

Supplementary Information for

Catalytic Manganese Oxide Nanostructures for The Reverse Water Gas Shift Reaction

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Characterization details

Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM). SEM and TEM images were collected on a Hitachi SU-70 and FEI Tecnai Osiris, respectively. The acceleration voltage was 10 kV for SEM and 200 kV for TEM. For SEM, powder samples were pressed onto double-sided carbon tape, while TEM samples were dispersed in ethanol via sonication and then added dropwise to a holey carbon-coated gold grid. In all cases multiple spots were examined to ensure sample uniformity.

Atomic Force Microscopy (AFM). AFM images were collected on a Bruker Dimension Fastscan using a ScanAsyst Air probe tips. Samples were dispersed in ethanol and then drop cast on silicon wafer. Multiple regions of the sample were scanned to ensure sample uniformity.

X-ray Diffraction (XRD). XRD patterns were collected on a Rigaku SmartLab X-Ray diffractometer using a Cu K α source with a beam energy of 8.04 eV ($\lambda = 1.5406\text{\AA}$). Powder samples were measured on glass slides and data analysis was performed using PDXL-2 Rigaku software.

Fourier Transform Infrared Spectroscopy (FTIR-ATR). Powder samples were measured using a Thermo Nicolet 6700 FTIR with a diamond ATR attachment and KBr beam splitter. Transmission measurements were conducted at room temperature using a deuterated triglycine sulfate (DTGS) detector and data analysis was performed using the Origin software package. Plots shown are the average of 64 scans collected over the range of 500-4000 cm^{-1} . An additional 8 scans were acquired as background before loading each sample. The noise region around 1900-2300 cm^{-1} is caused by the instrumental defects.

X-ray Photoelectron Spectroscopy (XPS). The XPS spectra were collected using a monochromatic 1486.7 eV Al K α X-ray source on PHI VersaProbe II X-ray Photoelectron Spectrometer with a 0.47 eV system resolution. The energy scale has been calibrated using Cu 2p $_{3/2}$ (932.67 eV) and Au 4f $_{7/2}$ (84.00 eV) peaks on a clean copper plate and a clean gold foil, respectively. Powder samples were pressed onto a double-sided scotch tape on a substrate. For region scan, high power (100u100W20kV_HP), 23.500 eV Pass Energy and 0.1000 eV step size were used, and each spectrum was swept for 10 times to improve the accuracy. Data analysis was performed with a software package in MultiPak and CasaXPS. Atomic concentrations were calculated as suggested by the following Eqn (S1):

$$AC_1(\%) = \frac{A_1/R.S.F}{A_1/R.S.F + A_n/R.S.F} \quad (S1)$$

where AC_1 is the atomic concentration for element 1, A_n is the integrated peak area for element n and R.S.F is the relative structural factor.

Brunauer-Emmet-Teller (BET)-N $_2$ Physisorption and Chemisorption. Surface area measurements were performed using a Quantachrome autosorb. Adsorption-Desorption isotherms were constructed using an 11-point Brunauer, Emmett and Teller (BET) measurements protocol with N $_2$ as the adsorbate. Typically, 50-100 mg of sample was used and outgassed at 200°C for 12-18 hours. Measurements of each sample were performed in triplicate and their average and standard deviation were calculated. The CO $_2$ adsorption isotherms of all materials were obtained with an Autosorb iQ2-Quanta Chrome up to 1 bar at 298K. 100 mg of sample were used and were degassed with the following procedure: heat to 60°C for 30 min, heat to 90 °C for 30 min, and heat to 150 °C for 4 hours.

Thermogravimetric Analysis. Thermogravimetric analysis was conducted by TGA in air atmosphere, TA Instruments Q50. The flow rate of air was 100 ml/min. 10-20 mg of sample was loaded into an alumina crucible and heated in the instrument to 40 °C for 1 hour. After 1 hour, the samples were heated at 10 °C/min to 600 °C and left to equilibrate for 1 hour before being allowed to cool to room temperature.

Atomic Force Microscopy

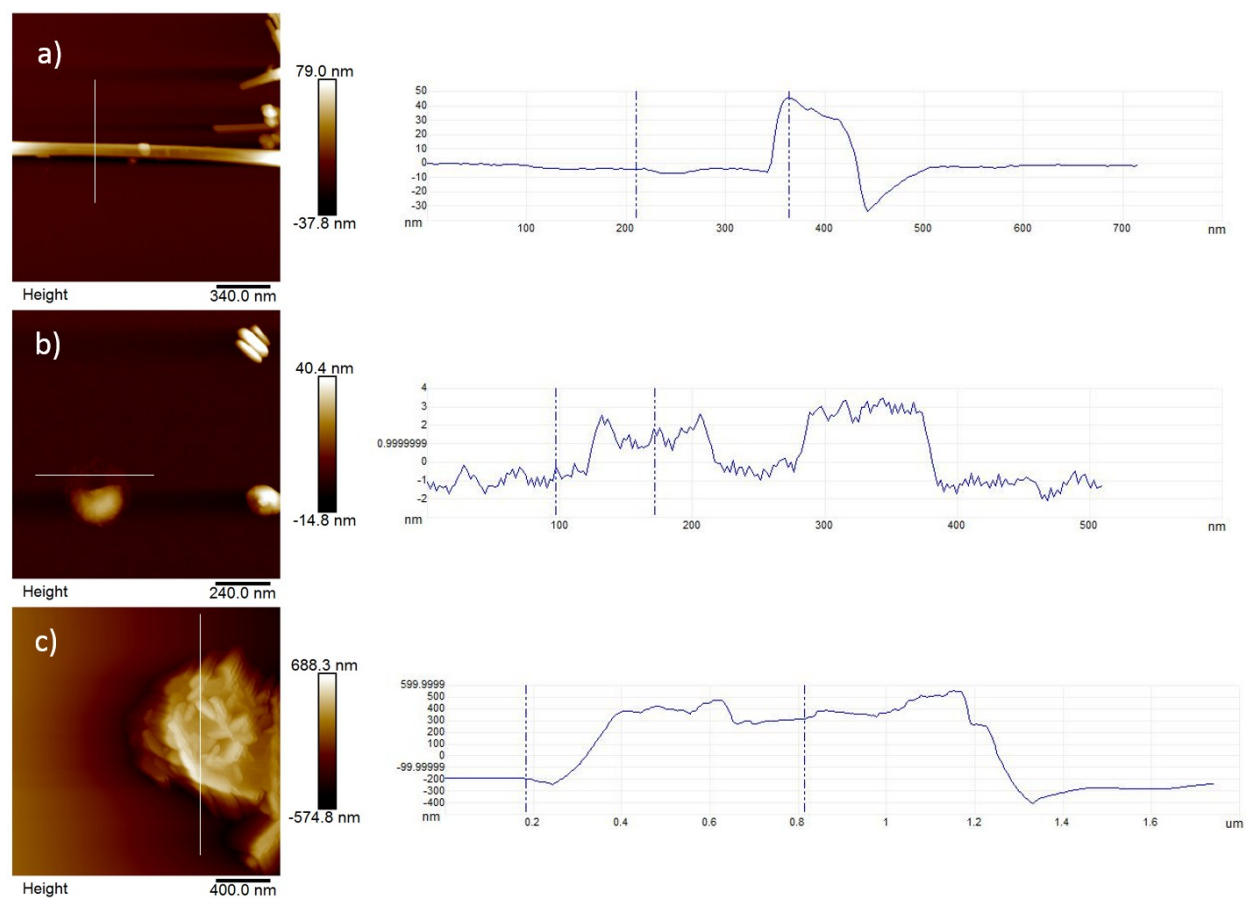


Figure S1 Atomic force microscopy images showing the thicknesses of a) nanowires, b) nanosheets and c) nanoflowers are approximately 30-40 nm, 2-4 nm and 400-500 nm, respectively.

X-ray diffraction patterns

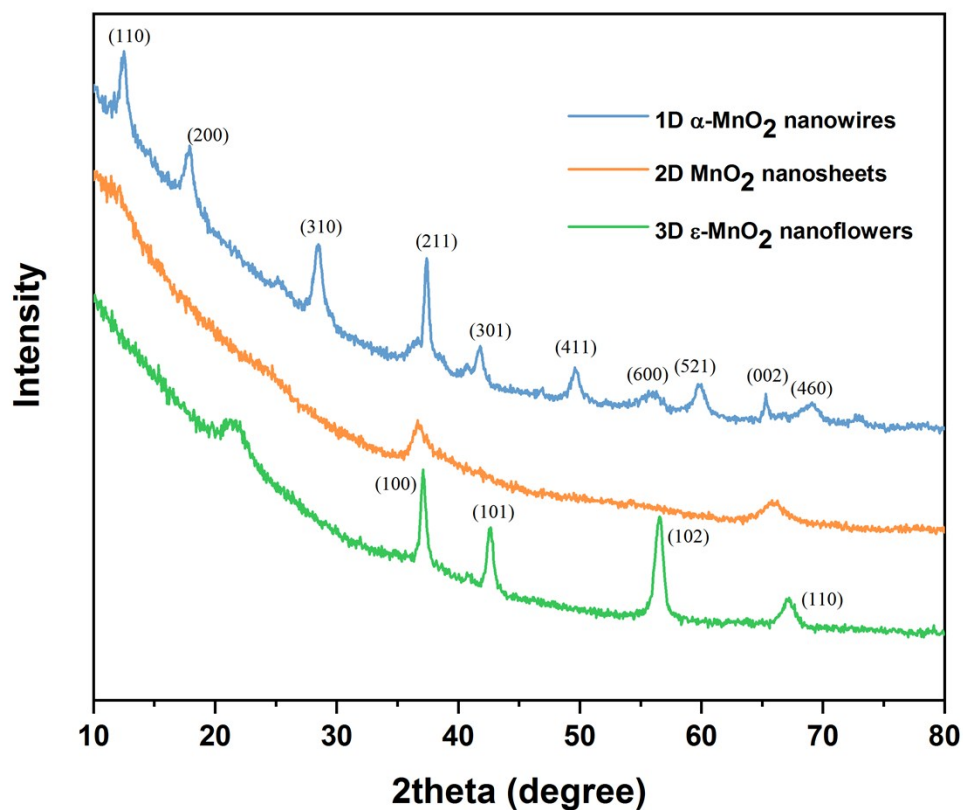


Figure S2 X-ray diffraction patterns. The crystallinities and the chemical compositions of nanowires, nanosheets and nanoflowers were found to be α -MnO₂ (PDF No.: 01-072-1982), polycrystalline/amorphous MnO₂ and ϵ -MnO₂ (PDF No.: 9014106), respectively.

Synthesis sensitivity of α -MnO₂ nanowires growth

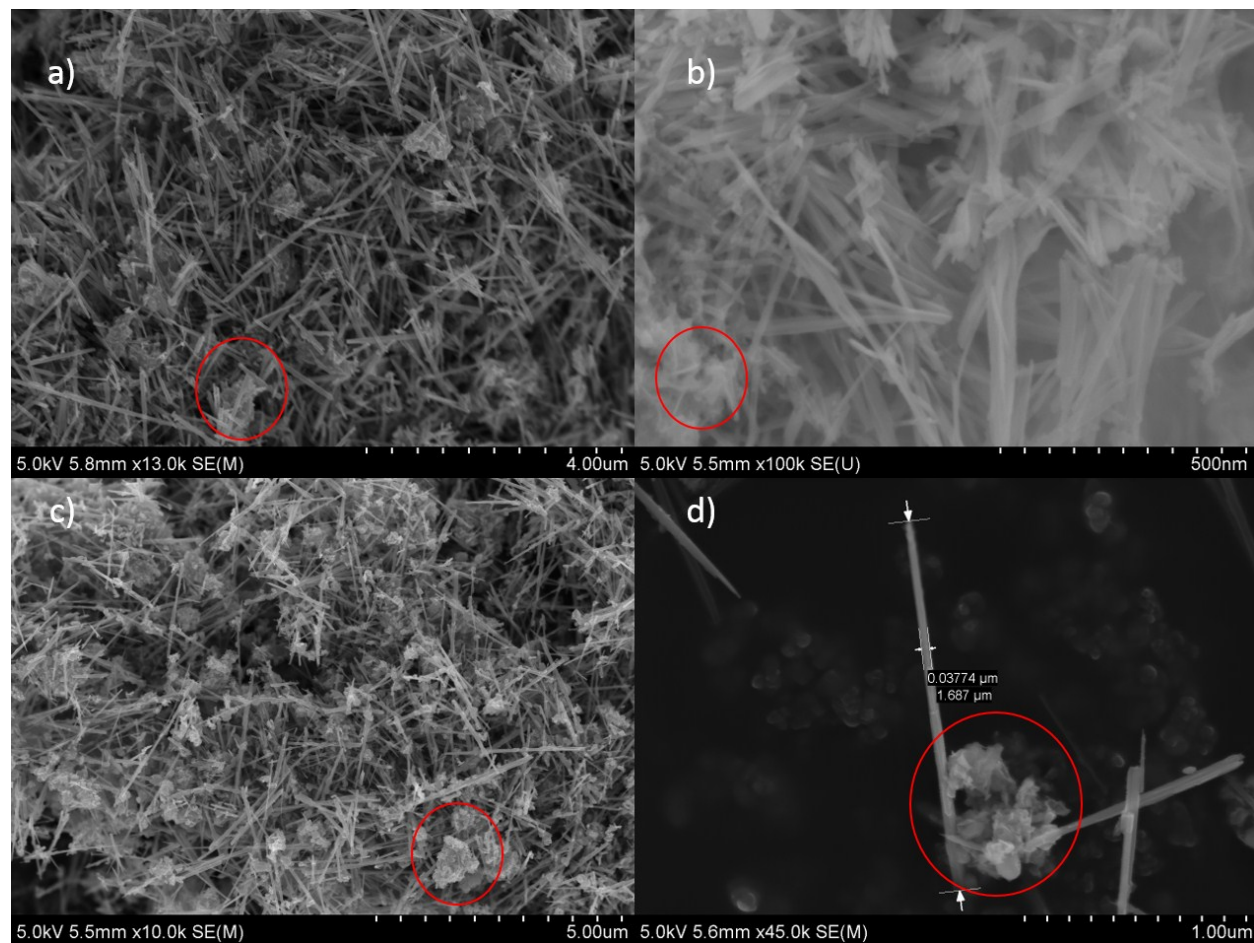


Figure S3 a)-d) The crystal growth of α -MnO₂ nanowires accompanied by side products formation (highlighted by red circles) when the synthetic parameters such as a) mass loading, b) acidity, c) time and d) temperature are perturbed from the optimal values.

X-ray Photoelectron Spectroscopy analysis at C 1s

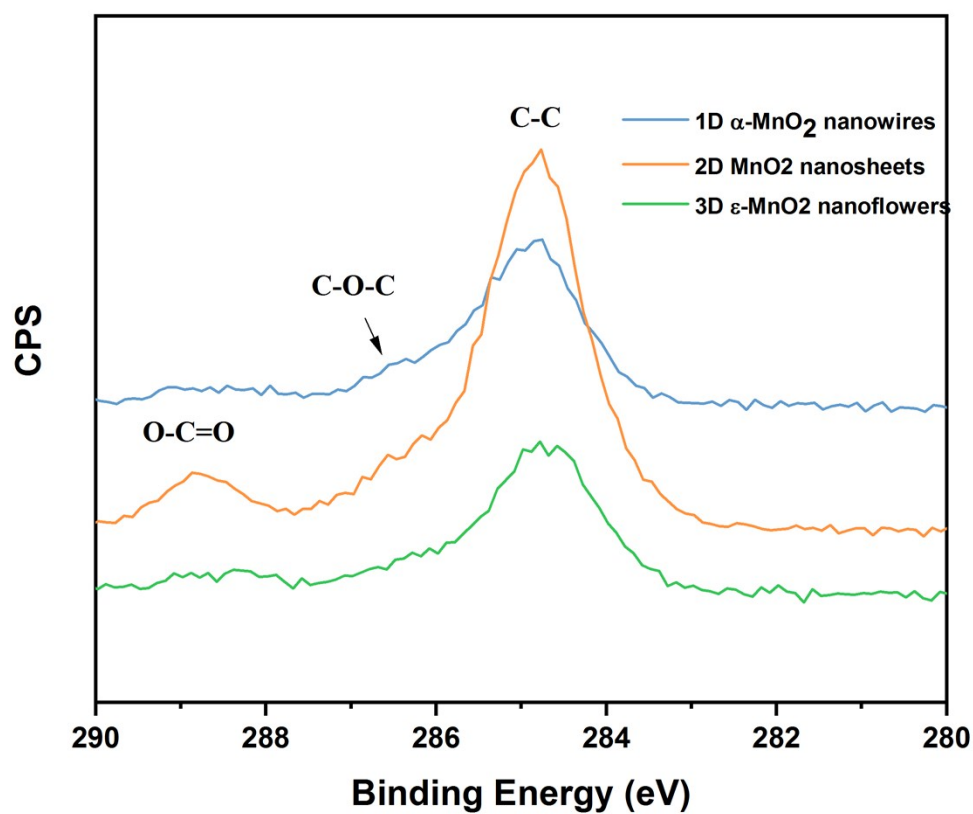


Figure S4 X-ray Photoelectron Spectroscopy spectra for all samples at C 1s. The primary peaks were fixed at 284.4eV for calibration.

Mn 2p3 fitting analysis

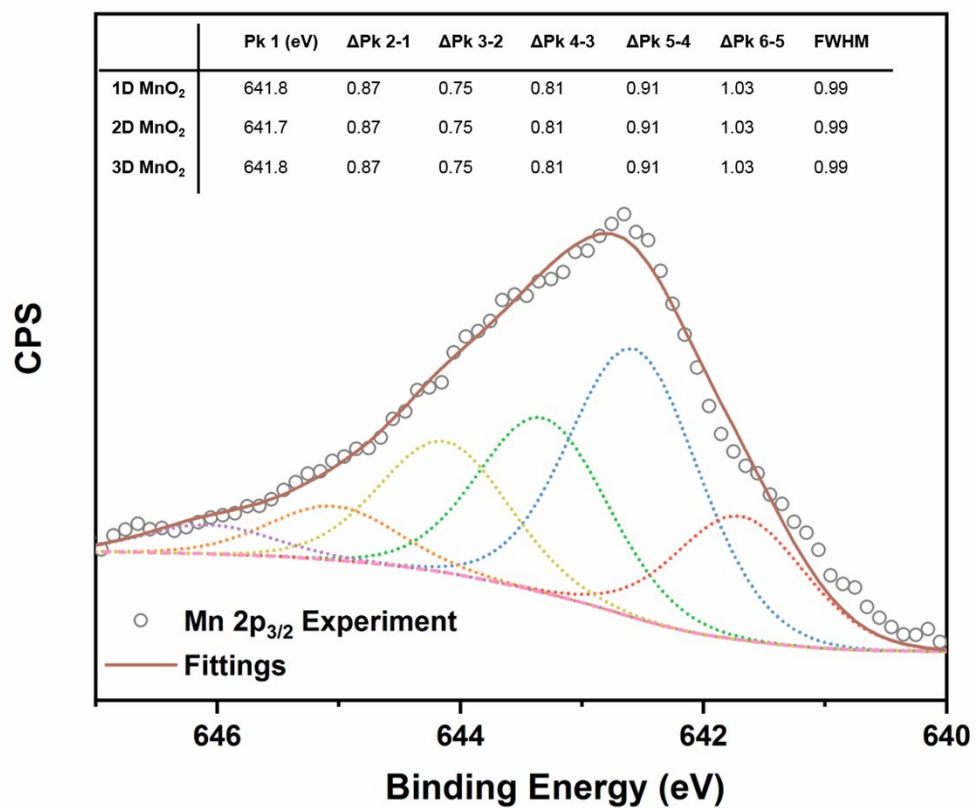


Figure S5 Mn 2p_{3/2} fitting using the models from Beisinger et al.⁴⁵ data, the FWHM was constrained in fit as well as the ΔPk x-1 (x = 2, 3, 4, 5, 6) spacings, only peak 1 was allowed to change.

Fourier-Transformed Infrared Spectroscopy

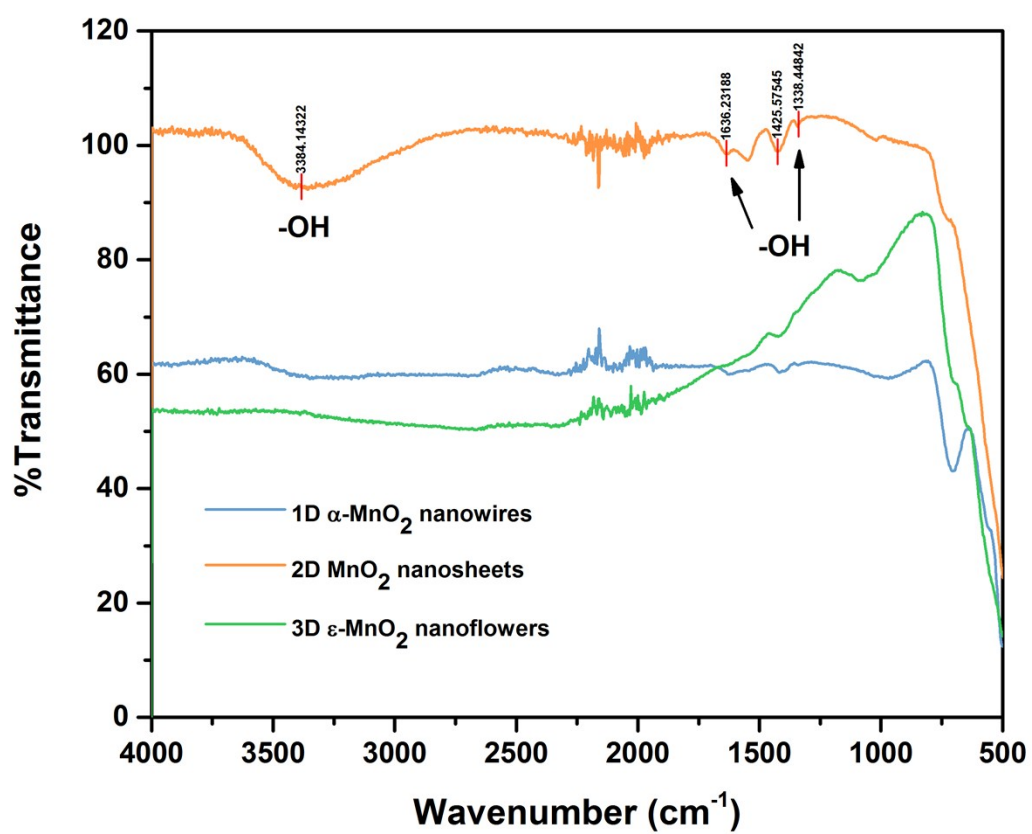


Figure S6 Fourier-Transformed Infrared Spectroscopy (FTIR) studies on all samples showing the 2D MnO_2 nanosheets possess rich hydroxyl groups in the structures.

HAADF elemental mappings

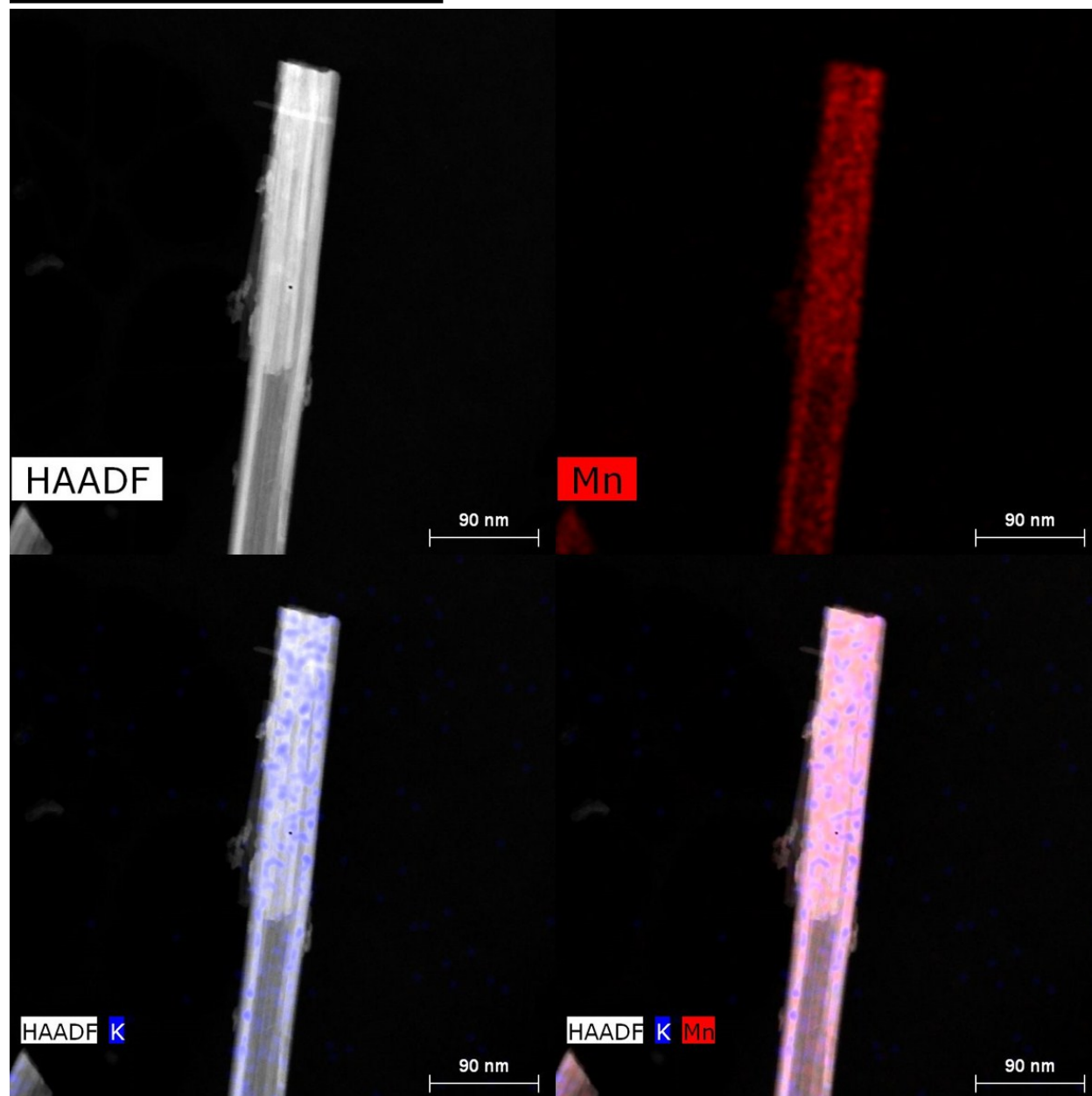


Figure S7 HAADF image example of MnO₂ nanowires showing the distribution of K⁺ ions in the structure.

X-ray diffraction studies during TPR reactions

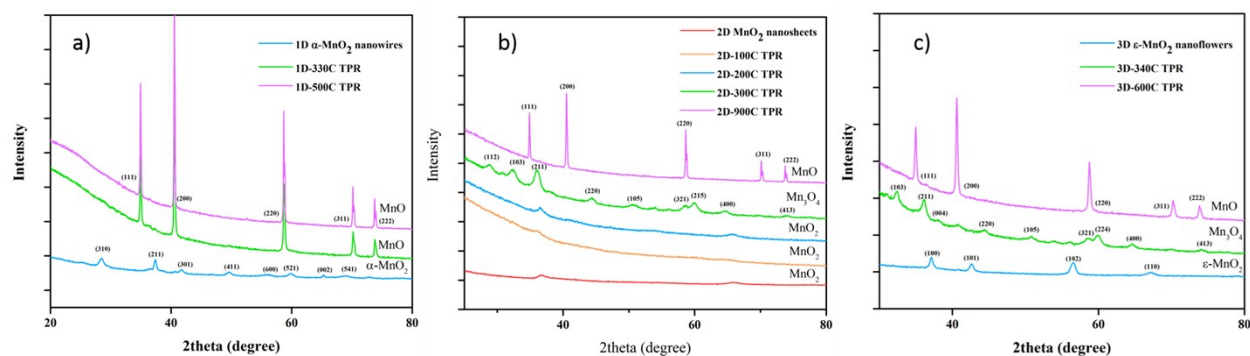


Figure S8 X-ray diffraction analysis of all samples during TPR reactions. a) nanowires; b) nanosheets and c) nanoflowers. The results revealed that regardless of structures, the reduction of MnO_2 in H_2 atmosphere is stepwise, first from MnO_2 to Mn_3O_4 , then Mn_3O_4 to MnO .

SEM images of all samples after TPR and rWGS reactions

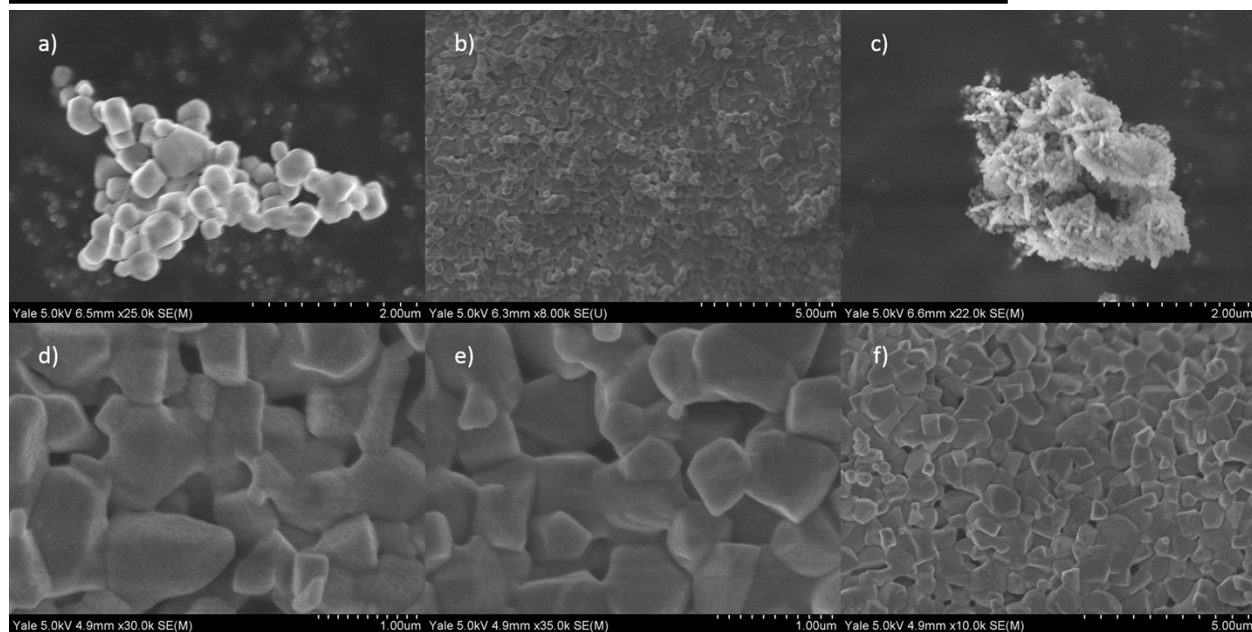


Figure S9 SEM images of a) MnO₂ nanowires, b) MnO₂ nanosheets, c) MnO₂ nanoflowers after TPR treatment and d) MnO₂ nanowires, e) MnO₂ nanosheets and f) MnO₂ nanoflowers after rWGS reaction. The nanostructures were perturbed and became more crystalline at high temperatures.

Complete mass spectrum data for selectivity

Reverse water gas shift was performed on MnO₂ nanowires, nanosheets and nanoflowers and their associated complete mass spectrum are shown below. The right column displays the “zoomed-in” portion of graphs on the left in order to enhance visibility. The SRS RGA 100 mass spectrometer, used here, acquires data every 3 seconds on up to 10 separate mass to charge (m/z) channels. Argon, measured using $m/z=40$, was used as an inert carrier gas and its signal intensity remained relatively constant for the duration of the experiment. No other product besides CO and H₂O were detected.

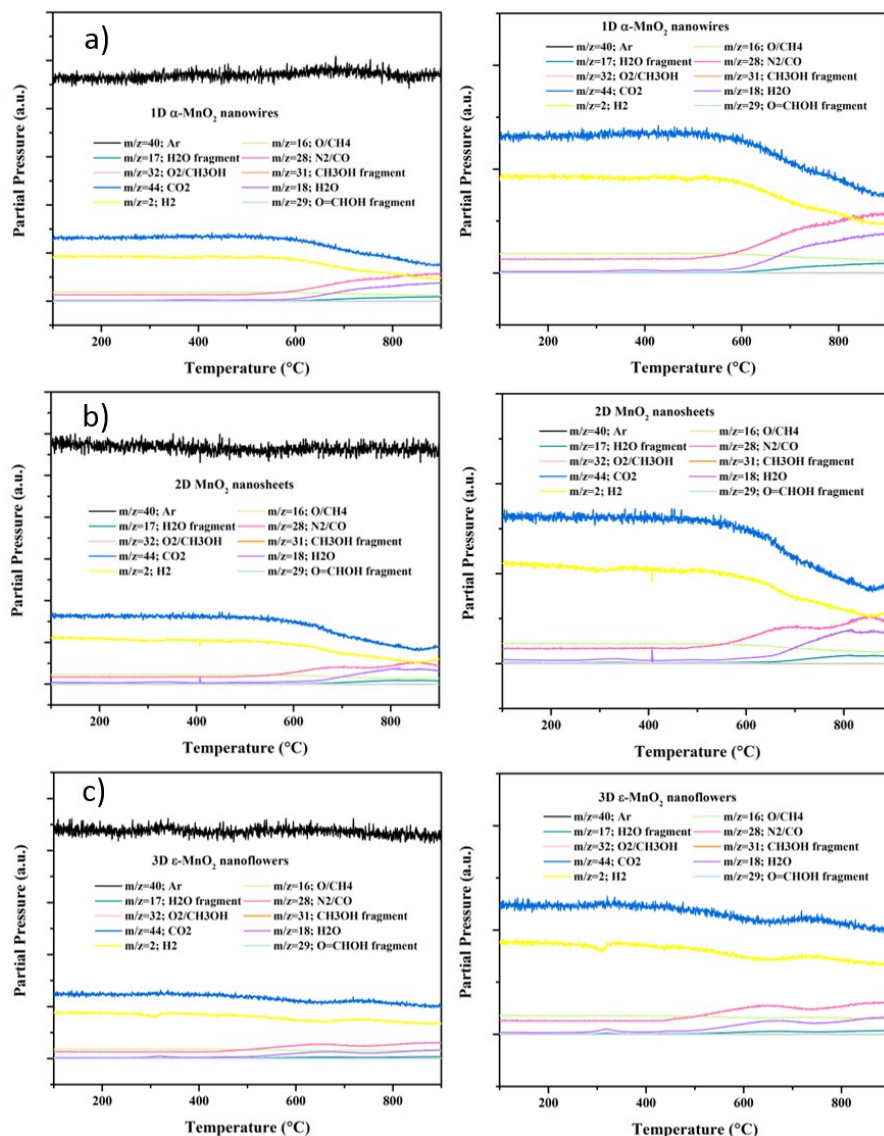


Figure S10 Partial pressure of each species listed is plotted as a function of temperature as by the mass spectrometer during rWGS for a) MnO₂ nanowires, b) MnO₂ nanosheets and c) MnO₂ nanoflowers. In this mode data can be collected every 3 seconds from up to 10 m/z channels. The m/z channels are listed on the figure and color coded for each run. Species that appear at that m/z are listed for convenience; note that this is not an exhaustive list.

XRD studies during and after rWGS reactions

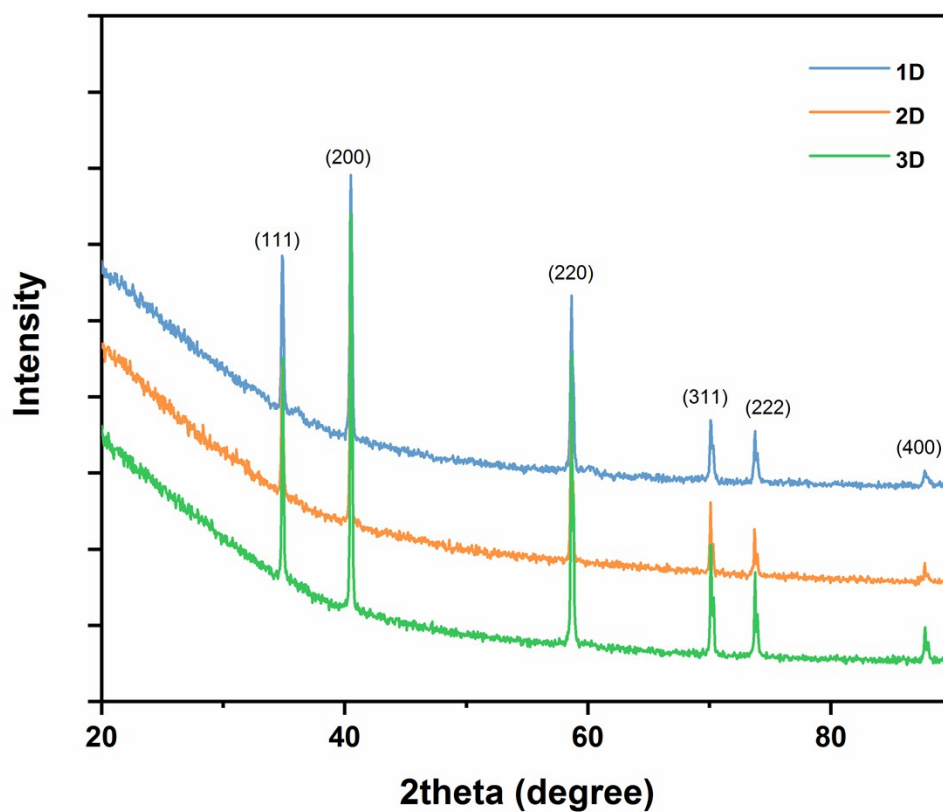


Figure S11 XRD studies on all MnO₂ nanocatalysts during and after rWGS reactions. Results suggested that the most thermodynamically stable form of manganese oxides under rWGS conditions is MnO.

rWGS reaction on commercial MnO catalyst

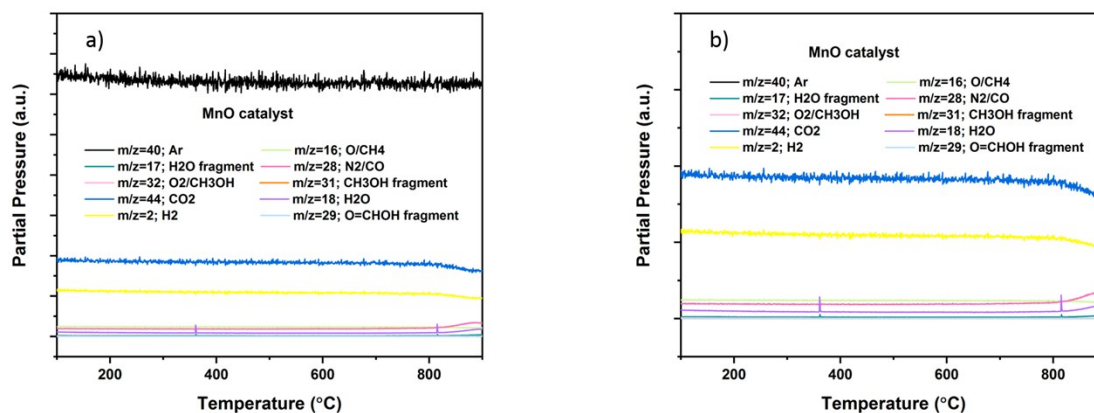


Figure S12 Complete mass spectra for MnO catalyst (nano or bulk, with or without K⁺) in rWGS reaction. Simply starting with MnO catalyst in the rWGS gave almost no conversion, indicating that the transition from MnO₂ pre-catalyst to MnO is essential for the reaction to occur.

Stability tests at 600°C

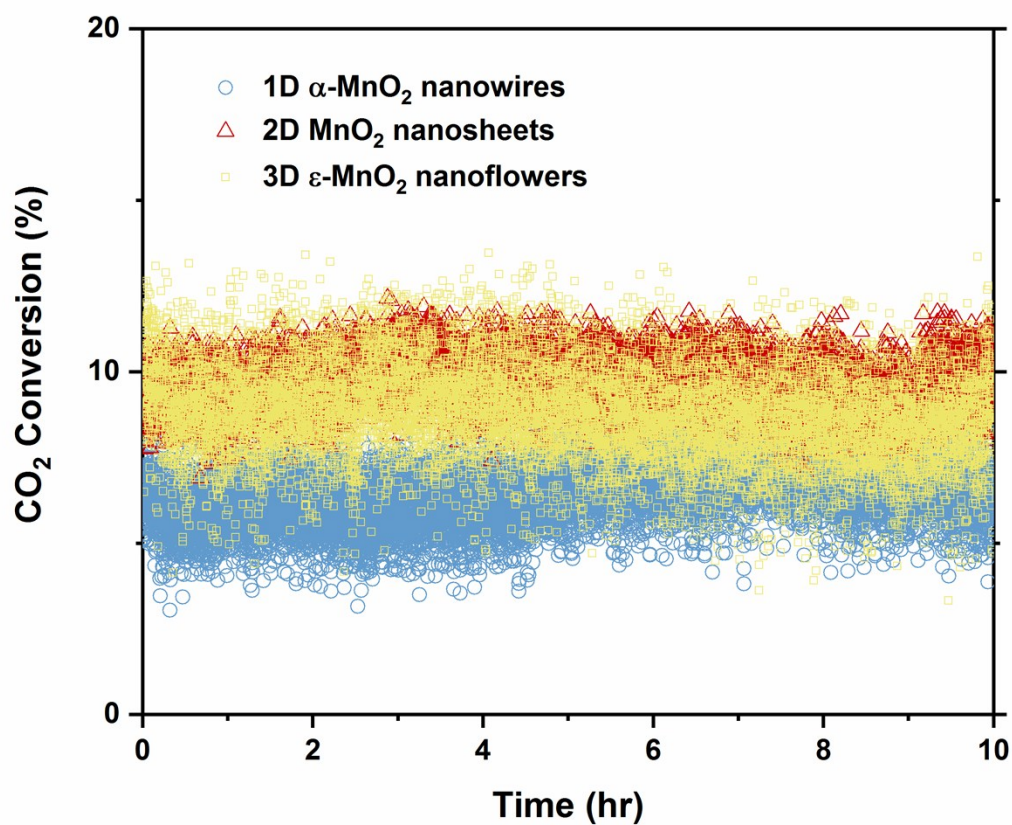


Figure S13 Stability tests at 600°C away from the equilibrium limits, all three nanostructures exhibited high stability over the course of 10 hours.

Comparative table over rWGS catalysts

Table S1 Comparative table on relevant parameters of the catalysts in this work to other reports

Catalyst	Temperature (°C)	CO ₂ WHSV (mL g ⁻¹ h ⁻¹)	H ₂ : CO ₂	CO Selectivity (%)	CO ₂ Conversion (%)	Reference*
1D MnO ₂	850	40,000	1:1	100	43 %	This work
2D MnO ₂	850	40,000	1:1	100	50 %	This work
3D MnO ₂	850	40,000	1:1	100	20 %	This work
MnO ₂ bulk	850	40,000	1:1	100	12 %	This work
1D Hematite	850	24,000	1:1	100	55 %	8
NiO on SBA-15	900	72,000	1:1	100	55 %	22
Cs-Mo ₂ C	750	12,000	1:1	97	40 %	18
Pt/CeO ₂	225	750	4:1	100	13.7 %	13

*References are listed in the main text of the article.

Carbon deposition analysis

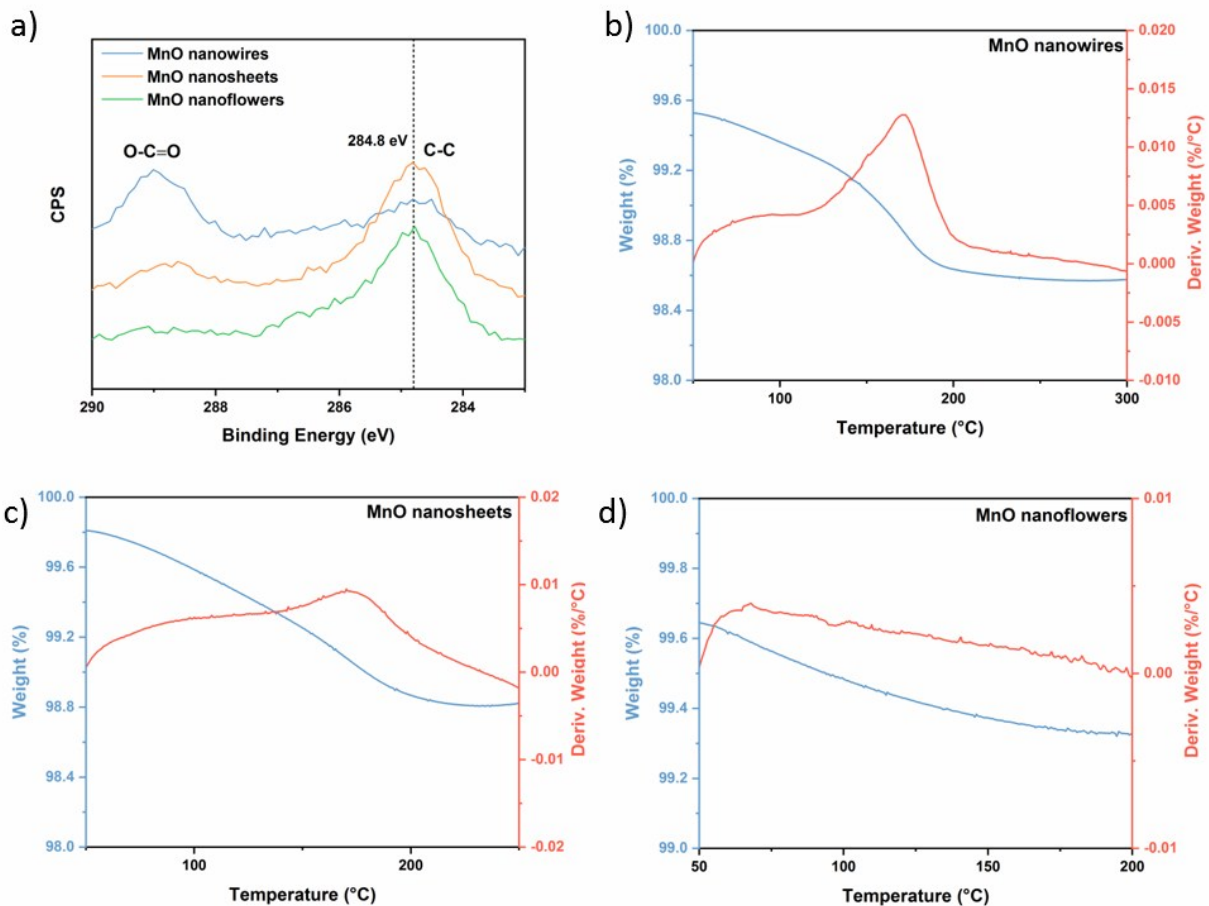


Figure S14 a) XPS analysis on MnO structures post reaction at C1s showing the formation of carbonate species on the surface; TGA analysis in air on MnO derived from b) nanowires, c) nanosheets, d) nanoflowers. The weight loss of all samples is negligible indicating the high resistance to carbon coking.

The effect of K promotion

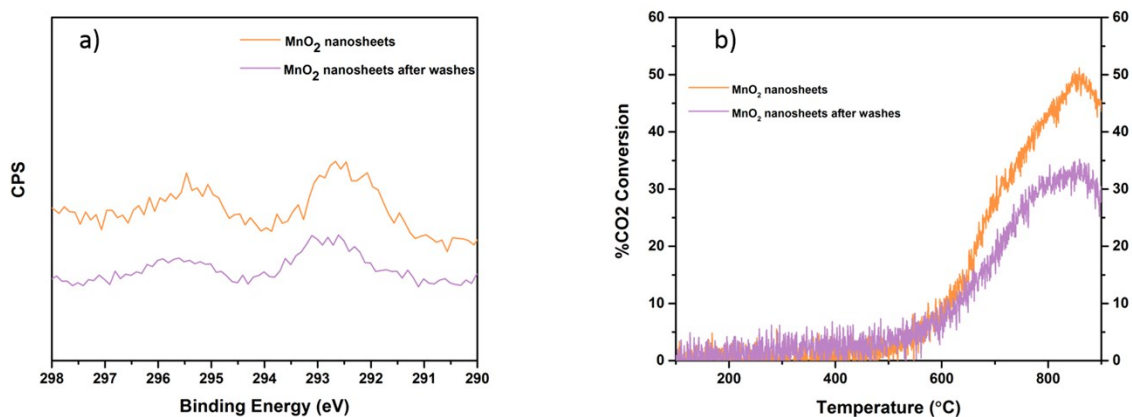


Figure S15 a) XPS K 2p spectra for MnO₂ nanosheets before and after DI water washes, the intensity of K 2p decreased after sonication; b) The “cleaned” sample showed a lower CO₂ conversion, suggesting that the presence of K⁺ has enhanced the catalytic performance of the nanosheets.

BET surface areas

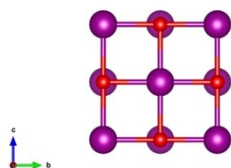
Table S2 BET surface areas measurements*

Samples	Surface Area/ ($\text{m}^2\cdot\text{g}^{-1}$)
MnO nanowires	9.05
MnO nanosheets	16.7
MnO nanoflowers	22.5
Commercial MnO	12.0

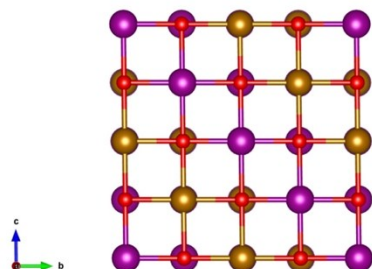
*The surface area measurements were conducted on the actual active species MnO that were taking out at 500°C from the reaction conditions in order to calculate the specific STY.

MnO bulk structures

a) Ferromagnetic phase



b) Antiferromagnetic phase



c) Magnetic moments along (111) plane

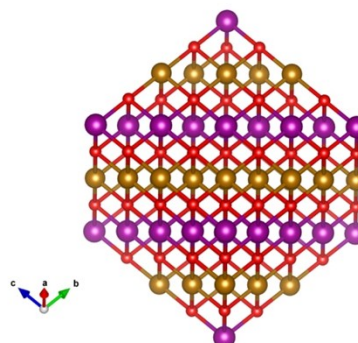


Figure S16 Unit cells and atomic magnetic moments of MnO. Unit cells of MnO in (a) ferromagnetic phase and (b) antiferromagnetic phase; (c) atomic magnetic moments along (111) plane. Purple, brown, and red balls represent spin-up Mn²⁺ ion, spin-down Mn²⁺ ions and O²⁻ ion, respectively.

Pristine and K-doped MnO surfaces

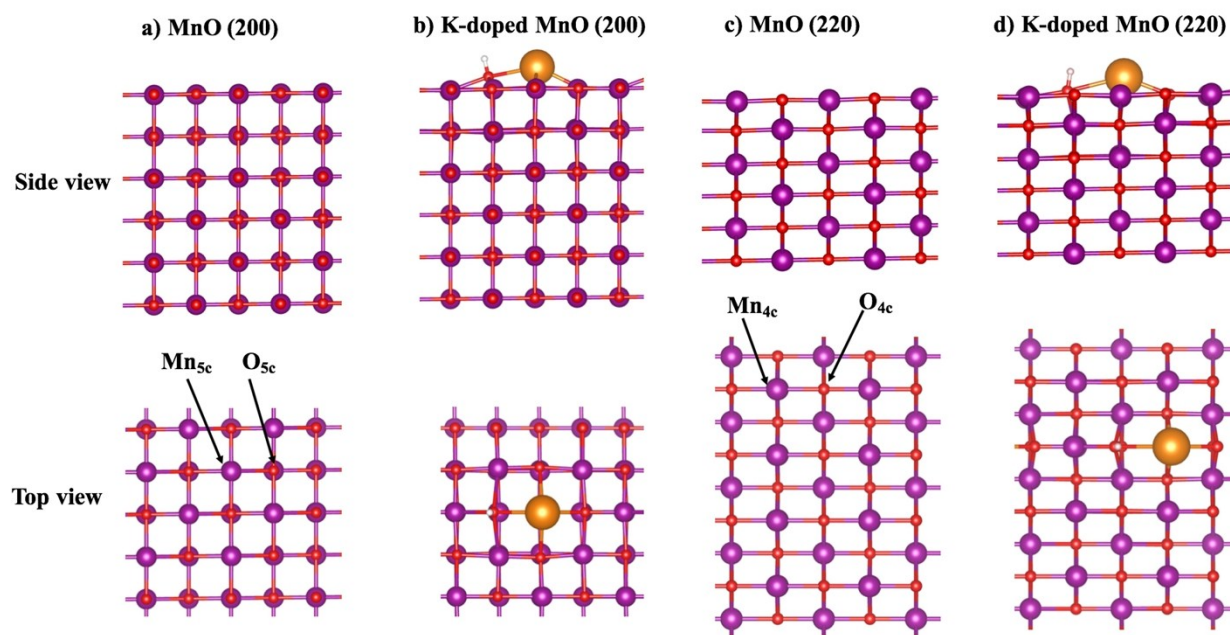


Figure S17 Optimized structures of pristine and K-doped MnO surfaces. (a) MnO (200) surface, (b) K-doped MnO (200) surface, (c) MnO (220) surfaces, and (d) K-doped MnO (220) surface. Purple, red, orange, and white balls represent Mn, O, K, and H atoms, respectively.

Calculated H₂ adsorption on MnO

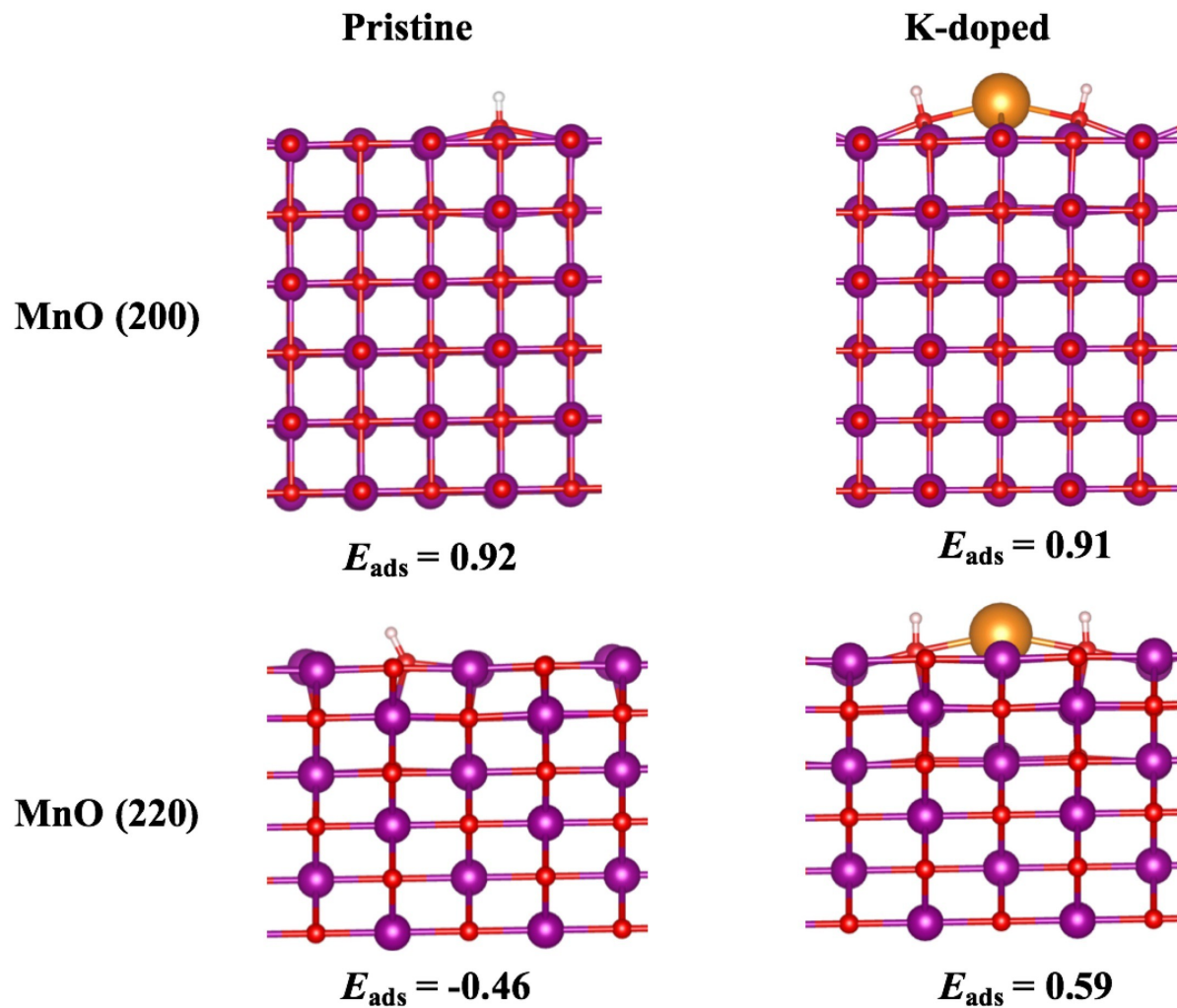


Figure S18 Optimized structures of H atom adsorption on pristine and K-doped MnO surfaces and the calculated adsorption energies in the unit of eV. The adsorption energy of H is calculated according to $E_{\text{ads}} = E_{\text{slab} + \text{H}} - E_{\text{slab}} - \frac{1}{2}E_{\text{H}_2}$. Purple, red, orange, and white balls represent Mn, O, K, and H atoms, respectively.

X-ray Photoelectron Spectroscopy studies on MnO at K2p

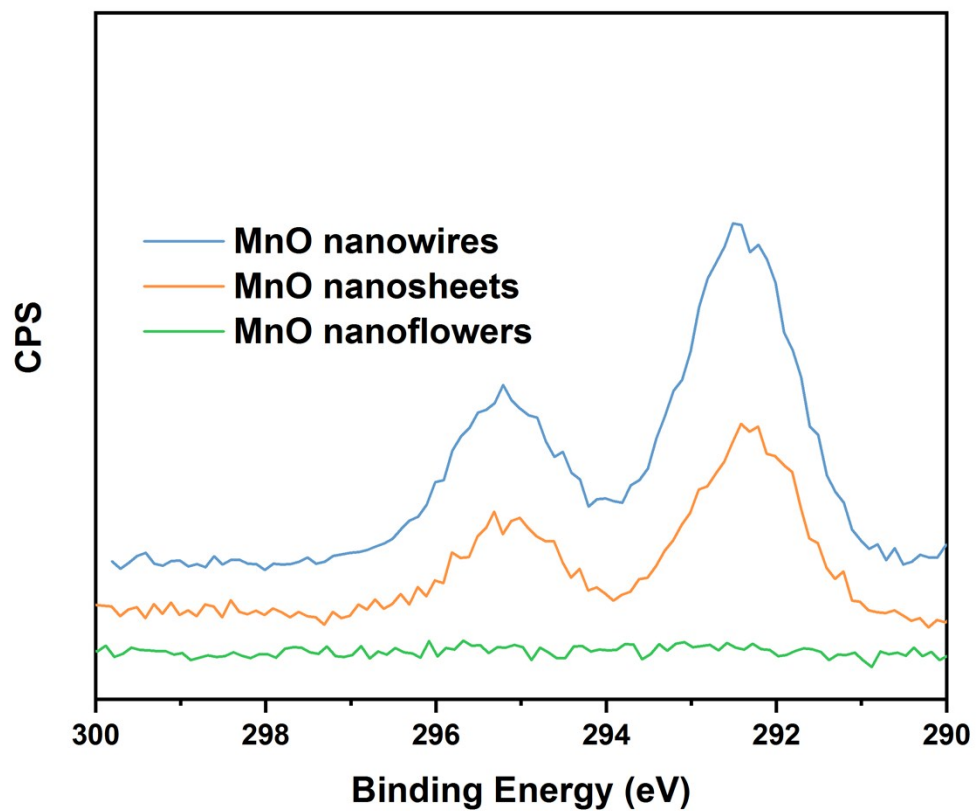


Figure S19 X-ray Photoelectron Spectroscopy studies on MnO catalysts show that the K⁺ remains in the nanowires and nanosheets derivatives.

Correlations between catalytic activities and adsorption energies at different temperatures

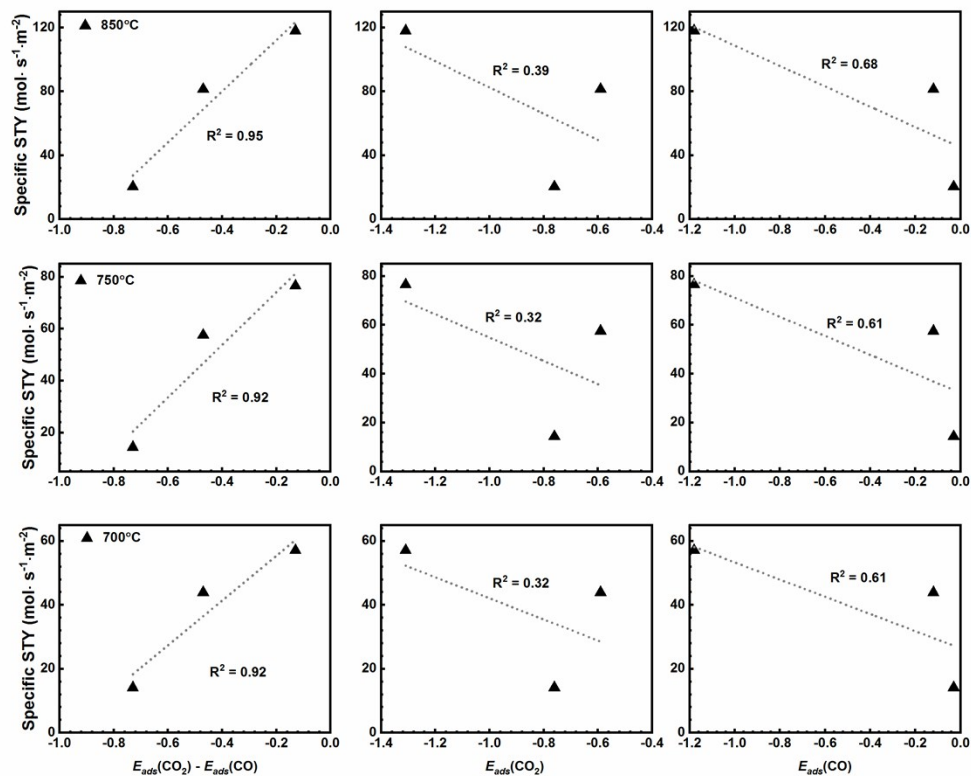


Figure S20 Correlations between the measured specific STY at 850 °C (top), 750 °C (middle), 700 °C (bottom) and the calculated absorption energies of CO₂ and CO and their differences.

Coordinates of optimized structures

All optimized coordinates are given the VASP POSCAR format.

CO:

Title

```
1.0000000000000000
15.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 15.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.0000000000000000
```

```
C O
1 1
```

Direct

```
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0.4666666666666686 0.3885563517862096 0.4666666666666686
```

CO₂:

Title

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0.0000000000000000 15.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.0000000000000000
```

```
C O
1 2
```

Direct

```
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0.4666666666666686 0.5450973883053941 0.4666666666666686
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H₂:

Title

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0.0000000000000000 15.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.0000000000000000
```

```
H
2
```

Direct

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0.4666666666666686 0.4016527872477938 0.4666666666666686
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MnO bulk:

MnO bulk calculation ! title

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-0.0489862487715852 8.9582019290186885 -0.0489862487715852
-0.0489862487715852 -0.0489862487715852 8.9582019290186885

Mn O
32 32

Direct

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0.5000000000000000	0.7500000000000000	0.5000000000000000
0.5000000000000000	0.5000000000000000	0.7500000000000000

MnO (200):

Title

1.0000000000000000

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-0.0977017000000000 8.9579370100000002 0.0000000000000000

-0.0977017000000000 -0.0987731200000000 8.9573924399999996

Mn O

48 48

Selective dynamics

Direct

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0.2406729548883888	0.2499999997209201	0.0000000000000000	F	F	F
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0.1604486363560582	0.5000000005581668	0.5000000000000000	F	F	F
0.2406729548883888	0.2499999997209201	0.5000000000000000	F	F	F
0.1604486363531308	0.2499999997209201	0.7500000000000000	F	F	F
0.2406729548893694	0.0000000000000000	0.7500000000000000	F	F	F
0.3208972734265814	0.5000000005581668	0.0000000000000000	F	F	F
0.4001785589442202	0.2499826359026759	0.9999826361817558	T	T	T
0.4796984207062139	0.0001399133805653	0.0001399133805653	T	T	T
0.3208972734236539	0.2499999997209201	0.2500000000000000	F	F	F
0.4001785589451937	0.9999826361817558	0.2499826361817558	T	T	T
0.3208972734246274	0.0000000000000000	0.5000000000000000	F	F	F
0.5581477170494231	0.7488420369823605	0.9988420367032806	T	T	T
0.4796984203489885	0.7501399136596452	0.2501399133805653	T	T	T
0.4001785589461742	0.7499826364608356	0.4999826361817558	T	T	T
0.3208972730673949	0.7500000002790799	0.7500000000000000	F	F	F
0.5581477170504037	0.4988420372614476	0.2488420367032807	T	T	T
0.4796984203499620	0.5001399139387321	0.5001399133805653	T	T	T
0.4001785589471477	0.4999826367399227	0.7499826361817558	T	T	T
0.5581477170474691	0.2488420364242009	0.4988420367032808	T	T	T
0.4796984203470345	0.2501399131014855	0.7501399133805653	T	T	T
0.5581477170484497	0.9988420367032806	0.7488420367032806	T	T	T
0.2406729550674953	0.2499999997209201	0.2500000000000000	F	F	F
0.2406729550684688	0.0000000000000000	0.0000000000000000	F	F	F
0.1604486365322373	0.2499999997209201	0.0000000000000000	F	F	F
0.1604486365332107	0.0000000000000000	0.2500000000000000	F	F	F
0.2406729547112434	0.7500000002790799	0.2500000000000000	F	F	F
0.2406729550704227	0.5000000005581668	0.0000000000000000	F	F	F
0.1604486365341842	0.7500000002790799	0.0000000000000000	F	F	F
0.1604486365351647	0.5000000005581668	0.2500000000000000	F	F	F
0.2406729547092894	0.2499999997209201	0.7500000000000000	F	F	F
0.2406729550684688	0.0000000000000000	0.5000000000000000	F	F	F
0.1604486365322373	0.2499999997209201	0.5000000000000000	F	F	F
0.1604486365332107	0.0000000000000000	0.7500000000000000	F	F	F
0.2406729547112434	0.7500000002790799	0.7500000000000000	F	F	F
0.2406729547122168	0.5000000005581668	0.5000000000000000	F	F	F
0.1604486365341842	0.7500000002790799	0.5000000000000000	F	F	F

0.1604486365351647	0.5000000005581668	0.7500000000000000	F	F	F
0.4002902715084650	0.2499214691836833	0.2499214694627632	T	T	T
0.4002902715094456	0.9999214694627632	0.9999214694627632	T	T	T
0.3208972732445474	0.2499999997209201	0.0000000000000000	F	F	F
0.3208972732455209	0.0000000000000000	0.2500000000000000	F	F	F
0.5594092109710795	0.2495477115208747	0.2495477117999546	T	T	T
0.5594092109720530	0.9995477117999546	0.9995477117999546	T	T	T
0.4794549738717479	0.2500623352270401	0.0000623355061199	T	T	T
0.4794549738727213	0.0000623355061199	0.2500623355061199	T	T	T
0.4002902715104190	0.7499214697418430	0.2499214694627632	T	T	T
0.4002902715113996	0.4999214700209301	0.9999214694627632	T	T	T
0.3208972732465014	0.7500000002790799	0.0000000000000000	F	F	F
0.3208972732474749	0.5000000005581668	0.2500000000000000	F	F	F
0.5594092106148276	0.7495477120790345	0.2495477117999546	T	T	T
0.5594092109740070	0.4995477123581215	0.9995477117999546	T	T	T
0.4794549738736948	0.7500623357851998	0.0000623355061199	T	T	T
0.4794549738746753	0.5000623360642867	0.2500623355061199	T	T	T
0.4002902715084650	0.2499214691836833	0.7499214694627632	T	T	T
0.4002902715094456	0.9999214694627632	0.4999214694627632	T	T	T
0.3208972732445474	0.2499999997209201	0.5000000000000000	F	F	F
0.3208972732455209	0.0000000000000000	0.7500000000000000	F	F	F
0.5594092106128736	0.2495477115208747	0.7495477117999546	T	T	T
0.5594092109720530	0.9995477117999546	0.4995477117999546	T	T	T
0.4794549738717479	0.2500623352270401	0.5000623355061199	T	T	T
0.4794549738727213	0.0000623355061199	0.7500623355061199	T	T	T
0.4002902711522131	0.7499214697418430	0.7499214694627632	T	T	T
0.4002902715113996	0.4999214700209301	0.4999214694627632	T	T	T
0.3208972732465014	0.7500000002790799	0.5000000000000000	F	F	F
0.3208972732474749	0.5000000005581668	0.7500000000000000	F	F	F
0.5594092106148276	0.7495477120790345	0.7495477117999546	T	T	T
0.5594092106158011	0.4995477123581215	0.4995477117999546	T	T	T
0.4794549738736948	0.7500623357851998	0.5000623355061199	T	T	T
0.4794549738746753	0.5000623360642867	0.7500623355061199	T	T	T

MnO (220):

Title

1.0000000000000000

12.7380876799999996 0.0000000000000000 0.0000000000000000

0.0000000000000000 25.5999145599999984 0.0000000000000000

0.0000000000000000 -0.1389307400000000 8.9573924399999996

Mn O

48 48

Selective dynamics

Direct

0.1250000000000000 0.1845696767434859 0.2500000000000000 F F F

0.3750000000000000 0.1845696767434859 0.2500000000000000 F F F

0.2500000000000000 0.2460929021944338 0.0000000000000000 F F F

0.6250000000000000	0.1845696767434859	0.2500000000000000	F	F	F
0.8749999992149498	0.1845696767434859	0.2500000000000000	F	F	F
0.7500000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.0000000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.0000000000000000	0.1230464509019029	0.5000000000000000	F	F	F
0.2500000000000000	0.1230464512925309	0.5000000000000000	F	F	F
0.7500000000000000	0.1230464512925309	0.5000000000000000	F	F	F
0.8750000000000000	0.3053589899215600	0.7500230609497104	T	T	T
0.1250000000000000	0.3053589903121880	0.7500230609497104	T	T	T
0.0000000000000000	0.3704351884034811	0.4999565243326085	T	T	T
0.5000000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.6250000000000000	0.4240619140726881	0.2463374651901237	T	T	T
0.8750000000000000	0.4240619144633160	0.2463374651901237	T	T	T
0.1250000000000000	0.4240619140726881	0.2463374651901237	T	T	T
0.3750000000000000	0.4240619144633160	0.2463374651901237	T	T	T
0.3750000000000000	0.3053589899215600	0.7500230609497104	T	T	T
0.6250000000000000	0.3053589903121880	0.7500230609497104	T	T	T
0.5000000000000000	0.3704351884034811	0.4999565243326085	T	T	T
0.7500000000000000	0.3704351884034811	0.4999565243326085	T	T	T
0.2499999992149498	0.3704351884034811	0.4999565243326085	T	T	T
0.5000000000000000	0.1230464512925309	0.5000000000000000	F	F	F
0.7500000000000000	0.1230464512925309	0.0000000000000000	F	F	F
0.0000000000000000	0.1230464509019029	0.0000000000000000	F	F	F
0.2500000000000000	0.1230464512925309	0.0000000000000000	F	F	F
0.0000000000000000	0.3704351884034811	0.9999565243326085	T	T	T
0.8749999992149498	0.3053589903121880	0.2500230609497104	T	T	T
0.7500000000000000	0.2460929021944338	0.5000000000000000	F	F	F
0.6249999992149498	0.1845696767434859	0.7500000000000000	F	F	F
0.1250000000000000	0.3053589903121880	0.2500230609497104	T	T	T
0.9999999992149498	0.2460929021944338	0.5000000000000000	F	F	F
0.8750000000000000	0.1845696767434859	0.7500000000000000	F	F	F
0.2500000000000000	0.2460929021944338	0.5000000000000000	F	F	F
0.1250000000000000	0.1845696763528579	0.7500000000000000	F	F	F
0.3750000000000000	0.1845696767434859	0.7500000000000000	F	F	F
0.2500000000000000	0.3704351887941090	0.9999565243326085	T	T	T
0.5000000000000000	0.3704351884034811	0.9999565243326085	T	T	T
0.7500000000000000	0.3704351887941090	0.9999565243326085	T	T	T
0.3750000000000000	0.3053589903121880	0.2500230609497104	T	T	T
0.6250000000000000	0.3053589903121880	0.2500230609497104	T	T	T
0.5000000000000000	0.2460929025850618	0.5000000000000000	F	F	F
0.5000000000000000	0.1230464512925309	0.0000000000000000	F	F	F
0.1250000000000000	0.4240619140726881	0.7463374651901237	T	T	T
0.3750000000000000	0.4240619144633160	0.7463374651901237	T	T	T
0.6250000000000000	0.4240619140726881	0.7463374651901237	T	T	T
0.8750000000000000	0.4240619140726881	0.7463374651901237	T	T	T
0.0000000000000000	0.1230464510972169	0.2500000000000000	F	F	F
0.2500000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.3750000000000000	0.1845696769387999	0.0000000000000000	F	F	F

0.1250000000000000	0.1845696765481719	0.0000000000000000	F	F	F
0.2500000000000000	0.1230464510972169	0.2500000000000000	F	F	F
0.7500000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.8750000000000000	0.1845696769387999	0.0000000000000000	F	F	F
0.6250000000000000	0.1845696769387999	0.0000000000000000	F	F	F
0.7499999992149498	0.1230464510972169	0.2500000000000000	F	F	F
0.0000000000000000	0.3687832437364919	0.2506927423906321	T	T	T
0.1250000000000000	0.3057023170350683	0.0003326658090947	T	T	T
0.8750000000000000	0.3057023170350683	0.0003326658090947	T	T	T
0.0000000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.0000000007850502	0.1230464510972169	0.7500000000000000	F	F	F
0.2500000000000000	0.2460929019991198	0.7500000000000000	F	F	F
0.3750000000000000	0.1845696769387999	0.5000000000000000	F	F	F
0.1250000000000000	0.1845696765481719	0.5000000000000000	F	F	F
0.2500000000000000	0.1230464510972169	0.7500000000000000	F	F	F
0.7499999992149498	0.2460929019991198	0.7500000000000000	F	F	F
0.8750000000000000	0.1845696769387999	0.5000000000000000	F	F	F
0.6250000000000000	0.1845696765481719	0.5000000000000000	F	F	F
0.7500000000000000	0.1230464510972169	0.7500000000000000	F	F	F
0.0000000000000000	0.3687832433458639	0.7506927423906321	T	T	T
0.1249999992149498	0.3057023166444404	0.5003326658090947	T	T	T
0.8750000000000000	0.3057023166444404	0.5003326658090947	T	T	T
0.0000000000000000	0.2460929023897478	0.7500000000000000	F	F	F
0.5000000000000000	0.3687832433458639	0.2506927423906321	T	T	T
0.6250000000000000	0.3057023170350683	0.0003326658090947	T	T	T
0.3750000000000000	0.3057023166444404	0.0003326658090947	T	T	T
0.5000000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.8750000000000000	0.4259526217032074	0.0007456157926321	T	T	T
0.6250000000000000	0.4259526217032074	0.0007456157926321	T	T	T
0.7500000000000000	0.3687832437364919	0.2506927423906321	T	T	T
0.3749999992149498	0.4259526217032074	0.0007456157926321	T	T	T
0.1250000000000000	0.4259526217032074	0.0007456157926321	T	T	T
0.2500000000000000	0.3687832437364919	0.2506927423906321	T	T	T
0.4999999992149498	0.1230464510972169	0.2500000000000000	F	F	F
0.5000000000000000	0.3687832433458639	0.7506927423906321	T	T	T
0.6250000000000000	0.3057023166444404	0.5003326658090947	T	T	T
0.3750000000000000	0.3057023166444404	0.5003326658090947	T	T	T
0.5000000000000000	0.2460929023897478	0.7500000000000000	F	F	F
0.8750000000000000	0.4259526217032074	0.5007456157926321	T	T	T
0.6250000000000000	0.4259526217032074	0.5007456157926321	T	T	T
0.7500000000000000	0.3687832437364919	0.7506927423906321	T	T	T
0.3749999992149498	0.4259526217032074	0.5007456157926321	T	T	T
0.1250000000000000	0.4259526217032074	0.5007456157926321	T	T	T
0.2500000000000000	0.3687832437364919	0.7506927423906321	T	T	T
0.4999999992149498	0.1230464510972169	0.7500000000000000	F	F	F

K-MnO (200):

Title

1.0000000000000000

27.9169395999999992 0.0000000000000000 0.0000000000000000

-0.0977017000000000 8.9579370100000002 0.0000000000000000

-0.0977017000000000 -0.0987731200000000 8.9573924399999996

Mn O H K

47 48 1 1

Selective dynamics

Direct

0.1604486367113367	0.2499999997209201	0.2500000000000000	F	F	F
0.2406729548893694	0.0000000000000000	0.2500000000000000	F	F	F
0.2406729548883888	0.2499999997209201	0.0000000000000000	F	F	F
0.1604486367142641	0.5000000005581668	0.0000000000000000	F	F	F
0.1604486367123101	0.0000000000000000	0.5000000000000000	F	F	F
0.1604486363550848	0.7500000002790799	0.7500000000000000	F	F	F
0.2406729548913233	0.5000000005581668	0.7500000000000000	F	F	F
0.2406729548903428	0.7500000002790799	0.5000000000000000	F	F	F
0.3208972734246274	0.0000000000000000	0.0000000000000000	F	F	F
0.4796775591375297	0.2483996707366558	0.2498932599036429	T	T	T
0.5587078729324328	0.9955846771576782	0.2368001519630616	T	T	T
0.5574888637148618	0.2498155836365302	0.9981886241394051	T	T	T
0.3208972734256008	0.7500000002790799	0.2500000000000000	F	F	F
0.4003978319433154	0.5001722546545557	0.2497113608431801	T	T	T
0.4006685315081842	0.7487777311170317	0.9993296796218450	T	T	T
0.4793537671346822	0.5002918093847011	0.9993417547964909	T	T	T
0.3208972734236539	0.2499999997209201	0.7500000000000000	F	F	F
0.3999817306631532	0.9983654382252483	0.7509318942753883	T	T	T
0.4002623412106381	0.2510957939331991	0.4997567008864860	T	T	T
0.4754200415414397	0.9935807368962973	0.4993237028943715	T	T	T
0.3208972734265814	0.5000000005581668	0.5000000000000000	F	F	F
0.4825729696118911	0.7496188146767313	0.7440836225476314	T	T	T
0.5575303952141720	0.4976244593683567	0.7480001950901096	T	T	T
0.1604486367123101	0.0000000000000000	0.0000000000000000	F	F	F
0.2406729548903428	0.7500000002790799	0.0000000000000000	F	F	F
0.1604486363550848	0.7500000002790799	0.2500000000000000	F	F	F
0.2406729548913233	0.5000000005581668	0.2500000000000000	F	F	F
0.1604486363560582	0.5000000005581668	0.5000000000000000	F	F	F
0.2406729548883888	0.2499999997209201	0.5000000000000000	F	F	F
0.1604486363531308	0.2499999997209201	0.7500000000000000	F	F	F
0.2406729548893694	0.0000000000000000	0.7500000000000000	F	F	F
0.3208972734265814	0.5000000005581668	0.0000000000000000	F	F	F
0.4000639559582573	0.2497439066180768	0.9996378943959967	T	T	T
0.4793572072428512	0.9972376426179511	0.9999132931844217	T	T	T
0.3208972734236539	0.2499999997209201	0.2500000000000000	F	F	F
0.4000096074348459	0.9982835200078508	0.2488760503911423	T	T	T
0.3208972734246274	0.0000000000000000	0.5000000000000000	F	F	F
0.5588330853711844	0.7433931244198093	0.9987225929695374	T	T	T
0.4823870363821146	0.7494728643303291	0.2545921215635259	T	T	T

0.3998957674389381	0.7476657600459521	0.4993989844647583	T	T	T
0.3208972730673949	0.7500000002790799	0.7500000000000000	F	F	F
0.5574059992367759	0.4963607130777967	0.2465595590114528	T	T	T
0.4816546216013141	0.5083988492714648	0.4996792861195347	T	T	T
0.4004094930475867	0.5003741774965863	0.7495411725049967	T	T	T
0.5568326627731468	0.2545038427833641	0.4979196184999414	T	T	T
0.4796573978625220	0.2487831969084073	0.7490940739391542	T	T	T
0.5585604377938026	0.9972531178219326	0.7606719867559212	T	T	T
0.2406729550674953	0.2499999997209201	0.2500000000000000	F	F	F
0.2406729550684688	0.0000000000000000	0.0000000000000000	F	F	F
0.1604486365322373	0.2499999997209201	0.0000000000000000	F	F	F
0.1604486365332107	0.0000000000000000	0.2500000000000000	F	F	F
0.2406729547112434	0.7500000002790799	0.2500000000000000	F	F	F
0.2406729550704227	0.5000000005581668	0.0000000000000000	F	F	F
0.1604486365341842	0.7500000002790799	0.0000000000000000	F	F	F
0.1604486365351647	0.5000000005581668	0.2500000000000000	F	F	F
0.2406729547092894	0.2499999997209201	0.7500000000000000	F	F	F
0.2406729550684688	0.0000000000000000	0.5000000000000000	F	F	F
0.1604486365322373	0.2499999997209201	0.5000000000000000	F	F	F
0.1604486365332107	0.0000000000000000	0.7500000000000000	F	F	F
0.2406729547112434	0.7500000002790799	0.7500000000000000	F	F	F
0.2406729547122168	0.5000000005581668	0.5000000000000000	F	F	F
0.1604486365341842	0.7500000002790799	0.5000000000000000	F	F	F
0.1604486365351647	0.5000000005581668	0.7500000000000000	F	F	F
0.4003187475894140	0.2484366102165911	0.2498433234856325	T	T	T
0.4005291749816925	0.9997451638113238	0.9996486043619567	T	T	T
0.3208972732445474	0.2499999997209201	0.0000000000000000	F	F	F
0.3208972732455209	0.0000000000000000	0.2500000000000000	F	F	F
0.5590704422415482	0.2446755497223011	0.2468523542044993	T	T	T
0.5589876254710748	0.0062915418094492	0.9990022684891053	T	T	T
0.4783763143155134	0.2474260399078044	0.9994568661121226	T	T	T
0.4810210437096279	0.9982456948402717	0.2552149242763567	T	T	T
0.4003663110581623	0.7499682775097918	0.2485931413522115	T	T	T
0.4002115989454756	0.4987632324417068	0.9995991070105218	T	T	T
0.3208972732465014	0.7500000002790799	0.0000000000000000	F	F	F
0.3208972732474749	0.5000000005581668	0.2500000000000000	F	F	F
0.5615740754718406	0.7506457213596514	0.2315201031493337	T	T	T
0.5587778507112461	0.4917082326094980	0.9986270671960518	T	T	T
0.4789021434498696	0.7500212568998200	0.9997491319596367	T	T	T
0.4796547893686200	0.4989718578410284	0.2506680812690414	T	T	T
0.4003444681381199	0.2485631697278276	0.7494467302810653	T	T	T
0.3988197530809984	0.0011809668251415	0.4996024439028438	T	T	T
0.3208972732445474	0.2499999997209201	0.5000000000000000	F	F	F
0.3208972732455209	0.0000000000000000	0.7500000000000000	F	F	F
0.5589923288936207	0.2447329967042772	0.7511839748513873	T	T	T
0.5827950873409423	0.0253031025159324	0.4987142240100130	T	T	T
0.4796729653345179	0.2388966885321779	0.4993367553126907	T	T	T
0.4809777992717651	0.9981724012138605	0.7434738937652349	T	T	T

0.4003249259475271	0.7499854510512209	0.7506517110960862	T	T	T
0.4008621912062186	0.4974884446995822	0.4996795537481890	T	T	T
0.3208972732465014	0.7500000002790799	0.5000000000000000	F	F	F
0.3208972732474749	0.5000000005581668	0.7500000000000000	F	F	F
0.5617358808893783	0.7517554457093713	0.7669938478769779	T	T	T
0.5597078991381365	0.4832907544060641	0.4990884767799149	T	T	T
0.4777054268941175	0.7546473895483691	0.4995165806813339	T	T	T
0.4797235076137194	0.4993466334750029	0.7482679619165332	T	T	T
0.6170058211415307	0.0487934122719326	0.5011278828152425	T	T	T
0.6003047495284323	0.7364317432203341	0.5002514185612672	T	T	T

K-MnO (220):

Title

1.0000000000000000

12.7380876799999996 0.0000000000000000 0.0000000000000000

0.0000000000000000 25.5999145599999984 0.0000000000000000

0.0000000000000000 -0.1389307400000000 8.9573924399999996

Mn O H K

47 48 1 1

Selective dynamics

Direct

0.1250000000000000	0.1845696767434859	0.2500000000000000	F	F	F
0.3750000000000000	0.1845696767434859	0.2500000000000000	F	F	F
0.2500000000000000	0.2460929021944338	0.0000000000000000	F	F	F
0.6250000000000000	0.1845696767434859	0.2500000000000000	F	F	F
0.8749999992149498	0.1845696767434859	0.2500000000000000	F	F	F
0.7500000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.0000000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.0000000000000000	0.1230464509019029	0.5000000000000000	F	F	F
0.2500000000000000	0.1230464512925309	0.5000000000000000	F	F	F
0.7500000000000000	0.1230464512925309	0.5000000000000000	F	F	F
0.8750000000000000	0.3056273532035129	0.7492071836896667	T	T	T
0.1249337452376233	0.3053120926486845	0.7498944164367914	T	T	T
0.9997447679588809	0.3712450966444090	0.5001156659632564	T	T	T
0.5000000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.6253683268467798	0.4221460469132097	0.2447220186796867	T	T	T
0.8750000000000000	0.4247481354040024	0.2457367319304641	T	T	T
0.1246316731532202	0.4221460469132097	0.2447220186796867	T	T	T
0.3750000000000000	0.3056228637219620	0.7504399401832509	T	T	T
0.6250662547623768	0.3053120926486845	0.7498944164367914	T	T	T
0.5029407242320773	0.3694110009942937	0.4948403925978417	T	T	T
0.7502552320411191	0.3712450966444090	0.5001156659632564	T	T	T
0.2470592749828723	0.3694110009942937	0.4948403925978417	T	T	T
0.5000000000000000	0.1230464512925309	0.5000000000000000	F	F	F
0.7500000000000000	0.1230464512925309	0.0000000000000000	F	F	F
0.0000000000000000	0.1230464509019029	0.0000000000000000	F	F	F
0.2500000000000000	0.1230464512925309	0.0000000000000000	F	F	F

0.9998925414314839	0.3705369393820059	0.9993722659440335	T	T	T
0.8749999992149498	0.3055223470429384	0.2499860062859864	T	T	T
0.7500000000000000	0.2460929021944338	0.5000000000000000	F	F	F
0.6249999992149498	0.1845696767434859	0.7500000000000000	F	F	F
0.1254981054881749	0.3051328079866078	0.2488122848217544	T	T	T
0.9999999992149498	0.2460929021944338	0.5000000000000000	F	F	F
0.8750000000000000	0.1845696767434859	0.7500000000000000	F	F	F
0.2500000000000000	0.2460929021944338	0.5000000000000000	F	F	F
0.1250000000000000	0.1845696763528579	0.7500000000000000	F	F	F
0.3750000000000000	0.1845696767434859	0.7500000000000000	F	F	F
0.2510525890909570	0.3701197843615356	0.0046163076972867	T	T	T
0.4989474109090430	0.3701197839709147	0.0046163076972867	T	T	T
0.7501074585685161	0.3705369397726267	0.9993722659440335	T	T	T
0.3750000000000000	0.3091507347102755	0.2485820896441590	T	T	T
0.6245018945118251	0.3051328079866078	0.2488122848217544	T	T	T
0.5000000000000000	0.2460929025850618	0.5000000000000000	F	F	F
0.5000000000000000	0.1230464512925309	0.0000000000000000	F	F	F
0.1271449616748825	0.4235447237432446	0.7495421899548123	T	T	T
0.3750000000000000	0.4225955327040142	0.7619949977772050	T	T	T
0.6228550383251177	0.4235447237432446	0.7495421899548123	T	T	T
0.8750000000000000	0.4248866802273919	0.7471636970363671	T	T	T
0.0000000000000000	0.1230464510972169	0.2500000000000000	F	F	F
0.2500000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.3750000000000000	0.1845696769387999	0.0000000000000000	F	F	F
0.1250000000000000	0.1845696765481719	0.0000000000000000	F	F	F
0.2500000000000000	0.1230464510972169	0.2500000000000000	F	F	F
0.7500000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.8750000000000000	0.1845696769387999	0.0000000000000000	F	F	F
0.6250000000000000	0.1845696769387999	0.0000000000000000	F	F	F
0.7499999992149498	0.1230464510972169	0.2500000000000000	F	F	F
0.9978908365241034	0.3688332899395076	0.2499893097575605	T	T	T
0.1243207151047004	0.3060204538783232	0.9987595655286762	T	T	T
0.8750000000000000	0.3061204048087015	0.9987456439475821	T	T	T
0.0000000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.0000000007850502	0.1230464510972169	0.7500000000000000	F	F	F
0.2500000000000000	0.2460929019991198	0.7500000000000000	F	F	F
0.3750000000000000	0.1845696769387999	0.5000000000000000	F	F	F
0.1250000000000000	0.1845696765481719	0.5000000000000000	F	F	F
0.2500000000000000	0.1230464510972169	0.7500000000000000	F	F	F
0.7499999992149498	0.2460929019991198	0.7500000000000000	F	F	F
0.8750000000000000	0.1845696769387999	0.5000000000000000	F	F	F
0.6250000000000000	0.1845696765481719	0.5000000000000000	F	F	F
0.7500000000000000	0.1230464510972169	0.7500000000000000	F	F	F
0.0000018291225105	0.3697315664855049	0.7493639615167095	T	T	T
0.1236009390068282	0.3055610275099798	0.5003792704549697	T	T	T
0.8750000000000000	0.3062655267673893	0.5006778647879804	T	T	T
0.0000000000000000	0.2460929023897478	0.7500000000000000	F	F	F
0.5032840051691615	0.3678379210630052	0.2511187388216850	T	T	T

0.6256792848952996	0.3060204538783232	0.9987595655286762	T	T	T
0.3750000000000000	0.3057663804622788	0.9994183960844384	T	T	T
0.5000000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.8750000000000000	0.4266101889319232	0.9987541821749836	T	T	T
0.6237182755001150	0.4265955162661550	0.0007614209709164	T	T	T
0.7521091634758966	0.3688332899395076	0.2499893097575605	T	T	T
0.3749999992149498	0.4246188527684570	0.9759172118739471	T	T	T
0.1262817244998849	0.4265955162661550	0.0007614209709164	T	T	T
0.2467159948308385	0.3678379214536331	0.2511187388216850	T	T	T
0.4999999992149498	0.1230464510972169	0.2500000000000000	F	F	F
0.5019457260088528	0.3669682813313911	0.7455830497855092	T	T	T
0.6263990602081216	0.3055610275099798	0.5003792704549697	T	T	T
0.3750000000000000	0.3087037236600684	0.4998066200187077	T	T	T
0.5000000000000000	0.2460929023897478	0.7500000000000000	F	F	F
0.8750000000000000	0.4269960664422046	0.5001456045799761	T	T	T
0.6223194289949089	0.4272204841857697	0.4971271359764153	T	T	T
0.7499981708774897	0.3697315668761329	0.7493639615167095	T	T	T
0.3749999992149498	0.4343812935571318	0.5365329190740258	T	T	T
0.1276805710050912	0.4272204841857697	0.4971271359764153	T	T	T
0.2480542739911471	0.3669682817220191	0.7455830497855092	T	T	T
0.4999999992149498	0.1230464510972169	0.7500000000000000	F	F	F
0.3749999984299066	0.4717467460444780	0.5201237903065985	T	T	T
0.3750000000000000	0.4595008178564112	0.2270579098027055	T	T	T

CO adsorbed on MnO (200):

Title

1.0000000000000000

27.916939599999992 0.0000000000000000 0.0000000000000000

-0.0977017000000000 8.9579370100000002 0.0000000000000000

-0.0977017000000000 -0.0987731200000000 8.9573924399999996

Mn C O

48 1 49

Selective dynamics

Direct

0.1604486367113367	0.2499999997209201	0.2500000000000000	F	F	F
0.2406729548893694	0.0000000000000000	0.2500000000000000	F	F	F
0.2406729548883888	0.2499999997209201	0.0000000000000000	F	F	F
0.1604486367142641	0.5000000005581668	0.0000000000000000	F	F	F
0.1604486367123101	0.0000000000000000	0.5000000000000000	F	F	F
0.1604486363550848	0.7500000002790799	0.7500000000000000	F	F	F
0.2406729548913233	0.5000000005581668	0.7500000000000000	F	F	F
0.2406729548903428	0.7500000002790799	0.5000000000000000	F	F	F
0.3208972734246274	0.0000000000000000	0.0000000000000000	F	F	F
0.4799933316950865	0.2505514002343525	0.2501809298631845	T	T	T
0.5579181828264447	-0.0000531499046185	0.2426425645480365	T	T	T
0.5577218643427245	0.2472311146235157	0.9982576373650383	T	T	T
0.3208972734256008	0.7500000002790799	0.2500000000000000	F	F	F

0.3999816572473466	0.5002856105922238	0.2494144234400963	T	T	T
0.3999725406115328	0.7504573750333409	0.9993046670128067	T	T	T
0.4785267346871343	0.5004360757489957	0.9988029579588960	T	T	T
0.3208972734236539	0.2499999997209201	0.7500000000000000	F	F	F
0.4000604027610648	0.0002145210671749	0.7491954728735971	T	T	T
0.4004577540324921	0.2501402380958242	0.4994335385165678	T	T	T
0.4796974433801801	0.0020346833292216	0.4989442671239803	T	T	T
0.3208972734265814	0.5000000005581668	0.5000000000000000	F	F	F
0.4798716148330892	0.7507206791385179	0.7476745365307631	T	T	T
0.5581715849523262	0.5000933396136240	0.7608260868867788	T	T	T
0.5606975111820200	0.7637199856339260	0.4983588994917068	T	T	T
0.1604486367123101	0.0000000000000000	0.0000000000000000	F	F	F
0.2406729548903428	0.7500000002790799	0.0000000000000000	F	F	F
0.1604486363550848	0.7500000002790799	0.2500000000000000	F	F	F
0.2406729548913233	0.5000000005581668	0.2500000000000000	F	F	F
0.1604486363560582	0.5000000005581668	0.5000000000000000	F	F	F
0.2406729548883888	0.2499999997209201	0.5000000000000000	F	F	F
0.1604486363531308	0.2499999997209201	0.7500000000000000	F	F	F
0.2406729548893694	0.0000000000000000	0.7500000000000000	F	F	F
0.3208972734265814	0.5000000005581668	0.0000000000000000	F	F	F
0.4000112485980011	0.2499957512291075	0.9992716346261049	T	T	T
0.4788088958823169	0.0008670364297469	0.9987765594540536	T	T	T
0.3208972734236539	0.2499999997209201	0.2500000000000000	F	F	F
0.4000381223345313	0.0002778674337418	0.2495797248470346	T	T	T
0.3208972734246274	0.0000000000000000	0.5000000000000000	F	F	F
0.5579052656015049	0.7530358327440605	0.9977934697339679	T	T	T
0.4798746663396972	0.7511095266832426	0.2499146660062042	T	T	T
0.4003765407836855	0.7509324209497261	0.4994053694087365	T	T	T
0.3208972730673949	0.7500000002790799	0.7500000000000000	F	F	F
0.5577235871723947	0.5005829526310879	0.2357134926413326	T	T	T
0.4787608375206914	0.4992544942988503	0.4986500030201638	T	T	T
0.4000291486806949	0.5002379497233650	0.7493454652969147	T	T	T
0.5645755696340135	0.2337008729506884	0.4979398323099304	T	T	T
0.4800491632101028	0.2505027775015592	0.7471243138535937	T	T	T
0.5579746453247101	0.9998808227897408	0.7528425426594196	T	T	T
0.6073341277521128	0.4435084070111051	0.5046168970720371	T	T	T
0.2406729550674953	0.2499999997209201	0.2500000000000000	F	F	F
0.2406729550684688	0.0000000000000000	0.0000000000000000	F	F	F
0.1604486365322373	0.2499999997209201	0.0000000000000000	F	F	F
0.1604486365332107	0.0000000000000000	0.2500000000000000	F	F	F
0.2406729547112434	0.7500000002790799	0.2500000000000000	F	F	F
0.2406729550704227	0.5000000005581668	0.0000000000000000	F	F	F
0.1604486365341842	0.7500000002790799	0.0000000000000000	F	F	F
0.1604486365351647	0.5000000005581668	0.2500000000000000	F	F	F
0.2406729547092894	0.2499999997209201	0.7500000000000000	F	F	F
0.2406729550684688	0.0000000000000000	0.5000000000000000	F	F	F
0.1604486365322373	0.2499999997209201	0.5000000000000000	F	F	F
0.1604486365332107	0.0000000000000000	0.7500000000000000	F	F	F

0.2406729547112434	0.7500000002790799	0.7500000000000000	F	F	F
0.2406729547122168	0.5000000005581668	0.5000000000000000	F	F	F
0.1604486365341842	0.7500000002790799	0.5000000000000000	F	F	F
0.1604486365351647	0.5000000005581668	0.7500000000000000	F	F	F
0.4002864996630089	0.2505906231852367	0.2503227352239525	T	T	T
0.3999328126005700	0.0003143247206436	0.9992141178044742	T	T	T
0.3208972732445474	0.2499999997209201	0.0000000000000000	F	F	F
0.3208972732455209	0.0000000000000000	0.2500000000000000	F	F	F
0.5585139471101477	0.2495504676032131	0.2426636058604687	T	T	T
0.5586999233474861	0.0002557624816623	0.9975938041902135	T	T	T
0.4785265771992286	0.2511379568902996	0.9988159588893765	T	T	T
0.4792102030212940	0.0007055134637605	0.2492629802624209	T	T	T
0.4002117136438511	0.7499505176802410	0.2498285888051781	T	T	T
0.3999836985210448	0.5002368720626362	0.9990350360675786	T	T	T
0.3208972732465014	0.7500000002790799	0.0000000000000000	F	F	F
0.3208972732474749	0.5000000005581668	0.2500000000000000	F	F	F
0.5591425796012877	0.7532691586698043	0.2441884412654495	T	T	T
0.5588025967594893	0.5021208837812011	0.9987614579714017	T	T	T
0.4787185398236377	0.7502841834667976	0.9986659867019531	T	T	T
0.4796844441454889	0.5010092602376609	0.2497223514476544	T	T	T
0.4003662751271677	0.2506983666453262	0.7482054679025449	T	T	T
0.4003848542096350	0.0009847589315885	0.4993592128796907	T	T	T
0.3208972732445474	0.2499999997209201	0.5000000000000000	F	F	F
0.3208972732455209	0.0000000000000000	0.7500000000000000	F	F	F
0.5583873890554395	0.2506783512736864	0.7553245879139383	T	T	T
0.5602019868123227	0.9992498689416245	0.4993456079844081	T	T	T
0.4817936438582175	0.2521032724935957	0.4986398755732159	T	T	T
0.4792631824307265	0.0004612050858305	0.7481381889384311	T	T	T
0.4002261921260060	0.7498268320485285	0.7487516167445972	T	T	T
0.4003217684965371	0.5000232161336241	0.4993370216710978	T	T	T
0.3208972732465014	0.7500000002790799	0.5000000000000000	F	F	F
0.3208972732474749	0.5000000005581668	0.7500000000000000	F	F	F
0.5591551786944754	0.7507029744821662	0.7519688195043183	T	T	T
0.5600601244212691	0.5230290204046364	0.4925539083431496	T	T	T
0.4801259866682988	0.7507881233181989	0.4986882202508295	T	T	T
0.4800757753662789	0.5010408093016774	0.7465566273579488	T	T	T
0.6419001981187656	0.5270003498097293	0.5127708354944249	T	T	T

CO adsorbed on MnO (220):

Title

1.0000000000000000

12.7380876799999996 0.0000000000000000 0.0000000000000000

0.0000000000000000 25.5999145599999984 0.0000000000000000

0.0000000000000000 -0.1389307400000000 8.9573924399999996

Mn C O

48 1 49

Selective dynamics

Direct

0.1250000000000000	0.1845696767434859	0.2500000000000000	F	F	F
0.3750000000000000	0.1845696767434859	0.2500000000000000	F	F	F
0.2500000000000000	0.2460929021944338	0.0000000000000000	F	F	F
0.6250000000000000	0.1845696767434859	0.2500000000000000	F	F	F
0.8749999992149498	0.1845696767434859	0.2500000000000000	F	F	F
0.7500000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.0000000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.0000000000000000	0.1230464509019029	0.5000000000000000	F	F	F
0.2500000000000000	0.1230464512925309	0.5000000000000000	F	F	F
0.7500000000000000	0.1230464512925309	0.5000000000000000	F	F	F
0.8750000000000000	0.3057524880179209	0.7495007786628970	T	T	T
0.1244764797169786	0.3054466493040703	0.7487136022084314	T	T	T
0.9997961204701692	0.3709491966929572	0.4985715618867976	T	T	T
0.5000000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.6221756598595457	0.4250620985427865	0.2478571118726293	T	T	T
0.8750000000000000	0.4245831733590854	0.2452534287815561	T	T	T
0.1278243401404541	0.4250620985427865	0.2478571118726293	T	T	T
0.3750000000000000	0.4308819875173349	0.2122057173183964	T	T	T
0.3750000000000000	0.3058809457875480	0.7488056475691810	T	T	T
0.6255235202830214	0.3054466493040703	0.7487136022084314	T	T	T
0.5015795764041209	0.3686570759250546	0.4972898537007654	T	T	T
0.7502038795298379	0.3709491966929572	0.4985715618867976	T	T	T
0.2484204228108289	0.3686570759250546	0.4972898537007654	T	T	T
0.5000000000000000	0.1230464512925309	0.5000000000000000	F	F	F
0.7500000000000000	0.1230464512925309	0.0000000000000000	F	F	F
0.0000000000000000	0.1230464509019029	0.0000000000000000	F	F	F
0.2500000000000000	0.1230464512925309	0.0000000000000000	F	F	F
0.9997845437385132	0.3712555967885315	0.9990728735369765	T	T	T
0.8749999992149498	0.3057436129347634	0.2490924864450849	T	T	T
0.7500000000000000	0.2460929021944338	0.5000000000000000	F	F	F
0.6249999992149498	0.1845696767434859	0.7500000000000000	F	F	F
0.1247633158051757	0.3056265858586728	0.2492862451533134	T	T	T
0.9999999992149498	0.2460929021944338	0.5000000000000000	F	F	F
0.8750000000000000	0.1845696767434859	0.7500000000000000	F	F	F
0.2500000000000000	0.2460929021944338	0.5000000000000000	F	F	F
0.1250000000000000	0.1845696763528579	0.7500000000000000	F	F	F
0.3750000000000000	0.1845696767434859	0.7500000000000000	F	F	F
0.2469687671067511	0.3685500489926726	0.9977111792959875	T	T	T
0.5030312328932489	0.3685500486020518	0.9977111792959875	T	T	T
0.7502154562614868	0.3712555971791524	0.9990728735369765	T	T	T
0.3750000000000000	0.3066767837326898	0.2486086134669464	T	T	T
0.6252366841948241	0.3056265858586728	0.2492862451533134	T	T	T
0.5000000000000000	0.2460929025850618	0.5000000000000000	F	F	F
0.5000000000000000	0.1230464512925309	0.0000000000000000	F	F	F
0.1262980438251698	0.4243734454099438	0.7439556650001961	T	T	T
0.3750000000000000	0.4268305292238112	0.7663825804104821	T	T	T
0.6237019561748303	0.4243734454099438	0.7439556650001961	T	T	T

0.8750000000000000	0.4245544670689438	0.7456357260400392	T	T	T
0.3749999984299066	0.4705326238782130	0.4314635237405053	T	T	T
0.0000000000000000	0.1230464510972169	0.2500000000000000	F	F	F
0.2500000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.3750000000000000	0.1845696769387999	0.0000000000000000	F	F	F
0.1250000000000000	0.1845696765481719	0.0000000000000000	F	F	F
0.2500000000000000	0.1230464510972169	0.2500000000000000	F	F	F
0.7500000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.8750000000000000	0.1845696769387999	0.0000000000000000	F	F	F
0.6250000000000000	0.1845696769387999	0.0000000000000000	F	F	F
0.7499999992149498	0.1230464510972169	0.2500000000000000	F	F	F
0.0009635041622324	0.3695100417662759	0.2491842202981661	T	T	T
0.1242938441721198	0.3054581455521860	0.9996909674655106	T	T	T
0.8750000000000000	0.3061313024927333	0.9998214835888544	T	T	T
0.0000000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.0000000007850502	0.1230464510972169	0.7500000000000000	F	F	F
0.2500000000000000	0.2460929019991198	0.7500000000000000	F	F	F
0.3750000000000000	0.1845696769387999	0.5000000000000000	F	F	F
0.1250000000000000	0.1845696765481719	0.5000000000000000	F	F	F
0.2500000000000000	0.1230464510972169	0.7500000000000000	F	F	F
0.7499999992149498	0.2460929019991198	0.7500000000000000	F	F	F
0.8750000000000000	0.1845696769387999	0.5000000000000000	F	F	F
0.6250000000000000	0.1845696765481719	0.5000000000000000	F	F	F
0.7500000000000000	0.1230464510972169	0.7500000000000000	F	F	F
0.0001503173952664	0.3690496756347847	0.7487556328625881	T	T	T
0.1251797197712804	0.3055810957662800	0.4985613694951280	T	T	T
0.8750000000000000	0.3060538389230489	0.4991292049359981	T	T	T
0.0000000000000000	0.2460929023897478	0.7500000000000000	F	F	F
0.4970098502595581	0.3699626839912489	0.2497323344597013	T	T	T
0.6257061558278803	0.3054581455521860	0.9996909674655106	T	T	T
0.3750000000000000	0.3055427342466753	0.9989890146412330	T	T	T
0.5000000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.8750000000000000	0.4265414069768842	0.9983983340401679	T	T	T
0.6237088693142399	0.4260127036577180	0.9975686643216938	T	T	T
0.7490364958377673	0.3695100417662759	0.2491842202981661	T	T	T
0.3749999992149498	0.4253217141912740	0.9887132303210029	T	T	T
0.1262911306857603	0.4260127036577180	0.9975686643216938	T	T	T
0.2529901497404419	0.3699626843818769	0.2497323344597013	T	T	T
0.4999999992149498	0.1230464510972169	0.2500000000000000	F	F	F
0.4996513035461729	0.3682931184202197	0.7465885711039515	T	T	T
0.6248202794436694	0.3055810957662800	0.4985613694951280	T	T	T
0.3750000000000000	0.3075816552791205	0.4986492451536785	T	T	T
0.5000000000000000	0.2460929023897478	0.7500000000000000	F	F	F
0.8750000000000000	0.4264597479257043	0.4986519198525637	T	T	T
0.6223016217305137	0.4253231567970299	0.4990408910451979	T	T	T
0.7498496826047335	0.3690496760254127	0.7487556328625881	T	T	T
0.3749999992149498	0.4299460203272206	0.5343868470321870	T	T	T
0.1276983782694863	0.4253231567970299	0.4990408910451979	T	T	T

0.2503486964538271	0.3682931188108476	0.7465885711039515	T	T	T
0.4999999992149498	0.1230464510972169	0.7500000000000000	F	F	F
0.3749999976448564	0.5156654323035611	0.4773103284187215	T	T	T

CO adsorbed on K-MnO (200):

Title

1.0000000000000000		
27.916939599999992	0.0000000000000000	0.0000000000000000
-0.0977017000000000	8.9579370100000002	0.0000000000000000
-0.0977017000000000	-0.0987731200000000	8.9573924399999996

Mn	C	O	H	K
47	1	49	1	1

Selective dynamics

Direct

0.1604486367113367	0.2499999997209201	0.2500000000000000	F	F	F
0.2406729548893694	0.0000000000000000	0.2500000000000000	F	F	F
0.2406729548883888	0.2499999997209201	0.0000000000000000	F	F	F
0.1604486367142641	0.5000000005581668	0.0000000000000000	F	F	F
0.1604486367123101	0.0000000000000000	0.5000000000000000	F	F	F
0.1604486363550848	0.7500000002790799	0.7500000000000000	F	F	F
0.2406729548913233	0.5000000005581668	0.7500000000000000	F	F	F
0.2406729548903428	0.7500000002790799	0.5000000000000000	F	F	F
0.3208972734246274	0.0000000000000000	0.0000000000000000	F	F	F
0.4831858970770803	0.2509994242596340	0.2554150349747235	T	T	T
0.5585467953646371	0.0003266381807954	0.2363809856407515	T	T	T
0.5588544461749995	0.2435358256607408	0.9981208304042428	T	T	T
0.3208972734256008	0.7500000002790799	0.2500000000000000	F	F	F
0.4008513381152025	0.4987089337157936	0.2497423235134208	T	T	T
0.3998956653445429	0.7491214060836324	0.9995512569804302	T	T	T
0.4795218198582866	0.4977340374979595	0.0004913187159485	T	T	T
0.3208972734236539	0.2499999997209201	0.7500000000000000	F	F	F
0.3999972779111321	0.0011898972968545	0.7511911098758143	T	T	T
0.3998094429305605	0.2519716921664193	0.4996617681102819	T	T	T
0.4749419829779014	0.0065522939333720	0.4994490003687708	T	T	T
0.3208972734265814	0.5000000005581668	0.5000000000000000	F	F	F
0.4796563104639294	0.7491283267710862	0.7501141537617971	T	T	T
0.5601448869371676	0.4994209822072926	0.7638700156505350	T	T	T
0.5551041278965815	0.7502936010196994	0.4963756569379862	T	T	T
0.1604486367123101	0.0000000000000000	0.0000000000000000	F	F	F
0.2406729548903428	0.7500000002790799	0.0000000000000000	F	F	F
0.1604486363550848	0.7500000002790799	0.2500000000000000	F	F	F
0.2406729548913233	0.5000000005581668	0.2500000000000000	F	F	F
0.1604486363560582	0.5000000005581668	0.5000000000000000	F	F	F
0.2406729548883888	0.2499999997209201	0.5000000000000000	F	F	F
0.1604486363531308	0.2499999997209201	0.7500000000000000	F	F	F
0.2406729548893694	0.0000000000000000	0.7500000000000000	F	F	F
0.3208972734265814	0.5000000005581668	0.0000000000000000	F	F	F

0.4007209298436052	0.2504735878313470	0.9995766718483802	T	T	T
0.4788829639856533	0.0016064135058070	0.0001615056300000	T	T	T
0.3208972734236539	0.2499999997209201	0.2500000000000000	F	F	F
0.4000720008501106	0.0011726152252253	0.2490523169547610	T	T	T
0.3208972734246274	0.0000000000000000	0.5000000000000000	F	F	F
0.5570640359543499	0.7517575285851924	0.9990586624092349	T	T	T
0.4796626445273792	0.7485843153967485	0.2488268078921644	T	T	T
0.4001076627220649	0.7484415212459210	0.4997510797770559	T	T	T
0.3208972730673949	0.7500000002790799	0.7500000000000000	F	F	F
0.5639694573760192	0.4931553559531210	0.2280965314733929	T	T	T
0.4806771240937239	0.4905578395285975	0.4981174112447275	T	T	T
0.4008021718076942	0.4985646294866589	0.7497613680447343	T	T	T
0.4832092201376688	0.2503409792870305	0.7439121477014380	T	T	T
0.5586766071775890	0.9984472088058240	0.7588015253611919	T	T	T
0.6069894110261368	0.5280869239711496	0.4319892116113864	T	T	T
0.2406729550674953	0.2499999997209201	0.2500000000000000	F	F	F
0.2406729550684688	0.0000000000000000	0.0000000000000000	F	F	F
0.1604486365322373	0.2499999997209201	0.0000000000000000	F	F	F
0.1604486365332107	0.0000000000000000	0.2500000000000000	F	F	F
0.2406729547112434	0.7500000002790799	0.2500000000000000	F	F	F
0.2406729550704227	0.5000000005581668	0.0000000000000000	F	F	F
0.1604486365341842	0.7500000002790799	0.0000000000000000	F	F	F
0.1604486365351647	0.5000000005581668	0.2500000000000000	F	F	F
0.2406729547092894	0.2499999997209201	0.7500000000000000	F	F	F
0.2406729550684688	0.0000000000000000	0.5000000000000000	F	F	F
0.1604486365322373	0.2499999997209201	0.5000000000000000	F	F	F
0.1604486365332107	0.0000000000000000	0.7500000000000000	F	F	F
0.2406729547112434	0.7500000002790799	0.7500000000000000	F	F	F
0.2406729547122168	0.5000000005581668	0.5000000000000000	F	F	F
0.1604486365341842	0.7500000002790799	0.5000000000000000	F	F	F
0.1604486365351647	0.5000000005581668	0.7500000000000000	F	F	F
0.4005040238681797	0.2505798416721676	0.2488940463727824	T	T	T
0.4005139559038228	0.9993773041419197	0.9997078797408498	T	T	T
0.3208972732445474	0.2499999997209201	0.0000000000000000	F	F	F
0.3208972732455209	0.0000000000000000	0.2500000000000000	F	F	F
0.5614463905919996	0.2400369496026994	0.2305700073515596	T	T	T
0.5581039892626023	0.9926615558069738	0.9972722485257219	T	T	T
0.4789992361212020	0.2493848732899199	0.9998311449462941	T	T	T
0.4800002588102189	0.0019297662657033	0.2569173300876947	T	T	T
0.4004066729902494	0.7493948365177765	0.2501021001173776	T	T	T
0.4006531572612836	0.5001909215911050	0.0001091869117367	T	T	T
0.3208972732465014	0.7500000002790799	0.0000000000000000	F	F	F
0.3208972732474749	0.5000000005581668	0.2500000000000000	F	F	F
0.5568006019250215	0.7630567572596264	0.2468538830022348	T	T	T
0.5592539579834204	0.5080772517201563	0.9968203162513223	T	T	T
0.4780344341007257	0.7501944024496072	0.9990930611997184	T	T	T
0.4827510083161879	0.4990658576405764	0.2534593132104533	T	T	T
0.4004183366291414	0.2498342460528737	0.7507478904228460	T	T	T

0.3988058080048277	0.9979863061197524	0.4998782297085854	T	T	T
0.3208972732445474	0.2499999997209201	0.5000000000000000	F	F	F
0.3208972732455209	0.0000000000000000	0.7500000000000000	F	F	F
0.5615921768540501	0.2436188442522317	0.7678008635874973	T	T	T
0.5852495953164751	0.9681406570373182	0.5054512512400841	T	T	T
0.4778057163219337	0.2472627150345920	0.4998004345627992	T	T	T
0.4805421893734603	0.0008724720081324	0.7414967185170440	T	T	T
0.4003316631993710	0.7499312793612700	0.7491873251056729	T	T	T
0.4009075979776202	0.5018457359256450	0.4991102664124192	T	T	T
0.3208972732465014	0.7500000002790799	0.5000000000000000	F	F	F
0.3208972732474749	0.5000000005581668	0.7500000000000000	F	F	F
0.5578407000099804	0.7555877084504748	0.7517297840685410	T	T	T
0.5646606364871128	0.5146411922767415	0.5252845273946204	T	T	T
0.4797247422256700	0.7548774280152288	0.4996141341771522	T	T	T
0.4809336485283437	0.4989604146065166	0.7454900812790397	T	T	T
0.6455419672256980	0.5309221052623593	0.4998995938559422	T	T	T
0.6188500571809225	0.9389270243061031	0.5043631497750591	T	T	T
0.6054415404486467	0.2430358768052998	0.5087779036825363	T	T	T

CO adsorbed on K-MnO (220):

Title

1.0000000000000000

12.7380876799999996 0.0000000000000000 0.0000000000000000

0.0000000000000000 25.5999145599999984 0.0000000000000000

0.0000000000000000 -0.1389307400000000 8.9573924399999996

Mn C O H K

47 1 49 1 1

Selective dynamics

Direct

0.1250000000000000	0.1845696767434859	0.2500000000000000	F	F	F
0.3750000000000000	0.1845696767434859	0.2500000000000000	F	F	F
0.2500000000000000	0.2460929021944338	0.0000000000000000	F	F	F
0.6250000000000000	0.1845696767434859	0.2500000000000000	F	F	F
0.8749999992149498	0.1845696767434859	0.2500000000000000	F	F	F
0.7500000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.0000000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.0000000000000000	0.1230464509019029	0.5000000000000000	F	F	F
0.2500000000000000	0.1230464512925309	0.5000000000000000	F	F	F
0.7500000000000000	0.1230464512925309	0.5000000000000000	F	F	F
0.8750026577825279	0.3058529406589083	0.7497476855056362	T	T	T
0.1245009944165351	0.3056236264276329	0.7491433693588918	T	T	T
0.9994043090656687	0.3709852676681762	0.4992349851204914	T	T	T
0.5000000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.6231865398794458	0.4224282508327047	0.2471347829322027	T	T	T
0.8750516195193312	0.4251833391561464	0.2453719317588656	T	T	T
0.1269515888781726	0.4224473555275270	0.2472120021746919	T	T	T
0.3750021926561931	0.3052114686308668	0.7489082346204529	T	T	T

0.6254912819492116	0.3056480353329468	0.7490776521823647	T	T	T
0.5015722632443537	0.3686708757690673	0.4911895158784039	T	T	T
0.7505451254974369	0.3710187160803705	0.4991578493586890	T	T	T
0.2483656539539852	0.3685950118311120	0.4912497632902906	T	T	T
0.5000000000000000	0.1230464512925309	0.5000000000000000	F	F	F
0.7500000000000000	0.1230464512925309	0.0000000000000000	F	F	F
0.0000000000000000	0.1230464509019029	0.0000000000000000	F	F	F
0.2500000000000000	0.1230464512925309	0.0000000000000000	F	F	F
0.0000584100656636	0.3716808533160256	0.9982959285438615	T	T	T
0.8749983880977185	0.3059871798623809	0.2487059999619264	T	T	T
0.7500000000000000	0.2460929021944338	0.5000000000000000	F	F	F
0.6249999992149498	0.1845696767434859	0.7500000000000000	F	F	F
0.1244322913161024	0.3049164960469800	0.2490945105888540	T	T	T
0.9999999992149498	0.2460929021944338	0.5000000000000000	F	F	F
0.8750000000000000	0.1845696767434859	0.7500000000000000	F	F	F
0.2500000000000000	0.2460929021944338	0.5000000000000000	F	F	F
0.1250000000000000	0.1845696763528579	0.7500000000000000	F	F	F
0.3750000000000000	0.1845696767434859	0.7500000000000000	F	F	F
0.2467371470880712	0.3691316501540385	0.0060659948086330	T	T	T
0.5033394305023345	0.3691475025733570	0.0060175897610837	T	T	T
0.7500066913600477	0.3716539734418560	0.9981987125215728	T	T	T
0.3749553294337875	0.3094135574677933	0.2486711542882755	T	T	T
0.6255217038266129	0.3049061012636703	0.2490673292582331	T	T	T
0.5000000000000000	0.2460929025850618	0.5000000000000000	F	F	F
0.5000000000000000	0.1230464512925309	0.0000000000000000	F	F	F
0.1285321796887939	0.4247519010793169	0.7427513276980854	T	T	T
0.3749719204120332	0.4212219677596103	0.7524631287600816	T	T	T
0.6214942567937712	0.4247817880066811	0.7426963493047712	T	T	T
0.8750710794640372	0.4251442468772815	0.7454611785559454	T	T	T
0.3744643477602404	0.4756511778192339	0.5789394140500819	T	T	T
0.0000000000000000	0.1230464510972169	0.2500000000000000	F	F	F
0.2500000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.3750000000000000	0.1845696769387999	0.0000000000000000	F	F	F
0.1250000000000000	0.1845696765481719	0.0000000000000000	F	F	F
0.2500000000000000	0.1230464510972169	0.2500000000000000	F	F	F
0.7500000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.8750000000000000	0.1845696769387999	0.0000000000000000	F	F	F
0.6250000000000000	0.1845696769387999	0.0000000000000000	F	F	F
0.7499999992149498	0.1230464510972169	0.2500000000000000	F	F	F
0.9979506102847857	0.3693903853277691	0.2486291920575322	T	T	T
0.1240692456232537	0.3056901921733947	0.9966010134319212	T	T	T
0.8750399947743138	0.3063440472187028	0.9983539624397606	T	T	T
0.0000000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.0000000007850502	0.1230464510972169	0.7500000000000000	F	F	F
0.2500000000000000	0.2460929019991198	0.7500000000000000	F	F	F
0.3750000000000000	0.1845696769387999	0.5000000000000000	F	F	F
0.1250000000000000	0.1845696765481719	0.5000000000000000	F	F	F
0.2500000000000000	0.1230464510972169	0.7500000000000000	F	F	F

0.7499999992149498	0.2460929019991198	0.7500000000000000	F	F	F
0.8750000000000000	0.1845696769387999	0.5000000000000000	F	F	F
0.6250000000000000	0.1845696765481719	0.5000000000000000	F	F	F
0.7500000000000000	0.1230464510972169	0.7500000000000000	F	F	F
0.0009719381400198	0.3702658111665498	0.7491787823751679	T	T	T
0.1241408108952543	0.3054449292222096	0.5019230150194087	T	T	T
0.8750631174339135	0.3062817153932249	0.5004682943178842	T	T	T
0.0000000000000000	0.2460929023897478	0.7500000000000000	F	F	F
0.5048962241835749	0.3660506933550313	0.2481657927703826	T	T	T
0.6259113872672569	0.3056997578406926	0.9965122929407224	T	T	T
0.3750126119661826	0.3087192585377457	0.9976026891579935	T	T	T
0.5000000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.8750246005223273	0.4271190619393064	0.9972834598728045	T	T	T
0.6214855263121997	0.4270757214227920	0.0007581296813723	T	T	T
0.7520849612878132	0.3693854388991201	0.2485454224597478	T	T	T
0.3748987341424326	0.4307001954319146	0.9861519682269311	T	T	T
0.1285622768094184	0.4270471924703619	0.0006604984015612	T	T	T
0.2451348764734973	0.3660526435178054	0.2482106874589442	T	T	T
0.4999999992149498	0.1230464510972169	0.2500000000000000	F	F	F
0.4998073512455425	0.3678882817547273	0.7484194021458314	T	T	T
0.6258801597426858	0.3054862359385769	0.5018593331787085	T	T	T
0.3750532123971442	0.3078236938299787	0.4999731465379539	T	T	T
0.5000000000000000	0.2460929023897478	0.7500000000000000	F	F	F
0.8750034306957137	0.4269636558607322	0.4994915193308620	T	T	T
0.6219665176908917	0.4258015106290173	0.4964257664756820	T	T	T
0.7490097425212116	0.3703375724485923	0.7491007515046648	T	T	T
0.3748205289751116	0.4308672806999290	0.4905011078786206	T	T	T
0.1279830739160872	0.4257122776448035	0.4966742003392658	T	T	T
0.2502235359943278	0.3678332769173291	0.7485243406209182	T	T	T
0.4999999992149498	0.1230464510972169	0.7500000000000000	F	F	F
0.3741445814778354	0.5191552245172598	0.5210611370498958	T	T	T
0.3738603128321974	0.4684009948941847	0.9726404801413857	T	T	T
0.3757398163506050	0.4800144266584486	0.2486499669933978	T	T	T

CO₂ adsorbed on MnO (200):

Title

1.0000000000000000

27.916939599999992 0.0000000000000000 0.0000000000000000

-0.0977017000000000 8.9579370100000002 0.0000000000000000

-0.0977017000000000 -0.0987731200000000 8.9573924399999996

Mn C O

48 1 50

Selective dynamics

Direct

0.1604486367113367 0.2499999997209201 0.2500000000000000 F F F

0.2406729548893694 0.0000000000000000 0.2500000000000000 F F F

0.2406729548883888 0.2499999997209201 0.0000000000000000 F F F

0.1604486367142641	0.5000000005581668	0.0000000000000000	F	F	F
0.1604486367123101	0.0000000000000000	0.5000000000000000	F	F	F
0.1604486363550848	0.7500000002790799	0.7500000000000000	F	F	F
0.2406729548913233	0.5000000005581668	0.7500000000000000	F	F	F
0.2406729548903428	0.7500000002790799	0.5000000000000000	F	F	F
0.3208972734246274	0.0000000000000000	0.0000000000000000	F	F	F
0.4800277888062657	0.2490907278033948	0.2514507582826303	T	T	T
0.5582240498103923	0.9983791120910963	0.2448981337557972	T	T	T
0.5576757946334456	0.2453292529771921	0.9985746893238800	T	T	T
0.3208972734256008	0.7500000002790799	0.2500000000000000	F	F	F
0.3998853922090031	0.4997437136983992	0.2499798215621287	T	T	T
0.4000293766308761	0.7502795563463832	0.9996773834527930	T	T	T
0.4781561653483934	0.4995212505391334	0.9996873966230158	T	T	T
0.3208972734236539	0.2499999997209201	0.7500000000000000	F	F	F
0.4001841765919301	0.9997707627464113	0.7494145370515229	T	T	T
0.4005572847859972	0.2491620019554003	0.4998155844607897	T	T	T
0.4805114277020633	0.9997212841500051	0.4996397544108626	T	T	T
0.3208972734265814	0.5000000005581668	0.5000000000000000	F	F	F
0.4801329343640249	0.7500740834326287	0.7471893249307204	T	T	T
0.5573613360967089	0.4987286284693190	0.7635748186873367	T	T	T
0.5649380137217771	0.7622034990098129	0.4990519094897172	T	T	T
0.1604486367123101	0.0000000000000000	0.0000000000000000	F	F	F
0.2406729548903428	0.7500000002790799	0.0000000000000000	F	F	F
0.1604486363550848	0.7500000002790799	0.2500000000000000	F	F	F
0.2406729548913233	0.5000000005581668	0.2500000000000000	F	F	F
0.1604486363560582	0.5000000005581668	0.5000000000000000	F	F	F
0.2406729548883888	0.2499999997209201	0.5000000000000000	F	F	F
0.1604486363531308	0.2499999997209201	0.7500000000000000	F	F	F
0.2406729548893694	0.0000000000000000	0.7500000000000000	F	F	F
0.3208972734265814	0.5000000005581668	0.0000000000000000	F	F	F
0.4000182532839027	0.2492338289747056	0.9995575192339445	T	T	T
0.4789331438955937	0.9995389451748748	0.9994820012131256	T	T	T
0.3208972734236539	0.2499999997209201	0.2500000000000000	F	F	F
0.4001664141971276	0.9997406591871943	0.2500928538884954	T	T	T
0.3208972734246274	0.0000000000000000	0.5000000000000000	F	F	F
0.5577307465334126	0.7518117687250587	0.9988215135484422	T	T	T
0.4800750697407324	0.7501453884969815	0.2516936419410475	T	T	T
0.4005523036710547	0.7506991787111482	0.4998959123569663	T	T	T
0.3208972730673949	0.7500000002790799	0.7500000000000000	F	F	F
0.5571697194801263	0.4979866214517628	0.2340639128428680	T	T	T
0.4780472360996630	0.4992997017066703	0.4995772827553758	T	T	T
0.3999191961147749	0.4997671016969008	0.7497164706683067	T	T	T
0.5650096562446957	0.2364078200197736	0.4985091463444113	T	T	T
0.4801431293200359	0.2491285676314075	0.7470479083629082	T	T	T
0.5583066331316238	0.9987038679436727	0.7522997440024954	T	T	T
0.6151464485292946	0.5012404409551918	0.5013883865204345	T	T	T
0.2406729550674953	0.2499999997209201	0.2500000000000000	F	F	F
0.2406729550684688	0.0000000000000000	0.0000000000000000	F	F	F

0.1604486365322373	0.2499999997209201	0.0000000000000000	F	F	F
0.1604486365332107	0.0000000000000000	0.2500000000000000	F	F	F
0.2406729547112434	0.7500000002790799	0.2500000000000000	F	F	F
0.2406729550704227	0.5000000005581668	0.0000000000000000	F	F	F
0.1604486365341842	0.7500000002790799	0.0000000000000000	F	F	F
0.1604486365351647	0.5000000005581668	0.2500000000000000	F	F	F
0.2406729547092894	0.2499999997209201	0.7500000000000000	F	F	F
0.2406729550684688	0.0000000000000000	0.5000000000000000	F	F	F
0.1604486365322373	0.2499999997209201	0.5000000000000000	F	F	F
0.1604486365332107	0.0000000000000000	0.7500000000000000	F	F	F
0.2406729547112434	0.7500000002790799	0.7500000000000000	F	F	F
0.2406729547122168	0.5000000005581668	0.5000000000000000	F	F	F
0.1604486365341842	0.7500000002790799	0.5000000000000000	F	F	F
0.1604486365351647	0.5000000005581668	0.7500000000000000	F	F	F
0.4002946880852843	0.2499250179051145	0.2505861725850365	T	T	T
0.4000863420814901	0.9997088365191356	0.9996613501148193	T	T	T
0.3208972732445474	0.2499999997209201	0.0000000000000000	F	F	F
0.3208972732455209	0.0000000000000000	0.2500000000000000	F	F	F
0.5586636143498599	0.2499375120742030	0.2445439586554992	T	T	T
0.5585114195180682	0.9991298618431819	0.9990836315049004	T	T	T
0.4785705420441211	0.2502177487155842	0.9994628566504752	T	T	T
0.4794823562472624	0.9995561191967159	0.2504137025598258	T	T	T
0.4003283292730377	0.7494072643051924	0.2507172731770099	T	T	T
0.4000228940815256	0.4997133085366249	0.9995718507470286	T	T	T
0.3208972732465014	0.7500000002790799	0.0000000000000000	F	F	F
0.3208972732474749	0.5000000005581668	0.2500000000000000	F	F	F
0.5586135068725824	0.7481852982926303	0.2448642705118139	T	T	T
0.5580935481686129	0.4992611322980116	0.9991867046724435	T	T	T
0.4785544578285489	0.7488058181087063	0.9995148172571942	T	T	T
0.4796982622021326	0.4994552828868626	0.2528264066953958	T	T	T
0.4003376273592933	0.2500280111799551	0.7487942793960211	T	T	T
0.4008136753269519	0.9997660807336696	0.4997190407469664	T	T	T
0.3208972732445474	0.2499999997209201	0.5000000000000000	F	F	F
0.3208972732455209	0.0000000000000000	0.7500000000000000	F	F	F
0.5587330846751999	0.2505246651814619	0.7538106096290532	T	T	T
0.5602345666988620	0.9995226587492267	0.4994133029319033	T	T	T
0.4813810360970970	0.2526421675404826	0.4993751967741939	T	T	T
0.4795304591623335	0.9997009880812060	0.7485781164115193	T	T	T
0.4003390370358552	0.7494873855313219	0.7488205327088044	T	T	T
0.4000528878163640	0.4997907219467820	0.4997315356626634	T	T	T
0.3208972732465014	0.7500000002790799	0.5000000000000000	F	F	F
0.3208972732474749	0.5000000005581668	0.7500000000000000	F	F	F
0.5587318966955640	0.7482205944808922	0.7539609863827996	T	T	T
0.5636040257914521	0.4991905492981755	0.4982940176090394	T	T	T
0.4814386295822912	0.7465556986764169	0.4996171847305944	T	T	T
0.4798505166053472	0.4995472031393751	0.7457951062156524	T	T	T
0.6335963264521216	0.6303524239176785	0.5012645219038521	T	T	T
0.6336738875717656	0.3735236892914787	0.5038371268548686	T	T	T

CO₂ adsorbed on MnO (220):

Title

1.0000000000000000
12.7380876799999996 0.0000000000000000 0.0000000000000000
0.0000000000000000 25.5999145599999984 0.0000000000000000
0.0000000000000000 -0.1389307400000000 8.9573924399999996

Mn C O

48 1 50

Selective dynamics

Direct

0.1250000000000000	0.1845696767434859	0.2500000000000000	F	F	F
0.3750000000000000	0.1845696767434859	0.2500000000000000	F	F	F
0.2500000000000000	0.2460929021944338	0.0000000000000000	F	F	F
0.6250000000000000	0.1845696767434859	0.2500000000000000	F	F	F
0.8749999992149498	0.1845696767434859	0.2500000000000000	F	F	F
0.7500000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.0000000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.0000000000000000	0.1230464509019029	0.5000000000000000	F	F	F
0.2500000000000000	0.1230464512925309	0.5000000000000000	F	F	F
0.7500000000000000	0.1230464512925309	0.5000000000000000	F	F	F
0.8749914584165220	0.3056614887862779	0.7495723504829954	T	T	T
0.1246261628036480	0.3055489184556953	0.7506504485789863	T	T	T
0.9993660080059946	0.3710779550436947	0.4995134001388793	T	T	T
0.5000000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.6235004550889126	0.4248488683883567	0.2472736083723231	T	T	T
0.8750533000033550	0.4244535437790007	0.2450465219949734	T	T	T
0.1265103205762298	0.4248426981387809	0.2476083697181266	T	T	T
0.3750362982940875	0.4292908647260514	0.2248175060718792	T	T	T
0.3749213188637803	0.3068378492780569	0.7499963930621016	T	T	T
0.6253352322456034	0.3055479588723929	0.7505654654344610	T	T	T
0.5049370377230750	0.3666695538081183	0.4990005271927339	T	T	T
0.7505830807224464	0.3710980172423466	0.4993368870588958	T	T	T
0.2450637351054057	0.3666917822401616	0.4990721517395105	T	T	T
0.5000000000000000	0.1230464512925309	0.5000000000000000	F	F	F
0.7500000000000000	0.1230464512925309	0.0000000000000000	F	F	F
0.0000000000000000	0.1230464509019029	0.0000000000000000	F	F	F
0.2500000000000000	0.1230464512925309	0.0000000000000000	F	F	F
0.9999290212149911	0.3709939737840828	0.9994474934131538	T	T	T
0.8749943795847278	0.3056676011041506	0.2494928795465025	T	T	T
0.7500000000000000	0.2460929021944338	0.5000000000000000	F	F	F
0.6249999992149498	0.1845696767434859	0.7500000000000000	F	F	F
0.1245776373983416	0.3055291950604397	0.2489539949454942	T	T	T
0.9999999992149498	0.2460929021944338	0.5000000000000000	F	F	F
0.8750000000000000	0.1845696767434859	0.7500000000000000	F	F	F
0.2500000000000000	0.2460929021944338	0.5000000000000000	F	F	F
0.1250000000000000	0.1845696763528579	0.7500000000000000	F	F	F

0.3750000000000000	0.1845696767434859	0.7500000000000000	F	F	F
0.2477893686028624	0.3691229201873413	0.9996341197653034	T	T	T
0.5022188647733018	0.3691066906889818	0.9995677199432151	T	T	T
0.7500892916756874	0.3710144656906497	0.9992863263514700	T	T	T
0.3749477317538831	0.3066477686527034	0.2490939934431173	T	T	T
0.6253970834071712	0.3055319495573753	0.2488680978670077	T	T	T
0.5000000000000000	0.2460929025850618	0.5000000000000000	F	F	F
0.5000000000000000	0.1230464512925309	0.0000000000000000	F	F	F
0.1265496946746924	0.4247918757337833	0.7452465571779489	T	T	T
0.3750193340614288	0.4300834013028354	0.7744324932080505	T	T	T
0.6234324578780038	0.4247873186282165	0.7449595648209798	T	T	T
0.8750071238878090	0.4245131235211398	0.7467551304183447	T	T	T
0.3749585492912184	0.4737858642717796	0.5016052754388473	T	T	T
0.0000000000000000	0.1230464510972169	0.2500000000000000	F	F	F
0.2500000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.3750000000000000	0.1845696769387999	0.0000000000000000	F	F	F
0.1250000000000000	0.1845696765481719	0.0000000000000000	F	F	F
0.2500000000000000	0.1230464510972169	0.2500000000000000	F	F	F
0.7500000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.8750000000000000	0.1845696769387999	0.0000000000000000	F	F	F
0.6250000000000000	0.1845696769387999	0.0000000000000000	F	F	F
0.7499999992149498	0.1230464510972169	0.2500000000000000	F	F	F
0.0003772370710493	0.3691336987979469	0.2501695139273886	T	T	T
0.1244693236539615	0.3055742651524054	0.9998494879843929	T	T	T
0.8750444918344991	0.3060175027919337	0.9997262936585192	T	T	T
0.0000000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.0000000007850502	0.1230464510972169	0.7500000000000000	F	F	F
0.2500000000000000	0.2460929019991198	0.7500000000000000	F	F	F
0.3750000000000000	0.1845696769387999	0.5000000000000000	F	F	F
0.1250000000000000	0.1845696765481719	0.5000000000000000	F	F	F
0.2500000000000000	0.1230464510972169	0.7500000000000000	F	F	F
0.7499999992149498	0.2460929019991198	0.7500000000000000	F	F	F
0.8750000000000000	0.1845696769387999	0.5000000000000000	F	F	F
0.6250000000000000	0.1845696765481719	0.5000000000000000	F	F	F
0.7500000000000000	0.1230464510972169	0.7500000000000000	F	F	F
0.0004905925083073	0.3691589853748929	0.7493426376251741	T	T	T
0.1243005157303381	0.3053101664170206	0.4999927607689150	T	T	T
0.8750419609514369	0.3060356874665708	0.4997716772647693	T	T	T
0.0000000000000000	0.2460929023897478	0.7500000000000000	F	F	F
0.4989170359094708	0.3695250136118358	0.2510434935180677	T	T	T
0.6255040233916906	0.3055775367137302	0.9997425665675063	T	T	T
0.3749773871729280	0.3055068073585441	0.9997833195127436	T	T	T
0.5000000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.8750152304507482	0.4262667821163222	0.9989713380777913	T	T	T
0.6243018411622392	0.4260161482319865	0.9995994552905982	T	T	T
0.7496843714093568	0.3691900290083164	0.2499822730321228	T	T	T
0.3750334084376990	0.4247569526489173	0.9998660726138568	T	T	T
0.1257471133275424	0.4260045792451360	0.9998211910783364	T	T	T

0.2511398406533891	0.3696082178249344	0.2510869145358480	T	T	T
0.4999999992149498	0.1230464510972169	0.2500000000000000	F	F	F
0.4985706665974104	0.3698502460376037	0.7482003505493724	T	T	T
0.6256898008547687	0.3052941586917886	0.4998712491545408	T	T	T
0.3749628882540006	0.3066884166474374	0.4996609316180832	T	T	T
0.5000000000000000	0.2460929023897478	0.7500000000000000	F	F	F
0.8749890640242741	0.4264917125374556	0.4995103590003886	T	T	T
0.6222185220159112	0.4254663518122321	0.4988900288839727	T	T	T
0.7495346138958322	0.3691903165519878	0.7491954207265155	T	T	T
0.3750598963904497	0.4211399951462496	0.5005956649054711	T	T	T
0.1277495603256472	0.4254726850346919	0.4990733484068312	T	T	T
0.2514079339326145	0.3698654718392281	0.7482496430561378	T	T	T
0.4999999992149498	0.1230464510972169	0.7500000000000000	F	F	F
0.3749264413423450	0.4955719389452509	0.3739143029513826	T	T	T
0.3749205206249463	0.4962160005702525	0.6303385977331875	T	T	T

CO₂ adsorbed on K-MnO (200):

Title

1.0000000000000000

27.916939599999992 0.0000000000000000 0.0000000000000000

-0.0977017000000000 8.9579370100000002 0.0000000000000000

-0.0977017000000000 -0.0987731200000000 8.9573924399999996

Mn C O H K

47 1 50 1 1

Selective dynamics

Direct

0.1604486367113367	0.2499999997209201	0.2500000000000000	F	F	F
0.2406729548893694	0.0000000000000000	0.2500000000000000	F	F	F
0.2406729548883888	0.2499999997209201	0.0000000000000000	F	F	F
0.1604486367142641	0.5000000005581668	0.0000000000000000	F	F	F
0.1604486367123101	0.0000000000000000	0.5000000000000000	F	F	F
0.1604486363550848	0.7500000002790799	0.7500000000000000	F	F	F
0.2406729548913233	0.5000000005581668	0.7500000000000000	F	F	F
0.2406729548903428	0.7500000002790799	0.5000000000000000	F	F	F
0.3208972734246274	0.0000000000000000	0.0000000000000000	F	F	F
0.4796922245878031	0.2517196897891502	0.2485973724164881	T	T	T
0.5590198359226333	0.9989677495093666	0.2386911430204166	T	T	T
0.5575367543037272	0.2516273123066527	0.9983908471997287	T	T	T
0.3208972734256008	0.7500000002790799	0.2500000000000000	F	F	F
0.4003548240361011	0.5020896912442332	0.2488129445547080	T	T	T
0.4008661303499440	0.7508207839332005	0.9992897030384309	T	T	T
0.4798234298246227	0.5039244062595568	0.0000507638951159	T	T	T
0.3208972734236539	0.2499999997209201	0.7500000000000000	F	F	F
0.4002467455457248	0.9995918154427031	0.7507912174314968	T	T	T
0.3999353371273863	0.2510183071335919	0.4996755607110574	T	T	T
0.4769466373601154	0.9954267722784388	0.4991436574749687	T	T	T
0.3208972734265814	0.5000000005581668	0.5000000000000000	F	F	F

0.4835039180611733	0.7519686098469345	0.7430448231016860	T	T	T
0.5598006665940702	0.5036491858431491	0.7578510547895850	T	T	T
0.1604486367123101	0.0000000000000000	0.0000000000000000	F	F	F
0.2406729548903428	0.7500000002790799	0.0000000000000000	F	F	F
0.1604486363550848	0.7500000002790799	0.2500000000000000	F	F	F
0.2406729548913233	0.5000000005581668	0.2500000000000000	F	F	F
0.1604486363560582	0.5000000005581668	0.5000000000000000	F	F	F
0.2406729548883888	0.2499999997209201	0.5000000000000000	F	F	F
0.1604486363531308	0.2499999997209201	0.7500000000000000	F	F	F
0.2406729548893694	0.0000000000000000	0.7500000000000000	F	F	F
0.3208972734265814	0.5000000005581668	0.0000000000000000	F	F	F
0.3999671583984543	0.2506906384466565	0.9995740297665731	T	T	T
0.4795527953079962	0.9997725900974815	0.9996233437446302	T	T	T
0.3208972734236539	0.2499999997209201	0.2500000000000000	F	F	F
0.4002224269300950	0.9994272134915448	0.2487554770449394	T	T	T
0.3208972734246274	0.0000000000000000	0.5000000000000000	F	F	F
0.5595593554845830	0.7512508944900498	0.9984257360724608	T	T	T
0.4833752525169926	0.7519828440944766	0.2555723304485226	T	T	T
0.3996764872149570	0.7513605317177150	0.4994084017626672	T	T	T
0.3208972730673949	0.7500000002790799	0.7500000000000000	F	F	F
0.5602165581617268	0.5032106079834237	0.2396513567171185	T	T	T
0.4766511327228479	0.5087257040792806	0.4997188829241492	T	T	T
0.4002578784174300	0.5023676880292777	0.7511608052449059	T	T	T
0.5562218432448945	0.2528758592538349	0.4975718101811798	T	T	T
0.4796535762861810	0.2523978153434921	0.7500957335796793	T	T	T
0.5588615242953210	0.0006901064015741	0.7575208352969753	T	T	T
0.6320129427650196	0.4268796152845148	0.4976335925069731	T	T	T
0.2406729550674953	0.2499999997209201	0.2500000000000000	F	F	F
0.2406729550684688	0.0000000000000000	0.0000000000000000	F	F	F
0.1604486365322373	0.2499999997209201	0.0000000000000000	F	F	F
0.1604486365332107	0.0000000000000000	0.2500000000000000	F	F	F
0.2406729547112434	0.7500000002790799	0.2500000000000000	F	F	F
0.2406729550704227	0.5000000005581668	0.0000000000000000	F	F	F
0.1604486365341842	0.7500000002790799	0.0000000000000000	F	F	F
0.1604486365351647	0.5000000005581668	0.2500000000000000	F	F	F
0.2406729547092894	0.2499999997209201	0.7500000000000000	F	F	F
0.2406729550684688	0.0000000000000000	0.5000000000000000	F	F	F
0.1604486365322373	0.2499999997209201	0.5000000000000000	F	F	F
0.1604486365332107	0.0000000000000000	0.7500000000000000	F	F	F
0.2406729547112434	0.7500000002790799	0.7500000000000000	F	F	F
0.2406729547122168	0.5000000005581668	0.5000000000000000	F	F	F
0.1604486365341842	0.7500000002790799	0.5000000000000000	F	F	F
0.1604486365351647	0.5000000005581668	0.7500000000000000	F	F	F
0.4003678434557288	0.2510165674587636	0.2499652637768245	T	T	T
0.4008347472089567	0.0012015188399349	0.9993885380877856	T	T	T
0.3208972732445474	0.2499999997209201	0.0000000000000000	F	F	F
0.3208972732455209	0.0000000000000000	0.2500000000000000	F	F	F
0.5570765167353852	0.2504086790470420	0.2435740983554607	T	T	T

0.5583458927087656	0.0080111860612570	0.9977722991736955	T	T	T
0.4778342681223690	0.2521093387074254	0.9992860397538337	T	T	T
0.4809489744237507	0.0007504886046337	0.2567812531177676	T	T	T
0.4005612675082596	0.7506574592445588	0.2482950668998547	T	T	T
0.4009767711448761	0.5005672062544184	0.9996211476979646	T	T	T
0.3208972732465014	0.7500000002790799	0.0000000000000000	F	F	F
0.3208972732474749	0.5000000005581668	0.2500000000000000	F	F	F
0.5617029929870608	0.7532388763187915	0.2317074661115451	T	T	T
0.5584778094748836	0.4963516316135464	0.9997328759946102	T	T	T
0.4790320662473433	0.7517251230032507	0.9996567754209591	T	T	T
0.4815762070023013	0.5028729787516510	0.2581052121328969	T	T	T
0.4003646174054377	0.2511061817742081	0.7491488879314415	T	T	T
0.3996018081280249	0.0032310276392286	0.4995557375642165	T	T	T
0.3208972732445474	0.2499999997209201	0.5000000000000000	F	F	F
0.3208972732455209	0.0000000000000000	0.7500000000000000	F	F	F
0.5569145999740441	0.2540889499503927	0.7541092651653860	T	T	T
0.5769372479616368	0.0193544296700906	0.5021217230384863	T	T	T
0.4797461850619788	0.2518028860614375	0.4992666029584389	T	T	T
0.4810126897197655	0.0008231520843704	0.7412839009872143	T	T	T
0.4004763579943681	0.7508071992191468	0.7507842668486864	T	T	T
0.3996225311280996	0.4988384734560027	0.4997756517935044	T	T	T
0.3208972732465014	0.7500000002790799	0.5000000000000000	F	F	F
0.3208972732474749	0.5000000005581668	0.7500000000000000	F	F	F
0.5617308242926903	0.7513377062303154	0.7659716011086495	T	T	T
0.5828742351666576	0.4809353212658959	0.4954021575046357	T	T	T
0.4774495408556511	0.7521952879308139	0.4993281025436138	T	T	T
0.4813880714315444	0.5033686189973590	0.7409430060429908	T	T	T
0.6646212467899097	0.5222628233358253	0.4937532004489741	T	T	T
0.6347145523901517	0.2852852071763523	0.5034280430090455	T	T	T
0.6086770714765926	0.0686902089462978	0.5037586002549707	T	T	T
0.6126034130848473	0.7569044393149904	0.5006321224416567	T	T	T

CO₂ adsorbed on K-MnO (220):

Title

1.0000000000000000

12.7380876799999996 0.0000000000000000 0.0000000000000000

0.0000000000000000 25.5999145599999984 0.0000000000000000

0.0000000000000000 -0.1389307400000000 8.9573924399999996

Mn C O H K

47 1 50 1 1

Selective dynamics

Direct

0.1250000000000000 0.1845696767434859 0.2500000000000000 F F F

0.3750000000000000 0.1845696767434859 0.2500000000000000 F F F

0.2500000000000000 0.2460929021944338 0.0000000000000000 F F F

0.6250000000000000 0.1845696767434859 0.2500000000000000 F F F

0.8749999992149498 0.1845696767434859 0.2500000000000000 F F F

0.7500000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.0000000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.0000000000000000	0.1230464509019029	0.5000000000000000	F	F	F
0.2500000000000000	0.1230464512925309	0.5000000000000000	F	F	F
0.7500000000000000	0.1230464512925309	0.5000000000000000	F	F	F
0.8750068594226235	0.3058022005847140	0.7495695619684166	T	T	T
0.1240999272109991	0.3055238546338517	0.7487599025601405	T	T	T
0.9991923816860516	0.3708732152463100	0.4991812956869675	T	T	T
0.5000000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.6244275167513985	0.4229222923028117	0.2457262106587357	T	T	T
0.8750705048418239	0.4252766898451296	0.2457548351063635	T	T	T
0.1256699863900566	0.4229564920833179	0.2458355103314268	T	T	T
0.3749850359087376	0.3045615375327118	0.7488552087427844	T	T	T
0.6258780049007655	0.3055152202807077	0.7487463604578285	T	T	T
0.5030731082815955	0.3692779666787145	0.4914376883829324	T	T	T
0.7508375201864236	0.3709019350627323	0.4991419572841055	T	T	T
0.2470458583750466	0.3692913770661468	0.4914036303622243	T	T	T
0.5000000000000000	0.1230464512925309	0.5000000000000000	F	F	F
0.7500000000000000	0.1230464512925309	0.0000000000000000	F	F	F
0.0000000000000000	0.1230464509019029	0.0000000000000000	F	F	F
0.2500000000000000	0.1230464512925309	0.0000000000000000	F	F	F
0.9995167976529790	0.3712829331749711	0.9985855171694972	T	T	T
0.8750045060890993	0.3058065017426892	0.2489908183396116	T	T	T
0.7500000000000000	0.2460929021944338	0.5000000000000000	F	F	F
0.6249999992149498	0.1845696767434859	0.7500000000000000	F	F	F
0.1245636499961055	0.3050826658157669	0.2493002196773666	T	T	T
0.9999999992149498	0.2460929021944338	0.5000000000000000	F	F	F
0.8750000000000000	0.1845696767434859	0.7500000000000000	F	F	F
0.2500000000000000	0.2460929021944338	0.5000000000000000	F	F	F
0.1250000000000000	0.1845696763528579	0.7500000000000000	F	F	F
0.3750000000000000	0.1845696767434859	0.7500000000000000	F	F	F
0.2459072095154393	0.3684845411263909	0.0047779269648557	T	T	T
0.5041621782776174	0.3684585828522288	0.0047447006021046	T	T	T
0.7505441540012204	0.3712783429096833	0.9984667535785193	T	T	T
0.3749638074383708	0.3094246207279006	0.2482803058210821	T	T	T
0.6254140505412658	0.3050742499972417	0.2492960460842946	T	T	T
0.5000000000000000	0.2460929025850618	0.5000000000000000	F	F	F
0.5000000000000000	0.1230464512925309	0.0000000000000000	F	F	F
0.1263576482434965	0.4246736186076484	0.7446906933103037	T	T	T
0.3750511127543287	0.4205974533156845	0.7473516192241761	T	T	T
0.6237972220370853	0.4246454866987825	0.7447359981269974	T	T	T
0.8750804130721545	0.4252404350946431	0.7454201766385451	T	T	T
0.3743129092232106	0.4924120682641054	0.5529852508890893	T	T	T
0.0000000000000000	0.1230464510972169	0.2500000000000000	F	F	F
0.2500000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.3750000000000000	0.1845696769387999	0.0000000000000000	F	F	F
0.1250000000000000	0.1845696765481719	0.0000000000000000	F	F	F
0.2500000000000000	0.1230464510972169	0.2500000000000000	F	F	F

0.7500000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.8750000000000000	0.1845696769387999	0.0000000000000000	F	F	F
0.6250000000000000	0.1845696769387999	0.0000000000000000	F	F	F
0.7499999992149498	0.1230464510972169	0.2500000000000000	F	F	F
0.9980997043932738	0.3692572133473927	0.2486938396734545	T	T	T
0.1242065393029558	0.3055625398202603	0.9978681322863669	T	T	T
0.8750669162853277	0.3062070408864861	0.9987883921190924	T	T	T
0.0000000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.0000000007850502	0.1230464510972169	0.7500000000000000	F	F	F
0.2500000000000000	0.2460929019991198	0.7500000000000000	F	F	F
0.3750000000000000	0.1845696769387999	0.5000000000000000	F	F	F
0.1250000000000000	0.1845696765481719	0.5000000000000000	F	F	F
0.2500000000000000	0.1230464510972169	0.7500000000000000	F	F	F
0.7499999992149498	0.2460929019991198	0.7500000000000000	F	F	F
0.8750000000000000	0.1845696769387999	0.5000000000000000	F	F	F
0.6250000000000000	0.1845696765481719	0.5000000000000000	F	F	F
0.7500000000000000	0.1230464510972169	0.7500000000000000	F	F	F
0.9997796205595796	0.3698108459432052	0.7492510020523869	T	T	T
0.1241110332525091	0.3053240612705741	0.5003911081392478	T	T	T
0.8750248224022922	0.3061893040226991	0.5000714476680090	T	T	T
0.0000000000000000	0.2460929023897478	0.7500000000000000	F	F	F
0.5038449865049079	0.3672710019779418	0.2486783599952699	T	T	T
0.6257793851205747	0.3055447969310345	0.9978229576859725	T	T	T
0.3750120830390745	0.3084926912584661	0.9976780572106214	T	T	T
0.5000000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.8749886594416008	0.4269799645003336	0.9979662089832502	T	T	T
0.6220491959434074	0.4264709403889596	0.9993110300734339	T	T	T
0.7518969456263092	0.3692916217566359	0.2486302302315573	T	T	T
0.3751061055153838	0.4277361425992128	0.9800988410687400	T	T	T
0.1279748036046052	0.4264593139823138	0.9995297050723977	T	T	T
0.2461484772346443	0.3672658825420147	0.2486731414881160	T	T	T
0.4999999992149498	0.1230464510972169	0.2500000000000000	F	F	F
0.5030484616041038	0.3667888556978844	0.7468989443376681	T	T	T
0.6259106480144960	0.3053056435234701	0.5003447758620923	T	T	T
0.3750411058251064	0.3093517206681693	0.4995779369406982	T	T	T
0.5000000000000000	0.2460929023897478	0.7500000000000000	F	F	F
0.8750277554779630	0.4268314336857137	0.4991174441761542	T	T	T
0.6228738678438444	0.4257814905972591	0.4975665450638657	T	T	T
0.7503299325888770	0.3698134773325799	0.7492096710055872	T	T	T
0.3748095065915578	0.4392768957479712	0.5109221012747236	T	T	T
0.1272126436737190	0.4257637019328662	0.4975522758149465	T	T	T
0.2469853481675750	0.3667775034683969	0.7470146089199505	T	T	T
0.4999999992149498	0.1230464510972169	0.7500000000000000	F	F	F
0.3746233735282226	0.5267778016849608	0.4565097253230315	T	T	T
0.3736056667247401	0.5002662008616153	0.6968978808149153	T	T	T
0.3747334121910697	0.4656228752692109	0.9704982069866145	T	T	T
0.3752939984589493	0.4650195295344942	0.2411329153398224	T	T	T

H adsorbed on MnO (200):

Title

1.0000000000000000
27.916939599999992 0.0000000000000000 0.0000000000000000
-0.0977017000000000 8.9579370100000002 0.0000000000000000
-0.0977017000000000 -0.0987731200000000 8.9573924399999996

Mn O H
48 48 1

Selective dynamics

Direct

0.1604486367113367	0.2499999997209201	0.2500000000000000	F	F	F
0.2406729548893694	0.0000000000000000	0.2500000000000000	F	F	F
0.2406729548883888	0.2499999997209201	0.0000000000000000	F	F	F
0.1604486367142641	0.5000000005581668	0.0000000000000000	F	F	F
0.1604486367123101	0.0000000000000000	0.5000000000000000	F	F	F
0.1604486363550848	0.7500000002790799	0.7500000000000000	F	F	F
0.2406729548913233	0.5000000005581668	0.7500000000000000	F	F	F
0.2406729548903428	0.7500000002790799	0.5000000000000000	F	F	F
0.3208972734246274	0.0000000000000000	0.0000000000000000	F	F	F
0.4795264707643311	0.2492586465841931	0.2492586458118687	T	T	T
0.5582676269435186	0.9984881050136416	0.2462863810998031	T	T	T
0.5582676269425452	0.2462863810518557	0.9984881047825092	T	T	T
0.3208972734256008	0.7500000002790799	0.2500000000000000	F	F	F
0.3995111857142862	0.4996243176834095	0.2488899524369697	T	T	T
0.3998080951259314	0.7502191063496968	0.9998135619270083	T	T	T
0.4788745064656824	0.4995903840208262	0.9999652226466211	T	T	T
0.3208972734236539	0.2499999997209201	0.7500000000000000	F	F	F
0.3998080951249508	0.9998135624649389	0.7502191055326863	T	T	T
0.3995111857113588	0.2488899526958133	0.4996243165873192	T	T	T
0.4788745064637284	0.9999652236980254	0.4995903824112550	T	T	T
0.3208972734265814	0.5000000005581668	0.5000000000000000	F	F	F
0.4795937274080340	0.7498165915268447	0.7498165901963605	T	T	T
0.5584664527226635	0.4987245666634514	0.7587915118342069	T	T	T
0.5584664527216900	0.7587915123444192	0.4987245658741521	T	T	T
0.1604486367123101	0.0000000000000000	0.0000000000000000	F	F	F
0.2406729548903428	0.7500000002790799	0.0000000000000000	F	F	F
0.1604486363550848	0.7500000002790799	0.2500000000000000	F	F	F
0.2406729548913233	0.5000000005581668	0.2500000000000000	F	F	F
0.1604486363560582	0.5000000005581668	0.5000000000000000	F	F	F
0.2406729548883888	0.2499999997209201	0.5000000000000000	F	F	F
0.1604486363531308	0.2499999997209201	0.7500000000000000	F	F	F
0.2406729548893694	0.0000000000000000	0.7500000000000000	F	F	F
0.3208972734265814	0.5000000005581668	0.0000000000000000	F	F	F
0.3997798165482985	0.2492021587286200	0.9995409246741751	T	T	T
0.4791862369059204	0.9995347575677394	0.9995347565163351	T	T	T
0.3208972734236539	0.2499999997209201	0.2500000000000000	F	F	F
0.3997798165492719	0.9995409252121057	0.2492021584697764	T	T	T

0.3208972734246274	0.0000000000000000	0.5000000000000000	F	F	F
0.5583517842223834	0.7509045815723177	0.9987170412797227	T	T	T
0.4796367444458836	0.7495079407219623	0.2496877028553579	T	T	T
0.3994736231507875	0.7509898805196923	0.4997796677788949	T	T	T
0.3208972730673949	0.7500000002790799	0.7500000000000000	F	F	F
0.5586322937834723	0.4982236206031561	0.2386449658795972	T	T	T
0.4753591648887519	0.4996407132790910	0.4996407116695198	T	T	T
0.3994736231517610	0.4997796688749852	0.7509898797026818	T	T	T
0.5586322937805449	0.2386449658316498	0.4982236198138639	T	T	T
0.4796367444439296	0.2496877036276823	0.7495079393914781	T	T	T
0.5583517842214029	0.9987170415108552	0.7509045810621053	T	T	T
0.2406729550674953	0.2499999997209201	0.2500000000000000	F	F	F
0.2406729550684688	0.0000000000000000	0.0000000000000000	F	F	F
0.1604486365322373	0.2499999997209201	0.0000000000000000	F	F	F
0.1604486365332107	0.0000000000000000	0.2500000000000000	F	F	F
0.2406729547112434	0.7500000002790799	0.2500000000000000	F	F	F
0.2406729550704227	0.5000000005581668	0.0000000000000000	F	F	F
0.1604486365341842	0.7500000002790799	0.0000000000000000	F	F	F
0.1604486365351647	0.5000000005581668	0.2500000000000000	F	F	F
0.2406729547092894	0.2499999997209201	0.7500000000000000	F	F	F
0.2406729550684688	0.0000000000000000	0.5000000000000000	F	F	F
0.1604486365322373	0.2499999997209201	0.5000000000000000	F	F	F
0.1604486365332107	0.0000000000000000	0.7500000000000000	F	F	F
0.2406729547112434	0.7500000002790799	0.7500000000000000	F	F	F
0.2406729547122168	0.5000000005581668	0.5000000000000000	F	F	F
0.1604486365341842	0.7500000002790799	0.5000000000000000	F	F	F
0.1604486365351647	0.5000000005581668	0.7500000000000000	F	F	F
0.4003872526643720	0.2500222004633128	0.2500221997735108	T	T	T
0.4003490167239244	0.9996313997206845	0.9996313987517955	T	T	T
0.3208972732445474	0.2499999997209201	0.0000000000000000	F	F	F
0.3208972732455209	0.0000000000000000	0.2500000000000000	F	F	F
0.5591167180068866	0.2499350283616609	0.2499350284473879	T	T	T
0.5589691733990426	0.9989869490438058	0.9989869488504529	T	T	T
0.4792443256715431	0.2505256440771446	0.9992665734176264	T	T	T
0.4792443256725236	0.9992665725310964	0.2505256452427544	T	T	T
0.4004206357577124	0.7490651269367021	0.2501989798456957	T	T	T
0.4005630508709602	0.4996714462099066	0.9996768669706029	T	T	T
0.3208972732465014	0.7500000002790799	0.0000000000000000	F	F	F
0.3208972732474749	0.5000000005581668	0.2500000000000000	F	F	F
0.5592404317408710	0.7475489417019419	0.2509982010200938	T	T	T
0.5585574511513649	0.4993107691558463	0.9991704388716079	T	T	T
0.4793057192234130	0.7485425535863516	0.9997712350560511	T	T	T
0.4802239260037222	0.4992658063304851	0.2548732439593128	T	T	T
0.4004206357557584	0.2501989805354977	0.7490651256887333	T	T	T
0.4005630508690062	0.9996768679394918	0.4996714446828579	T	T	T
0.3208972732445474	0.2499999997209201	0.5000000000000000	F	F	F
0.3208972732455209	0.0000000000000000	0.7500000000000000	F	F	F
0.5592404317389170	0.2509982009343669	0.7475489412295020	T	T	T

0.5585574511494109	0.9991704390649608	0.4993107684043266	T	T	T
0.4802239260007877	0.2548732427937030	0.4992658066588553	T	T	T
0.4793057192224395	0.9997712341695212	0.7485425541938017	T	T	T
0.4004269908931569	0.7492620683793997	0.7492620671314308	T	T	T
0.3992241022995509	0.4996756581481679	0.4996756566211192	T	T	T
0.3208972732465014	0.7500000002790799	0.5000000000000000	F	F	F
0.3208972732474749	0.5000000005581668	0.7500000000000000	F	F	F
0.5591379127551125	0.7476334590051678	0.7476334585327279	T	T	T
0.5758787579138770	0.4986398345739676	0.4986398338224479	T	T	T
0.4801469596016844	0.7440356934475297	0.4995401852793917	T	T	T
0.4801469596026650	0.4995401849510215	0.7440356940549798	T	T	T
0.6111936089261000	0.5011478040828702	0.5011478041571645	T	T	T

H adsorbed on MnO (220):

Title

1.0000000000000000		
12.7380876799999996	0.0000000000000000	0.0000000000000000
0.0000000000000000	25.5999145599999984	0.0000000000000000
0.0000000000000000	-0.1389307400000000	8.9573924399999996

Mn	O	H
48	48	1

Selective dynamics

Direct

0.1250000000000000	0.1845696767434859	0.2500000000000000	F	F	F
0.3750000000000000	0.1845696767434859	0.2500000000000000	F	F	F
0.2500000000000000	0.2460929021944338	0.0000000000000000	F	F	F
0.6250000000000000	0.1845696767434859	0.2500000000000000	F	F	F
0.8749999992149498	0.1845696767434859	0.2500000000000000	F	F	F
0.7500000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.0000000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.0000000000000000	0.1230464509019029	0.5000000000000000	F	F	F
0.2500000000000000	0.1230464512925309	0.5000000000000000	F	F	F
0.7500000000000000	0.1230464512925309	0.5000000000000000	F	F	F
0.8750000000000000	0.3058096333285278	0.7497133844399547	T	T	T
0.1242690358619988	0.3055857483096898	0.7488719909642481	T	T	T
0.9998653972408995	0.3712343984441733	0.4998578338434392	T	T	T
0.5000000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.6245777735602681	0.4244127878943800	0.2481333174038678	T	T	T
0.8750000000000000	0.4245278496002838	0.2462598169145628	T	T	T
0.1254222264397177	0.4244127878943800	0.2481333174038678	T	T	T
0.3750000000000000	0.4236088326725599	0.2274057893990662	T	T	T
0.3750000000000000	0.3062151840719619	0.7488475514263435	T	T	T
0.6257309641380012	0.3055857483096898	0.7488719909642481	T	T	T
0.5015579890546135	0.3702620341382561	0.4999517079331388	T	T	T
0.7501346027591005	0.3712343984441733	0.4998578338434392	T	T	T
0.2484420101603362	0.3702620341382561	0.4999517079331388	T	T	T
0.5000000000000000	0.1230464512925309	0.5000000000000000	F	F	F

0.7500000000000000	0.1230464512925309	0.0000000000000000	F	F	F
0.0000000000000000	0.1230464509019029	0.0000000000000000	F	F	F
0.2500000000000000	0.1230464512925309	0.0000000000000000	F	F	F
0.9993305894475301	0.3712955133590699	0.9997889873507624	T	T	T
0.8749999992149498	0.3057204203011454	0.2497596921940694	T	T	T
0.7500000000000000	0.2460929021944338	0.5000000000000000	F	F	F
0.6249999992149498	0.1845696767434859	0.7500000000000000	F	F	F
0.1241905297336298	0.3053658805415452	0.2508254071299303	T	T	T
0.9999999992149498	0.2460929021944338	0.5000000000000000	F	F	F
0.8750000000000000	0.1845696767434859	0.7500000000000000	F	F	F
0.2500000000000000	0.2460929021944338	0.5000000000000000	F	F	F
0.1250000000000000	0.1845696763528579	0.7500000000000000	F	F	F
0.3750000000000000	0.1845696767434859	0.7500000000000000	F	F	F
0.2457675978099332	0.3681756120898578	0.0007763743169961	T	T	T
0.5042324021900668	0.3681756116992369	0.0007763743169961	T	T	T
0.7506694105524699	0.3712955137496908	0.9997889873507624	T	T	T
0.3750000000000000	0.3052105513610059	0.2498365312564081	T	T	T
0.6258094702663772	0.3053658805415452	0.2508254071299303	T	T	T
0.5000000000000000	0.2460929025850618	0.5000000000000000	F	F	F
0.5000000000000000	0.1230464512925309	0.0000000000000000	F	F	F
0.1276635116834655	0.4260883330359285	0.7456402831842550	T	T	T
0.3750000000000000	0.4290620607289814	0.7821519732076608	T	T	T
0.6223364883165343	0.4260883330359285	0.7456402831842550	T	T	T
0.8750000000000000	0.4249801737324519	0.7465347694221631	T	T	T
0.0000000000000000	0.1230464510972169	0.2500000000000000	F	F	F
0.2500000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.3750000000000000	0.1845696769387999	0.0000000000000000	F	F	F
0.1250000000000000	0.1845696765481719	0.0000000000000000	F	F	F
0.2500000000000000	0.1230464510972169	0.2500000000000000	F	F	F
0.7500000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.8750000000000000	0.1845696769387999	0.0000000000000000	F	F	F
0.6250000000000000	0.1845696769387999	0.0000000000000000	F	F	F
0.7499999992149498	0.1230464510972169	0.2500000000000000	F	F	F
0.9995283693098913	0.3685902715880937	0.2505671116272249	T	T	T
0.1241531412624675	0.3054848064910358	0.9982439259662043	T	T	T
0.8750000000000000	0.3062862740315446	0.9985892081412129	T	T	T
0.0000000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.0000000007850502	0.1230464510972169	0.7500000000000000	F	F	F
0.2500000000000000	0.2460929019991198	0.7500000000000000	F	F	F
0.3750000000000000	0.1845696769387999	0.5000000000000000	F	F	F
0.1250000000000000	0.1845696765481719	0.5000000000000000	F	F	F
0.2500000000000000	0.1230464510972169	0.7500000000000000	F	F	F
0.7499999992149498	0.2460929019991198	0.7500000000000000	F	F	F
0.8750000000000000	0.1845696769387999	0.5000000000000000	F	F	F
0.6250000000000000	0.1845696765481719	0.5000000000000000	F	F	F
0.7500000000000000	0.1230464510972169	0.7500000000000000	F	F	F
0.0018102680534279	0.3702625469652009	0.7495178518596898	T	T	T
0.1253038858100529	0.3059807427088954	0.5013138871924412	T	T	T

0.8750000000000000	0.3061183126923831	0.5012481081717464	T	T	T
0.0000000000000000	0.2460929023897478	0.7500000000000000	F	F	F
0.5003404877101973	0.3673158675805319	0.2523156311064950	T	T	T
0.6258468587375325	0.3054848064910358	0.9982439259662043	T	T	T
0.3750000000000000	0.3054579091862594	0.9986464352999959	T	T	T
0.5000000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.8750000000000000	0.4267936805904389	0.9999694745517599	T	T	T
0.6241375653517688	0.4260784278114447	0.0051365620642436	T	T	T
0.7504716306901087	0.3685902715880937	0.2505671116272249	T	T	T
0.3749999992149498	0.4244628229639019	0.0073950260985462	T	T	T
0.1258624346482312	0.4260784278114447	0.0051365620642436	T	T	T
0.2496595122898027	0.3673158679711599	0.2523156311064950	T	T	T
0.4999999992149498	0.1230464510972169	0.2500000000000000	F	F	F
0.4964624320407693	0.3709161656947048	0.7465717385671106	T	T	T
0.6246961134048968	0.3059807427088954	0.5013138871924412	T	T	T
0.3750000000000000	0.3086928302667929	0.5000490019959688	T	T	T
0.5000000000000000	0.2460929023897478	0.7500000000000000	F	F	F
0.8750000000000000	0.4266351876543968	0.4990898684097739	T	T	T
0.6229307220548834	0.4264329927402793	0.4954727358434233	T	T	T
0.7481897319465721	0.3702625473558289	0.7495178518596898	T	T	T
0.3749999992149498	0.4323441803054096	0.4558228799168940	T	T	T
0.1270692779451165	0.4264329927402793	0.4954727358434233	T	T	T
0.2535375679592307	0.3709161660853328	0.7465717385671106	T	T	T
0.4999999992149498	0.1230464510972169	0.7500000000000000	F	F	F
0.3749999984299066	0.4667570095680939	0.5043779299912564	T	T	T

H adsorbed on K-MnO (200):

Title

1.0000000000000000

27.916939599999992 0.0000000000000000 0.0000000000000000

-0.0977017000000000 8.9579370100000002 0.0000000000000000

-0.0977017000000000 -0.0987731200000000 8.9573924399999996

Mn O H K

47 48 2 1

Selective dynamics

Direct

0.1604486367113367	0.2499999997209201	0.2500000000000000	F	F	F
0.2406729548893694	0.0000000000000000	0.2500000000000000	F	F	F
0.2406729548883888	0.2499999997209201	0.0000000000000000	F	F	F
0.1604486367142641	0.5000000005581668	0.0000000000000000	F	F	F
0.1604486367123101	0.0000000000000000	0.5000000000000000	F	F	F
0.1604486363550848	0.7500000002790799	0.7500000000000000	F	F	F
0.2406729548913233	0.5000000005581668	0.7500000000000000	F	F	F
0.2406729548903428	0.7500000002790799	0.5000000000000000	F	F	F
0.3208972734246274	0.0000000000000000	0.0000000000000000	F	F	F
0.4797276728302970	0.2489090154502705	0.2486618324274238	T	T	T
0.5595333877476681	0.9962075139899096	0.2373032840883081	T	T	T

0.5579064379972937	0.2480982736523169	0.9980300887359095	T	T	T
0.3208972734256008	0.7500000002790799	0.2500000000000000	F	F	F
0.4000698168926553	0.5005441537147903	0.2485427737637339	T	T	T
0.4007052870743559	0.7495386422893702	0.9993596364959770	T	T	T
0.4795498368366979	0.5012140477451824	0.9999214348867005	T	T	T
0.3208972734236539	0.2499999997209201	0.7500000000000000	F	F	F
0.4000144945101429	0.9985260130154217	0.7511217459247850	T	T	T
0.3996681101877804	0.2498487356751776	0.4996489895008530	T	T	T
0.4761232178047128	0.9925301449600670	0.4991834877997314	T	T	T
0.3208972734265814	0.5000000005581668	0.5000000000000000	F	F	F
0.4832319517505012	0.7495154928577054	0.7436568198527067	T	T	T
0.5595598941629828	0.4991943810103604	0.7588659148571680	T	T	T
0.1604486367123101	0.0000000000000000	0.0000000000000000	F	F	F
0.2406729548903428	0.7500000002790799	0.0000000000000000	F	F	F
0.1604486363550848	0.7500000002790799	0.2500000000000000	F	F	F
0.2406729548913233	0.5000000005581668	0.2500000000000000	F	F	F
0.1604486363560582	0.5000000005581668	0.5000000000000000	F	F	F
0.2406729548883888	0.2499999997209201	0.5000000000000000	F	F	F
0.1604486363531308	0.2499999997209201	0.7500000000000000	F	F	F
0.2406729548893694	0.0000000000000000	0.7500000000000000	F	F	F
0.3208972734265814	0.5000000005581668	0.0000000000000000	F	F	F
0.3998861548159947	0.2494347886654557	0.9995326284970846	T	T	T
0.4794387823282986	0.9971666826994796	0.9997169018395656	T	T	T
0.3208972734236539	0.2499999997209201	0.2500000000000000	F	F	F
0.4000083581163940	0.9983685938754737	0.2484805836054823	T	T	T
0.3208972734246274	0.0000000000000000	0.5000000000000000	F	F	F
0.5596137057545331	0.7479573752197749	0.9984541298913385	T	T	T
0.4830813454365767	0.7493072232828949	0.2549903526351566	T	T	T
0.3994871517242014	0.7500369975070692	0.4994400368987975	T	T	T
0.3208972730673949	0.7500000002790799	0.7500000000000000	F	F	F
0.5598294741353302	0.4976795826421948	0.2372798629050710	T	T	T
0.4760736187891503	0.5064629928783774	0.4996403370149630	T	T	T
0.4000164666603171	0.5009191030628635	0.7513852445237500	T	T	T
0.5557173070643400	0.2477480058156225	0.4974051676972060	T	T	T
0.4797517816949037	0.2496202728612411	0.7501741873137063	T	T	T
0.5593648177995914	0.9981925008589357	0.7591378843324229	T	T	T
0.2406729550674953	0.2499999997209201	0.2500000000000000	F	F	F
0.2406729550684688	0.0000000000000000	0.0000000000000000	F	F	F
0.1604486365322373	0.2499999997209201	0.0000000000000000	F	F	F
0.1604486365332107	0.0000000000000000	0.2500000000000000	F	F	F
0.2406729547112434	0.7500000002790799	0.2500000000000000	F	F	F
0.2406729550704227	0.5000000005581668	0.0000000000000000	F	F	F
0.1604486365341842	0.7500000002790799	0.0000000000000000	F	F	F
0.1604486365351647	0.5000000005581668	0.2500000000000000	F	F	F
0.2406729547092894	0.2499999997209201	0.7500000000000000	F	F	F
0.2406729550684688	0.0000000000000000	0.5000000000000000	F	F	F
0.1604486365322373	0.2499999997209201	0.5000000000000000	F	F	F
0.1604486365332107	0.0000000000000000	0.7500000000000000	F	F	F

0.2406729547112434	0.7500000002790799	0.7500000000000000	F	F	F
0.2406729547122168	0.5000000005581668	0.5000000000000000	F	F	F
0.1604486365341842	0.7500000002790799	0.5000000000000000	F	F	F
0.1604486365351647	0.5000000005581668	0.7500000000000000	F	F	F
0.4005936292841549	0.2494678308326228	0.2500120040774901	T	T	T
0.4010394870443406	0.0000161418056663	0.9993870854071851	T	T	T
0.3208972732445474	0.2499999997209201	0.0000000000000000	F	F	F
0.3208972732455209	0.0000000000000000	0.2500000000000000	F	F	F
0.5584535512233675	0.2472336421556895	0.2474412878128069	T	T	T
0.5585668205966983	0.0058936988866036	0.9981197285311790	T	T	T
0.4784490728860734	0.2493160905734367	0.9992394537492897	T	T	T
0.4813239274257925	0.9986297187922442	0.2568410282147648	T	T	T
0.4008600871335853	0.7494154586390943	0.2483644856909765	T	T	T
0.4010841216074907	0.4988506062793926	0.9997087493556176	T	T	T
0.3208972732465014	0.7500000002790799	0.0000000000000000	F	F	F
0.3208972732474749	0.5000000005581668	0.2500000000000000	F	F	F
0.5618881866553774	0.7488088960381136	0.2320904432372989	T	T	T
0.5587198665183091	0.4915605570643953	0.9988457836233455	T	T	T
0.4793159702981633	0.7490359083789249	0.9996636646640393	T	T	T
0.4815966701923889	0.4993908116461598	0.2574566489988142	T	T	T
0.4006517644526796	0.2496118965150906	0.7490212109495654	T	T	T
0.3996193534055796	0.0017187874703808	0.4995198331288868	T	T	T
0.3208972732445474	0.2499999997209201	0.5000000000000000	F	F	F
0.3208972732455209	0.0000000000000000	0.7500000000000000	F	F	F
0.5584739841884521	0.2498486568182112	0.7493248113645286	T	T	T
0.5824069315633629	0.0255677179425444	0.4998185944113747	T	T	T
0.4799756564044655	0.2487439848319418	0.4991699778481068	T	T	T
0.4813972756375959	0.9987583140902943	0.7412283557260532	T	T	T
0.4008062068295004	0.7495438730577112	0.7507884464360745	T	T	T
0.3996744523518659	0.4974608595435926	0.4996857159169849	T	T	T
0.3208972732465014	0.7500000002790799	0.5000000000000000	F	F	F
0.3208972732474749	0.5000000005581668	0.7500000000000000	F	F	F
0.5619086425471795	0.7483992157361730	0.7656548509266949	T	T	T
0.5832772494620756	0.4711979132861255	0.4972314504199662	T	T	T
0.4780637909604624	0.7497306729600381	0.4992907086901535	T	T	T
0.4814296089832493	0.4999316912004399	0.7412395190805912	T	T	T
0.6175430857764957	0.4459503786216681	0.4986617054454477	T	T	T
0.6167094114212335	0.0524631376678582	0.5019819155013934	T	T	T
0.6036030194357991	0.7494502256474823	0.5003759874669428	T	T	T

H adsorbed on K-MnO (220):

Title

1.0000000000000000

12.7380876799999996 0.0000000000000000 0.0000000000000000

0.0000000000000000 25.5999145599999984 0.0000000000000000

0.0000000000000000 -0.1389307400000000 8.9573924399999996

Mn O H K

47 48 2 1
 Selective dynamics
 Direct

0.1250000000000000	0.1845696767434859	0.2500000000000000	F	F	F
0.3750000000000000	0.1845696767434859	0.2500000000000000	F	F	F
0.2500000000000000	0.2460929021944338	0.0000000000000000	F	F	F
0.6250000000000000	0.1845696767434859	0.2500000000000000	F	F	F
0.8749999992149498	0.1845696767434859	0.2500000000000000	F	F	F
0.7500000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.0000000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.0000000000000000	0.1230464509019029	0.5000000000000000	F	F	F
0.2500000000000000	0.1230464512925309	0.5000000000000000	F	F	F
0.7500000000000000	0.1230464512925309	0.5000000000000000	F	F	F
0.8750000000000000	0.3057229606135713	0.7496192457562179	T	T	T
0.1233574344541224	0.3052135024713399	0.7494799312200615	T	T	T
0.9988477161676970	0.3712808378051871	0.4999801937836362	T	T	T
0.5000000000000000	0.2460929025850618	0.0000000000000000	F	F	F
0.6265831635172665	0.4230680824614987	0.2465346255044704	T	T	T
0.8750000000000000	0.4255833449161318	0.2469889711246342	T	T	T
0.1234168364827336	0.4230680824614987	0.2465346255044704	T	T	T
0.3750000000000000	0.3040932383395406	0.7490671611803518	T	T	T
0.6266425655458704	0.3052135024713399	0.7494799312200615	T	T	T
0.5051188004292606	0.3685168956128417	0.4939560331797629	T	T	T
0.7511522838323030	0.3712808378051871	0.4999801937836362	T	T	T
0.2448811987856893	0.3685168956128417	0.4939560331797629	T	T	T
0.5000000000000000	0.1230464512925309	0.5000000000000000	F	F	F
0.7500000000000000	0.1230464512925309	0.0000000000000000	F	F	F
0.0000000000000000	0.1230464509019029	0.0000000000000000	F	F	F
0.2500000000000000	0.1230464512925309	0.0000000000000000	F	F	F
0.9988582508004474	0.3713645143609004	0.9994239440158841	T	T	T
0.8749999992149498	0.3055690525074921	0.2494091766621676	T	T	T
0.7500000000000000	0.2460929021944338	0.5000000000000000	F	F	F
0.6249999992149498	0.1845696767434859	0.7500000000000000	F	F	F
0.1241819180087777	0.3050099900912847	0.2497491937263316	T	T	T
0.9999999992149498	0.2460929021944338	0.5000000000000000	F	F	F
0.8750000000000000	0.1845696767434859	0.7500000000000000	F	F	F
0.2500000000000000	0.2460929021944338	0.5000000000000000	F	F	F
0.1250000000000000	0.1845696763528579	0.7500000000000000	F	F	F
0.3750000000000000	0.1845696767434859	0.7500000000000000	F	F	F
0.2446897470293196	0.3683992857505107	0.0049803576799903	T	T	T
0.5053102529706804	0.3683992853598828	0.0049803576799903	T	T	T
0.7511417491995526	0.3713645147515284	0.9994239440158841	T	T	T
0.3750000000000000	0.3089232622289292	0.2495685160805741	T	T	T
0.6258180819912221	0.3050099900912847	0.2497491937263316	T	T	T
0.5000000000000000	0.2460929025850618	0.5000000000000000	F	F	F
0.5000000000000000	0.1230464512925309	0.0000000000000000	F	F	F
0.1256767336904214	0.4248449446564046	0.7464594512621920	T	T	T
0.3750000000000000	0.4176123545508734	0.7484194509554912	T	T	T

0.6243232663095788	0.4248449446564046	0.7464594512621920	T	T	T
0.8750000000000000	0.4258740572290774	0.7467005756188176	T	T	T
0.0000000000000000	0.1230464510972169	0.2500000000000000	F	F	F
0.2500000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.3750000000000000	0.1845696769387999	0.0000000000000000	F	F	F
0.1250000000000000	0.1845696765481719	0.0000000000000000	F	F	F
0.2500000000000000	0.1230464510972169	0.2500000000000000	F	F	F
0.7500000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.8750000000000000	0.1845696769387999	0.0000000000000000	F	F	F
0.6250000000000000	0.1845696769387999	0.0000000000000000	F	F	F
0.7499999992149498	0.1230464510972169	0.2500000000000000	F	F	F
0.9983377036031765	0.3687357239170659	0.2496278910052324	T	T	T
0.1245336023220378	0.3059235238183329	0.9985857514890266	T	T	T
0.8750000000000000	0.3065042030612132	0.9984727301650482	T	T	T
0.0000000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.0000000007850502	0.1230464510972169	0.7500000000000000	F	F	F
0.2500000000000000	0.2460929019991198	0.7500000000000000	F	F	F
0.3750000000000000	0.1845696769387999	0.5000000000000000	F	F	F
0.1250000000000000	0.1845696765481719	0.5000000000000000	F	F	F
0.2500000000000000	0.1230464510972169	0.7500000000000000	F	F	F
0.7499999992149498	0.2460929019991198	0.7500000000000000	F	F	F
0.8750000000000000	0.1845696769387999	0.5000000000000000	F	F	F
0.6250000000000000	0.1845696765481719	0.5000000000000000	F	F	F
0.7500000000000000	0.1230464510972169	0.7500000000000000	F	F	F
0.0000991621296006	0.3699987164132564	0.7495326758780076	T	T	T
0.1245968547272951	0.3058814762287193	0.5006725031965721	T	T	T
0.8750000000000000	0.3064704776069653	0.5007520190298583	T	T	T
0.0000000000000000	0.2460929023897478	0.7500000000000000	F	F	F
0.5028950238053759	0.3684015813270446	0.2496419497476632	T	T	T
0.6254663976779623	0.3059235238183329	0.9985857514890266	T	T	T
0.3750000000000000	0.3102053990768314	0.9978836952133138	T	T	T
0.5000000000000000	0.2460929023897478	0.2500000000000000	F	F	F
0.8750000000000000	0.4271536258307342	0.0002057300490619	T	T	T
0.6216333843107704	0.4267188826451145	0.0005384749740754	T	T	T
0.7516622963968235	0.3687357239170659	0.2496278910052324	T	T	T
0.3749999992149498	0.4339019718280471	0.9703618808537117	T	T	T
0.1283666156892296	0.4267188826451145	0.0005384749740754	T	T	T
0.2471049761946242	0.3684015817176726	0.2496419497476632	T	T	T
0.4999999992149498	0.1230464510972169	0.2500000000000000	F	F	F
0.5023375707076089	0.3671333426664579	0.7489841432420234	T	T	T
0.6254031444876549	0.3058814762287193	0.5006725031965721	T	T	T
0.3750000000000000	0.3104018547301081	0.5006185922073724	T	T	T
0.5000000000000000	0.2460929023897478	0.7500000000000000	F	F	F
0.8750000000000000	0.4271354050083384	0.4986216275105944	T	T	T
0.6215784817433180	0.4266664820519291	0.4971737222912359	T	T	T
0.7499008378703993	0.3699987168038844	0.7495326758780076	T	T	T
0.3749999992149498	0.4355990866108498	0.5298921247436893	T	T	T
0.1284215182566678	0.4266664820519291	0.4971737222912359	T	T	T

0.2476624292923910	0.3671333430570859	0.7489841432420234	T	T	T
0.4999999992149498	0.1230464510972169	0.7500000000000000	F	F	F
0.3749999984299066	0.4737150027503584	0.5306911370103745	T	T	T
0.3749999992149498	0.4719783891292620	0.9752621880275117	T	T	T
0.3750000000000000	0.4538912037508247	0.2516642923035083	T	T	T