269664429025	T	T	T
0.2994185346765873	0.2440898270922204	0.6486825836786543	T	T	T
0.9636277930384918	0.5736001264470283	0.4941805411266417	T	T	T
0.9400239819013956	0.0296230158065278	0.5117568456013856	T	T	T
0.9297812916412743	0.7886504009166112	0.4857570701919922	T	T	T
0.4746501867876229	0.3091671195606882	0.5084695467361637	T	T	T
0.1439384934055953	0.6445332513653993	0.3473676619052482	T	T	T
0.8013208728071494	0.9779865928061375	0.6775322901047478	T	T	T
0.5872232220995527	0.1183648900778692	0.3239624775928554	T	T	T
0.2635002998753211	0.4535944230198924	0.6638437721714692	T	T	T
0.7100689456516137	0.0412322450261486	0.4861936525219969	T	T	T
0.1893286360670394	0.0638482596497393	0.5024593535492562	T	T	T
0.8535559519396178	0.3985379084293219	0.3465755871509579	T	T	T
0.5176916456182520	0.7334542353369848	0.6761557689536770	T	T	T
0.3810050863791231	0.3682623138817439	0.3270661708947529	T	T	T
0.0466377418046490	0.7044703962584329	0.6647427140936432	T	T	T
0.4589123579967720	0.5676654795195424	0.4901506090373737	T	T	T
0.4339033121019489	0.0244755210503092	0.5015706302136774	T	T	T
0.0989136080667375	0.3538002037155324	0.3465422185386012	T	T	T
0.7884336271631772	0.7040776592012689	0.6766366281037549	T	T	T
0.1293426063458059	0.9104796894000814	0.3235017180583006	T	T	T
0.7945776806286130	0.2411934784229532	0.6668934045070518	T	T	T
0.6998150364432509	0.2996046643738524	0.4991016777944716	T	T	T
0.6995305741110628	0.8000601298399939	0.4993907191463888	T	T	T
0.1977841959855510	0.2977815800272360	0.4982100348023693	T	T	T
0.1993455962288345	0.7995724380931782	0.4984810584625400	T	T	T
0.8692655281032230	0.1276817522277415	0.3340185868468798	T	T	T
0.3720096634473116	0.6414156269757963	0.3363846103228927	T	T	T
0.0300440726588670	0.9599980023876221	0.6635351418793465	T	T	T
0.3658665642966584	0.1326476388605406	0.3136512188541009	T	T	T
0.0331952072782412	0.4658701858374837	0.6847999150767650	T	T	T
0.8548170158323051	0.6281330780072339	0.3362255672994355	T	T	T
0.5410235295100712	0.9735362246516569	0.6635522278378088	T	T	T
0.5247201919573232	0.4550809830597815	0.6638779308656353	T	T	T
0.5709136222332652	0.5628353587607250	0.7370436106726301	T	T	T

The perfect Ni₁₁-O_{V6}-[CO₂+H]* surface

O In Ni C H

1.0000000000000000
12.5091304782646002 -7.2221498489373399 0.0000000000000000
0.0000000000000000 14.4442996978254001 0.0000000000000000
0.0000000000000000 0.0000000000000000 17.9855003356999994

O In Ni C H
73 47 1 1 1

Direct

0.8392794958290841 0.6126838986705962 0.4583422127389687
0.5151214435299188 0.9518081412620679 0.2869941258291001
0.1722249632906055 0.2810544842860815 0.6194612987210437
0.7916852237483916 0.9604156419182955 0.2972645056638126
0.4694758800964899 0.2917337648008497 0.6395341556814123
0.1324677473228412 0.6252278831359414 0.4691613996447623
0.2994896137425863 0.7294732468471351 0.2989499133122608
0.9796436243335224 0.0732410496868039 0.6321939239749611
0.6400351353325913 0.4053470681066669 0.4677785638694837
0.5286897555117536 0.2105342107918490 0.2683107599667258
0.1848495872011194 0.5400972984704624 0.6100307763908391
0.8553889808274520 0.8824373587288638 0.4410027801254470
0.8841953453608046 0.1269382547559864 0.4556887169136596
0.5467010555864282 0.4623062458069592 0.2901497986998573
0.2203451308655522 0.7912078956394336 0.6196568555286985
0.5381584524168110 0.7309013012074049 0.2985071200039219
0.2058363524860348 0.0774952541720694 0.6546528039328798
0.8736133800799055 0.4056801016393289 0.4685324881314593
0.7665133887629058 0.4680381351640500 0.3003345394666614
0.4314891720830432 0.8094289056455338 0.6384491350235950
0.0929673892614272 0.1335299733871788 0.4616732414392314
0.2898885932042279 0.2191133868539959 0.2688407022015600
0.9561136939238147 0.5416297407417470 0.6105192925986273
0.6172023969875690 0.8738297738741181 0.4411030921055608
0.3731651244767599 0.6579241666795782 0.4575987983381688
0.0353775916097251 0.9828221832145474 0.2877787318117093
0.7078225318505968 0.3284996498895790 0.6203508364472419
0.7665539823838319 0.7063655837946782 0.2986868791039568
0.4187750098589014 0.0319294350251805 0.6601283252680122
0.0901101584806126 0.3644102292073278 0.4685004261587148
0.0296496713480949 0.1979767299716587 0.2984133612870662
0.6858791510577493 0.5277635517249142 0.6436343588127504
0.3641116212755685 0.8588965869257210 0.4636154159598287
0.2788150618830854 0.9694330216875319 0.2662430846618470

0.9553347440453764	0.3146893735076803	0.6112974479159569
0.6253702393306715	0.6434726855014247	0.4432379852983880
0.2258768553956578	0.3173086637466379	0.3772614998255696
0.8872577304043425	0.6454792494855695	0.7116257712065281
0.5553044363132952	0.9855717273805372	0.5426421176580004
0.2671687523054005	0.9745966911028506	0.5296616805627226
0.9270028964349953	0.3050472174249479	0.3440053632392603
0.7586324878818902	0.1938849228316860	0.5357762765237627
0.4226664830942046	0.5281107028145335	0.3658051974798183
0.0972932902580650	0.8654630054385395	0.6980739522001144
0.5450354724781230	0.7193137317879889	0.5611335133275293
0.2148979868406810	0.0577905032089562	0.3855921646744092
0.8693864360149030	0.3885266663750273	0.7294490931909237
0.1815843887215857	0.8088680683014832	0.3773570866858776
0.8534651791409322	0.1369137679541583	0.7114564641559320
0.5145037307358097	0.4737509598285611	0.5486079292707723
0.5266621274280134	0.1882122946356613	0.5283384886358127
0.1937169887786353	0.5216205364446529	0.3495594470154901
0.8651665996151909	0.8710387595797640	0.7025533168213473
0.3028565916991894	0.4629595443672020	0.5331719021433839
0.9697365560022029	0.7928944784550435	0.3642825669159187
0.6315419468997876	0.1309826035789631	0.6989715302512856
0.7836239816557399	0.7280045172045214	0.5597125050444222
0.4378008613574420	0.0538435995556551	0.3836302368854440
0.1126488112341056	0.3826984290149663	0.7287107010850793
0.6891916413654289	0.2715072947853417	0.3784549627736560
0.3591793707465996	0.6135636373710102	0.7120099835472860
0.0290020126476858	0.9418494200580406	0.5419339706541091
0.3038381851627083	0.2305887021473113	0.5270804015452766
0.9761058157404177	0.5710402292595904	0.3483598509404682
0.6333579158940976	0.8930569264200320	0.7127016373712234
0.0352588032920397	0.7398459978502815	0.5345402528103467
0.7042929528244156	0.0762410456168919	0.3637653303943120
0.3767208455394507	0.4026522933680124	0.6910545616978597
0.7699239796313759	0.9549169042126451	0.5600822684799024
0.4438881230810862	0.2833857841279643	0.3900958810683512
0.1166883482767620	0.6276248540066832	0.7292567446124009
0.6190740220816110	0.6668844209648279	0.7213604343366498
0.5653431317119885	0.5227836175350282	0.7980313694429025
0.1391131696667972	0.1447488499052411	0.3302061836117930
0.8078209638653856	0.4795916666298528	0.6757856610495383
0.5977624676766655	0.6223522551931597	0.3224640028934807
0.2531414139783180	0.9539597873972482	0.6515847173456093
0.9243726250101989	0.2894210052331470	0.4950743489579936

0.4698383282752442	0.8115502670398986	0.5097463341071397
0.3525106726349256	0.8929791858869158	0.3275242191262673
0.0209396837790726	0.2328167638570435	0.6743766982245428
0.8752068607959704	0.8746072678394622	0.3201040178313432
0.5448767053600283	0.2022378130392349	0.6504875697895310
0.2081186200986675	0.5334778237396756	0.4931566589587610
0.6859299530353680	0.5574452352825762	0.5175030793028313
0.6039182707896643	0.3588067654830596	0.3334997764300406
0.2653070058291429	0.6858536617607459	0.6741656154214216
0.6235805512594872	0.9002442332334420	0.3198925804239618
0.2997929499532491	0.2445324004889830	0.6489318561406050
0.9633814084499933	0.5730857095129860	0.4941845576197963
0.9409778837870899	0.0298967776629706	0.5098202593466566
0.9305931396994161	0.7887139445099838	0.4858582756605470
0.4744814448587236	0.3096783479191128	0.5078861813298666
0.1435917518538947	0.6445316325168208	0.3471721573320864
0.8129863417473993	0.9829712154172768	0.6750498593898515
0.5875462302941815	0.1185839658909152	0.3224928957559794
0.2617831296348720	0.4523013189887663	0.6635978925582134
0.7094515055027553	0.0414684923756551	0.4859847128035729
0.1899901421119695	0.0641498646273058	0.5007594387470706
0.8531363064141080	0.3981908480998910	0.3465656472460001
0.5112242898313545	0.7214572429495302	0.6745641532751211
0.3810396801028619	0.3681716095791403	0.3261982146433292
0.0459824696726690	0.7039845382416223	0.6643679812604616
0.4583118477540734	0.5664355895131795	0.4885893234673674
0.4329197733080760	0.0254903326146786	0.4983350833894996
0.0990759568610048	0.3538086124007322	0.3463603488592413
0.7891367062879076	0.7042103723880466	0.6765667835725289
0.1291450399740696	0.9101891367854982	0.3227464288340084
0.7942028924926776	0.2403047814124128	0.6659835706174559
0.6993030587711934	0.2992607212225714	0.4988719591620643
0.7000801826537877	0.7999475628467325	0.4987893591442616
0.1982445569879104	0.2979996394712405	0.4977395999941190
0.1994988507306048	0.7993886034866121	0.4982944846672681
0.8689305640925952	0.1275421111233812	0.3335363535337713
0.3717645801830282	0.6412181919673765	0.3357299735437375
0.0326443729665250	0.9609010127757822	0.6630316607318660
0.3657195340957606	0.1327075915209172	0.3115062670370905
0.0320304073326845	0.4655018187524227	0.6849951900788821
0.8548616092975974	0.6281455048416663	0.3362884792185096
0.5315017901379607	0.9751938030155263	0.6615936924848245
0.5246763668488511	0.4556264875250917	0.6642841355797985
0.5712599129897800	0.5626770127165893	0.7377798964336795

0.6360767554959385 0.9000025170164536 0.7666081771165068

The perfect Ni₁₁-O_{V6}-[CO+OH]* surface

O In Ni C H

1.000000000000000				
12.5091304782646002	-7.2221498489373399	0.000000000000000		
0.000000000000000	14.4442996978254001	0.000000000000000		
0.000000000000000	0.000000000000000	17.9855003356999994		

O	In	Ni	C	H
73	47	1	1	1

Direct

0.8393055849270264	0.6128362269445918	0.4574642069539501
0.5148206762553641	0.9512966537561200	0.2878554499081374
0.1726220225462194	0.2819814508179204	0.6192461424418203
0.7910738281003111	0.9601690949241836	0.2972888062583056
0.4628470986216587	0.2794337734072422	0.6390014666033834
0.1320520634684815	0.6252086009626834	0.4681296603053371
0.3000285380580222	0.7292279226508508	0.2993677757672950
0.9773357560325251	0.0742912403157114	0.6321883266304508
0.6391151672261483	0.4050953507862341	0.4674960686103687
0.5281292643393665	0.2100020109194883	0.2697641474577320
0.1851443840573882	0.5415503466411803	0.6084544775118410
0.8552784137987435	0.8821203275893816	0.4404120886771349
0.8849783738432024	0.1290488838046111	0.4551762516543514
0.5459219323070802	0.4613483915203826	0.2913859278793625
0.2178184966771249	0.7904486533215405	0.6184628623370332
0.5379375686832915	0.7301430971305889	0.2988890790210193
0.2050966150842929	0.0770365852923098	0.6554251075617874
0.8745715351762570	0.4067178919168865	0.4676259812036062
0.7657438535186464	0.4680803619609495	0.3005269081198481
0.4284015279302197	0.8072457183605638	0.6343382317381393
0.0915009444581448	0.1328700644349587	0.4611523805090469
0.2898057059838660	0.2186461321486333	0.2699086050916742
0.9564896529168758	0.5436760956254212	0.6096310205917461
0.6163131675988521	0.8722306896845872	0.4414361706779633
0.3731962272790322	0.6581450020952082	0.4581440304462054
0.0347642685105301	0.9823022005533273	0.2869094040558714
0.7076057441440884	0.3315322870928560	0.6198466578206040
0.7653584229216952	0.7058664741458794	0.2990090583505635
0.4209133763534728	0.0247090270999226	0.6553570774952768
0.0890181472397517	0.3642014669378642	0.4678737600802225
0.0286863552673260	0.1971249671432608	0.2980722794773101
0.6820682725742269	0.5330859815751303	0.6405069871632634
0.3641803117314192	0.8579998626500593	0.4635486330566054
0.2793787640459459	0.9692523215983507	0.2668677475324683
0.9562893519751378	0.3179523382027538	0.6114710523881827

0.6241980023924352	0.6411980954461906	0.4441747741871173
0.2244520133795254	0.3169036590580059	0.3768129122543811
0.8832898277902967	0.6465003959496023	0.7080710214285169
0.5575084298968240	0.9858514836674707	0.5424657062355089
0.2672107930206333	0.9751217046765461	0.5292734374853744
0.9266952418825842	0.3055574260502589	0.3406350795042313
0.7592635954757202	0.1950033913563275	0.5360098358361218
0.4224537075804875	0.5277468184979205	0.3671597729958127
0.0972630955381877	0.8664137274018687	0.6970317594615271
0.5457478134899477	0.7163169881598098	0.5619933418425075
0.2132148391112696	0.0565501085777824	0.3854290834876915
0.8704309800167745	0.3925677163734368	0.7291174658826005
0.1812602911274237	0.8084670340823514	0.3769101773448789
0.8547113449516440	0.1404649519287800	0.7108334254141998
0.5128126759963746	0.4697528396602342	0.5505116639076466
0.5291793933329666	0.1876780551051436	0.5272214480687145
0.1934196600804936	0.5211775000780894	0.3496864833793776
0.8670542144761560	0.8756741140118013	0.7029143290280091
0.3018741183068773	0.4623022461660004	0.5314942104107678
0.9694123189885729	0.7925760858841134	0.3632568609093942
0.6330263259911363	0.1340404337339039	0.6992079187574710
0.7845310739912937	0.7293433307893843	0.5592162096995269
0.4375431498698510	0.0531754514183245	0.3856397870978721
0.1142151848932469	0.3847183842853128	0.7274697510343752
0.6898748854202272	0.2718047451229519	0.3785457877470191
0.3641772623388159	0.6164622041927721	0.7090199242646908
0.0286868347367678	0.9425820571548598	0.5420658186276484
0.3020303154750604	0.2296957200758648	0.5255788153418838
0.9762756532725995	0.5711982598486006	0.3463116748004524
0.6327578298195355	0.9001084485037235	0.7019099266824637
0.0351385339944494	0.7407154879226225	0.5324876749522723
0.7040069844984136	0.0758146540473196	0.3641926858987960
0.3781469787121384	0.4060951679349358	0.6826790452767711
0.7731357027432850	0.9568496141032364	0.5578172400059180
0.4430732769333304	0.2824169516898478	0.3914729610764237
0.1185221872968838	0.6296341349358369	0.7278673198643310
0.6407470565977317	0.6983312399721999	0.7308164369199887
0.5400842613345186	0.4711951249347814	0.8195568449203298
0.1380872009772463	0.1440213094286266	0.3303228875043290
0.8077299232666686	0.4818191973595055	0.6737116328346766
0.5968069235360980	0.6212940055042964	0.3235721597012886
0.2544057460800630	0.9541268416532604	0.6512199780799406
0.9241171823176251	0.2899409660511905	0.4961144563376949
0.4696419386958279	0.8106650031093996	0.5124208004014777

0.3527396957557688	0.8927682517556638	0.3295446337489034
0.0204419213391065	0.2333420731296924	0.6738741515311584
0.8747789036379722	0.8744878032803599	0.3202737788461103
0.5434695472475389	0.1971149633678536	0.6500518972199075
0.2078004093187495	0.5335579181297351	0.4918618091875241
0.6866237043685665	0.5582117503699268	0.5160707412555608
0.6034708378997931	0.3583047960977225	0.3351780149674184
0.2683392972908272	0.6878224815122418	0.6723285992472698
0.6230777815084411	0.8996408063179538	0.3210308148856508
0.2994035256427433	0.2438544343920999	0.6472371207048393
0.9638372422307834	0.5741668807179726	0.4934124620956335
0.9400270479666412	0.0304323380580489	0.5111407283526673
0.9301736759799304	0.7896624656061906	0.4858376039338937
0.4737367808374125	0.3056869915070305	0.5096327744772533
0.1436334625299327	0.6445659182826204	0.3466566267734359
0.8028311253799135	0.9808309862023510	0.6770374829370694
0.5866863858013155	0.1178973677555962	0.3241119718119895
0.2627579770122933	0.4561072967374858	0.6613596994447979
0.7099200703687982	0.0414227713227024	0.4865158735880011
0.1886734602082004	0.0631377879246693	0.5005782133296239
0.8530769650319712	0.3984137968676736	0.3459140308222253
0.5216430617907311	0.7318275072684969	0.6781739800368867
0.3804112225119849	0.3674152553092802	0.3278343037402734
0.0456678863055499	0.7054204073108343	0.6636465884331897
0.4585159616293286	0.5672899612920045	0.4909682880092912
0.4340452734644539	0.0234445627464413	0.5013655241961577
0.0977321904498998	0.3531364968123524	0.3460182021232295
0.7829606715458227	0.7069826404023881	0.6777406703586877
0.1287930495168417	0.9097049072568232	0.3220446846558647
0.7950107771860336	0.2428899334930367	0.6675686287046479
0.7001364948235986	0.3000256544086706	0.4990722615334266
0.6998510052822642	0.8001503778735489	0.4998553998662957
0.1968581779150509	0.2970952739694125	0.4973849939126964
0.1998155988116746	0.7999522359983675	0.4979673852920194
0.8683440038294580	0.1275806519710871	0.3337050231727427
0.3720875429459138	0.6412143757315030	0.3369452825135021
0.0312141529809853	0.9625028886065620	0.6634237984063668
0.3653546876528096	0.1319786200466894	0.3132433711099061
0.0332304980505981	0.4677170766249966	0.6844397991172952
0.8547205584552274	0.6282476392222834	0.3358197982472329
0.5419590437896554	0.9729842271633014	0.6638929120640165
0.5279712804045669	0.4663487104654347	0.6577982002759403
0.5389542493902740	0.4722672064972624	0.7554880725228237
0.6670454424158136	0.7456279726018933	0.7735401689341705

The perfect Ni₁₁-O_{v6}-[TS-CO-O]* surface

O	In	Ni	C
1.000000000000000			
12.5091304782646002	-7.2221498489373399	0.000000000000000	
0.000000000000000	14.4442996978254001	0.000000000000000	
0.000000000000000	0.000000000000000	17.9855003356999994	

O	In	Ni	C
73	47	1	1

Direct

0.8404532892070208	0.6124917440539849	0.4568810436792198
0.5148269473730843	0.9515102096666952	0.2886609040966141
0.1744295797056133	0.2828128399234854	0.6206269723655053
0.7917374672773353	0.9603127078608621	0.2977804344568825
0.4729561821658210	0.2945779329771785	0.6433352321160228
0.1321617989642371	0.6253905495526513	0.4684928495410244
0.3002197564985568	0.7302768963765238	0.2996644601029200
0.9778637569050832	0.0726962895808085	0.6344475777427717
0.6399952942776823	0.4047590113451332	0.4654674359657506
0.5283646892649320	0.2096844652019999	0.2695362209734051
0.1848545407226120	0.5415224514486279	0.6091600658593475
0.8553629990776385	0.8820340957835016	0.4413533890713314
0.8857225963984126	0.1284626901174134	0.4557559731734183
0.5464305708879758	0.4620549727313445	0.2902666648144608
0.2180653850988762	0.7913448966922955	0.6198304382298935
0.5383044055499210	0.7308623021828430	0.2988788729758068
0.2072783156667843	0.0790236574402060	0.6548300259035541
0.8747309933787824	0.4067709651499211	0.4679882442245789
0.7668761096393866	0.4683564702486678	0.2999355219937219
0.4287406116206969	0.8066666881658939	0.6361196378582565
0.0927985571265562	0.1338514439794633	0.4638327880795261
0.2897096850782317	0.2187554429628662	0.2696398762333170
0.9573220346490507	0.5429448196210911	0.6099468620758874
0.6166893043731277	0.8730016763938405	0.4417773858043311
0.3719814778271762	0.6581386986988853	0.4574925723124231
0.0354690826733446	0.9830700464994506	0.2884360641253960
0.7090974957363210	0.3285584255697380	0.6196326254341632
0.7662674949426014	0.7062078668048160	0.2991012498508388
0.4219051432878549	0.0286147631894154	0.6556126778842254
0.0901693506560468	0.3648226536543790	0.4685460278571296
0.0296638617995851	0.1977372581297612	0.2989638994179000
0.6840490609549226	0.5226980477400047	0.6362346857898605
0.3643269601075810	0.8584622351219433	0.4647780317157669
0.2797963167701581	0.9699363528017904	0.2683434006476723
0.9563110951466859	0.3160678128172333	0.6114419081547962

0.6241385023055909	0.6409537104879378	0.4435208371369665
0.2255517718878373	0.3169503837940515	0.3778366334726622
0.8810744929838930	0.6460070063666408	0.7064094550683035
0.5574356986782983	0.9862422084129283	0.5434312299417010
0.2671865752280438	0.9750391291037509	0.5300773732079318
0.9273779933920601	0.3055653987953723	0.3426322564806249
0.7591187598424609	0.1943933724019969	0.5349710055507687
0.4225053759961482	0.5281049479077032	0.3662829478581182
0.0978329866493765	0.8673324485297775	0.6985245999219616
0.5434316655912153	0.7168968307029200	0.5602907838492230
0.2141629585617446	0.0580518129826991	0.3870068009423720
0.8705205528688559	0.3912103203418839	0.7291367647635635
0.1816435554195611	0.8089946209771424	0.3781128646145532
0.8541545770696666	0.1386700635101761	0.7109428580768213
0.5131278787709480	0.4689889210724377	0.5485584900162259
0.5267204159421301	0.1896078325288216	0.5290815124323531
0.1935614316625108	0.5214742170363174	0.3489570808011694
0.8627175905706231	0.8708818949556204	0.7020101508677231
0.3029453315103679	0.4631535408324425	0.5322698591891054
0.9698457008089161	0.7929522929042220	0.3640637271648668
0.6327222855770428	0.1325828570813306	0.6995181190473519
0.7829071916910111	0.7266732236624113	0.5589205037322361
0.4388198021603754	0.0544451271544709	0.3870554521557432
0.1134435804746360	0.3835903221728074	0.7280711705349660
0.6902571210447301	0.2718327351716261	0.3783078463516818
0.3618889622982190	0.6155951912416987	0.7103757349281234
0.0285561291056753	0.9419006054913056	0.5430060493469684
0.3052699029802744	0.2308352838485375	0.5274948295700062
0.9769486585934317	0.5714025017888268	0.3459868041246530
0.6319709607996680	0.8951535246320400	0.7019915687210574
0.0350041738829879	0.7404255583917778	0.5336498257065461
0.7047999200882185	0.0760949410828409	0.3642658470445871
0.3814331081214397	0.4091761785550178	0.6840190510283465
0.7735170426755151	0.9567884522941388	0.5587172561052087
0.4434360786667148	0.2832122924679144	0.3897663542945297
0.1175286409461135	0.6293530562457091	0.7282979970906879
0.6120514038170054	0.6486290366884098	0.7095389076345160
0.5618996950002636	0.4996420237871201	0.8189410783537656
0.1390197578599715	0.1446739573328189	0.3312586410279423
0.8085704785137869	0.4804871696618008	0.6733076274650139
0.5973528447825623	0.6219883080551737	0.3229496025302360
0.2547826536696261	0.9548585924851314	0.6520329515432846
0.9245073185051497	0.2896663402618807	0.4958107043992546
0.4693065875594694	0.8103368885006766	0.5135601143173489

0.3532472789802590	0.8934766557538576	0.3309522249275627
0.0204744092265840	0.2321249828991048	0.6746481715051018
0.8752221239648250	0.8747188872717668	0.3212562841428029
0.5457082483580653	0.2002768054368447	0.6509670191718588
0.2081514975037433	0.5340182650778452	0.4927147721553715
0.6877130667524012	0.5578336154174904	0.5143113419203106
0.6043669745773835	0.3588746102550663	0.3335727796801720
0.2683467990253929	0.6881526041240303	0.6737031454590645
0.6236396747885520	0.9001732332295682	0.3215393118779728
0.3020878886447786	0.2465917309986868	0.6485144441466126
0.9642481621691432	0.5740254875117989	0.4940319532585565
0.9401371337999376	0.0300246758353107	0.5125196185821228
0.9296029059307623	0.7889597685383458	0.4867106032018518
0.4748933432666131	0.3079428987955191	0.5068241080691005
0.1441459194728749	0.6450964880670158	0.3469947941289080
0.8014219288398768	0.9780173510420501	0.6787942126138903
0.5871494917206240	0.1179732406335044	0.3244108032582064
0.2629183037601001	0.4566576684235822	0.6627581408721501
0.7100594010600594	0.0407154829517524	0.4869038610275823
0.1893102060795621	0.0638364449547862	0.5025760660717915
0.8537964860001207	0.3987124204115651	0.3462761374804085
0.5223584532858717	0.7259102759029122	0.6798284968718059
0.3807003223747421	0.3682644299863005	0.3264639588639144
0.0445349275958442	0.7053040006523859	0.6644156249252148
0.4586156212168278	0.5682886118088761	0.4900277860401140
0.4343809637533792	0.0241524597299238	0.5028178843368919
0.0988139557541697	0.3536879215779385	0.3467384838227428
0.7749361110932548	0.7016865153938667	0.6785043020591994
0.1294305532210317	0.9106625665291318	0.3238774917203762
0.7952057786957416	0.2411300677820692	0.6675506450231758
0.7000648526673563	0.2995115839722028	0.4988079586778984
0.6993384347589009	0.7996216241169908	0.5006912224276968
0.1983645318689679	0.2981909032482187	0.4984813609819226
0.1998521552214339	0.7999673855444824	0.4991016458560605
0.8690967238806494	0.1275036693951064	0.3344091804728406
0.3721116247844166	0.6417844673400009	0.3365793633677679
0.0293794197570363	0.9599327401068458	0.6642685619643026
0.3658425669542814	0.1325973526968917	0.3136017008682906
0.0333234302142109	0.4671836189544038	0.6845698490569027
0.8559113007916876	0.6286896750930575	0.3355009366962877
0.5419586584277976	0.9713738251761749	0.6648778076355895
0.5309200764664137	0.4650422464094694	0.6565524995225563
0.5565164212638434	0.5003755804385593	0.7548895860266873

The perfect Ni₁₁-CO*_P surface

O In Ni C

1.000000000000000			
12.5091304782646002	-7.2221498489373399	0.000000000000000	
0.000000000000000	14.4442996978254001	0.000000000000000	
0.000000000000000	0.000000000000000	17.9855003356999994	

O	In	Ni	C
73	47	1	1

Direct

0.8405395172021309	0.6122814290975738	0.4569848785098583
0.5148107373587357	0.9515440564256944	0.2887106882798791
0.1750409074180941	0.2834163218318130	0.6208349186113351
0.7916448828303213	0.9602342421132395	0.2977192932319117
0.4723967843954643	0.2930943066340454	0.6424669061018846
0.1320449442480646	0.6253182938808693	0.4684546470641511
0.3001011122784201	0.7301305374253017	0.2996282607203758
0.9782254674622328	0.0732492738137896	0.6344054727266419
0.6396494135665067	0.4051469672494710	0.4663728567409104
0.5281537098660546	0.2096330307532081	0.2698049923415029
0.1849627440258001	0.5415933487236042	0.6091275893106998
0.8553969040934332	0.8821003100079654	0.4413775274151343
0.8857840616467842	0.1284577864886971	0.4557568067230529
0.5461225105619896	0.4618186631522964	0.2902989851347541
0.2181363562833872	0.7913910226592851	0.6197259380094050
0.5381232611206510	0.7305715345516933	0.2990630071134488
0.2073003073493636	0.0790609821012151	0.6548271859804596
0.8746859041449716	0.4066951705464313	0.4680006469543690
0.7665785130689776	0.4682836708066353	0.3001380987556362
0.4289110412652553	0.8065572729111510	0.6361088920759549
0.0929660667508699	0.1340002176102687	0.4639734127565612
0.2897670664043926	0.2187024036980988	0.2699896481691769
0.9576715657696024	0.5430285063559104	0.6099121702227659
0.6169399923028075	0.8733090534220043	0.4415632334677007
0.3714714938215466	0.6580236198827945	0.4574493478171685
0.0353818231079037	0.9830060091167859	0.2885048232285072
0.7093215837818317	0.3283698002896087	0.6197682691227927
0.7660597328955199	0.7060765017801169	0.2993723251300791
0.4220110527570624	0.0282700018575143	0.6557034481584002
0.0902386162819919	0.3648252139318930	0.4686332613644835
0.0295587227892003	0.1975967652640530	0.2989924419215200
0.6842628346317631	0.5217006668305987	0.6368534984183138
0.3642732822448013	0.8584578477522397	0.4646333674450589
0.2797038122740282	0.9698154849902653	0.2684464848870870
0.9564248241688276	0.3161589615094469	0.6114078862474811

0.6239485189176942	0.6401900653019973	0.4438326613256346
0.2254073573027137	0.3168989745004174	0.3778919580050142
0.8810167273319711	0.6466063361736472	0.7055703867572458
0.5573833009043769	0.9861504676086600	0.5434629937213348
0.2673017904660092	0.9751670422067352	0.5301306506605117
0.9272819452656937	0.3055320531850368	0.3426853439154695
0.7592714019606008	0.1944035710118200	0.5350558672567918
0.4224853406684275	0.5279910391010326	0.3668073300060515
0.0981084421856583	0.8675972512441477	0.6986462723500555
0.5431644244827312	0.7177937956200040	0.5592343093630529
0.2140658048150345	0.0579209258911251	0.3871427778295022
0.8708204949871566	0.3914000886091675	0.7292564989882605
0.1815235744201399	0.8088841505933074	0.3781016776054352
0.8545974688094073	0.1389670863112877	0.7110976344142286
0.5143153900085178	0.4710273034308212	0.5513838627842818
0.5271436623342786	0.1895150771905542	0.5288738414188355
0.1933679355512882	0.5212438963633408	0.3488101573106885
0.8629509810302356	0.8713700555509828	0.7021954498617705
0.3033995022436495	0.4631913193052075	0.5325055308097252
0.9697890723114637	0.7928722940040924	0.3641083270526581
0.6329075406847656	0.1323943627159765	0.6996556085783798
0.7832218935062788	0.7267224369621946	0.5587236802540597
0.4386591175751430	0.0543273616382705	0.3870213911321855
0.1136569191392681	0.3838414815970613	0.7281771764290832
0.6899912877309123	0.2720585568734212	0.3785335323904514
0.3618425769144639	0.6155731889189088	0.7101978822235507
0.0286801121475529	0.9420117221916057	0.5431213983680279
0.3054016995378915	0.2314069632354072	0.5275364467385472
0.9768503371476712	0.5712780240511628	0.3458092504523407
0.6322386112216791	0.8954216472594969	0.7020599387466346
0.0351362653393820	0.7404613830998362	0.5336633597314764
0.7047834014833435	0.0762885454729909	0.3642212524433351
0.3820027328455825	0.4088372191626553	0.6853571718379825
0.7736700852777548	0.9568304377134347	0.5588490016797114
0.4435764180179529	0.2835385254095519	0.3905543503086812
0.1176707953047627	0.6295816622416569	0.7281725193346104
0.6111302887505855	0.6480515095558874	0.7044072588026780
0.5605309893275905	0.4820450825584153	0.8221065600158511
0.1389157888944637	0.1445623209616404	0.3313946151596026
0.8091484892000040	0.4806591243208341	0.6733249354243318
0.5971464482463277	0.6216932765809953	0.3232258702736467
0.2549503058800279	0.9548903596754907	0.6520463307807836
0.9244788340264243	0.2895809248774869	0.4958482326471091
0.4692389522537829	0.8104861166712443	0.5134468676420300

0.3531584729437064	0.8933160763945213	0.3309170408867041
0.0206945310394082	0.2324341190616568	0.6747627045128792
0.8751347264479316	0.8746407412083427	0.3213283862420935
0.5458773122711467	0.1994666209330770	0.6507062423036254
0.2081387114215698	0.5339951720437955	0.4928329918661104
0.6882191397494011	0.5583330966162897	0.5149964554798095
0.6040981212138180	0.3588489840924979	0.3338582358502010
0.2685847036736053	0.6882551876681592	0.6736547187537077
0.6235429759360671	0.9000831619890143	0.3214992209449111
0.3020365625714295	0.2465018317897034	0.6485125079327423
0.9643084116200150	0.5739940420191805	0.4939665212421345
0.9401981052256039	0.0300816449538013	0.5126161128583906
0.9297216358815373	0.7890092435458788	0.4868300834747306
0.4752296726151288	0.3083301634943100	0.5077691560986555
0.1440669253000183	0.6449395050969953	0.3469448063588259
0.8014612167766083	0.9781932007237248	0.6789511617175338
0.5870774780082697	0.1179746194729412	0.3245427509955597
0.2634167437290906	0.4569911866090219	0.6630242572098012
0.7100636525298887	0.0406649262272783	0.4869458163724194
0.1894356803310105	0.0639582327522600	0.5027112092353309
0.8536392135159085	0.3986503934769955	0.3463166201133143
0.5230983348724416	0.7256670774275844	0.6792928703635875
0.3806149902468213	0.3681696391013486	0.3268806213501927
0.0445869133596682	0.7056051180456693	0.6642187576551628
0.4588930092919702	0.5690013043665607	0.4905578535355860
0.4343918106291872	0.0240590604834848	0.5027956298906187
0.0986188130179316	0.3535689114239883	0.3467344108116671
0.7737155825818254	0.7019928336446813	0.6786884995847016
0.1293560360497054	0.9105453039157488	0.3239449370087503
0.7953587451067172	0.2411918282687422	0.6677195307467079
0.7001682572624239	0.2995651503161693	0.4989496736236058
0.6993424237891983	0.7996469062363315	0.5007118893654544
0.1984015325346689	0.2983532325595684	0.4984858313006921
0.1998722713995090	0.7999490720379930	0.4990636571735853
0.8689933594080362	0.1274235956275313	0.3344374657609442
0.3719518254434073	0.6415415749933150	0.3366903971268435
0.0292065666337447	0.9599006862609784	0.6643913453573400
0.3657519319182840	0.1324654953152521	0.3139220548906468
0.0337149339532355	0.4674405208631045	0.6844522033847045
0.8557946963360351	0.6286195175036021	0.3356431358153508
0.5421020625557348	0.9710015195756772	0.6649964958906872
0.5322123479271920	0.4651957911269762	0.6580247349552012
0.5521934395947334	0.4786853030618360	0.7585678189924260

The perfect Ni₁₁-H₂*_P surface

O In Ni In H

1.000000000000000		
14.4442996979000000	0.0000000000000000	0.0000000000000000
-7.2221498489000000	12.5091304781999995	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.9855003356999994

O	In	Ni	In	H
72	41	1	6	2

Direct

0.8415250841955469	0.6126335779342137	0.4569954452129636
0.5152019538351936	0.9522212319533802	0.2893930573402997
0.1770615732984705	0.2839301899989081	0.6228517867503921
0.7927675930791831	0.9609330283251620	0.2978922775498749
0.4808194172439588	0.3063129061523863	0.6450889155133418
0.1327409874402389	0.6257783568815948	0.4694943273739373
0.3004302849591811	0.7314570375774678	0.2998569151165268
0.9775501984440650	0.0703076187828836	0.6369492418827185
0.6418433907247030	0.4053553830673552	0.4653673960484080
0.5290741739968823	0.2102792194124297	0.2701692140636662
0.1850628844707480	0.5410803339817686	0.6105612809417750
0.8565968311559524	0.8829580472453235	0.4416761457543994
0.8867884041420239	0.1286001771160571	0.4563494244195557
0.5474403773070088	0.4628927914173310	0.2901889864445424
0.2181251704837247	0.7923739699954030	0.6212407184161695
0.5387528983422367	0.7317667988382819	0.2979794422229622
0.2093061238046260	0.0813405668781669	0.6529900800798430
0.8754948527660216	0.4069008095242000	0.4687715755624723
0.7681017331052349	0.4687305506076739	0.300038882586610
0.4280969431644451	0.8056102613860033	0.6353906411763149
0.0944653282471764	0.1354990419915842	0.4667956731243234
0.2901098551187561	0.2191418899517235	0.2708457668359191
0.9578963980663783	0.5422090896767323	0.6107186806738107
0.6172912910909419	0.8743256697205568	0.4413578555554235
0.3714203331323866	0.6585850113444480	0.4567124126380304
0.0368544550120704	0.9843303067825924	0.2901142465419473
0.7101089941783773	0.3274877550540896	0.6202773545944980
0.7680084050215840	0.7070533045421136	0.2981629832513715
0.4226453448058037	0.0310417590825991	0.6569197682679109
0.0916956333490341	0.3660181143135871	0.4695784519481624
0.0311800338277370	0.1985750469192246	0.3001350330226131
0.6829039977929118	0.5182239865345020	0.6368812489382861
0.3645974098569768	0.8596065330013920	0.4651356543712421
0.2805795901094627	0.9709911831448558	0.2702955951026998
0.9569833824587564	0.3144627985604508	0.6120486816093825

0.6259258822715842	0.6431929595857397	0.4414169058244364
0.2269525414969830	0.3178612945126024	0.3794300884697610
0.8796871053482173	0.6449705904656234	0.7054736989479929
0.5577173128520571	0.9867911168697776	0.5438842964794697
0.2678141283659548	0.9753336584678181	0.5310748995117480
0.9285608151547492	0.3059850702339737	0.3441380487660606
0.5943131664552433	0.6206260081035765	0.6943010930045637
0.7598045297236105	0.1944490093779455	0.5350363490146877
0.4229287070362330	0.5291637560605001	0.3651286739146891
0.0980813101417392	0.8681385298980356	0.6999779627854592
0.5432522320284765	0.7180856953155724	0.5577397478519837
0.2151493775952006	0.0594445610392570	0.3896215064416562
0.8708830929477580	0.3896240336901961	0.7296175491050366
0.1817215379232804	0.8092387603444802	0.3794101634854862
0.8532627621342375	0.1361315612955171	0.7109215757137030
0.5152149658134054	0.4726410341369684	0.5452247170233792
0.5261744528717616	0.1913141718412367	0.5307513635442029
0.1939324229186511	0.5221095399970068	0.3483179497652933
0.8565747321864525	0.8639413449648733	0.7011550294796804
0.3047090103791990	0.4649058529631306	0.5336959327268538
0.9705034541006904	0.7934630979276266	0.3649320518225718
0.6325612814224381	0.1309920651554436	0.6993787877099250
0.7818457186759792	0.7252716431589771	0.5581549360357395
0.4403876029996823	0.0559371222722092	0.3882435069608124
0.1135264704647171	0.3827137731342533	0.7292440638887925
0.6912071825757435	0.2722999632537674	0.3788279471643225
0.3607115479868455	0.6156043892571298	0.7117348958862476
0.0284032066113921	0.9414456624875470	0.5439472728742701
0.3084588008084734	0.2339046666567987	0.5293317666323420
0.9777307455219333	0.5717539735121189	0.3464266729687968
0.6297654277113122	0.8884839025036235	0.7016774725886493
0.0349863834387813	0.7402941065485475	0.5350263521259119
0.7060791361749623	0.0770152548285694	0.3642137651247488
0.3882657909988758	0.4139785366550052	0.6885169067865268
0.7739648990844452	0.9569448083161992	0.5587713169295625
0.4448297038924566	0.2846572332726992	0.3899488687101920
0.1170079694571429	0.6291725876687883	0.7289614141983798
0.1402362491560895	0.1456077256621983	0.3334591930906289
0.8091249781580485	0.4791919714895518	0.6740674076993465
0.5986771008653208	0.6233935638185576	0.3216325780839116
0.2552725182711020	0.9562211281367555	0.6529772982634804
0.9256488386250250	0.2898947985006802	0.4961682712937727
0.4693662243073354	0.8110757735360944	0.5129494497323766
0.3539102066723768	0.8942437716617588	0.3324857486513921

0.0209813726203254	0.2310080033629445	0.6758921718548407
0.8762666918676502	0.8753649346995096	0.3216200223540390
0.5469434636851650	0.2024986043647730	0.6518970914253279
0.2090360600369786	0.5349270778562412	0.4942204174822783
0.6880618888653505	0.5583265606766724	0.5135434545090667
0.6056339464776536	0.3598189883919204	0.3335660734281394
0.2680044148348673	0.6883321197112066	0.6744685767860829
0.6244573956191389	0.9009786933989971	0.3212667023431564
0.3065602929110199	0.2506704692525653	0.6503905619629766
0.9647363284742346	0.5740004131172198	0.4949449949509173
0.9408526196181105	0.0301553415242806	0.5134443748769432
0.9298822761568424	0.7887650536144588	0.4872927977539872
0.4768838838751504	0.3112499721077493	0.5066980386098986
0.1447673382229410	0.6456703873832425	0.3478091511670839
0.7994859516975265	0.9748838310602030	0.6790634057857911
0.5880535513521669	0.1186709486147241	0.3248725855323762
0.2646927660555038	0.4568234106117354	0.6649340048639442
0.7106592191113611	0.0411051783909092	0.4869639783469353
0.1910267068050185	0.0658806674052394	0.5058784303656140
0.8548649633125288	0.3992382366396508	0.3469929736352043
0.5203086034036877	0.7189967982404976	0.6769765884886449
0.3815398367413004	0.3691575847778750	0.3266267123778961
0.0440451543353626	0.7052059034268847	0.6651673740124032
0.4593109785431293	0.5695262733936298	0.4882534655420475
0.4349967734786052	0.0255001344202738	0.5038576240862382
0.1002382270801395	0.3545855818614175	0.3476824958837642
0.7670522294868765	0.6937022124105181	0.6772525549101274
0.1304724250933491	0.9119763509545638	0.3259500809071734
0.7954233863417270	0.2394282582917251	0.6676028592872205
0.7006815511160340	0.2995517208492705	0.4993160019435576
0.6999191654673834	0.8001531337894578	0.4996255541034998
0.2003407018068370	0.3000545617627070	0.5002027622022267
0.2001133555265227	0.8004838640629124	0.5002560830696191
0.8703542336749757	0.1280407012916401	0.3349879738950283
0.5337424052264333	0.4693106781311353	0.6581197330419871
0.3721543537248080	0.6424103182484874	0.3358409562021823
0.0263799043987664	0.9562899017949065	0.6650050269092370
0.3667321054224534	0.1335313879206591	0.3149877489497470
0.0338777594326700	0.4665106140612481	0.6851119015072666
0.8571612956011639	0.6292253206127508	0.3356102974972628
0.5416116218082860	0.9694054300358574	0.6652149678905528
0.5662753645475636	0.6618035591232442	0.8413256869346720
0.5631189983888552	0.7012295953764354	0.8657454449072518

The perfect Ni₁₁-[TS-2H]* surface

O	In	Ni	In	H
1.000000000000000				
14.4442996979000000		0.0000000000000000		0.0000000000000000
-7.2221498489000000		12.5091304781999995		0.0000000000000000
0.0000000000000000		0.0000000000000000		17.9855003356999994

O	In	Ni	In	H
72	41	1	6	2

Direct

0.8410938331808180	0.6125355506456196	0.4570857054185783
0.5151833933013223	0.9519056068297878	0.2896891505157209
0.1768132320338839	0.2833233273259047	0.6227329632058036
0.7923233832736792	0.9604474606927588	0.2989672514326926
0.4801679659539935	0.3048496830004296	0.6435688453195213
0.1326001081702197	0.6261309602917764	0.4694949685264303
0.3008754610382232	0.7308473258065215	0.3010314513761086
0.9775471458572030	0.0704032502870787	0.6374866652008214
0.6413924415616999	0.4051571121863503	0.4646494619558856
0.5288871112511595	0.2100912740095428	0.2700482164316140
0.1829919055657920	0.5404876953990857	0.6097667613777473
0.8556268683859529	0.8818277260567273	0.4427642312941863
0.8866767025200167	0.1284183092497088	0.4564243455847500
0.5472996453090657	0.4632822194050356	0.2913721739206963
0.2173648667102194	0.7925168599046349	0.6210542957135261
0.5387087934980624	0.7317095728104386	0.3000008481839888
0.2084855184115625	0.0805868143776947	0.6535142134029215
0.8757146722234235	0.4068765612383541	0.4682707247759870
0.7678584658337972	0.4686507052922101	0.2999045524084903
0.4271883105361354	0.8091185318002825	0.6379918975932197
0.0940303293698419	0.1350257637423156	0.4666684355510650
0.2902257404268306	0.2195316998096197	0.2706927664422368
0.9578484215901095	0.5426367626772660	0.6105588459453042
0.6166932869419861	0.8737804685145013	0.4432303870983620
0.3726279441054233	0.6591014952681246	0.4593964915947349
0.0360850597520972	0.9838297183282402	0.2901054586750658
0.7116493058659898	0.3280404467314617	0.6193758698656493
0.7669182320492502	0.7065514626214295	0.2998796755013201
0.4225998606808441	0.0330290922161301	0.6568679680068105
0.0913062308890670	0.3650096807001130	0.4697608546105067
0.0308833567668691	0.1982196989073987	0.3001649178338202
0.6846397189882563	0.5162633297629605	0.6366728247148495
0.3645577393654982	0.8594482522315832	0.4659738132873228
0.2802748081475285	0.9707950955973124	0.2698214975428682
0.9571908077793372	0.3146492433454235	0.6120734136207078

0.6251284679057485	0.6442192326279629	0.4441178032475704
0.2265734198517174	0.3173870667585413	0.3795175583297243
0.8807201807434559	0.6440275552594908	0.7079434509803963
0.5575417053247157	0.9880061931787539	0.5443812861731652
0.2675581425233066	0.9753970193680062	0.5309686169671516
0.9284644393989536	0.3058866902964402	0.3434432520994244
0.5931777888172520	0.6108800305541829	0.6966964614676526
0.7598820980622418	0.1943764002001470	0.5350527920438640
0.4230215689987847	0.5289182790398321	0.3677194685111711
0.0976339646602297	0.8678180150837391	0.7000777822761736
0.5440220851644029	0.7198836117496978	0.5632295347142798
0.2147746655374219	0.0591069117780314	0.3890884027646694
0.8719706436080730	0.3899625913005197	0.7299656059603163
0.1819890139072520	0.8095459116887274	0.3791822941651893
0.8548626406956107	0.1380981662777842	0.7117605076341935
0.5155129656558507	0.4722659413152937	0.5461949831127333
0.5267894030619017	0.1916031030633418	0.5300898679496515
0.1943700573316002	0.5219935244533961	0.3508271504160232
0.8556517727557608	0.8633591676257334	0.7010425261192121
0.3040659937611929	0.4642868730509657	0.5347267669218098
0.9703447342739632	0.7931882325115235	0.3649685497324917
0.6332843344179053	0.1348024479886308	0.7009138538926051
0.7814706520500656	0.7241297021185255	0.5595169059659511
0.4397699408033408	0.0555417043959137	0.3878960637640448
0.1147368728953861	0.3833476404394714	0.7291006351061948
0.6913172707364933	0.2721416170309306	0.3783523767158765
0.3579905970857795	0.6151483699978764	0.7093524692657375
0.0282235690844933	0.9413150384702333	0.5441601667480606
0.3078374875101863	0.2331198700554865	0.5292808617228076
0.9777281712449446	0.5717191992402287	0.3459827860750297
0.6320859566487423	0.8980719429483552	0.7010449493496581
0.0346544046432251	0.7403380689314863	0.5348723889318294
0.7056282384492737	0.0765466949129026	0.3648742033435370
0.3879902280829495	0.4109204675632438	0.6898676269823183
0.7748268233574498	0.9577734514083405	0.5594064863129701
0.4441430663296195	0.2838068200245834	0.3898580922569564
0.1161792875893283	0.6289590528641956	0.7291378890271721
0.1400848725036330	0.1453341277983297	0.3328747487157470
0.8100065155495242	0.4786939181496871	0.6743056647377519
0.5979939129491174	0.6231864005341979	0.3241409207045857
0.2550584806250972	0.9563137708094837	0.6529264386039099
0.9253885173579888	0.2896152477256614	0.4963905491496340
0.4695554185951574	0.8119813224040492	0.5151974922016470
0.3537423063123490	0.8941176949272116	0.3322388264989188

0.0217633293438436	0.2317479959879693	0.6761627644309295
0.8756909769031077	0.8748499740670859	0.3225595755980571
0.5482526988284914	0.2042738539461146	0.6512522433379923
0.2083780540913573	0.5343145558207824	0.4940851863122488
0.6878367801434160	0.5574466417600817	0.5139979224455852
0.6053221301734327	0.3595587307397571	0.3335552155295290
0.2658796182314146	0.6876410360345125	0.6737911644108215
0.6241814946373965	0.9007557268896111	0.3228174114556856
0.3053896704525870	0.2491669157844156	0.6505355971566589
0.9645672493583327	0.5739705474432854	0.4949163438760368
0.9407568345100421	0.0300383267608097	0.5136441806741482
0.9294020711570364	0.7885657353289752	0.4874428028173238
0.4764034638740962	0.3108287036635185	0.5063569897964950
0.1448028936546506	0.6456644758916036	0.3480496951100090
0.8007595666274890	0.9770412884568476	0.6796116573202478
0.5877765768888612	0.1183549344169623	0.3248878167521155
0.2654158559049351	0.4565765235288678	0.6644356078291258
0.7104940432852264	0.0409641809041129	0.4875809058515221
0.1904240974681082	0.0653595905304600	0.5053393453133205
0.8549095521259733	0.3991632579537409	0.3465233724419058
0.5184628373943239	0.7289735833524525	0.6823585642397324
0.3814499527348739	0.3693478289393574	0.3274339994448743
0.0438645322326085	0.7051083492480991	0.6654665308124050
0.4597728854067899	0.5706370629182581	0.4917853544583914
0.4347381115768285	0.0258007554235100	0.5036040825563121
0.0999398572304136	0.3541625138643718	0.3479912021613921
0.7703524030315443	0.6929912203220184	0.6777317650436747
0.1301201479657577	0.9117080470439793	0.3255634380798333
0.7961328003588450	0.2401722977149780	0.6681158958613698
0.7008902924663963	0.2995589887565365	0.4987258763038295
0.6995568239438010	0.8003766619304220	0.5023851408290652
0.2000788331229737	0.2994886518260760	0.5003068824144082
0.1998170966942188	0.8006523961752560	0.5001031884639051
0.8700159462763659	0.1277511891521644	0.3352406105826250
0.5341142173167557	0.4634921500121594	0.6592221672746921
0.3727557612359775	0.6425282526886286	0.3382261113986156
0.0261460355190241	0.9562035213459107	0.6652061365117182
0.3664500886799916	0.1334189800962156	0.3146125784128624
0.0343886760060844	0.4665536091564922	0.6849388386062936
0.8567449791458034	0.6290025608509222	0.3357176979558960
0.5418145884929780	0.9742819579458865	0.6657641817275419
0.5749607120950121	0.6441310347197103	0.7548746176948911
0.5638685138366430	0.6948169768950000	0.7852300180155229

The perfect Ni₁₁-2H* surface

O In Ni In H

1.000000000000000

14.4442996979000000 0.0000000000000000 0.0000000000000000

-7.2221498489000000 12.5091304781999995 0.0000000000000000

0.0000000000000000 0.0000000000000000 17.9855003356999994

O In Ni In H

72 41 1 6 2

Direct

0.8409581174749957 0.6127245882079342 0.4562877133351564

0.5150684201474424 0.9515802516445413 0.2893878736255236

0.1770171827495124 0.2832261736758963 0.6224168618042523

0.7920567570049809 0.9601771858300365 0.2989212635026450

0.4798229921296333 0.3037207426383665 0.6410606405404743

0.1322520298293156 0.6264338069690240 0.4685507458104922

0.3011439753641464 0.7307201868758101 0.3010096198696534

0.9780179559216163 0.0706655785780282 0.6373519932290715

0.6411613392573817 0.4050714806831308 0.4634112314768686

0.5289430292498553 0.2098481711856758 0.2691429752015919

0.1798580516867236 0.5394608029049157 0.6078440522333012

0.8549970197696903 0.8804744829458313 0.4424914399867225

0.8869802198102366 0.1286558496646527 0.4556759829520579

0.5474056549484745 0.4636585479589141 0.2908685781625924

0.2171821164476968 0.7922367608826796 0.6205209436212858

0.5387739833294301 0.7318315120036384 0.3002354466588144

0.2080832737666091 0.0795918880210445 0.6537488298622415

0.8758194963641025 0.4069471833910202 0.4675049154290061

0.7680291296513707 0.4685366383104456 0.2990240595175390

0.4275895904992178 0.8104165477658508 0.6402583719281881

0.0941984727010212 0.1349984808947122 0.4661577904506091

0.2904475467796118 0.2199977169497523 0.2698155733032930

0.9573589840404184 0.5431068559838234 0.6098023581192636

0.6158171441911525 0.8728638516908539 0.4440810067094620

0.3735651235187932 0.6595101625618522 0.4604648179639987

0.0357519926998856 0.9838664860442102 0.2898922439652698

0.7121946205867804 0.3285587589634069 0.6178327381762678

0.7663116106597287 0.7061281298636243 0.2998025994099005

0.4227360509423284 0.0345184657736687 0.6561717189281355

0.0912188505732455 0.3643594736259668 0.4692064656656256

0.0309794561998366 0.1984439993197898 0.2995512056049771

0.6851803322560039 0.5148288169420402 0.6353578996310002

0.3646013658002127 0.8586179063733657 0.4664710921856218

0.2801912374987676 0.9706869620857836 0.2690145459484460

0.9571253420941697 0.3146893495163454 0.6113926638206374

0.6244410114968683	0.6444421908308440	0.4449580586193185
0.2267167545056202	0.3173312787597641	0.3789150020027889
0.8812558816130478	0.6431031500303991	0.7091840272704184
0.5571595287001304	0.9889441910664060	0.5436828741475498
0.2673611258621321	0.9753592656284884	0.5304691268181400
0.9285118170897214	0.3058207803202559	0.3429103232002962
0.5931025167474343	0.6042953130236225	0.6974915582961768
0.7598210034030553	0.1942325822906340	0.5345466656279396
0.4232550811095504	0.5290539547715173	0.3682754802835851
0.0972733240875811	0.8673460115028834	0.6994836097366550
0.5447998504836506	0.7202625763002322	0.5675637113155748
0.2149463929442489	0.0594220736219792	0.3881697839223874
0.8720172544524056	0.3902832163309182	0.7294785063759009
0.1823897843605420	0.8100932699522071	0.3786632990761805
0.8573642204087003	0.1408596548118533	0.7126495463629230
0.5154677837966843	0.4715067487199108	0.5461480103416375
0.5267892820287399	0.1915305562577784	0.5287244792867903
0.1946723883497378	0.5222202067752951	0.3516346704127269
0.8556347335911783	0.8634593778856162	0.7003168579709251
0.3037305127120962	0.4637933349749128	0.5346573197790454
0.9704249265659840	0.7929639868804103	0.3639706544049179
0.6338481800533953	0.1382190262496467	0.7015875549404992
0.7810466193072348	0.7231721152228361	0.5598095796866870
0.4393070977485934	0.0552583781666806	0.3872094814318303
0.1147325280013513	0.3835565011422483	0.7285698340596017
0.6913176444870356	0.2720580890755142	0.3774821611140320
0.3544351534558675	0.6118443945666230	0.7059537733208102
0.0281939173971323	0.9412713408132761	0.5435736986458104
0.3076163667646039	0.2325625626041464	0.5286987849569453
0.9777740500294863	0.5717994419892001	0.3450552710864082
0.6372390551899234	0.9099497337178918	0.6958348814088903
0.0344723373571923	0.7404095517466227	0.5342629868550300
0.7053155820043251	0.0760579353362797	0.3647857783116884
0.3896187907545015	0.4081076323237189	0.6902018172886639
0.7768519968278285	0.9588454309304940	0.5581901258653157
0.4440292891516934	0.2835114757573959	0.3885735724455348
0.1156687630564842	0.6285187248228387	0.7285937846930887
0.1403264682362390	0.1456572609702614	0.3319446094654660
0.8102838546719378	0.4782413349510136	0.6735143114750182
0.5975643181751100	0.6231461925846146	0.3245803010662661
0.2550122569130584	0.9556466555131843	0.6524549988666339
0.9253235878515939	0.2893972624835833	0.4958969410858599
0.4696510288306309	0.8117283419141166	0.5180794344350407
0.3537070636883646	0.8940635448389309	0.3318498008624309

0.0220579069164966	0.2323073484837275	0.6762494144134553
0.8752841497822486	0.8745252259119968	0.3222565732449273
0.5494240542232303	0.2050564629973881	0.6497915503250448
0.2078859694633602	0.5341262709346416	0.4930450883904955
0.6878122993246337	0.5570256158161582	0.5131201252407792
0.6054398199047470	0.3595315182080866	0.3322616692771764
0.2651003493358683	0.6863386061048707	0.6727424302061339
0.6239247772607327	0.9005308905699246	0.3234162676785583
0.3039446231175429	0.2472402669068657	0.6498620821768540
0.9645465741341617	0.5740652413770380	0.4941977199894685
0.9409124547207957	0.0298874379248212	0.5126940212791231
0.9295224871721496	0.7885719744886551	0.4865570239201002
0.4760215209494968	0.3100293397812845	0.5046233066359153
0.1447976552103077	0.6460055419581723	0.3474574734990711
0.8024918008576064	0.9801049512634927	0.6787206371423078
0.5875800824077202	0.1180232558149319	0.3243946296656085
0.2641360983357198	0.4557825045688350	0.6629741573590615
0.7102613457305513	0.0406432685562114	0.4874420650101722
0.1902068436016911	0.0648910403469119	0.5042706677673046
0.8550703640955484	0.3991474848395144	0.3458505010742190
0.5196586341809240	0.7344540432454164	0.6893259212336453
0.3815466872645113	0.3698677591952701	0.3267564690584406
0.0442888082667157	0.7048590299097879	0.6651392786030370
0.4601707937536414	0.5720283812336892	0.4937558656673450
0.4344152873884445	0.0253004666193508	0.5028274618521507
0.0999308115970754	0.3541221578552978	0.3476378691705537
0.7746270228018953	0.6943471391649710	0.6771318909282084
0.1301113265128418	0.9118388819906844	0.3248242880184148
0.7965861860767202	0.2403867766742152	0.6680440584451846
0.7011062021758123	0.2995317898740681	0.4977053736543449
0.6987980678369339	0.8004186871184695	0.5037286451888131
0.2001609261839431	0.2994424341584122	0.4995962129741096
0.1998482993382233	0.8004536932773368	0.4996194209410031
0.8699997660729304	0.1276345825410857	0.3347991241633715
0.5328149992509393	0.4567211872243901	0.6579903877558351
0.3733701734765914	0.6430237702305076	0.3391080100279250
0.0263875602963270	0.9562982626372313	0.6646705422780453
0.3664202890502577	0.1334091940636097	0.3136029066433292
0.0342029151700438	0.4664400441357591	0.6840382062727494
0.8566861619344318	0.6288735621837971	0.3348653035263318
0.5424959729146644	0.9777587744110553	0.6652173369247522
0.5705107821530109	0.6007199134648156	0.7490029192574493
0.5603439445321194	0.7267313270144652	0.7816591310842033

The perfect Ni₁₁-[TS-H₂O]* surface

O In Ni In H

1.000000000000000				
14.4442996979000000	0.0000000000000000	0.0000000000000000		
-7.2221498489000000	12.5091304781999995	0.0000000000000000		
0.0000000000000000	0.0000000000000000	17.9855003356999994		

O	In	Ni	In	H
72	41	1	6	2

Direct

0.8394440419759265	0.6122706119392499	0.4573696075851838
0.5148712295553678	0.9512415044416334	0.2886101244172840
0.1722724062093683	0.2816715800234684	0.6195258875667629
0.7916746086828848	0.9601742337684986	0.2981386327727887
0.4682490406421350	0.2895043168916923	0.6424811834097645
0.1326115812096189	0.6250596707174936	0.4688973893017725
0.3001958003240812	0.7299354300105745	0.2998478726220572
0.9773891277681538	0.0723748348432931	0.6342130946705882
0.6402318210119260	0.4043542536286348	0.4651085537543456
0.5286530574343129	0.2094198064807759	0.2685948229921379
0.1840487322607595	0.5396123797105374	0.6098034949369153
0.8550126365066806	0.8813349884446581	0.4416161301143701
0.8857952696697337	0.1287216169929714	0.4557308445425367
0.5469695530323810	0.4625636963769201	0.2904979702107244
0.2172992149629307	0.7903963745206541	0.6196016195002478
0.5383472771829229	0.7310497785517693	0.2992603098067639
0.2053148786062745	0.0770719092622150	0.6546017303229706
0.8747362300134365	0.4062893863927884	0.4676609266288109
0.7673462721834194	0.4683009696404657	0.2994072364912935
0.4264841251486024	0.8089880798000676	0.6361710711881254
0.0927885154735241	0.1335602245209254	0.4629638385874870
0.2894077255623723	0.2187600906221405	0.2689589134571326
0.9568593902610276	0.5429280146714572	0.6097995342799132
0.6159113786289235	0.8722355800504481	0.4427181010912616
0.3730064456553284	0.6581039028040584	0.4584413189510829
0.0353027146376689	0.9828413207820463	0.2885850310872547
0.7082673346150337	0.3296990828638649	0.6187845954516052
0.7660535540760278	0.7060110876099005	0.2992562865072660
0.4213977511907742	0.0295786480175758	0.6559291719481961
0.0903986564564758	0.3647363978048553	0.4684113348360936
0.0298460756007669	0.1976721079058030	0.2990118246434914
0.6837297164278827	0.5260357287488697	0.6412697069667949
0.3639441630885413	0.8580942834629816	0.4644335248871230
0.2793206216211691	0.9693611585449111	0.2676953767469938
0.9560173864961903	0.3162504686454880	0.6113825066258807

0.6248809018196734	0.6432982910742139	0.4443927341195867
0.2260870223240435	0.3171374029766128	0.3777165142652049
0.8856644765539341	0.6453961342412544	0.7109598254536065
0.5567821663976085	0.9868912778688953	0.5427816197038409
0.2669210221100271	0.9745224357525424	0.5299682502925659
0.9275619430658356	0.3054568970692443	0.3420881288141464
0.6292889643109582	0.6732127650082228	0.7285822418963999
0.7589437636698675	0.1943734844881543	0.5353202537740243
0.4227780348376809	0.5282381425298341	0.3663216259035574
0.0975236263854064	0.8664358085552566	0.6984242572668522
0.5441756331819906	0.7167823361478660	0.5643574669731686
0.2146608951653464	0.0579675127497308	0.3866773073648385
0.8699282997304779	0.3910341167436393	0.7289264873636784
0.1814234923193584	0.8086707162878547	0.3778523277607290
0.8544413681759241	0.1395091406307427	0.7111092779163590
0.5130213226446126	0.4677935707404754	0.5436928731049457
0.5264705078328439	0.1892377202250882	0.5281642691539249
0.1939626959038505	0.5214576819216874	0.3491654355593850
0.8631947087133580	0.8705740606867404	0.7015938136602543
0.3035283994947668	0.4628685881025461	0.5334470130340210
0.9696336793169201	0.7925316730473942	0.3639620786348114
0.6328459923635495	0.1351789070657880	0.7001198664838576
0.7831346905020906	0.7265473924645742	0.5603468861077554
0.4383729216867222	0.0542360054171053	0.3861120154079292
0.1131348141170674	0.3827805418674177	0.7285907619098954
0.6903466518201452	0.2715154447023091	0.3776352966935638
0.3610365709368624	0.6148966711928903	0.7096239066210651
0.0285642733565169	0.9417386445826521	0.5426713866118618
0.3044542538639072	0.2302535926665051	0.5280725737447286
0.9768371708831362	0.5712756338264765	0.3471390086447355
0.6337883430302467	0.9021827642857795	0.6990611893658306
0.0346689405714074	0.7400862620378186	0.5332769792042050
0.7045654103529129	0.0756357057979491	0.3646131980697573
0.3794317083213401	0.4037868431989598	0.6918465647492722
0.7741414890326156	0.9572575375541597	0.5582231930118929
0.4431170894673430	0.2820769590105112	0.3880593556686907
0.1173071659321699	0.6280844386297512	0.7288810077280297
0.1391219726445593	0.1445615640917175	0.3312629134093497
0.8079149866675422	0.4807709185467537	0.6735158632667714
0.5975615392348532	0.6224090219109435	0.3239511606629829
0.2542758856710673	0.9540821938438888	0.6519211372614805
0.9246964074099192	0.2896799215802340	0.4958961445574159
0.4692387959369425	0.8107495051782374	0.5136244496516063
0.3529533904851592	0.8931604108519867	0.3304707672964797

0.0200362695576467	0.2321888341130177	0.6745809015485474
0.8750714414171106	0.8744219246604632	0.3214226537778356
0.5457746756671867	0.2010028041649511	0.6500661193230717
0.2083528465010004	0.5334683187306439	0.4937607345679453
0.6869846845547102	0.5567143871142165	0.5163009353823068
0.6047323412892082	0.3587410322442864	0.3326858548301186
0.2663350398774595	0.6863303096517741	0.6732633511209467
0.6235711334791975	0.8999628851233124	0.3221075500767909
0.2977476218467268	0.2442301792872532	0.6503916653379231
0.9640060404985590	0.5736885141669750	0.4938069965601968
0.9405166484257416	0.0300652802958634	0.5119163252199861
0.9294508128933153	0.7886554648708857	0.4865028100302211
0.4732138385895573	0.3060473890521193	0.5044495075502857
0.1441613500238184	0.6446489046206894	0.3474121883356974
0.8030843146038459	0.9796790419644665	0.6778891377714679
0.5870766693391142	0.1176536687268756	0.3239584080554910
0.2635959674491787	0.4539475431610605	0.6644571352464467
0.7099889558204673	0.0408714973407786	0.4870004137868226
0.1892746310771096	0.0635966207376912	0.5022841096519148
0.8540080238989487	0.3984874445107707	0.3459853480508241
0.5180741376944142	0.7342584445131772	0.6811716446432518
0.3808230837781021	0.3684669247142939	0.3258460690286352
0.0455196247017053	0.7045195571692677	0.6648544067343056
0.4588787787659773	0.5683960046087045	0.4904143382723086
0.4335590854216582	0.0240159965538574	0.5016920775463561
0.0990775827843740	0.3536593645530834	0.3467185425164654
0.7837457255117085	0.7018848781637245	0.6787757759852868
0.1292446707216278	0.9103937551483745	0.3237623332940164
0.7950314724670914	0.2416473143191957	0.6674391110733696
0.7000736245809431	0.2994693491931076	0.4982775871353329
0.6993573208043496	0.7997064590506716	0.5018880009638192
0.1986091141936039	0.2980954294729269	0.4983132093889959
0.1994074644395150	0.7995625503040094	0.4988572926779841
0.8692048224508171	0.1275062335818968	0.3344172230492998
0.5208566378647230	0.4455891812251597	0.6524383090167090
0.3722351363418736	0.6417455894009155	0.3369750348352192
0.0295392842074096	0.9596818870517052	0.6639627851203147
0.3656984257865190	0.1322930499269178	0.3122692617510241
0.0329131610998806	0.4662772689964806	0.6847260190599789
0.8552694821804998	0.6282614930888543	0.3358783201804200
0.5415012318109682	0.9751696732290687	0.6639771473947026
0.5872580793616456	0.6039250216534167	0.7526165161662453
0.5881321526368024	0.7368700421450056	0.7844047958613570

The perfect Ni₁₁-H₂O* surface

O In Ni In H

1.000000000000000				
14.4442996979000000	0.0000000000000000	0.0000000000000000		
-7.2221498489000000	12.5091304781999995	0.0000000000000000		
0.0000000000000000	0.0000000000000000	17.9855003356999994		

O	In	Ni	In	H
72	41	1	6	2

Direct

0.8399886306229825	0.6131128915850588	0.4561618668699216
0.5152190971124784	0.9523087720281901	0.2871175502478772
0.1724366792282934	0.2809347703808429	0.6195938124919229
0.7917584438287985	0.9611957359824788	0.2970904596634557
0.4682124606884677	0.2907908602840087	0.6438560442647473
0.1340786190274805	0.6264894431376611	0.4687808268292545
0.3002706192619881	0.7305662876587349	0.2988821875087092
0.9750577820721066	0.0692768636897007	0.6354395145509455
0.6403635906958205	0.4050332992541128	0.4645734088152565
0.5292191344548344	0.2103725445764359	0.2666911799149911
0.1862514720117586	0.5404011986280342	0.6097730572665404
0.8561889268918262	0.8832305809457707	0.4402464799722376
0.8853256182839221	0.1287553150921981	0.4557642212245102
0.5470415969497148	0.4629813905121566	0.2886707267507879
0.2174772749703991	0.7914419313819057	0.6192976932750772
0.5384889228336247	0.7315708912900504	0.2978827857189643
0.2055945914749127	0.0777001352785647	0.6577211012193294
0.8741999491841632	0.4065476062335444	0.4676453943843563
0.7679356865926193	0.4687538106803906	0.2982454841805915
0.4244949312112433	0.8092069466922059	0.6319202097781235
0.0927336514472137	0.1339184254752129	0.4626839918895186
0.2896135880092927	0.2196216969786785	0.2672326106276009
0.9577271570902051	0.5428744001974763	0.6088893103865367
0.6159604108437967	0.8728013682555550	0.4413821608476444
0.3741318059486731	0.6586034983427130	0.4574006314318272
0.0356579468426628	0.9836459700913724	0.2867527324763118
0.7068642502382125	0.3317525656510454	0.6188355442423022
0.7666860436721974	0.7069566790155362	0.2977003692223373
0.4211355706684787	0.0300427734991308	0.6587936653404515
0.0913633675096548	0.3654192031513039	0.4683203735974686
0.0300368407642148	0.1985409809369081	0.2983768806116073
0.6835130628198819	0.5331849874160850	0.6430145373522481
0.3640642813232780	0.8599606977858305	0.4621375221973788
0.2795642332714077	0.9700757411834087	0.2658428835619985
0.9569809896251822	0.3156508068154089	0.6108070942161977

0.6252831119501772	0.6439409033799821	0.4424492591983298
0.2265440579497364	0.3171481338153943	0.3772975178064699
0.8877818202102868	0.6437899894557786	0.7114570860095107
0.5565579639376554	0.9874665042916423	0.5422317678363220
0.2678248669361743	0.9760403051486075	0.5299839077776470
0.9277988502526375	0.3058018449938837	0.3436206129011439
0.6000195268618047	0.6597489871323954	0.7572006266617594
0.7591312241580451	0.1957516815145640	0.5355079494276874
0.4229523839312129	0.5284478296652588	0.3650439326781286
0.0958988472921399	0.8654117853968860	0.6976853713128095
0.5465332423402600	0.7154475712513565	0.5627983721089879
0.2148242118259861	0.0587273354446846	0.3850251763800922
0.8703846453340122	0.3897118784503800	0.7280867099769270
0.1814645165202631	0.8097447800213219	0.3768270554355134
0.8529757879283484	0.1378302096822120	0.7102209212673659
0.5139766195153799	0.4683567011429497	0.5427424356094067
0.5260605175774928	0.1899547926865044	0.5284363754592747
0.1945882543768714	0.5221966910754730	0.3491912078603807
0.8571175330380737	0.8654969117852054	0.7028937412392704
0.3042259375860156	0.4632103996226090	0.5332627685677425
0.9700926360310189	0.7935536618401876	0.3625762009662414
0.6335899349943883	0.1349376637487474	0.6987450730267893
0.7850870194389025	0.7282137211883698	0.5574943205902225
0.4385156693325609	0.0556620465531362	0.3842362836087069
0.1137702387373022	0.3825615587128000	0.7282778067548833
0.6898130474053740	0.2720769162559732	0.3771230043404404
0.3637809944996347	0.6174233788623832	0.7113118584524946
0.0290154548350082	0.9424500044975169	0.5425025423257115
0.3047116362462980	0.2300710647462124	0.5282935406441615
0.9770325643323957	0.5717953370773359	0.3481440275332048
0.6291217855612424	0.8959421391248288	0.7030694566560221
0.0349893808741339	0.7405283917018097	0.5326407060417718
0.7043787651082049	0.0763032634067884	0.3642431671760392
0.3805975213164262	0.4065782578858768	0.6924477604097287
0.7723408637579869	0.9565957189261625	0.5580346973925220
0.4434886946038191	0.2826918778788400	0.3866255621984759
0.1175580658141976	0.6275184329668752	0.7285763835672552
0.1393258421129052	0.1452692959695251	0.3295780040009805
0.8093062749474831	0.4803032484101428	0.6734121757841653
0.5980048322586832	0.6230656828995190	0.3216279804026706
0.2542367471777894	0.9553573732914505	0.6522328040957845
0.9252236527095437	0.2906129223107818	0.4948817388432317
0.4691544953737101	0.8124219932618008	0.5097734544692486
0.3530332536333848	0.8940700997154558	0.3286400841581824

0.0199051256594791	0.2311172883461981	0.6746816077328910
0.8754496241961840	0.8755686617568568	0.3196077412853823
0.5449704334806638	0.2011827591450911	0.6505018133393408
0.2091056319197955	0.5341082230480929	0.4929200459356294
0.6872375412695265	0.5579667370516667	0.5138219131314893
0.6050049161751512	0.3594132806725499	0.3308070102280239
0.2658462843359605	0.6869082018354709	0.6727796820675618
0.6236959676758222	0.9008373361025028	0.3203402264124335
0.2983590682489359	0.2447199012269222	0.6509838156644713
0.9645680882160198	0.5742802897201831	0.4924569034855625
0.9404710078092751	0.0304373327515943	0.5115975225808403
0.9315950505689434	0.7903435704916278	0.4841915133997871
0.4730036976769368	0.3063955461942557	0.5030575854907742
0.1446151726844139	0.6455660228342770	0.3469454711691367
0.8002135200264331	0.9780011519075226	0.6771553446331978
0.5875364500865654	0.1187593078421397	0.3224755113664598
0.2636532959215517	0.4540706043088936	0.6636775331425651
0.7099312715028662	0.0422177077051102	0.4862837080212729
0.1894622619751883	0.0639662767506962	0.5004351228287459
0.8539112397713200	0.3988033315431622	0.3457649342539096
0.5140878996261360	0.7358946594886482	0.6747091767486320
0.3808799363717871	0.3689133701701380	0.3244324123478706
0.0470421592059198	0.7044061723438945	0.6636526299330863
0.4589105223779473	0.5675448380631865	0.4881864329252818
0.4338784542231088	0.0257344653689741	0.4995195716330139
0.0997876582080135	0.3543312558933536	0.3464304710292084
0.7913505641181285	0.7026289860862129	0.6738865633713733
0.1295323580262269	0.9111258009064278	0.3217310702611178
0.7951541149437795	0.2411805265505849	0.6657018113617871
0.6998901703417524	0.3003777811026626	0.4978675664238978
0.7004285873340228	0.8007806169528898	0.4989378223659450
0.1988950645685522	0.2981484882916014	0.4980031836427753
0.1998619271630007	0.8009777341926805	0.4979363827158215
0.8692688756675534	0.1281260777839804	0.3340058727120924
0.5209398431436746	0.4466633616143175	0.6515439445207707
0.3723662094548978	0.6421067476507494	0.3354594326085568
0.0299352955908579	0.9599984585415181	0.6640385362572843
0.3660170720973604	0.1331770579086779	0.3098846864439405
0.0333525493467351	0.4655284747957693	0.6842570242676896
0.8556126631487897	0.6289024237583181	0.3345573877510129
0.5398864856751600	0.9750443914805520	0.6634840181653757
0.5413185839890075	0.5877154424364278	0.7678521360503829
0.6198453967244947	0.6970930480697090	0.8046000755725047

The perfect Rh₁₁ doped c-In₂O₃(111) surface

O In Rh In

1.000000000000000			
14.4442996979000000	0.0000000000000000	0.0000000000000000	
-7.2221498489000000	12.5091304781999995	0.0000000000000000	
0.0000000000000000	0.0000000000000000	17.9855003356999994	

O	In	Rh	In
72	41	1	6

Direct

0.8429951473932705	0.6133972114326701	0.4561902481338506
0.5153837125177070	0.9524656281671411	0.2897957095500316
0.1727929364298390	0.2829879863282423	0.6207951087330127
0.7925994406385073	0.9609994036266417	0.2973752208017680
0.4748852646018101	0.3017801928317078	0.6422725821377420
0.1333812393427218	0.6255436086643706	0.4693358965134689
0.3012435451415245	0.7318723379579103	0.3004758096818688
0.9768384163407973	0.0701917722068007	0.6366467552976952
0.6399348302272000	0.4055565940899382	0.4657154654173203
0.5286276535652854	0.2103694073952572	0.2710546874064632
0.1858495959509545	0.5409421115919704	0.6107997355643318
0.8563904408833064	0.8831129749616604	0.4409601373536490
0.8866022051921411	0.1286714843355470	0.4564617604860166
0.5465714146394686	0.4623256833948280	0.2900430630565314
0.2183750858182271	0.7919053863881433	0.6211100086959781
0.5389722764013802	0.7313456188375645	0.2988923094810655
0.2062486085256843	0.0788314826220250	0.6520280045489706
0.8747736916179333	0.4079974519103214	0.4691480952566515
0.7674796236381790	0.4688058131366685	0.3002182025484047
0.4287639458590853	0.8062416839100742	0.6358590672432015
0.0933711804662652	0.1347425372654562	0.4654448931925586
0.2899890286377668	0.2188511055786559	0.2710488134317495
0.9591554658032874	0.5435315904512741	0.6108068375727201
0.6176067694279991	0.8739325745340571	0.4414716880362485
0.3717222157358739	0.6587512709576266	0.4573025134437406
0.0367949332417921	0.9844498264720813	0.2894561491647350
0.7091211365933707	0.3282502928711437	0.6207351887508274
0.7670070655439861	0.7066744628041853	0.2993164531571839
0.4223833061844050	0.0306693457164128	0.6550880949487747
0.0922254345336202	0.3671003531551372	0.4693355562420617
0.0306794432525634	0.1990073705907301	0.2996725615138608
0.6925439147884522	0.5246886277160335	0.6351213712662371
0.3647859419188590	0.8593327203780067	0.4655877798943538
0.2810404490987748	0.9711214940293706	0.2704646466261804
0.9563083019026555	0.3155472120783909	0.6110636144856771

0.6244407525665424	0.6400326508201228	0.4434590314561608
0.2262569947276750	0.3176845334963214	0.3789312000556671
0.8839218500715040	0.6472264596726283	0.7089530506893856
0.5583091262692337	0.9867120732033398	0.5440554897284493
0.2673228268940838	0.9750863305876069	0.5307404932679056
0.9281588039880855	0.3060975522152137	0.3466280369310082
0.5988042332631575	0.6266988276711852	0.6965545309853336
0.7594939127923984	0.1949687856370904	0.5346840238243461
0.4231292885703714	0.5288407913338599	0.3665594121941643
0.0988986535735173	0.8684130276694969	0.7003604999657480
0.5438678378363847	0.7184428613718994	0.5586462315861183
0.2146832397963825	0.0589656205512315	0.3893044576531812
0.8710388768249114	0.3899804805465828	0.7294155120163611
0.1817684847224708	0.8091558955213012	0.3793174911880723
0.8520842459360478	0.1366590879353481	0.7099478075329112
0.5182405736461537	0.4732491081905720	0.5516719605254288
0.5266775333920874	0.1908399631318956	0.5303034961511435
0.1945025631606438	0.5222767187744615	0.3473496407380124
0.8584552929836293	0.8659046664111875	0.7022012013311323
0.3062885463102140	0.4643247664730273	0.5339743813395774
0.9706375151387784	0.7935871799306624	0.3637139598229615
0.6319928829117084	0.1315676362356842	0.6996356735899339
0.7846541845481260	0.7281631535062996	0.5579618175298204
0.4402794237252555	0.0557961152447861	0.3889272281137905
0.1113047600270585	0.3816557086340674	0.7295622747532601
0.6909743012295242	0.2727851184394678	0.3792662487096434
0.3616201017024253	0.6158270558672391	0.7120097711057978
0.0280510493385237	0.9415641970763267	0.5437771373296841
0.3062415406159445	0.2333813580223908	0.5291887093573678
0.9779681706039044	0.5716413572921047	0.3459518360875399
0.6306867148493005	0.8902522740422213	0.7021895617375691
0.0356207791130773	0.7410280018081588	0.5344770873530394
0.7062025681001977	0.0771555797868084	0.3642727723904539
0.3774011081439462	0.4060488329635064	0.6948562645632846
0.7738102881693495	0.9567796780128356	0.5587449564177704
0.4439771166097983	0.2848848773042247	0.3908575628329143
0.1183109302188118	0.6290200299857513	0.7292441599836236
0.1396424919806153	0.1453922623528415	0.3331631911366643
0.8113207880032700	0.4813894074177609	0.6746565773826899
0.5979608546739038	0.6223127686722049	0.3227066337627182
0.2549651811445419	0.9555405993610130	0.6524967045362056
0.9252716451979202	0.2905779786888026	0.4950044361320009
0.4700000768299258	0.8113172094908476	0.5134219430941680
0.3541208559567939	0.8944031956527362	0.3330467997868302

0.0189496085539058	0.2308783569202580	0.6748629874160872
0.8761529167222010	0.8754790754042387	0.3211149621017012
0.5463498767026250	0.2022733567229618	0.6513887010582613
0.2100005607009008	0.5349382017893778	0.4947622071892209
0.6922188735293181	0.5598100061128379	0.5141152490309651
0.6049492493001219	0.3598717331898057	0.3342872384833249
0.2689473540776652	0.6884589122766391	0.6747059050625013
0.6245202786125366	0.9009985050646687	0.3213525333723184
0.2996245816479188	0.2470629025594613	0.6507734796531959
0.9658260185309969	0.5749014639380126	0.4950576217793827
0.9405121470027337	0.0300673188596211	0.5133773070098983
0.9308739831143411	0.7898127588128953	0.4864371487224187
0.4751273366175264	0.3085921310227396	0.5076782010874239
0.1451692933705522	0.6456292157128423	0.3476417938325601
0.8000792043882947	0.9755468399506306	0.6789160329223366
0.5879035238714042	0.1188282908356631	0.3255196120030451
0.2623221290232307	0.4555149604453591	0.6668419113063714
0.7108244409546787	0.0412482000064402	0.4869956841464946
0.1898979652957897	0.0652172936016212	0.5053989194761760
0.8544373675050211	0.3995669658748056	0.3474001890791483
0.5215695676683658	0.7208406460791870	0.6783535505617526
0.3809381296459554	0.3689219600148604	0.3267922321354474
0.0453737854035895	0.7057139502926871	0.6663573192061862
0.4598167221627487	0.5706953836299720	0.4898244165207755
0.4347750988114435	0.0248176210327387	0.5046975620261469
0.1002139428883755	0.3549846132942823	0.3474443759895096
0.7723688666032030	0.6965996058774853	0.6778003972714985
0.1306085893000542	0.9119734164863227	0.3253854711060145
0.7947237962973652	0.2403389945971010	0.6667998753323442
0.7004938053492775	0.3004349349217282	0.4996659838329079
0.7004310922842429	0.8001154226458862	0.5001179941688061
0.1990654055619178	0.2995693088226060	0.4995465133084233
0.2002267794091006	0.8003553238278753	0.5001405620412009
0.8702846479552967	0.1277998352495215	0.3351808758397812
0.5325265881167729	0.4681259364309731	0.6616111566308273
0.3724411175812888	0.6423244489378150	0.3363211966159339
0.0266152003269709	0.9563816401295937	0.6650388843188531
0.3664228795476444	0.1333742746833805	0.3157415388197700
0.0337543385470123	0.4667287333511924	0.6848404985661429
0.8574212369497271	0.6293880565814756	0.3350440941846698
0.5423592460549974	0.9701530336213131	0.6653525174854049

The perfect Rh₁₁-O_{V6} surface

O In Rh In

1.000000000000000			
14.4442996979000000	0.0000000000000000	0.0000000000000000	
-7.2221498489000000	12.5091304781999995	0.0000000000000000	
0.0000000000000000	0.0000000000000000	17.9855003356999994	

O	In	Rh	In
71	41	1	6

Direct

0.8427777684636694	0.6135718203946008	0.4565295542072229
0.5157375022519645	0.9527075198526506	0.2892253620154666
0.1719467619636791	0.2821057368789276	0.6203171239907171
0.7923678369038203	0.9611679770924947	0.2978859950645423
0.4719226958093884	0.2986176468958281	0.6445570895835689
0.1333545729425302	0.6252596445099655	0.4689414462823938
0.3015538352501349	0.7315958181516916	0.3002398263182890
0.9766828695861812	0.0702161173969803	0.6364960041233373
0.6396903814163595	0.4058304265475335	0.4665944071386756
0.5288712432383547	0.2102864039492238	0.2702167486793590
0.1850649308309623	0.5402799428472359	0.6107888253330284
0.8568726678423834	0.8832904013148261	0.4408118772403191
0.8865256264720185	0.1292959864100406	0.4568071939521064
0.5465990180725178	0.4624037302905832	0.2897763377720683
0.2192578491229082	0.7908168649683724	0.6203583795613170
0.5390826447440550	0.7312559981965683	0.2992542470286573
0.2051352432075625	0.0761742077936473	0.6537186397704294
0.8749293358130544	0.4078401162691909	0.4687625933004596
0.7674095317528585	0.4688108761061728	0.3001637162376705
0.4297563381566970	0.8050619307479829	0.6360631888081726
0.0935720691011402	0.1343669653322256	0.4647773133490885
0.2901335935114138	0.2190467068154560	0.2703530754632840
0.9584980110631459	0.5432683476271386	0.6106906380139734
0.6172302469223185	0.8736721544357641	0.4419478476462398
0.3719940091642984	0.6582438194435156	0.4579498175736998
0.0367814960307436	0.9840762894753514	0.2885781805569070
0.7076244175079339	0.3310299594291494	0.6204898351088796
0.7672839544594979	0.7068205781005277	0.2990478648605808
0.4222216877443682	0.0296712896638579	0.6571648083047708
0.0921141591231296	0.3667400064965931	0.4691383073684015
0.0304412675026329	0.1986345093582270	0.2997656760499223
0.6887064111518826	0.5316464245688872	0.6394600086175413
0.3653458692373874	0.8593416534207602	0.4649661105536204
0.2809954796098194	0.9708122584426454	0.2692019627089002
0.9562869855643188	0.3161960331908199	0.6114701193449241

0.6250737057047809	0.6402703656169842	0.4436236516061423
0.2264887617386884	0.3176467222437381	0.3785675680645683
0.8859667585157978	0.6465966596768152	0.7093005538121779
0.5578857191154090	0.9868461744519271	0.5443563269666069
0.2679179038348295	0.9750200961752171	0.5308487664388073
0.9280169057324513	0.3060601216433636	0.3454320848132559
0.7593009454586092	0.1957422481293483	0.5355815984971448
0.4234154929853172	0.5286789348959476	0.3667847155617591
0.0985367777347132	0.8665960233405346	0.6995194228260667
0.5457978950917262	0.7173578096909603	0.5595038961550604
0.2148989869790528	0.0586966413012411	0.3880438376305858
0.8702601246201853	0.3904727764307864	0.7294763634225484
0.1821873386428225	0.8092198425164469	0.3785816841139921
0.8526434487191621	0.1378322444096693	0.7106098166948932
0.5174835842846971	0.4725042934878911	0.5504288550721399
0.5260722557908035	0.1905256630577600	0.5310005966416443
0.1946417802444887	0.5220927491623487	0.3471603029169109
0.8605204499676232	0.8679685332952696	0.7032209486843908
0.3060515564702077	0.4635487535976287	0.5345304399762512
0.9709953961363690	0.7937334273717975	0.3635625074442260
0.6328617402325762	0.1330961660559993	0.6995894579260007
0.7863118567971563	0.7292694445861265	0.5580097616207335
0.4399216886004481	0.0558292746342937	0.3880146977268767
0.1109272872653887	0.3812233603148376	0.7299143336927462
0.6904555135310848	0.2730429193310374	0.3792574113969144
0.3615863861407261	0.6136497019105102	0.7115647117397265
0.0287994918737678	0.9419658021752951	0.5435469845682150
0.3058179157673046	0.2318861859680188	0.5295708992087680
0.9780219682287858	0.5717756295674061	0.3453162679081038
0.6314850395984181	0.8931350563094371	0.7029919697319000
0.0363364227230067	0.7409660528694204	0.5340724625568546
0.7056890277299332	0.0770945919286259	0.3651219346917904
0.3724005519790802	0.4001809987497894	0.6972764653193307
0.7739871439574477	0.9569385987196407	0.5587593236982601
0.4439489684728427	0.2844256841624034	0.3901815510001690
0.1189395886800259	0.6285182641937221	0.7294632087183874
0.1395850820854472	0.1451770291166907	0.3321677830662689
0.8100844738891646	0.4814835054869299	0.6746354249818852
0.5983334274154574	0.6223832498067856	0.3227746436491284
0.2551364921520969	0.9538574078391033	0.6526578563318400
0.9253511504850883	0.2908743014289478	0.4955362333791848
0.4701486291802949	0.8113239754774024	0.5135057679548007
0.3542624738895459	0.8943351191888173	0.3318973132400861
0.0184513885442752	0.2307379218419179	0.6750940078622575

0.8762231738469799	0.8756898135868052	0.3207124737387854
0.5457246147739269	0.2016018174694450	0.6523705088798770
0.2096694850763743	0.5345112249641040	0.4947914163980727
0.6917494917352033	0.5600749207609721	0.5147445408514852
0.6048840562992337	0.3596822061748922	0.3334213829334357
0.2692658127081751	0.6876432436170282	0.6746435945927085
0.6242633434209640	0.9009409219474958	0.3216931873831101
0.2957638223098391	0.2426384455171889	0.6511000083920319
0.9657965136157096	0.5747606033723426	0.4948508340064682
0.9408170975563301	0.0304898232168113	0.5132272720185520
0.9324055373573175	0.7904610810802902	0.4857064666669817
0.4744154157518639	0.3074742454777424	0.5069291197977256
0.1452077622163920	0.6453999728789510	0.3472201981018897
0.8003474004627550	0.9769984019450990	0.6789899649221288
0.5880446090318967	0.1189441705057559	0.3252315815246100
0.2603033954809604	0.4540555275313377	0.6663305728084666
0.7106582176832359	0.0417699599583724	0.4876294645895606
0.1899383690520718	0.0641473687648767	0.5038043123624697
0.8544881094655600	0.3995868255028718	0.3470364476496224
0.5218762166387844	0.7232153010181541	0.6783594013186953
0.3810390129980950	0.3688809172984870	0.3264257616133998
0.0471536467325443	0.7049999987284447	0.6656777529214397
0.4595049167997305	0.5702417539964018	0.4895769110375915
0.4350648006969581	0.0248470728563940	0.5036493931372502
0.0999997536348267	0.3547976979660317	0.3471434637519449
0.7819125604235814	0.7017944575169583	0.6765298640375507
0.1306497880896485	0.9115555207139719	0.3243214242967860
0.7948173280984009	0.2410954694890071	0.6672120866310948
0.7003548708976219	0.3007663391351594	0.4996865573421279
0.7012305146761686	0.8009060570831251	0.4995428506546614
0.1990421664634404	0.2990761385480666	0.4989736880196437
0.2008458083408938	0.8001058424498800	0.4994086476385100
0.8699123508188893	0.1280285693289767	0.3353733384455050
0.5218022371522241	0.4627503031525870	0.6606842912474120
0.3725154791272194	0.6421793090001059	0.3364887612037075
0.0287947823787274	0.9578595817716563	0.6649579695582896
0.3664614540020927	0.1331735726128545	0.3142895334669267
0.0331019723610721	0.4664004857635616	0.6855064917215827
0.8574329962302694	0.6293823468303489	0.3350427146333953
0.5419234700717921	0.9709862288932073	0.6659511784665635

The perfect Rh₁₁-O_{V6}-bt-CO₂ surface

O In Rh In C O

1.000000000000000

14.4443000000000001 0.000000000000000 0.000000000000000

-7.22214999999999965 12.5091307398835685 0.000000000000000

0.00000000000000011 0.00000000000000019 17.9854999999999983

O In Rh In C O

71 41 1 6 1 2

Direct

0.8409254182705290 0.6141109757976276 0.4566997232364212

0.5154759116852123 0.9523995413900704 0.2893555489909997

0.1715436198788450 0.2815383497026996 0.6198272881301607

0.7928634230051611 0.9611350001112836 0.2976804189057740

0.4764842728302038 0.3048897331637569 0.6494015124954766

0.1341232416733504 0.6268079613739026 0.4698942754906651

0.3012431181532663 0.7318286303861326 0.3005778275405194

0.9763116984703287 0.0704049748298488 0.6362402764713632

0.6423632356256204 0.4054690216009255 0.4628467167112655

0.5295559382897921 0.2101436458261903 0.2690316499862253

0.1862340815929341 0.5424177199375199 0.6105240155137016

0.8566849551639083 0.8835986462853189 0.4410672838133952

0.8863487808383840 0.1288645856070233 0.4564386665172754

0.5482813656236226 0.4636361604019239 0.2900466180463086

0.2189946338636100 0.7929320087362129 0.6210521355768681

0.5394722159875924 0.7325863785747231 0.2982401168695180

0.2070629698718966 0.0796969195495593 0.6538073517677883

0.8748223042632989 0.4081154004968833 0.4688355575722058

0.7691091013969960 0.4692200576470732 0.2990040987696418

0.4283903134644270 0.8092825507376379 0.6362630733782909

0.0936328887464930 0.1347516769158483 0.4643510647761204

0.2899339047035530 0.2194316289003595 0.2691729000176171

0.9591629346175400 0.5444622680932688 0.6103618364833500

0.6167433127565577 0.8740453174090421 0.4423047981297302

0.3742708073873710 0.6592656422514344 0.4578592691728469

0.0368621308294608 0.9843812334756368 0.2887173488703554

0.7093325078572275 0.3303153127861923 0.6200010913402062

0.7677938468756955 0.7072157410511312 0.2980095704338644

0.4229757100385796 0.0332290238126195 0.6562618329846898

0.0918239961669857 0.3664300341906612 0.4691483956127556

0.0310016700216404 0.1993458567415992 0.2993584160396467

0.6936132456174978 0.5292174730085017 0.6354902123101775

0.3653700519670715 0.8603776287899353 0.4656403111797500

0.2812444898727846 0.9709934056446874 0.2693660251016644

0.9560979660652871 0.3163128083673468 0.6106682534019864

0.6263481417438557	0.6457851087666627	0.4421083886984840
0.2273072546587134	0.3179376951697742	0.3784914192052322
0.8872057063937863	0.6470187652305965	0.7111015774158731
0.5581829618103477	0.9880729424291280	0.5441363159001490
0.2677634436311648	0.9757564562379130	0.5307234852572709
0.9285830431723375	0.3062233244280698	0.3461771808169579
0.7590631819162617	0.1956716320267727	0.5345371095489014
0.4233287681793487	0.5293686156528880	0.3646230444989249
0.0988191730976422	0.8686917923991058	0.6995537071459578
0.5450675428033950	0.7171717101363030	0.5623184745774058
0.2154614857339141	0.0594591386484857	0.3878339133992709
0.8712958448357785	0.3906720456803387	0.7290504205565023
0.1824781904649211	0.8101463414780604	0.3790353370205793
0.8523175477565840	0.1377016089262650	0.7096582134938563
0.5131371646204850	0.4677577593586426	0.5402611632746489
0.5249815512528804	0.1931680956577171	0.5313064626108666
0.1948240967135885	0.5228314928549102	0.3493428546455839
0.8600644897289681	0.8674484993413570	0.7024194197255300
0.3040612919639814	0.4642796972954630	0.5337316035819735
0.9708339670574514	0.7938484833658025	0.3637078874208319
0.6328153968647982	0.1346482129153411	0.6998062849700738
0.7837862213363058	0.7284700965781513	0.5584134347614328
0.4408517451206043	0.0566271478557932	0.3881269706105095
0.1118796597259600	0.3827952146981473	0.7284440683742013
0.6914482802464467	0.2720726119450839	0.3781264770021569
0.3624291526058385	0.6171870238306976	0.7120558002800356
0.0288852654523727	0.9423370553202148	0.5434836642124030
0.3065376603426285	0.2317719154861860	0.5294298287819872
0.9781049130366127	0.5724753938386657	0.3483121435218553
0.6310571065982399	0.8934124046652264	0.7030230867762305
0.0356052319881387	0.7415339663890728	0.5340995112949525
0.7060734117042404	0.0765763651599149	0.3642421031513181
0.3731503233348453	0.4047118090661667	0.6934089584776761
0.7736281137219909	0.9574186690177932	0.5588578558507761
0.4439439499292158	0.2832817286352486	0.3873807615998687
0.1184566345625754	0.6293770045375909	0.7294400898049902
0.1402161867635242	0.1457660078592122	0.3317099973724468
0.8112459993924691	0.4817794255236283	0.6745513990083332
0.5987834206679918	0.6238431213697081	0.3219600597948253
0.2556453615689890	0.9568000182559443	0.6526815176206900
0.9252518190865312	0.2910132384639238	0.4946529546968667
0.4702226706409915	0.8118205638082671	0.5133790524025497
0.3544937405061812	0.8948898213552228	0.3324513725679074
0.0191748018794929	0.2317876639031557	0.6742349932293162

0.8763821338545221	0.8755234219406894	0.3207918900673118
0.5467571223855243	0.2058489326802627	0.6527269565081542
0.2098601180153580	0.5351498400717001	0.4939857383134923
0.6866599089409168	0.5578371133418122	0.5126762346351275
0.6061821070546716	0.3599010776604081	0.3322857189035510
0.2681808650247886	0.6888749227278795	0.6746877248975333
0.6247265794238878	0.9012557945623557	0.3214722643495503
0.3002541613324171	0.2475848475869382	0.6508565567839626
0.9650894145847134	0.5753402245090816	0.4942481642043163
0.9409997066018501	0.0305901357655981	0.5127931939464417
0.9305817995422928	0.7900456571089088	0.4860498925498285
0.4746063853013066	0.3104022684943260	0.5032872966702756
0.1454287023192193	0.6462739184198408	0.3482023355849315
0.8009934547696905	0.9771552269622136	0.6785662926126308
0.5882781789865252	0.1188309064243263	0.3244198805701918
0.2618841334245945	0.4556106575044277	0.6646413960952632
0.7107227103823333	0.0420251000668362	0.4869195429351238
0.1903268079032023	0.0652739046153238	0.5036404009703392
0.8548082786271817	0.3995796565105166	0.3471477080401722
0.5182525048971881	0.7283066477071024	0.6790354399287688
0.3817386640478591	0.3695714791858759	0.3250898209681272
0.0470232019448470	0.7063956751289000	0.6657109510302175
0.4593887838149830	0.5677232698357212	0.4888445868529540
0.4353407010751380	0.0269059583722507	0.5038717514402229
0.1007629101868340	0.3550856177792174	0.3475716815173670
0.7841198125387510	0.7014392950201732	0.6761319463599824
0.1307414733113688	0.9120978994994844	0.3245971209552229
0.7950217224146223	0.2416810982102065	0.6662473588819090
0.7000572748474637	0.3008413769406253	0.4989699259796510
0.7003527683972459	0.8011165821217696	0.5002665104034381
0.1994813608648704	0.2993373886575724	0.4991865696082430
0.2006431615314606	0.8012734166391310	0.4999339242613546
0.8705313514002018	0.1279737232810881	0.3349823197800286
0.5334799287528658	0.4678865089850156	0.6672235415010815
0.3732801368771743	0.6432023028975918	0.3363359283933544
0.0295720662200979	0.9597209790715489	0.6646655061824156
0.3669582064931263	0.1337706133673694	0.3132670852551041
0.0337234369157626	0.4672902825874535	0.6846697573244507
0.8567121348965353	0.6294229520952216	0.3352926274462668
0.5422078385557283	0.9742329674907052	0.6651728098895202
0.5708863858644577	0.5350437841304424	0.7616833648210999
0.5769813028220978	0.5374875055423701	0.8276888257612002
0.6023912444731756	0.6294039087506205	0.7117756791674339

The perfect Rh₁₁-O_{V6}-[CO₂+H]* surface

O In Rh In C O H

1.000000000000000

14.4443000000000001 0.000000000000000 0.000000000000000

-7.2221499999999965 12.5091307398835685 0.000000000000000

0.00000000000000011 0.00000000000000019 17.985499999999983

O In Rh In C O H

71 41 1 6 1 2 1

Direct

0.8418441607944394 0.6153884840261522 0.4568633488951508

0.5160854412487600 0.9547897709717266 0.2882841623906212

0.1702470534630502 0.2810785107459393 0.6178153139981457

0.7927033824835241 0.9631857398578687 0.2974519880007407

0.4751544070706087 0.3039394910541222 0.6446567843128590

0.1343541535091245 0.6288259191482219 0.4700588765652585

0.3010726971687085 0.7329054733310124 0.2996424746999265

0.9769499697946212 0.0732163293414176 0.6349474743746811

0.6399808061937962 0.4079375580269210 0.4668049110561986

0.5294814962934763 0.2125493843475764 0.2700556512793699

0.1975582921926662 0.5502298816878753 0.6106443755870130

0.8572767313335777 0.8855371208062660 0.4404502033071445

0.8865092295839547 0.1309810401444662 0.4565740025524401

0.5475336160045208 0.4644125376270332 0.2893179932026522

0.2191770953753782 0.7972488088850171 0.6197062869998798

0.5395516876091417 0.7333640385258233 0.2979759688509460

0.2068096455335432 0.0814657384371590 0.6588255907771631

0.8742850391988835 0.4093039735602373 0.4697578107805013

0.7679215620862763 0.4706651475109683 0.3002704022603656

0.4289100056403007 0.8013501868865077 0.6400830724149846

0.0932176410490185 0.1351103425295865 0.4621730090168851

0.2910788557705065 0.2214062619549579 0.2687027650290979

0.9617801906039481 0.5466073170056807 0.6108364356695916

0.6173106386655706 0.8762157866699390 0.4410747135358991

0.3734164762503378 0.6599494760044113 0.4566707092554583

0.0367451741929788 0.9856343598458046 0.2868099007710224

0.7097440965670634 0.3311197942698491 0.6215864096185867

0.7679061426014896 0.7089586555506914 0.2982115733854475

0.4226995755740035 0.0318936968578867 0.6591265495051596

0.0920118603531786 0.3683420473690491 0.4692852911392487

0.0301413367368288 0.2009406369807582 0.2984207812157449

0.6929647704337955 0.5264259046731988 0.6370279231451107

0.3648727907025854 0.8613375561410601 0.4658646623688046

0.2814089413647584 0.9726651891215443 0.2676390394046933

0.9579595750556312 0.3199715475416042 0.6112785450502861

0.6257521275476569	0.6437805200900434	0.4423272321076729
0.2262443966576583	0.3193127636370355	0.3767647947743829
0.8848793342327310	0.6496288315893259	0.7086738686858122
0.5561895643972872	0.9862025515504701	0.5458745020597950
0.2688019348544893	0.9793760565924994	0.5311527335973482
0.9278335938363310	0.3079273274005116	0.3461538582292872
0.7591297421470292	0.1965455413024720	0.5361111776333203
0.4236530841272418	0.5302713520419564	0.3658144054082043
0.0986662133650331	0.8701007519398186	0.6998078365724335
0.5438723440139216	0.7209128392248683	0.5577385635516131
0.2154721586415756	0.0607619093883869	0.3856731431722569
0.8733411105325901	0.3935072709602762	0.7301947537137821
0.1830045912653488	0.8122800439890194	0.3781047153967795
0.8543521007465962	0.1410019338093269	0.7110271115383681
0.5164250481076003	0.4765016632213126	0.5520668778007037
0.5253174628088481	0.1931803923884851	0.5317213839028223
0.1948556911835350	0.5244031651638154	0.3500628270397589
0.8605644278132719	0.8705139889310136	0.7024347909384996
0.3046215487070777	0.4641014710112035	0.5322852512188344
0.9714362483821107	0.7960541699241994	0.3637043659512115
0.633554686496161	0.1348908753719939	0.7007744982522208
0.7845406995352868	0.7300622615774074	0.5579885652717208
0.4398648525683876	0.0570604219213715	0.3874058078941625
0.1155182262763494	0.3864754474804497	0.7269159804934939
0.6900546608589686	0.2745560248944248	0.3799649649026375
0.3676816069622258	0.6163511709335197	0.7212910813649404
0.0300738928401471	0.9447999460795914	0.5434011230525480
0.3057948774957850	0.2330015246200220	0.5289302052760700
0.9779667614225284	0.5738513912329182	0.3485448458811813
0.6337203393437748	0.8977086453708135	0.7033546522520173
0.0356805467090487	0.7430900230826502	0.5343187194913883
0.7055952609098509	0.0790043873572366	0.3650216481390152
0.3721750200302070	0.4061449935721613	0.6923061485230122
0.7733321428767130	0.9582444235769750	0.5585831624900510
0.4440083859144790	0.2867517556168999	0.3902798307885205
0.1204254185537425	0.6324987735749088	0.7289297885971485
0.1396358828599321	0.1471061221763212	0.3292810910772185
0.8131558056822800	0.4838577951336984	0.6748960454040751
0.5989599516871481	0.6246181273608327	0.3215492179171078
0.2556284749692696	0.9599791662916891	0.6534229517369177
0.9249548940985256	0.2923263269944127	0.4952021815171796
0.4699392047540271	0.8127312383625505	0.5118314915646232
0.3545359839008118	0.8963713811836707	0.3301289922652386
0.0189500155779215	0.2331323872633793	0.6742107207116443

0.8765571791642649	0.8775429620293982	0.3200639323530153
0.5468349956112669	0.2038804040383709	0.6525882180219944
0.2107743051551695	0.5373559936294313	0.4914106564852012
0.6896130356209601	0.5616687935376985	0.5145886575238855
0.6051453179782826	0.3616647182119796	0.3337058315039365
0.2676475435435415	0.6961105245225110	0.6729138732458052
0.6246686420896735	0.9030267099261988	0.3207065696571532
0.2984857550362001	0.2470428796958582	0.6498337390452636
0.9656092197655994	0.5768991375916390	0.4939491813638030
0.9410104782783064	0.0322548646607579	0.5122413723352671
0.9311565348298002	0.7920732688572093	0.4861082969345948
0.4754161396392713	0.3135119037487703	0.5072266332982863
0.1453992336719283	0.6480896890680909	0.3477212968774672
0.8031383218412323	0.9806970730744097	0.6782451482134984
0.5884707754388839	0.1209794874715732	0.3248510585700603
0.2582568956883103	0.4507446818899520	0.6573498897333673
0.7102882111834519	0.0431195796289084	0.4875716633825734
0.1899816065259602	0.0659525126796208	0.5008605116607823
0.8539337410580512	0.4010825754171068	0.3476911038514898
0.5335575425881846	0.7323105996488766	0.6757187900458995
0.3817221689779856	0.3708769349858322	0.3253338561349689
0.0452442462590864	0.7093372766181225	0.6645815170869962
0.4606001573712754	0.5705287917966118	0.4887358665823756
0.4354330607188381	0.0276732256572329	0.5030334307643619
0.0994404134508273	0.3565440111155724	0.3467093530698688
0.7764057506231934	0.7021021908140544	0.6773638326330375
0.1305383678443013	0.9131680033590641	0.3224675652174305
0.7955415847798695	0.2434297030822460	0.6676296053942146
0.6999982629737679	0.3023823437689157	0.5003244716861658
0.7011798050211179	0.8026876218468577	0.4983998714584778
0.1981685442002020	0.2990050175850488	0.4964280536310091
0.2002956830083514	0.8041854562051024	0.4987703298284221
0.8697952598347712	0.1297522584539098	0.3349551646381293
0.5352577295925777	0.4675173684544088	0.6688979432861560
0.3735581997296870	0.6443373062432699	0.3354343951527692
0.0285575993336885	0.9606898488188116	0.6649715623929718
0.3669337688457084	0.1352638962479467	0.3132233875315497
0.0349267307283413	0.4698171732715553	0.6849347094975975
0.8571714920010762	0.6314549161429857	0.3353949917326859
0.5415570115184057	0.9732276571461888	0.6668845462010076
0.5528745418036427	0.4557802926207942	0.7687835763830028
0.5609927732312533	0.4493899229386141	0.8323038428829744
0.6048453724771247	0.6369979768517975	0.6959328931535961
0.3666807166468646	0.5960299496005680	0.7728707270927163

The perfect Rh₁₁-O_{V6}-[CO+OH]* surface

O In Rh In C O H

1.000000000000000

14.4443000000000001 0.000000000000000 0.000000000000000

-7.2221499999999965 12.5091307398835685 0.000000000000000

0.0000000000000011 0.0000000000000019 17.985499999999983

O In Rh In C O H

71 41 1 6 1 2 1

Direct

0.8418252568324881 0.6163146294470615 0.4573868814238930

0.5159156888029419 0.9552696845142644 0.2883795455750320

0.1722230257850309 0.2842486272581851 0.6189994040939172

0.7924037536013312 0.9634947738546200 0.2978574566138119

0.4760366167076469 0.3036936479495112 0.6426979721705047

0.1345071160069969 0.6292663928001241 0.4692414836254512

0.3012344158931422 0.7332391219163246 0.2998659036570501

0.9775434373639803 0.0730494377968271 0.6356197507097018

0.6399939629897686 0.4090434765741225 0.4674013566144128

0.5295548912898691 0.2134816095440269 0.2688818385344378

0.1867273499031895 0.5436879338160214 0.6096298428306813

0.8569547533078758 0.8852151358843356 0.4413861493728097

0.8865735301762911 0.1314327645479430 0.4562626559111340

0.5469973806866423 0.4653227998735480 0.2895554764645507

0.2199415307752503 0.7948570630182935 0.6200093101390107

0.5391282525047436 0.7337116377105346 0.2992800311551294

0.2075195919357443 0.0806069999387159 0.6579423197048554

0.8746554238209985 0.4097420183899762 0.4691995119557093

0.7676499906030928 0.4713028421580652 0.3001890463538973

0.4278573556606607 0.8112039765163626 0.6339752381676611

0.0939454300626656 0.1363240323036075 0.4632518323853456

0.2908432448140666 0.2221892430935684 0.2689978251984939

0.9608382631666017 0.5463252624403058 0.6103584401658538

0.6176123435299171 0.8767308518072536 0.4415624158109800

0.3735175898317336 0.6611698773467728 0.4583037690059509

0.0364037585501081 0.9861605250991421 0.2875898074820926

0.7097554075999273 0.3321621760985430 0.6214068402933194

0.7669939488694545 0.7092144111713602 0.2994269696925131

0.4234259082535100 0.0346729409822392 0.6602989769282335

0.0916200586466357 0.3682165314292099 0.4687573844058829

0.0304117406600521 0.2012407554924780 0.2986605742114568

0.6949682274103706 0.5295709750964672 0.6394069761039356

0.3654228284590389 0.8632325232304667 0.4632174555151599

0.2808960152203284 0.9730013627501339 0.2672917399561336

0.9575628371018317	0.3182803203750728	0.6116538003921056
0.6254044689330412	0.6438393630796918	0.4442356770519822
0.2263313256713509	0.3197985288268055	0.3775342180668089
0.8884002931924875	0.6483989769673189	0.7118819263226942
0.5576029593381674	0.9906892344629640	0.5434988616466186
0.2693654430390408	0.9792566370406038	0.5311361028112440
0.9278828237191249	0.3085587875729059	0.3445597303101026
0.7597375128022605	0.1979911231897429	0.5359264503354425
0.4238939328225254	0.5309072895890984	0.3676913197125031
0.0988050423471319	0.8694470969925682	0.6990275771477906
0.5462016347370177	0.7213277345682478	0.5599797388434388
0.2156178103313193	0.0612554688138085	0.3858310533003078
0.8737509641780719	0.3924177280229607	0.7302120488536574
0.1823542077433613	0.8125058308801807	0.3779170881397100
0.8546200891711772	0.1399971942134202	0.7114482344195353
0.5174141798833423	0.4773938223428796	0.5552562917324995
0.5255464895443811	0.1941463141077315	0.5311924807389672
0.1949834955583642	0.5247984118371762	0.3499312132985385
0.8612644464421045	0.8703683412056752	0.7032157146832296
0.3052370934622880	0.4655171155962833	0.5337224839502763
0.9710549251170963	0.7963635815171785	0.3636172271641884
0.6351083622946571	0.1357976178800706	0.7005556100324507
0.7846909192240336	0.7302329643171875	0.5593518125253921
0.4397664536270539	0.0589743180847926	0.3860039589604405
0.1151896993738043	0.3852749710908426	0.7286293197955589
0.6896112833124913	0.2754621503503312	0.3795661127624081
0.3644765390040454	0.6184682829781578	0.7100266246330861
0.0303027531284297	0.9451048273215701	0.5432805262690190
0.3062527435980548	0.2335671620726213	0.5289206518713319
0.9776075121649584	0.5742705328918846	0.3482399554156676
0.6313703556897035	0.8963039509138648	0.7028002589963074
0.0364069167468627	0.7435770372757888	0.5341995311038962
0.7056390294455491	0.0798820704703180	0.3645626859655494
0.3737102905067072	0.4022747893165429	0.6937789594529604
0.7739555187131224	0.9595052915950274	0.5588598092802695
0.4444883178651413	0.2874435321867454	0.3899579225936364
0.1202263014385894	0.6314048270087825	0.7291956822715829
0.1397509253739285	0.1477881474764484	0.3301433435816036
0.8146883946173029	0.4832667298815296	0.6752833489577211
0.5982836559136981	0.6249944980628576	0.3232244631145544
0.2564078729450120	0.9581695159940069	0.6532518817079142
0.9254944397573657	0.2929926353803963	0.4957312517014454
0.4702786764473375	0.8152898239287539	0.5110092222523728
0.3540763906199146	0.8966678334325092	0.3300492464471627

0.0205304572502613	0.2336645791559206	0.6752281776892579
0.8760952847157460	0.8779117665163896	0.3206615919209433
0.5482370541798465	0.2038711286762121	0.6518235293938603
0.2096959534063078	0.5368419670019241	0.4928877684635966
0.6898292067581249	0.5620488898521133	0.5153076720611458
0.6048158786664022	0.3622047704354100	0.3326253997992663
0.2689011735097265	0.6904855525065479	0.6734269899836921
0.6243425638806978	0.9034591848828877	0.3208867001155165
0.2958318382250412	0.2458759792897833	0.6495317068738340
0.9660488509115540	0.5773672644385266	0.4939437090156720
0.9415004785143458	0.0331884349991638	0.5126246250848374
0.9323432713486108	0.7928092921160589	0.4858271982564851
0.4753945219851869	0.3138981487649164	0.5066183721423949
0.1452428421058060	0.6483625523999924	0.3473982488041219
0.8018270329238008	0.9799080320238061	0.6784391194160274
0.5884872082946108	0.1218724817423630	0.3240293845224522
0.2634070277070604	0.4577724557057496	0.6631112607425349
0.7110144530217190	0.0447885485947162	0.4869490714626027
0.1904930516941860	0.0663202681491827	0.5010471703078971
0.8539870690033601	0.4015379859204704	0.3472065110570777
0.5185827033116021	0.7335367577507550	0.6749162009481581
0.3813757593928571	0.3716647170193244	0.3259737379309386
0.0486993589015853	0.7083428523049001	0.6650818037391797
0.4603104123405650	0.5716097530078065	0.4909448181611905
0.4355711211188151	0.0292539397401020	0.5011780160673113
0.0996364525312959	0.3570753791677221	0.3466246347033400
0.7877969613094474	0.7052567688196573	0.6764346340110846
0.1303945528930215	0.9136163712109776	0.3225521492584528
0.7968523433675061	0.2431579851154349	0.6676249565281143
0.7005549470727612	0.3034550853203032	0.4999762047990219
0.7012224195248727	0.8037142810031250	0.4995413162165387
0.1986406478836641	0.3009166391488108	0.4977556176535768
0.2011683310253322	0.8038189393307429	0.4989313599187110
0.8699484798776821	0.1306831022643279	0.3345491477783375
0.5342193784433715	0.4608181202053174	0.6703693384414200
0.3730631227068600	0.6444899376340705	0.3368307089407417
0.0307551026766376	0.9621484838153068	0.6648141817187873
0.3667367131907770	0.1358503299581211	0.3122006483490935
0.0359393130201979	0.4691331064776303	0.6850368449387785
0.8567445819193326	0.6317475392399631	0.3356451709289464
0.5421539162291937	0.9758350548258510	0.6650167366721312
0.5500042112766209	0.4323953719949554	0.7679182862936303
0.5554883344736196	0.4080503347034483	0.8284011798910068
0.6034525824691729	0.6379542639464538	0.7054451127020303

0.5939718881338950 0.6310199972129243 0.7591142115632130

The perfect Rh₁₁-O_{V6}-[TS-CO-O]* surface

O In Rh In C O

1.000000000000000					
14.4443000000000001		0.000000000000000		0.000000000000000	
-7.2221500000000001		12.5091307398836005		0.000000000000000	
0.00000000000000011		0.00000000000000019		17.9855000000000018	
O	In	Rh	In	C	O
71	41	1	6	1	2

Selective dynamics

Direct

0.8411133314316217	0.6141337019463435	0.4567350005237145
0.5155439746105159	0.9524946744561902	0.2893669655768463
0.1716211241737540	0.2816726700617380	0.6198166491003860
0.7928469233485060	0.9612097927362768	0.2979069723460839
0.4767000632793881	0.3050784325077629	0.6488142294408235
0.1340698559789004	0.6267993924245090	0.4698077023452498
0.3013833497078267	0.7318724995565802	0.3006630764445291
0.9764995827785796	0.0706458697161167	0.6361384146092846
0.6421873063748720	0.4054936524132557	0.4629385644029753
0.5295689615895327	0.2102090755886650	0.2691160858546411
0.1861001661539348	0.5424523575723370	0.6104539782356966
0.8567690980782317	0.8836679848449194	0.4411067179513566
0.8863687750549119	0.1290544760382417	0.4565140405619488
0.5481587099344765	0.4635751502128400	0.2900060581918140
0.2189772737559750	0.7930044604623987	0.6210786162971189
0.5394652023182971	0.7325470087060566	0.2985010754634416
0.2071981723940013	0.0798417187877973	0.6541807813519114
0.8748603430822683	0.4082015323459416	0.4688166420976572
0.7690250240503431	0.4693341196483942	0.2991484192254532
0.4284794191369699	0.8090076562054023	0.6361959439762046
0.0936198582877097	0.1347605632200697	0.4643440341429681
0.2900360600178686	0.2195475567049812	0.2691717376026048
0.9592989234805955	0.5444755941528001	0.6104073722821610
0.6167185499374881	0.8740696746072842	0.4423178648292350
0.3741335722859276	0.6591885776539073	0.4579210097541591
0.0369010409121984	0.9844433090558837	0.2888075745294216
0.7092908002854017	0.3302497462755127	0.6200043527289907
0.7678193903145996	0.7073032396042080	0.2983182463826282
0.4229300755680470	0.0331180201394901	0.6564205153084046
0.0916369614631094	0.3664566671327947	0.4691143574699623
0.0309205980921590	0.1992723554256912	0.2994741362897670
0.6934788876994631	0.5289250364452016	0.6352343374684750
0.3653254033863931	0.8603422243322640	0.4656664776510979
0.2811735903732853	0.9710224224741779	0.2693223844487775

0.9560660457306227	0.3163433449260040	0.6108406846492471
0.6261431868419081	0.6454280289643251	0.4421516688666287
0.2271871462200821	0.3179480014373368	0.3784532697225984
0.8869159539862039	0.6471978642501881	0.7107380923407902
0.5580766200853517	0.9880164745505127	0.5440821053839429
0.2677827989251469	0.9759020392200810	0.5307854034349688
0.9285695651466028	0.3063552260040510	0.3458578489470554
0.7590637572288230	0.1956944092664941	0.5346066667753533
0.4232677029465250	0.5292417035808654	0.3648493530280703
0.0987238025888146	0.8687313051132293	0.6994738400879115
0.5450124197349737	0.7170955806118400	0.5620925570479685
0.2155087749470823	0.0595453642952464	0.3877775647056367
0.8711880599524235	0.3907977833802008	0.7291576188681148
0.1825326440013058	0.8101757352333507	0.3790445715482491
0.8524554462566840	0.1377534105292142	0.7097425623058058
0.5133622369267812	0.4679911559652723	0.5411168879863766
0.5249752880836667	0.1929656994208386	0.5312483265725589
0.1947884287536468	0.5228158466752362	0.3492221429699356
0.8601304955704094	0.8676580705857262	0.7021137051911737
0.3039589590317817	0.4642043530968252	0.5336142108030373
0.9709421637245441	0.7939066540824129	0.3638352434517458
0.6328336332793256	0.1343734404268560	0.6997383008695266
0.7836292210909690	0.7283755959105349	0.5583120851820595
0.4407763987075555	0.0565873974905173	0.3880631710987075
0.1118592038258726	0.3828095345196445	0.7285076428104063
0.6914652996909254	0.2721869341240932	0.3781473105107409
0.3623619364427881	0.6170601761798054	0.7118469282481783
0.0289466893387882	0.9424487588226285	0.5434613797087451
0.3065047504206078	0.2317871294233314	0.5293429221575678
0.9781686841922763	0.5725225009101607	0.3480859401499075
0.6311184695544867	0.8932679869135995	0.7027390205452377
0.0356197158043798	0.7415186458109417	0.5341200087887543
0.7060428808453381	0.0766963345981893	0.3644079810360878
0.3733166831878734	0.4049729992010285	0.6929394308498686
0.7736874479291203	0.9574713545394786	0.5587773743508251
0.4439160688499939	0.2834490587590537	0.3875777352239069
0.1185735992401717	0.6295309496661403	0.7295010238226922
0.1402674148276333	0.1458667629972794	0.3317095600150850
0.8112328626337799	0.4818917020997517	0.6744582735989937
0.5987348285130878	0.6237447657964097	0.3220358363611737
0.2556047632402354	0.9568817390702407	0.6527392277270039
0.9251830842613842	0.2910824703296626	0.4948776801572947
0.4701738258323402	0.8117212854804379	0.5134512128607511
0.3544622211009312	0.8949152411687251	0.3323630921709295

0.0192610819539496	0.2317984749320274	0.6743239590218764
0.8764595072301589	0.8756450644006435	0.3208982220412864
0.5467649431404880	0.2056139648827724	0.6526074471923309
0.2097516564632542	0.5351093986169460	0.4939615621026476
0.6869452950158390	0.5580321120225591	0.5126494012458309
0.6061124904623796	0.3599532265596821	0.3323986655895723
0.2683388728054794	0.6889783454310887	0.6746512820324995
0.6247122800597396	0.9013103829619737	0.3215627557621801
0.3003365069612940	0.2476904239886153	0.6506946112155276
0.9651798636506257	0.5753945917628016	0.4943247987929738
0.9409826382358233	0.0306709296266874	0.5127729556450760
0.9305790331964943	0.7900828782832789	0.4862046181093689
0.4747247449757239	0.3104466215271415	0.5035994160360175
0.1454813229482070	0.6463064861244092	0.3481445105216352
0.8009996093041067	0.9771992344254059	0.6785035757856761
0.5883199236538559	0.1188913950319019	0.3244579477370877
0.2617597496987329	0.4556842215503423	0.6645408449028309
0.7106840350068708	0.0420295620748306	0.4870368806115266
0.1903165959236688	0.0653037928166569	0.5035541128249008
0.8548575552638411	0.3997120456413796	0.3471090461180211
0.5187402572087123	0.7276553975620317	0.6790597199369444
0.3816999780203503	0.3695859552727043	0.3251713336081679
0.0469571649842138	0.7064507362199350	0.6658030420189647
0.4594380405342235	0.5678402849476853	0.4890474691802211
0.4352505601033272	0.0267987916894228	0.5038082488564939
0.1006235590778388	0.3550924631926335	0.3475323457905120
0.7831724449341522	0.7013433977891950	0.6762090834142782
0.1307516797485206	0.9121016802175177	0.3245967837278698
0.7950321418158168	0.2416838444747356	0.6664587083688076
0.7000388749989384	0.3008355947572454	0.4989569127876337
0.7003058043316699	0.8010741151363021	0.5001578612228244
0.1993462993252848	0.2993319378393622	0.4991370151239991
0.2006567577815517	0.8012947766316714	0.4999774247503055
0.8704721157683935	0.1281294647744318	0.3350848658628252
0.5338373802274461	0.4684703641477199	0.6667920529307807
0.3732420151371301	0.6430988462449108	0.3364697164316226
0.0295144083015160	0.9597853799003744	0.6646478875971127
0.3669727507802278	0.1338420584477831	0.3133232149390395
0.0337292826507962	0.4673893437378140	0.6847888701636720
0.8568814767378541	0.6295427223260930	0.3353715171425193
0.5421609718616480	0.9738861875181613	0.6651457237267806
0.5662959505545615	0.5240396661014088	0.7619362449676714
0.5730009450337405	0.5284768039567851	0.8276714577864510
0.6032986444132789	0.6305825237934783	0.7083441437139466

The perfect Rh₁₁-CO* _P surface

O In Rh In C O

1.000000000000000					
14.444300000000001	0.000000000000000	0.000000000000000			
-7.2221499999999965	12.5091307398835685	0.000000000000000			
0.0000000000000011	0.0000000000000019	17.985499999999983			
O	In	Rh	In	C	O
71	41	1	6	1	2

Direct

0.8418463829459132	0.6140456475885971	0.4568706895242353
0.5154670144429725	0.9538189113437211	0.2890526847654824
0.1718647693760041	0.2833034172524017	0.6197832514039672
0.7924425173607568	0.9621952277345259	0.2975625477163475
0.4752523652842063	0.3017348284444614	0.6446184142059085
0.1328036224846185	0.6268215790338985	0.4690131033951017
0.3011244432011557	0.7324903850545970	0.3002031609638474
0.9770605582872496	0.0717327458592577	0.6357614428556330
0.6403831294597132	0.4073011313980565	0.4667493616014353
0.5288868278951282	0.2119154277986105	0.2705074748038073
0.1850647700145001	0.5422758133613814	0.6101779141183837
0.8564488280058618	0.8843445900153156	0.4409976205218116
0.8864626343678389	0.1301753221775138	0.4561851158014512
0.5469586905083744	0.4639280473600677	0.2904120799147122
0.2187370603316252	0.7929830064119314	0.6206606418586333
0.5388244656282636	0.7325321771656620	0.2988760830735455
0.2065368023970893	0.0798052651385041	0.6524537293973270
0.8747732360633498	0.4088324504160075	0.4691038471312192
0.7671473223594376	0.4698265593276955	0.3005083772390273
0.4288881510968887	0.8076765704959588	0.6357097162340444
0.0936450140824482	0.1356203633897768	0.4646126543231998
0.2903885133584641	0.2204743057264005	0.2706454163922384
0.9597394840341160	0.5447093652982581	0.6110369156330003
0.6175012360487887	0.8757836861244347	0.4412107407417136
0.3714004246394904	0.6593711797841731	0.4575680065978971
0.0366144306269826	0.9852175237508265	0.2889633816061504
0.7095601427135448	0.3289833081064428	0.6214508447404657
0.7673102100452505	0.7080433532571588	0.2989750047659788
0.4225374729819045	0.0317798656261907	0.6571569051613670
0.0909905503004059	0.3674679964066082	0.4688227580787497
0.0304061589330372	0.1997775056878583	0.2993856683655801
0.6937001245508237	0.5247095401456338	0.6364053177188165
0.3648933940307684	0.8609545485550145	0.4648849200878594
0.2809011931649445	0.9722268465026529	0.2695098660350125
0.9559127741910036	0.3166169140159734	0.6116180950494894

0.6253359712669604	0.6428691877792950	0.4430905058475036
0.2260087371170471	0.3188944633994076	0.3782987577311908
0.8849362924535763	0.6489563104735955	0.7090076419866632
0.5577137372437754	0.9883682547291498	0.5438581252107850
0.2680396294824305	0.9766356333201375	0.5306578745069814
0.9276721629278021	0.3072225486809729	0.3444283107846497
0.7590456112635724	0.1959980482248258	0.5348555699731101
0.4232193211891322	0.5299378426715479	0.3668675214586148
0.0993793059662453	0.8697638683800223	0.6998794537443823
0.5438786021181921	0.7204998654923541	0.5577999702659994
0.2150583354547723	0.0601334854576864	0.3883184193126446
0.8719492570813767	0.3914117324471414	0.7302836972819995
0.1819779663722655	0.8105306679808656	0.3787239283510380
0.8529513353687542	0.1379658252459723	0.7107436429103814
0.5165851871057752	0.4754247042751995	0.5523431886301761
0.5254740575157644	0.1927886624542389	0.5309506572514842
0.1941125492703581	0.5232333146019933	0.3479437222135874
0.8602394431836751	0.8685482295825601	0.7021175781710061
0.3044416831369446	0.4648351435740891	0.5335754679438068
0.9706549920170442	0.7947510053705069	0.3641024326978182
0.6326853180764792	0.1321497098862074	0.7000220626562955
0.7845558141266261	0.7289012141512896	0.5580282252185441
0.4401552762330554	0.0570837575494679	0.3878919627536884
0.1123649862373559	0.3830664151804982	0.7289750353322278
0.6902993992109391	0.2739469620599616	0.3796297763956347
0.3624273150095949	0.6162736716166226	0.7102365089827652
0.0288293357095936	0.9430697827407970	0.5432279209900062
0.3066153803978486	0.2342873797379506	0.5288517997818646
0.9776727468920028	0.5729065955493898	0.3455623743266131
0.6311794064117306	0.8917540449232844	0.7017702350527841
0.0357305062729909	0.7421644167598554	0.5344749468171788
0.7058873238330816	0.0785321593071563	0.3640590577365453
0.3738678843832555	0.4041342015054696	0.6928546796056184
0.7738598382869992	0.9582317480373438	0.5584956972172800
0.4442046455015359	0.2861953197104795	0.3909877566773399
0.1192607825549660	0.6305620661768475	0.7293702871700248
0.1396744043163611	0.1465025463524690	0.3322438311346437
0.8127655269862850	0.4825473445025619	0.6751643462160866
0.5982576118848553	0.6239711071054519	0.3228875983490418
0.2555017583540742	0.9565935148847527	0.6524492771135867
0.9248170867347130	0.2914521600173233	0.4957424540827356
0.4696396462262755	0.8125410343814974	0.5128204261416340
0.3540507184597849	0.8954045566744018	0.3318555339857306
0.0192213929397291	0.2320183328666658	0.6748396333143305

0.8760583928489080	0.8765383661259974	0.3210544577455083
0.5467383727335531	0.2022358672262101	0.6517685102168745
0.2091464539127247	0.5358064420768384	0.4939192980415261
0.6893990070772209	0.5608199520738999	0.5148219722102410
0.6048075680329867	0.3609672762579214	0.3343677627299909
0.2693976798849299	0.6894773973704754	0.6742240867794870
0.6242855135302906	0.9021420866541622	0.3211425066196553
0.2982790543637308	0.2470740230093901	0.6497648279450947
0.9652005909281428	0.5759082655289064	0.4951973539577711
0.9407052048463657	0.0314038056327854	0.5127850388623743
0.9306629797482944	0.7906257329788569	0.4864978030997446
0.4758020829779465	0.3132267072861951	0.5079282128885176
0.1448396329523237	0.6467378675964718	0.3473447231401510
0.8006337141845312	0.9771861495848096	0.6786274100417722
0.5880795675275984	0.1202577426938622	0.3249325742417341
0.2620441559109914	0.4565808236487225	0.6645086092312305
0.7105051308351444	0.0425433612222330	0.4868533478034152
0.1904274170272872	0.0662279794088822	0.5041727467132708
0.8541863818127581	0.4006023622902174	0.3472670180732549
0.5221846756129808	0.7228988018139560	0.6771117809935716
0.3812784888374836	0.3703373694422063	0.3268930973440085
0.0463583113385102	0.7072267659231085	0.6662565924894350
0.4598193702396368	0.5703739828764330	0.4905245497346834
0.4351259812105809	0.0269087224316299	0.5034263138155030
0.0994353605949873	0.3558392415898204	0.3469522917774451
0.7751833075504636	0.6999417318548542	0.6775399565717990
0.1304368912676202	0.9128246054198098	0.3247780920653391
0.7951496613028914	0.2414675288178476	0.6677305823469513
0.7000934186060315	0.3016403615428340	0.5000610029021074
0.7003003158100674	0.8016103811668646	0.4997445924108329
0.1985544048614144	0.3003686688852616	0.4986886910383626
0.2003312362202454	0.8015624362367182	0.4996922259020601
0.8699042837207542	0.1291843445682135	0.3348027338627026
0.5359273012371492	0.4659242741173816	0.6692777345463232
0.3724405511192215	0.6432297324343744	0.3367160601519498
0.0277452193478445	0.9585091287491208	0.6644117187563323
0.3665742925054390	0.1346678395901289	0.3147992957743915
0.0345217481557004	0.4681225807815332	0.6852643872412569
0.8569917627914748	0.6304210512583936	0.3355570555572061
0.5422055741094997	0.9711577956104620	0.6652633459377342
0.5539100352720528	0.4541184658742617	0.7690780660122287
0.5626489442824824	0.4470654819459774	0.8324220224681473
0.6043807606417259	0.6343598479482432	0.6938781116418430

The perfect Rh₁₁-H₂*_P surface

O In Rh In H

1.000000000000000				
14.4442996979000000	0.0000000000000000	0.0000000000000000		
-7.2221498489000000	12.5091304781999995	0.0000000000000000		
0.0000000000000000	0.0000000000000000	17.9855003356999994		

O	In	Rh	In	H
72	41	1	6	2

Direct

0.8431470315038997	0.6131003124191680	0.4557280946570610
0.5154656600330294	0.9523397313010036	0.2887911316848026
0.1726535373176806	0.2829101531843343	0.6201569695272199
0.7923619243873360	0.9609120744490423	0.2971910451956535
0.4748242090059032	0.3016095632363078	0.6413932953286324
0.1329368425906036	0.6252844596136578	0.4686413086743194
0.3012282789573692	0.7314277424026873	0.2996769632880278
0.9767767663315275	0.0701922233110735	0.6359602651528193
0.6398302775962745	0.4052323161369039	0.4651411678861347
0.5287296137460464	0.2102863349087997	0.2700563070332924
0.1853737584261219	0.5406909101223901	0.6104632533847806
0.8562903812616787	0.8830594787517686	0.4404884471086288
0.8865050125028507	0.1289024263621883	0.4560270085459530
0.5465531715615962	0.4622280103711293	0.2897248490566685
0.2182312801049633	0.7916587909005064	0.6205319469161518
0.5388044544487813	0.7310320323772144	0.2985425374702638
0.2061862931647763	0.0786530521662891	0.6509152708066648
0.8750721075131765	0.4078623458318446	0.4684263309267384
0.7673413890203097	0.4687000056103667	0.2998131261141865
0.4286458440797246	0.8062036047135519	0.6353516159623724
0.0933591235933667	0.1345705372352954	0.4646908830583736
0.2899911481607517	0.2189380980686348	0.2703047295829356
0.9592124038019236	0.5434138493942258	0.6107504917233971
0.6173760768106353	0.8737943531451614	0.4410860050049626
0.3712562798879553	0.6583437589564924	0.4569830093425503
0.0366644289761076	0.9841580023009281	0.2888195609889376
0.7089765823245050	0.3281240448262192	0.6202277518466901
0.7671503536829628	0.7066017179284262	0.2987519067216195
0.4222345670551335	0.0308326895404682	0.6559203594722630
0.0917766426956488	0.3668453757648419	0.4687347315809814
0.0304438870319768	0.1985448969453127	0.2993065667246217
0.6925369111866476	0.5245020082471393	0.6342584810987437
0.3647564865042712	0.8590947517504736	0.4647078360296603
0.2807082944615301	0.9708700733554633	0.2691940856584999
0.9560484177832071	0.3155381960334416	0.6111607140425027

0.6244373041847493	0.6398501571753695	0.4429983659770221
0.2261159606294658	0.3176363838915838	0.3782446573335202
0.8837235435668105	0.6472627469392900	0.7084345473381249
0.5578897455321253	0.9866767404778429	0.5436081655351114
0.2676692044553338	0.9750120491650995	0.5300118849087849
0.9279457914278427	0.3059490583349135	0.3447945175058006
0.5985120151230573	0.6262780020206327	0.6955438342113329
0.7593761306880199	0.1948913921993811	0.5344783411622114
0.4230809674641693	0.5285899295782206	0.3662944696687416
0.0989267484269362	0.8684656232775917	0.6997762074308287
0.5437486508042517	0.7183151572769446	0.5579794998748503
0.2148583071194651	0.0588698250762696	0.3884591324755063
0.8706493180063102	0.3900580118415376	0.7293409201567619
0.1819658136659762	0.8091004185427770	0.3784762701914115
0.8522445028698614	0.1366228052761678	0.7099302634156616
0.5179672693967903	0.4728806852295159	0.5508359636743756
0.5265004999471906	0.1903357401682963	0.5296878378102007
0.1942791471191295	0.5220151801212269	0.3467550436857522
0.8584467885578297	0.8658625890005646	0.7015416169497075
0.3058865861299395	0.4641030014221554	0.5335256033920318
0.9707150663037143	0.7935824660812441	0.3635150203492752
0.6320219546583311	0.1315494616577047	0.6992704463289536
0.7846068194856021	0.7280537300619124	0.5573011207291179
0.4399652137228410	0.0554898317868778	0.3876201871137137
0.1113959413149689	0.3815198112953704	0.7293030851092276
0.6908843098443970	0.2726529565115184	0.3786411970397331
0.3617043638483066	0.6156553276215979	0.7112817667448101
0.0282831982183784	0.9416045977876356	0.5430178963766105
0.3062351379341292	0.2334407145614781	0.5283267844896369
0.9780618096010090	0.5716304642296528	0.3443095084966008
0.6305719782046121	0.8902538878291213	0.7016721891026381
0.0356412185253918	0.7409182603163468	0.5341364392407062
0.7057603166127395	0.0769070123027391	0.3640452242240170
0.3774532092347749	0.4058856580403636	0.6940933260734938
0.7737193544788411	0.9568010551934136	0.5582450701896244
0.4439112192395483	0.2843321058930229	0.3901060843060931
0.1184417280477753	0.6291235369711153	0.7291146040152919
0.1395340740441908	0.1451989990339443	0.3323980330541265
0.8110413088278382	0.4813051575229317	0.6741785080849366
0.5980855287211835	0.6222445271375326	0.3223189271065620
0.2550015313520065	0.9554257746581286	0.6518918733160645
0.9251955697769935	0.2904317302947664	0.4952209471773510
0.4697773638721534	0.8111792868395269	0.5129318275225012
0.3539544311851278	0.8941113096474494	0.3315323715878848

0.0189669990422668	0.2307150851469700	0.6746217777379576
0.8760678398296676	0.8753743760562472	0.3206659569448374
0.5461391329887385	0.2020121003333613	0.6508851153987240
0.2094987699393986	0.5347010614186216	0.4944484133991962
0.6921511257595787	0.5595608518114310	0.5133805402383139
0.6049390409175366	0.3596308270402715	0.3335719712552887
0.2689225484898760	0.6883380286141985	0.6742462631223312
0.6242580190377229	0.9007099438464461	0.3209973419364073
0.2995460038709424	0.2469116356602562	0.6498886874268658
0.9657065586449999	0.5746953391606496	0.4951020117919827
0.9404592956422985	0.0300658599278536	0.5127139550339841
0.9309270248314399	0.7897082270445924	0.4860018852617616
0.4750778231476813	0.3082265714733055	0.5069648757767553
0.1450525912374927	0.6453775940846164	0.3468726475830110
0.8000381835825219	0.9756092868901719	0.6784397771287914
0.5879320834992398	0.1187292129608776	0.3246612103933434
0.2622295402818950	0.4553116292882698	0.6661711206368494
0.7105756447136656	0.0411652287382822	0.4867048106154304
0.1900838890094227	0.0651838633239142	0.5045761748614669
0.8546525148496444	0.3996371743886475	0.3465985216442990
0.5216312704381906	0.7209185350516270	0.6775902195561065
0.3809008855839248	0.3687548863152516	0.3264186177327735
0.0454157151252967	0.7057408100129376	0.6662451245826850
0.4595537790664006	0.5703896736687154	0.4894064667845202
0.4347866806723900	0.0246406652230133	0.5032160404123840
0.0997629853650651	0.3547086810696780	0.3467620704411682
0.7722038961554109	0.6965342287396500	0.6770979489982775
0.1305321673812463	0.9117621539211521	0.3247160438857099
0.7945899807327785	0.2402915156193038	0.6668772426088385
0.7005276725187164	0.3002368677850876	0.4990480902918804
0.7003946987953459	0.8000564849466076	0.4995272021560966
0.1988879688007550	0.2994155792689621	0.4987840720145443
0.2002050161344529	0.8001899743813898	0.4994360319367103
0.8699137310878117	0.1278387425945189	0.3346820274061811
0.5324166861278167	0.4678963881582772	0.6607392388591007
0.3721395854119195	0.6418315651345571	0.3360175328627761
0.0265356663056825	0.9563056646435366	0.6642279400704338
0.3663372143857976	0.1331856722869947	0.3144741423919349
0.0336296709677737	0.4666588539927009	0.6850998324259662
0.8577633588328843	0.6293956443263159	0.3344807705436459
0.5419774863657766	0.9701317586568503	0.6650062732903257
0.5919616906174759	0.6463481795345161	0.8643836181108864
0.6422105369224633	0.6815748850076105	0.8842431326431557

The perfect Rh₁₁-[TS-2H]* surface

O	In	Rh	In	H
1.000000000000000				
14.4442996979000000		0.0000000000000000		0.0000000000000000
-7.2221498489000000		12.5091304781999995		0.0000000000000000
0.0000000000000000		0.0000000000000000		17.9855003356999994

O	In	Rh	In	H
72	41	1	6	2

Direct

0.8428534233100469	0.6129717873972244	0.4562032415688924
0.5159864596597904	0.9521550815938385	0.2892394111835903
0.1735947998149167	0.2830319720897162	0.6211011690961541
0.7922023794067388	0.9604156473353206	0.2982602862135000
0.4739405439234789	0.2989357890663967	0.6409368960654023
0.1335570283803293	0.6254532272459850	0.4688171689879830
0.3019233989360515	0.7310027124598614	0.3006759351970060
0.9775685055611278	0.0707671813911980	0.6365748023885489
0.6395570966200840	0.4051579637350745	0.4655088457963503
0.5290850125282898	0.2102886201597737	0.2704726332089402
0.1834232834040634	0.5393889253388524	0.6104335272283063
0.8557190222942044	0.8819364715685011	0.4416280006646453
0.8869865719278126	0.1287609456624388	0.4564068480767048
0.5468055242191868	0.4625427827562856	0.2913788908050973
0.2180058416044072	0.7912555702985776	0.6204700587577225
0.5387912919069977	0.7308126353325157	0.3000724463344561
0.2058827476434213	0.0776634022249579	0.6508494367494180
0.8753881935012084	0.4076866114725757	0.4686218132547414
0.7675883196835841	0.4684481221281085	0.3001465738725365
0.4281329538143829	0.8090892317749870	0.6383837484305355
0.0939171730896623	0.1345537271050941	0.4652669493636554
0.2902853755488954	0.2192862961203911	0.2710875364403465
0.9598227621479213	0.5436523212660240	0.6105730091468050
0.6170550214486187	0.8730945209646859	0.4429129742576088
0.3724105289574538	0.6586122165276820	0.4594078540105441
0.0364229845240765	0.9839916021186867	0.2896795809073724
0.7103150819021253	0.3282144543393692	0.6197894740900578
0.7663560721331923	0.7060925334855085	0.3003851128877072
0.4225788762260695	0.0322219674466894	0.6574832656494494
0.0922584075406477	0.3665540699672074	0.4692790554332906
0.0307101858883168	0.1983794085890774	0.2998782684518452
0.6943961006999104	0.5220081201197848	0.6350434996062418
0.3652724026534679	0.8588277351791743	0.4654817857031756
0.2806581401860917	0.9707580884913535	0.2691929108278936
0.9568056142136326	0.3155931496587135	0.6113280054634760

0.6238405235787251	0.6404022584568384	0.4460376227269597
0.2264152950363072	0.3176326861866272	0.3791036507932886
0.8857723512343029	0.6465191639930705	0.7103784162841580
0.5578518204224916	0.9875607031790311	0.5442850600823927
0.2684188483444649	0.9751683055047865	0.5304517591291050
0.9282567979341484	0.3057261498250191	0.3453486960712729
0.6011948165575962	0.6211170863266958	0.6969438044755809
0.7599337397880973	0.1947412014995744	0.5348124607558701
0.4236610236679400	0.5286100390731051	0.3689281408938882
0.0992399608783059	0.8682342087344264	0.6998795105410536
0.5444134615510011	0.7200946593950992	0.5635936305753292
0.2149835032187023	0.0584537143788710	0.3889324470482672
0.8720139211696155	0.3900332844109863	0.7298852272409793
0.1824494709574091	0.8091445568666368	0.3784751457954478
0.8543495886834009	0.1385301438574650	0.7111131497566349
0.5194226793329004	0.4733253077543014	0.5537337701136690
0.5270668495134533	0.1901856920054047	0.5296341627345955
0.1948381308025760	0.5218299908474993	0.3477279745102334
0.8591176500185254	0.8661276991779500	0.7016478008877602
0.3061943202708061	0.4637713478921936	0.5353047885529308
0.9707114232474422	0.7931791998226055	0.3635853003502535
0.6332768906733655	0.1348173383344258	0.7009796514905882
0.7850718247782984	0.7271741204805331	0.5588635669421805
0.4398461210030123	0.0549554347856973	0.3873982517855535
0.1126443551696668	0.3818456344785404	0.7300445645808200
0.6911353578164013	0.2725160437019788	0.3789353828529213
0.3589454447477540	0.6143801707747581	0.7092525337725685
0.0284924513333029	0.9414519113614699	0.5433579539973094
0.3064001012185072	0.2334228390472647	0.5289943438990110
0.9782787482438621	0.5715082446684472	0.3452630020295336
0.6338346636963328	0.9000215748764914	0.7004832824480438
0.0359849516280175	0.7409312475678907	0.5339128524181648
0.7057295920775378	0.0763975282250321	0.3649952327744207
0.3790275837316549	0.4034435401262672	0.6960854080675595
0.7751240432987290	0.9576083898193876	0.5589089834056258
0.4437932320817077	0.2836531471070288	0.3906743476767839
0.1178721990759712	0.6287256439974367	0.7296784542093451
0.1398169574291769	0.1450775304462110	0.3331143564372152
0.8127396977684067	0.4806230579259498	0.6745460530883448
0.5977663354293387	0.6222122277870820	0.3247946955202682
0.2553505058953303	0.9549451983196519	0.6522556016079617
0.9255723856050095	0.2902590389488841	0.4955423923785072
0.4701202359673291	0.8117065088784302	0.5154625699476438
0.3541774873410432	0.8939143102333128	0.3313345528894774

0.0200351510096614	0.2315172873823952	0.6754540576485564
0.8758314147188064	0.8749910535002060	0.3216499647132859
0.5474768423448274	0.2027278030586978	0.6509166611274166
0.2095178680805265	0.5343959254025755	0.4952085523483840
0.6925227780873021	0.5589362468100275	0.5146947476877900
0.6050655455045966	0.3594549504810841	0.3341346473621158
0.2672064444439132	0.6871855404335631	0.6742068578727729
0.6242129388325228	0.9002990611318142	0.3225494994845241
0.2988421885441443	0.2453491239436235	0.6507342059540031
0.9660992821206575	0.5746929144130735	0.4948961841662604
0.9410006824976834	0.0299833288907420	0.5130770968240654
0.9311134025858484	0.7895638416985301	0.4862296130208562
0.4750618248198304	0.3077875172956145	0.5072802187018135
0.1454219098191038	0.6452051149144488	0.3472826042694592
0.8018319222075260	0.9778141283541713	0.6791221213417237
0.5882538049743925	0.1185355442329951	0.3249631580770956
0.2634137765863864	0.4548965681051966	0.6666633661569445
0.7108241519005610	0.0409978052217071	0.4875936863982281
0.1904358813880909	0.0648868882558606	0.5050644982329495
0.8548493720239886	0.3994028096541699	0.3469108372212558
0.5201753332044586	0.7302248580660057	0.6840927115385371
0.3812387370601080	0.3690093665391511	0.3277483890450949
0.0462076282821857	0.7056393831842428	0.6663101748285239
0.4604444800814640	0.5717918032127618	0.4933234827155159
0.4350963886680026	0.0247292118986306	0.5028867701916269
0.1000928316618728	0.3544658987538061	0.3473182731204479
0.7773044780768963	0.6968208186930581	0.6776533099343838
0.1305861460117026	0.9116092245725007	0.3249363108857838
0.7957133080673385	0.2406819735020256	0.6673963857625290
0.7009954662894911	0.3001670752689916	0.4992256148877099
0.7002337214683844	0.8001954490579104	0.5025174315211258
0.1992724212258739	0.2993320129744086	0.4995273474701273
0.2006404847086148	0.8002305775135589	0.4994174870724232
0.8700984069896165	0.1275049317236927	0.3353107561468582
0.5335696688493066	0.4619745598175058	0.6630071478842454
0.3727570334200918	0.6416793132657848	0.3380402126173331
0.0271679655224799	0.9565765560979183	0.6646334494182805
0.3664346506759247	0.1330728470446312	0.3146265126013065
0.0345353773264598	0.4664882490273471	0.6852471285205550
0.8574490755529216	0.6290161672156519	0.3350019081509161
0.5425511759688988	0.9743050143845152	0.6658676241321867
0.5649878807253187	0.7001246583410580	0.7863943639446885
0.5817189046824597	0.6518032152043047	0.7548394278182863

The perfect Rh₁₁-2H* surface

O In Rh In H

1.000000000000000				
14.4442996979000000	0.0000000000000000	0.0000000000000000		
-7.2221498489000000	12.5091304781999995	0.0000000000000000		
0.0000000000000000	0.0000000000000000	17.9855003356999994		

O	In	Rh	In	H
72	41	1	6	2

Direct

0.8427794187600809	0.6129816606730148	0.4555473341533221
0.5153871278551841	0.9518308687594244	0.2892604287105727
0.1734995081798368	0.2824552511236054	0.6199976469687902
0.7917439790291679	0.9603532049510504	0.2983522939280694
0.4731437109541211	0.2983433563347864	0.6386136834071413
0.1326499694303346	0.6258402379528949	0.4680971384329112
0.3019304212139651	0.7306878467321180	0.3010751631442518
0.9780156847061809	0.0710309784409904	0.6363209843578677
0.6392711081311048	0.4051855093695845	0.4642671981275450
0.5287347759876370	0.2098986875874948	0.2696441219572999
0.1795514034652290	0.5382946709035222	0.6078530875241502
0.8551937744021505	0.8809043701714078	0.4414745927475538
0.8869656568969507	0.1291292540472221	0.4554287582670124
0.5466258658402922	0.4631196577360008	0.2910917467713792
0.2175128410434747	0.7912311408352384	0.6199298308828487
0.5388932707751505	0.7311893406093655	0.3011377537911664
0.2055092010141389	0.0769263373294353	0.6523011498368215
0.8758047478369706	0.4075889163076240	0.4676905905157461
0.7673965289827340	0.4684826785394927	0.2993047780215677
0.4283765726575229	0.8111784907417970	0.6406277360755389
0.0937706616838376	0.1344867681888233	0.4641591829892805
0.2903524347609834	0.2199606136847903	0.2698546667137908
0.9589688078295499	0.5438886945970739	0.6101062635279365
0.6161698372284095	0.8725690460431949	0.4440389700433131
0.3732048376081581	0.6595363348063038	0.4610821082961313
0.0356663228865410	0.9838182664815208	0.2889351011790676
0.7110890769171427	0.3291669925027602	0.6183236964714752
0.7657233512631172	0.7057386713451711	0.3007202684807604
0.4226119757244699	0.0342944350337160	0.6554327530045239
0.0916794306786889	0.3650849744087017	0.4687210493342737
0.0303699197726581	0.1986243585445723	0.2987660769374462
0.6947175566045853	0.5218894137000246	0.6343746760713591
0.3650148174793971	0.8583473049220007	0.4663469944841511
0.2804773246713331	0.9706516975190369	0.2682639839097061
0.9565468401629948	0.3152049959569905	0.6110066303036986

0.6234205843982114	0.6409851679931506	0.4471518973324236
0.2260472766214399	0.3174655016475314	0.3779680185363642
0.8859715868942153	0.6452257858693559	0.7118469191558150
0.5576345458538160	0.9890405158572926	0.5435208633944861
0.2674546276882734	0.9750638303455562	0.5298355209958030
0.9281032505887218	0.3059246920825314	0.3435892456655209
0.6026127289199164	0.6186510082954527	0.6979579048667935
0.7598723692079333	0.1946505653613337	0.5346867886834860
0.4237752522090514	0.5288561218074321	0.3702051531802568
0.0983537544318141	0.8673715537180419	0.6992837465080001
0.5454700632971556	0.7208959090471079	0.5677868477907498
0.2148207923740400	0.0589077398923892	0.3872563535978991
0.8722362877172335	0.3902804534364698	0.7295658565933598
0.1825527165138380	0.8098145609969737	0.3779223646620226
0.8567413275279101	0.1410620804987917	0.7124211141350998
0.5197859192762025	0.4730489586650513	0.5534662210202210
0.5273225659208005	0.1908539482373870	0.5283887688029607
0.1951358120250418	0.5221277094649543	0.3503760246810633
0.8589897562551881	0.8660870274324347	0.7009081000010089
0.3055266952839062	0.4631459853142825	0.5348376919186919
0.9707962642580812	0.7931190992285670	0.3628326019298086
0.6335012176505642	0.1383439230940956	0.7018489409544131
0.7852209729322505	0.7267324187666280	0.5588615879956064
0.4388849871425393	0.0549229656749037	0.3870692582872822
0.1132284547928399	0.3821498957325922	0.7289331246200985
0.6911379893579179	0.2726654765434414	0.3779769502392213
0.3552077868095961	0.6110105303901603	0.7044144953954754
0.0289439281276601	0.9419177924778478	0.5426302174176489
0.3059007083743492	0.2321766309029893	0.5281431079080601
0.9781973520117341	0.5715429021575931	0.3434783217834849
0.6385922908691035	0.9107006591890902	0.6951412682247395
0.0354200812200900	0.7409773222089023	0.5334409602118012
0.7052538512107739	0.0762432643568152	0.3648723553491084
0.3793903766133415	0.4007839929933401	0.6957540627301356
0.7772644495956895	0.9589659234043031	0.5577076283120860
0.4433628285251789	0.2834672693885241	0.3893144282099821
0.1174349808161202	0.6280610006580950	0.7290199138368332
0.1395021357996700	0.1453415926831451	0.3313462369186229
0.8126099454903232	0.4800284847654490	0.6741929701788164
0.5973068594543393	0.6222797929491698	0.3258123185790089
0.2549834457845074	0.9546055452849019	0.6517102639219785
0.9254450525529728	0.2898803954404232	0.4955153991808643
0.4702463992936626	0.8120918633742509	0.5184482787736406
0.3538345380264514	0.8939489648182833	0.3313147802681088

0.0205899150565805	0.2317941546321038	0.6755098964121384
0.8752081050501680	0.8747406472683423	0.3215561602829513
0.5488426272309697	0.2043996489197074	0.6493785361402572
0.2085021467228804	0.5338592014025746	0.4934742734647231
0.6925885679542392	0.5586092671682570	0.5139642167593933
0.6048933016819580	0.3594395715550466	0.3328128794434551
0.2661092829740694	0.6858927585106277	0.6723467103981104
0.6238214312889165	0.9003707132754732	0.3234903050050529
0.2971000818979725	0.2435029439551564	0.6499441826720580
0.9657507073564975	0.5745872721138785	0.4946632542377104
0.9412198839625648	0.0302137839997122	0.5120128046726586
0.9312698781102062	0.7897838419352857	0.4853995943735994
0.4745684555444451	0.3073103558635664	0.5053918131993139
0.1451409487402818	0.6455889161835332	0.3469723640712707
0.8035640172781767	0.9807213316173516	0.6781658157959877
0.5875665270865716	0.1181837822474736	0.3247822659739393
0.2621694430802966	0.4539478793714994	0.6642020587662455
0.7106437673857141	0.0409253379094604	0.4874712808781447
0.1899849574385113	0.0643358622163662	0.5030728602133050
0.8549530877732464	0.3995788200362860	0.3459586494058702
0.5202964934486111	0.7357472819000695	0.6907820233602407
0.3810817567744235	0.3696909091974118	0.3271057388615278
0.0461582988198173	0.7050201465720543	0.6664306957752989
0.4608175791383871	0.5737037439590142	0.4956914108524511
0.4344511315816409	0.0246909567840053	0.5026409474041527
0.0994614955253786	0.3543207169285670	0.3469517994835519
0.7816844076575713	0.6980334309640188	0.6764458482624235
0.1302861827476669	0.9116145383414637	0.3237456180479383
0.7962171920618505	0.2408226543310827	0.6678387364116798
0.7012945185316752	0.3002006187530339	0.4981051171547257
0.6996420454197647	0.8005498639325312	0.5038807629547124
0.1993657354592900	0.2990466116300801	0.4983929501482603
0.2001795821555206	0.8001380440754327	0.4989472344973119
0.8697313025107186	0.1277067273266777	0.3345798953349906
0.5318930018724061	0.4565774903942355	0.6620908076654691
0.3734752022047721	0.6425514683122305	0.3396953471458024
0.0274810500945581	0.9567866498528457	0.6639932480649192
0.3660450529848211	0.1331538840270258	0.3133910052736132
0.0345475492505680	0.4662755396880729	0.6842390500349055
0.8573713154794208	0.6289523267057011	0.3342929072291864
0.5432525762725329	0.9781231076311891	0.6652071238047546
0.5536277292686677	0.7292993702739882	0.7856063590011442
0.5852782403739709	0.6188491722073405	0.7503315085303199

The perfect Rh₁₁-[TS-H₂O]* surface

O	In	Rh	In	H
1.000000000000000				
14.4442996979000000		0.0000000000000000		0.0000000000000000
-7.2221498489000000		12.5091304781999995		0.0000000000000000
0.0000000000000000		0.0000000000000000		17.9855003356999994

O	In	Rh	In	H
72	41	1	6	2

Direct

0.8420923373890826	0.6141702989641120	0.4567884171764828
0.5152198072052649	0.9525751692503874	0.2883271301576048
0.1733469974977568	0.2840155563419928	0.6203397145360378
0.7916698988400055	0.9610132764817181	0.2984876247902969
0.4731448378885437	0.2999498464407216	0.6366579181892468
0.1333049249768741	0.6266083915580497	0.4683568255355073
0.3011691804980621	0.7311853889803548	0.2999650140759151
0.9766524764700192	0.0713354690044080	0.6364217358826896
0.6385894724996265	0.4063465790950949	0.4639148202553625
0.5286364616531523	0.2108953029467641	0.2683639059674780
0.1832562732024037	0.5399331664098435	0.6095828769898355
0.8544923277595416	0.8814572339587065	0.4423565394129741
0.8857936263185108	0.1293954342744726	0.4560446473829354
0.5459587947966628	0.4632407895788656	0.2897185038405285
0.2191278852834672	0.7928234481348001	0.6197797039169702
0.5384430771487246	0.7313335665118014	0.3005824099277296
0.2054809895960114	0.0780166401654784	0.6543350668990930
0.8749591993518425	0.4080842338887277	0.4675123469662250
0.7674632448999867	0.4697555667848791	0.2993043918921276
0.4282149397785736	0.8110740704177634	0.6372709459805853
0.0922081912652526	0.1343406505295873	0.4640260689437690
0.2893407143500796	0.2199021006164963	0.2688456368622620
0.9600316249976748	0.5442622200075492	0.6095339050412750
0.6168516047338798	0.8746552978724805	0.4426816293290089
0.3713431745132108	0.6587725029810824	0.4590792822101489
0.0350587310039506	0.9837862776815597	0.2884738918632414
0.7105572538610152	0.3311549064248998	0.6179104817149640
0.7657520551334761	0.7066544008624099	0.3005098666704286
0.4223916194625750	0.0355263242602026	0.6576599576431112
0.0912945756862295	0.3663368533662847	0.4684459316195660
0.0296111741307002	0.1987223934007049	0.2988701929095396
0.6956660125026914	0.5250087825245709	0.6346764507305236
0.3646556055274228	0.8600548413312346	0.4641028053552492
0.2795080925888481	0.9706855271901693	0.2674029585270811
0.9569314058718726	0.3164133714516060	0.6110324023369682

0.6236537801062617	0.6400937101406935	0.4462184246227191
0.2255225498503927	0.3175082260583736	0.3778279547033767
0.8890283755941142	0.6452781113848924	0.7127358163460658
0.5564657591185239	0.9894869297014279	0.5433028778778570
0.2678103705956738	0.9763765999635809	0.5298972675519775
0.9276078263652765	0.3065314191769691	0.3433160485659322
0.6170031398168154	0.5957268851508333	0.7353274113998661
0.7590845309289966	0.1959289287172666	0.5347135480921353
0.4231227599524269	0.5286536732344000	0.3687712044749520
0.0981382743161286	0.8678490461287195	0.6987439746098806
0.5438908378503504	0.7203030858981462	0.5616755761655786
0.2143627790663193	0.0591878084853632	0.3865886875654457
0.8724369552942560	0.3908409166491851	0.7293349365946015
0.1819361450194151	0.8100909597801063	0.3776060653393727
0.8555624861150842	0.1410375955538052	0.7117940483591719
0.5176665185858372	0.4722819875761980	0.5553062660283019
0.5261723979510406	0.1916205530257883	0.5281058375212622
0.1942118925184002	0.5222442752481434	0.3482478869752115
0.8594413412042921	0.8675106077171402	0.7029510436256862
0.3053991979696919	0.4634065495080590	0.5350254128647466
0.9702080490800155	0.7941566167540385	0.3640215787930973
0.6338297685981529	0.1399721050896986	0.7012254843639260
0.7837666779508722	0.7274995704537627	0.5613284114735386
0.4386631283922342	0.0559737620570704	0.3855108995962346
0.1137035488924014	0.3829685596575052	0.7295408263917583
0.6902184049155743	0.2733718070961657	0.3775242111689381
0.3572278434655785	0.6151567205251149	0.7100378082731824
0.0284173356640252	0.9426165611380145	0.5433383942579963
0.3042785083409142	0.2316286774465948	0.5280699582612105
0.9776464305877498	0.5725305191474289	0.3456620065981763
0.6340986495493930	0.9105886184498422	0.7025615309092320
0.0358044055787335	0.7416723848315299	0.5338071011983537
0.7048046986384883	0.0774108648358312	0.3643402561594971
0.3791775977799605	0.3990383576461245	0.6992437917179440
0.7740026566943420	0.9583520011031672	0.5592028494011958
0.4427525061534908	0.2836962079535471	0.3883422257600758
0.1175832381784916	0.6290845694376461	0.7291689979677587
0.1388211427190755	0.1454345975967109	0.3308870069740180
0.8135297219575782	0.4809890004662781	0.6737879389512554
0.5971600553735971	0.6223646769569140	0.3248711350293796
0.2550171779128774	0.9560713833547799	0.6519071842959354
0.9249261011647293	0.2908812122192106	0.4955451196264299
0.4694689266414497	0.8129597081660418	0.5138486926379168
0.3533167386393034	0.8943434906801137	0.3300006264719995

0.0202584878317855	0.2325753466574870	0.6755618278329607
0.8749469570922259	0.8753981808376132	0.3219469851396515
0.5489410432721775	0.2054836887109530	0.6487769674274863
0.2085831094658728	0.5344417241116491	0.4943716245382279
0.6910047543164874	0.5589566652289931	0.5148740993164423
0.6044998021018199	0.3602123214313868	0.3320309972109512
0.2664923524734240	0.6874352221012334	0.6735872304458655
0.6235754181595452	0.9010535690853307	0.3223183864369414
0.2959283502798472	0.2443191112163320	0.6498379234943116
0.9657430391054554	0.5752530441293822	0.4939226612878618
0.9398700357038672	0.0307033325199814	0.5131038562276689
0.9305336238822852	0.7901557157492765	0.4867208484647252
0.4734497438498311	0.3089047384493687	0.5044722288949262
0.1449547971589996	0.6458797115497834	0.3468927083848342
0.8006031210353800	0.9797568594585425	0.6794324440291593
0.5875300848413977	0.1192143160375331	0.3235387127994991
0.2645007867661039	0.4559484647742405	0.6664825210421856
0.7099047439606937	0.0421592936089377	0.4872668646252202
0.1888727271307199	0.0644061294990729	0.5022007819889591
0.8543914137604059	0.4000786398146287	0.3457649561438998
0.5194340572134071	0.7388510286688541	0.6819800529142607
0.3802447445978493	0.3695254003013712	0.3259981417503292
0.0476880491228234	0.7060822902578909	0.6652552268600038
0.4594237861452397	0.5715975291691368	0.4930821677477321
0.4342820302903836	0.0262270723367752	0.5008724152752757
0.0991231049149989	0.3547833807667976	0.3464956218259497
0.7869929620111664	0.7001444614676720	0.6795994044570280
0.1295020858472898	0.9116177783246634	0.3234745412430628
0.7961243780602248	0.2418425576977464	0.6673203969933110
0.7005987245747836	0.3016369334419277	0.4976320999590324
0.6993518369588962	0.8007328401436885	0.5026801443452894
0.1981859593315379	0.2991895675199808	0.4983795536137031
0.2002825386184315	0.8011169878526885	0.4986306666573653
0.8691472313484364	0.1283535758775770	0.3347440940052803
0.5332490454236292	0.4539445044200187	0.6655949913512007
0.3722125796163390	0.6421022481731942	0.3378942779866653
0.0281339122329913	0.9589084057655500	0.6647771429340203
0.3656085616051731	0.1335107775589091	0.3119483349091891
0.0350897287633446	0.4671027069632103	0.6847280299364229
0.8567316063914058	0.6298813445845501	0.3353138859995979
0.5417226891392912	0.9793684810405373	0.6651865311216733
0.5914779116260379	0.6780712380138564	0.7240034057247527
0.5981689658813469	0.5818636430904225	0.7877572719596228

The perfect Rh₁₁-H₂O* surface

O In Rh In H

1.000000000000000				
14.4442996979000000	0.0000000000000000	0.0000000000000000		
-7.2221498489000000	12.5091304781999995	0.0000000000000000		
0.0000000000000000	0.0000000000000000	17.9855003356999994		

O	In	Rh	In	H
72	41	1	6	2

Direct

0.8405297843886046	0.6129987384717573	0.4553904919694805
0.5142653871270917	0.9515935133967823	0.2872059754323011
0.1698081261612136	0.2796600037700143	0.6183373880883744
0.7906848661989933	0.9603188950891819	0.2967110422146959
0.4677226761580122	0.2944489622094473	0.6446943026537053
0.1327536817140819	0.6252814278733411	0.4680311151084531
0.2996341723613962	0.7297904499072573	0.2987038536331453
0.9745261966660753	0.0693810791808203	0.6335813449080381
0.6380170933847106	0.4046020858082977	0.4650409019425016
0.5280976960474656	0.2097719145373111	0.2672200468824668
0.1839810769750495	0.5389874369535759	0.6090563838742347
0.8552724786657200	0.8822910284323610	0.4396643000343145
0.8843995627250471	0.1282366321161799	0.4553905454239571
0.5453653777901938	0.4617696765497899	0.2885372921214382
0.2169703797862667	0.7896469628305662	0.6187171415826700
0.5375848676953036	0.7301802694683791	0.2982085994708152
0.2030270057205729	0.0741583313093711	0.6583584463436331
0.8727704192465429	0.4060781861901989	0.4676055531594230
0.7662660636102162	0.4677908470009049	0.2983924276475030
0.4250803997029677	0.8059934968029044	0.6330992249822248
0.0920592825339321	0.1328468669156417	0.4615107622847660
0.2888725467904870	0.2188249298901876	0.2673375078645699
0.9565822260212911	0.5417920207545938	0.6087520575122730
0.6150263034921555	0.8719359917449921	0.4410525204645513
0.3720112569630238	0.6576432581502530	0.4574666378633379
0.0348279909610141	0.9828201269177075	0.2860518402831281
0.7048114034423395	0.3299897806501680	0.6192326321611836
0.7655118301437326	0.7059413052547981	0.2979668217683653
0.4197140639669313	0.0284893702277846	0.6589670677713879
0.0903798765751811	0.3646797656423832	0.4679852149446792
0.0288298059305122	0.1978683799814576	0.2977913549179881
0.6867867566969073	0.5337252042421353	0.6396715877255208
0.3633411746481507	0.8590399786394173	0.4622267242859228
0.2792700193027140	0.9692825405675506	0.2656385720918588
0.9549509860623631	0.3146773656780510	0.6103794979360919

0.6239607153236435	0.6404282370606884	0.4434438396802147
0.2252640051949065	0.3165185252089232	0.3768005479311176
0.8865453017442527	0.6423121042154832	0.7118475204052908
0.5554259517629381	0.9862093712952978	0.5428125780775813
0.2666179132162045	0.9748033681280631	0.5299726312925530
0.9264895410408208	0.3050556434684165	0.3439276725021766
0.6695567757810443	0.6854310962296873	0.7757010951552118
0.7576424426849317	0.1948077656542312	0.5351618839105007
0.4223867908150377	0.5276491875043090	0.3663268279204945
0.0942055070223700	0.8631722831966164	0.6969455027512756
0.5454235044416466	0.7153572128496204	0.5612477961239807
0.2139436518718116	0.0575794948616380	0.3842198700886197
0.8687714313798408	0.3882667209547077	0.7280814345396858
0.1806173208265726	0.8088512895931811	0.3764761664432080
0.8514356029523503	0.1363669739544844	0.7099951420315050
0.5155518517843498	0.4698252683578610	0.5478941285649471
0.5239800510572443	0.1890766266256352	0.5298662396947411
0.1936788649553707	0.5212690341010244	0.3486612569394590
0.8602935720870174	0.8680880783704371	0.7036325684334869
0.3042108919623898	0.4619480508448748	0.5334560899606077
0.9695703520939108	0.7930100995282540	0.3618737093249283
0.6319105288990624	0.1328215313794331	0.6989742660894838
0.7863132179180220	0.7297005312001696	0.5577167560431477
0.4377418719028581	0.0550914197288312	0.3848579016183264
0.1107814433332975	0.3803140571545699	0.7281285071336892
0.6882864246999770	0.2715870611620491	0.3777634558292184
0.3606703858708570	0.6133417695966061	0.7108329884753021
0.0286149028938557	0.9420404043037762	0.5417208138545979
0.3032598497083128	0.2285324673083228	0.5283779115628675
0.9761421845031334	0.5707753533117988	0.3466575392827235
0.6290419944074456	0.8920842243227719	0.7028912046272179
0.0344039308733176	0.7396527527595961	0.5324245687404257
0.7034801266689624	0.0757373774562424	0.3640240548999210
0.3703422620219023	0.3981046735646604	0.6951992873105728
0.7715663702354797	0.9558118820449957	0.5573420066553538
0.4421244958441288	0.2823856012352255	0.3876939130985059
0.1166698641406781	0.6261106958567711	0.7283292582389272
0.1381418251803815	0.1443414033529619	0.3290398155426479
0.8084015926512270	0.4789128711904319	0.6730873586745673
0.5969586931165726	0.6215910992167407	0.3220820860699365
0.2527650394659954	0.9526268101802760	0.6522285494750111
0.9237590568741165	0.2898028823931201	0.4943655006481872
0.4682939121262035	0.8114858787928476	0.5105431483169011
0.3523898553735429	0.8931881149861564	0.3289862382817307

0.0172795279040989	0.2294463992427073	0.6737891150528684
0.8745876096309110	0.8748494732212436	0.3192179472530990
0.5431482066313497	0.1999523623365745	0.6519102192631590
0.2079836119618552	0.5330409486099325	0.4924395056737391
0.6900257823274620	0.5587960878483037	0.5138346932195512
0.6035049305686153	0.3586109529409331	0.3312752784524708
0.2653689920351902	0.6857658889714568	0.6726154518220200
0.6226065980711374	0.8998696762294890	0.3202735853523673
0.2925688006458982	0.2393415418546376	0.6501724987952162
0.9641635130238948	0.5735733618413352	0.4923891800978030
0.9396746208223218	0.0299086347422280	0.5108357323141115
0.9317418443067766	0.7902397502945329	0.4837003728349454
0.4719369670532865	0.3050898309420237	0.5041984785756709
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0.2589728144287798	0.4522004660003171	0.6633166627304030
0.7086553926347653	0.0412027481478753	0.4861741264423327
0.1882448643145405	0.0621750264661728	0.4992883761756329
0.8524696422898081	0.3980310288667842	0.3457608161834735
0.5136987313212977	0.7295848308410280	0.6756048266300487
0.3796902201944784	0.3680222769250308	0.3247239102675280
0.0460045689077532	0.7028303073618124	0.6635678264968429
0.4580834887511950	0.5686438878132033	0.4888791857922031
0.4330410912381705	0.0245816977481341	0.5002756983310244
0.0984040504898321	0.3535368930211644	0.3458831051654446
0.7924256319000303	0.7039192666933769	0.6742991013404138
0.1288319099585963	0.9101290240446231	0.3208448601545160
0.7932066456408680	0.2394026569375848	0.6656440839920484
0.6983304276616960	0.2995101999402600	0.4983387996561369
0.6998506191160424	0.8001058684591059	0.4986920440252611
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0.1990533755948257	0.7997823602975103	0.4975694855054118
0.8681583324702087	0.1272678168456140	0.3337223830742772
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0.3714381069219203	0.6411849006760494	0.3355964219618513
0.0287662613178572	0.9590098278269987	0.6634207898789305
0.3650505926404732	0.1322132151387655	0.3101201225821328
0.0313389341264572	0.4642210085397994	0.6841732994821470
0.8553525557662824	0.6283190567223625	0.3338188505152764
0.5389234629891050	0.9720970181018728	0.6644215356727901
0.7107407835657873	0.7484383053434297	0.8065157780270649
0.6413591158085128	0.6237857757372162	0.8085535227928643