Thermodynamics and Catalytic Activity of Ruthenium Oxides Grown on Ruthenium Metal from Machine Learning Atomic Simulation

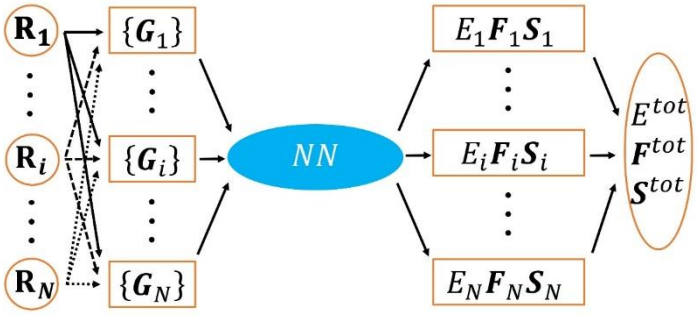
Ze-Yi Zhu, Ye-Fei Li*, Cheng Shang, Zhi-Pan Liu*

[a]Collaborative Innovation Center of Chemistry for Energy Material, Shanghai Key Laboratory of Molecular Catalysis and Innovative Materials, Key Laboratory of Computational Physical Science, Department of Chemistry, Fudan University, Shanghai 200433, China

Table of Contents

1. Theoretical methodology and construction of the quaternary Ru-C-H-O G-NN potential

1.1 Architecture of neural network potential



Scheme S1. Scheme of the HDNN architecture. The subscripts (1, *i*,⋯, *N*) are atom indices and represent the total atoms in a structure. The inputs of NN are a set of structural descriptors {$\boldsymbol{G}$}, which are constructed from the Cartesian coordinates {**R**} of the structure, while the outputs of NN are the atomic properties { E_i, $\boldsymbol{F}_i$, $\boldsymbol{S}_i$ }, i.e., energies, forces, and stresses. The overall properties, E^{tot}, $\boldsymbol{F}^{tot}$, and $\boldsymbol{S}^{tot}$, can be calculated from the individual atomic contributions.

In this work, we utilized the high dimensional neural network (HDNN) scheme to construct the global NN (G-NN) potential, as shown in Scheme S1. The input nodes to NN are a set of structural descriptors of a structure, as detailedly discussed in our previous works.[1-3] The total energy E^{tot} of the structure can be composed as a linear combination of its atomic energy E^i from the output of NN

$$E^{tot} = \sum_i E_i \tag{1}$$

Consistently, the atomic force can be analytically derived from the total energy, i.e., the force component $F_{k,\alpha}$ (α = *x*, *y*, or *z*) acting on atom *k* is the derivative of the total energy E^{tot} with respect to coordinate $R_{k,\alpha}$. In combination with Eq. 1, the force component $F_{k,\alpha}$ then is related to the derivatives of the atomic energy E^i with respect to the j^{th} structural descriptors of atom *i*, $G_{j,i}$

$$F_{k,\alpha} = -\frac{\partial E^{tot}}{\partial R_{k,\alpha}} = -\sum_{i,j} \frac{\partial E_i}{\partial G_{j,i}} \frac{\partial G_{j,i}}{\partial R_{k,\alpha}} \tag{2}$$

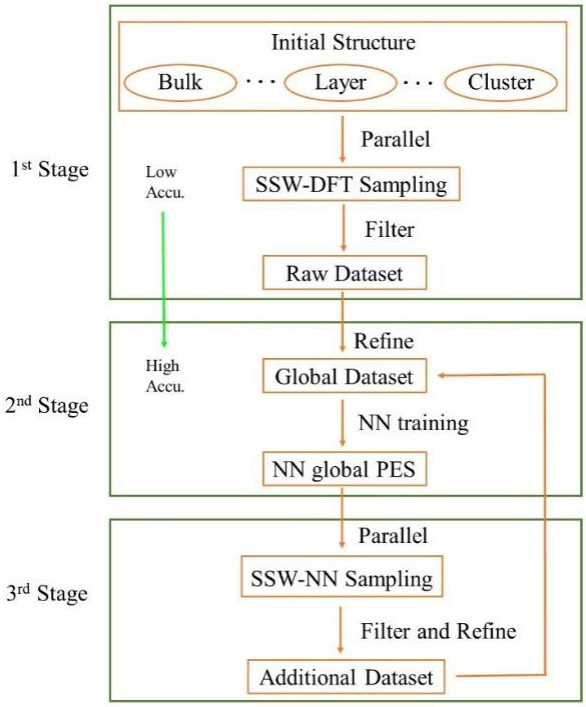
Similarly, the element $\sigma_{\alpha\beta}$ of static stress tensor matrix can be analytically derived as

$$\sigma_{\alpha\beta} = -\frac{1}{V}\sum_{i,j,d} \frac{(r_d)_\alpha (r_d)_\beta}{r_d} \frac{\partial E_i}{\partial G_{j,i}} \frac{\partial G_{j,i}}{\partial r_d} \tag{3}$$

where $\boldsymbol{r}_d$ and r_d are the distance vector, constituted by $G_{j,i}$ and its module, respectively, and *V* is the volume of the structure.

1.2 Generation of global dataset using SSW-NN

Undoubtedly, the quality of the potential energy surface (PES) of G-NN is largely determined by its training dataset. Here we utilized the stochastic surface walking (SSW) global optimzation[4-6] to generate a global dataset, which is fully automated and does not need a priori knowledge on the system, such as the structural motif, e.g. bonding patterns and symmetry. The final obtained Ru-C-H-O global dataset contains a variety of structural patterns on the global PES, as summarized in Table S1.



Scheme S2. Procedure for the generation of the global training dataset by SSW global optimization. In the first stage, the SSW sampling is typically performed by low accuracy DFT calculations. In the second stage, the global dataset is first refined with high accuracy DFT setups, and then a NN training is performed based on the accurate global dataset. In the third stage, an additional dataset is generated by SSW sampling utilizing the previously obtained NN PES, and is fed into the global dataset. A new cycle of NN training then starts based on the new global dataset (back to stage 2).

In brief, the SSW-NN method involves three stages to generate the global dataset (see Scheme S2), as described below.

(i) **The first stage** generates a raw dataset, which contains the most common atomic environment and serves to build an initial NN PES. This is done by performing density functional theory (DFT) SSW global optimization in a massively parallel way. In this stage, the DFT calculations have low accuracy setups and small unit cells to speed up the SSW search. By collecting and screening the structures from SSW trajectories, a raw dataset is obtained.

(ii) **The second stage** trains a NN global PES. This is done by refining the dataset using DFT calculations with high accuracy setups, followed by NN training on the accurate global dataset (see our previous work[7] for details). The NN architecture applied in this stage utilizes a small set of structural descriptors and a small network size.

(iii) **The third stage** iteratively expands the global dataset. It targets to increase the predictive power of NN PES by incorporating more structural patterns into the dataset. This is done by performing SSW PES search using the NN PES obtained in the second stage, starting from a variety of initial structures. These initial structures are randomly constructed, and also include large systems with many atoms per unit cell. The structures from all the SSW trajectories are collected and filtered to generate an additional dataset. The new dataset is then fed to the global dataset to start a new cycle of NN training (back to stage 2).

Table S1. Structural information of the global PES dataset for G-NN potential training. The listed data is the number of structures in the dataset, as distinguished by chemical formula, the number of atoms per cell (N_{atm}), and the type of the structure, including cluster (N_{cls}), layer (N_{lay}), and bulk (N_{bul}). The total number of the structures (N_{tot}) is also summarized.

Chem. Formula	N_{atm}	N_{cls}	N_{lay}	N_{bul}	N_{tot}
Ru12	12	0	0	17	17
Ru16	16	267	2	946	1215
Ru31	31	0	0	6	6
Ru32	32	0	6	19	25
O1-Ru12	13	0	52	0	52
O1-Ru16	17	0	0	10	10
O1-Ru30	31	51	0	0	51
O2-Ru10	12	0	45	0	45
O2-Ru16	18	0	0	8	8
O2-Ru29	31	27	0	20	47
O2-Ru62	64	0	83	0	83
O2-Ru64	66	0	84	0	84
O4	4	0	31	0	31
O4-Ru8	12	0	0	759	759
O4-Ru16	20	54	1	5	60
O4-Ru27	31	113	2	10	125
O4-Ru60	64	0	41	0	41
O4-Ru64	68	0	83	0	83
O6-Ru4	10	0	32	759	791
O6-Ru8	14	1	0	0	1
O6-Ru25	31	0	0	18	18
O6-Ru26	32	0	0	16	16
O7-Ru8	15	0	0	1225	1225

O7-Ru16	23	0	1	7	8
O8-Ru4	12	0	1691	4228	5919
O8-Ru6	14	0	4	24	28
O8-Ru8	16	0	0	1464	1464
O8-Ru52	60	0	38	19	57
O8-Ru56	64	0	41	0	41
O9-Ru9	18	0	0	6	6
O9-Ru16	25	62	0	0	62
O10-Ru6	16	0	17	22	39
O10-Ru16	26	0	0	6	6
O11	11	0	224	69	293
O12-Ru8	20	16	4	4	24
O12-Ru16	28	0	0	4	4
O12-Ru28	40	230	0	0	230
O14-Ru7	21	0	10	27	37
O14-Ru8	22	0	0	10	10
O14-Ru16	30	0	2	4	6
O14-Ru50	64	0	82	0	82
O14-Ru64	78	0	72	0	72
O15-Ru8	23	0	0	8	8
O16-Ru8	24	6	4	9	19
O16-Ru16	32	0	12	5	17
O16-Ru48	64	0	121	0	121
O16-Ru64	80	0	178	0	178
O18-Ru7	25	0	20	21	41
O18-Ru8	26	0	12	18	30
O18-Ru9	27	0	11	14	25
O18-Ru12	30	0	0	36	36
O18-Ru22	40	12	0	0	12
O18-Ru46	64	0	41	0	41
O18-Ru64	82	0	105	0	105
O20-Ru12	32	0	0	5	5
O20-Ru20	40	0	0	1	1
O20-Ru44	64	0	117	0	117
O22-Ru16	38	0	0	45	45
O22-Ru64	86	0	104	0	104
O24-Ru12	36	0	44	0	44
O24-Ru16	40	0	0	3	3
O24-Ru64	88	0	41	0	41
O30-Ru10	40	0	0	1	1
O32-Ru20	52	0	0	76	76
O33-Ru14	47	0	188	58	246
O33-Ru15	48	0	191	73	264
O34-Ru14	48	0	220	81	301

O34-Ru16	50	0	401	171	572
O35-Ru16	51	0	326	120	446
O36-Ru16	52	0	200	80	280
O40-Ru10	50	0	273	78	351
O40-Ru40	80	0	0	114	114
O44-Ru20	64	0	0	121	121
O46-Ru20	66	0	0	42	42
O60-Ru20	80	0	0	249	249
C1-O2-Ru31	34	0	19	0	19
C1-O3-Ru33	37	0	26	0	26
C1-O4-Ru36	41	0	32	0	32
C1-O5-Ru36	42	0	22	0	22
C1-O6-Ru34	41	0	56	0	56
C1-O6-Ru36	43	0	144	0	144
C1-O9-Ru31	41	0	18	0	18
C1-O9-Ru32	42	0	32	0	32
C1-O9-Ru33	43	0	12	0	12
C1-O10-Ru29	40	0	31	0	31
C1-O10-Ru32	43	0	33	0	33
C1-O11-Ru31	43	0	58	0	58
C1-O12-Ru30	43	0	41	0	41
C1-O13-Ru29	43	0	52	0	52
C1-O15-Ru64	80	0	20	0	20
C1-O22-Ru40	63	0	231	0	231
C1-O41-Ru20	62	0	122	0	122
C1-O45-Ru24	70	0	13	0	13
C1-O46-Ru24	71	0	9	0	9
C1-O47-Ru24	72	0	15	0	15
C1-O49-Ru24	74	0	23	0	23
C1-O51-Ru24	76	0	15	0	15
C1-O53-Ru24	78	0	37	0	37
C1-O73-Ru36	110	0	40	0	40
C1-O89-Ru48	138	0	35	0	35
C1-O96-Ru48	145	0	21	0	21
C2-O4-Ru62	68	0	1	0	1
C2-O6-Ru66	74	0	2	0	2
C2-O12-Ru68	82	0	1	0	1
C2-O12-Ru72	86	0	7	0	7
C2-O18-Ru62	82	0	2	0	2
C2-O18-Ru64	84	0	4	0	4
C2-O20-Ru58	80	0	5	0	5
C2-O22-Ru62	86	0	7	0	7
C2-O24-Ru60	86	0	1	0	1
C2-O26-Ru58	86	0	3	0	3

H1-Ru15	16	0	0	18	18
H1-O1	2	0	3	0	3
H1-O8-Ru4	13	0	7	492	499
H1-O12-Ru6	19	0	4	9	13
H1-O23-Ru12	36	0	28	0	28
H2	2	4	0	0	4
H2-Ru14	16	0	0	27	27
H2-O1	3	3	0	0	3
H2-O4-Ru23	29	0	1	0	1
H2-O6-Ru4	12	0	26	9	35
H2-O7-Ru4	13	0	74	53	127
H2-O8-Ru4	14	3	68	529	600
H2-O12-Ru6	20	0	10	4	14
H2-O14-Ru8	24	0	4	0	4
H2-O15-Ru8	25	0	6	0	6
H2-O16-Ru8	26	0	9	19	28
H2-O34-Ru16	52	0	213	116	329
H2-O36-Ru16	54	0	227	126	353
H2-C1-O2-Ru12	17	0	157	5	162
H2-C1-O2-Ru16	21	0	139	0	139
H2-C1-O2-Ru20	25	0	41	0	41
H2-C1-O2-Ru27	32	0	1	0	1
H2-C1-O2-Ru36	41	0	131	0	131
H2-C1-O3-Ru36	42	0	33	0	33
H2-C2-O3-Ru26	33	0	16	0	16
H2-C2-O3-Ru27	34	0	42	1	43
H2-C2-O3-Ru36	43	0	2	0	2
H2-C3-O2-Ru25	32	0	1	0	1
H2-C3-O2-Ru26	33	0	57	0	57
H2-C3-O2-Ru27	34	0	44	0	44
H2-C3-O4-Ru33	42	0	2	0	2
H2-C3-O4-Ru35	44	0	3	0	3
H2-C3-O4-Ru36	45	0	4	0	4
H2-C4-O1-Ru26	33	0	9	0	9
H2-C4-O1-Ru27	34	0	55	1	56
H2-C4-O2-Ru25	33	0	9	0	9
H3-Ru26	29	0	40	240	280
H3-O6-Ru15	24	101	0	0	101
H3-O6-Ru16	25	62	2	19	83
H3-O6-Ru20	29	0	15	272	287
H3-O8-Ru4	15	0	29	130	159
H3-O9-Ru28	40	42	0	0	42
H3-O10-Ru16	29	0	18	211	229
H3-O12-Ru6	21	0	8	2	10

H3-O15-Ru8	26	0	6	0	6
H3-O15-Ru22	40	115	0	0	115
H3-O16-Ru8	27	0	8	0	8
H3-O19-Ru8	30	0	624	111	735
H3-C1-O1-Ru15	20	0	195	1	196
H3-C1-O1-Ru16	21	0	223	2	225
H3-C1-O1-Ru20	25	0	39	0	39
H3-C1-O2-Ru15	21	0	120	0	120
H3-C1-O2-Ru16	22	0	136	0	136
H3-C1-O2-Ru36	42	0	65	0	65
H3-C1-O3-Ru35	42	0	9	0	9
H3-C2-O2-Ru26	33	0	7	0	7
H3-C2-O2-Ru27	34	0	29	0	29
H3-C2-O2-Ru36	43	0	3	0	3
H3-C2-O3-Ru34	42	0	62	0	62
H3-C2-O3-Ru36	44	0	109	0	109
H3-C2-O4-Ru32	41	0	6	3	9
H3-C2-O4-Ru33	42	0	15	0	15
H3-C2-O4-Ru35	44	0	48	0	48
H3-C3-O1-Ru26	33	0	3	0	3
H3-C3-O1-Ru27	34	0	21	0	21
H3-C3-O2-Ru25	33	0	29	0	29
H3-C3-O3-Ru35	44	0	35	0	35
H4-Ru12	16	4	0	21	25
H4-Ru16	20	114	0	0	114
H4-Ru17	21	0	0	18	18
H4-O4-Ru8	16	0	0	12	12
H4-O5-Ru20	29	0	4	0	4
H4-O6-Ru4	14	0	43	28	71
H4-O8-Ru4	16	0	54	96	150
H4-O11-Ru8	23	0	1	9	10
H4-O12-Ru8	24	0	3	10	13
H4-O13-Ru8	25	0	13	10	23
H4-O14-Ru8	26	0	26	3	29
H4-O15-Ru8	27	0	10	1	11
H4-O16-Ru8	28	0	38	22	60
H4-O19-Ru8	31	0	305	54	359
H4-O28-Ru16	48	0	12	0	12
H4-O30-Ru16	50	0	6	29	35
H4-O32-Ru16	52	0	0	45	45
H4-O34-Ru15	53	0	170	91	261
H4-O35-Ru16	55	0	316	194	510
H4-O36-Ru16	56	0	235	126	361
H4-O37-Ru16	57	0	143	66	209

H4-C1-O1-Ru16	22	0	180	0	180
H4-C1-O2-Ru36	43	0	11	0	11
H4-C1-O3-Ru27	35	0	3	0	3
H4-C1-O3-Ru36	44	0	23	0	23
H4-C2-O1-Ru15	22	0	32	1	33
H4-C2-O2-Ru33	41	0	197	7	204
H4-C2-O3-Ru32	41	0	37	5	42
H4-C2-O3-Ru34	43	0	2	0	2
H4-C2-O3-Ru36	45	0	5	0	5
H4-C2-O4-Ru12	22	0	15	33	48
H4-C2-O4-Ru24	34	0	9	0	9
H4-C2-O4-Ru26	36	0	1	0	1
H4-C2-O4-Ru32	42	0	2	0	2
H4-C2-O4-Ru36	46	0	42	0	42
H4-C2-O4-Ru72	82	0	3	0	3
H4-C2-O7-Ru41	54	0	2	0	2
H4-C2-O7-Ru43	56	0	21	0	21
H4-C2-O8-Ru45	59	0	14	0	14
H4-C2-O10-Ru41	57	0	30	0	30
H4-C2-O10-Ru43	59	0	25	0	25
H4-C2-O10-Ru45	61	0	24	0	24
H4-C2-O11-Ru42	59	0	51	1	52
H4-C2-O11-Ru43	60	0	84	1	85
H4-C2-O11-Ru44	61	0	18	0	18
H4-C2-O11-Ru45	62	0	45	2	47
H4-C2-O12-Ru41	59	0	61	0	61
H4-C2-O12-Ru42	60	0	23	0	23
H4-C2-O12-Ru43	61	0	26	1	27
H4-C2-O12-Ru44	62	0	1	0	1
H4-C2-O13-Ru41	60	0	25	1	26
H4-C2-O13-Ru45	64	0	67	0	67
H4-C4-O4-Ru36	48	0	2	5	7
H4-C6-O4-Ru50	64	0	7	0	7
H4-C6-O4-Ru52	66	0	1	0	1
H4-C6-O8-Ru66	84	0	2	0	2
H4-C8-O2-Ru52	66	0	2	0	2
H4-C8-O2-Ru54	68	0	10	0	10
H4-C8-O4-Ru50	66	0	4	0	4
H5-Ru16	21	0	0	1	1
H5-O19-Ru8	32	0	330	27	357
H5-C1-O2-Ru35	43	0	143	9	152
H5-C1-O3-Ru36	45	0	8	2	10
H6-Ru10	16	0	0	11	11
H6-Ru26	32	1	1	4	6

H6-Ru52	58	0	14	1	15
H6-O7-Ru16	29	0	1	3	4
H6-O10-Ru8	24	0	10	1	11
H6-O15-Ru8	29	0	1	6	7
H6-O16-Ru8	30	0	9	4	13
H6-O19-Ru8	33	0	391	21	412
H6-O28-Ru16	50	0	7	21	28
H6-O30-Ru16	52	0	20	0	20
H6-O32-Ru16	54	0	18	0	18
H6-C1-O1-Ru33	41	0	23	0	23
H6-C1-O1-Ru35	43	0	43	0	43
H6-C1-O2-Ru36	45	0	11	3	14
H6-C1-O3-Ru12	22	0	5	9	14
H6-C1-O3-Ru36	46	0	27	5	32
H6-C2-O2-Ru30	40	0	28	7	35
H6-C2-O2-Ru31	41	0	60	13	73
H6-C2-O2-Ru32	42	0	420	39	459
H6-C2-O3-Ru36	47	0	1409	0	1409
H6-C3-O2-Ru36	47	0	1162	0	1162
H6-C4-O4-Ru54	68	0	3	0	3
H6-C4-O6-Ru72	88	0	1	0	1
H6-C6-O6-Ru70	88	0	9	0	9
H7-O16-Ru8	31	0	8	0	8
H7-C1-O4-Ru34	46	0	4	4	8
H7-C1-O4-Ru36	48	0	12	10	22
H7-C2-O2-Ru31	42	0	88	11	99
H7-C2-O2-Ru32	43	0	97	13	110
H7-C2-O2-Ru36	47	0	45	0	45
H7-C2-O5-Ru34	48	0	8	7	15
H8-Ru8	16	3	0	57	60
H8-Ru21	29	0	0	190	190
H8-Ru32	40	46	0	0	46
H8-O3-Ru18	29	0	3	10	13
H8-O8-Ru8	24	0	10	2	12
H8-O10-Ru40	58	0	22	0	22
H8-O11-Ru8	27	0	11	5	16
H8-O12-Ru8	28	0	23	2	25
H8-O15-Ru8	31	0	3	2	5
H8-O16-Ru8	32	0	8	7	15
H8-O19-Ru8	35	0	0	1	1
H8-O22-Ru16	46	0	27	0	27
H8-O26-Ru16	50	0	37	31	68
H8-O30-Ru16	54	0	22	27	49
H8-C1-O5-Ru36	50	0	10	3	13

H8-C2-O2-Ru23	35	0	4	0	4
H8-C2-O2-Ru32	44	0	30	6	36
H8-C2-O2-Ru36	48	0	1455	0	1455
H8-C2-O4-Ru34	48	0	55	10	65
H8-C2-O4-Ru35	49	0	19	6	25
H8-C2-O4-Ru36	50	0	67	6	73
H8-C3-O1-Ru36	48	0	40	0	40
H8-C4-O4-Ru66	82	0	6	0	6
H8-C4-O6-Ru64	82	0	1	0	1
H8-C4-O8-Ru72	92	0	3	1	4
H9-Ru16	25	75	0	0	75
H9-O13-Ru8	30	0	34	0	34
H9-C2-O1-Ru34	46	0	3	0	3
H9-C2-O1-Ru35	47	0	4	1	5
H9-C2-O1-Ru36	48	0	50	0	50
H9-C3-O1-Ru35	48	0	34	0	34
H10-O1-Ru18	29	0	8	0	8
H10-O10-Ru8	28	0	14	22	36
H10-O12-Ru8	30	0	22	12	34
H10-O13-Ru6	29	0	15	13	28
H10-O13-Ru7	30	0	33	0	33
H10-O13-Ru8	31	0	12	18	30
H10-O20-Ru8	38	0	2	2	4
H10-C2-O2-Ru36	50	0	1190	0	1190
H10-C2-O4-Ru70	86	0	1	0	1
H10-C2-O6-Ru72	90	0	1	0	1
H10-C3-O2-Ru36	51	0	1407	0	1407
H11-Ru5	16	0	0	24	24
H11-Ru18	29	0	28	287	315
H11-O12-Ru8	31	0	34	0	34
H12-Ru28	40	14	0	0	14
H12-O14-Ru32	58	0	12	3	15
H12-O20-Ru16	48	0	33	12	45
H12-O30-Ru16	58	0	5	12	17
H12-C2-O3-Ru36	53	0	1144	0	1144
H12-C2-O4-Ru12	30	0	3	25	28
H12-C4-O4-Ru64	84	0	3	1	4
H13-Ru19	32	0	0	2	2
H13-O3-Ru11	27	0	8	15	23
H14-Ru18	32	0	0	3	3
H14-O7	21	0	1	985	986
H14-O21-Ru8	43	0	2	0	2
H14-C3-O3-Ru36	56	0	734	0	734
H14-C4-O4-Ru64	86	0	1	0	1

H15-Ru6	21	0	20	0	20
H15-Ru14	29	0	0	208	208
H15-Ru17	32	0	0	6	6
H16-Ru5	21	0	14	0	14
H16-Ru16	32	0	0	9	9
H16-O8	24	0	15	4738	4753
H16-O16-Ru16	48	0	30	1	31
H16-O22-Ru16	54	0	28	0	28
H16-C4-O4-Ru64	88	0	0	1	1
H16-C4-O8-Ru72	100	0	2	6	8
H16-C6-O2-Ru72	96	0	1	0	1
H17-Ru15	32	0	0	2	2
H19-Ru21	40	69	0	0	69
H20-O2-Ru36	58	0	17	0	17
H22-Ru30	52	0	19	1	20
H22-Ru36	58	0	11	0	11
H23-Ru8	31	0	1	0	1
H23-Ru9	32	0	1	1	2
H24-Ru8	32	0	0	2	2
H30-O15	45	146	4	111	261
total	--	1641	23536	21554	46731

1.3 Benchmark of G-NN potential against DFT calculations

To examine the accuracy of the G-NN potential, we have calculated the energy difference between G-NN and DFT for the representative bulk structures of RuO_x, which shows a low root mean square error (RMSE) of only 8.343 meV/atom, as seen in **Table S2**.

Table S2. Benchmark of NN calculations for RuO_x systems as compared with DFT results. Listed data includes the compositions, O%, NN energy, DFT energy and errors between NN energy and DFT energy.

Chem. Formula	O%	E_{NN}(eV/atom)	E_{DFT}(eV/atom)	Error(meV/atom)
Ru20O5	0.200	-0.670	-0.666	4.226
Ru20O10	0.333	-1.037	-1.037	0.051
Ru20O16	0.444	-1.092	-1.083	-8.896
Ru20O20	0.500	-1.148	-1.145	-2.627
Ru20O28	0.583	-1.242	-1.245	3.066
Ru20O30	0.600	-1.280	-1.278	-1.866
Ru20O32	0.615	-1.319	-1.320	0.623
Ru20O34	0.630	-1.336	-1.343	7.690
Ru20O36	0.643	-1.391	-1.394	3.217
Ru20O38	0.655	-1.426	-1.424	-1.686
Ru20O40	0.667	-1.510	-1.509	-1.130
Ru20O42	0.677	-1.399	-1.399	-0.171

Ru20O44	0.688	-1.368	-1.372	3.860
Ru20O46	0.697	-1.296	-1.296	-0.221
Ru20O48	0.706	-1.217	-1.224	7.144
Ru20O50	0.714	-1.154	-1.146	-7.650
Ru20O60	0.750	-0.907	-0.897	-9.776
Ru10O40	0.800	-0.698	-0.669	-29.00

Ru_xO_y means a unit cell consists of x Ru atom and y O atom.

2. Modified Phenomenal Theory of Martensitic Crystallography, M-PTMC

2.1 Phenomenal Theory of Martensitic Crystallography

PTMC is one of the oldest phase transformation theories, which is developed to explain the phase transition between face-centered cubic austenite (γ-Fe) and body-centered cubic martensite (α–Fe) discovered by Bain in 1924.[8] PTMC takes the existence of invariant plane as the basic geometric constraint. In the invariant plane, the lattice is neither stretched nor compressed during phase transition. The key step of PTMC is to determine the orientation of the invariant plane through the lattice correspondence. The basic idea of PTMC and corresponding mathematical methods have been adopted by other crystallographic theories. Here, we briefly review the algorithm of PTMC.

(a) Determine the Deformation Gradient F

Let us first define the lattice parameters **T** and **M** of two crystals, which are two (3×3) matrices. Each row in **T** and **M** represents a basis vector of the unit cell. The lattice correspondence between two crystals is described by the deformation gradient **F** in Eq. (4).

$$\mathbf{TF} = \mathbf{M} \tag{4}$$

According to the polar decomposition, **F** can be decomposed into rotation and stretching. The Cauchy-Green deformation tensor **C** is then constructed to eliminate the rotation in **F**.

$$\mathbf{C} = \mathbf{F}^{\mathrm{T}}\mathbf{F} \tag{5}$$

It should be noticed that if you define the columns of **T** and **M** to represent the basis vectors, formulas (4)-(5) need to be modified accordingly.

(b) Calculate the orientation of invariant plane

Next, we perform an eigendecomposition of the Cauchy-Green deformation tensor **C**:

$$\mathbf{Ce_i} = I_i\mathbf{e_i} \quad (i=1,2,3) \tag{6}$$

Where I_i and $\mathbf{e_i}$ are the eigenvalues and eigenvectors, which represent the magnitude and direction of strain during phase transition. For clarity, we set $I_1 < I_2 < I_3$ in the following discussions. In a martensitic transformation, the eigenvalues should satisfy the conditions of $I_2 = 1$, $I_1 < 1$, and $I_3 > 1$, while $\mathbf{e_2}$ is the direction of a strain invariant line (**sil**). The lattice along $\mathbf{e_2}$ is neither stretched nor compressed. The direction of another strain invariant line ($\mathbf{sil_2}$) can be calculated by the linear combination of $\mathbf{e_1}$ and $\mathbf{e_3}$ through formulas (7)-(9):

$$a^2 + c^2 = 1 \tag{7}$$

$$a^2I_1 + c^2I_3 = 1 \tag{8}$$

$$\mathbf{sil_2} = a\mathbf{e_1} + c\mathbf{e_3} \quad (9)$$

where a and c are the coefficients of linear combination. The normal vector of strain invariant plane (**sip**) is given by

$$\mathbf{sip} = \mathbf{e_2} \times \mathbf{sil_2} \quad (10)$$

The **sip**, **T**, and **M** define the orientations of the invariant plane.

2.2 Determination of orientation relations in heterojunctions using PTMC

The idea of invariant plane and corresponding mathematical methods in PTMC can be adapted to predict the OR in heterojunctions since a good interface also requires the match of lattice. The difference is the definition of lattice correspondence. In martensitic transformation, the lattice correspondence is explicitly defined by the phase transition channel with the lowest barrier. While in heterojunction, any lattice correspondence is allowed since it is independent of a specific phase transition. Since the definition of a unit cell is not unique, a pair of crystals can generate an infinite number of lattice correspondences. Therefore, the basic idea to predict the OR in heterojunctions is to sample numerous lattice correspondences by changing the definition of the unit cell and then calculate the orientation of invariant plane through PTMC. The calculation details of OR in heterojunctions are described as follows.

First, we produce a set of lattice correspondence. Mathematically, the definition of lattice parameters for a crystal can be generally denoted by the product of the lattice parameters of primitive cell and a transformation matrix, as shown in Eq. (11)-(12).

$$\mathbf{T} = \mathbf{AT'} \quad (11)$$

$$\mathbf{M} = \mathbf{BM'} \quad (12)$$

where **A** and **B** represent the transformation matrices; **T'** and **M'** the lattice parameters of primitive cell for two materials. All matrix elements of A_{ij} and B_{ij} are integers due to the translational symmetry of lattice. Any transformation matrices **A** and **B** are allowed if their determinants are positive. Therefore, a set of deformation gradient **F** can be obtained by exhausting matrices **A** and **B**.

With deformation gradient **F**, we can calculate **sip** with Eq. (4)-(10). According to PTMC, the existence of invariant plane requires the eigenvalue I_2 of the Cauchy-Green deformation tensor **C** close to 1.[9-11] Otherwise, no invariant plane exists for this lattice correspondence. Thus, we screen out the lattice correspondence with $I_2 > 1.05$ or $I_2 < 0.95$.

On the other hand, since there is an infinite number of transformation matrices **A** and **B**, a cutoff for the matrix elements A_{ij} and B_{ij} must be applied. In our implementation, we set $A_{ij} \in \{-2, -1, 0, 1, 2\}$ and $B_{ij} \in \{-2, -1, 0, 1, 2\}$. Our test shows that this criterion can correctly produce the OR observed in experiments for a series of heterojunctions. It should be noted that the simultaneous enumeration of both **A** and **B** matrices is necessary. Otherwise, some OR observed in experiments might be missed.

3. Structures for the GM of RuO_X

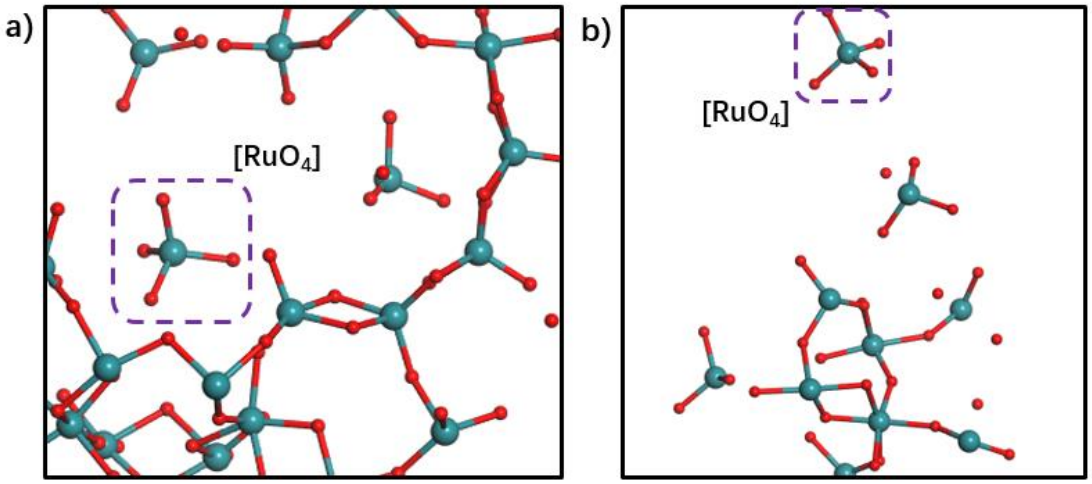


Figure S1. The GM of RuO_x at high O% content obtained from SSW-NN search (a) $Ru_{20}O_{60}$ (O%=0.75), and (b) $Ru_{10}O_{40}$ (O%=0.8) per unit cell. [RuO_4] indicates the four-coordinated Ru monomer in the gas phase. Ru atoms, green balls; O atoms, red balls.

Reference

(1) Huang, S.-D.; Shang, C.; Zhang, X.-J.; Liu, Z.-P. Material Discovery by Combining Stochastic Surface Walking Global Optimization with a Neural Network. *Chem. Sci.* **2017**, *8*, 6327-6337.

(2) Huang, S.-D.; Shang, C.; Kang, P.-L.; Liu, Z.-P. Atomic Structure of Boron Resolved Using Machine Learning and Global Sampling. *Chem. Sci.* **2018**, *9*, 8644-8655.

(3) Shang, C.; Huang, S.-D.; Liu, Z.-P. Massively Parallelization Strategy for Material Simulation Using High-Dimensional Neural Network Potential. *J. Comput. Chem.* **2019**, *40*, 1091-1096.

(4) Shang, C.; Liu, Z.-P. Stochastic Surface Walking Method for Structure Prediction and Pathway Searching. *J. Chem. Theory Comput.* **2013**, *9*, 1838-1845.

(5) Zhang, X.-J.; Shang, C.; Liu, Z.-P. From Atoms to Fullerene: Stochastic Surface Walking Solution for Automated Structure Prediction of Complex Material. *J. Chem. Theory Comput.* **2013**, *9*, 3252-3260.

(6) Shang, C.; Zhang, X.-J.; Liu, Z.-P. Stochastic Surface Walking Method for Crystal Structure and Phase Transition Pathway Prediction. *Phys. Chem. Chem. Phys.* **2014**, *16*, 17845-17856.

(7) Ma, S.; Shang, C.; Liu, Z.-P. Heterogeneous Catalysis from Structure to Activity via SSW-NN Method. *J. Chem. Phys.* **2019**, *151*, 050901.

(8) Bain, E. C.; Dunkirk, N. Y., The nature of martensite. Trans. AIME 1924, 70, 25-46.

(9) Bowles, J. S.; Mackenzie, J. K., The crystallography of martensite transformations I. Acta Metallurgica 1954, 2 (1), 129-137.

(10) Mackenzie, J. K.; Bowles, J. S., The crystallography of martensite transformations II. Acta Metallurgica 1954, 2 (1), 138-147.

(11) Wayman, C. M., The phenomenological theory of martensite crystallography: Inter-

relationships. Metallurgical and Materials Transactions A 1994, 25 (9), 1787-1795.
(12) Knapp M , Seitsonen A P , Kim Y D , et al. Catalytic activity of the RuO2(100) surface in the oxidation of CO. J.phys.chem.b, 2004, 108(38):14392-14397.

4. XYZ coordinates for important structures of RuO_X

VASP POSCAR format

POSCAR (Ru_2O)

1.00000000

16.25024 0.00000 0.00000

-0.54122 5.49747 0.00000

-0.47735 -0.05345 4.24686

O Ru

10 20

D

0.861211 0.766355 0.155897

0.584515 0.480570 0.580921

0.695544 0.492904 0.129961

0.750010 0.752469 0.606524

0.530543 0.713419 0.046409

0.583411 0.983513 0.559692

0.751392 0.251616 0.640746

0.915047 0.533992 0.688105

0.694143 0.993726 0.094228

0.862289 0.263492 0.174570

0.975407 0.299272 0.010550

0.469984 0.443417 0.723661

0.173434 0.362103 0.595081

0.031945 0.068833 0.536390

0.124060 0.095791 0.075711

0.639672 0.741884 0.339804

0.805925 0.504056 0.395814

0.802951 0.001962 0.905302

0.030133 0.568891 0.532533

0.413591 0.180043 0.196115

0.123323 0.595587 0.074882

0.642685 0.244083 0.830415

0.173396 0.858298 0.595170
0.322220 0.653709 0.657172
0.415453 0.680277 0.200320
0.272112 0.887213 0.136577
0.470219 0.949298 0.722722
0.321487 0.153362 0.656191
0.272123 0.390999 0.136514
0.975440 0.805414 0.009281

POSCAR (RuO)
1.00000000
18.92066 0.00000 0.00000
-0.34916 5.57247 0.00000
0.00001 -0.00018 4.37444
O Ru
20 20
D
0.073700 0.536384 0.414872
0.024246 0.775482 0.914869
0.164781 0.491783 0.917859
0.305210 0.732171 0.977408
0.212706 0.747645 0.498245
0.024224 0.276677 0.003525
0.885660 0.063305 0.927390
0.355393 0.989739 0.420995
0.352924 0.491438 0.481027
0.305629 0.230300 0.950344
0.934944 0.319462 0.499623
0.742519 0.322208 0.920627
0.792310 0.081695 0.450159
0.933155 0.820141 0.417841
0.163010 0.992469 0.999529
0.792743 0.579805 0.477396
0.212285 0.248561 0.427454
0.073717 0.035243 0.503490
0.885230 0.564204 0.998360

0.744998 0.820522 0.980804
0.647184 0.803006 0.174224
0.694918 0.046507 0.670541
0.118810 0.762222 0.707848
0.254796 0.980113 0.208736
0.404021 0.736124 0.173875
0.450756 0.509030 0.674371
0.529832 0.523946 0.168928
0.528841 0.029574 0.170705
0.568105 0.788120 0.668829
0.449031 0.010840 0.679275
0.259344 0.482191 0.710838
0.693899 0.575871 0.673575
0.118524 0.264756 0.211548
0.403012 0.265410 0.170789
0.569083 0.282539 0.670682
0.838598 0.829737 0.210776
0.843145 0.331798 0.708719
0.979423 0.047143 0.711566
0.979132 0.549675 0.207886
0.648911 0.301189 0.179130

POSCAR (Ru_2O_3)
1.00000000
4.42767 0.00000 0.00000
-0.04467 12.93535 0.00000
0.02683 -3.01506 9.69459
O Ru
30 20
D
0.554325 0.299300 0.651232
0.015660 0.156601 0.623261
0.025769 0.638704 0.996099
0.514460 0.652519 0.435962
0.503250 0.413975 0.242977
0.025878 0.399732 0.810207

0.033696	0.985514	0.749419
0.068992	0.812335	0.880763
0.050374	0.039546	0.039956
0.081056	0.220020	0.915523
0.583150	0.473236	0.542208
0.514855	0.536090	0.841822
0.547482	0.773366	0.023538
0.090595	0.575825	0.697834
0.007973	0.516192	0.398965
0.087848	0.695763	0.291814
0.084146	0.335491	0.504961
0.586645	0.359910	0.950146
0.027728	0.753487	0.585932
0.582564	0.711017	0.729622
0.030983	0.277880	0.211317
0.525992	0.177552	0.050383
0.520339	0.948763	0.884434
0.557090	0.123621	0.759529
0.581729	0.833775	0.317488
0.022919	0.880517	0.171568
0.549694	0.886298	0.603581
0.085045	0.459093	0.102301
0.087002	0.934505	0.463789
0.583757	0.593614	0.141704
0.766689	0.020119	0.602790
0.804190	0.730617	0.163596
0.785036	0.982176	0.332656
0.312765	0.076279	0.464193
0.299919	0.222229	0.342777
0.309265	0.017248	0.202213
0.301190	0.679471	0.865780
0.308967	0.434400	0.675739
0.296145	0.078999	0.890182
0.804094	0.613348	0.565847
0.294962	0.554915	0.270856
0.306486	0.318545	0.073704
0.803717	0.850533	0.748101

0.753796 0.910774 0.024782
0.800237 0.262116 0.793753
0.307443 0.793997 0.453411
0.763429 0.371185 0.372651
0.779732 0.136655 0.197800
0.778938 0.205371 0.476889
0.803574 0.499828 0.973063

POSCAR (RuO_2)
1.00000000
8.47231 6.10322 -0.00387
-1.97071 6.10824 0.00259
-1.10871 2.99517 10.12217
O Ru
40 20
D
0.511867 0.295154 0.839590
0.512088 0.907642 0.838762
0.212086 0.107607 0.738782
0.923115 0.263194 0.105611
0.711863 0.495108 0.239606
0.200821 0.539495 0.272779
0.412092 0.307619 0.138755
0.023128 0.863202 0.805615
0.423114 0.263241 0.605591
0.811862 0.095119 0.939614
0.700821 0.539536 0.772786
0.011865 0.295076 0.339616
0.723127 0.063216 0.705598
0.823119 0.663178 0.405601
0.612082 0.507611 0.538782
0.123134 0.463190 0.505612
0.211858 0.495139 0.739604
0.111862 0.895099 0.039625
0.411867 0.695142 0.139590
0.611874 0.895131 0.539588

0.712076	0.107594	0.238779
0.323119	0.663251	0.905596
0.300824	0.139504	0.972778
0.000830	0.339477	0.872787
0.812075	0.707607	0.938781
0.223132	0.063210	0.205603
0.400826	0.739537	0.672770
0.523121	0.863238	0.305593
0.311857	0.095137	0.439591
0.911871	0.695110	0.639604
0.623128	0.463256	0.005587
0.012087	0.907559	0.338794
0.312081	0.707605	0.438776
0.500825	0.339528	0.372769
0.600823	0.939524	0.072773
0.112090	0.507576	0.038786
0.100824	0.939502	0.572785
0.900828	0.739449	0.172798
0.912083	0.307589	0.638795
0.800828	0.139492	0.472793
0.111969	0.201341	0.039198
0.261974	0.601364	0.089189
0.961973	0.801339	0.989205
0.611973	0.201374	0.539186
0.711972	0.801348	0.239191
0.061974	0.401355	0.689200
0.311973	0.401368	0.439185
0.761975	0.601360	0.589195
0.461975	0.801378	0.489180
0.861971	0.201325	0.289204
0.661976	0.001383	0.889183
0.511971	0.601402	0.839180
0.361973	0.201388	0.789185
0.011976	0.601313	0.339204
0.211974	0.801374	0.739190
0.161975	0.001342	0.389192
0.411978	0.001382	0.139182

0.561976 0.401376 0.189179
0.811979 0.401358 0.939197
0.911978 0.001352 0.639200

5. XYZ coordinates for important structures of interfaces between Ru and RuO_2

VASP POSCAR format
POSCAR (OR_1)
1.00000000
4.32289 -0.00376 0.00830
-0.00294 5.49117 -0.00211
0.00160 -0.00050 22.54204
O Ru
12 22
D
0.212404 0.994697 0.091215
0.189635 0.412683 0.819928
0.234410 0.493107 0.588624
0.191203 0.717008 0.705901
0.250613 0.217689 0.704951
0.692602 0.494459 0.087909
0.242769 0.910746 0.819544
0.684696 0.457959 0.743704
0.739247 0.248307 0.627365
0.716769 0.749678 0.626740
0.743732 0.958927 0.747056
0.195653 0.993489 0.591612
0.460401 0.994919 0.169101
0.986340 0.494514 0.237686
0.472872 0.242159 0.270102
0.957805 0.994853 0.236055
0.471430 0.743718 0.477474
0.967719 0.993911 0.446680
0.973717 0.243014 0.340804
0.973956 0.745578 0.340849

0.467316 0.994536 0.377473
0.964743 0.494269 0.446825
0.471467 0.244195 0.477616
0.472643 0.494111 0.377165
0.980000 0.723910 0.133275
0.472903 0.747075 0.270084
0.484211 0.494457 0.169002
0.979783 0.265324 0.133178
0.990046 0.676359 0.783184
0.964724 0.249238 0.545918
0.436880 0.178941 0.783195
0.964931 0.988688 0.669711
0.966442 0.738039 0.545915
0.474484 0.488779 0.663903

POSCAR (OR_2)
1.00000000
5.43512 -0.00030 0.00060
-0.00039 4.70390 -0.01804
0.00008 -0.00341 25.98838
O Ru
12 30
D
0.840716 0.337673 0.669873
0.610117 0.831545 0.628432
0.110095 0.950901 0.628434
0.341100 0.445565 0.669679
0.179214 0.330539 0.475875
0.925393 0.853577 0.724829
0.425307 0.932351 0.724672
0.677737 0.448761 0.474569
0.509648 0.323753 0.571582
0.281867 0.821088 0.531564
0.782336 0.961385 0.531158
0.008143 0.457252 0.572109
0.194620 0.558852 0.165070

0.945308	0.059673	0.164890
0.194508	0.890903	0.082212
0.444592	0.059972	0.164443
0.444982	0.391514	0.081988
0.695477	0.559011	0.164746
0.945630	0.391632	0.081811
0.695224	0.891135	0.082162
0.693066	0.561927	0.330928
0.446909	0.061682	0.330474
0.695189	0.894778	0.247674
0.945682	0.054477	0.331430
0.944633	0.394200	0.248321
0.196153	0.561466	0.331338
0.444580	0.392766	0.247908
0.195799	0.896271	0.248149
0.695857	0.555352	0.002188
0.445527	0.057856	0.002167
0.192017	0.889021	0.412579
0.945737	0.056771	0.002253
0.441852	0.394067	0.411752
0.195044	0.554876	0.002189
0.946464	0.387616	0.410718
0.709899	0.885265	0.412943
0.811197	0.148135	0.600788
0.310943	0.633428	0.600847
0.149424	0.115755	0.696622
0.649657	0.669302	0.696638
0.480431	0.115793	0.500304
0.981123	0.665925	0.500993

POSCAR (OR_3)

1.00000000

4.26570	0.00000	0.00000
0.00000	4.74630	0.00000
0.00000	0.00000	22.70751

O Ru

12 18

D

0.812096	0.386470	0.719531
0.232375	0.027267	0.580216
0.728947	0.874260	0.648806
0.297789	0.521599	0.648781
0.667005	0.960133	0.118396
0.797782	0.372195	0.579654
0.240352	0.969666	0.827078
0.212520	0.011194	0.719678
0.737863	0.869138	0.512400
0.286481	0.537466	0.512822
0.785817	0.428164	0.826981
0.264777	0.410064	0.087877
0.532652	0.053221	0.203753
0.037192	0.222174	0.385224
0.530372	0.575781	0.146431
0.035708	0.719070	0.326125
0.536699	0.547249	0.385262
0.534866	0.551388	0.266246
0.037782	0.221894	0.264080
0.512347	0.698759	0.719917
0.536104	0.055774	0.325179
0.029814	0.211512	0.145628
0.533553	0.057846	0.441361
0.030546	0.709461	0.446912
0.022867	0.203444	0.507254
0.012582	0.198790	0.648378
0.012212	0.699656	0.781241
0.036962	0.723323	0.208260
0.513489	0.198262	0.780429
0.511961	0.697199	0.580975

POSCAR (OR_4)

1.00000000

6.43425 -0.17809 -0.03319

0.49456 6.30969 0.17123

-0.00507 0.04581 24.26186

O Ru

24 36

D

0.703746 0.712972 0.629559

0.392259 0.459844 0.576177

0.392473 0.959652 0.576260

0.894286 0.957029 0.545116

0.894547 0.456585 0.545094

0.587134 0.203931 0.494242

0.703847 0.212975 0.629555

0.587125 0.703882 0.494064

0.700699 0.726771 0.359665

0.392387 0.482611 0.320642

0.389473 0.974492 0.312834

0.393842 0.454754 0.676608

0.393787 0.954733 0.676323

0.082281 0.703173 0.629812

0.696915 0.229874 0.360479

0.082430 0.203173 0.629844

0.200494 0.215205 0.493854

0.891723 0.961816 0.445407

0.893391 0.463190 0.442413

0.395888 0.461782 0.416879

0.394182 0.964118 0.416474

0.087894 0.715451 0.360329

0.200772 0.715469 0.493898

0.081280 0.209409 0.362636

0.922917 0.223058 0.112294

0.340843 0.140919 0.113571

0.424527 0.722361 0.113167

0.842245 0.640154 0.112907

0.175831 0.472250 0.168270

0.591838 0.384557 0.168641

0.674557 0.972889 0.167681

0.091552 0.887120 0.168173

0.434509	0.706217	0.221157
0.838080	0.636248	0.222768
0.934901	0.208336	0.220852
0.338209	0.133849	0.223355
0.683764	0.948077	0.275036
0.094710	0.873171	0.277160
0.140437	0.457887	0.273790
0.639112	0.358013	0.277066
0.424024	0.728173	0.004153
0.842367	0.643420	0.004414
0.923196	0.227095	0.004200
0.342910	0.142033	0.004317
0.678794	0.976625	0.055846
0.088305	0.888976	0.055800
0.179073	0.475981	0.055532
0.587257	0.389975	0.055572
0.394176	0.960097	0.496212
0.393777	0.459572	0.496074
0.893715	0.210500	0.494240
0.894506	0.707922	0.494381
0.892816	0.458539	0.623021
0.892966	0.958607	0.623079
0.392778	0.708668	0.631312
0.393233	0.209242	0.631349
0.891549	0.469728	0.359100
0.892839	0.973379	0.364442
0.399302	0.719045	0.369786
0.383189	0.215017	0.367952

POSCAR (OR_5)

1.00000000

5.01227	-0.10926	0.02582
0.78944	9.17156	-0.08277
0.00222	-0.02613	29.20289

O Ru

24 60

D

0.797691	0.565585	0.607002
0.800775	0.236109	0.608272
0.802226	0.903774	0.609969
0.672292	0.729553	0.682917
0.301495	0.735646	0.621758
0.671949	0.398930	0.683260
0.300329	0.401746	0.620549
0.671021	0.066222	0.683621
0.305186	0.069896	0.622768
0.192329	0.899556	0.697099
0.193233	0.566179	0.696640
0.194124	0.233873	0.697068
0.866235	0.905173	0.758406
0.868376	0.571897	0.758660
0.868316	0.239336	0.758732
0.703501	0.386871	0.527673
0.262357	0.388348	0.484248
0.719522	0.055889	0.532882
0.199783	0.038289	0.468376
0.694270	0.732168	0.532702
0.288172	0.745553	0.477322
0.176938	0.564555	0.550050
0.196253	0.220396	0.548342
0.187312	0.895460	0.551654
0.099995	0.732217	0.079191
0.599394	0.732903	0.106473
0.849917	0.482416	0.079263
0.349724	0.982549	0.079235
0.849135	0.982956	0.106355
0.349172	0.482810	0.106453
0.599683	0.232091	0.079226
0.098879	0.232970	0.106385
0.722701	0.359117	0.161072
0.222347	0.359802	0.188043
0.472747	0.109039	0.161013
0.973193	0.609466	0.161159

0.472316	0.610196	0.188167
0.972436	0.109362	0.188475
0.222696	0.859282	0.161086
0.722002	0.859815	0.188244
0.346549	0.986091	0.242174
0.844653	0.986792	0.269634
0.095600	0.736439	0.241821
0.595437	0.236244	0.241775
0.094442	0.236568	0.269203
0.595427	0.738773	0.269415
0.845133	0.486755	0.241772
0.343722	0.486916	0.269202
0.969674	0.614972	0.324010
0.467604	0.616828	0.349213
0.717954	0.365448	0.322761
0.217684	0.864965	0.324408
0.717102	0.866049	0.353557
0.218740	0.364111	0.349760
0.468340	0.114138	0.323851
0.966742	0.116533	0.350111
0.598015	0.244466	0.404330
0.094643	0.239339	0.433453
0.331299	0.992472	0.403142
0.840913	0.491201	0.402133
0.346724	0.492225	0.427909
0.822863	0.004080	0.434305
0.090284	0.739674	0.405412
0.588034	0.733942	0.431078
0.477052	0.105011	0.001569
0.976352	0.105690	0.025734
0.227243	0.854693	0.001543
0.726817	0.355273	0.001584
0.226096	0.355787	0.025698
0.726147	0.855781	0.025743
0.977091	0.605091	0.001527
0.476475	0.605726	0.025697
0.488313	0.565862	0.650901

0.490338 0.234848 0.651640
0.993728 0.394503 0.576351
0.004094 0.065976 0.579842
0.490347 0.900070 0.652375
0.988941 0.733743 0.578860
0.506494 0.210418 0.501236
0.491193 0.908244 0.506265
0.972312 0.734903 0.723404
0.971740 0.402162 0.723437
0.487513 0.562909 0.508286
0.972558 0.068800 0.723770

6. XYZ coordinates for important structures of $RuO_X/Ru(10\bar{1}0)$

VASP POSCAR format
POSCAR (0.5ML)
1.00000000
10.90720 0.00000 0.00000
0.00000 8.57660 0.00000
0.00000 0.00000 35.76230
O Ru
4 64
D
0.243933 0.246848 0.748273
0.753126 0.744788 0.748183
0.494741 0.001845 0.747738
0.502981 0.502099 0.747759
0.123560 0.125000 0.500000
0.998557 0.375000 0.522059
0.248973 0.125000 0.566105
0.123970 0.375000 0.588165
0.373561 0.125000 0.500000
0.248559 0.375000 0.522059
0.498974 0.125000 0.566105
0.373971 0.375000 0.588165
0.123560 0.625000 0.500000

0.998557	0.875000	0.522059
0.248973	0.625000	0.566105
0.123970	0.875000	0.588165
0.373561	0.625000	0.500000
0.248559	0.875000	0.522059
0.498974	0.625000	0.566105
0.373971	0.875000	0.588165
0.623560	0.125000	0.500000
0.498557	0.375000	0.522059
0.748973	0.125000	0.566105
0.623970	0.375000	0.588165
0.873561	0.125000	0.500000
0.748559	0.375000	0.522059
0.998974	0.125000	0.566105
0.873971	0.375000	0.588165
0.623560	0.625000	0.500000
0.498557	0.875000	0.522059
0.748973	0.625000	0.566105
0.623970	0.875000	0.588165
0.873561	0.625000	0.500000
0.748559	0.875000	0.522059
0.998974	0.625000	0.566105
0.873971	0.875000	0.588165
0.124032	0.124971	0.633015
0.999402	0.375042	0.654579
0.248834	0.877499	0.654963
0.500874	0.121679	0.697986
0.373960	0.124219	0.633357
0.249093	0.376675	0.653669
0.245665	0.627937	0.697758
0.626296	0.875852	0.720258
0.123854	0.625663	0.632693
0.998246	0.875107	0.654634
0.246288	0.127692	0.698289
0.874420	0.373193	0.717438
0.497755	0.371490	0.654037
0.373904	0.625412	0.632967

0.373366 0.873823 0.718808
0.748827 0.377319 0.654885
0.623673 0.125364 0.632970
0.123796 0.376488 0.718840
0.872979 0.876003 0.718828
0.371382 0.376152 0.720177
0.873868 0.125547 0.632696
0.496593 0.621738 0.697961
0.751103 0.627303 0.698114
0.000384 0.623967 0.697905
0.623665 0.624174 0.633297
0.499895 0.871488 0.654032
0.122910 0.873138 0.717499
0.996967 0.123837 0.697937
0.873662 0.625051 0.632981
0.748594 0.876687 0.653691
0.751824 0.127708 0.697783
0.623967 0.373861 0.718802

POSCAR (1ML)
1.00000000
8.53140 0.00000 0.00000
0.00000 10.96120 0.00000
0.00000 0.00000 21.39580
O Ru
8 64
D
0.933581 0.497853 0.688931
0.665786 0.746181 0.690940
0.449287 0.998402 0.690980
0.678153 0.747517 0.229729
0.189510 0.744621 0.688730
0.189431 0.252182 0.688463
0.665725 0.248956 0.690959
0.924679 0.997786 0.687791
0.056899 0.122939 0.280796

0.056903	0.372924	0.280796
0.306719	0.122681	0.422114
0.306830	0.372722	0.422125
0.056793	0.997591	0.385525
0.056806	0.247586	0.385541
0.306462	0.998311	0.533903
0.306964	0.248269	0.533849
0.056934	0.372813	0.498252
0.056517	0.122764	0.498241
0.306867	0.247907	0.313006
0.306868	0.997904	0.312997
0.556899	0.122939	0.280796
0.556903	0.372924	0.280796
0.806719	0.122681	0.422114
0.806830	0.372722	0.422125
0.556793	0.997591	0.385525
0.556806	0.247586	0.385541
0.806462	0.998311	0.533903
0.806964	0.248269	0.533849
0.556934	0.372813	0.498252
0.556517	0.122764	0.498241
0.806867	0.247907	0.313006
0.806868	0.997904	0.312997
0.056899	0.622939	0.280796
0.056903	0.872924	0.280796
0.306719	0.622681	0.422114
0.306830	0.872722	0.422125
0.056793	0.497591	0.385525
0.056806	0.747586	0.385541
0.306462	0.498311	0.533903
0.306964	0.748269	0.533849
0.056972	0.873275	0.498647
0.057187	0.623144	0.498303
0.304295	0.747678	0.313902
0.306995	0.497594	0.312644
0.556214	0.620518	0.278276
0.555425	0.874497	0.278196

0.807007 0.623005 0.421790
0.806877 0.872765 0.422214
0.556694 0.498115 0.385287
0.555121 0.747774 0.387333
0.805664 0.498014 0.531943
0.810038 0.747665 0.533611
0.557298 0.872982 0.498594
0.556552 0.623491 0.497695
0.804775 0.747870 0.312507
0.808066 0.495215 0.313615
0.307243 0.880298 0.644095
0.805144 0.625527 0.643368
0.557848 0.745502 0.605983
0.554638 0.498213 0.605734
0.061028 0.747777 0.607047
0.307547 0.615986 0.642118
0.806236 0.864110 0.643889
0.052665 0.497993 0.605915
0.804631 0.370462 0.643471
0.806307 0.131736 0.643738
0.557276 0.250207 0.606074
0.555519 0.998067 0.605948
0.307679 0.380832 0.642066
0.307148 0.116087 0.644124
0.060586 0.248461 0.606880
0.053027 0.998133 0.606968

POSCAR (1.75ML)
1.00000000
10.90720 0.00000 0.00000
0.00000 8.57660 0.00000
0.00000 0.00000 35.76230
O Ru
14 64
D
0.746914 0.371676 0.760918

0.744071	0.723449	0.749379
0.255921	0.717666	0.747608
0.254890	0.033782	0.747808
0.496724	0.879950	0.761521
0.004371	0.723007	0.748589
0.252192	0.375910	0.759317
0.877102	0.877307	0.811361
0.501175	0.218784	0.747919
0.999954	0.022133	0.746678
0.749483	0.023491	0.747527
0.999455	0.373931	0.760501
0.872678	0.835382	0.694561
0.501230	0.533385	0.748019
0.123560	0.125000	0.500000
0.998557	0.375000	0.522059
0.248973	0.125000	0.566105
0.123970	0.375000	0.588165
0.373561	0.125000	0.500000
0.248559	0.375000	0.522059
0.498974	0.125000	0.566105
0.373971	0.375000	0.588165
0.123560	0.625000	0.500000
0.998557	0.875000	0.522059
0.248973	0.625000	0.566105
0.123970	0.875000	0.588165
0.373561	0.625000	0.500000
0.248559	0.875000	0.522059
0.498974	0.625000	0.566105
0.373971	0.875000	0.588165
0.623560	0.125000	0.500000
0.498557	0.375000	0.522059
0.748973	0.125000	0.566105
0.623970	0.375000	0.588165
0.873561	0.125000	0.500000
0.748559	0.375000	0.522059
0.998974	0.125000	0.566105
0.873971	0.375000	0.588165

0.623560	0.625000	0.500000
0.498557	0.875000	0.522059
0.748973	0.625000	0.566105
0.623970	0.875000	0.588165
0.873561	0.625000	0.500000
0.748559	0.875000	0.522059
0.998974	0.625000	0.566105
0.873971	0.875000	0.588165
0.123696	0.126360	0.633075
0.000018	0.376793	0.654183
0.617191	0.876188	0.722864
0.998170	0.131429	0.697332
0.373761	0.124078	0.633114
0.250352	0.375351	0.654418
0.133993	0.875283	0.727105
0.124965	0.376168	0.722911
0.124939	0.623978	0.632809
0.003292	0.876045	0.654151
0.371677	0.876291	0.723003
0.248513	0.626570	0.696754
0.373868	0.626767	0.633204
0.246001	0.875598	0.653763
0.500687	0.620118	0.696530
0.747159	0.376999	0.655126
0.624321	0.125478	0.632896
0.498870	0.375481	0.652627
0.871785	0.375554	0.723568
0.751036	0.125225	0.697274
0.874204	0.128129	0.633309
0.997586	0.622699	0.697438
0.500087	0.131676	0.696548
0.383388	0.376284	0.722764
0.623229	0.625100	0.632701
0.500085	0.875704	0.655732
0.618834	0.376195	0.722958
0.874277	0.871954	0.763557
0.874130	0.622376	0.632280

0.746052 0.876892 0.653305
0.248590 0.124647 0.696886
0.751809 0.629923 0.697476

POSCAR (4ML)
1.00000000
8.53140 0.00000 0.00000
0.00000 10.96120 0.00000
0.00000 0.00000 22.98250
O Ru
32 80
D
0.820451 0.642666 0.840866
0.101804 0.942904 0.647969
0.010256 0.692842 0.647981
0.570691 0.622010 0.769779
0.320453 0.642635 0.840890
0.791612 0.392666 0.840833
0.791608 0.892720 0.840831
0.541353 0.871987 0.769799
0.273870 0.242271 0.724784
0.601490 0.443065 0.647933
0.510339 0.192970 0.647947
0.291564 0.892718 0.840874
0.774002 0.242238 0.724763
0.338276 0.992318 0.724770
0.041404 0.372021 0.769775
0.291656 0.392655 0.840886
0.570653 0.122020 0.769767
0.101733 0.442924 0.647990
0.010263 0.192863 0.647965
0.320370 0.142660 0.840900
0.041428 0.872032 0.769782
0.820401 0.142683 0.840864
0.541408 0.371998 0.769743
0.838207 0.492268 0.724743

0.273908	0.742279	0.724797
0.601773	0.942901	0.647986
0.510238	0.692917	0.647971
0.070663	0.622046	0.769785
0.774058	0.742225	0.724789
0.338183	0.492263	0.724793
0.070649	0.122064	0.769771
0.838311	0.992303	0.724733
0.056170	0.121709	0.257553
0.056174	0.371711	0.257554
0.305795	0.120329	0.389016
0.305897	0.370323	0.389013
0.055944	0.995507	0.354960
0.055954	0.245501	0.354958
0.306108	0.246517	0.287477
0.306111	0.996519	0.287479
0.556170	0.121709	0.257553
0.556174	0.371711	0.257554
0.805795	0.120329	0.389016
0.805897	0.370323	0.389013
0.555944	0.995507	0.354960
0.555954	0.245501	0.354958
0.806108	0.246517	0.287477
0.806111	0.996519	0.287479
0.056170	0.621709	0.257553
0.056174	0.871711	0.257554
0.305795	0.620329	0.389016
0.305897	0.870323	0.389013
0.055944	0.495507	0.354960
0.055954	0.745501	0.354958
0.306108	0.746517	0.287477
0.306111	0.496519	0.287479
0.556170	0.621709	0.257553
0.556174	0.871711	0.257554
0.805795	0.620329	0.389016
0.805897	0.870323	0.389013
0.555944	0.495507	0.354960

0.555954	0.745501	0.354958
0.806108	0.746517	0.287477
0.806111	0.496519	0.287479
0.806246	0.496440	0.492971
0.805480	0.746426	0.492985
0.555709	0.870744	0.459742
0.555961	0.620783	0.459755
0.557446	0.742303	0.559962
0.554203	0.492383	0.559942
0.920030	0.509987	0.804770
0.192103	0.760024	0.804822
0.928737	0.844094	0.688129
0.183520	0.594132	0.688145
0.794228	0.871885	0.595259
0.817408	0.621954	0.595224
0.306254	0.996364	0.493031
0.305518	0.246446	0.493043
0.055785	0.370613	0.459796
0.056031	0.120667	0.459864
0.057445	0.242238	0.559989
0.054121	0.992065	0.559960
0.419988	0.010050	0.804808
0.692046	0.260020	0.804765
0.428504	0.344132	0.688107
0.683595	0.094140	0.688091
0.294270	0.371946	0.595260
0.317462	0.121933	0.595240
0.806135	0.996409	0.492982
0.805431	0.246447	0.492998
0.555697	0.370798	0.459749
0.555946	0.120762	0.459742
0.557482	0.242287	0.559968
0.554252	0.992321	0.559980
0.920040	0.010040	0.804762
0.192035	0.260026	0.804808
0.928589	0.344130	0.688091
0.183566	0.094144	0.688113

0.794153	0.371952	0.595250
0.817460	0.121902	0.595214
0.306230	0.496417	0.493041
0.305461	0.746504	0.493013
0.055674	0.870723	0.459752
0.056133	0.620665	0.459803
0.057456	0.742247	0.559995
0.054111	0.492174	0.559989
0.420052	0.509997	0.804805
0.692088	0.760014	0.804779
0.428667	0.844111	0.688153
0.683503	0.594146	0.688119
0.294349	0.871951	0.595266
0.317399	0.621989	0.595248

7. XYZ coordinates for important structures of initial and transition states on CO oxidation

VASP POSCAR format

POSCAR (IS: CO + O_h on Ru($10\bar{1}0$))

1.00000000

10.90720	0.00000	0.00000
0.00000	8.57660	0.00000
0.00000	0.00000	35.76230

C O Ru

1 2 64

D

0.751461	0.792035	0.758825
0.752000	0.746692	0.790281
0.373140	0.655757	0.741894
0.123560	0.125000	0.500000
0.998557	0.375000	0.522059
0.248973	0.125000	0.566105
0.123970	0.375000	0.588165
0.373561	0.125000	0.500000
0.248559	0.375000	0.522059
0.498974	0.125000	0.566105
0.373971	0.375000	0.588165
0.123560	0.625000	0.500000

0.998557	0.875000	0.522059
0.248973	0.625000	0.566105
0.123970	0.875000	0.588165
0.373561	0.625000	0.500000
0.248559	0.875000	0.522059
0.498974	0.625000	0.566105
0.373971	0.875000	0.588165
0.623560	0.125000	0.500000
0.498557	0.375000	0.522059
0.748973	0.125000	0.566105
0.623970	0.375000	0.588165
0.873561	0.125000	0.500000
0.748559	0.375000	0.522059
0.998974	0.125000	0.566105
0.873971	0.375000	0.588165
0.623560	0.625000	0.500000
0.498557	0.875000	0.522059
0.748973	0.625000	0.566105
0.623970	0.875000	0.588165
0.873561	0.625000	0.500000
0.748559	0.875000	0.522059
0.998974	0.625000	0.566105
0.873971	0.875000	0.588165
0.124594	0.125431	0.632709
0.999361	0.375161	0.654412
0.373726	0.874548	0.718126
0.750415	0.125240	0.698175
0.374116	0.125221	0.632778
0.248982	0.375938	0.655098
0.874211	0.874898	0.718825
0.875483	0.374545	0.717398
0.124034	0.624650	0.632777
0.000360	0.874574	0.653772
0.120538	0.878761	0.717482
0.001139	0.625697	0.698067
0.374149	0.624648	0.632564
0.248850	0.874774	0.654599
0.249414	0.623194	0.699443
0.749099	0.375783	0.654608
0.623927	0.124370	0.632963
0.498961	0.375974	0.655060
0.625454	0.369555	0.717569
0.498286	0.123447	0.698294
0.873891	0.124389	0.632706

0.747582 0.622740 0.698649
0.249676 0.123873 0.698319
0.121899 0.371692 0.717486
0.624269 0.625110 0.632855
0.498666 0.874558 0.654067
0.498409 0.623989 0.699418
0.373745 0.368948 0.718312
0.874094 0.625234 0.632897
0.748854 0.874095 0.654900
0.998583 0.124824 0.698035
0.629677 0.878612 0.719316

POSCAR (TS: CO + O_h on Ru(10$\bar{1}$0))
1.00000000
10.90720 0.00000 0.00000
0.00000 8.57660 0.00000
0.00000 0.00000 35.76230
C O Ru
1 2 64
D
0.587661 0.756692 0.765089
0.619259 0.714353 0.795030
0.441533 0.690157 0.751561
0.123560 0.125000 0.500000
0.998557 0.375000 0.522059
0.248973 0.125000 0.566105
0.123970 0.375000 0.588165
0.373561 0.125000 0.500000
0.248559 0.375000 0.522059
0.498974 0.125000 0.566105
0.373971 0.375000 0.588165
0.123560 0.625000 0.500000
0.998557 0.875000 0.522059
0.248973 0.625000 0.566105
0.123970 0.875000 0.588165
0.373561 0.625000 0.500000
0.248559 0.875000 0.522059
0.498974 0.625000 0.566105
0.373971 0.875000 0.588165
0.623560 0.125000 0.500000
0.498557 0.375000 0.522059
0.748973 0.125000 0.566105
0.623970 0.375000 0.588165
0.873561 0.125000 0.500000

0.748559	0.375000	0.522059
0.998974	0.125000	0.566105
0.873971	0.375000	0.588165
0.623560	0.625000	0.500000
0.498557	0.875000	0.522059
0.748973	0.625000	0.566105
0.623970	0.875000	0.588165
0.873561	0.625000	0.500000
0.748559	0.875000	0.522059
0.998974	0.625000	0.566105
0.873971	0.875000	0.588165
0.124502	0.124565	0.632861
0.999182	0.374491	0.654508
0.372937	0.869321	0.719166
0.751279	0.126206	0.698298
0.374621	0.124795	0.632922
0.249021	0.374031	0.654803
0.874938	0.875424	0.717242
0.874299	0.375795	0.717607
0.124465	0.624867	0.632903
0.999058	0.875144	0.654533
0.123995	0.875681	0.717330
0.999539	0.624865	0.698177
0.374108	0.624557	0.633009
0.250230	0.875016	0.654951
0.246490	0.623264	0.697492
0.749371	0.375252	0.654592
0.623995	0.124777	0.633057
0.498850	0.376149	0.655171
0.625696	0.372107	0.717540
0.497511	0.123521	0.698595
0.874307	0.125092	0.632761
0.749527	0.624612	0.698118
0.250717	0.123420	0.698630
0.123704	0.374135	0.717540
0.623782	0.624986	0.633166
0.498661	0.875477	0.654219
0.497360	0.624898	0.698546
0.372421	0.372559	0.718043
0.874032	0.624747	0.632867
0.750542	0.874408	0.653946
0.999318	0.124929	0.698302
0.626812	0.878549	0.718775

POSCAR (IS: CO + O_t on RuO_2(101))

1.00000000

11.05460	0.00000	0.00000
0.00000	9.07380	0.00000
0.00000	0.00000	21.13440

C	O	Ru
1	66	32

D

0.271244	0.665550	0.724121
0.700210	0.404656	0.434104
0.493856	0.097591	0.360481
0.743856	0.152412	0.360481
0.610651	0.349421	0.311165
0.360651	0.400582	0.311165
0.146345	0.104055	0.242141
0.396346	0.145948	0.242141
0.950210	0.345349	0.434103
0.700211	0.904656	0.434104
0.493856	0.597591	0.360481
0.743855	0.652413	0.360481
0.610651	0.849422	0.311165
0.360651	0.900582	0.311165
0.146345	0.604056	0.242141
0.396344	0.645949	0.242141
0.950211	0.845348	0.434104
0.860651	0.400582	0.311165
0.646345	0.104055	0.242141
0.896345	0.145948	0.242141
0.450211	0.345348	0.434104
0.200211	0.404657	0.434104
0.243856	0.152413	0.360481
0.110651	0.349421	0.311165
0.860651	0.900582	0.311165
0.646345	0.604055	0.242141
0.896344	0.645949	0.242141
0.450210	0.845348	0.434103
0.200211	0.904655	0.434103
0.243856	0.652412	0.360481
0.110651	0.849421	0.311165
0.993856	0.097591	0.360481
0.993855	0.597591	0.360481
0.389116	0.390595	0.672342
0.171325	0.102505	0.602879

0.421917	0.147737	0.603131
0.289510	0.349229	0.554455
0.831597	0.094986	0.481031
0.390558	0.897733	0.676195
0.169658	0.597646	0.602478
0.419151	0.647534	0.602970
0.288935	0.847797	0.554511
0.831466	0.595159	0.481375
0.538393	0.405470	0.557046
0.333092	0.097075	0.481034
0.581962	0.155033	0.481252
0.886994	0.393020	0.672034
0.672180	0.096809	0.602868
0.922726	0.148940	0.603134
0.788589	0.346901	0.554252
0.538877	0.899228	0.554717
0.331169	0.595414	0.481020
0.581278	0.653940	0.481263
0.887906	0.896516	0.673374
0.673435	0.598612	0.604050
0.922921	0.650872	0.603896
0.789555	0.847354	0.554744
0.634645	0.343521	0.671181
0.640363	0.858510	0.673434
0.139751	0.357322	0.672076
0.134708	0.861341	0.675463
0.039007	0.401077	0.554320
0.082203	0.154297	0.480832
0.039460	0.902462	0.554233
0.081514	0.653624	0.480637
0.262844	0.623816	0.775327
0.547848	0.607549	0.714624
0.596984	0.252020	0.396545
0.509194	0.010851	0.275992
0.259193	0.239152	0.275993
0.846986	0.997982	0.396545
0.596987	0.752020	0.396544
0.509194	0.510851	0.275992
0.259196	0.739151	0.275991
0.846988	0.497982	0.396544
0.759196	0.239152	0.275992
0.346986	0.997983	0.396544
0.096986	0.252021	0.396544
0.009194	0.010853	0.275991

0.759196 0.739151 0.275991
0.346985 0.497982 0.396545
0.096984 0.752020 0.396546
0.009194 0.510851 0.275992
0.275767 0.259909 0.637759
0.186346 0.002715 0.518313
0.935523 0.247265 0.518231
0.275263 0.754373 0.642812
0.185285 0.502242 0.518326
0.935795 0.747724 0.518400
0.436996 0.250736 0.519180
0.773666 0.257364 0.637917
0.684902 0.000771 0.518334
0.434267 0.745988 0.518933
0.775217 0.761683 0.638997
0.684284 0.501876 0.519461
0.523305 0.986680 0.638589
0.527892 0.499931 0.647169
0.024640 0.989036 0.638291
0.023281 0.488125 0.638200

POSCAR (TS: CO + O_t on RuO_2(101))
1.00000000
11.05460 0.00000 0.00000
0.00000 9.07380 0.00000
0.00000 0.00000 21.13440
C O Ru
1 66 32
D
0.321247 0.639714 0.725677
0.700210 0.404656 0.434104
0.493856 0.097591 0.360481
0.743856 0.152412 0.360481
0.610651 0.349421 0.311165
0.360651 0.400582 0.311165
0.146345 0.104055 0.242141
0.396346 0.145948 0.242141
0.950210 0.345349 0.434103
0.700211 0.904656 0.434104
0.493856 0.597591 0.360481
0.743855 0.652413 0.360481
0.610651 0.849422 0.311165
0.360651 0.900582 0.311165
0.146345 0.604056 0.242141

0.396344	0.645949	0.242141
0.950211	0.845348	0.434104
0.860651	0.400582	0.311165
0.646345	0.104055	0.242141
0.896345	0.145948	0.242141
0.450211	0.345348	0.434104
0.200211	0.404657	0.434104
0.243856	0.152413	0.360481
0.110651	0.349421	0.311165
0.860651	0.900582	0.311165
0.646345	0.604055	0.242141
0.896344	0.645949	0.242141
0.450210	0.845348	0.434103
0.200211	0.904655	0.434103
0.243856	0.652412	0.360481
0.110651	0.849421	0.311165
0.993856	0.097591	0.360481
0.993855	0.597591	0.360481
0.375325	0.395736	0.672180
0.172572	0.095581	0.603460
0.422357	0.151479	0.602954
0.287102	0.344167	0.553476
0.833049	0.095522	0.481143
0.391032	0.907020	0.673660
0.174438	0.594041	0.605149
0.422275	0.652638	0.600578
0.288523	0.844579	0.556036
0.831396	0.595421	0.481318
0.539801	0.403555	0.556375
0.333663	0.094826	0.481328
0.582738	0.155771	0.481161
0.886553	0.396810	0.673336
0.673495	0.103086	0.602567
0.924350	0.148527	0.604743
0.790482	0.349100	0.554926
0.539592	0.902367	0.553913
0.332061	0.595027	0.481185
0.582259	0.654122	0.480966
0.890025	0.892389	0.673747
0.671711	0.601063	0.604963
0.923712	0.649877	0.603913
0.789944	0.848386	0.554675
0.637397	0.354909	0.673401
0.643346	0.863891	0.672252

0.134227 0.348848 0.672617
0.140315 0.855841 0.675690
0.039758 0.402052 0.554809
0.083500 0.153532 0.481322
0.039850 0.900556 0.554553
0.082403 0.653814 0.481075
0.283241 0.608817 0.775663
0.484371 0.609551 0.717300
0.596984 0.252020 0.396545
0.509194 0.010851 0.275992
0.259193 0.239152 0.275993
0.846986 0.997982 0.396545
0.596987 0.752020 0.396544
0.509194 0.510851 0.275992
0.259196 0.739151 0.275991
0.846988 0.497982 0.396544
0.759196 0.239152 0.275992
0.346986 0.997983 0.396544
0.096986 0.252021 0.396544
0.009194 0.010853 0.275991
0.759196 0.739151 0.275991
0.346985 0.497982 0.396545
0.096984 0.752020 0.396546
0.009194 0.510851 0.275992
0.271223 0.256130 0.637521
0.186991 0.999278 0.518763
0.936968 0.246992 0.519061
0.282767 0.752738 0.644622
0.186209 0.502291 0.518966
0.935753 0.747180 0.518388
0.436671 0.250239 0.518838
0.773885 0.262656 0.638873
0.686288 0.002640 0.518220
0.435443 0.747747 0.517883
0.775289 0.760860 0.638735
0.684763 0.502050 0.519692
0.526585 0.992046 0.637524
0.521564 0.499245 0.644665
0.027338 0.983830 0.639348
0.024481 0.488718 0.639127

POSCAR (IS: CO + O_b on RuO_2(101))
1.00000000
11.05460 0.00000 0.00000

0.00000 9.07380 0.00000
0.00000 0.00000 21.13440
C O Ru
1 65 32
D
0.277275 0.667600 0.725567
0.700210 0.404656 0.434104
0.493856 0.097591 0.360481
0.743856 0.152412 0.360481
0.610651 0.349421 0.311165
0.360651 0.400582 0.311165
0.146345 0.104055 0.242141
0.396346 0.145948 0.242141
0.950210 0.345349 0.434103
0.700211 0.904656 0.434104
0.493856 0.597591 0.360481
0.743855 0.652413 0.360481
0.610651 0.849422 0.311165
0.360651 0.900582 0.311165
0.146345 0.604056 0.242141
0.396344 0.645949 0.242141
0.950211 0.845348 0.434104
0.860651 0.400582 0.311165
0.646345 0.104055 0.242141
0.896345 0.145948 0.242141
0.450211 0.345348 0.434104
0.200211 0.404657 0.434104
0.243856 0.152413 0.360481
0.110651 0.349421 0.311165
0.860651 0.900582 0.311165
0.646345 0.604055 0.242141
0.896344 0.645949 0.242141
0.450210 0.845348 0.434103
0.200211 0.904655 0.434103
0.243856 0.652412 0.360481
0.110651 0.849421 0.311165
0.993856 0.097591 0.360481
0.993855 0.597591 0.360481
0.388007 0.391846 0.671473
0.170188 0.100335 0.603305
0.421972 0.149440 0.603075
0.289109 0.347937 0.554316
0.831812 0.095063 0.481215
0.389626 0.902892 0.676357

0.170819	0.597423	0.603078
0.421611	0.650949	0.603986
0.288620	0.847121	0.555317
0.831867	0.595479	0.481093
0.538635	0.402027	0.554047
0.331830	0.095082	0.481014
0.581844	0.153999	0.481063
0.887590	0.394840	0.672851
0.672216	0.098653	0.604109
0.922161	0.149424	0.603740
0.788977	0.347673	0.554577
0.538963	0.900735	0.555010
0.332037	0.595621	0.481312
0.581398	0.654504	0.481163
0.885647	0.895381	0.673470
0.672409	0.599262	0.603940
0.922171	0.650812	0.604015
0.789089	0.847175	0.554879
0.636709	0.354503	0.672554
0.636651	0.853822	0.673560
0.139231	0.357092	0.672473
0.133177	0.860159	0.676459
0.039196	0.401667	0.554589
0.082180	0.154048	0.481008
0.038657	0.901917	0.554650
0.081666	0.653778	0.480792
0.274160	0.628062	0.777472
0.596984	0.252020	0.396545
0.509194	0.010851	0.275992
0.259193	0.239152	0.275993
0.846986	0.997982	0.396545
0.596987	0.752020	0.396544
0.509194	0.510851	0.275992
0.259196	0.739151	0.275991
0.846988	0.497982	0.396544
0.759196	0.239152	0.275992
0.346986	0.997983	0.396544
0.096986	0.252021	0.396544
0.009194	0.010853	0.275991
0.759196	0.739151	0.275991
0.346985	0.497982	0.396545
0.096984	0.752020	0.396546
0.009194	0.510851	0.275992
0.273729	0.258460	0.637791

0.185494 0.001245 0.518612
0.935712 0.247561 0.518564
0.275577 0.754649 0.644317
0.185937 0.502662 0.518574
0.935564 0.747668 0.518475
0.435247 0.247637 0.518221
0.773818 0.260479 0.638844
0.685315 0.001278 0.518754
0.434780 0.747661 0.519159
0.773395 0.760152 0.639174
0.685398 0.502046 0.518406
0.523624 0.988653 0.638902
0.523701 0.488609 0.638045
0.023090 0.987450 0.638838
0.023673 0.489324 0.638493

POSCAR (TS: CO + O_b on RuO_2(101))
1.00000000
11.05460 0.00000 0.00000
0.00000 9.07380 0.00000
0.00000 0.00000 21.13440
C O Ru
1 65 32
D
0.303082 0.597355 0.714473
0.700210 0.404656 0.434104
0.493856 0.097591 0.360481
0.743856 0.152412 0.360481
0.610651 0.349421 0.311165
0.360651 0.400582 0.311165
0.146345 0.104055 0.242141
0.396346 0.145948 0.242141
0.950210 0.345349 0.434103
0.700211 0.904656 0.434104
0.493856 0.597591 0.360481
0.743855 0.652413 0.360481
0.610651 0.849422 0.311165
0.360651 0.900582 0.311165
0.146345 0.604056 0.242141
0.396344 0.645949 0.242141
0.950211 0.845348 0.434104
0.860651 0.400582 0.311165
0.646345 0.104055 0.242141
0.896345 0.145948 0.242141

0.450211	0.345348	0.434104
0.200211	0.404657	0.434104
0.243856	0.152413	0.360481
0.110651	0.349421	0.311165
0.860651	0.900582	0.311165
0.646345	0.604055	0.242141
0.896344	0.645949	0.242141
0.450210	0.845348	0.434103
0.200211	0.904655	0.434103
0.243856	0.652412	0.360481
0.110651	0.849421	0.311165
0.993856	0.097591	0.360481
0.993855	0.597591	0.360481
0.366626	0.441658	0.680088
0.175207	0.100222	0.605216
0.423645	0.162630	0.607481
0.290443	0.352368	0.556009
0.832676	0.095505	0.481240
0.389693	0.896782	0.674819
0.167418	0.597877	0.601500
0.422761	0.652602	0.600989
0.290196	0.848235	0.556845
0.832709	0.595951	0.481114
0.539618	0.405957	0.555022
0.333827	0.096313	0.482050
0.582193	0.156153	0.481551
0.882695	0.397541	0.672768
0.671583	0.099788	0.603769
0.923860	0.150309	0.604838
0.789386	0.347281	0.554672
0.538198	0.904688	0.554539
0.331743	0.596919	0.480721
0.582697	0.655173	0.480940
0.887589	0.897035	0.673336
0.674178	0.599379	0.604084
0.921635	0.653421	0.603890
0.789223	0.849093	0.554619
0.632261	0.355007	0.672279
0.636719	0.857321	0.672698
0.134285	0.358377	0.673301
0.137483	0.852350	0.675158
0.038597	0.402818	0.554641
0.083718	0.154568	0.481588
0.039787	0.903139	0.554758

0.081372 0.654347 0.480619
0.283572 0.587292 0.769023
0.596984 0.252020 0.396545
0.509194 0.010851 0.275992
0.259193 0.239152 0.275993
0.846986 0.997982 0.396545
0.596987 0.752020 0.396544
0.509194 0.510851 0.275992
0.259196 0.739151 0.275991
0.846988 0.497982 0.396544
0.759196 0.239152 0.275992
0.346986 0.997983 0.396544
0.096986 0.252021 0.396544
0.009194 0.010853 0.275991
0.759196 0.739151 0.275991
0.346985 0.497982 0.396545
0.096984 0.752020 0.396546
0.009194 0.510851 0.275992
0.270613 0.264117 0.639826
0.187663 0.002010 0.519634
0.936682 0.247006 0.519112
0.277816 0.747150 0.642907
0.185361 0.502789 0.518049
0.935744 0.749451 0.518441
0.436418 0.251387 0.519508
0.770901 0.261277 0.638780
0.685404 0.002880 0.518523
0.435955 0.749157 0.518132
0.773721 0.763479 0.639135
0.686573 0.502486 0.518598
0.521543 0.991272 0.638881
0.525632 0.498750 0.639133
0.027520 0.986211 0.639648
0.019560 0.490932 0.638376

POSCAR (IS: CO + O_t on RuO_2(110))
1.00000000
6.28540 0.00000 0.00000
0.00000 12.84640 0.00000
0.00000 0.00000 23.56790
C O Ru
1 66 32
D

0.249092	0.492561	0.829136
0.250002	0.997666	0.390854
0.000000	0.901431	0.474485
0.250002	0.748484	0.421466
0.000000	0.844720	0.337835
0.000000	0.650880	0.338215
0.250002	0.248214	0.527124
0.250002	0.248483	0.421466
0.000000	0.344718	0.337835
0.000000	0.150878	0.338215
0.250002	0.748216	0.527124
0.250002	0.497665	0.390854
0.000000	0.595269	0.474105
0.000000	0.401429	0.474485
0.750002	0.997666	0.390854
0.500000	0.901431	0.474485
0.750002	0.748484	0.421466
0.500000	0.844720	0.337835
0.500000	0.650880	0.338215
0.750002	0.248483	0.421466
0.500000	0.344718	0.337835
0.500000	0.150878	0.338215
0.750002	0.748216	0.527124
0.750002	0.248214	0.527124
0.750002	0.497665	0.390854
0.500000	0.595269	0.474105
0.500000	0.401429	0.474485
0.250002	0.497933	0.285196
0.250002	0.997935	0.285196
0.750002	0.497933	0.285196
0.750002	0.997935	0.285196
0.000000	0.095268	0.474105
0.500000	0.095268	0.474105
0.249568	0.999439	0.556924
0.248785	0.499481	0.660656
0.996453	0.595412	0.744833
0.995674	0.402323	0.743980
0.248636	0.247034	0.694137
0.998562	0.346121	0.610753
0.999675	0.152752	0.610366
0.248585	0.751865	0.694360
0.999561	0.846302	0.610197
0.998467	0.653019	0.611114
0.249090	0.499508	0.557714

0.249405	0.999382	0.661772
0.999119	0.904286	0.749530
0.749560	0.999458	0.556934
0.748727	0.499608	0.664244
0.499566	0.595357	0.744915
0.500365	0.402361	0.744090
0.748598	0.245399	0.693849
0.499829	0.346121	0.610748
0.498952	0.152752	0.610366
0.748556	0.753243	0.694151
0.498989	0.846320	0.610197
0.499842	0.653000	0.611108
0.749092	0.499500	0.557315
0.749426	0.999418	0.661818
0.498849	0.904299	0.749512
0.248420	0.746148	0.796944
0.248460	0.253070	0.796247
0.748424	0.748948	0.796789
0.748484	0.249176	0.796808
0.999305	0.093815	0.749449
0.498684	0.093796	0.749430
0.250421	0.485501	0.877810
0.748754	0.498272	0.826180
0.250002	0.998351	0.474295
0.000000	0.997801	0.338024
0.250002	0.747800	0.338025
0.000000	0.248350	0.474295
0.250002	0.247798	0.338025
0.000000	0.748351	0.474295
0.250002	0.498349	0.474295
0.000000	0.497800	0.338024
0.750002	0.998351	0.474295
0.500000	0.997801	0.338024
0.750002	0.747800	0.338025
0.500000	0.248350	0.474295
0.750002	0.247798	0.338025
0.500000	0.748351	0.474295
0.750002	0.498349	0.474295
0.500000	0.497800	0.338024
0.247847	0.498715	0.747889
0.996586	0.499625	0.610364
0.249289	0.249696	0.611196
0.249149	0.749386	0.611312
0.249039	0.998911	0.742127

0.999596 0.999563 0.609298
0.747805 0.498717 0.752095
0.501228 0.499618 0.610359
0.749237 0.249330 0.610914
0.749297 0.749762 0.611054
0.749053 0.998952 0.742217
0.499349 0.999571 0.609300
0.997828 0.747955 0.749633
0.997599 0.249822 0.749244
0.499021 0.748003 0.749633
0.499356 0.249767 0.749249

POSCAR (TS: CO + O_t on RuO_2(110))
1.00000000
6.28540 0.00000 0.00000
0.00000 12.84640 0.00000
0.00000 0.00000 23.56790
C O Ru
1 66 32
D
0.142251 0.484446 0.830567
0.250002 0.997666 0.390854
0.000000 0.901431 0.474485
0.250002 0.748484 0.421466
0.000000 0.844720 0.337835
0.000000 0.650880 0.338215
0.250002 0.248214 0.527124
0.250002 0.248483 0.421466
0.000000 0.344718 0.337835
0.000000 0.150878 0.338215
0.250002 0.748216 0.527124
0.250002 0.497665 0.390854
0.000000 0.595269 0.474105
0.000000 0.401429 0.474485
0.750002 0.997666 0.390854
0.500000 0.901431 0.474485
0.750002 0.748484 0.421466
0.500000 0.844720 0.337835
0.500000 0.650880 0.338215
0.750002 0.248483 0.421466
0.500000 0.344718 0.337835
0.500000 0.150878 0.338215
0.750002 0.748216 0.527124
0.750002 0.248214 0.527124

0.750002	0.497665	0.390854
0.500000	0.595269	0.474105
0.500000	0.401429	0.474485
0.250002	0.497933	0.285196
0.250002	0.997935	0.285196
0.750002	0.497933	0.285196
0.750002	0.997935	0.285196
0.000000	0.095268	0.474105
0.500000	0.095268	0.474105
0.249585	0.999050	0.556837
0.255353	0.499301	0.661804
0.000828	0.598487	0.738619
0.999927	0.397888	0.737062
0.251872	0.245545	0.693883
0.999408	0.345850	0.610948
0.999883	0.152483	0.610507
0.253413	0.751732	0.694157
0.000337	0.845837	0.610513
0.999954	0.652534	0.610993
0.249440	0.499092	0.557859
0.250288	0.999192	0.661441
0.999128	0.904713	0.748492
0.750209	0.999089	0.556842
0.745752	0.499490	0.663969
0.499714	0.592763	0.753409
0.499323	0.403929	0.752036
0.743995	0.244804	0.693653
0.500367	0.345808	0.610824
0.499412	0.152232	0.609761
0.746494	0.751853	0.694031
0.500148	0.846048	0.609921
0.500929	0.652479	0.610955
0.751187	0.499076	0.557579
0.749313	0.999256	0.661515
0.499573	0.903945	0.749286
0.247663	0.751150	0.796648
0.244262	0.249753	0.796061
0.751454	0.751301	0.796830
0.748654	0.245900	0.796178
0.999344	0.092370	0.748864
0.498586	0.093521	0.749554
0.201113	0.463864	0.876480
0.857365	0.493630	0.824615
0.250002	0.998351	0.474295

0.000000 0.997801 0.338024
0.250002 0.747800 0.338025
0.000000 0.248350 0.474295
0.250002 0.247798 0.338025
0.000000 0.748351 0.474295
0.250002 0.498349 0.474295
0.000000 0.497800 0.338024
0.750002 0.998351 0.474295
0.500000 0.997801 0.338024
0.750002 0.747800 0.338025
0.500000 0.248350 0.474295
0.750002 0.247798 0.338025
0.500000 0.748351 0.474295
0.750002 0.498349 0.474295
0.500000 0.497800 0.338024
0.239838 0.497541 0.747768
0.999095 0.499321 0.610820
0.249885 0.249227 0.611018
0.250496 0.749015 0.611216
0.249991 0.998489 0.741721
0.999876 0.999214 0.609182
0.757800 0.498114 0.749261
0.501908 0.499214 0.610524
0.749517 0.249003 0.610853
0.750213 0.749191 0.611041
0.748423 0.998610 0.741869
0.499893 0.999203 0.608949
0.998850 0.749758 0.748956
0.996391 0.246769 0.748275
0.500509 0.747864 0.750559
0.497278 0.249917 0.750225

POSCAR (IS: CO + O_b on RuO_2(110))
1.00000000
6.28540 0.00000 0.00000
0.00000 12.84640 0.00000
0.00000 0.00000 23.56790
C O Ru
1 65 32
D
0.242974 0.496047 0.831451
0.250002 0.997666 0.390854
0.000000 0.901431 0.474485
0.250002 0.748484 0.421466

0.000000	0.844720	0.337835
0.000000	0.650880	0.338215
0.250002	0.248214	0.527124
0.250002	0.248483	0.421466
0.000000	0.344718	0.337835
0.000000	0.150878	0.338215
0.250002	0.748216	0.527124
0.250002	0.497665	0.390854
0.000000	0.595269	0.474105
0.000000	0.401429	0.474485
0.750002	0.997666	0.390854
0.500000	0.901431	0.474485
0.750002	0.748484	0.421466
0.500000	0.844720	0.337835
0.500000	0.650880	0.338215
0.750002	0.248483	0.421466
0.500000	0.344718	0.337835
0.500000	0.150878	0.338215
0.750002	0.748216	0.527124
0.750002	0.248214	0.527124
0.750002	0.497665	0.390854
0.500000	0.595269	0.474105
0.500000	0.401429	0.474485
0.250002	0.497933	0.285196
0.250002	0.997935	0.285196
0.750002	0.497933	0.285196
0.750002	0.997935	0.285196
0.000000	0.095268	0.474105
0.500000	0.095268	0.474105
0.249446	0.999267	0.557010
0.248779	0.499470	0.662189
0.991479	0.593970	0.748089
0.991577	0.402211	0.747385
0.248393	0.247316	0.694969
0.999333	0.346022	0.610798
0.999420	0.152735	0.610775
0.248343	0.749734	0.695151
0.999370	0.846079	0.610900
0.999282	0.652868	0.610894
0.249069	0.499388	0.557118
0.249300	0.999373	0.661893
0.998829	0.903248	0.749330
0.749478	0.999267	0.557025
0.748673	0.499482	0.660435

0.503754	0.593946	0.748166
0.503675	0.402215	0.747436
0.748218	0.247021	0.694488
0.498896	0.346008	0.610775
0.498992	0.152732	0.610747
0.748162	0.749995	0.694662
0.498978	0.846087	0.610867
0.498876	0.652874	0.610872
0.749115	0.499374	0.557002
0.749227	0.999391	0.661957
0.498515	0.903186	0.749386
0.247845	0.742750	0.797255
0.247918	0.254461	0.796927
0.748080	0.749738	0.798665
0.748143	0.246838	0.798516
0.998958	0.093018	0.749646
0.498419	0.093078	0.749699
0.233795	0.493758	0.880551
0.250002	0.998351	0.474295
0.000000	0.997801	0.338024
0.250002	0.747800	0.338025
0.000000	0.248350	0.474295
0.250002	0.247798	0.338025
0.000000	0.748351	0.474295
0.250002	0.498349	0.474295
0.000000	0.497800	0.338024
0.750002	0.998351	0.474295
0.500000	0.997801	0.338024
0.750002	0.747800	0.338025
0.500000	0.248350	0.474295
0.750002	0.247798	0.338025
0.500000	0.748351	0.474295
0.750002	0.498349	0.474295
0.500000	0.497800	0.338024
0.247591	0.498038	0.750988
0.000757	0.499543	0.609416
0.249166	0.249500	0.611744
0.249132	0.749276	0.611872
0.248790	0.998092	0.742251
0.999399	0.999475	0.609399
0.747609	0.498055	0.740005
0.497056	0.499540	0.609427
0.749171	0.249354	0.611293
0.749131	0.749432	0.611404

0.748689 0.998115 0.742389
0.499297 0.999479 0.609386
0.996133 0.747414 0.750652
0.996198 0.248733 0.750425
0.499828 0.747236 0.750732
0.499893 0.248914 0.750503

POSCAR (TS: CO + O_b on RuO_2(110))
1.00000000
6.28540 0.00000 0.00000
0.00000 12.84640 0.00000
0.00000 0.00000 23.56790
C O Ru
1 65 32
D
0.238152 0.570827 0.824545
0.250002 0.997666 0.390854
0.000000 0.901431 0.474485
0.250002 0.748484 0.421466
0.000000 0.844720 0.337835
0.000000 0.650880 0.338215
0.250002 0.248214 0.527124
0.250002 0.248483 0.421466
0.000000 0.344718 0.337835
0.000000 0.150878 0.338215
0.250002 0.748216 0.527124
0.250002 0.497665 0.390854
0.000000 0.595269 0.474105
0.000000 0.401429 0.474485
0.750002 0.997666 0.390854
0.500000 0.901431 0.474485
0.750002 0.748484 0.421466
0.500000 0.844720 0.337835
0.500000 0.650880 0.338215
0.750002 0.248483 0.421466
0.500000 0.344718 0.337835
0.500000 0.150878 0.338215
0.750002 0.748216 0.527124
0.750002 0.248214 0.527124
0.750002 0.497665 0.390854
0.500000 0.595269 0.474105
0.500000 0.401429 0.474485
0.250002 0.497933 0.285196
0.250002 0.997935 0.285196

0.750002	0.497933	0.285196
0.750002	0.997935	0.285196
0.000000	0.095268	0.474105
0.500000	0.095268	0.474105
0.248658	0.997018	0.557298
0.248276	0.489891	0.661308
0.988745	0.591378	0.738736
0.996686	0.401609	0.752016
0.247650	0.244829	0.694992
0.998744	0.341238	0.610244
0.998344	0.148223	0.611405
0.247060	0.748658	0.694284
0.998718	0.842070	0.610259
0.998338	0.648301	0.611344
0.248661	0.497004	0.556850
0.248217	0.993268	0.662627
0.000991	0.898124	0.752672
0.748677	0.996766	0.557287
0.748084	0.489401	0.659754
0.505499	0.590924	0.738966
0.498016	0.401543	0.752339
0.747451	0.246203	0.694769
0.498364	0.341218	0.610272
0.498741	0.148225	0.611395
0.746659	0.753007	0.694203
0.497885	0.842107	0.610203
0.498270	0.648307	0.611344
0.748670	0.497132	0.556746
0.748163	0.992410	0.662926
0.492790	0.897874	0.752709
0.245941	0.702027	0.801988
0.247302	0.240958	0.798196
0.746744	0.740516	0.796003
0.747330	0.240991	0.797524
0.996126	0.088611	0.749142
0.498113	0.088585	0.749183
0.204145	0.555784	0.872987
0.250002	0.998351	0.474295
0.000000	0.997801	0.338024
0.250002	0.747800	0.338025
0.000000	0.248350	0.474295
0.250002	0.247798	0.338025
0.000000	0.748351	0.474295
0.250002	0.498349	0.474295

0.000000 0.497800 0.338024
0.750002 0.998351 0.474295
0.500000 0.997801 0.338024
0.750002 0.747800 0.338025
0.500000 0.248350 0.474295
0.750002 0.247798 0.338025
0.500000 0.748351 0.474295
0.750002 0.498349 0.474295
0.500000 0.497800 0.338024
0.247153 0.500770 0.746479
0.999633 0.494064 0.608881
0.248572 0.245027 0.611643
0.248314 0.745396 0.611182
0.247095 0.994207 0.743102
0.998272 0.994957 0.609950
0.747238 0.494259 0.739517
0.497148 0.494075 0.608917
0.748568 0.244908 0.611507
0.748265 0.745640 0.611133
0.746962 0.992552 0.743520
0.498529 0.994976 0.609941
0.994857 0.743118 0.748440
0.997900 0.245432 0.751243
0.498357 0.742498 0.748496
0.496765 0.245331 0.751316

POSCAR (IS: CO + O_h on Ru(10$\bar{1}$0) with 0.5ML O)
1.00000000
17.06280 0.00000 0.00000
0.00000 10.96120 0.00000
0.00000 0.00000 22.98250
C O Ru
1 9 128
D
0.433711 0.801006 0.671357
0.343074 0.492004 0.637851
0.205784 0.745700 0.637143
0.210910 0.245553 0.637009
0.340592 0.004985 0.637529
0.844901 0.245810 0.637352
0.712635 0.996534 0.637319
0.845311 0.745860 0.637257
0.710758 0.495583 0.637295

0.451031	0.773935	0.718802
0.028066	0.121524	0.257497
0.028066	0.371527	0.257499
0.153001	0.120395	0.388995
0.153024	0.370695	0.388992
0.028042	0.995622	0.355052
0.027890	0.245624	0.355051
0.153032	0.246347	0.287479
0.153040	0.996350	0.287329
0.278065	0.121526	0.257575
0.278068	0.371527	0.257577
0.402838	0.120699	0.388990
0.402856	0.370391	0.388998
0.277924	0.995627	0.355047
0.278008	0.245621	0.355045
0.403034	0.246350	0.287329
0.403044	0.996347	0.287480
0.028066	0.621525	0.257498
0.028066	0.871527	0.257498
0.153006	0.620395	0.388996
0.153024	0.870693	0.388990
0.028043	0.495624	0.355053
0.027891	0.745621	0.355051
0.153031	0.746345	0.287479
0.153041	0.496351	0.287330
0.278066	0.621525	0.257577
0.278068	0.871525	0.257577
0.402838	0.620699	0.388995
0.402856	0.870391	0.388994
0.277924	0.495625	0.355049
0.278010	0.745622	0.355045
0.403035	0.746349	0.287329
0.403044	0.496347	0.287481
0.528066	0.121524	0.257497
0.528066	0.371527	0.257499
0.653001	0.120395	0.388995
0.653024	0.370695	0.388992
0.528042	0.995622	0.355052
0.527890	0.245624	0.355051
0.653032	0.246347	0.287479
0.653040	0.996350	0.287329
0.778065	0.121526	0.257575
0.778068	0.371527	0.257577
0.902838	0.120699	0.388990

0.902856	0.370391	0.388998
0.777924	0.995627	0.355047
0.778008	0.245621	0.355045
0.903034	0.246350	0.287329
0.903044	0.996347	0.287480
0.528066	0.621525	0.257498
0.528066	0.871527	0.257498
0.653006	0.620395	0.388996
0.653024	0.870693	0.388990
0.528043	0.495624	0.355053
0.527891	0.745621	0.355051
0.653031	0.746345	0.287479
0.653041	0.496351	0.287330
0.778066	0.621525	0.257577
0.778068	0.871525	0.257577
0.902838	0.620699	0.388995
0.902856	0.870391	0.388994
0.777924	0.495625	0.355049
0.778010	0.745622	0.355045
0.903035	0.746349	0.287329
0.903044	0.496347	0.287481
0.028025	0.620325	0.459535
0.401791	0.245195	0.493747
0.275665	0.245499	0.560470
0.277799	0.120961	0.460206
0.404380	0.621371	0.593864
0.275176	0.745210	0.561774
0.404749	0.367151	0.593103
0.150931	0.879207	0.593851
0.151393	0.115678	0.593388
0.027789	0.495572	0.561542
0.154178	0.495711	0.493817
0.027771	0.995998	0.561504
0.027784	0.245756	0.559141
0.280615	0.495736	0.560895
0.404830	0.124789	0.593236
0.403538	0.866010	0.598057
0.152038	0.745805	0.491105
0.402010	0.746052	0.494232
0.278007	0.621167	0.460481
0.027867	0.371411	0.459433
0.028026	0.871187	0.459490
0.151062	0.612051	0.593913
0.403973	0.997327	0.489730

0.278021	0.370691	0.460234
0.154137	0.995755	0.493821
0.278186	0.870540	0.460483
0.027861	0.120250	0.459400
0.151767	0.245875	0.490830
0.403981	0.496496	0.491305
0.151451	0.375603	0.593489
0.280639	0.995251	0.560731
0.027943	0.745732	0.559194
0.527887	0.621930	0.459623
0.904081	0.245818	0.490852
0.780549	0.245744	0.560727
0.777936	0.120775	0.460209
0.904398	0.615180	0.593682
0.780534	0.745798	0.560785
0.904356	0.375986	0.593657
0.652037	0.867368	0.593438
0.651596	0.124824	0.593367
0.527971	0.495692	0.559249
0.651873	0.495816	0.490807
0.527167	0.995507	0.559516
0.528394	0.245729	0.561390
0.775400	0.495732	0.560765
0.904392	0.115656	0.593664
0.904416	0.876432	0.593670
0.654116	0.745818	0.493991
0.904168	0.745814	0.490951
0.777962	0.620876	0.460297
0.527958	0.370184	0.459468
0.527732	0.869881	0.459539
0.651482	0.625785	0.593644
0.901736	0.995771	0.493734
0.777987	0.370840	0.460246
0.651557	0.995802	0.491124
0.777916	0.870778	0.460254
0.528139	0.121658	0.459524
0.654287	0.245958	0.493877
0.901658	0.495884	0.493854
0.651627	0.365117	0.593666
0.775711	0.995989	0.560521
0.527987	0.745808	0.561241

POSCAR (TS: CO + O_h on Ru(10$\bar{1}$0) with 0.5ML O)
1.00000000

```
  17.06280      0.00000      0.00000
   0.00000     10.96120      0.00000
   0.00000      0.00000     22.98250
     C         O          Ru
     1         9         128
D
      0.428860       0.791500       0.677160
      0.389588       0.645655       0.675105
      0.205498       0.746322       0.636407
      0.211515       0.243825       0.637280
      0.338230       0.003019       0.638123
      0.845084       0.245634       0.637217
      0.711276       0.995853       0.636920
      0.844882       0.745269       0.637171
      0.711003       0.495283       0.637122
      0.454691       0.815539       0.723442
      0.028066       0.121524       0.257497
      0.028066       0.371527       0.257499
      0.153001       0.120395       0.388995
      0.153024       0.370695       0.388992
      0.028042       0.995622       0.355052
      0.027890       0.245624       0.355051
      0.153032       0.246347       0.287479
      0.153040       0.996350       0.287329
      0.278065       0.121526       0.257575
      0.278068       0.371527       0.257577
      0.402838       0.120699       0.388990
      0.402856       0.370391       0.388998
      0.277924       0.995627       0.355047
      0.278008       0.245621       0.355045
      0.403034       0.246350       0.287329
      0.403044       0.996347       0.287480
      0.028066       0.621525       0.257498
      0.028066       0.871527       0.257498
      0.153006       0.620395       0.388996
      0.153024       0.870693       0.388990
      0.028043       0.495624       0.355053
      0.027891       0.745621       0.355051
      0.153031       0.746345       0.287479
      0.153041       0.496351       0.287330
      0.278066       0.621525       0.257577
      0.278068       0.871525       0.257577
      0.402838       0.620699       0.388995
      0.402856       0.870391       0.388994
```

0.277924	0.495625	0.355049
0.278010	0.745622	0.355045
0.403035	0.746349	0.287329
0.403044	0.496347	0.287481
0.528066	0.121524	0.257497
0.528066	0.371527	0.257499
0.653001	0.120395	0.388995
0.653024	0.370695	0.388992
0.528042	0.995622	0.355052
0.527890	0.245624	0.355051
0.653032	0.246347	0.287479
0.653040	0.996350	0.287329
0.778065	0.121526	0.257575
0.778068	0.371527	0.257577
0.902838	0.120699	0.388990
0.902856	0.370391	0.388998
0.777924	0.995627	0.355047
0.778008	0.245621	0.355045
0.903034	0.246350	0.287329
0.903044	0.996347	0.287480
0.528066	0.621525	0.257498
0.528066	0.871527	0.257498
0.653006	0.620395	0.388996
0.653024	0.870693	0.388990
0.528043	0.495624	0.355053
0.527891	0.745621	0.355051
0.653031	0.746345	0.287479
0.653041	0.496351	0.287330
0.778066	0.621525	0.257577
0.778068	0.871525	0.257577
0.902838	0.620699	0.388995
0.902856	0.870391	0.388994
0.777924	0.495625	0.355049
0.778010	0.745622	0.355045
0.903035	0.746349	0.287329
0.903044	0.496347	0.287481
0.027968	0.620335	0.459503
0.401933	0.244537	0.493449
0.276679	0.247248	0.560999
0.277795	0.120467	0.460198
0.405132	0.618110	0.596296
0.276261	0.743459	0.561591
0.404386	0.366429	0.590611
0.151058	0.879633	0.593651

0.151972	0.115475	0.593178
0.028174	0.495303	0.561572
0.153561	0.495366	0.493013
0.027850	0.995902	0.561497
0.028237	0.245591	0.559151
0.280202	0.494812	0.559491
0.404610	0.119583	0.593072
0.402850	0.868868	0.598807
0.152215	0.745193	0.491034
0.402069	0.745875	0.494476
0.278427	0.620906	0.460057
0.027804	0.370866	0.459440
0.028108	0.870936	0.459542
0.152664	0.610087	0.593775
0.403868	0.996207	0.489844
0.277987	0.370067	0.459723
0.154302	0.995526	0.493782
0.278232	0.869879	0.460456
0.027922	0.120159	0.459458
0.152035	0.245825	0.490875
0.403033	0.494407	0.492111
0.152868	0.375442	0.593473
0.280681	0.994138	0.560596
0.028427	0.745118	0.559180
0.527240	0.621472	0.459725
0.904001	0.245532	0.490962
0.780401	0.245427	0.560779
0.777846	0.120593	0.460285
0.904648	0.615408	0.593454
0.780265	0.745399	0.560782
0.904630	0.375636	0.593486
0.651228	0.866068	0.593273
0.650902	0.125096	0.593291
0.526215	0.495049	0.559730
0.651371	0.495624	0.490977
0.526606	0.994552	0.559630
0.527571	0.245842	0.561201
0.775354	0.495444	0.560640
0.904423	0.115279	0.593542
0.904455	0.875442	0.593448
0.653736	0.745240	0.494045
0.904129	0.745696	0.491067
0.777821	0.620579	0.460326
0.527885	0.369806	0.459368

0.527588 0.869184 0.459644
0.650933 0.624703 0.593406
0.901724 0.995513 0.493744
0.777842 0.370663 0.460313
0.651567 0.995523 0.491062
0.777788 0.870484 0.460306
0.528174 0.121118 0.459419
0.653918 0.245723 0.494021
0.901650 0.495633 0.493829
0.651311 0.365450 0.593439
0.775415 0.995569 0.560599
0.526921 0.744966 0.561457

POSCAR (IS: CO + O_h on Ru(10$\bar{1}$0) with 1ML O)
1.00000000
10.90720 0.00000 0.00000
0.00000 8.57660 0.00000
0.00000 0.00000 35.76230
C O Ru
1 9 64
D
0.307598 0.284021 0.776316
0.248087 0.989998 0.746460
0.748383 0.999687 0.746746
0.997704 0.247196 0.747731
0.755149 0.519792 0.747905
0.514576 0.247659 0.745842
0.500977 0.736081 0.748542
0.232317 0.536257 0.747080
0.996586 0.734028 0.747612
0.285489 0.247191 0.806599
0.123560 0.125000 0.500000
0.998557 0.375000 0.522059
0.248973 0.125000 0.566105
0.123970 0.375000 0.588165
0.373561 0.125000 0.500000
0.248559 0.375000 0.522059
0.498974 0.125000 0.566105
0.373971 0.375000 0.588165
0.123560 0.625000 0.500000
0.998557 0.875000 0.522059
0.248973 0.625000 0.566105
0.123970 0.875000 0.588165

0.373561	0.625000	0.500000
0.248559	0.875000	0.522059
0.498974	0.625000	0.566105
0.373971	0.875000	0.588165
0.623560	0.125000	0.500000
0.498557	0.375000	0.522059
0.748973	0.125000	0.566105
0.623970	0.375000	0.588165
0.873561	0.125000	0.500000
0.748559	0.375000	0.522059
0.998974	0.125000	0.566105
0.873971	0.375000	0.588165
0.623560	0.625000	0.500000
0.498557	0.875000	0.522059
0.748973	0.625000	0.566105
0.623970	0.875000	0.588165
0.873561	0.625000	0.500000
0.748559	0.875000	0.522059
0.998974	0.625000	0.566105
0.873971	0.875000	0.588165
0.623627	0.125191	0.633069
0.498857	0.377132	0.653935
0.998209	0.627732	0.696927
0.124527	0.125701	0.633097
0.872127	0.376404	0.719791
0.358675	0.368577	0.728619
0.999060	0.878471	0.653968
0.115606	0.874489	0.719678
0.623895	0.624815	0.633067
0.498222	0.623795	0.698219
0.381817	0.873588	0.719626
0.619292	0.874273	0.719649
0.874152	0.625203	0.632730
0.874050	0.125406	0.632864
0.499041	0.876985	0.654439
0.124781	0.624742	0.632995
0.249179	0.873629	0.653900
0.998732	0.128865	0.698047
0.748949	0.372512	0.654182
0.749000	0.873273	0.653716
0.498710	0.129795	0.697603
0.636265	0.377909	0.720063
0.374190	0.125808	0.633292
0.121451	0.378360	0.719789

0.750165 0.624809 0.697096
0.247962 0.121973 0.698368
0.250151 0.623094 0.696730
0.250284 0.372262 0.654863
0.374254 0.623904 0.633176
0.749210 0.122353 0.697721
0.999526 0.377520 0.654181
0.878044 0.875365 0.719943

POSCAR (IS: CO + O_h on Ru(10$\bar{1}$0) with 1ML O)
1.00000000
10.90720 0.00000 0.00000
0.00000 8.57660 0.00000
0.00000 0.00000 35.76230
C O Ru
1 9 64
D
0.451481 0.454760 0.778179
0.245183 0.013980 0.748381
0.752117 0.011599 0.748095
0.991620 0.234830 0.747702
0.627917 0.481136 0.764152
0.506495 0.206799 0.746291
0.495927 0.762557 0.745864
0.235885 0.510726 0.746111
0.001232 0.747730 0.747002
0.448556 0.472353 0.810321
0.123560 0.125000 0.500000
0.998557 0.375000 0.522059
0.248973 0.125000 0.566105
0.123970 0.375000 0.588165
0.373561 0.125000 0.500000
0.248559 0.375000 0.522059
0.498974 0.125000 0.566105
0.373971 0.375000 0.588165
0.123560 0.625000 0.500000
0.998557 0.875000 0.522059
0.248973 0.625000 0.566105
0.123970 0.875000 0.588165
0.373561 0.625000 0.500000
0.248559 0.875000 0.522059
0.498974 0.625000 0.566105
0.373971 0.875000 0.588165
0.623560 0.125000 0.500000

0.498557	0.375000	0.522059
0.748973	0.125000	0.566105
0.623970	0.375000	0.588165
0.873561	0.125000	0.500000
0.748559	0.375000	0.522059
0.998974	0.125000	0.566105
0.873971	0.375000	0.588165
0.623560	0.625000	0.500000
0.498557	0.875000	0.522059
0.748973	0.625000	0.566105
0.623970	0.875000	0.588165
0.873561	0.625000	0.500000
0.748559	0.875000	0.522059
0.998974	0.625000	0.566105
0.873971	0.875000	0.588165
0.623219	0.125422	0.632998
0.497571	0.376768	0.654963
0.996811	0.625977	0.697838
0.123820	0.125012	0.632976
0.877221	0.373844	0.718370
0.384372	0.381143	0.729142
0.998557	0.876907	0.653730
0.127184	0.875545	0.719460
0.623485	0.623115	0.633132
0.500272	0.626347	0.698403
0.363503	0.876811	0.719529
0.634195	0.871185	0.719972
0.873372	0.623949	0.632904
0.873671	0.125149	0.632893
0.498818	0.875322	0.653738
0.124052	0.624874	0.632971
0.248546	0.872982	0.654277
0.998184	0.125990	0.697175
0.747871	0.372533	0.655321
0.748719	0.872180	0.653766
0.497857	0.124222	0.695921
0.628565	0.366683	0.721019
0.373793	0.125820	0.633069
0.116978	0.372475	0.720461
0.749347	0.621785	0.697423
0.249419	0.126731	0.698164
0.249116	0.621207	0.697134
0.248928	0.372969	0.653799
0.373883	0.623861	0.633312

0.749587 0.121213 0.697564
0.999748 0.377288 0.654118
0.870822 0.872316 0.719729

POSCAR (IS: CO + O_t on Ru(10$\bar{1}$0) with 1.75ML O)
1.00000000
10.90720 0.00000 0.00000
0.00000 8.57660 0.00000
0.00000 0.00000 35.76230
C O Ru
1 15 64
D
0.375906 0.392701 0.804985
0.749098 0.719472 0.747834
0.995676 0.870483 0.762040
0.249682 0.868961 0.757685
0.502434 0.869602 0.761540
0.512976 0.220399 0.747878
0.749015 0.028424 0.748004
0.509835 0.525032 0.746761
0.246903 0.193469 0.751349
0.241804 0.538746 0.747386
0.991304 0.221502 0.748498
0.999135 0.516812 0.745903
0.750137 0.379825 0.762571
0.133213 0.324319 0.698380
0.123775 0.376563 0.808891
0.384614 0.412839 0.837016
0.123560 0.125000 0.500000
0.998557 0.375000 0.522059
0.248973 0.125000 0.566105
0.123970 0.375000 0.588165
0.373561 0.125000 0.500000
0.248559 0.375000 0.522059
0.498974 0.125000 0.566105
0.373971 0.375000 0.588165
0.123560 0.625000 0.500000
0.998557 0.875000 0.522059
0.248973 0.625000 0.566105
0.123970 0.875000 0.588165
0.373561 0.625000 0.500000
0.248559 0.875000 0.522059
0.498974 0.625000 0.566105

0.373971	0.875000	0.588165
0.623560	0.125000	0.500000
0.498557	0.375000	0.522059
0.748973	0.125000	0.566105
0.623970	0.375000	0.588165
0.873561	0.125000	0.500000
0.748559	0.375000	0.522059
0.998974	0.125000	0.566105
0.873971	0.375000	0.588165
0.623560	0.625000	0.500000
0.498557	0.875000	0.522059
0.748973	0.625000	0.566105
0.623970	0.875000	0.588165
0.873561	0.625000	0.500000
0.748559	0.875000	0.522059
0.998974	0.625000	0.566105
0.873971	0.875000	0.588165
0.873876	0.125104	0.632596
0.750165	0.374417	0.655936
0.113516	0.873098	0.723193
0.249430	0.119138	0.697829
0.124026	0.121930	0.631980
0.000095	0.375217	0.653941
0.496839	0.620331	0.696997
0.862926	0.373895	0.721533
0.874961	0.623712	0.632730
0.749273	0.874500	0.652095
0.870242	0.874450	0.722666
0.129080	0.367166	0.760194
0.124213	0.627841	0.633024
0.996938	0.876162	0.655121
0.749796	0.628668	0.696751
0.497382	0.374848	0.653147
0.375277	0.124060	0.632969
0.252749	0.375803	0.654097
0.000633	0.126301	0.697404
0.634088	0.373786	0.721110
0.624295	0.125691	0.632935
0.249044	0.633856	0.697136
0.750410	0.119619	0.696867
0.999497	0.625416	0.696816
0.373895	0.625564	0.633097
0.249982	0.876417	0.653827
0.384492	0.874202	0.722718

0.370644 0.370560 0.753497
0.624251 0.623884 0.632791
0.501233 0.875009 0.655200
0.497024 0.129041 0.697373
0.628292 0.874233 0.722571

POSCAR (TS: CO + O_t on Ru(10$\bar{1}$0) with 1.75ML O)
1.00000000
10.90720 0.00000 0.00000
0.00000 8.57660 0.00000
0.00000 0.00000 35.76230
C O Ru
1 15 64
D
0.360235 0.394976 0.807041
0.751281 0.721491 0.747821
0.997050 0.873669 0.762071
0.251155 0.871881 0.756415
0.504689 0.872159 0.761601
0.515402 0.222367 0.748572
0.750880 0.029981 0.747997
0.512738 0.527831 0.747598
0.255150 0.192672 0.749805
0.251002 0.547233 0.746359
0.993976 0.224659 0.749062
0.001503 0.520457 0.746676
0.753062 0.381744 0.762927
0.132590 0.324131 0.697845
0.181268 0.383115 0.806614
0.391634 0.420359 0.837575
0.123560 0.125000 0.500000
0.998557 0.375000 0.522059
0.248973 0.125000 0.566105
0.123970 0.375000 0.588165
0.373561 0.125000 0.500000
0.248559 0.375000 0.522059
0.498974 0.125000 0.566105
0.373971 0.375000 0.588165
0.123560 0.625000 0.500000
0.998557 0.875000 0.522059
0.248973 0.625000 0.566105
0.123970 0.875000 0.588165
0.373561 0.625000 0.500000
0.248559 0.875000 0.522059

0.498974	0.625000	0.566105
0.373971	0.875000	0.588165
0.623560	0.125000	0.500000
0.498557	0.375000	0.522059
0.748973	0.125000	0.566105
0.623970	0.375000	0.588165
0.873561	0.125000	0.500000
0.748559	0.375000	0.522059
0.998974	0.125000	0.566105
0.873971	0.375000	0.588165
0.623560	0.625000	0.500000
0.498557	0.875000	0.522059
0.748973	0.625000	0.566105
0.623970	0.875000	0.588165
0.873561	0.625000	0.500000
0.748559	0.875000	0.522059
0.998974	0.625000	0.566105
0.873971	0.875000	0.588165
0.874416	0.125657	0.632588
0.751360	0.375435	0.656035
0.113429	0.874878	0.722833
0.251647	0.119062	0.696914
0.124440	0.122595	0.631883
0.000103	0.376334	0.653731
0.498661	0.620661	0.697252
0.865901	0.375654	0.722065
0.875541	0.624533	0.632727
0.749826	0.875374	0.652080
0.872038	0.876175	0.722669
0.138323	0.371104	0.757561
0.124607	0.628544	0.632890
0.997462	0.877130	0.655289
0.751368	0.629844	0.696829
0.498200	0.375673	0.653263
0.376375	0.124755	0.632843
0.253631	0.376773	0.653891
0.001539	0.128450	0.697733
0.636623	0.375667	0.721535
0.625115	0.126556	0.632988
0.251082	0.636781	0.696274
0.751889	0.121337	0.696909
0.000697	0.626078	0.697105
0.374992	0.626140	0.632931
0.250811	0.877402	0.653389

0.388294 0.876100 0.722337
0.374557 0.373427 0.752804
0.625012 0.624328 0.632840
0.502363 0.875840 0.655300
0.499133 0.131264 0.697606
0.629933 0.875724 0.722593

POSCAR (IS: CO + O_b on Ru(10$\bar{1}$0) with 1.75ML O)
1.00000000
10.90720 0.00000 0.00000
0.00000 8.57660 0.00000
0.00000 0.00000 35.76230
C O Ru
1 15 64
D
0.376481 0.367713 0.805135
0.748751 0.719411 0.747863
0.995676 0.869650 0.762050
0.249537 0.868423 0.757694
0.502287 0.872093 0.761516
0.513811 0.218568 0.747630
0.749014 0.028371 0.747958
0.508635 0.523201 0.746984
0.245284 0.191489 0.751157
0.242781 0.537136 0.747595
0.990909 0.221078 0.748538
0.999295 0.516294 0.745846
0.749995 0.380132 0.762563
0.132812 0.324276 0.698311
0.124161 0.377017 0.808872
0.386181 0.365758 0.837501
0.123560 0.125000 0.500000
0.998557 0.375000 0.522059
0.248973 0.125000 0.566105
0.123970 0.375000 0.588165
0.373561 0.125000 0.500000
0.248559 0.375000 0.522059
0.498974 0.125000 0.566105
0.373971 0.375000 0.588165
0.123560 0.625000 0.500000
0.998557 0.875000 0.522059
0.248973 0.625000 0.566105
0.123970 0.875000 0.588165
0.373561 0.625000 0.500000

0.248559	0.875000	0.522059
0.498974	0.625000	0.566105
0.373971	0.875000	0.588165
0.623560	0.125000	0.500000
0.498557	0.375000	0.522059
0.748973	0.125000	0.566105
0.623970	0.375000	0.588165
0.873561	0.125000	0.500000
0.748559	0.375000	0.522059
0.998974	0.125000	0.566105
0.873971	0.375000	0.588165
0.623560	0.625000	0.500000
0.498557	0.875000	0.522059
0.748973	0.625000	0.566105
0.623970	0.875000	0.588165
0.873561	0.625000	0.500000
0.748559	0.875000	0.522059
0.998974	0.625000	0.566105
0.873971	0.875000	0.588165
0.873771	0.125036	0.632585
0.750063	0.374402	0.655930
0.113413	0.872608	0.723175
0.249121	0.118845	0.697732
0.123962	0.121791	0.631971
0.999969	0.375121	0.653931
0.496685	0.619713	0.697166
0.862746	0.373770	0.721532
0.874897	0.623651	0.632729
0.749216	0.874419	0.652096
0.870128	0.874217	0.722677
0.128924	0.366364	0.760189
0.124157	0.627715	0.633036
0.996859	0.876009	0.655116
0.749639	0.628669	0.696789
0.497297	0.374656	0.653131
0.375176	0.123861	0.632926
0.252653	0.375649	0.654084
0.000373	0.126039	0.697393
0.633855	0.373814	0.721113
0.624224	0.125568	0.632918
0.249076	0.633305	0.697239
0.750345	0.119548	0.696837
0.999429	0.625261	0.696797
0.373837	0.625387	0.633131

0.249905 0.876093 0.653837
0.384250 0.873869 0.722687
0.370345 0.367103 0.753403
0.624183 0.623773 0.632805
0.501147 0.874608 0.655199
0.496871 0.128496 0.697211
0.628210 0.874098 0.722556

POSCAR (TS: CO + O_b on Ru(10$\bar{1}$0) with 1.75ML O)
1.00000000
10.90720 0.00000 0.00000
0.00000 8.57660 0.00000
0.00000 0.00000 35.76230
C O Ru
1 15 64
D
0.448583 0.370874 0.803159
0.750724 0.718772 0.748132
0.997035 0.871722 0.760206
0.246924 0.871447 0.761243
0.499255 0.872964 0.757100
0.518466 0.193631 0.745120
0.750145 0.029312 0.748048
0.514140 0.548213 0.744423
0.255753 0.215146 0.751128
0.251587 0.515683 0.747665
0.984618 0.220909 0.748818
0.994141 0.519186 0.746412
0.624763 0.374075 0.789422
0.128968 0.325510 0.698118
0.117785 0.372952 0.810223
0.442815 0.369295 0.835596
0.123560 0.125000 0.500000
0.998557 0.375000 0.522059
0.248973 0.125000 0.566105
0.123970 0.375000 0.588165
0.373561 0.125000 0.500000
0.248559 0.375000 0.522059
0.498974 0.125000 0.566105
0.373971 0.375000 0.588165
0.123560 0.625000 0.500000
0.998557 0.875000 0.522059
0.248973 0.625000 0.566105
0.123970 0.875000 0.588165

0.373561	0.625000	0.500000
0.248559	0.875000	0.522059
0.498974	0.625000	0.566105
0.373971	0.875000	0.588165
0.623560	0.125000	0.500000
0.498557	0.375000	0.522059
0.748973	0.125000	0.566105
0.623970	0.375000	0.588165
0.873561	0.125000	0.500000
0.748559	0.375000	0.522059
0.998974	0.125000	0.566105
0.873971	0.375000	0.588165
0.623560	0.625000	0.500000
0.498557	0.875000	0.522059
0.748973	0.625000	0.566105
0.623970	0.875000	0.588165
0.873561	0.625000	0.500000
0.748559	0.875000	0.522059
0.998974	0.625000	0.566105
0.873971	0.875000	0.588165
0.872594	0.125443	0.632803
0.747858	0.374666	0.655798
0.122090	0.873814	0.723224
0.248638	0.124465	0.698429
0.122969	0.121699	0.632011
0.998874	0.375326	0.654088
0.496453	0.626476	0.694816
0.866727	0.374825	0.721106
0.873930	0.623458	0.632990
0.748314	0.874341	0.652384
0.868732	0.874680	0.721697
0.119663	0.367433	0.762084
0.123127	0.627974	0.633139
0.995693	0.876129	0.654685
0.746940	0.623398	0.697349
0.497002	0.374712	0.653492
0.373094	0.124416	0.632356
0.250544	0.375308	0.653782
0.000219	0.125279	0.697364
0.642352	0.373003	0.738717
0.624094	0.126474	0.632651
0.247957	0.628617	0.698142
0.747843	0.124890	0.697219
0.999541	0.626844	0.696863

0.371650 0.625023 0.632656
0.248905 0.876330 0.654437
0.367996 0.874422 0.722214
0.398475 0.368779 0.750685
0.624016 0.623040 0.632524
0.500028 0.874673 0.653524
0.496826 0.122391 0.694872
0.633886 0.874232 0.721249

POSCAR (IS: CO + O_t on Ru(10$\bar{1}$0) with 4ML O)
1.00000000
8.53140 0.00000 0.00000
0.00000 10.96120 0.00000
0.00000 0.00000 22.98250
C O Ru
1 34 80
D
0.591790 0.768193 0.886195
0.831371 0.639984 0.842369
0.098454 0.941990 0.647319
0.010940 0.691403 0.647622
0.564552 0.619808 0.773388
0.300630 0.638542 0.839501
0.805324 0.386489 0.839612
0.807588 0.892980 0.841514
0.536101 0.871416 0.770568
0.273739 0.241649 0.723588
0.598301 0.445348 0.648375
0.508299 0.195581 0.647924
0.286132 0.890431 0.838532
0.770143 0.241846 0.724964
0.335827 0.992647 0.724564
0.041878 0.376251 0.763802
0.266933 0.396381 0.839003
0.570058 0.119683 0.770686
0.097994 0.443023 0.647378
0.008247 0.193453 0.647351
0.311474 0.142709 0.838598
0.045673 0.876328 0.764829
0.822376 0.140773 0.840649
0.535873 0.369267 0.774034
0.827690 0.490666 0.725326
0.278149 0.739466 0.724779

0.600141	0.943530	0.647547
0.508195	0.694279	0.648064
0.060761	0.625969	0.764336
0.770392	0.742287	0.725458
0.339292	0.492300	0.727219
0.064558	0.123973	0.766184
0.832987	0.990820	0.723786
0.551662	0.778732	0.933854
0.540668	0.490192	0.877892
0.056170	0.121709	0.257553
0.056174	0.371711	0.257554
0.305795	0.120329	0.389016
0.305897	0.370323	0.389013
0.055944	0.995507	0.354960
0.055954	0.245501	0.354958
0.306108	0.246517	0.287477
0.306111	0.996519	0.287479
0.556170	0.121709	0.257553
0.556174	0.371711	0.257554
0.805795	0.120329	0.389016
0.805897	0.370323	0.389013
0.555944	0.995507	0.354960
0.555954	0.245501	0.354958
0.806108	0.246517	0.287477
0.806111	0.996519	0.287479
0.056170	0.621709	0.257553
0.056174	0.871711	0.257554
0.305795	0.620329	0.389016
0.305897	0.870323	0.389013
0.055944	0.495507	0.354960
0.055954	0.745501	0.354958
0.306108	0.746517	0.287477
0.306111	0.496519	0.287479
0.556170	0.621709	0.257553
0.556174	0.871711	0.257554
0.805795	0.620329	0.389016
0.805897	0.870323	0.389013
0.555944	0.495507	0.354960
0.555954	0.745501	0.354958
0.806108	0.746517	0.287477
0.806111	0.496519	0.287479
0.805332	0.496621	0.492872
0.804856	0.746031	0.492974
0.555194	0.870618	0.459654

0.555414	0.620754	0.459675
0.556421	0.742175	0.559749
0.553052	0.492571	0.559972
0.919848	0.510520	0.802667
0.184083	0.758901	0.801580
0.923815	0.841816	0.687435
0.187232	0.591196	0.688057
0.793143	0.871808	0.594677
0.815853	0.621435	0.595635
0.305486	0.996165	0.492896
0.304771	0.246545	0.492838
0.055065	0.370688	0.459650
0.055533	0.120701	0.459633
0.056365	0.242237	0.559635
0.053151	0.992031	0.559696
0.415412	0.009985	0.804403
0.692882	0.258102	0.805066
0.426885	0.347879	0.689120
0.679265	0.094699	0.687752
0.292651	0.371872	0.595438
0.316350	0.122062	0.594781
0.805481	0.996533	0.492792
0.804573	0.246279	0.492851
0.555061	0.370785	0.459688
0.555409	0.120743	0.459644
0.556219	0.242553	0.559851
0.553079	0.992284	0.559755
0.920553	0.009831	0.802383
0.184057	0.260450	0.801859
0.922096	0.344173	0.687170
0.182333	0.093314	0.686681
0.792339	0.372362	0.594784
0.816045	0.121849	0.595009
0.305493	0.496223	0.492953
0.304707	0.746529	0.492849
0.055070	0.870593	0.459658
0.055508	0.620604	0.459653
0.056434	0.741624	0.559864
0.052892	0.492102	0.559688
0.427777	0.505558	0.815037
0.683148	0.757798	0.810597
0.431150	0.844457	0.688865
0.675678	0.596751	0.689925
0.293026	0.871667	0.595162

0.316155 0.621954 0.595007

POSCAR (TS: CO + O_t on Ru(10$\bar{1}$0) with 4ML O)
1.00000000
8.53140 0.00000 0.00000
0.00000 10.96120 0.00000
0.00000 0.00000 22.98250
C O Ru
1 34 80
D
0.572431 0.709518 0.886912
0.841131 0.641133 0.840023
0.098811 0.942660 0.647920
0.011216 0.692591 0.647628
0.570862 0.618690 0.768345
0.306126 0.648081 0.839583
0.805917 0.385890 0.839458
0.798844 0.888902 0.841894
0.533689 0.867572 0.772816
0.275402 0.240784 0.724928
0.599153 0.444477 0.648411
0.508883 0.195500 0.647975
0.283023 0.892727 0.839681
0.772440 0.242246 0.725025
0.337397 0.992530 0.725124
0.046119 0.372709 0.766390
0.286382 0.390703 0.841651
0.568842 0.120426 0.770852
0.100095 0.443095 0.647646
0.009696 0.192572 0.647871
0.315770 0.141365 0.840679
0.041324 0.876725 0.765841
0.817688 0.139698 0.841457
0.540795 0.371077 0.772799
0.833966 0.490545 0.724751
0.274852 0.742257 0.724220
0.600825 0.944157 0.647919
0.509826 0.694223 0.648298
0.064641 0.625206 0.764427
0.770906 0.743088 0.725999
0.336447 0.490636 0.727182
0.065271 0.122728 0.769129
0.833082 0.991819 0.724128
0.548124 0.742920 0.934537

0.543882 0.545047 0.878182
0.056170 0.121709 0.257553
0.056174 0.371711 0.257554
0.305795 0.120329 0.389016
0.305897 0.370323 0.389013
0.055944 0.995507 0.354960
0.055954 0.245501 0.354958
0.306108 0.246517 0.287477
0.306111 0.996519 0.287479
0.556170 0.121709 0.257553
0.556174 0.371711 0.257554
0.805795 0.120329 0.389016
0.805897 0.370323 0.389013
0.555944 0.995507 0.354960
0.555954 0.245501 0.354958
0.806108 0.246517 0.287477
0.806111 0.996519 0.287479
0.056170 0.621709 0.257553
0.056174 0.871711 0.257554
0.305795 0.620329 0.389016
0.305897 0.870323 0.389013
0.055944 0.495507 0.354960
0.055954 0.745501 0.354958
0.306108 0.746517 0.287477
0.306111 0.496519 0.287479
0.556170 0.621709 0.257553
0.556174 0.871711 0.257554
0.805795 0.620329 0.389016
0.805897 0.870323 0.389013
0.555944 0.495507 0.354960
0.555954 0.745501 0.354958
0.806108 0.746517 0.287477
0.806111 0.496519 0.287479
0.805874 0.496684 0.492950
0.805240 0.746401 0.493013
0.555446 0.870847 0.459753
0.555763 0.620887 0.459751
0.557037 0.742417 0.559907
0.553813 0.492666 0.560058
0.924795 0.507453 0.802537
0.182269 0.761890 0.801769
0.923676 0.842613 0.687943
0.186891 0.592485 0.688123
0.793396 0.872147 0.594902

0.817464 0.622155 0.595220
0.305827 0.996410 0.493069
0.305122 0.246611 0.492967
0.055461 0.370812 0.459729
0.055814 0.120809 0.459744
0.057035 0.242369 0.559861
0.053680 0.992233 0.559947
0.417496 0.008814 0.805308
0.692146 0.258708 0.805050
0.427222 0.346656 0.689376
0.680683 0.095977 0.687688
0.293620 0.372081 0.595519
0.316621 0.122178 0.595301
0.805850 0.996658 0.492906
0.805043 0.246471 0.492959
0.555405 0.370886 0.459753
0.555642 0.120871 0.459744
0.556659 0.242686 0.559904
0.553446 0.992586 0.559941
0.915136 0.008244 0.803749
0.190435 0.259736 0.804034
0.925578 0.343638 0.687181
0.182537 0.093408 0.688039
0.793494 0.372301 0.594977
0.816708 0.122045 0.595099
0.306015 0.496422 0.493006
0.305230 0.746696 0.492936
0.055468 0.870833 0.459730
0.055879 0.620793 0.459721
0.057395 0.742301 0.559885
0.053888 0.492315 0.559762
0.427478 0.510024 0.811257
0.683880 0.752184 0.810369
0.431223 0.845003 0.688770
0.679284 0.595101 0.689362
0.293576 0.871954 0.595477
0.317121 0.622221 0.595076

POSCAR (IS: CO + O_b on Ru(10$\bar{1}$0) with 4ML O)
1.00000000
8.53140 0.00000 0.00000
0.00000 10.96120 0.00000
0.00000 0.00000 22.98250
C O Ru

1 33 80

D

0.589626	0.760510	0.886096
0.832170	0.640394	0.842789
0.098594	0.942485	0.647606
0.008978	0.693382	0.647372
0.568595	0.619694	0.772121
0.301863	0.637841	0.838523
0.792411	0.391993	0.840594
0.802468	0.895685	0.842275
0.536735	0.871204	0.770030
0.273636	0.241199	0.724453
0.598935	0.444918	0.648139
0.508330	0.193355	0.647784
0.287729	0.889201	0.838872
0.771184	0.242297	0.724953
0.335624	0.991800	0.724851
0.041131	0.373341	0.768578
0.287829	0.390952	0.840930
0.568646	0.120882	0.770659
0.098764	0.442728	0.647721
0.008785	0.193183	0.647807
0.313383	0.139863	0.840146
0.043015	0.877246	0.766173
0.819978	0.143999	0.840572
0.538497	0.371445	0.770458
0.832221	0.491065	0.725199
0.275663	0.740209	0.724767
0.599884	0.943729	0.647820
0.509186	0.693336	0.648465
0.061227	0.624803	0.765348
0.772046	0.742382	0.725918
0.335276	0.491710	0.724748
0.065957	0.123917	0.767704
0.833592	0.992221	0.724430
0.548260	0.765220	0.933952
0.056170	0.121709	0.257553
0.056174	0.371711	0.257554
0.305795	0.120329	0.389016
0.305897	0.370323	0.389013
0.055944	0.995507	0.354960
0.055954	0.245501	0.354958
0.306108	0.246517	0.287477
0.306111	0.996519	0.287479

0.556170	0.121709	0.257553
0.556174	0.371711	0.257554
0.805795	0.120329	0.389016
0.805897	0.370323	0.389013
0.555944	0.995507	0.354960
0.555954	0.245501	0.354958
0.806108	0.246517	0.287477
0.806111	0.996519	0.287479
0.056170	0.621709	0.257553
0.056174	0.871711	0.257554
0.305795	0.620329	0.389016
0.305897	0.870323	0.389013
0.055944	0.495507	0.354960
0.055954	0.745501	0.354958
0.306108	0.746517	0.287477
0.306111	0.496519	0.287479
0.556170	0.621709	0.257553
0.556174	0.871711	0.257554
0.805795	0.620329	0.389016
0.805897	0.870323	0.389013
0.555944	0.495507	0.354960
0.555954	0.745501	0.354958
0.806108	0.746517	0.287477
0.806111	0.496519	0.287479
0.805488	0.496412	0.492963
0.804756	0.746165	0.492958
0.555227	0.870611	0.459713
0.555553	0.620656	0.459712
0.556468	0.742127	0.559943
0.553318	0.492419	0.559966
0.919115	0.509914	0.803762
0.181957	0.759851	0.801948
0.923704	0.843485	0.687939
0.182647	0.593599	0.687186
0.792919	0.872011	0.594932
0.816196	0.621682	0.595386
0.305511	0.996149	0.492920
0.304810	0.246375	0.492868
0.055113	0.370621	0.459698
0.055532	0.120662	0.459677
0.056408	0.242115	0.559797
0.053247	0.992050	0.559816
0.416833	0.008801	0.804515
0.689335	0.260316	0.804940

0.426936 0.344481 0.687773
0.680323 0.095007 0.687928
0.292994 0.371651 0.595071
0.316128 0.121685 0.594912
0.805542 0.996429 0.492885
0.804761 0.246275 0.492946
0.555234 0.370681 0.459721
0.555512 0.120645 0.459681
0.556435 0.242238 0.559834
0.553079 0.992177 0.559808
0.918531 0.011733 0.803368
0.188655 0.259323 0.804018
0.924699 0.344185 0.687762
0.182154 0.093369 0.687533
0.792727 0.372043 0.595200
0.816277 0.121801 0.595153
0.305614 0.496238 0.492911
0.304872 0.746419 0.492906
0.055128 0.870588 0.459662
0.055520 0.620613 0.459679
0.056415 0.742064 0.559671
0.053129 0.492093 0.559807
0.414448 0.508939 0.804609
0.682526 0.758256 0.811009
0.430503 0.843607 0.688774
0.679528 0.596326 0.689696
0.293104 0.871594 0.595226
0.316125 0.621893 0.594851

POSCAR (TS: CO + O_b on Ru(10$\bar{1}$0) with 4ML O)
1.00000000
8.53140 0.00000 0.00000
0.00000 10.96120 0.00000
0.00000 0.00000 22.98250
C O Ru
1 33 80
D
0.474451 0.704403 0.872768
0.823166 0.640377 0.841293
0.100698 0.942850 0.648332
0.013288 0.692380 0.649340
0.578454 0.617513 0.769775
0.355344 0.656656 0.852949
0.791977 0.392771 0.839936

0.791795	0.893888	0.841093
0.539097	0.871853	0.769956
0.275013	0.242135	0.724651
0.602902	0.443083	0.647971
0.510704	0.191812	0.647640
0.289799	0.895739	0.841565
0.777729	0.241754	0.724364
0.337753	0.992806	0.725459
0.041971	0.370981	0.769983
0.292260	0.399408	0.839967
0.574532	0.120725	0.769847
0.103824	0.444594	0.648338
0.011604	0.193460	0.648090
0.326534	0.147598	0.840830
0.039312	0.873438	0.767766
0.824033	0.143489	0.841954
0.543942	0.366420	0.767955
0.841141	0.493232	0.725284
0.280811	0.739816	0.727974
0.601649	0.943419	0.648111
0.511269	0.692833	0.649011
0.084517	0.618051	0.774861
0.774082	0.741705	0.726805
0.343425	0.491303	0.724981
0.073725	0.121159	0.771230
0.838102	0.992685	0.724571
0.560622	0.743130	0.909002
0.056170	0.121709	0.257553
0.056174	0.371711	0.257554
0.305795	0.120329	0.389016
0.305897	0.370323	0.389013
0.055944	0.995507	0.354960
0.055954	0.245501	0.354958
0.306108	0.246517	0.287477
0.306111	0.996519	0.287479
0.556170	0.121709	0.257553
0.556174	0.371711	0.257554
0.805795	0.120329	0.389016
0.805897	0.370323	0.389013
0.555944	0.995507	0.354960
0.555954	0.245501	0.354958
0.806108	0.246517	0.287477
0.806111	0.996519	0.287479
0.056170	0.621709	0.257553

0.056174	0.871711	0.257554
0.305795	0.620329	0.389016
0.305897	0.870323	0.389013
0.055944	0.495507	0.354960
0.055954	0.745501	0.354958
0.306108	0.746517	0.287477
0.306111	0.496519	0.287479
0.556170	0.621709	0.257553
0.556174	0.871711	0.257554
0.805795	0.620329	0.389016
0.805897	0.870323	0.389013
0.555944	0.495507	0.354960
0.555954	0.745501	0.354958
0.806108	0.746517	0.287477
0.806111	0.496519	0.287479
0.806654	0.496456	0.493094
0.805812	0.746274	0.493284
0.555828	0.870494	0.459897
0.556242	0.620769	0.459872
0.557598	0.742102	0.560298
0.554974	0.492607	0.560034
0.923872	0.509825	0.805117
0.181982	0.768565	0.805106
0.926731	0.842543	0.688415
0.187448	0.594646	0.689801
0.794205	0.871679	0.595375
0.818347	0.622217	0.595492
0.306249	0.996131	0.493117
0.305645	0.246294	0.492982
0.055903	0.370769	0.459823
0.056183	0.120560	0.459803
0.057875	0.242239	0.560006
0.054540	0.991820	0.560165
0.422687	0.012502	0.805080
0.695733	0.258206	0.804511
0.428483	0.343038	0.686688
0.685146	0.094823	0.687463
0.294522	0.372110	0.594953
0.317528	0.121533	0.595227
0.806433	0.996243	0.493038
0.805794	0.246375	0.492988
0.555919	0.370733	0.459815
0.556118	0.120553	0.459785
0.557800	0.242125	0.559810

0.554161	0.991936	0.559974
0.919618	0.009850	0.804759
0.194457	0.262295	0.804915
0.930793	0.345469	0.687925
0.183237	0.094105	0.688529
0.794975	0.372028	0.595278
0.818114	0.121856	0.595032
0.306623	0.496535	0.493073
0.305708	0.746276	0.493266
0.055879	0.870464	0.459914
0.056264	0.620732	0.459896
0.058110	0.741996	0.560463
0.054708	0.492663	0.560100
0.437469	0.500525	0.803854
0.686280	0.757986	0.807750
0.431816	0.843627	0.689562
0.683193	0.593940	0.689135
0.294559	0.871674	0.595666
0.318301	0.621799	0.595810