

Supporting Information

In Situ Surfaced Mn-Mn Dimeric Sites Dictate CO Hydrogenation Activity and C₂ Selectivity over MnRh Binary Catalysts

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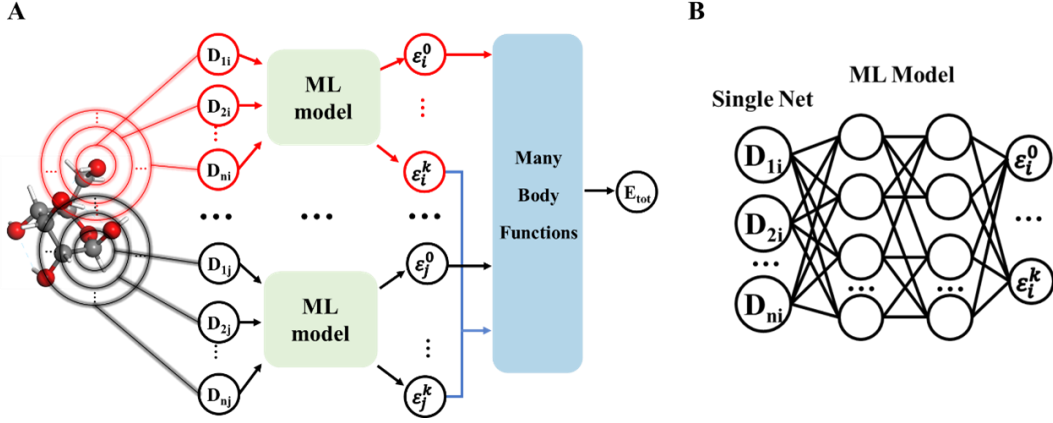
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1. Theoretical Methods

1.1 Construction of Rh-Mn-C-H-O G-NN Potential

Architecture of neural network potential



Scheme S1. Architecture of the many-body function corrected neural network potential (MBNN). (A) Each atomic ML model, the feed-forward neural network (NN) utilized in this work as shown in (B), outputs a series of coefficients ε_i^k that acts as the parameters for different many-body functions. The total energy of system is written as the sum of these many-body functions. (B) The implementations of the atomic ML model with the feed-forward NN.

In this work, the many-body function corrected global neural network (G-MBNN)¹ was utilized to establish the global neural network (G-NN) potential. This is an upgraded framework of the high-dimensional neural network (HDNN)²⁻⁵ as implemented in LASP code⁶. The neural network (NN) architecture is schematically shown in Scheme S1. As shown in Scheme 1A, the input nodes are a set of power-type structural descriptors (PTSD)² $\{D_i\}$, which are calculated from the Cartesian coordinates $\{R_i\}$. Two typical PTSDs are given in Eqs. S3 and S4, while others can be seen in Ref. S2.

$$f_c(r_{ij}) = \begin{cases} 0.5 \times \tanh^3 \left[1 - \frac{r_{ij}}{r_c} \right], & \text{for } r_{ij} \leq r_c \\ 0 & \text{for } r_{ij} > r_c \end{cases} \quad (\text{S1})$$

$$R^n(r_{ij}) = r_{ij}^n \cdot f_c(r_{ij}) \quad (\text{S2})$$

$$D_i^2 = \left[\sum_{m=-L}^L \left| \sum_{j \neq i} R^n(r_{ij}) Y_{Lm}(\mathbf{r}_{ij}) \right|^2 \right]^{\frac{1}{2}} \quad (\text{S3})$$

$$D_i^5 = \left[\sum_{m=-L}^L \left| \sum_{j,k \neq i} R^n(r_{ij}) \cdot R^m(r_{ik}) \cdot R^p(r_{jk}) \cdot (Y_{Lm}(\mathbf{r}_{ij}) + Y_{Lm}(\mathbf{r}_{ik})) \right|^2 \right]^{\frac{1}{2}} \quad (\text{S4})$$

In the Eqs, r_{ij} is the distance between atom i and j . θ_{ijk} is the angle centered at atom i with j and k as neighbors (where i, j , and k are atom indices). f_c is the cut-off function, which decays to zero beyond the cut-off distance r_c . The combination of the power function and the spherical harmonic function (Y_{Lm}), similar to atomic wavefunctions, provides a convenient way to couple the radial and angular information of atoms.

As shown in Scheme 1B, the feed-forward NN outputs a vector, including the atomic energy ε_i^0 and a series of coefficients ε_i^k (where $k=1, 2, 3, \dots$). These coefficients ε_i^k are used to build different many-body functions, including single-body (f_s), two-body (f_d) and three-body (f_t) functions. The total energy E^{tot} can thus be expressed as the sum of both atomic energies and many-body functions as shown in Eq. S5, with these many-body functions defined in Eqs. S6-S9:

$$E^{\text{tot}} = \sum_{s=1}^{\text{ns}} \sum_{i=1}^{\text{na}} f_s(\varepsilon_i^s) + \sum_{d=1}^{\text{nd}} \sum_{i=1}^{\text{na}} \sum_{j>i}^{\text{na}} f_d(\varepsilon_i^d, \varepsilon_j^d, r_{ij}) + \sum_{t=1}^{\text{nt}} \sum_{i=1}^{\text{na}} \sum_{j>i}^{\text{na}} \sum_{k>j}^{\text{na}} \sum_{\text{ang}=1}^3 f_t(\varepsilon_i^t, \varepsilon_j^t, \varepsilon_k^t, r_{ij}, r_{ik}, r_{jk}, \theta_{\text{ang}}) + \dots \quad (\text{S5})$$

$$f_s = \lambda \varepsilon_i^s \quad (\text{S6})$$

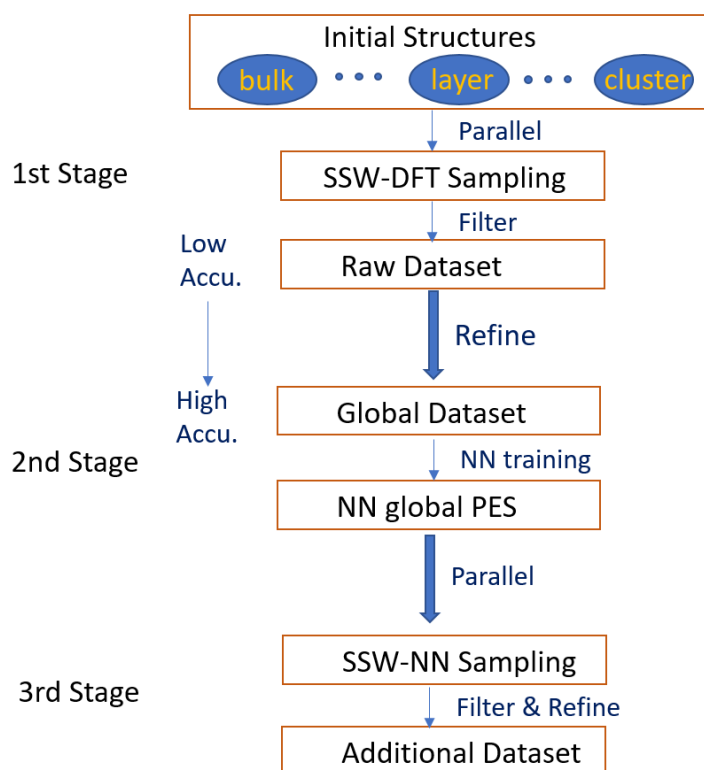
$$f_d = \lambda \frac{\varepsilon_i^d \varepsilon_j^d}{r_{ij}^{m_d}} f_c(r_{ij}) \quad (\text{S7})$$

$$f_t = \lambda \frac{\varepsilon_i^t (\varepsilon_j^t + \varepsilon_k^t) (2 + \cos(\theta_{ijk}))^{l_t}}{r_{ij}^{m_t} \cdot r_{ik}^{m_t} \cdot r_{jk}^{m_t}} f_c(r_{ij}) f_c(r_{ik}) f_c(r_{jk}) \quad (\text{S8})$$

$$f_c(r_{ij}) = 0.5 * \left(1 - \tanh \left(\alpha (r_{ij} - (r_{\text{cut}} - \beta)) \right) \right) \quad (\text{S9})$$

where ε_i^k generated from the NN act as the parameters; na is the total atom number of atoms in the system; ns, nd, and nt are the number of single-body, two-body, three-body functions in the MBNN architecture, respectively (with s, d and t are function indices). λ , m_d , m_t and l_t are adjustable parameters of these functions. The f_c in all the equations is the cut-off function with the cut-off radius r_{cut} and the adjustable parameters α and β , as defined in Eq. S9.

The atomic force in the MBNN architecture is analytically derived based on Eq. S5, where the force component F_u acting on the atom u is the derivative of the total energy with respect to its coordinate vector \mathbf{r}_u . This is further related to the derivatives of the atomic coefficients ε_i^k and the pairwise distance r_{iu} .



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

Construction of the global dataset using SSW-NN

The stochastic surface walking (SSW) global optimization is utilized to construct the global dataset. The SSW global optimization can rapidly generate a global dataset, incorporating different structural patterns on the global potential energy surface (PES), as demonstrated in previous works⁷⁻⁹. The fully automated SSW PES search does not require prior knowledge of the system, such as the structure motif (e.g., bonding patterns, symmetry) of materials. A brief description of the Rh-Mn-C-H-O global dataset is provided in Table S1. The G-NN dataset and potential can be openly downloaded from http://www.lasphub.com/supportings/Trainfile_RhMnCHO.tar.gz and <http://www.lasphub.com/supportings/RhMnCHO.pot>.

Briefly, the global dataset is constructed following three stages by using the

SSW-NN method, as described below.

- (i) **The first stage** constructs a raw dataset. This dataset contains the most common atomic environments and serves as the training dataset for building an initial NN PES. This construction is done by performing density functional theory (DFT) SSW global optimization in a massively parallel manner. To speed up the SSW search, the DFT calculations are typically performed with low accuracy setups and restricted to small unit cells. After collecting and screening the structures from the SSW trajectories, a raw dataset is finally obtained. The low accuracy calculations use a setup with 300 eV kinetics energy cutoff and 15 \AA^{-1} k -point auto-mesh (15 \AA^{-1} auto-mesh means that the first Brillouin zone k -point sampling adopted the Monkhorst-Pack scheme with an automated mesh determined by 15 times the reciprocal lattice vectors).
- (ii) **The second stage** involves training an NN global PES. This is accomplished by first refining the dataset using DFT calculations with high accuracy setups (450 eV kinetics energy cutoff and 25 \AA^{-1} k -point auto-mesh). Subsequently, the NN is trained on the accurate global dataset. In this stage, the NN architecture employs a small scale of structural descriptors and a small network size.
- (iii) **The third stage** expands the global dataset in an iterative manner, aiming to enhance the predictive power of the NN PES by incorporating more structural patterns. This is achieved through an SSW PES search using the NN potential obtained in the second stage, starting from a variety of initial structures. These initial structures are typically randomly configured and include large systems with a substantial number of atoms per unit cell. Structures from all SSW trajectories are collected and filtered to generate the additional dataset. This new dataset is then added to the global dataset, initiating a new cycle of NN training starting again from stage 2.

Table S1. Structure information of the global PES dataset for Rh-Mn-C-H-O G-NN potential training. The listed data is the number of structures in the dataset, as distinguished by the chemical formula, the number of atoms per cell (N_{atom}) and the type of structure, including cluster (N_{cluster}), layer (N_{layer}) and bulk (N_{bulk}). The total numbers of the structure (N_{total}) are also summarized.

Species	N_{atom}	N_{cluster}	N_{layer}	N_{bulk}	N_{total}
Rh4	4	0	0	18	18
Rh16	16	199	1	765	965
Rh31	31	0	0	4	4
Rh32	32	0	0	72	72
Rh38	38	859	0	0	859
Rh76	76	0	3	0	3
Mn1-Rh23	24	0	13	0	13

Mn1-Rh31	32	0	37	23	60
Mn1-Rh59	60	0	63	11	74
Mn1-Rh60	61	0	53	45	98
Mn1-Rh61	62	0	73	25	98
Mn2-Rh30	32	0	4	0	4
Mn2-Rh59	61	0	56	5	61
Mn2-Rh62	64	0	0	12	12
Mn3-Rh29	32	0	17	14	31
Mn3-Rh57	60	0	87	23	110
Mn3-Rh58	61	0	66	14	80
Mn4	4	0	308	18	326
Mn4-Rh28	32	0	8	18	26
Mn4-Rh58	62	0	73	14	87
Mn4-Rh60	64	0	0	37	37
Mn5-Rh27	32	0	9	13	22
Mn5-Rh57	62	0	19	6	25
Mn6-Rh26	32	0	6	1	7
Mn6-Rh58	64	0	0	32	32
Mn7-Rh25	32	0	12	0	12
Mn7-Rh53	60	0	33	7	40
Mn8-Rh24	32	0	14	0	14
Mn8-Rh53	61	0	12	2	14
Mn8-Rh54	62	0	133	41	174
Mn8-Rh56	64	0	0	8	8
Mn9-Rh23	32	0	11	1	12
Mn10-Rh22	32	0	50	17	67
Mn10-Rh48	58	0	60	20	80
Mn10-Rh52	62	0	83	4	87
Mn10-Rh54	64	0	0	46	46
Mn11-Rh21	32	0	32	2	34
Mn11-Rh49	60	0	34	16	50
Mn12-Rh19	31	0	2	1	3
Mn12-Rh20	32	0	108	41	149
Mn12-Rh52	64	0	0	17	17
Mn13-Rh18	31	0	0	1	1
Mn13-Rh19	32	0	3	0	3
Mn13-Rh48	61	4	91	31	126
Mn14-Rh17	31	0	96	27	123
Mn14-Rh18	32	0	94	33	127
Mn14-Rh45	59	7	63	25	95
Mn14-Rh50	64	0	0	13	13
Mn15-Rh16	31	0	1	1	2
Mn15-Rh17	32	0	7	0	7
Mn16	16	0	636	213	849

Mn16-Rh15	31	0	32	26	58
Mn16-Rh16	32	0	191	61	252
Mn16-Rh48	64	0	0	12	12
Mn17-Rh15	32	0	29	23	52
Mn17-Rh43	60	0	58	13	71
Mn17-Rh44	61	3	47	20	70
Mn18-Rh13	31	0	25	9	34
Mn18-Rh14	32	0	1	0	1
Mn19-Rh42	61	4	39	22	65
Mn20-Rh11	31	0	2	0	2
Mn20-Rh12	32	0	22	7	29
Mn20-Rh40	60	0	58	33	91
Mn20-Rh41	61	4	110	24	138
Mn21-Rh11	32	0	1	0	1
Mn21-Rh40	61	6	123	15	144
Mn22-Rh10	32	0	0	1	1
Mn22-Rh36	58	7	26	12	45
Mn22-Rh42	64	0	0	27	27
Mn23-Rh9	32	0	3	0	3
Mn23-Rh38	61	7	14	16	37
Mn23-Rh39	62	0	18	9	27
Mn24-Rh7	31	0	1	0	1
Mn24-Rh8	32	0	5	4	9
Mn24-Rh34	58	0	13	17	30
Mn24-Rh40	64	0	0	18	18
Mn25-Rh7	32	0	11	3	14
Mn25-Rh36	61	11	16	4	31
Mn25-Rh37	62	0	41	8	49
Mn28-Rh4	32	0	6	4	10
Mn29-Rh33	62	0	11	1	12
Mn30-Rh2	32	0	2	0	2
Mn30-Rh31	61	13	4	0	17
Mn30-Rh32	62	0	5	2	7
Mn30-Rh34	64	0	0	1	1
Mn31	31	0	2	0	2
Mn31-Rh1	32	0	1	5	6
Mn32	32	0	12	17	29
Mn32-Rh30	62	0	2	1	3
Mn32-Rh32	64	0	0	2	2
Mn33-Rh28	61	21	2	0	23
Mn34-Rh25	59	0	1	0	1
Mn34-Rh27	61	23	5	0	28
Mn35-Rh26	61	14	7	0	21
Mn37-Rh24	61	6	2	0	8

Mn38-Rh24	62	0	3	0	3
Mn40-Rh21	61	13	3	0	16
Mn42-Rh17	59	8	3	0	11
Mn42-Rh19	61	12	2	1	15
Mn43-Rh17	60	0	4	1	5
Mn46-Rh16	62	0	0	2	2
Mn47-Rh13	60	0	1	0	1
Mn48-Rh12	60	0	0	3	3
Mn50-Rh12	62	0	1	0	1
Mn50-Rh14	64	0	0	1	1
Mn51-Rh10	61	3	3	0	6
Mn52-Rh9	61	2	5	0	7
Mn54-Rh10	64	0	0	1	1
Mn56-Rh3	59	0	0	1	1
Mn56-Rh6	62	0	0	1	1
Mn56-Rh8	64	0	0	2	2
Mn57-Rh3	60	0	1	0	1
Mn58-Rh3	61	0	1	0	1
Mn58-Rh6	64	0	0	6	6
Mn59-Rh1	60	0	0	1	1
Mn59-Rh2	61	0	3	0	3
Mn62-Rh2	64	0	0	2	2
Mn64	64	0	0	6	6
O1-Rh12	13	0	51	0	51
O1-Mn1-Rh11	13	0	2	0	2
O1-Mn1-Rh23	25	0	26	0	26
O1-Mn3-Rh61	65	0	45	0	45
O2-Rh10	12	0	37	0	37
O2-Mn1-Rh9	12	0	1	0	1
O2-Mn1-Rh14	17	0	8	9	17
O2-Mn2-Rh13	17	0	17	17	34
O2-Mn3-Rh27	32	0	1	28	29
O3-Rh16	19	21	0	0	21
O3-Mn1-Rh15	19	2	0	0	2
O3-Mn3-Rh27	33	0	0	107	107
O4	4	0	37	0	37
O4-Rh40	44	0	0	1	1
O4-Rh48	52	0	0	5	5
O5-Rh27	32	0	1	12	13
O5-Mn2-Rh25	32	0	0	1	1
O5-Mn3-Rh24	32	0	0	1	1
O6-Rh4	10	0	19	75	94
O6-Rh20	26	0	0	1	1
O6-Rh40	46	0	10	17	27

06-Mn1-Rh3	10	0	1	3	4
06-Mn1-Rh39	46	0	0	1	1
06-Mn2-Rh38	46	0	0	10	10
06-Mn4-Rh36	46	0	0	1	1
07-Rh20	27	0	0	1	1
07-Mn7-Rh57	71	0	36	0	36
08-Rh4	12	0	838	4181	5019
08-Rh6	14	0	0	9	9
08-Rh8	16	17	1	45	63
08-Rh16	24	35	0	0	35
08-Rh20	28	0	0	3	3
08-Mn1-Rh3	12	0	58	181	239
08-Mn1-Rh5	14	0	1	2	3
08-Mn1-Rh7	16	2	0	1	3
08-Mn1-Rh15	24	1	0	0	1
08-Mn2-Rh2	12	0	4	13	17
08-Mn2-Rh14	24	1	0	0	1
08-Mn3-Rh13	24	1	0	0	1
09-Rh20	29	0	0	11	11
09-Rh23	32	0	1	7	8
09-Mn1-Rh19	29	0	0	4	4
09-Mn2-Rh21	32	0	0	1	1
010-Rh6	16	0	3	15	18
010-Rh20	30	0	0	27	27
010-Rh40	50	0	0	5	5
010-Mn1-Rh19	30	0	0	1	1
010-Mn10-Rh54	74	0	66	0	66
011	11	0	179	98	277
012-Rh20	32	0	1	5	6
012-Rh30	42	0	0	3	3
012-Rh64	76	0	0	1	1
012-Mn2-Rh28	42	0	0	2	2
014-Rh7	21	0	4	19	23
014-Rh20	34	0	0	1	1
014-Mn1-Rh6	21	0	1	1	2
014-Mn2-Rh5	21	0	0	1	1
016-Rh16	32	17	0	13	30
016-Rh20	36	0	0	2	2
016-Rh32	48	0	2	4	6
016-Mn1-Rh15	32	1	0	0	1
017-Rh20	37	0	0	5	5
018-Rh7	25	0	16	35	51
018-Rh8	26	0	11	23	34
018-Rh9	27	0	1	21	22

018-Rh12	30	0	2	37	39
018-Rh20	38	0	0	8	8
018-Rh36	54	0	27	20	47
018-Rh40	58	0	18	28	46
018-Rh46	64	0	0	8	8
018-Mn1-Rh8	27	0	0	3	3
018-Mn1-Rh11	30	0	0	1	1
018-Mn1-Rh35	54	0	0	3	3
018-Mn1-Rh39	58	0	1	1	2
018-Mn1-Rh45	64	0	0	1	1
018-Mn2-Rh5	25	0	0	1	1
018-Mn2-Rh10	30	0	1	2	3
018-Mn2-Rh34	54	0	1	2	3
018-Mn2-Rh38	58	0	3	0	3
018-Mn2-Rh44	64	0	0	3	3
018-Mn3-Rh37	58	0	0	2	2
018-Mn4-Rh36	58	0	0	1	1
019-Rh20	39	0	0	4	4
020-Rh12	32	0	0	1	1
020-Rh20	40	0	0	20	20
020-Mn1-Rh19	40	0	0	3	3
020-Mn2-Rh18	40	0	1	4	5
020-Mn4-Rh16	40	0	0	1	1
021-Rh20	41	0	29	42	71
021-Mn1-Rh19	41	0	1	4	5
021-Mn2-Rh18	41	0	2	6	8
021-Mn3-Rh17	41	0	0	1	1
022-Rh18	40	0	28	26	54
022-Rh20	42	0	0	22	22
022-Rh40	62	0	20	35	55
022-Mn1-Rh17	40	0	0	2	2
022-Mn1-Rh19	42	0	0	2	2
022-Mn1-Rh39	62	0	3	1	4
022-Mn2-Rh16	40	0	0	1	1
022-Mn2-Rh38	62	0	1	3	4
023-Rh20	43	0	0	2	2
023-Mn1-Rh19	43	0	1	1	2
024-Rh16	40	0	0	4	4
024-Rh20	44	0	0	16	16
024-Mn2-Rh18	44	0	0	1	1
026-Rh20	46	0	0	1	1
028-Rh14	42	0	0	1	1
028-Rh20	48	0	0	7	7
029-Rh19	48	0	0	1	1

029-Rh20	49	0	0	1	1
030-Rh20	50	0	0	7	7
030-Rh34	64	0	0	3	3
030-Rh40	70	0	28	19	47
030-Mn1-Rh39	70	0	1	1	2
030-Mn2-Rh32	64	0	0	1	1
030-Mn2-Rh38	70	0	2	1	3
031-Rh20	51	0	23	31	54
031-Mn1-Rh19	51	0	0	3	3
031-Mn2-Rh18	51	0	0	1	1
031-Mn3-Rh17	51	0	3	3	6
031-Mn4-Rh16	51	0	0	1	1
032-Rh16	48	26	46	164	236
032-Rh20	52	0	15	42	57
032-Rh32	64	0	0	4	4
032-Rh40	72	0	9	11	20
032-Mn1-Rh15	48	3	0	12	15
032-Mn1-Rh19	52	0	1	0	1
032-Mn1-Rh39	72	0	1	0	1
032-Mn2-Rh14	48	0	1	3	4
032-Mn2-Rh18	52	0	1	1	2
033-Rh18	51	0	15	21	36
033-Rh20	53	0	0	4	4
033-Mn2-Rh16	51	0	0	1	1
034-Rh20	54	0	21	57	78
034-Mn1-Rh19	54	0	0	1	1
034-Mn2-Rh18	54	0	0	1	1
034-Mn3-Rh17	54	0	0	1	1
034-Mn4-Rh16	54	0	0	1	1
035-Rh20	55	0	39	44	83
035-Mn1-Rh19	55	0	3	3	6
035-Mn2-Rh18	55	0	4	0	4
035-Mn3-Rh17	55	0	1	0	1
036-Rh18	54	0	1	4	5
036-Rh20	56	0	12	23	35
036-Rh24	60	0	0	2	2
036-Mn1-Rh17	54	0	0	1	1
036-Mn1-Rh19	56	0	1	0	1
036-Mn3-Rh17	56	0	0	1	1
038-Rh20	58	0	0	16	16
038-Mn1-Rh19	58	0	0	1	1
039-Rh18	57	0	23	30	53
039-Mn1-Rh17	57	0	1	4	5
039-Mn2-Rh16	57	0	0	1	1

O40-Rh20	60	0	32	18	50
O40-Rh24	64	0	0	2	2
O40-Mn1-Rh19	60	0	3	1	4
O41-Rh20	61	0	23	24	47
O41-Mn1-Rh19	61	0	1	2	3
O41-Mn2-Rh18	61	0	2	1	3
O44-Rh16	60	0	24	31	55
O44-Rh17	61	0	1	46	47
O44-Rh18	62	0	18	10	28
O44-Rh19	63	0	13	21	34
O44-Rh20	64	0	19	25	44
O44-Mn1-Rh15	60	0	2	2	4
O44-Mn1-Rh16	61	0	0	2	2
O44-Mn1-Rh17	62	0	2	5	7
O44-Mn1-Rh18	63	0	1	0	1
O44-Mn1-Rh19	64	0	1	5	6
O44-Mn2-Rh15	61	0	0	3	3
O44-Mn2-Rh16	62	0	0	1	1
O44-Mn2-Rh17	63	0	1	0	1
O44-Mn2-Rh18	64	0	0	1	1
O44-Mn3-Rh14	61	0	0	1	1
O44-Mn3-Rh16	63	0	0	3	3
O45-Rh16	61	0	0	2	2
O46-Rh20	66	0	1	0	1
C1-Rh12	13	0	131	0	131
C1-Rh18	19	0	0	104	104
C1-Mn1-Rh11	13	0	5	11	16
C1-Mn1-Rh17	19	0	0	11	11
C1-Mn1-Rh23	25	0	36	0	36
C1-Mn2-Rh10	13	0	3	0	3
C1-Mn2-Rh16	19	0	0	5	5
C1-Mn3-Rh15	19	0	0	1	1
C1-O1-Rh48	50	0	14	0	14
C1-O1-Mn1-Rh23	26	0	85	2	87
C1-O1-Mn4-Rh44	50	0	14	0	14
C2-Rh10	12	0	153	0	153
C2-Rh17	19	0	1	257	258
C2-Rh25	27	0	0	44	44
C2-Rh29	31	0	5	77	82
C2-Mn1-Rh9	12	0	8	16	24
C2-Mn1-Rh16	19	0	0	25	25
C2-Mn1-Rh24	27	0	0	4	4
C2-Mn1-Rh28	31	0	1	5	6
C2-Mn2-Rh8	12	0	1	0	1

C2-Mn2-Rh15	19	0	0	15	15
C2-Mn2-Rh27	31	0	0	7	7
C2-Mn3-Rh14	19	0	0	1	1
C2-Mn3-Rh22	27	0	0	1	1
C2-Mn3-Rh26	31	0	1	1	2
C2-Mn4-Rh25	31	0	0	2	2
C2-O1-Rh48	51	0	16	0	16
C2-O1-Mn1-Rh23	27	0	12	0	12
C2-O1-Mn4-Rh44	51	0	887	0	887
C3-Rh16	19	14	0	0	14
C3-Mn1-Rh15	19	2	0	0	2
C4-Rh8	12	0	0	435	435
C4-Rh25	29	0	2	40	42
C4-Mn1-Rh7	12	0	0	69	69
C4-Mn1-Rh24	29	0	0	3	3
C4-Mn2-Rh6	12	0	0	1	1
C4-Mn2-Rh23	29	0	0	2	2
C4-Mn3-Rh22	29	0	1	0	1
C6-Rh10	16	0	6	87	93
C6-Rh25	31	0	154	101	255
C6-Mn1-Rh9	16	0	0	4	4
C6-Mn1-Rh24	31	0	2	4	6
C6-Mn2-Rh8	16	0	0	1	1
C6-Mn2-Rh23	31	0	5	3	8
C6-Mn3-Rh22	31	0	5	1	6
C6-Mn4-Rh21	31	0	1	0	1
C7-Rh16	23	0	1	320	321
C7-Mn1-Rh15	23	0	1	26	27
C7-Mn2-Rh14	23	0	0	6	6
C7-Mn3-Rh13	23	0	0	2	2
C8	8	0	48	331	379
C8-Rh16	24	7	0	0	7
C8-Mn2-Rh14	24	1	0	0	1
C10-Rh13	23	0	0	131	131
C10-Mn1-Rh12	23	0	0	12	12
C10-Mn2-Rh11	23	0	0	3	3
C10-Mn3-Rh10	23	0	0	4	4
C12-Rh50	62	0	1	0	1
H1-Rh15	16	0	0	320	320
H1-Rh16	17	0	0	1	1
H1-Rh23	24	0	28	16	44
H1-Rh26	27	0	73	0	73
H1-Rh27	28	0	29	0	29
H1-Rh31	32	1	0	14	15

H1-Rh38	39	726	0	0	726
H1-Mn1-Rh14	16	0	1	19	20
H1-Mn1-Rh22	24	0	4	3	7
H1-Mn1-Rh23	25	0	37	0	37
H1-Mn1-Rh25	27	0	2	1	3
H1-Mn1-Rh26	28	0	2	0	2
H1-Mn2-Rh13	16	0	0	5	5
H1-Mn2-Rh21	24	0	1	1	2
H1-Mn2-Rh24	27	0	2	0	2
H1-Mn2-Rh25	28	0	1	0	1
H1-Mn2-Rh29	32	0	0	2	2
H1-Mn3-Rh12	16	0	1	2	3
H1-Mn3-Rh23	27	0	2	0	2
H1-Mn3-Rh28	32	0	0	3	3
H1-Mn4-Rh22	27	0	2	0	2
H1-O1-Rh48	50	0	104	0	104
H1-O1-Rh64	66	0	79	0	79
H1-O1-Mn4-Rh44	50	0	15	0	15
H1-C1-Rh48	50	0	11	0	11
H1-C1-Mn1-Rh23	26	0	21	0	21
H1-C1-Mn4-Rh44	50	0	8	0	8
H1-C1-O1-Rh48	51	0	59	0	59
H1-C1-O1-Mn1-Rh23	27	0	129	6	135
H1-C1-O1-Mn4-Rh44	51	0	61	0	61
H1-C2-O1-Rh48	52	0	111	0	111
H1-C2-O1-Mn4-Rh44	52	0	1308	0	1308
H1-C5-Rh18	24	0	0	125	125
H1-C5-Mn1-Rh17	24	0	0	5	5
H1-C5-Mn3-Rh15	24	0	0	1	1
H2	2	1	0	0	1
H2-Rh14	16	0	65	548	613
H2-Rh16	18	0	0	1	1
H2-Rh21	23	0	0	121	121
H2-Rh22	24	0	25	0	25
H2-Rh27	29	3	51	69	123
H2-Rh28	30	0	55	0	55
H2-Rh30	32	1	0	14	15
H2-Rh38	40	648	0	0	648
H2-Rh76	78	0	5	0	5
H2-Mn1-Rh13	16	0	3	32	35
H2-Mn1-Rh20	23	0	0	3	3
H2-Mn1-Rh21	24	0	2	0	2
H2-Mn1-Rh26	29	1	2	5	8
H2-Mn1-Rh27	30	0	5	2	7

H2-Mn1-Rh29	32	0	0	1	1
H2-Mn2-Rh12	16	0	3	18	21
H2-Mn2-Rh19	23	0	1	8	9
H2-Mn2-Rh25	29	0	0	5	5
H2-Mn2-Rh26	30	0	1	0	1
H2-Mn2-Rh28	32	0	1	1	2
H2-Mn3-Rh11	16	0	0	4	4
H2-Mn3-Rh18	23	0	0	1	1
H2-Mn3-Rh24	29	0	1	7	8
H2-Mn4-Rh26	32	0	0	1	1
H2-O1-Rh27	30	0	457	81	538
H2-O1-Rh48	51	0	13	0	13
H2-O1-Mn1-Rh26	30	0	38	19	57
H2-O1-Mn2-Rh25	30	0	17	11	28
H2-O1-Mn3-Rh24	30	0	10	2	12
H2-O1-Mn4-Rh23	30	0	6	4	10
H2-O1-Mn4-Rh44	51	0	16	0	16
H2-O2-Rh64	68	0	18	0	18
H2-O4-Mn4-Rh44	54	0	20	0	20
H2-O5-Rh23	30	0	3	0	3
H2-O6-Rh22	30	0	1	0	1
H2-O6-Mn1-Rh21	30	0	4	0	4
H2-O7-Rh21	30	0	1	0	1
H2-O8-Rh20	30	0	3	0	3
H2-O8-Mn2-Rh18	30	0	1	0	1
H2-O13-Rh15	30	0	7	0	7
H2-O14-Rh14	30	0	11	0	11
H2-O15-Rh13	30	0	4	0	4
H2-O16-Rh12	30	0	3	0	3
H2-O17-Rh11	30	0	2	0	2
H2-O20-Rh8	30	0	3	0	3
H2-O20-Mn1-Rh7	30	0	1	0	1
H2-O22-Rh6	30	0	1	0	1
H2-O24-Rh4	30	0	4	0	4
H2-C1	3	4	0	0	4
H2-C1-Rh48	51	0	30	0	30
H2-C1-Mn1-Rh23	27	0	71	0	71
H2-C1-Mn4-Rh44	51	0	15	0	15
H2-C1-O1	4	102	0	0	102
H2-C1-O1-Rh48	52	0	62	0	62
H2-C1-O1-Mn4-Rh44	52	0	35	0	35
H2-C1-O2	5	38	0	0	38
H2-C1-O2-Rh12	17	0	302	9	311
H2-C1-O2-Rh16	21	0	252	0	252

H2-C1-02-Rh20	25	0	99	0	99
H2-C1-02-Rh27	32	0	1	0	1
H2-C1-02-Rh36	41	0	358	0	358
H2-C1-02-Mn1-Rh11	17	0	29	4	33
H2-C1-02-Mn1-Rh15	21	0	21	10	31
H2-C1-02-Mn1-Rh19	25	0	6	0	6
H2-C1-02-Mn1-Rh35	41	0	16	0	16
H2-C1-02-Mn2-Rh10	17	0	2	1	3
H2-C1-02-Mn2-Rh14	21	0	12	0	12
H2-C1-02-Mn2-Rh18	25	0	2	0	2
H2-C1-02-Mn2-Rh34	41	0	18	3	21
H2-C1-02-Mn3-Rh13	21	0	1	0	1
H2-C1-02-Mn3-Rh33	41	0	11	1	12
H2-C1-02-Mn4-Rh32	41	0	2	0	2
H2-C1-03	6	11	0	0	11
H2-C1-03-Rh36	42	0	82	0	82
H2-C1-03-Mn1-Rh35	42	0	2	0	2
H2-C1-03-Mn2-Rh34	42	0	2	0	2
H2-C2	4	86	0	0	86
H2-C2-Rh18	22	0	0	122	122
H2-C2-Mn1-Rh17	22	0	0	7	7
H2-C2-Mn2-Rh16	22	0	0	2	2
H2-C2-Mn3-Rh15	22	0	0	2	2
H2-C2-01-Rh48	53	0	101	0	101
H2-C2-01-Mn4-Rh44	53	0	705	0	705
H2-C2-03-Rh26	33	0	19	0	19
H2-C2-03-Rh27	34	0	91	1	92
H2-C2-03-Rh36	43	0	3	0	3
H2-C2-03-Mn1-Rh26	34	0	3	1	4
H2-C2-03-Mn2-Rh24	33	0	2	3	5
H2-C2-03-Mn2-Rh25	34	0	4	0	4
H2-C2-03-Mn3-Rh23	33	0	1	0	1
H2-C2-03-Mn3-Rh24	34	0	2	0	2
H2-C2-03-Mn4-Rh23	34	0	1	0	1
H2-C3-Rh17	22	0	0	177	177
H2-C3-Mn1-Rh16	22	0	1	10	11
H2-C3-Mn2-Rh15	22	0	0	5	5
H2-C3-Mn3-Rh14	22	0	0	1	1
H2-C3-02-Rh25	32	0	4	0	4
H2-C3-02-Rh26	33	0	114	0	114
H2-C3-02-Rh27	34	0	98	0	98
H2-C3-02-Mn1-Rh25	33	0	9	2	11
H2-C3-02-Mn1-Rh26	34	0	15	13	28
H2-C3-02-Mn2-Rh24	33	0	6	0	6

H2-C3-02-Mn2-Rh25	34	0	4	3	7
H2-C3-02-Mn4-Rh22	33	0	1	0	1
H2-C3-04-Rh33	42	0	272	4	276
H2-C3-04-Rh35	44	0	301	3	304
H2-C3-04-Rh36	45	0	507	10	517
H2-C3-04-Mn1-Rh32	42	0	1	0	1
H2-C3-04-Mn1-Rh34	44	0	1	0	1
H2-C3-04-Mn2-Rh33	44	0	1	0	1
H2-C3-04-Mn4-Rh31	44	0	1	0	1
H2-C4-Rh18	24	0	0	138	138
H2-C4-Rh23	29	0	0	108	108
H2-C4-Mn1-Rh17	24	0	0	11	11
H2-C4-Mn1-Rh22	29	0	0	8	8
H2-C4-Mn2-Rh16	24	0	0	2	2
H2-C4-Mn2-Rh21	29	0	0	5	5
H2-C4-Mn3-Rh20	29	0	0	7	7
H2-C4-01-Rh26	33	0	18	0	18
H2-C4-01-Rh27	34	0	114	1	115
H2-C4-01-Mn1-Rh25	33	0	1	0	1
H2-C4-01-Mn1-Rh26	34	0	6	2	8
H2-C4-01-Mn2-Rh25	34	0	6	0	6
H2-C4-01-Mn3-Rh24	34	0	1	0	1
H2-C4-01-Mn4-Rh23	34	0	3	0	3
H2-C4-02-Rh25	33	0	34	0	34
H2-C4-02-Mn1-Rh24	33	0	1	0	1
H2-C4-02-Mn2-Rh23	33	0	1	0	1
H2-C4-03	9	60	0	0	60
H2-C4-04	10	2	0	0	2
H2-C4-05	11	8	0	0	8
H2-C5-Rh18	25	0	0	129	129
H2-C5-Mn1-Rh17	25	0	0	13	13
H2-C5-Mn2-Rh16	25	0	0	7	7
H2-C5-Mn3-Rh15	25	0	0	1	1
H2-C5-03	10	6	0	0	6
H2-C5-04	11	4	0	0	4
H2-C6-Rh16	24	0	0	173	173
H2-C6-Mn1-Rh15	24	0	0	16	16
H2-C6-Mn2-Rh14	24	0	0	10	10
H2-C6-Mn3-Rh13	24	0	0	2	2
H2-C6-02	10	2	0	0	2
H2-C7-Rh13	22	0	0	137	137
H2-C7-Rh18	27	0	1	300	301
H2-C7-Mn1-Rh12	22	0	0	12	12
H2-C7-Mn1-Rh17	27	0	1	26	27

H2-C7-Mn2-Rh11	22	0	0	7	7
H2-C7-Mn2-Rh16	27	0	0	12	12
H2-C7-Mn3-Rh15	27	0	0	10	10
H2-C7-O1	10	2	0	0	2
H2-C9-Rh13	24	0	0	141	141
H2-C9-Rh16	27	0	0	119	119
H2-C9-Mn1-Rh12	24	0	2	12	14
H2-C9-Mn1-Rh15	27	0	0	10	10
H2-C9-Mn2-Rh11	24	0	0	4	4
H2-C9-Mn2-Rh14	27	0	0	8	8
H2-C9-Mn4-Rh12	27	0	0	1	1
H3-Rh16	19	0	0	1	1
H3-Rh26	29	0	106	0	106
H3-Rh28	31	1	0	10	11
H3-Rh29	32	0	0	20	20
H3-Rh38	41	201	0	0	201
H3-Mn1-Rh25	29	0	5	3	8
H3-Mn1-Rh27	31	1	0	0	1
H3-Mn1-Rh28	32	0	0	1	1
H3-Mn2-Rh24	29	0	2	0	2
H3-Mn3-Rh23	29	0	2	0	2
H3-Mn3-Rh26	32	0	0	1	1
H3-Mn4-Rh24	31	0	0	1	1
H3-O3-Rh48	54	0	68	0	68
H3-O4-Mn4-Rh44	55	0	38	0	38
H3-C1	4	7	0	0	7
H3-C1-Rh48	52	0	21	0	21
H3-C1-Mn1-Rh23	28	0	85	0	85
H3-C1-Mn4-Rh44	52	0	15	0	15
H3-C1-O1-Rh15	20	0	468	7	475
H3-C1-O1-Rh16	21	0	438	6	444
H3-C1-O1-Rh20	25	0	91	0	91
H3-C1-O1-Rh48	53	0	29	0	29
H3-C1-O1-Mn1-Rh14	20	0	29	7	36
H3-C1-O1-Mn1-Rh15	21	0	21	4	25
H3-C1-O1-Mn1-Rh19	25	0	5	0	5
H3-C1-O1-Mn2-Rh13	20	0	13	4	17
H3-C1-O1-Mn2-Rh14	21	0	13	4	17
H3-C1-O1-Mn2-Rh18	25	0	1	0	1
H3-C1-O1-Mn3-Rh12	20	0	2	8	10
H3-C1-O1-Mn3-Rh13	21	0	5	13	18
H3-C1-O1-Mn4-Rh11	20	0	1	0	1
H3-C1-O1-Mn4-Rh44	53	0	40	0	40
H3-C1-O2-Rh15	21	0	215	0	215

H3-C1-02-Rh16	22	0	263	0	263
H3-C1-02-Rh36	42	0	146	0	146
H3-C1-02-Mn1-Rh14	21	0	14	0	14
H3-C1-02-Mn1-Rh15	22	0	18	11	29
H3-C1-02-Mn1-Rh35	42	0	10	0	10
H3-C1-02-Mn2-Rh13	21	0	5	0	5
H3-C1-02-Mn2-Rh14	22	0	5	0	5
H3-C1-02-Mn2-Rh34	42	0	1	0	1
H3-C1-02-Mn3-Rh13	22	0	4	4	8
H3-C1-02-Mn3-Rh33	42	0	11	3	14
H3-C1-02-Mn4-Rh12	22	0	1	0	1
H3-C1-03-Rh35	42	0	23	8	31
H3-C1-03-Mn2-Rh33	42	0	0	3	3
H3-C1-03-Mn3-Rh32	42	0	0	1	1
H3-C2-Rh22	27	0	0	133	133
H3-C2-Mn1-Rh21	27	0	0	11	11
H3-C2-Mn2-Rh20	27	0	0	11	11
H3-C2-Mn3-Rh19	27	0	0	3	3
H3-C2-Mn4-Rh18	27	0	0	1	1
H3-C2-01-Rh48	54	0	189	0	189
H3-C2-01-Mn1-Rh23	30	0	30	0	30
H3-C2-01-Mn4-Rh44	54	0	409	0	409
H3-C2-02-Rh26	33	0	14	0	14
H3-C2-02-Rh27	34	0	80	0	80
H3-C2-02-Rh36	43	0	3	0	3
H3-C2-02-Mn1-Rh25	33	0	1	0	1
H3-C2-02-Mn1-Rh26	34	0	3	0	3
H3-C2-02-Mn2-Rh24	33	0	2	0	2
H3-C2-02-Mn2-Rh25	34	0	2	0	2
H3-C2-02-Mn3-Rh24	34	0	3	0	3
H3-C2-03-Rh24	32	0	1	0	1
H3-C2-03-Rh34	42	0	148	0	148
H3-C2-03-Rh36	44	0	219	1	220
H3-C2-03-Mn1-Rh33	42	0	11	0	11
H3-C2-03-Mn1-Rh35	44	0	11	3	14
H3-C2-03-Mn2-Rh32	42	0	7	4	11
H3-C2-03-Mn2-Rh34	44	0	15	4	19
H3-C2-03-Mn3-Rh31	42	0	6	0	6
H3-C2-03-Mn3-Rh33	44	0	4	0	4
H3-C2-03-Mn4-Rh30	42	0	1	0	1
H3-C2-03-Mn4-Rh32	44	0	2	1	3
H3-C2-04-Rh32	41	0	17	4	21
H3-C2-04-Rh33	42	0	27	0	27
H3-C2-04-Rh35	44	0	108	2	110

H3-C2-04-Mn1-Rh34	44	0	3	0	3
H3-C2-04-Mn2-Rh30	41	0	1	0	1
H3-C2-04-Mn2-Rh31	42	0	1	0	1
H3-C2-04-Mn2-Rh33	44	0	4	0	4
H3-C2-04-Mn3-Rh29	41	0	0	1	1
H3-C2-04-Mn3-Rh32	44	0	1	0	1
H3-C2-04-Mn4-Rh31	44	0	1	0	1
H3-C3-01-Rh26	33	0	3	0	3
H3-C3-01-Rh27	34	0	56	3	59
H3-C3-01-Mn1-Rh26	34	0	5	0	5
H3-C3-01-Mn2-Rh25	34	0	1	0	1
H3-C3-01-Mn3-Rh24	34	0	1	0	1
H3-C3-02-Rh25	33	0	60	0	60
H3-C3-02-Mn1-Rh24	33	0	3	0	3
H3-C3-02-Mn2-Rh23	33	0	1	0	1
H3-C3-03-Rh35	44	0	114	1	115
H3-C3-03-Mn1-Rh34	44	0	4	3	7
H3-C3-03-Mn2-Rh33	44	0	3	0	3
H3-C3-03-Mn3-Rh32	44	0	3	0	3
H3-C3-03-Mn4-Rh31	44	0	1	0	1
H3-C6-Rh16	25	0	0	162	162
H3-C6-Rh22	31	0	0	68	68
H3-C6-Mn1-Rh15	25	0	0	8	8
H3-C6-Mn1-Rh21	31	0	0	4	4
H3-C6-Mn2-Rh14	25	0	0	5	5
H3-C6-Mn3-Rh13	25	0	0	1	1
H3-C6-Mn3-Rh19	31	0	0	1	1
H3-C8-Rh14	25	0	0	114	114
H3-C8-Mn1-Rh13	25	0	0	5	5
H3-C8-Mn2-Rh12	25	0	0	1	1
H3-C8-Mn3-Rh11	25	0	0	1	1
H4-Rh12	16	1880	0	232	2112
H4-Rh16	20	0	0	1	1
H4-Rh17	21	0	0	157	157
H4-Rh20	24	0	21	0	21
H4-Rh24	28	0	36	0	36
H4-Rh38	42	39	0	0	39
H4-Rh76	80	0	1	0	1
H4-Mn1-Rh11	16	97	8	38	143
H4-Mn1-Rh16	21	0	1	13	14
H4-Mn1-Rh19	24	0	2	0	2
H4-Mn1-Rh23	28	0	3	0	3
H4-Mn2-Rh10	16	32	1	16	49
H4-Mn2-Rh15	21	0	1	7	8

H4-Mn2-Rh22	28	0	1	0	1
H4-Mn3-Rh9	16	8	0	5	13
H4-Mn3-Rh21	28	0	2	0	2
H4-O4-Rh48	56	0	67	0	67
H4-O4-Mn4-Rh44	56	0	76	0	76
H4-C1	5	128	0	0	128
H4-C1-Rh36	41	0	293	0	293
H4-C1-Rh48	53	0	21	0	21
H4-C1-Mn1-Rh35	41	0	14	7	21
H4-C1-Mn2-Rh34	41	0	18	10	28
H4-C1-Mn3-Rh33	41	0	8	3	11
H4-C1-Mn4-Rh32	41	0	1	0	1
H4-C1-Mn4-Rh44	53	0	13	0	13
H4-C1-O1	6	35	0	0	35
H4-C1-O1-Rh12	18	0	3	0	3
H4-C1-O1-Rh16	22	0	459	3	462
H4-C1-O1-Rh48	54	0	27	0	27
H4-C1-O1-Mn1-Rh15	22	0	25	0	25
H4-C1-O1-Mn2-Rh14	22	0	13	1	14
H4-C1-O1-Mn3-Rh13	22	0	2	0	2
H4-C1-O1-Mn4-Rh44	54	0	49	0	49
H4-C1-O2	7	0	7	0	7
H4-C1-O2-Rh36	43	0	40	0	40
H4-C1-O2-Mn1-Rh35	43	0	1	0	1
H4-C1-O3-Rh27	35	0	14	0	14
H4-C1-O3-Rh36	44	0	40	1	41
H4-C1-O3-Mn1-Rh26	35	0	2	0	2
H4-C1-O3-Mn1-Rh35	44	0	1	1	2
H4-C1-O3-Mn2-Rh34	44	0	1	0	1
H4-C1-O3-Mn3-Rh24	35	0	1	0	1
H4-C1-O3-Mn3-Rh33	44	0	1	0	1
H4-C2	6	34	0	0	34
H4-C2-O1	7	156	0	0	156
H4-C2-O1-Rh15	22	0	81	4	85
H4-C2-O1-Rh48	55	0	133	0	133
H4-C2-O1-Mn1-Rh14	22	0	4	1	5
H4-C2-O1-Mn1-Rh23	31	0	46	2	48
H4-C2-O1-Mn2-Rh13	22	0	1	0	1
H4-C2-O1-Mn3-Rh12	22	0	2	0	2
H4-C2-O1-Mn4-Rh44	55	0	510	0	510
H4-C2-O2	8	51	3	4	58
H4-C2-O2-Rh27	35	0	2	0	2
H4-C2-O2-Rh33	41	0	489	48	537
H4-C2-O2-Rh36	44	0	1	0	1

H4-C2-02-Mn1-Rh32	41	0	21	1	22
H4-C2-02-Mn2-Rh31	41	0	18	5	23
H4-C2-02-Mn3-Rh30	41	0	15	4	19
H4-C2-02-Mn4-Rh23	35	0	1	0	1
H4-C2-02-Mn4-Rh29	41	0	3	0	3
H4-C2-03-Rh32	41	0	81	17	98
H4-C2-03-Rh34	43	0	8	0	8
H4-C2-03-Rh36	45	0	1	0	1
H4-C2-03-Mn1-Rh31	41	0	3	0	3
H4-C2-03-Mn1-Rh33	43	0	1	0	1
H4-C2-03-Mn2-Rh30	41	0	2	4	6
H4-C2-03-Mn3-Rh29	41	0	3	1	4
H4-C2-04-Rh12	22	0	1	64	65
H4-C2-04-Rh24	34	0	2	0	2
H4-C2-04-Rh26	36	0	1	0	1
H4-C2-04-Rh36	46	0	595	0	595
H4-C2-04-Mn1-Rh11	22	0	0	3	3
H4-C2-04-Mn1-Rh25	36	0	1	0	1
H4-C2-04-Mn1-Rh35	46	0	37	11	48
H4-C2-04-Mn2-Rh34	46	0	19	1	20
H4-C2-04-Mn3-Rh9	22	0	0	1	1
H4-C2-04-Mn3-Rh33	46	0	17	1	18
H4-C2-04-Mn4-Rh32	46	0	3	0	3
H4-C3	7	52	0	0	52
H4-C3-01	8	12	0	0	12
H4-C3-02	9	1	0	0	1
H4-C3-05-Rh36	48	0	10	0	10
H4-C4	8	381	0	0	381
H4-C4-Rh16	24	0	0	182	182
H4-C4-Mn1-Rh15	24	0	0	9	9
H4-C4-Mn2-Rh14	24	0	0	10	10
H4-C4-02	10	6	0	0	6
H4-C4-03	11	2	0	0	2
H4-C4-04	12	4	0	0	4
H4-C4-04-Rh36	48	0	0	19	19
H4-C4-04-Mn2-Rh34	48	0	0	1	1
H4-C4-04-Mn3-Rh33	48	0	0	4	4
H4-C4-04-Mn4-Rh32	48	0	0	1	1
H4-C4-05	13	1	0	0	1
H4-C5-02	11	3	0	0	3
H4-C5-03	12	21	0	0	21
H4-C5-04	13	26	0	0	26
H4-C6-Rh14	24	0	0	110	110
H4-C6-Mn1-Rh13	24	0	0	10	10

H4-C6-Mn2-Rh12	24	0	0	4	4
H4-C6-01	11	7	0	0	7
H4-C6-02	12	21	0	0	21
H4-C6-03	13	46	0	0	46
H4-C7	11	3	0	0	3
H4-C7-01	12	6	0	0	6
H4-C7-02	13	54	0	0	54
H4-C8-Rh46	58	0	0	2	2
H4-C8-01	13	23	0	0	23
H4-C9	13	1	0	0	1
H5-Rh16	21	0	165	36	201
H5-Rh20	25	0	2	0	2
H5-Rh27	32	0	90	2	92
H5-Mn1-Rh15	21	0	13	1	14
H5-Mn1-Rh26	32	0	4	0	4
H5-Mn2-Rh14	21	0	3	2	5
H5-Mn2-Rh25	32	0	2	1	3
H5-Mn3-Rh17	25	0	1	0	1
H5-Mn3-Rh24	32	0	1	0	1
H5-C1-02-Rh35	43	0	452	37	489
H5-C1-02-Mn1-Rh34	43	0	28	3	31
H5-C1-02-Mn2-Rh33	43	0	22	6	28
H5-C1-02-Mn3-Rh32	43	0	7	0	7
H5-C1-02-Mn4-Rh31	43	0	4	9	13
H5-C1-03-Rh36	45	0	17	1	18
H5-C1-03-Mn1-Rh35	45	0	1	1	2
H5-C1-03-Mn3-Rh33	45	0	2	1	3
H5-C2-Rh21	28	0	0	124	124
H5-C2-Rh36	43	0	275	0	275
H5-C2-Mn1-Rh20	28	0	0	9	9
H5-C2-Mn1-Rh35	43	0	14	2	16
H5-C2-Mn2-Rh19	28	0	0	12	12
H5-C2-Mn2-Rh34	43	0	17	2	19
H5-C2-Mn3-Rh18	28	0	0	1	1
H5-C2-Mn3-Rh33	43	0	8	0	8
H5-C2-Mn4-Rh17	28	0	0	1	1
H5-C2-Mn4-Rh32	43	0	4	0	4
H5-C2-01-Rh48	56	0	85	0	85
H5-C2-01-Mn4-Rh44	56	0	88	0	88
H5-C2-02-Rh44	53	0	51	0	51
H5-C2-02-Mn1-Rh43	53	0	4	0	4
H5-C2-02-Mn2-Rh42	53	0	4	1	5
H5-C2-02-Mn3-Rh41	53	0	1	0	1
H5-C2-02-Mn4-Rh40	53	0	2	0	2

H5-C4-Rh19	28	0	0	297	297
H5-C4-Mn1-Rh18	28	0	0	27	27
H5-C4-Mn2-Rh17	28	0	0	14	14
H5-C4-Mn3-Rh16	28	0	0	1	1
H5-C6-Rh20	31	0	0	65	65
H5-C6-Mn1-Rh19	31	0	0	3	3
H5-C6-Mn2-Rh18	31	0	0	5	5
H5-C6-Mn3-Rh17	31	0	0	1	1
H6-Rh10	16	0	0	325	325
H6-Rh15	21	0	255	3	258
H6-Rh16	22	0	0	1	1
H6-Rh20	26	0	12	0	12
H6-Rh25	31	0	66	0	66
H6-Rh26	32	100	69	95	264
H6-Mn1-Rh9	16	0	0	20	20
H6-Mn1-Rh14	21	0	8	3	11
H6-Mn1-Rh24	31	0	3	0	3
H6-Mn1-Rh25	32	5	4	18	27
H6-Mn2-Rh8	16	0	0	6	6
H6-Mn2-Rh13	21	0	10	0	10
H6-Mn2-Rh24	32	4	1	2	7
H6-Mn3-Rh7	16	0	0	1	1
H6-Mn3-Rh12	21	0	1	0	1
H6-Mn3-Rh22	31	0	1	0	1
H6-Mn3-Rh23	32	0	2	1	3
H6-C1-01-Rh33	41	0	54	0	54
H6-C1-01-Rh35	43	0	128	0	128
H6-C1-01-Rh36	44	0	575	0	575
H6-C1-01-Mn1-Rh32	41	0	9	0	9
H6-C1-01-Mn1-Rh34	43	0	4	0	4
H6-C1-01-Mn1-Rh35	44	0	27	3	30
H6-C1-01-Mn2-Rh31	41	0	3	0	3
H6-C1-01-Mn2-Rh33	43	0	9	3	12
H6-C1-01-Mn2-Rh34	44	0	24	4	28
H6-C1-01-Mn3-Rh30	41	0	4	0	4
H6-C1-01-Mn3-Rh32	43	0	3	0	3
H6-C1-01-Mn3-Rh33	44	0	11	5	16
H6-C1-01-Mn4-Rh32	44	0	4	0	4
H6-C1-02-Rh36	45	0	751	10	761
H6-C1-02-Mn1-Rh35	45	0	40	6	46
H6-C1-02-Mn2-Rh34	45	0	44	21	65
H6-C1-02-Mn3-Rh33	45	0	22	4	26
H6-C1-02-Mn4-Rh32	45	0	10	0	10
H6-C1-03-Rh12	22	0	0	22	22

H6-C1-03-Rh36	46	0	77	5	82
H6-C1-03-Mn1-Rh11	22	0	0	2	2
H6-C1-03-Mn1-Rh35	46	0	3	0	3
H6-C1-03-Mn2-Rh10	22	0	0	1	1
H6-C1-03-Mn2-Rh34	46	0	2	0	2
H6-C1-03-Mn3-Rh33	46	0	3	0	3
H6-C2	8	290	0	0	290
H6-C2-Rh36	44	0	307	0	307
H6-C2-Mn1-Rh35	44	0	14	2	16
H6-C2-Mn2-Rh34	44	0	11	4	15
H6-C2-Mn3-Rh33	44	0	5	1	6
H6-C2-Mn4-Rh32	44	0	4	0	4
H6-C2-01	9	23	15	20	58
H6-C2-01-Rh45	54	0	83	0	83
H6-C2-01-Rh48	57	0	33	0	33
H6-C2-01-Mn1-Rh44	54	0	2	0	2
H6-C2-01-Mn2-Rh43	54	0	2	0	2
H6-C2-01-Mn3-Rh42	54	0	4	0	4
H6-C2-01-Mn4-Rh41	54	0	2	0	2
H6-C2-01-Mn4-Rh44	57	0	43	0	43
H6-C2-02-Rh30	40	0	55	10	65
H6-C2-02-Rh31	41	0	125	50	175
H6-C2-02-Rh32	42	0	836	152	988
H6-C2-02-Mn1-Rh29	40	0	3	1	4
H6-C2-02-Mn1-Rh30	41	0	7	1	8
H6-C2-02-Mn1-Rh31	42	0	57	22	79
H6-C2-02-Mn2-Rh28	40	0	5	0	5
H6-C2-02-Mn2-Rh29	41	0	6	7	13
H6-C2-02-Mn2-Rh30	42	0	31	10	41
H6-C2-02-Mn3-Rh28	41	0	5	6	11
H6-C2-02-Mn3-Rh29	42	0	32	11	43
H6-C2-02-Mn4-Rh27	41	0	1	0	1
H6-C2-02-Mn4-Rh28	42	0	5	2	7
H6-C3	9	88	0	0	88
H6-C3-01	10	2	0	0	2
H6-C3-01-Rh48	58	0	4	1	5
H6-C3-01-Rh64	74	0	218	2	220
H6-C3-02	11	60	0	0	60
H6-C4	10	114	0	0	114
H6-C4-Rh44	54	0	0	5	5
H6-C4-Mn1-Rh43	54	0	0	1	1
H6-C4-Mn3-Rh41	54	0	0	2	2
H6-C4-Mn4-Rh40	54	0	0	1	1
H6-C4-01-Rh64	75	0	30	0	30

H6-C4-02	12	1	0	0	1
H6-C4-02-Rh64	76	0	67	1	68
H6-C4-03	13	4	0	0	4
H6-C4-04	14	3	0	0	3
H6-C5-02	13	18	0	0	18
H6-C5-03	14	40	0	0	40
H6-C5-04	15	51	0	0	51
H6-C6	12	76	0	0	76
H6-C6-01	13	419	0	0	419
H6-C6-02	14	75	0	0	75
H6-C6-03	15	29	0	0	29
H6-C7-01	14	8	0	0	8
H6-C7-02	15	19	0	0	19
H6-C7-04	17	0	3	0	3
H6-C8	14	3	0	0	3
H6-C8-01	15	7	0	0	7
H6-C9	15	2	0	0	2
H7-Rh16	23	0	0	1	1
H7-Rh20	27	0	23	0	23
H7-Rh25	32	0	0	64	64
H7-Mn1-Rh19	27	0	2	0	2
H7-Mn1-Rh24	32	0	0	5	5
H7-Mn2-Rh18	27	0	2	0	2
H7-Mn3-Rh17	27	0	1	0	1
H7-Mn3-Rh22	32	0	0	6	6
H7-C1-04-Rh34	46	0	16	10	26
H7-C1-04-Rh36	48	0	24	12	36
H7-C1-04-Mn1-Rh33	46	0	3	1	4
H7-C1-04-Mn1-Rh35	48	0	1	2	3
H7-C1-04-Mn2-Rh32	46	0	0	3	3
H7-C1-04-Mn2-Rh34	48	0	0	1	1
H7-C2-Rh35	44	0	171	0	171
H7-C2-Rh36	45	0	570	0	570
H7-C2-Mn1-Rh34	44	0	8	2	10
H7-C2-Mn1-Rh35	45	0	30	9	39
H7-C2-Mn2-Rh33	44	0	6	0	6
H7-C2-Mn2-Rh34	45	0	32	2	34
H7-C2-Mn3-Rh32	44	0	2	0	2
H7-C2-Mn3-Rh33	45	0	20	1	21
H7-C2-Mn4-Rh31	44	0	3	0	3
H7-C2-Mn4-Rh32	45	0	4	0	4
H7-C2-02-Rh31	42	0	219	43	262
H7-C2-02-Rh32	43	0	212	34	246
H7-C2-02-Rh36	47	0	120	0	120

H7-C2-02-Mn1-Rh30	42	0	15	8	23
H7-C2-02-Mn1-Rh31	43	0	11	2	13
H7-C2-02-Mn1-Rh35	47	0	3	0	3
H7-C2-02-Mn2-Rh29	42	0	4	2	6
H7-C2-02-Mn2-Rh30	43	0	7	1	8
H7-C2-02-Mn2-Rh34	47	0	6	0	6
H7-C2-02-Mn3-Rh28	42	0	5	2	7
H7-C2-02-Mn3-Rh29	43	0	8	5	13
H7-C2-02-Mn3-Rh33	47	0	2	0	2
H7-C2-02-Mn4-Rh27	42	0	1	1	2
H7-C2-02-Mn4-Rh28	43	0	2	3	5
H7-C2-02-Mn4-Rh32	47	0	0	1	1
H7-C2-05-Rh34	48	0	2	36	38
H7-C2-05-Mn1-Rh33	48	0	0	7	7
H7-C2-05-Mn2-Rh32	48	0	0	2	2
H7-C2-05-Mn3-Rh31	48	0	0	1	1
H8-Rh8	16	2657	0	1303	3960
H8-Rh16	24	0	44	1	45
H8-Rh20	28	0	134	0	134
H8-Mn1-Rh7	16	131	3	88	222
H8-Mn1-Rh15	24	0	3	0	3
H8-Mn1-Rh19	28	0	8	1	9
H8-Mn2-Rh6	16	39	7	18	64
H8-Mn2-Rh18	28	0	2	2	4
H8-Mn3-Rh5	16	13	0	9	22
H8-Mn3-Rh13	24	0	0	1	1
H8-C1-01-Rh36	46	0	994	0	994
H8-C1-01-Mn1-Rh35	46	0	50	8	58
H8-C1-01-Mn2-Rh34	46	0	56	6	62
H8-C1-01-Mn3-Rh33	46	0	25	7	32
H8-C1-01-Mn4-Rh32	46	0	13	0	13
H8-C1-05-Rh36	50	0	32	24	56
H8-C1-05-Mn1-Rh35	50	0	2	8	10
H8-C1-05-Mn2-Rh34	50	0	3	1	4
H8-C1-05-Mn3-Rh33	50	0	2	0	2
H8-C1-05-Mn4-Rh32	50	0	2	1	3
H8-C2	10	0	1	0	1
H8-C2-Rh16	26	0	7	0	7
H8-C2-Rh37	47	0	10	0	10
H8-C2-Mn1-Rh36	47	0	1	0	1
H8-C2-Mn2-Rh35	47	0	1	0	1
H8-C2-O2	12	0	7	0	7
H8-C2-02-Rh23	35	0	1	0	1
H8-C2-02-Rh32	44	0	63	11	74

H8-C2-02-Rh36	48	0	604	0	604
H8-C2-02-Rh64	76	0	98	0	98
H8-C2-02-Rh72	84	0	352	0	352
H8-C2-02-Mn1-Rh31	44	0	4	2	6
H8-C2-02-Mn1-Rh35	48	0	3	0	3
H8-C2-02-Mn2-Rh30	44	0	5	15	20
H8-C2-02-Mn2-Rh34	48	0	17	7	24
H8-C2-02-Mn3-Rh29	44	0	2	0	2
H8-C2-02-Mn3-Rh33	48	0	7	0	7
H8-C2-02-Mn4-Rh28	44	0	1	0	1
H8-C2-03	13	0	6	0	6
H8-C2-04-Rh34	48	0	76	33	109
H8-C2-04-Rh35	49	0	34	19	53
H8-C2-04-Rh36	50	0	161	1	162
H8-C2-04-Mn1-Rh33	48	0	1	2	3
H8-C2-04-Mn1-Rh34	49	0	1	1	2
H8-C2-04-Mn1-Rh35	50	0	9	1	10
H8-C2-04-Mn2-Rh32	48	0	6	2	8
H8-C2-04-Mn2-Rh33	49	0	1	1	2
H8-C2-04-Mn2-Rh34	50	0	10	3	13
H8-C2-04-Mn3-Rh31	48	0	2	1	3
H8-C2-04-Mn3-Rh32	49	0	1	1	2
H8-C2-04-Mn3-Rh33	50	0	4	0	4
H8-C2-04-Mn4-Rh31	49	0	1	0	1
H8-C3	11	4	0	0	4
H8-C3-01-Rh36	48	0	119	0	119
H8-C3-01-Mn1-Rh35	48	0	6	0	6
H8-C3-01-Mn2-Rh34	48	0	2	0	2
H8-C3-01-Mn3-Rh33	48	0	3	0	3
H8-C3-01-Mn4-Rh32	48	0	1	0	1
H8-C3-03	14	2	0	0	2
H8-C3-03-Rh64	78	0	3	0	3
H8-C4-01	13	4	0	0	4
H8-C5-01	14	165	0	0	165
H8-C5-03	16	10	0	0	10
H8-C5-04	17	13	0	0	13
H8-C6-01	15	8	0	0	8
H8-C6-02	16	10	0	0	10
H8-C6-03	17	27	0	0	27
H8-C7	15	3	0	0	3
H8-C7-Rh21	36	0	84	1	85
H8-C7-Mn1-Rh20	36	0	4	1	5
H8-C7-Mn2-Rh19	36	0	1	0	1
H8-C7-01	16	11	0	0	11

H8-C7-02	17	54	0	0	54
H8-C7-03	18	0	3	4	7
H8-C8	16	6	0	0	6
H8-C8-01	17	53	0	0	53
H8-C8-02	18	2	0	0	2
H8-C8-03	19	0	6	2	8
H8-C9	17	19	0	0	19
H8-C9-03	20	73	0	0	73
H8-C12-06	26	0	2	0	2
H9-Rh16	25	0	0	1	1
H9-Rh23	32	90	0	0	90
H9-Mn1-Rh22	32	5	0	2	7
H9-Mn2-Rh21	32	4	0	1	5
H9-C2-Rh16	27	0	21	0	21
H9-C2-Rh20	31	0	8	0	8
H9-C2-Mn1-Rh15	27	0	1	0	1
H9-C2-Mn1-Rh19	31	0	2	0	2
H9-C2-Mn2-Rh14	27	0	1	0	1
H9-C2-Mn3-Rh13	27	0	1	0	1
H9-C2-01-Rh34	46	0	24	0	24
H9-C2-01-Rh35	47	0	16	9	25
H9-C2-01-Rh36	48	0	114	1	115
H9-C2-01-Mn1-Rh33	46	0	1	0	1
H9-C2-01-Mn1-Rh34	47	0	1	1	2
H9-C2-01-Mn1-Rh35	48	0	7	2	9
H9-C2-01-Mn2-Rh33	47	0	1	0	1
H9-C2-01-Mn2-Rh34	48	0	4	0	4
H9-C2-01-Mn3-Rh33	48	0	1	0	1
H9-C2-01-Mn4-Rh30	46	0	1	0	1
H9-C3-01-Rh35	48	0	72	0	72
H9-C3-01-Mn1-Rh34	48	0	3	2	5
H9-C3-01-Mn2-Rh33	48	0	3	1	4
H9-C3-01-Mn3-Rh32	48	0	2	1	3
H9-C9-01	19	210	0	0	210
H10-Rh16	26	0	0	1	1
H10-Rh21	31	0	81	143	224
H10-Rh22	32	0	59	183	242
H10-Rh54	64	0	6	0	6
H10-Mn1-Rh20	31	0	1	7	8
H10-Mn1-Rh21	32	0	4	10	14
H10-Mn1-Rh53	64	0	1	0	1
H10-Mn2-Rh19	31	0	2	7	9
H10-Mn2-Rh20	32	0	0	16	16
H10-Mn3-Rh18	31	0	1	0	1

H10-Mn3-Rh19	32	0	0	1	1
H10-Mn3-Rh51	64	0	1	0	1
H10-Mn4-Rh17	31	0	0	1	1
H10-Mn4-Rh18	32	0	1	1	2
H10-O5-Rh12	27	0	256	7	263
H10-O5-Mn1-Rh11	27	0	10	1	11
H10-O5-Mn2-Rh10	27	0	2	0	2
H10-O6-Rh11	27	0	1	0	1
H10-O6-Mn1-Rh10	27	0	1	0	1
H10-O8-Rh9	27	0	2	0	2
H10-O11-Rh6	27	0	3	0	3
H10-C2-O4-Rh36	52	0	2625	0	2625
H10-C2-O4-Mn1-Rh35	52	0	161	24	185
H10-C2-O4-Mn2-Rh34	52	0	121	21	142
H10-C2-O4-Mn3-Rh33	52	0	64	5	69
H10-C2-O4-Mn4-Rh32	52	0	33	6	39
H10-C3-O3-Rh64	80	0	2178	68	2246
H10-C4-O3	17	0	7	0	7
H10-C5-O4	19	3	0	0	3
H10-C5-O5	20	3	0	0	3
H10-C6	16	26	0	0	26
H10-C6-O1	17	3	0	0	3
H10-C6-O2	18	7	0	0	7
H10-C6-O3	19	10	0	0	10
H10-C6-O4-Rh64	84	0	726	50	776
H10-C7	17	3	0	0	3
H10-C7-O1	18	52	0	0	52
H10-C7-O2	19	34	0	0	34
H10-C7-O3	20	0	1	0	1
H10-C8	18	12	0	0	12
H10-C8-O1	19	36	0	0	36
H10-C8-O2	20	0	12	1	13
H10-C8-O3	21	0	1	1	2
H10-C9	19	65	0	0	65
H10-C9-O2	21	0	5	3	8
H10-C10-O1	21	0	3	1	4
H10-C12-Rh40	62	0	0	4	4
H10-C12-Mn1-Rh39	62	0	0	1	1
H10-C12-Mn4-Rh36	62	0	0	1	1
H10-C12-O6	28	0	2	1	3
H10-C13-O5	28	0	6	7	13
H11-Rh5	16	0	34	1188	1222
H11-Rh16	27	0	0	1	1
H11-Rh21	32	0	0	151	151

H11-Mn1-Rh4	16	0	1	60	61
H11-Mn1-Rh20	32	0	0	11	11
H11-Mn2-Rh3	16	0	3	11	14
H11-Mn2-Rh19	32	0	0	14	14
H11-Mn3-Rh18	32	0	0	4	4
H11-O5-Rh12	28	0	77	11	88
H11-O5-Mn1-Rh11	28	0	8	2	10
H11-O5-Mn2-Rh10	28	0	1	0	1
H11-O5-Mn3-Rh9	28	0	1	0	1
H11-O11-Rh6	28	0	3	0	3
H11-O14-Rh3	28	0	5	0	5
H11-C4-O3-Rh41	59	0	11	2	13
H11-C4-O3-Rh42	60	0	20	8	28
H11-C4-O3-Rh43	61	0	26	13	39
H11-C4-O3-Rh44	62	0	18	0	18
H11-C4-O3-Mn1-Rh42	61	0	1	2	3
H11-C4-O3-Mn1-Rh43	62	0	2	0	2
H11-C4-O3-Mn2-Rh40	60	0	1	1	2
H11-C4-O3-Mn2-Rh41	61	0	1	1	2
H11-C4-O3-Mn3-Rh41	62	0	3	0	3
H11-C5-O2-Rh44	62	0	21	0	21
H11-C5-O2-Mn1-Rh43	62	0	2	0	2
H11-C5-O2-Mn2-Rh42	62	0	2	0	2
H11-C5-O2-Mn3-Rh41	62	0	1	0	1
H11-C5-O2-Mn4-Rh40	62	0	3	0	3
H12-Rh16	28	0	0	1	1
H12-Rh19	31	0	0	289	289
H12-Mn1-Rh18	31	0	0	27	27
H12-Mn2-Rh17	31	0	0	9	9
H12-Mn3-Rh16	31	0	0	7	7
H12-O5-Rh12	29	0	112	7	119
H12-O5-Mn1-Rh11	29	0	3	1	4
H12-O5-Mn2-Rh10	29	0	3	2	5
H12-O11-Rh6	29	0	2	0	2
H12-O11-Mn1-Rh5	29	0	1	0	1
H12-O12-Rh5	29	0	4	0	4
H12-C2-O4-Rh12	30	0	0	48	48
H12-C2-O4-Mn1-Rh11	30	0	0	2	2
H12-C2-O4-Mn2-Rh10	30	0	0	1	1
H12-C3-O3-Rh36	54	0	1232	0	1232
H12-C3-O3-Mn1-Rh35	54	0	74	10	84
H12-C3-O3-Mn2-Rh34	54	0	63	11	74
H12-C3-O3-Mn3-Rh33	54	0	37	3	40
H12-C3-O3-Mn4-Rh32	54	0	19	2	21

H12-C3-06	21	0	20	63	83
H12-C4-01	17	1	0	0	1
H12-C4-02	18	7	0	0	7
H12-C5-02-Rh43	62	0	11	8	19
H12-C5-02-Mn2-Rh41	62	0	1	0	1
H12-C6-03	21	0	0	1	1
H12-C6-06	24	5199	70	56	5325
H12-C7	19	8	0	0	8
H12-C7-01	20	27	0	0	27
H12-C7-02	21	46	0	0	46
H12-C7-03	22	0	1	1	2
H12-C8	20	10	0	0	10
H12-C8-01	21	28	0	0	28
H12-C8-03	23	0	3	1	4
H12-C9	21	45	0	0	45
H12-C9-01	22	0	7	2	9
H12-C10	22	0	4	1	5
H12-C12-04	28	0	0	1	1
H12-C12-06	30	0	2	0	2
H12-C13-05	30	0	5	6	11
H12-C14-04	30	0	16	5	21
H12-C15-03	30	0	7	1	8
H13-Rh16	29	0	0	1	1
H13-Rh19	32	0	0	47	47
H13-Mn1-Rh18	32	0	0	3	3
H13-Mn2-Rh17	32	0	0	2	2
H13-O5-Rh12	30	0	54	7	61
H13-O5-Mn1-Rh11	30	0	6	1	7
H13-O5-Mn3-Rh9	30	0	0	1	1
H13-O9-Rh8	30	0	2	0	2
H13-O13-Rh4	30	0	2	0	2
H13-C2-Rh16	31	0	78	0	78
H13-C2-Mn1-Rh15	31	0	6	5	11
H13-C2-Mn2-Rh14	31	0	3	0	3
H13-C5-Rh22	40	0	23	0	23
H13-C5-Mn1-Rh21	40	0	1	0	1
H14-Rh16	30	0	0	107	107
H14-Rh17	31	0	0	110	110
H14-Rh18	32	0	0	80	80
H14-Mn1-Rh15	30	0	0	11	11
H14-Mn1-Rh16	31	0	0	10	10
H14-Mn1-Rh17	32	0	0	16	16
H14-Mn2-Rh14	30	0	0	2	2
H14-Mn2-Rh15	31	0	0	2	2

H14-Mn3-Rh13	30	0	0	1	1
H14-O7	21	0	1	756	757
H14-C1-Rh21	36	0	0	136	136
H14-C1-Mn1-Rh20	36	0	0	9	9
H14-C1-Mn2-Rh19	36	0	0	6	6
H14-C1-Mn4-Rh17	36	0	0	1	1
H14-C2-Rh20	36	0	0	272	272
H14-C2-Rh40	56	0	12	0	12
H14-C2-Mn1-Rh19	36	0	0	20	20
H14-C2-Mn2-Rh18	36	0	0	14	14
H14-C2-Mn2-Rh38	56	0	1	0	1
H14-C2-Mn3-Rh17	36	0	0	3	3
H14-C2-Mn3-Rh37	56	0	1	0	1
H14-C3-O3-Rh36	56	0	767	0	767
H14-C3-O3-Mn1-Rh35	56	0	30	2	32
H14-C3-O3-Mn2-Rh34	56	0	34	3	37
H14-C3-O3-Mn3-Rh33	56	0	20	2	22
H14-C3-O3-Mn4-Rh32	56	0	13	0	13
H14-C3-O4-Rh36	57	0	842	0	842
H14-C3-O4-Mn1-Rh35	57	0	47	9	56
H14-C3-O4-Mn2-Rh34	57	0	39	4	43
H14-C3-O4-Mn3-Rh33	57	0	24	11	35
H14-C3-O4-Mn4-Rh32	57	0	6	0	6
H14-C4-O4	22	0	8	0	8
H14-C4-O4-Rh64	86	0	494	48	542
H14-C7-O3	24	0	1	0	1
H14-C8	22	2	0	0	2
H14-C8-O1	23	1	0	0	1
H14-C8-O2	24	0	3	1	4
H14-C8-O3	25	0	1	0	1
H14-C9	23	54	0	0	54
H14-C10-O4	28	0	1	0	1
H14-C12-O6	32	0	4	0	4
H14-C13-O5	32	0	7	1	8
H14-C14-O4	32	0	2	2	4
H14-C15-O3	32	0	7	14	21
H14-C16-O2	32	0	4	6	10
H15-Rh6	21	0	566	0	566
H15-Rh16	31	0	0	148	148
H15-Rh17	32	0	0	228	228
H15-Mn1-Rh5	21	0	17	6	23
H15-Mn1-Rh15	31	0	0	10	10
H15-Mn1-Rh16	32	0	0	15	15
H15-Mn2-Rh4	21	0	8	0	8

H15-Mn2-Rh15	32	0	0	6	6
H15-Mn3-Rh14	32	0	0	5	5
H15-C1-Rh16	32	0	0	88	88
H15-C1-Mn1-Rh15	32	0	0	5	5
H15-C1-Mn2-Rh14	32	0	0	1	1
H15-C1-Mn3-Rh13	32	0	0	4	4
H15-C2-Rh21	38	0	0	137	137
H15-C2-Mn1-Rh20	38	0	0	9	9
H15-C2-Mn2-Rh19	38	0	1	15	16
H15-C2-Mn4-Rh17	38	0	0	4	4
H15-C4-Rh19	38	0	0	301	301
H15-C4-Mn1-Rh18	38	0	1	38	39
H15-C4-Mn2-Rh17	38	0	0	12	12
H15-C4-Mn3-Rh16	38	0	0	2	2
H16-Rh5	21	0	845	51	896
H16-Rh16	32	0	32	438	470
H16-Mn1-Rh4	21	0	47	8	55
H16-Mn1-Rh15	32	0	0	28	28
H16-Mn2-Rh3	21	0	8	5	13
H16-Mn2-Rh14	32	0	1	11	12
H16-Mn3-Rh13	32	0	0	2	2
H16-O8	24	0	14	3911	3925
H16-C2-Rh16	34	0	148	0	148
H16-C2-Rh20	38	0	395	0	395
H16-C2-Mn1-Rh15	34	0	2	0	2
H16-C2-Mn1-Rh19	38	0	17	1	18
H16-C2-Mn2-Rh14	34	0	5	0	5
H16-C2-Mn2-Rh18	38	0	10	2	12
H16-C2-Mn3-Rh17	38	0	5	2	7
H16-C2-Mn4-Rh16	38	0	1	1	2
H16-C3-O5-Rh36	60	0	2509	0	2509
H16-C3-O5-Mn1-Rh35	60	0	108	9	117
H16-C3-O5-Mn2-Rh34	60	0	105	27	132
H16-C3-O5-Mn3-Rh33	60	0	63	8	71
H16-C3-O5-Mn4-Rh32	60	0	46	4	50
H16-C4-Rh20	40	0	158	1	159
H16-C4-Mn1-Rh19	40	0	8	0	8
H16-C4-Mn2-Rh18	40	0	8	1	9
H16-C4-Mn3-Rh17	40	0	1	0	1
H16-C7-O1	24	1	0	0	1
H16-C8-O1	25	38	0	0	38
H16-C8-O2	26	0	5	0	5
H16-C9	25	18	0	0	18
H16-C10	26	2	0	0	2

H16-C10-01	27	0	2	0	2
H16-C13-05	34	0	13	1	14
H16-C14-Rh42	72	0	3	0	3
H16-C14-Mn2-Rh40	72	0	3	0	3
H16-C14-04	34	0	18	4	22
H16-C16-02	34	0	2	3	5
H16-C17-01	34	0	6	3	9
H16-C18	34	0	3	0	3
H17-Rh15	32	0	0	96	96
H17-Mn1-Rh14	32	0	0	7	7
H17-Mn2-Rh13	32	0	0	8	8
H17-Mn3-Rh12	32	0	0	1	1
H17-C2-Rh16	35	0	161	0	161
H17-C2-Mn1-Rh15	35	0	11	0	11
H17-C2-Mn2-Rh14	35	0	8	0	8
H17-C2-Mn3-Rh13	35	0	3	0	3
H17-C3-Rh20	40	0	195	0	195
H17-C3-Mn1-Rh19	40	0	9	9	18
H17-C3-Mn2-Rh18	40	0	13	4	17
H17-C4-Rh21	42	0	0	288	288
H17-C4-Mn1-Rh20	42	0	3	23	26
H17-C4-Mn2-Rh19	42	0	0	11	11
H17-C4-Mn3-Rh18	42	0	0	5	5
H17-C5-Rh24	46	0	84	0	84
H17-C5-Mn1-Rh23	46	0	6	0	6
H17-C5-Mn2-Rh22	46	0	2	4	6
H18-Rh13	31	0	0	46	46
H18-Mn1-Rh12	31	0	0	3	3
H18-Mn2-Rh11	31	0	0	2	2
H18-C1-Rh21	40	0	0	288	288
H18-C1-Mn1-Rh20	40	0	0	28	28
H18-C1-Mn2-Rh19	40	0	0	13	13
H18-C1-Mn3-Rh18	40	0	0	1	1
H18-C2-Rh16	36	0	260	1	261
H18-C2-Rh20	40	0	240	0	240
H18-C2-Rh26	46	0	65	0	65
H18-C2-Mn1-Rh15	36	0	21	5	26
H18-C2-Mn1-Rh19	40	0	17	3	20
H18-C2-Mn1-Rh25	46	0	3	3	6
H18-C2-Mn2-Rh14	36	0	9	2	11
H18-C2-Mn2-Rh18	40	0	7	0	7
H18-C2-Mn2-Rh24	46	0	1	1	2
H18-C2-Mn3-Rh13	36	0	3	0	3
H18-C2-Mn3-Rh17	40	0	3	0	3

H18-C2-Mn3-Rh23	46	0	1	0	1
H18-C2-Mn4-Rh16	40	0	1	0	1
H18-C6-O4-Rh52	80	0	10	11	21
H18-C6-O4-Mn1-Rh51	80	0	2	2	4
H18-C6-O4-Mn2-Rh50	80	0	1	0	1
H18-C6-O4-Mn3-Rh49	80	0	0	1	1
H18-C6-O6-Rh52	82	0	8	9	17
H18-C6-O6-Mn2-Rh50	82	0	0	1	1
H18-C9	27	1	0	0	1
H18-C9-O5	32	0	1	0	1
H18-C10	28	0	3	0	3
H18-C13-O5	36	0	3	0	3
H18-C14-O4	36	0	10	2	12
H18-C15-O3	36	0	20	3	23
H18-C16-O2	36	0	4	1	5
H19-Rh13	32	0	0	55	55
H19-Rh21	40	0	0	158	158
H19-Mn1-Rh12	32	0	0	5	5
H19-Mn1-Rh20	40	0	0	7	7
H19-Mn2-Rh19	40	0	0	8	8
H19-Mn3-Rh18	40	0	0	2	2
H19-C2-Rh20	41	0	60	0	60
H19-C2-Rh21	42	0	2	117	119
H19-C2-Mn1-Rh19	41	0	2	0	2
H19-C2-Mn1-Rh20	42	0	0	11	11
H19-C2-Mn2-Rh18	41	0	1	0	1
H19-C2-Mn2-Rh19	42	0	0	10	10
H19-C2-Mn3-Rh17	41	0	1	0	1
H19-C2-Mn4-Rh17	42	0	0	1	1
H20-C2-Rh39	61	0	9	0	9
H20-C2-Rh67	89	0	12	0	12
H20-C2-Mn2-Rh65	89	0	1	0	1
H20-C2-Mn4-Rh63	89	0	1	0	1
H20-C6-O4-Rh52	82	0	13	13	26
H20-C6-O4-Mn3-Rh49	82	0	3	0	3
H20-C13-O5	38	0	1	0	1
H20-C14-O4	38	0	2	0	2
H20-C15-O3	38	0	4	1	5
H20-C16-O2	38	0	19	0	19
H22-C14-O4	40	0	1	2	3
H22-C17-O1	40	0	4	2	6
H22-C18	40	0	7	2	9
H23-Rh8	31	0	131	53	184
H23-Rh9	32	0	207	122	329

H23-Mn1-Rh7	31	0	7	20	27
H23-Mn1-Rh8	32	0	16	11	27
H23-Mn2-Rh7	32	0	2	0	2
H23-Mn3-Rh5	31	0	1	0	1
H23-O11-Rh16	50	0	288	189	477
H23-O11-Mn1-Rh15	50	0	12	13	25
H23-O11-Mn2-Rh14	50	0	6	10	16
H23-O13-Rh14	50	0	3	0	3
H23-O14-Rh13	50	0	6	0	6
H23-O14-Mn1-Rh12	50	0	1	0	1
H23-O14-Mn3-Rh10	50	0	1	0	1
H23-O15-Rh12	50	0	7	0	7
H23-O17-Rh10	50	0	5	0	5
H23-O18-Rh9	50	0	2	0	2
H23-O19-Rh8	50	0	9	0	9
H23-O20-Rh7	50	0	2	0	2
H23-O20-Mn1-Rh6	50	0	1	0	1
H23-O21-Rh6	50	0	4	0	4
H23-O22-Rh5	50	0	6	0	6
H23-O23-Rh4	50	0	4	0	4
H23-O24-Rh3	50	0	1	0	1
H24-Rh8	32	0	34	59	93
H24-Rh38	62	1	0	0	1
H24-Mn1-Rh7	32	0	2	3	5
H24-O11-Rh16	51	0	151	105	256
H24-O11-Mn1-Rh15	51	0	13	18	31
H24-O11-Mn2-Rh14	51	0	2	4	6
H24-O11-Mn3-Rh13	51	0	1	2	3
H24-O11-Mn4-Rh12	51	0	1	0	1
H24-O14-Rh13	51	0	1	0	1
H24-O16-Rh11	51	0	1	0	1
H24-O18-Rh9	51	0	2	0	2
H24-O19-Rh8	51	0	1	0	1
H24-O21-Rh6	51	0	2	0	2
H24-O22-Rh5	51	0	1	0	1
H24-O23-Rh4	51	0	1	0	1
H24-C2-Rh20	46	0	491	0	491
H24-C2-Mn1-Rh19	46	0	40	0	40
H24-C2-Mn2-Rh18	46	0	12	1	13
H24-C2-Mn3-Rh17	46	0	9	0	9
H24-C12-O12	48	1	0	0	1
H24-C16-O2	42	0	5	0	5
H25-O11-Rh16	52	0	105	70	175
H25-O11-Mn1-Rh15	52	0	11	5	16

H25-O11-Mn2-Rh14	52	0	6	3	9
H25-O11-Mn3-Rh13	52	0	0	1	1
H25-O13-Rh14	52	0	1	0	1
H25-O14-Rh13	52	0	3	0	3
H25-O15-Rh12	52	0	2	0	2
H25-O15-Mn1-Rh11	52	0	2	1	3
H25-O16-Rh11	52	0	3	0	3
H25-O17-Rh10	52	0	8	0	8
H25-O17-Mn1-Rh9	52	0	1	0	1
H25-O18-Rh9	52	0	1	0	1
H25-O19-Rh8	52	0	2	0	2
H25-O20-Rh7	52	0	2	0	2
H25-O21-Rh6	52	0	1	0	1
H25-O22-Rh5	52	0	2	0	2
H26-Rh38	64	2	0	0	2
H26-C2-Rh40	68	0	104	0	104
H26-C2-Mn1-Rh39	68	0	7	0	7
H26-C2-Mn2-Rh38	68	0	5	0	5
H26-C2-Mn3-Rh37	68	0	4	2	6
H26-C2-Mn4-Rh36	68	0	3	4	7
H26-C10-Rh44	80	0	3	0	3
H27-Rh38	65	12	0	0	12
H27-C2-Rh35	64	0	204	0	204
H27-C2-Rh36	65	0	333	0	333
H27-C2-Rh58	87	0	2	5	7
H27-C2-Mn1-Rh34	64	0	18	1	19
H27-C2-Mn1-Rh35	65	0	24	1	25
H27-C2-Mn1-Rh57	87	0	0	1	1
H27-C2-Mn2-Rh33	64	0	19	3	22
H27-C2-Mn2-Rh34	65	0	13	0	13
H27-C2-Mn3-Rh32	64	0	7	0	7
H27-C2-Mn3-Rh33	65	0	14	4	18
H27-C2-Mn4-Rh31	64	0	1	1	2
H27-C2-Mn4-Rh32	65	0	3	0	3
H28-Rh32	60	0	0	3	3
H28-Rh38	66	7	0	0	7
H28-Mn3-Rh29	60	0	0	1	1
H29-C2-Rh39	70	0	78	0	78
H29-C2-Mn1-Rh38	70	0	13	0	13
H29-C2-Mn2-Rh37	70	0	5	0	5
H29-C2-Mn3-Rh36	70	0	1	0	1
H29-C2-Mn4-Rh35	70	0	1	2	3
H30-O15	45	124	4	94	222
H30-C2-Rh32	64	0	0	4	4

H30-C2-Mn1-Rh31	64	0	0	2	2
H31-Rh38	69	1	0	0	1
H32-Rh38	70	7	0	0	7
H32-C1-018-Rh36	87	0	1	5	6
H32-C1-018-Mn1-Rh35	87	0	0	1	1
H32-C1-019-Rh35	87	0	7	45	52
H32-C1-019-Mn1-Rh34	87	0	2	0	2
H32-C1-019-Mn3-Rh32	87	0	1	3	4
H32-C2-016-Rh35	85	0	3	60	63
H32-C2-016-Rh36	86	0	3	48	51
H32-C2-016-Mn1-Rh34	85	0	1	5	6
H32-C2-016-Mn1-Rh35	86	0	0	5	5
H32-C2-016-Mn2-Rh33	85	0	0	2	2
H32-C2-016-Mn2-Rh34	86	0	0	2	2
H32-C2-016-Mn3-Rh32	85	0	0	2	2
H32-C2-016-Mn4-Rh32	86	0	0	1	1
H32-C2-017-Rh35	86	0	14	20	34
H32-C2-017-Mn1-Rh34	86	0	3	1	4
H32-C2-017-Mn2-Rh33	86	0	1	2	3
H32-C2-017-Mn3-Rh32	86	0	1	4	5
H32-C2-017-Mn4-Rh31	86	0	0	1	1
H32-C8-Rh40	80	0	2	0	2
H33-Rh38	71	9	0	0	9
H33-C1-017-Rh36	87	0	1	6	7
H33-C1-018-Rh35	87	0	3	34	37
H33-C1-018-Mn3-Rh32	87	0	0	1	1
H33-C2-Rh40	75	0	75	0	75
H33-C2-Mn1-Rh39	75	0	5	1	6
H33-C2-Mn2-Rh38	75	0	1	0	1
H33-C2-Mn3-Rh37	75	0	3	2	5
H33-C2-Mn4-Rh36	75	0	1	0	1
H34-Rh38	72	2	0	0	2
H34-C1-017-Rh35	87	0	7	23	30
H34-C1-017-Mn3-Rh32	87	0	0	1	1
H34-C6-Rh40	80	0	6	0	6
H34-C10-Rh48	92	0	7	0	7
H35-Rh38	73	1	0	0	1
H35-C2-Rh30	67	0	26	0	26
H35-C2-Mn1-Rh29	67	0	2	0	2
H35-C2-Mn4-Rh26	67	0	2	0	2
H36-C2-017-Rh35	90	0	0	7	7
H36-C4-Rh52	92	0	2	0	2
H37-C2-Rh30	69	0	25	0	25
H37-C2-Mn1-Rh29	69	0	1	0	1

H37-C2-Mn2-Rh28	69	0	2	0	2
H37-C2-Mn4-Rh26	69	0	1	0	1
H38-Rh38	76	2	0	0	2
H38-C2-Rh45	85	0	30	0	30
H38-C2-Mn1-Rh44	85	0	1	0	1
H38-C2-Mn2-Rh43	85	0	1	0	1
H38-C2-Mn3-Rh42	85	0	4	0	4
H38-C2-Mn4-Rh41	85	0	1	0	1
H38-C2-017-Rh35	92	0	0	8	8
H38-C2-017-Mn1-Rh34	92	0	0	1	1
H40-Rh38	78	1	0	0	1
H40-C2-Rh45	87	0	32	0	32
H40-C2-Mn2-Rh43	87	0	2	0	2
H40-C2-Mn3-Rh42	87	0	3	0	3
H40-C2-018-Rh29	89	0	187	106	293
H40-C2-018-Rh30	90	0	204	82	286
H40-C2-018-Rh32	92	0	217	133	350
H40-C2-018-Mn1-Rh28	89	0	13	10	23
H40-C2-018-Mn1-Rh29	90	0	5	14	19
H40-C2-018-Mn1-Rh31	92	0	13	15	28
H40-C2-018-Mn2-Rh27	89	0	9	6	15
H40-C2-018-Mn2-Rh28	90	0	9	1	10
H40-C2-018-Mn2-Rh30	92	0	13	14	27
H40-C2-018-Mn3-Rh26	89	0	1	3	4
H40-C2-018-Mn3-Rh27	90	0	6	4	10
H40-C2-018-Mn3-Rh29	92	0	9	4	13
H40-C2-018-Mn4-Rh25	89	0	1	4	5
H40-C2-018-Mn4-Rh26	90	0	1	1	2
H40-C3-017-Rh32	92	0	96	37	133
H40-C3-017-Mn1-Rh31	92	0	5	1	6
H40-C3-017-Mn2-Rh30	92	0	7	4	11
H40-C3-017-Mn3-Rh29	92	0	1	1	2
H41-C2-Rh39	82	0	284	0	284
H41-C2-Mn1-Rh38	82	0	14	1	15
H41-C2-Mn2-Rh37	82	0	24	2	26
H41-C2-Mn3-Rh36	82	0	6	1	7
H41-C2-Mn4-Rh35	82	0	3	0	3
H42-Rh38	80	1	0	0	1
H42-C2-Rh40	84	0	703	0	703
H42-C2-Mn1-Rh39	84	0	30	2	32
H42-C2-Mn2-Rh38	84	0	44	1	45
H42-C2-Mn3-Rh37	84	0	24	3	27
H42-C2-Mn4-Rh36	84	0	12	7	19
H42-C2-018-Rh32	94	0	369	204	573

H42-C2-O18-Mn1-Rh31	94	0	14	10	24
H42-C2-O18-Mn2-Rh30	94	0	14	28	42
H42-C2-O18-Mn3-Rh29	94	0	8	4	12
H42-C2-O18-Mn4-Rh28	94	0	2	5	7
H44-C2-Rh39	85	0	55	0	55
H44-C2-Mn2-Rh37	85	0	1	0	1
H44-C2-Mn3-Rh36	85	0	1	0	1
H44-C2-Mn4-Rh35	85	0	1	0	1
H45-O22-Rh32	99	0	56	20	76
H45-O22-Mn2-Rh30	99	0	3	2	5
H45-O22-Mn3-Rh29	99	0	3	5	8
H45-O22-Mn4-Rh28	99	0	1	0	1
H45-O29-Rh25	99	0	2	0	2
H45-O31-Rh23	99	0	5	0	5
H45-O32-Rh22	99	0	1	0	1
H45-O35-Rh19	99	0	2	0	2
H45-O36-Rh18	99	0	1	0	1
H45-O37-Rh17	99	0	3	0	3
H45-O39-Rh15	99	0	1	0	1
H45-O41-Rh13	99	0	1	0	1
H45-C2-Rh40	87	0	486	10	496
H45-C2-Mn1-Rh39	87	0	25	0	25
H45-C2-Mn2-Rh38	87	0	25	0	25
H45-C2-Mn3-Rh37	87	0	23	0	23
H45-C2-Mn4-Rh36	87	0	4	1	5
H46-C2-Rh40	88	0	69	0	69
H46-C2-Mn1-Rh39	88	0	3	0	3
H46-C2-Mn2-Rh38	88	0	1	0	1
H46-C2-Mn3-Rh37	88	0	2	1	3
H46-C2-Mn4-Rh36	88	0	1	1	2
H47-Rh38	85	1	0	0	1
H47-C2-Rh40	89	0	461	0	461
H47-C2-Mn1-Rh39	89	0	22	1	23
H47-C2-Mn2-Rh38	89	0	20	2	22
H47-C2-Mn3-Rh37	89	0	18	5	23
H47-C2-Mn4-Rh36	89	0	6	0	6
H48-Rh38	86	9	0	0	9
H48-O24-Rh24	96	0	11	15	26
H48-O24-Mn1-Rh23	96	0	0	3	3
H48-O24-Mn2-Rh22	96	0	0	1	1
H48-C2-Rh40	90	0	63	0	63
H48-C2-Mn1-Rh39	90	0	2	0	2
H48-C2-Mn3-Rh37	90	0	3	0	3
H48-C4-Rh40	92	0	2	0	2

H49-Rh38	87	5	0	0	5
H49-Mn3-Rh35	87	1	0	0	1
H50-Rh38	88	50	0	0	50
H50-Mn1-Rh37	88	4	0	0	4
H50-Mn3-Rh35	88	1	0	0	1
H50-Mn4-Rh34	88	1	0	0	1
H50-C2-Rh48	100	0	51	0	51
H50-C2-Mn2-Rh46	100	0	2	0	2
H50-C2-Mn4-Rh44	100	0	1	0	1
H51-Rh38	89	39	0	0	39
H51-Mn2-Rh36	89	5	1	0	6
H52-Rh38	90	53	0	0	53
H52-O22-Rh32	106	0	139	77	216
H52-O22-Mn1-Rh31	106	0	10	10	20
H52-O22-Mn2-Rh30	106	0	6	8	14
H52-O22-Mn3-Rh29	106	0	0	6	6
H52-O22-Mn4-Rh28	106	0	1	1	2
H52-O31-Rh23	106	0	1	0	1
H52-O33-Rh21	106	0	1	0	1
H52-O36-Rh18	106	0	1	0	1
H52-O38-Rh16	106	0	1	0	1
H52-O39-Rh15	106	0	1	0	1
H52-O40-Rh14	106	0	2	0	2
H52-O41-Rh13	106	0	2	0	2
H52-C2-Rh48	102	0	36	0	36
H52-C2-Mn1-Rh47	102	0	1	1	2
H52-C2-Mn2-Rh46	102	0	3	0	3
H53-Rh38	91	65	0	0	65
H53-Mn1-Rh37	91	1	0	0	1
H53-Mn2-Rh36	91	1	0	0	1
H53-Mn4-Rh34	91	1	0	0	1
H54-Rh38	92	22	0	0	22
H55-Rh38	93	18	0	0	18
H56-Rh38	94	28	0	0	28
H58-Rh38	96	42	0	0	42
H58-Mn1-Rh37	96	2	0	2	4
H58-Mn3-Rh35	96	1	0	0	1
H59-Rh38	97	1	0	0	1
H60-Rh38	98	42	0	0	42
H60-Mn1-Rh37	98	3	0	0	3
H60-Mn2-Rh36	98	3	0	1	4
H62-Rh38	100	55	0	0	55
H62-Mn1-Rh37	100	4	0	0	4
H62-Mn2-Rh36	100	2	0	0	2

H62-Mn3-Rh35	100	1	0	0	1
H64-Rh38	102	104	0	0	104
H64-Mn1-Rh37	102	2	1	0	3
H64-Mn2-Rh36	102	4	0	1	5
H64-Mn3-Rh35	102	1	0	0	1
H64-Mn4-Rh34	102	1	0	2	3
H66-Rh38	104	58	0	0	58
H66-Mn1-Rh37	104	2	0	0	2
H66-Mn2-Rh36	104	3	1	0	4
H66-Mn3-Rh35	104	1	0	0	1
H68-Rh38	106	61	0	0	61
H68-Mn2-Rh36	106	4	0	0	4
H70-Rh38	108	73	0	0	73
H70-Mn3-Rh35	108	2	0	0	2
H70-O32-Rh48	150	0	0	1	1
H71-Rh38	109	97	0	0	97
H71-Mn1-Rh37	109	6	0	2	8
H71-Mn2-Rh36	109	2	0	0	2
H71-Mn3-Rh35	109	1	0	0	1
H71-Mn4-Rh34	109	1	0	0	1
H72-Rh38	110	97	0	0	97
H72-Mn1-Rh37	110	3	0	0	3
H72-Mn2-Rh36	110	3	0	0	3
H72-Mn3-Rh35	110	4	1	0	5
H73-Rh38	111	72	0	0	72
H73-Mn1-Rh37	111	5	1	1	7
H73-Mn2-Rh36	111	2	0	0	2
H73-Mn3-Rh35	111	1	0	0	1
H73-Mn4-Rh34	111	2	0	0	2
H78-O32-Rh48	158	0	4	14	18
H78-O32-Mn3-Rh45	158	0	0	2	2
H80-O32-Rh48	160	0	1	5	6
H80-O32-Mn1-Rh47	160	0	1	0	1
H81-C1-O42-Rh64	188	0	4	0	4
H84-O50-Rh62	196	0	1	6	7
H84-O50-Rh64	198	0	2	7	9
H84-O50-Mn3-Rh59	196	0	0	2	2
H84-O50-Mn4-Rh60	198	0	0	2	2
H84-O64-Rh48	196	0	1	0	1
H84-C1-O45-Rh64	194	0	15	148	163
H84-C2-O50-Rh62	198	0	0	19	19
H84-C2-O50-Rh64	200	0	3	1	4
H84-C2-O50-Mn1-Rh61	198	0	0	1	1
H84-C2-O50-Mn2-Rh60	198	0	0	3	3

H84-C4-047-Rh64	199	0	0	2	2
H84-C4-047-Mn3-Rh61	199	0	0	1	1
H88-C3-052-Rh62	205	0	3	4	7
H88-C3-052-Rh64	207	0	2	4	6
H88-C3-052-Mn3-Rh59	205	0	0	6	6
H88-C3-052-Mn4-Rh58	205	0	0	1	1
H91-C4-054-Rh64	213	0	0	22	22
H92-C3-053-Rh62	210	0	0	14	14
H92-C3-053-Rh64	212	0	1	16	17
H92-C3-053-Mn2-Rh60	210	0	0	2	2
H92-C3-053-Mn3-Rh61	212	0	0	1	1
H93-Rh38	131	37	0	0	37
H93-Mn2-Rh36	131	2	0	0	2
H94-Rh38	132	46	0	0	46
H94-Mn1-Rh37	132	1	0	0	1
H94-Mn2-Rh36	132	5	1	0	6
H94-Mn3-Rh35	132	1	0	0	1
H94-042-Rh64	200	0	2	0	2
H94-C3-054-Rh64	215	0	0	5	5
H94-C3-054-Mn3-Rh61	215	0	0	1	1
H94-C4-054-Rh64	216	0	0	48	48
H94-C4-054-Mn1-Rh63	216	0	0	1	1
H94-C4-054-Mn2-Rh62	216	0	0	2	2
H94-C4-054-Mn3-Rh61	216	0	0	3	3
H94-C4-054-Mn4-Rh60	216	0	0	1	1
H95-Rh38	133	38	0	0	38
H95-Mn1-Rh37	133	1	0	0	1
H95-Mn2-Rh36	133	2	0	0	2
H96-Rh38	134	56	0	0	56
H96-Mn1-Rh37	134	1	0	0	1
H96-Mn2-Rh36	134	1	0	0	1
H96-Mn3-Rh35	134	1	0	0	1
H96-043-Rh64	203	0	4	0	4
H96-043-Mn2-Rh62	203	0	1	0	1
H96-056-Rh51	203	0	1	0	1
H97-Rh38	135	66	0	0	66
H97-Mn1-Rh37	135	2	0	0	2
H97-Mn2-Rh36	135	1	0	0	1
H97-Mn3-Rh35	135	1	0	0	1
H98-Rh38	136	36	0	0	36
H98-Mn1-Rh37	136	2	0	0	2
H98-044-Rh64	206	0	13	11	24
H98-044-Mn3-Rh61	206	0	0	1	1
total	--	18763	55864	32395	107022

Benchmark of G-NN potential against DFT calculations

Table S2. Benchmark of NN calculations for Rh-Mn-C-H-O systems against DFT results. Total atom number per cell (N_{atom}), DFT energy (E_{DFT}), NN energy (E_{NN}), and energy differences per atom (E_{diff}) between E_{DFT} and E_{NN} are included.

Surface	N_{atom}	E_{DFT} (eV)	E_{NN} (eV)	E_{diff} (meV/atom)
1	67	-459.56	-459.60	0.60
2	68	-462.71	-463.01	4.41
3	68	-463.28	-463.38	1.47
4	67	-459.56	-459.60	0.60
5	67	-469.18	-469.21	0.45
6	67	-469.38	-469.44	0.90
7	67	-469.18	-469.21	0.45
8	68	-472.79	-472.77	-0.29
9	67	-469.26	-469.33	1.04
10	67	-469.42	-469.37	-0.75
11	68	-472.53	-472.56	0.44
12	68	-473.07	-473.17	1.47
13	67	-459.34	-459.59	3.73
14	56	-380.63	-380.56	-1.25
15	56	-381.21	-381.20	-0.18
16	56	-381.10	-381.00	-1.79
17	56	-381.21	-381.09	-2.14
18	56	-380.86	-380.85	-0.18
19	56	-381.49	-381.46	-0.54
20	56	-380.95	-380.89	-1.07
21	56	-381.55	-381.55	0.00
22	56	-381.21	-381.14	-1.25
23	56	-381.90	-381.82	-1.43
24	57	-384.88	-384.82	-1.05
25	56	-381.90	-381.82	-1.43
26	56	-381.34	-381.30	-0.71
27	56	-381.92	-381.84	-1.43
28	55	-378.03	-377.88	-2.73
29	55	-377.74	-377.63	-2.00
30	55	-378.07	-377.99	-1.45
31	55	-377.70	-377.67	-0.55
32	55	-377.57	-377.51	-1.09
33	55	-377.47	-377.37	-1.82
34	55	-378.13	-378.00	-2.36
35	57	-384.89	-384.85	-0.70
36	55	-377.34	-377.28	-1.09
37	55	-377.54	-377.49	-0.91

38	55	-377.68	-377.68	0.00
39	55	-377.58	-377.57	-0.18
40	55	-377.65	-377.66	0.18
41	55	-377.38	-377.34	-0.73
42	55	-377.34	-377.28	-1.09
43	55	-377.64	-377.55	-1.64
44	55	-377.34	-377.23	-2.00
45	55	-378.09	-378.01	-1.45
46	57	-384.53	-384.47	-1.05
47	55	-377.51	-377.48	-0.55
48	55	-377.61	-377.58	-0.55
49	55	-376.91	-376.79	-2.18
50	55	-377.25	-377.17	-1.45
51	55	-376.71	-376.70	-0.18
52	55	-377.19	-377.11	-1.45
53	55	-377.12	-377.00	-2.18
54	54	-373.86	-373.72	-2.59
55	54	-374.06	-374.05	-0.19
56	54	-374.06	-373.96	-1.85
57	57	-384.85	-384.76	-1.58
58	54	-373.58	-373.54	-0.74
59	54	-373.54	-373.44	-1.85
60	54	-372.94	-373.00	1.11
61	54	-373.53	-373.41	-2.22
62	54	-374.12	-374.06	-1.11
63	54	-374.24	-374.15	-1.67
64	54	-373.97	-373.94	-0.56
65	54	-373.63	-373.63	0.00
66	54	-373.58	-373.61	0.56
67	54	-374.23	-374.13	-1.85
68	57	-385.80	-385.70	-1.75
69	54	-373.79	-373.71	-1.48
70	54	-373.69	-373.71	0.37
71	54	-373.07	-372.99	-1.48
72	54	-372.95	-372.95	0.00
73	54	-373.43	-373.36	-1.30
74	54	-373.29	-373.24	-0.93
75	54	-373.52	-373.41	-2.04
76	54	-373.82	-373.73	-1.67
77	54	-373.78	-373.78	0.00
78	54	-373.33	-373.27	-1.11
79	57	-385.01	-384.97	-0.70
80	54	-373.72	-373.71	-0.19
81	53	-370.33	-370.24	-1.70

82	53	-370.60	-370.50	-1.89
83	53	-370.39	-370.30	-1.70
84	53	-370.13	-369.98	-2.83
85	53	-370.06	-370.01	-0.94
86	53	-369.92	-369.73	-3.58
87	53	-369.93	-369.85	-1.51
88	53	-369.88	-369.79	-1.70
89	53	-370.20	-370.16	-0.75
90	56	-380.80	-380.77	-0.54
91	53	-370.20	-370.16	-0.75
92	53	-370.30	-370.23	-1.32
93	53	-370.06	-370.01	-0.94
94	53	-369.51	-369.44	-1.32
95	53	-369.41	-369.40	-0.19
96	52	-366.30	-366.22	-1.54
97	52	-366.23	-366.13	-1.92
98	52	-366.27	-366.16	-2.12
99	52	-366.02	-365.93	-1.73
100	52	-366.49	-366.36	-2.50
101	56	-380.76	-380.77	0.18
102	52	-366.01	-365.91	-1.92
103	56	-381.03	-380.98	-0.89
104	53	-360.81	-360.68	-2.45
105	53	-360.80	-360.75	-0.94
106	53	-360.83	-360.79	-0.75
107	53	-360.95	-360.87	-1.51
108	53	-360.75	-360.70	-0.94
109	53	-360.28	-360.19	-1.70
110	53	-360.21	-360.08	-2.45
111	53	-360.01	-359.88	-2.45
112	53	-360.76	-360.58	-3.40
113	53	-360.58	-360.49	-1.70
114	52	-357.00	-356.94	-1.15
115	53	-360.48	-360.34	-2.64
116	53	-360.16	-360.10	-1.13
117	53	-360.39	-360.25	-2.64
118	54	-364.34	-364.32	-0.37
119	54	-364.43	-364.32	-2.04
120	54	-364.48	-364.48	0.00
121	54	-364.34	-364.25	-1.67
122	54	-364.38	-364.31	-1.30
123	54	-363.60	-363.64	0.74
124	54	-364.36	-364.28	-1.48
125	52	-357.05	-357.00	-0.96

126	54	-364.13	-364.12	-0.19
127	54	-364.15	-364.21	1.11
128	54	-364.03	-364.09	1.11
129	54	-364.51	-364.44	-1.30
130	54	-364.28	-364.36	1.48
131	54	-364.75	-364.62	-2.41
132	54	-364.18	-364.16	-0.37
133	54	-364.10	-364.00	-1.85
134	54	-363.89	-363.83	-1.11
135	54	-363.67	-363.58	-1.67
136	52	-357.03	-357.07	0.77
137	54	-364.10	-364.00	-1.85
138	54	-364.05	-364.02	-0.56
139	54	-364.21	-364.19	-0.37
140	54	-363.84	-363.72	-2.22
141	54	-363.64	-363.59	-0.93
142	54	-363.96	-364.02	1.11
143	54	-364.42	-364.31	-2.04
144	55	-368.27	-368.25	-0.36
145	55	-368.58	-368.63	0.91
146	55	-368.30	-368.21	-1.64
147	52	-356.70	-356.60	-1.92
148	55	-367.98	-367.99	0.18
149	55	-367.51	-367.49	-0.36
150	55	-368.33	-368.40	1.27
151	55	-368.13	-368.12	-0.18
152	55	-368.41	-368.33	-1.45
153	55	-368.36	-368.41	0.91
154	55	-367.85	-367.89	0.73
155	55	-367.99	-367.98	-0.18
156	55	-367.41	-367.33	-1.45
157	55	-367.98	-367.91	-1.27
158	52	-356.15	-356.21	1.15
159	55	-368.12	-368.06	-1.09
160	55	-368.18	-368.06	-2.18
161	55	-368.27	-368.23	-0.73
162	55	-367.34	-367.32	-0.36
163	55	-367.42	-367.42	0.00
164	55	-368.02	-367.93	-1.64
165	55	-368.00	-367.90	-1.82
166	55	-368.05	-368.03	-0.36
167	55	-367.28	-367.20	-1.45
168	55	-367.46	-367.34	-2.18
169	52	-356.75	-356.66	-1.73

170	55	-367.63	-367.46	-3.09
171	56	-371.51	-371.48	-0.54
172	56	-371.86	-371.77	-1.61
173	56	-371.43	-371.48	0.89
174	56	-371.83	-371.76	-1.25
175	56	-372.24	-372.27	0.54
176	56	-371.90	-371.91	0.18
177	56	-371.50	-371.55	0.89
178	56	-371.86	-371.88	0.36
179	56	-371.36	-371.35	-0.18
180	53	-360.70	-360.68	-0.38
181	56	-371.28	-371.23	-0.89
182	56	-371.28	-371.23	-0.89
183	56	-371.55	-371.51	-0.71
184	56	-371.55	-371.51	-0.71
185	56	-371.75	-371.64	-1.96
186	56	-371.85	-371.74	-1.96
187	56	-371.49	-371.42	-1.25
188	57	-375.33	-375.35	0.35
189	57	-375.52	-375.47	-0.88
190	57	-375.73	-375.70	-0.53
191	53	-360.79	-360.65	-2.64
192	57	-375.42	-375.31	-1.93
193	57	-375.06	-374.94	-2.11
194	57	-375.34	-375.31	-0.53
195	53	-360.45	-360.43	-0.38

* Root mean square error between DFT energy and NN energy is 1.47 meV/atom.

Table S3. Comparison between the Gibbs free energies of TS (G_{TS} , see Eq.3) of key reactions on 0.17-0.17 ML(b) MnRh(211) and Rh(211) from DFT and NN calculations. The symbol * represents surface sites.

Reaction	G_{TS} (eV)		Diff (eV)
	DFT	NN	
0.17-0.17 ML(b) MnRh(211)			
$CO^* + H^* \rightarrow CHO^* + *$	-0.71	-0.66	-0.05
$CHO^* + * \rightarrow CH^* + O^*$	-0.39	-0.35	-0.04
$O^* + H^* \rightarrow OH^* + *$	0.61	0.74	-0.13
$OH^* + H^* \rightarrow H_2O + 2^*$	0.86	0.86	0.00
$CH^* + CO^* \rightarrow CHCO^* + *$	-1.64	-1.60	-0.04
$CHCO^* + H^* \rightarrow CH_2CO^* + *$	-1.61	-1.55	-0.06
$CH_2CO^* + H^* \rightarrow CH_3CO^* + *$	-1.87	1.88	0.01
$CH_3CO^* + H^* \rightarrow CH_3CHO^* + *$	-1.76	-1.69	-0.07
$CH_3CHO^* + H^* \rightarrow CH_3CH_2O^* + *$	-1.68	-1.62	-0.06
$CH_3CH_2O^* + H^* \rightarrow CH_3CH_2OH + 2^*$	-1.44	-1.38	-0.06
$CH^* + H^* \rightarrow CH_2^* + *$	-1.28	-1.23	-0.05
$CH_2^* + * \rightarrow CH_3^* + *$	-1.28	-1.23	-0.05
$CH_3^* + * \rightarrow CH_4 + 2^*$	-1.06	-1.07	0.01
Rh(211)			
$CO^* + H^* \rightarrow CHO^* + *$	-0.28	-0.14	-0.14
$CHO^* + * \rightarrow CH^* + O^*$	0.42	0.47	-0.05
$O^* + H^* \rightarrow OH^* + *$	1.45	1.60	-0.15
$OH^* + H^* \rightarrow H_2O + 2^*$	1.47	1.47	0.00
$CH^* + CO^* \rightarrow CHCO^* + *$	-1.54	-1.44	-0.10
$CHCO^* + H^* \rightarrow CH_2CO^* + *$	-1.31	-1.21	-0.10
$CH_2CO^* + H^* \rightarrow CH_2CHO^* + *$	-1.35	-1.24	-0.11
$CH_2CHO^* + H^* \rightarrow CH_3CHO^* + *$	-1.54	-1.50	-0.04
$CH_3CHO^* + H^* \rightarrow CH_3CH_2O^* + *$	-1.17	-1.06	-0.11
$CH_3CH_2O^* + H^* \rightarrow CH_3CH_2OH + 2^*$	-0.89	-0.76	-0.13
$CH^* + H^* \rightarrow CH_2^* + *$	-1.30	-1.24	-0.06
$CH_2^* + * \rightarrow CH_3^* + *$	-1.22	-1.24	0.02
$CH_3^* + * \rightarrow CH_4 + 2^*$	-1.04	-0.93	-0.11

1.2 Gibbs Free Energy Calculation

The Gibbs free energy (G) of surface/bulks is approximately as the zero-point energy (ZPE) corrected DFT total energy ($E(\text{DFT})$), as the translation and rotation entropy can be neglected for surface species, and the contributions of vibration entropy and the PV term are also small to G . Regarding the gas phase molecules, the chemical potential μ can be determined using the following equation:

$$\mu(T, P) = E(\text{DFT}) + \text{ZPE} + \Delta H(0 \rightarrow T, P_0) - TS(T, P_0) + k_B T \ln \frac{P}{P_0} \quad (\text{S10})$$

Here, P_0 is the standard state pressure (1 bar); the enthalpy (H) and entropy (S) terms are obtained from the standard thermodynamics data (e.g., NIST Chemistry WebBook, NIST-JANAF Thermochemical Tables), or vibrational analysis.

1.3 Derivation of the free energy of MnO in the Bulk Phase

The chemical potential of MnO in the bulk phase ($G_{\text{MnO}}^{\text{bulk}}$) is calculated using the standard Gibbs free energy of formation of MnO, which is -3.76 eV¹⁰. In this method, the chemical potential of Mn in the bulk phase ($\mu_{\text{Mn}}^{\text{bulk}}$) and O₂ in the gas phase (μ_{O_2}) under standard conditions are needed. We compute the Mn metal free energy by DFT. As for μ_{O_2} , it is calculated indirectly from the standard potential (1.23 V) of water splitting.

$$\mu_{\text{O}_2} = 2\mu_{\text{H}_2\text{O}} - 2\mu_{\text{H}_2} + 4.92 \quad (\text{S11})$$

Here, $\mu_{\text{H}_2\text{O}}$ and μ_{H_2} are the chemical potentials of water and hydrogen under the standard conditions, respectively, which can be calculated by DFT. It should be noted that the chemical potential of water in the liquid phase at the standard conditions equals to that of the gas phase water at the saturated vapor pressure.

Then, we can utilize Eq. S10 to compute $\mu_{\text{H}_2\text{O}}$.

1.4 Microkinetic Simulation

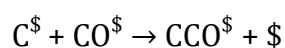
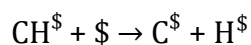
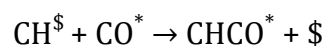
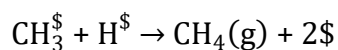
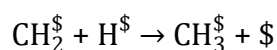
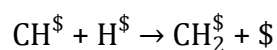
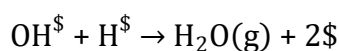
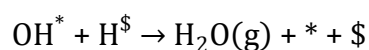
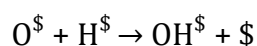
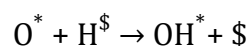
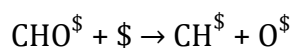
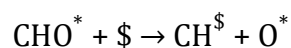
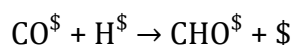
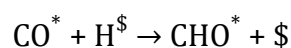
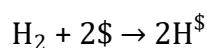
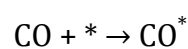
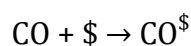
Our microkinetics simulation utilizes the following conditions.

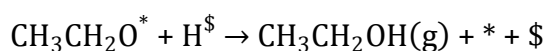
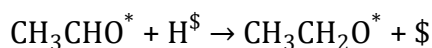
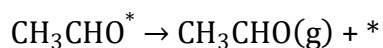
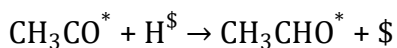
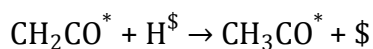
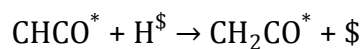
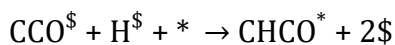
(i) To ensure consistency for the enthalpy changes of the gas-phase reaction $2\text{CO}(\text{g}) + 4\text{H}_2(\text{g}) \rightarrow \text{CH}_3\text{CH}_2\text{OH}(\text{g}) + \text{H}_2\text{O}(\text{g})$ (-2.65 eV from experiment¹¹ and -3.44 eV from PBE functional) between experiment and DFT calculations, we have made adjustments to the DFT gas-phase enthalpies of CO (-0.15 eV), H₂ (-0.10 eV), and H₂O (+0.09 eV), which effectively modifies the adsorption energy of the species.

(ii) Since our reaction pathway shows that the step-edge of (211) surface is the active site, our simulation exclusively considers reactions occurring at the step-edge and omits reactions taking place on the terrace.

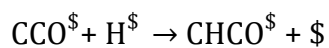
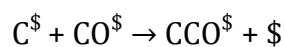
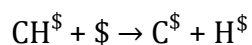
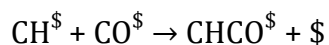
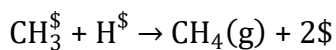
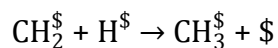
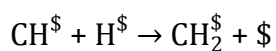
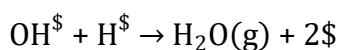
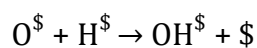
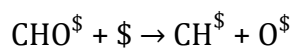
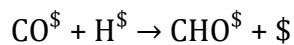
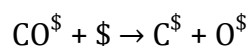
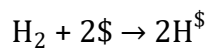
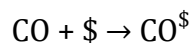
(iii) For MnRh(211), two types of active sites are considered in a 1:1 ratio: Rh_{sb} (denoted as \$) and Mn_{sb} or Mn_{B5} (denoted as *). The definition of these sites can be seen in Figure 1b or Figure S10. In the case of Rh(211), only \$ sites are available. The key elementary reactions incorporated in the microkinetic simulations are outlined as follows.

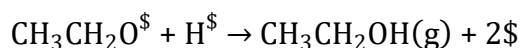
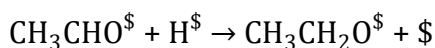
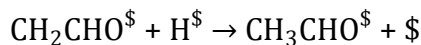
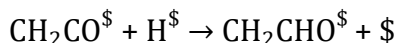
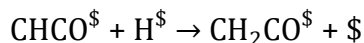
(a) Reactions on MnRh(211):





(b) Reactions on Rh(211):





(iv) The lateral adsorbate-adsorbate interaction is used to correct the free energies of adsorbates or transition states (TSs), using the following equation:

$$G_{\text{int}}(A) = G_0(A) + E_{\text{CO}}(A) - E_0(A) \quad (\text{S12})$$

Here, A represents the adsorbates or TSs undergoing correction. $G_{\text{int}}(A)$, $G_0(A)$, $E_{\text{CO}}(A)$, and $E_0(A)$, are the free energy of A after correction for lateral interaction, the free energy of A in the zero-coverage limit, the energy of A at high CO coverage at the step edge, and the energy of A in the zero-coverage limit, respectively.

For the * sites, Eq. S12 is applied to the 0.17-0.17 ML(b) MnRh(211) surface, while for \$ sites, we apply Eq. S12 to the Rh(211) surface, since the Rh_{sb} sites are sequential with high probability for real catalysts. As an example, the snapshots of the TSs for CH₃CH₂O-H under zero and high CO coverage on 0.17-0.17 ML(b) MnRh(211) and Rh(211) are shown in Figure S1. The free energies (Eq. 3) of the TSs on 0.17-0.17 ML(b) MnRh(211) are -1.37 eV with adsorbed CO and -1.44 eV without adsorbed CO, resulting in a lateral adsorbate-adsorbate interaction of 0.07 eV for the TS. Using the same method, the interaction is 0.03 eV for the TS on Rh(211).

In both cases, the application of Eq. S12 requires a high CO coverage on \$ sites, which is consistent with our microkinetic simulation results (see Tables S12 and S13). The corrected free energies for adsorbates and TSs on 0.17-0.17 ML(b) MnRh(211) and Rh(211) for adsorbates and TSs are listed in Tables S4-S7. It should be noted that since CO adsorption on the RhMn_{sb} site is unstable, with the adsorbed CO automatically migrating to the top site of the step-edge Rh atom, the lateral interactions for the adsorbates of TSs at * sites are small.

(v) The degrees of rate control (DRC) for species, and apparent activation energies are calculated using Eqs. S13 and S14, following the methodology outlined by Campbell et al:^{12, 13}

$$X_{i,p} = \left(\frac{\partial(\ln(r_p))}{\partial(-G_i^0/RT)} \right)_{G_{j \neq i}} \quad (\text{S13})$$

$$E_{\text{app},p} = RT + \sum_i X_{i,p} H_i^0 \quad (\text{S14})$$

Here, i and j represent the adsorbates or TSs; p represents the product (acetaldehyde or methane); X_i is the DRC of adsorbates or TSs; $E_{\text{app},p}$ is the apparent activation energy; r_p is the production rate; and G_i^0 and H_i^0 are the standard-state Gibbs free energy or enthalpy, respectively, which can be calculated using Eq. 3 (or in a similar way for H_i^0).

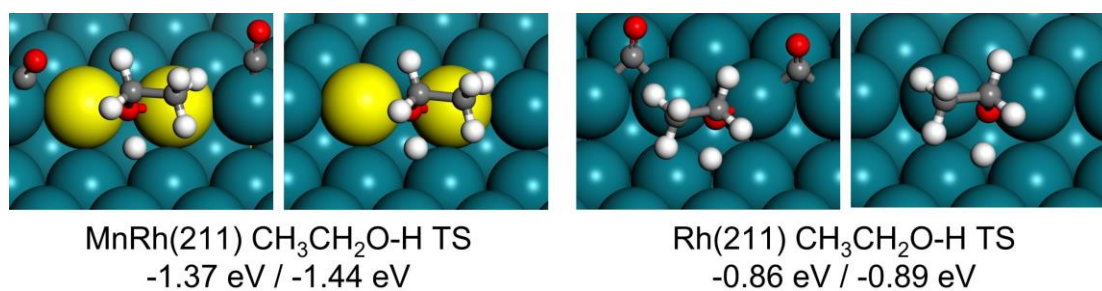


Figure S1. Transition state snapshots of CH₃CH₂O hydrogenation on 0.17-0.17 ML(b) MnRh(211) and Rh(211) under high or zero CO step edge coverage. Free energies (Eq. 3) are also provided.

Table S4. Free energy (Eq. 3, with respect to gas phase molecules and 0.17-0.17 ML(b) MnRh(211)) of adsorbates with and without the correction of lateral interaction on MnRh(211) at 523 K. The pressures of H₂, CO, and H₂O are set at 13.33, 6.67, and 10⁻⁵ bar, respectively.

Species	<i>G</i> on MnRh(211) (eV)	
	Without correction	With correction
CO ^{\$}	-1.18	-0.79
CO*(Mn _{B5})	-0.94	-0.91
CO*(Mn _{sb})	-0.12	-0.07
OH ^{\$}	0.71	0.93
OH*	-0.06	-0.02
O ^{\$}	0.97	1.53
O*	0.17	0.30
CHO ^{\$}	-0.38	0.00
CHO*	-0.85	-0.79
H ^{\$}	-0.30	-0.33
C ^{\$}	-1.55	-1.50
CH ^{\$}	-1.63	-1.44
CH ₂ ^{\$}	-1.37	-1.12
CH ₃ ^{\$}	-1.56	-1.21
CCO ^{\$}	-1.84	-1.50
CHCO*	-2.20	-2.15
CH ₂ CO*	-1.85	-1.68
CH ₃ CO*	-2.26	-2.19
CH ₃ CHO*	-1.93	-1.88
CH ₃ CH ₂ O*	-2.23	-2.24

Table S5. Free energies of TS (G_{TS}) for surface reaction considered in microkinetics simulation on 0.17-0.17 ML(b) MnRh(211) under typical reaction conditions. The results with or without correction of lateral interaction are both listed. G_{TS} is calculated using Eq. 3, with respect to gas phase molecules and 0.17-0.17 ML(b) MnRh(211), and the forward (ΔG_f) and reverse barriers (ΔG_r) are calculated with respect to the surface intermediates, whose free energies are listed in Table S4. It should be noted that the microkinetics simulation consider the specific reaction sites, so the barriers may different from those listed in Table S10, where the barriers are calculated with respect to the most stable adsorption states of the surface intermediates.

Elementary reaction	Without correction			With correction		
	G_{TS} (eV)	ΔG_f (eV)	ΔG_r (eV)	G_{TS} (eV)	ΔG_f (eV)	ΔG_r (eV)
$CO^* + H^\$ \rightarrow CHO^* + \$$	-0.71	0.53	0.14	-0.70	0.54	0.09
$CO^\$ + H^\$ \rightarrow CHO^\$ + \$$	-0.28	1.20	0.10	0.02	1.14	0.02
$CHO^* + \$ \rightarrow CH^\$ + O^*$	-0.39	0.46	1.07	-0.26	0.47	0.88
$CHO^\$ + \$ \rightarrow CH^\$ + O^\$$	0.42	0.80	1.08	0.74	0.74	0.65
$O^* + H^\$ \rightarrow OH^* + \$$	0.61	0.74	0.67	0.53	0.56	0.55
$O^\$ + H^\$ \rightarrow OH^\$ + \$$	1.45	0.78	0.86	2.04	0.84	1.11
$OH^* + H^\$ \rightarrow H_2O + * + \$$	0.86	1.22	0.86	0.83	1.19	0.83
$OH^\$ + H^\$ \rightarrow H_2O + 2\$$	1.47	1.18	1.47	1.58	0.98	1.58
$CH^\$ + H^\$ \rightarrow CH_2^\$ + \$$	-1.28	0.65	0.09	-1.10	0.67	0.02
$CH_2^\$ + H^\$ \rightarrow CH_3^\$ + \$$	-1.28	0.39	0.28	-1.19	0.26	0.02
$CH_3^\$ + H^\$ \rightarrow CH_4 + 2\$$	-1.06	0.80	1.75	-1.10	0.44	1.71
$CH^\$ + CO^* \rightarrow CHCO^* + \$$	-1.64	0.93	0.56	-1.61	0.74	0.54
$CH^\$ + \$ \rightarrow C^\$ + H^\$$	-1.02	0.61	0.83	-1.03	0.41	0.80
$C^\$ + CO^* \rightarrow CCO^* + \$$	-1.36	1.37	0.48	-1.08	1.33	0.42
$CCO^* + H^\$ \rightarrow CHCO^* + \$$	-1.48	0.66	0.72	-1.06	0.77	1.09
$CHCO^* + H^\$ \rightarrow CH_2CO^* + \$$	-1.61	0.89	0.24	-1.49	0.99	0.19
$CH_2CO^* + H^\$ \rightarrow CH_3CO^* + \$$	-1.87	0.28	0.39	-1.82	0.19	0.37
$CH_3CO^* + H^\$ \rightarrow CH_3CHO^* + \$$	-1.76	0.80	0.17	-1.68	0.84	0.20
$CH_3CHO^* + H^\$ \rightarrow CH_3CH_2O^* + \$$	-1.65	0.58	0.58	-1.66	0.55	0.58
$CH_3CH_2O^* + H^\$ \rightarrow CH_3CH_2OH + * + \$$	-1.44	1.09	1.12	-1.37	1.20	1.19

Table S6. Free energy (Eq. 3, with respect to gas phase molecules and Rh(211)) of CO^{\$}, CO^{*}, O^{\$}, O^{*}, OH^{\$} and OH^{*} with and without the correction of lateral interaction on Rh(211) at 523 K. The pressures of H₂, CO, and H₂O are set at 13.33, 6.67, and 10⁻⁵ bar, respectively.

Species	<i>G</i> on Rh(211) (eV)	
	Without correction	With correction
CO ^{\$}	-1.16	-0.77
OH ^{\$}	0.71	0.93
O ^{\$}	0.97	1.53
CHO ^{\$}	-0.38	0.00
H ^{\$}	-0.28	-0.31
C ^{\$}	-1.63	-1.58
CH ^{\$}	-1.69	-1.50
CH ₂ ^{\$}	-1.40	-1.15
CH ₃ ^{\$}	-1.51	-1.16
CCO ^{\$}	-1.87	-1.53
CHCO ^{\$}	-1.89	-1.65
CH ₂ CO ^{\$}	-1.62	-1.33
CH ₂ CHO ^{\$}	-1.79	-1.76
CH ₃ CHO ^{\$}	-1.63	-1.39
CH ₃ CH ₂ O ^{\$}	-1.56	-1.27

Table S7. Free energies of TS (G_{TS}) for surface reaction considered in microkinetics simulation on Rh(211) under typical reaction conditions. The results with or without lateral interaction are both listed. G_{TS} is calculated using Eq. 3, with respect to gas phase molecules and Rh(211), and the forward (ΔG_f) and reverse barriers (ΔG_r) are calculated with respect to the surface intermediates, whose free energies are listed in Table S6.

Elementary reaction	Without correction			With correction		
	G_{TS} (eV)	ΔG_f (eV)	ΔG_r (eV)	G_{TS} (eV)	ΔG_f (eV)	ΔG_r (eV)
$CO^{\$} + \$ \rightarrow C^{\$} + O^{\$}$	0.64	1.80	1.30	1.38	2.15	1.43
$CO^{\$} + H^{\$} \rightarrow CHO^{\$} + \$$	-0.28	1.16	0.10	0.02	1.10	0.02
$CHO^{\$} + \$ \rightarrow CH^{\$} + O^{\$}$	0.42	0.80	1.14	0.74	0.74	0.71
$O^{\$} + H^{\$} \rightarrow OH^{\$} + \$$	1.45	0.76	0.74	2.04	0.82	1.11
$OH^{\$} + H^{\$} \rightarrow H_2O + 2\$$	1.47	1.04	1.47	1.58	0.96	1.58
$CH^{\$} + H^{\$} \rightarrow CH_2^{\$} + \$$	-1.30	0.67	0.10	-1.12	0.69	0.03
$CH_2^{\$} + H^{\$} \rightarrow CH_3^{\$} + \$$	-1.22	0.46	0.29	-1.13	0.33	0.03
$CH_3^{\$} + H^{\$} \rightarrow CH_4 + 2\$$	-1.04	0.75	1.77	-1.08	0.39	1.73
$CH^{\$} + CO^{\$} \rightarrow CHCO^{\$} + \$$	-1.54	1.31	0.35	-1.03	1.24	0.62
$CH^{\$} + \$ \rightarrow C^{\$} + H^{\$}$	-1.10	0.59	0.81	-1.11	0.39	0.78
$C^{\$} + CO^{\$} \rightarrow CCO^{\$} + \$$	-1.40	1.39	0.47	-1.12	1.23	0.41
$CCO^{\$} + H^{\$} \rightarrow CHCO^{\$} + \$$	-1.54	0.61	0.35	-1.12	0.72	0.53
$CHCO^{\$} + H^{\$} \rightarrow CH_2CO^{\$} + \$$	-1.31	0.86	0.31	-1.28	0.68	0.05
$CH_2CO^{\$} + H^{\$} \rightarrow CH_2CHO^{\$} + \$$	-1.35	0.55	0.44	-1.00	0.64	0.76
$CH_2CHO^{\$} + H^{\$} \rightarrow CH_3CHO^{\$} + \$$	-1.54	0.53	0.09	-1.03	1.04	0.36
$CH_3CHO^{\$} + H^{\$} \rightarrow CH_3CH_2O^{\$} + \$$	-1.17	0.74	0.39	-0.77	0.93	0.50
$CH_3CH_2O^{\$} + H^{\$} \rightarrow CH_3CH_2OH + 2\$$	-0.89	0.95	1.67	-0.86	0.72	1.70

2. Thermodynamics of Mn-Promoted Rh Surfaces

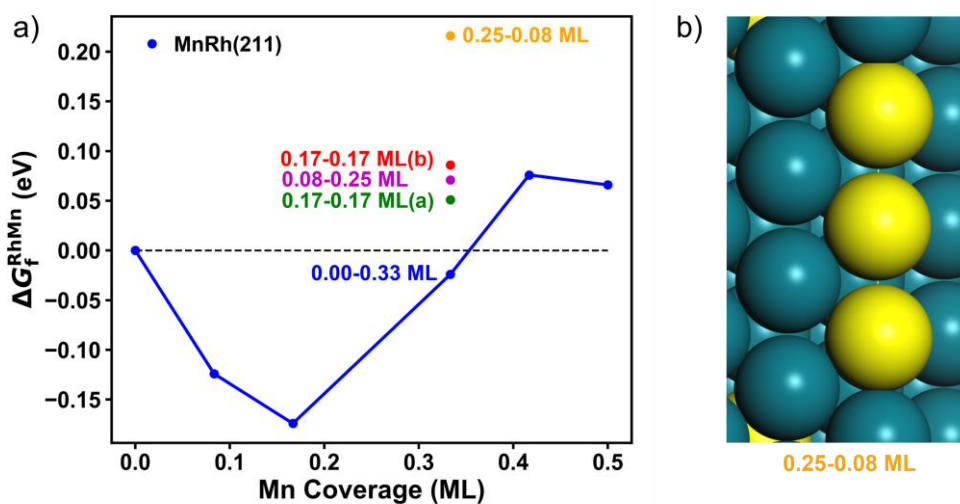


Figure S2. (a) The differential formation free energy (Eq. 2) for Mn on Rh(211) surface at 523 K. The pressures of H_2 , CO, and H_2O are set at 13.33, 6.67, and 10^{-5} bar, respectively. Points along the solid blue lines are taken from the GM, while the others are related to less stable structures. (b) Structure snapshots of 0.25-0.08 ML MnRh(211). Other configurations can be found in Figure 1b. Rh: dark green, Mn: yellow.

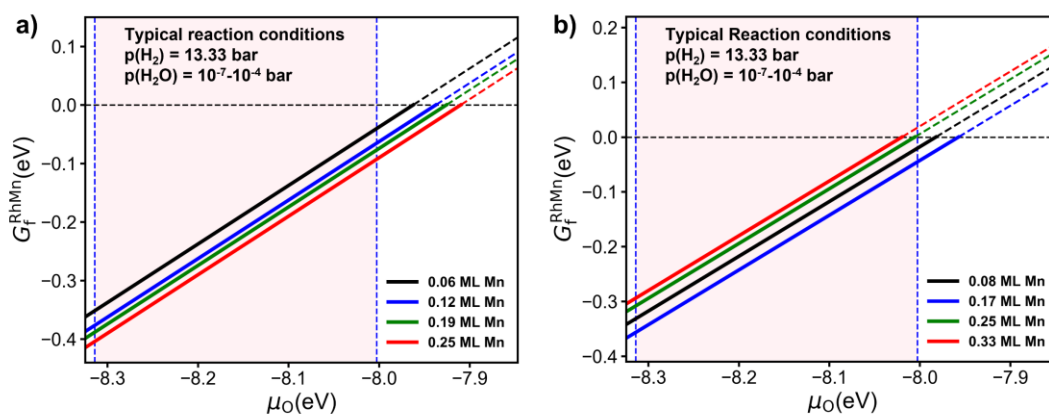


Figure S3. (a, b) Stability diagram of Mn-promoted Rh(111) and Rh(211) GM with various Mn content at 523 K, respectively, based on the formation free energy data (see Eq. 1). The typical reaction condition is in pink background framed by two blue dashed lines.

3. CO Dissociation on Mn-Promoted Rh Surfaces

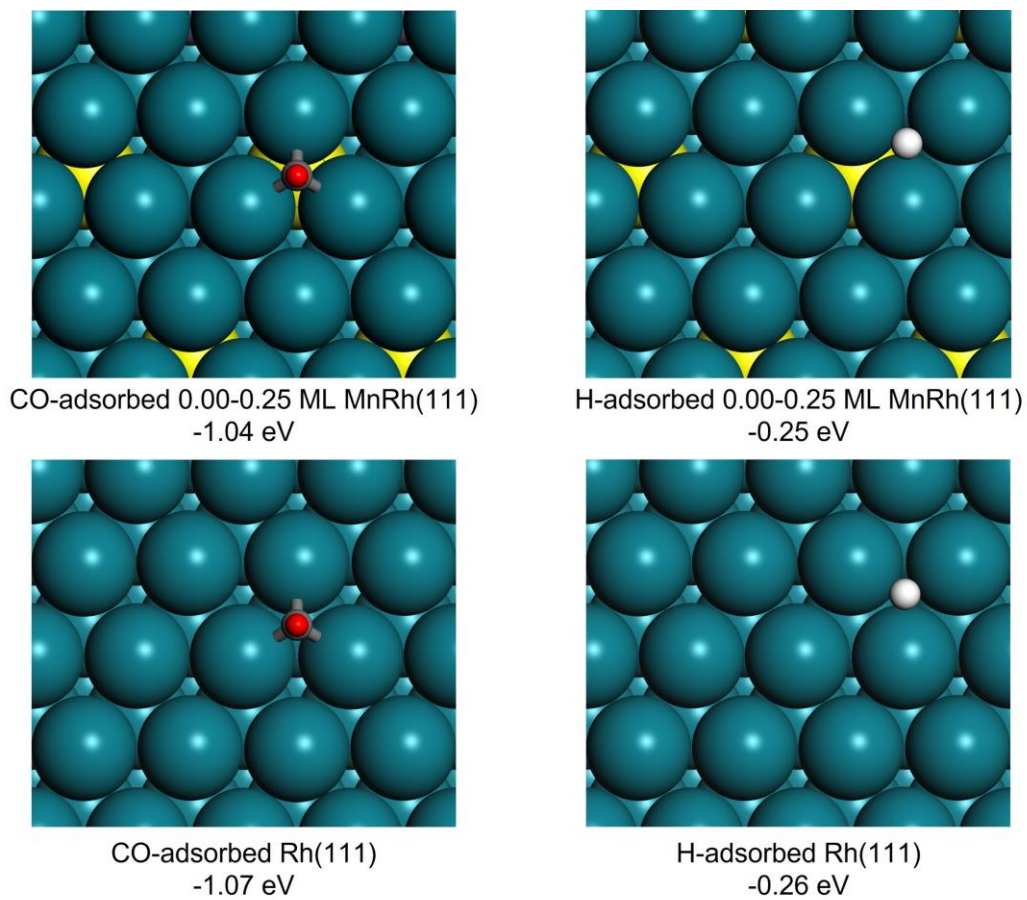


Figure S4. Snapshots for CO or H-adsorbed 0.00-0.25 ML MnRh(111) and Rh(111). The free energies (Eq.3, with respect to gas phase molecules and 0.00-0.25 ML MnRh(111) or Rh(111)) are also presented. Rh: dark green, Mn: yellow, O: red, C: grey, H: white.

Table S8. Free energy barriers for CO dissociation on Rh(111), MnRh(111), Rh(211), or MnRh(211) surfaces. The symbol * represents surface sites.

Reaction	G_b (eV) ^a			
	Rh(111)	MnRh(111)	Rh(211)	MnRh(211)
$\text{CO}^* + * \rightarrow \text{C}^* + \text{O}^*$	2.78	2.79	1.71	1.22
$\text{CHO}^* + * \rightarrow \text{CH}^* + \text{O}^*$	2.50	2.36	1.74	1.12
$\text{COH}^* + * \rightarrow \text{C}^* + \text{OH}^*$	2.49	2.62	1.87	1.68
$\text{CH}_2\text{O}^* + * \rightarrow \text{CH}_2^* + \text{O}^*$	2.97	2.93	2.52	1.93
$\text{CHOH}^* + * \rightarrow \text{CH}^* + \text{OH}^*$	2.41	2.34	2.36	2.18
$\text{CH}_3\text{O}^* + * \rightarrow \text{CH}_3^* + \text{O}^*$	3.55	3.35	3.08	2.56
$\text{CH}_2\text{OH}^* + * \rightarrow \text{CH}_2^* + \text{OH}^*$	3.11	2.93	2.62	2.35
$\text{CH}_3\text{OH}^* + * \rightarrow \text{CH}_3^* + \text{OH}^*$	3.83	3.86	3.51	3.33

^a For comparison, the effective free energy barrier (G_b) here is calculated with respect to adsorbed CO^* and H^* on Rh(111) for Rh surface and on 0.00-0.25 ML MnRh(111) for MnRh surfaces.

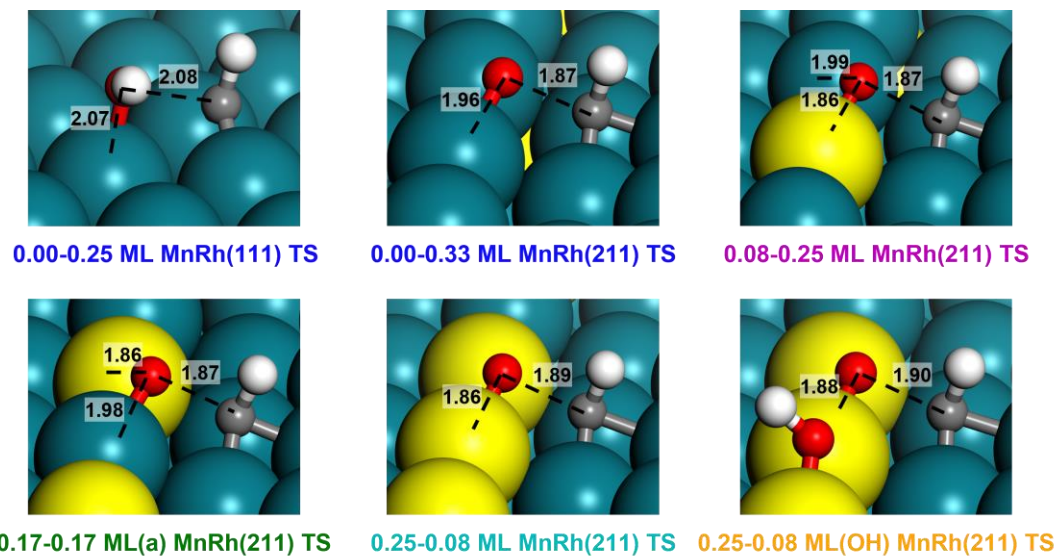


Figure S5. Enlarged snapshots for important TSs in Figure 2a, c and Figure S6. Rh: dark green, Mn: yellow, O: red, C: grey, H: white.

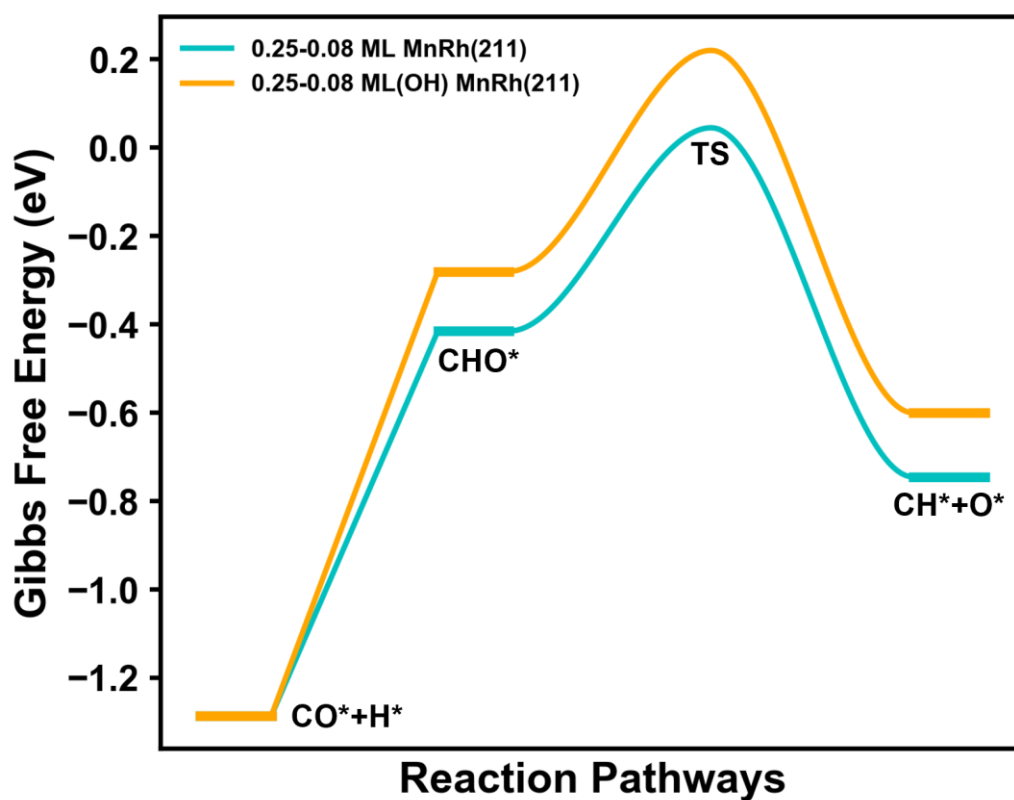


Figure S6. Free energy profile for C-O bond dissociation pathway on 0.25-0.08 ML MnRh(211) with or without pre-adsorbed OH*. The Gibbs free energies are calculated using Eq. 3 under the typical experimental conditions with respect to corresponding most stable clean surface and molecules (CO, H₂) in the gas phase. The initial structures are treated the adsorbed CO* and H* on 0.00-0.25 ML MnRh(111).

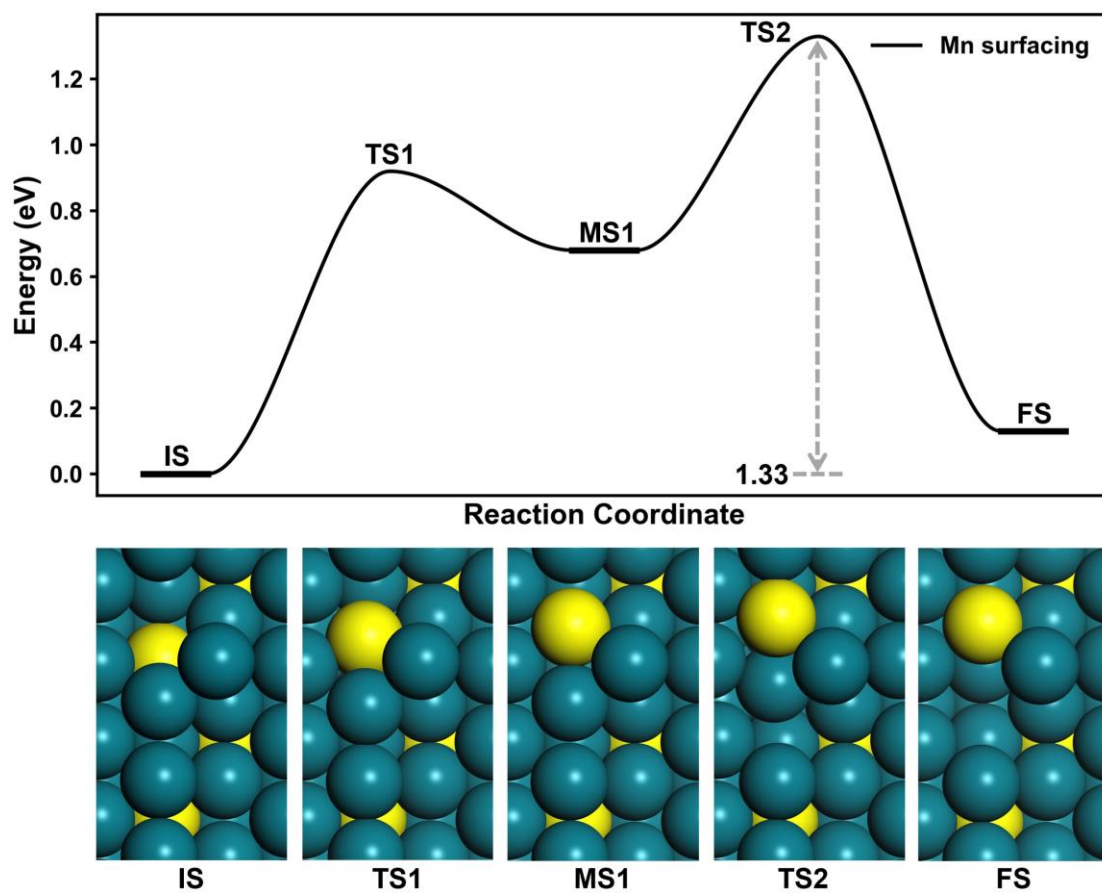


Figure S7. Energy profile for Mn surfacing to the first layer followed by surface Rh sinking to the second layer on 0.17-0.17(b) MnRh(211) with Rh defect. Rh: dark green, Mn: yellow, C: grey, H: white.

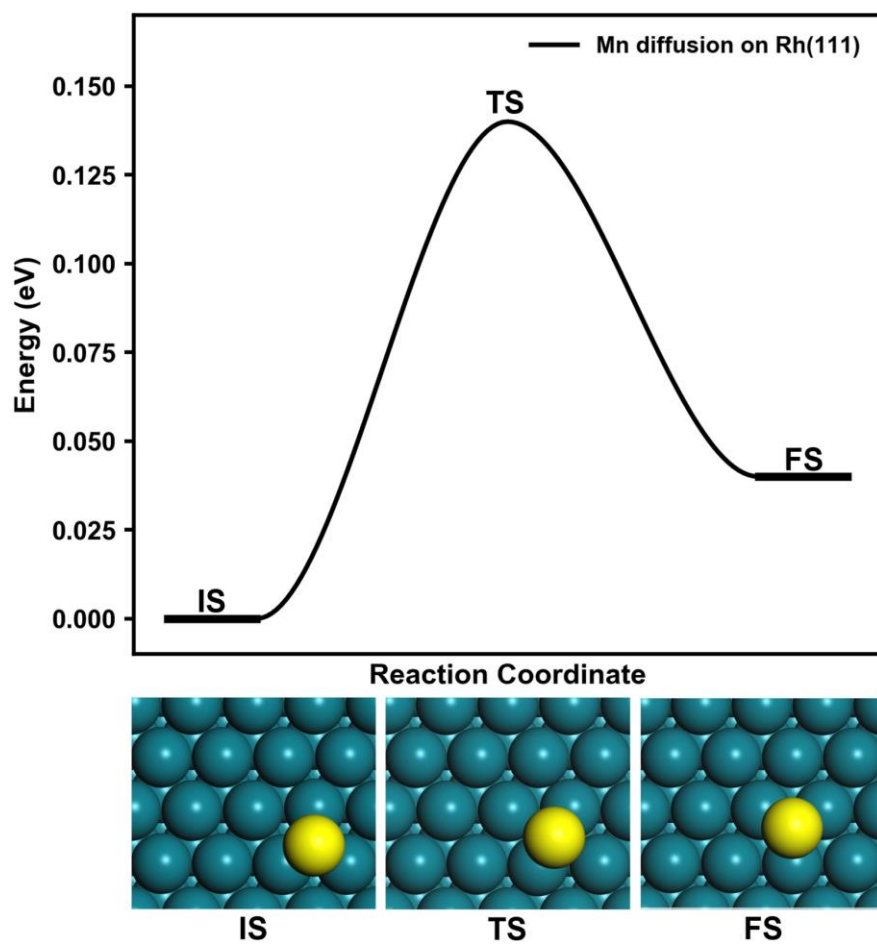


Figure S8. Energy profile for Mn diffusion on Rh(111). Rh: dark green, Mn: yellow, C: grey, H: white.

Table S9. Free energies (Eq. 3, with respect to gas phase molecules and 0.00-0.25 ML MnRh(111) or 0.17-0.17 ML(b) MnRh(211)) of different O or OH-adsorbed MnRh(111) or MnRh(211) surfaces at 523 K. Pressures of H₂, CO, and H₂O are set at 13.33, 6.67, and 10⁻⁵ bar, respectively.

Surface	<i>G</i> (eV)
MnRh(111)	
O-adsorbed 0.00-0.25 ML MnRh(111)	1.14
O-adsorbed 0.06-0.19 ML MnRh(111)	1.08
O-adsorbed 0.12-0.12 ML MnRh(111)	1.03
O-adsorbed 0.19-0.06 ML MnRh(111)	0.83
MnRh(211)	
OH-adsorbed 0.00-0.33 ML MnRh(211)	0.51
OH-adsorbed 0.08-0.25 ML MnRh(211)	0.31
OH-adsorbed 0.17-0.17(a) ML MnRh(211)	0.25
OH-adsorbed 0.17-0.17(b) ML MnRh(211)	-0.06
OH-adsorbed 0.25-0.08 ML MnRh(211)	0.19
2OH-adsorbed 0.25-0.08 ML MnRh(211)	0.35

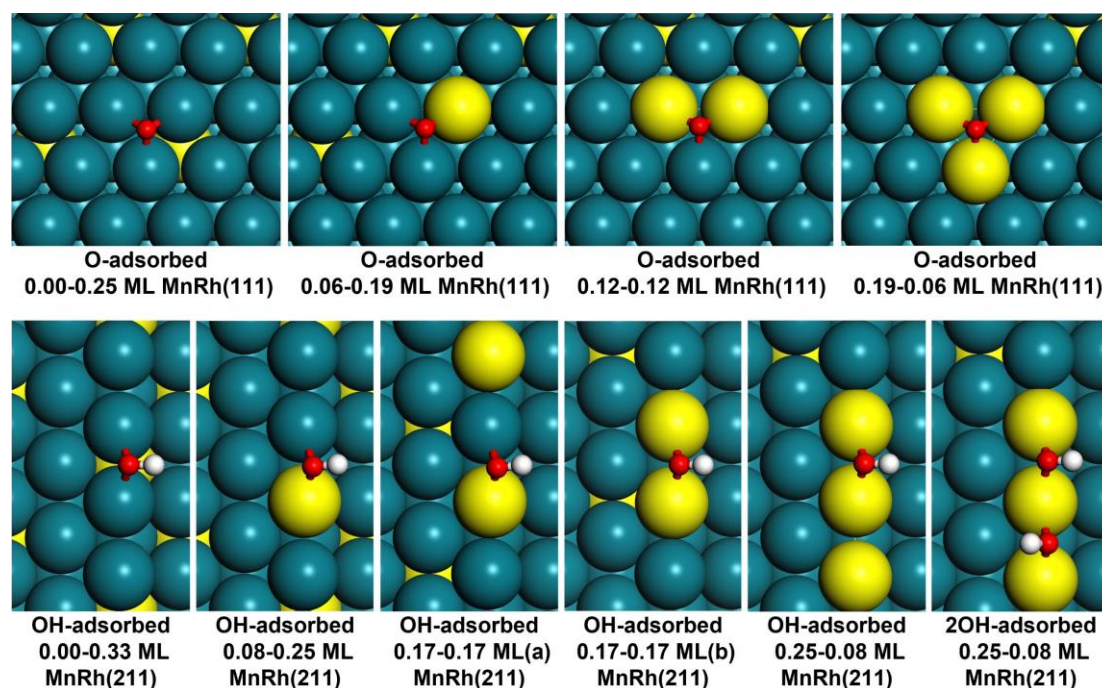


Figure S9. Spatial configurations of the surfaces in Table S9. Rh: dark green, Mn: yellow, O: red, H: white.

4. Reaction Networks and Mechanisms for CO Hydrogenation on MnRh(211) and Rh(211)

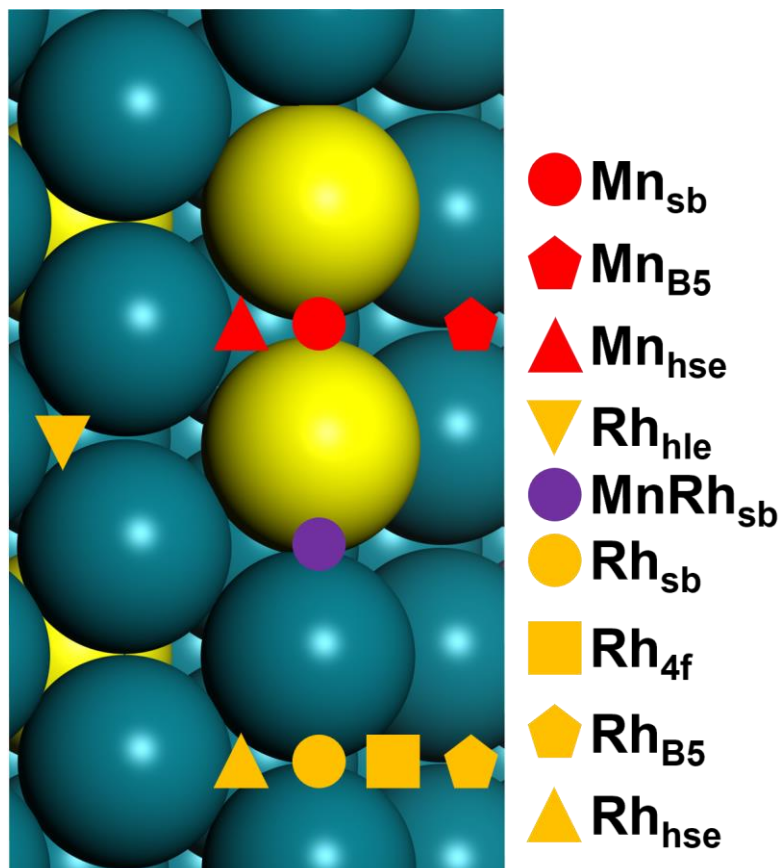


Figure S10. Schematic representation for key sites on MnRh(211) surface. Rh: dark green, Mn: yellow.

Table S10. Free energies of TS (G_{TS}) and free energy barriers for elementary reactions in the CO hydrogenation reaction network (Figure 3a, b), on 0.17-0.17 ML(b) MnRh(211) and Rh(211) under typical reaction conditions. G_{TS} is calculated using Eq. 3, with respect to gas phase molecules and 0.17-0.17 ML(b) MnRh(211) or Rh(211), and the forward (ΔG_f) and reverse barriers (ΔG_r) are calculated with respect to the most stable adsorption states of the surface intermediates, whose free energies are listed in Table S11. The symbol * represents surface sites.

Elementary reaction	MnRh(211)			Rh(211)		
	G_{TS} (eV)	ΔG_f (eV)	ΔG_r (eV)	G_{TS} (eV)	ΔG_f (eV)	ΔG_r (eV)
$CO^* + H^* \rightarrow CHO^* + *$	-0.71	0.77	0.14	-0.28	1.16	0.10
$CO^* + H^* \rightarrow COH^* + *$	-0.23	1.25	0.18	-0.27	1.17	0.19
$CHO^* + H^* \rightarrow CH_2O^* + *$	-0.24	0.91	0.16	-0.01	0.65	0.09
$CHO^* + H^* \rightarrow CHOH^* + *$	0.20	1.35	0.40	0.19	0.85	0.41
$COH^* + H^* \rightarrow CHOH^* + *$	0.18	0.89	0.38	0.17	0.91	0.39
$CH_2O^* + H^* \rightarrow CH_3O^* + *$	-0.02	0.68	0.79	0.35	0.73	0.48
$CH_2O^* + H^* \rightarrow CH_2OH^* + *$	0.17	0.87	0.29	0.44	0.82	0.39
$CHOH^* + H^* \rightarrow CH_2OH^* + *$	0.06	0.56	0.18	0.15	0.65	0.10
$CH_3O^* + H^* \rightarrow CH_3OH^* + *$	0.01	1.12	0.09	0.78	1.19	0.53
$CH_2OH^* + H^* \rightarrow CH_3OH^* + *$	0.53	0.95	0.61	0.59	0.82	0.34
$CO^* + * \rightarrow C^* + O^*$	-0.04	1.14	1.34	0.64	1.80	1.30
$CHO^* + * \rightarrow CH^* + O^*$	-0.39	0.46	1.07	0.42	0.80	1.14
$COH^* + * \rightarrow C^* + OH^*$	0.17	0.58	1.78	0.55	1.01	1.47
$CH_2O^* + * \rightarrow CH_2^* + O^*$	0.17	0.57	1.37	0.94	1.04	1.37
$CHOH^* + * \rightarrow CH^* + OH^*$	0.42	0.62	2.11	0.78	1.00	1.76
$CH_3O^* + * \rightarrow CH_3^* + O^*$	0.55	1.36	1.94	1.25	1.38	1.79
$CH_2OH^* + * \rightarrow CH_2^* + OH^*$	0.34	0.46	1.77	0.79	0.74	1.48
$CH_3OH^* + * \rightarrow CH_3^* + OH^*$	1.07	1.15	2.69	1.42	1.17	2.22
$O^* + H^* \rightarrow OH^* + *$	0.61	0.74	0.67	1.45	0.76	0.74
$OH^* + H^* \rightarrow H_2O + 2^*$	0.86	1.22	0.86	1.47	1.04	1.47
$C^* + H^* \rightarrow CH^* + *$	-1.02	0.83	0.61	-1.10	0.81	0.59
$CH^* + H^* \rightarrow CH_2^* + *$	-1.28	0.65	0.09	-1.30	0.67	0.10
$CH_2^* + H^* \rightarrow CH_3^* + *$	-1.28	0.39	0.28	-1.22	0.46	0.29
$CH_3^* + H^* \rightarrow CH_4 + 2^*$	-1.06	0.80	1.75	-1.04	0.75	1.77
$C^* + CO^* \rightarrow CCO^* + *$	-1.36	1.37	0.48	-1.40	1.39	0.47
$CH^* + CO^* \rightarrow CHCO^* + *$	-1.64	1.17	0.56	-1.54	1.31	0.35
$CH_2^* + CO^* \rightarrow CH_2CO^* + *$	-1.61	0.94	0.24	-1.53	1.03	0.09
$CH_3^* + CO^* \rightarrow CH_3CO^* + *$	-1.27	1.47	0.99	-1.25	1.42	0.78
$C^* + CHO^* \rightarrow CCHO^* + *$	-0.89	1.51	1.38	-0.70	1.31	1.10
$CH^* + CHO^* \rightarrow CHCHO^* + *$	-1.22	1.26	0.77	-0.91	1.16	0.53
$CH_2^* + CHO^* \rightarrow CH_2CHO^* + *$	-1.07	1.15	1.11	-0.79	0.99	1.00
$CH_3^* + CHO^* \rightarrow CH_3CHO^* + *$	-1.05	1.36	0.88	-0.80	1.09	0.83
$CCO^* + H^* \rightarrow CHCO^* + *$	-1.48	0.66	0.72	-1.54	0.61	0.35

$\text{CCO}^* + \text{H}^* \rightarrow \text{CCHO}^* + *$	-1.25	0.89	1.02	-1.20	0.95	0.60
$\text{CCO}^* + \text{H}^* \rightarrow \text{CCOH}^* + *$	-0.93	1.21	0.89	-0.96	1.19	0.91
$\text{CHCO}^* + \text{H}^* \rightarrow \text{CH}_2\text{CO}^* + *$	-1.61	0.89	0.24	-1.31	0.86	0.31
$\text{CHCO}^* + \text{H}^* \rightarrow \text{CHCHO}^* + *$	-1.44	1.06	0.55	-1.02	1.15	0.42
$\text{CHCO}^* + \text{H}^* \rightarrow \text{CHCOH}^* + *$	-1.05	1.45	0.59	-1.12	1.05	0.60
$\text{CCHO}^* + \text{H}^* \rightarrow \text{CHCHO}^* + *$	-1.95	0.62	0.04	-1.36	0.72	0.08
$\text{CCHO}^* + \text{H}^* \rightarrow \text{CCH}_2\text{O}^* + *$	-1.29	1.28	1.10	-1.09	0.99	0.69
$\text{CCHO}^* + \text{H}^* \rightarrow \text{CCHOH}^* + *$	-0.98	1.59	0.37	-1.08	1.00	0.38
$\text{CCOH}^* + \text{H}^* \rightarrow \text{CHCOH}^* + *$	-1.48	0.64	0.16	-1.56	0.59	0.16
$\text{CCOH}^* + \text{H}^* \rightarrow \text{CCHOH}^* + *$	-0.98	1.14	0.37	-1.18	0.97	0.28
$\text{CH}_2\text{CO}^* + \text{H}^* \rightarrow \text{CH}_3\text{CO}^* + *$	-1.87	0.28	0.39	-1.26	0.64	0.77
$\text{CH}_2\text{CO}^* + \text{H}^* \rightarrow \text{CH}_2\text{CHO}^* + *$	-1.60	0.55	0.58	-1.35	0.55	0.44
$\text{CH}_2\text{CO}^* + \text{H}^* \rightarrow \text{CH}_2\text{COH}^* + *$	-1.19	0.96	0.48	-1.21	0.69	0.47
$\text{CHCHO}^* + \text{H}^* \rightarrow \text{CH}_2\text{CHO}^* + *$	-1.65	0.64	0.53	-1.26	0.46	0.53
$\text{CHCHO}^* + \text{H}^* \rightarrow \text{CHCH}_2\text{O}^* + *$	-1.33	0.96	0.45	-0.93	0.79	0.19
$\text{CHCHO}^* + \text{H}^* \rightarrow \text{CHCHOH}^* + *$	-0.98	1.31	0.42	-1.02	0.70	0.41
$\text{CHCOH}^* + \text{H}^* \rightarrow \text{CH}_2\text{COH}^* + *$	-1.26	0.68	0.41	-1.29	0.71	0.39
$\text{CHCOH}^* + \text{H}^* \rightarrow \text{CHCHOH}^* + *$	-1.02	0.92	0.38	-1.07	0.93	0.36
$\text{CCH}_2\text{O}^* + \text{H}^* \rightarrow \text{CHCH}_2\text{O}^* + *$	-1.70	0.99	0.08	-0.97	1.09	0.15
$\text{CCH}_2\text{O}^* + \text{H}^* \rightarrow \text{CCH}_2\text{OH}^* + *$	-1.13	1.56	0.32	-0.93	1.13	0.51
$\text{CCHOH}^* + \text{H}^* \rightarrow \text{CHCHOH}^* + *$	-1.09	0.56	0.31	-1.15	0.59	0.28
$\text{CCHOH}^* + \text{H}^* \rightarrow \text{CCH}_2\text{OH}^* + *$	-0.99	0.66	0.46	-1.11	0.63	0.33
$\text{CH}_3\text{CO}^* + \text{H}^* \rightarrow \text{CH}_3\text{CHO}^* + *$	-1.76	0.80	0.17	-1.66	0.65	0.00
$\text{CH}_3\text{CO}^* + \text{H}^* \rightarrow \text{CH}_3\text{COH}^* + *$	-1.29	1.27	0.43	-1.31	1.00	0.43
$\text{CH}_2\text{CHO}^* + \text{H}^* \rightarrow \text{CH}_3\text{CHO}^* + *$	-1.88	0.60	0.05	-1.54	0.53	0.09
$\text{CH}_2\text{CHO}^* + \text{H}^* \rightarrow \text{CH}_2\text{CH}_2\text{O}^* + *$	-1.35	1.13	0.46	-0.92	1.15	0.28
$\text{CH}_2\text{CHO}^* + \text{H}^* \rightarrow \text{CH}_2\text{CHOH}^* + *$	-1.42	1.06	0.23	-1.15	0.92	0.34
$\text{CH}_2\text{COH}^* + \text{H}^* \rightarrow \text{CH}_3\text{COH}^* + *$	-1.46	0.51	0.26	-1.45	0.51	0.29
$\text{CH}_2\text{COH}^* + \text{H}^* \rightarrow \text{CH}_2\text{CHOH}^* + *$	-1.46	0.51	0.19	-1.45	0.51	0.04
$\text{CHCH}_2\text{O}^* + \text{H}^* \rightarrow \text{CH}_2\text{CH}_2\text{O}^* + *$	-1.32	0.76	0.49	-0.65	0.75	0.55
$\text{CHCH}_2\text{O}^* + \text{H}^* \rightarrow \text{CHCH}_2\text{OH}^* + *$	-0.85	1.23	0.40	-0.55	0.85	0.52
$\text{CHCHOH}^* + \text{H}^* \rightarrow \text{CH}_2\text{CHOH}^* + *$	-1.29	0.41	0.36	-1.25	0.46	0.24
$\text{CHCHOH}^* + \text{H}^* \rightarrow \text{CHCH}_2\text{OH}^* + *$	-0.92	0.78	0.33	-1.02	0.69	0.05
$\text{CCH}_2\text{OH}^* + \text{H}^* \rightarrow \text{CHCH}_2\text{OH}^* + *$	-1.13	0.62	0.12	-0.78	0.94	0.29
$\text{CH}_3\text{CHO}^* + \text{H}^* \rightarrow \text{CH}_3\text{CH}_2\text{O}^* + *$	-1.65	0.58	0.58	-1.17	0.74	0.39
$\text{CH}_3\text{CHO}^* + \text{H}^* \rightarrow \text{CH}_3\text{CHOH}^* + *$	-1.27	0.96	0.28	-1.03	0.88	0.37
$\text{CH}_3\text{COH}^* + \text{H}^* \rightarrow \text{CH}_3\text{CHOH}^* + *$	-1.39	0.63	0.16	-1.32	0.70	0.08
$\text{CH}_2\text{CH}_2\text{O}^* + \text{H}^* \rightarrow \text{CH}_3\text{CH}_2\text{O}^* + *$	-1.50	0.61	0.73	-0.85	0.63	0.71
$\text{CH}_2\text{CH}_2\text{O}^* + \text{H}^* \rightarrow \text{CH}_2\text{CH}_2\text{OH}^* + *$	-1.01	1.10	0.40	-0.66	0.82	0.76
$\text{CH}_2\text{CHOH}^* + \text{H}^* \rightarrow \text{CH}_3\text{CHOH}^* + *$	-1.28	0.67	0.27	-1.27	0.50	0.13
$\text{CH}_2\text{CHOH}^* + \text{H}^* \rightarrow \text{CH}_2\text{CH}_2\text{OH}^* + *$	-1.07	0.88	0.34	-1.07	0.70	0.35
$\text{CHCH}_2\text{OH}^* + \text{H}^* \rightarrow \text{CH}_2\text{CH}_2\text{OH}^* + *$	-0.91	0.64	0.50	-0.83	0.52	0.59
$\text{CH}_3\text{CH}_2\text{O}^* + \text{H}^* \rightarrow \text{CH}_3\text{CH}_2\text{OH} + 2^*$	-1.44	1.09	1.12	-0.89	0.95	1.67
$\text{CH}_3\text{CHOH}^* + \text{H}^* \rightarrow \text{CH}_3\text{CH}_2\text{OH} + 2^*$	-0.73	1.12	1.83	-0.80	0.88	1.76
$\text{CH}_2\text{CH}_2\text{OH}^* + \text{H}^* \rightarrow \text{CH}_3\text{CH}_2\text{OH} + 2^*$	-0.98	0.73	1.58	-0.82	0.88	1.74

Table S11. Free energies (Eq. 3, with respect to gas phase molecules and 0.17-0.17 ML(b) MnRh(211) or Rh(211)) for adsorbed species on 0.17-0.17 ML(b) MnRh(211) and Rh(211). The symbol * represents surface sites.

Speices	MnRh(211)		Rh(211)	
	G/eV	Geometries	G/eV	Geometries
C*	-1.55	Rh _{4f}	-1.63	Rh _{4f}
H*	-0.30	Rh _{sb}	-0.28	Rh _{sb}
O*	0.17	Mn _{sb}	0.97	Rh _{sb}
CO*	-1.18	Rh _{sb} via C	-1.16	Rh _{sb} via C
OH*	-0.06	Mn _{sb} via O	0.71	Rh _{sb} via O
CH*	-1.63	Rh _{4f} via C	-1.69	Rh _{4f} via C
CH ₂ *	-1.37	Rh _{sb} via C	-1.40	Rh _{sb} via C
CH ₃ *	-1.56	Rh _{sb} via C	-1.51	Rh _{sb} via C
CHO*	-0.85	Mn _{B5} via C and O	-0.38	Rh _{sb} via C and O
COH*	-0.41	Rh _{hse} via C	-0.46	Rh _{hse} via C
CHOH*	-0.20	Rh _{sb} via C	-0.22	Rh _{sb} via C
CH ₂ O*	-0.40	MnRh _{sb} via C and O	-0.10	Rh _{sb} via C and O
CH ₂ OH*	-0.12	MnRh _{sb} via C and O	0.05	Rh _{sb} via C and O
CH ₃ O*	-0.81	Mn _{sb} via O	-0.13	Rh _{sb} via O
CH ₃ OH*	-0.08	Mn _{sb} via O	0.25	Gas
CCO*	-1.84	Rh _{sb} via 2C	-1.87	Rh _{B5} via 2C
CHCO*	-2.20	Mn _{B5} via 2C and O	-1.89	Rh _{B5} via 2C and O
CCHO*	-2.27	Mn _{B5} via β -C and O	-1.80	Rh _{B5} via β -C and O
CCOH*	-1.82	Rh _{B5} via 2C	-1.87	Rh _{B5} via 2C
CH ₂ CO*	-1.85	MnRh _{sb} via α -C and O	-1.62	Rh _{sb} via α -C and O
CHCHO*	-1.99	Mn _{B5} via β -C and O	-1.44	Rh _{hse} via β -C and O
CHCOH*	-1.64	Rh _{B5} via 2C	-1.72	Rh _{ff} via 2C
CCH ₂ O*	-2.39	Mn _{B5} via β -C and O	-1.78	Rh _{B5} via β -C and O
CCHOH*	-1.35	Rh _{hse} via β -C	-1.46	Rh _{4f} via β -C
CH ₃ CO*	-2.26	MnRh _{sb} via α -C and O	-2.03	Rh _{sb} via α -C and O
CH ₂ CHO*	-2.18	MnRh _{sb} via 2C and O	-1.79	Rh _{sb} via 2C and O
CH ₂ COH*	-1.67	Rh _{sb} via 2C	-1.68	Rh _{sb} via 2C
CHCH ₂ O*	-1.78	Mn _{B5} via β -C and O	-1.12	Rh _{B5} via β -C and O
CHCHOH*	-1.40	Rh _{sb} via β -C	-1.43	Rh _{sb} via β -C
CCH ₂ OH*	-1.45	MnRh _{B5} via β -C and O	-1.44	Rh _{hle} via β -C
CH ₃ CHO*	-1.93	MnRh _{sb} via α -C and O	-1.63	Rh _{sb} via α -C and O
CH ₃ COH*	-1.72	Rh _{sb} via α -C	-1.74	Rh _{sb} via α -C
CH ₂ CH ₂ O*	-1.81	Mn _{hse} via β -C and O	-1.20	Rh _{hse} via β -C and O
CH ₂ CHOH*	-1.65	MnRh _{sb} via 2C and O	-1.49	Rh _{sb} via 2C
CHCH ₂ OH*	-1.25	MnRh _{4f} via β -C and O	-1.07	Rh _{4f} via β -C and O
CH ₃ CH ₂ O*	-2.23	Mn _{sb} via O	-1.56	Rh _{sb} via O
CH ₃ CHOH*	-1.55	MnRh _{sb} via α -C and O	-1.40	Rh _{sb} via α -C and O
CH ₂ CH ₂ OH*	-1.41	MnRh _{sb} via β -C and O	-1.42	Rh _{sb} via β -C and O

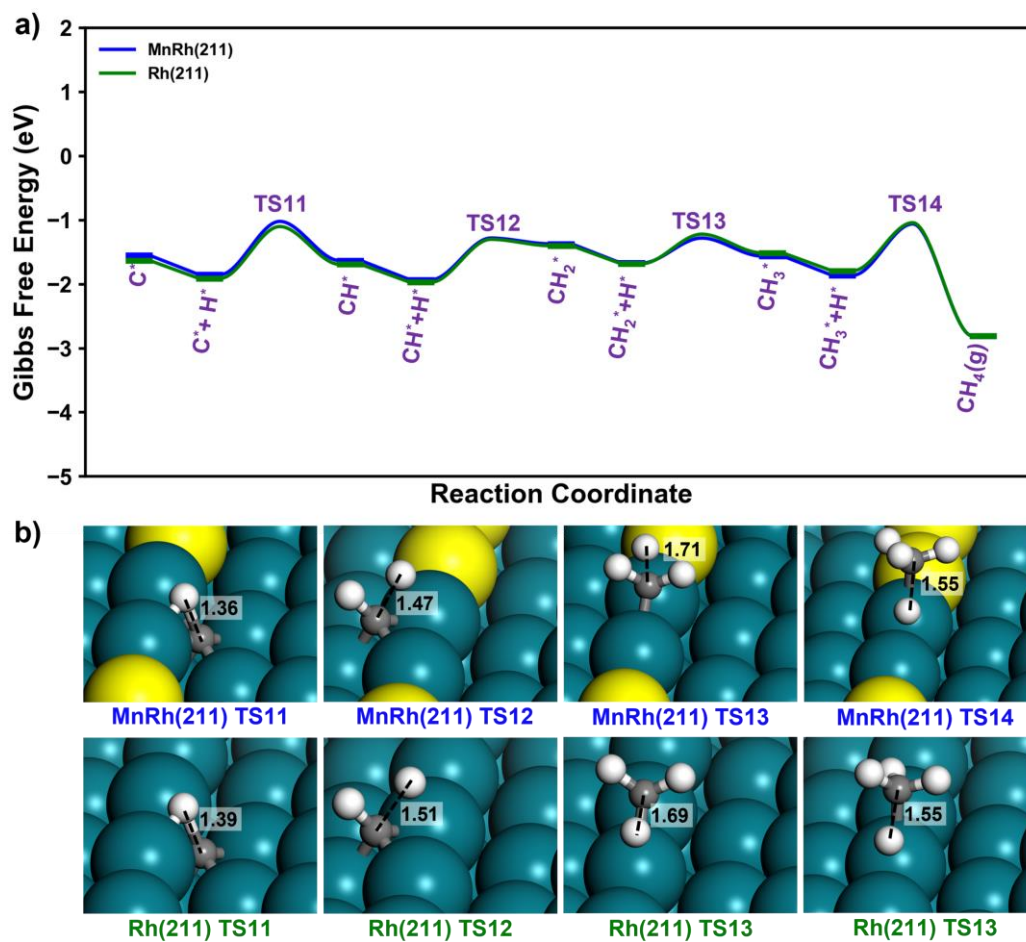


Figure S11. (a) Free energy profiles for C* hydrogenation to CH₄. The symbol * represents surface sites. (b) Local images of key TS structures in (a). Rh: dark green, Mn: yellow, C: grey, H: white.

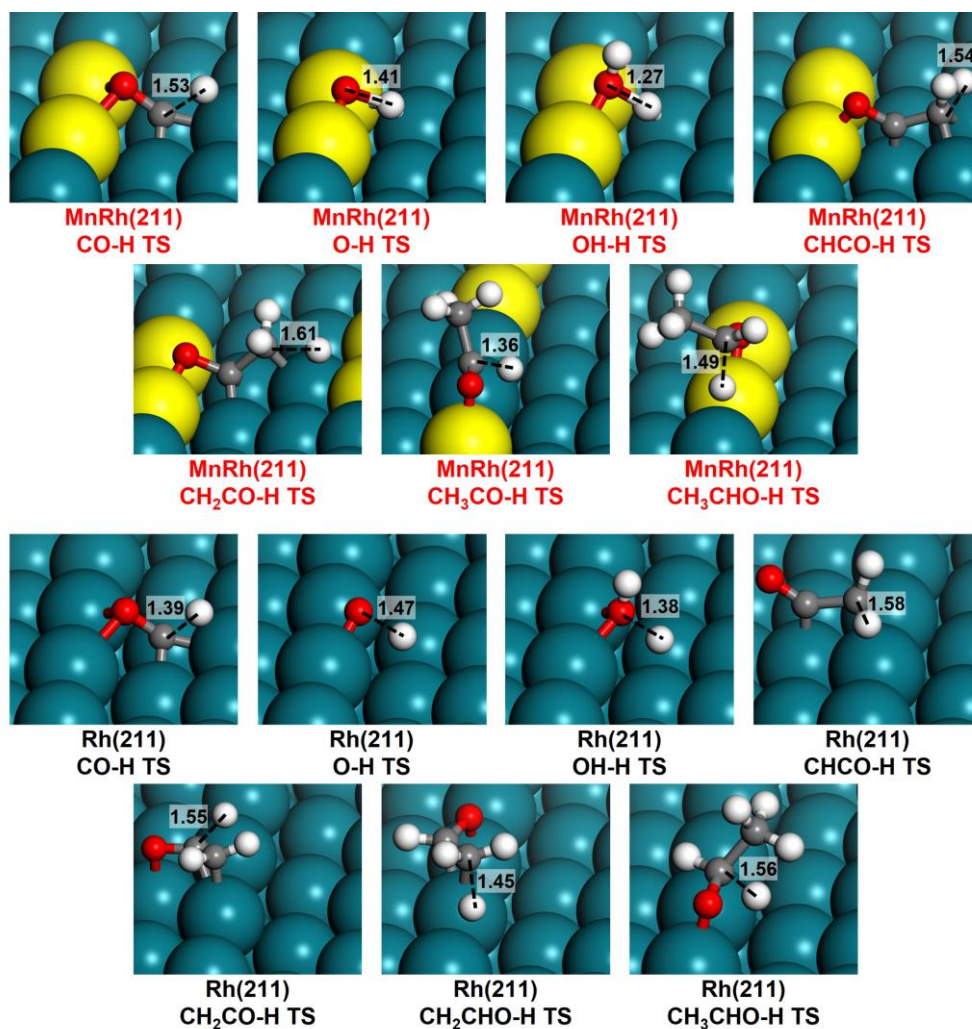


Figure S12. Snapshots for TS structures in profiles plotted in Figure 3c. The snapshots for TSs of CH-O, CH-CO, and CH₃CH₂O-H can be seen in Figure 2d or 3d. Rh: dark green, Mn: yellow, C: grey, O: red, H: white.

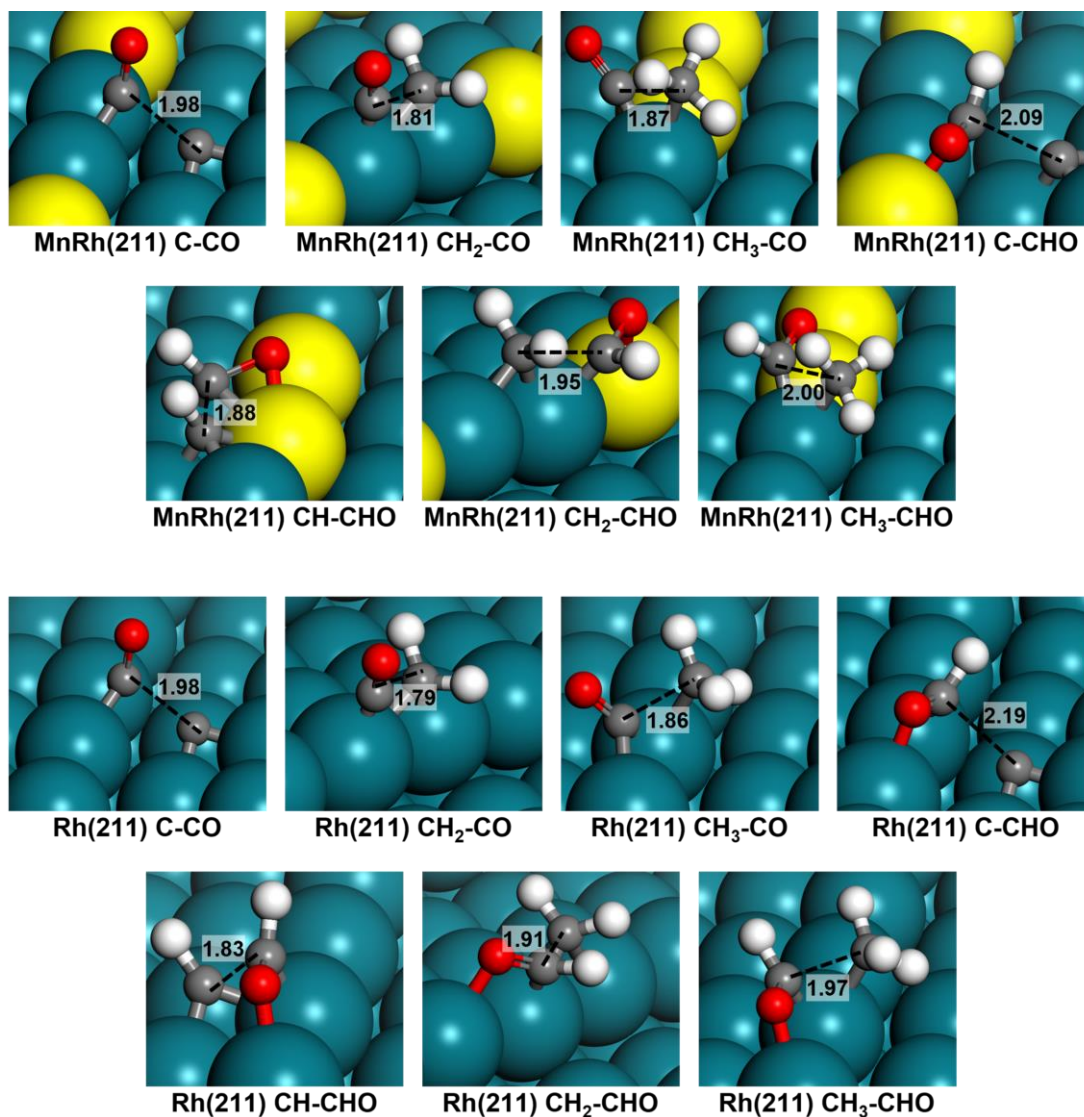


Figure S13. Snapshots of TS structures for C-C coupling. The images of CH-CO can be seen in Figure 3d. Rh: dark green, Mn: yellow, C: grey, O: red, H: white.

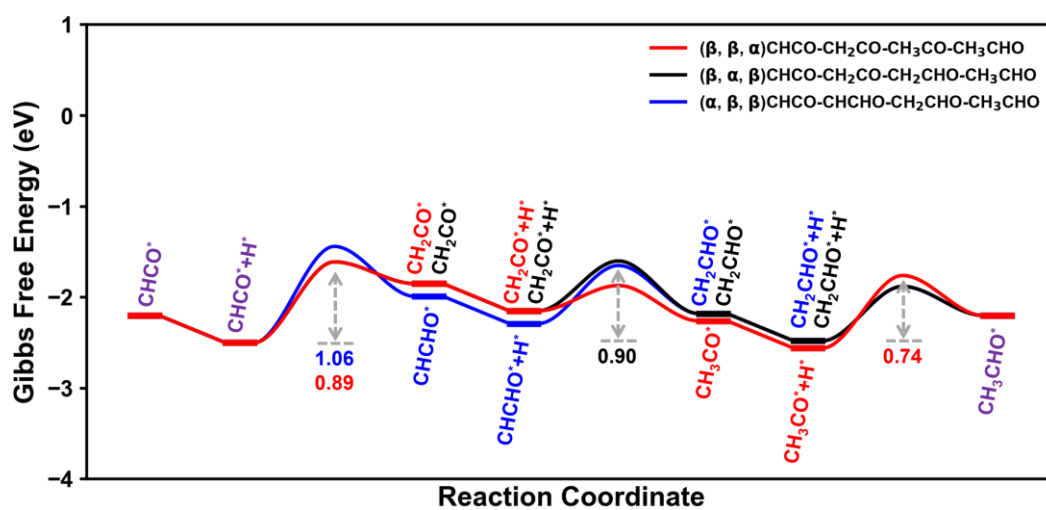


Figure S14. Free energy profiles for three different mechanisms from CHCO* hydrogenation to CH₃CHO* on MnRh(211). The symbol * represents surface sites.

5. Microkinetics

Table S12. Surface coverage of species on MnRh(211) at 523 K with or without artificial 0.05 eV increment to the free energy of H₂ gas. Pressures of H₂, CO, and H₂O are set at 13.33, 6.67, and 10⁻⁵ bar, respectively. The definition of coverage can be seen in Eq. 4.

Species	Coverage (ML)	
	Without increment	With 0.05 eV increment
\$	7.50E-07	7.51E-07
*	2.09E-10	1.44E-10
CO ^{\$}	9.99E-01	9.99E-01
CO [*]	3.98E-03	2.75E-03
OH ^{\$}	2.01E-10	5.84E-10
OH [*]	9.88E-01	9.94E-01
O ^{\$}	8.99E-12	2.61E-11
O [*]	2.71E-03	1.57E-03
CHO ^{\$}	7.33E-09	1.28E-08
CHO [*]	8.34E-05	1.00E-04
H ^{\$}	3.42E-04	5.95E-04
C ^{\$}	9.82E-04	2.96E-04
CH ^{\$}	7.80E-05	4.10E-05
CH ₂ ^{\$}	1.78E-08	1.41E-08
CH ₃ ^{\$}	3.79E-08	5.08E-08
CCO ^{\$}	2.22E-06	6.71E-07
CHCO [*]	4.80E-03	1.71E-03
CH ₂ CO [*]	6.06E-09	1.39E-09
CH ₃ CO [*]	1.48E-04	5.83E-05
CH ₃ CHO [*]	4.06E-16	2.79E-16
CH ₃ CH ₂ O [*]	3.60E-13	4.30E-13

Table S13. Surface coverage of species on Rh(211) at 523 K. Pressures of H₂, CO, and H₂O are set at 13.33, 6.67, and 10⁻⁵ bar, respectively. The definition of coverage can be seen in Eq. 4.

Species	Coverage (ML)
\$	1.17E-06
CO ^{\$}	9.99E-01
OH ^{\$}	5.16E-09
O ^{\$}	2.31E-10
CHO ^{\$}	1.21E-08
H ^{\$}	3.62E-04
C ^{\$}	6.55E-09
CH ^{\$}	3.53E-10
CH ₂ ^{\$}	4.58E-14
CH ₃ ^{\$}	1.65E-14
CCO ^{\$}	7.00E-11
CHCO ^{\$}	3.18E-10
CH ₂ CO ^{\$}	8.35E-14
CH ₂ CHO ^{\$}	2.28E-10
CH ₃ CHO ^{\$}	7.85E-24
CH ₃ CH ₂ O ^{\$}	5.21E-26

Table S14 Rates of all relevant elementary reactions on 0.17-0.17(b) ML MnRh(211) at 523 K. Pressures of H₂, CO, and H₂O are set at 13.33, 6.67, and 10⁻⁵ bar, respectively.

Elementary reaction	Forward rate (s ⁻¹)	Backward rate(s ⁻¹)
CO + \$ → CO ^{\$}	8.49E+07	8.49E+07
CO + * → CO*	2.31E+04	2.31E+04
H ₂ + 2\$ → 2H ^{\$}	1.98E+02	1.98E+02
CO* + H ^{\$} → CHO* + \$	1.49E+02	1.49E+02
CO ^{\$} + H ^{\$} → CHO ^{\$} + \$	6.32E-02	6.32E-02
CHO* + \$ → CH ^{\$} + O*	3.25E-02	1.19E-02
CHO ^{\$} + \$ → CH ^{\$} + O ^{\$}	1.98E-12	7.13E-18
O* + H ^{\$} → OH* + \$	6.31E+01	6.31E+01
O ^{\$} + H ^{\$} → OH ^{\$} + \$	2.06E-12	7.38E-14
OH* + H ^{\$} → H ₂ O + * + \$	2.07E-02	-
OH ^{\$} + H ^{\$} → H ₂ O + 2\$	1.98E-12	-
CH ^{\$} + H ^{\$} → CH ₂ ^{\$} + \$	2.75E-01	2.62E-01
CH ₂ ^{\$} + H ^{\$} → CH ₃ ^{\$} + \$	3.15E-01	3.02E-01
CH ₃ ^{\$} + H ^{\$} → CH ₄ + 2\$	1.30E-02	-
CH ^{\$} + CO* → CHCO* + \$	4.02E-01	3.95E-01
CH ^{\$} + \$ → C ^{\$} + H ^{\$}	1.83E-01	1.83E-01
C ^{\$} + CO ^{\$} → CCO ^{\$} + \$	2.53E-03	2.53E-03
CCO ^{\$} + H ^{\$} + * → CHCO* + 2\$	1.64E-13	2.31E-12
CHCO* + H ^{\$} → CH ₂ CO* + \$	8.76E-03	1.13E-03
CH ₂ CO* + H ^{\$} → CH ₃ CO* + \$	5.43E-01	5.36E-01
CH ₃ CO* + H ^{\$} → CH ₃ CHO* + \$	7.63E-03	1.05E-10
CH ₃ CHO* → CH ₃ CHO + *	7.63E-03	-
CH ₃ CHO* + H ^{\$} → CH ₃ CH ₂ O* + \$	2.15E-11	2.15E-11
CH ₃ CH ₂ O* + H ^{\$} → CH ₃ CH ₂ OH* + * + \$	1.10E-14	-

Table S15. Rates of all relevant elementary reactions on Rh(211) at 523 K. Pressures of H₂, CO, and H₂O are set at 13.33, 6.67, and 10⁻⁵ bar, respectively..

Elementary reaction	Forward rate (s ⁻¹)	Backward rate(s ⁻¹)
CO + \$ → CO ^{\$}	8.51E+07	8.51E+07
H ₂ + 2\$ → 2H ^{\$}	1.99E+02	1.99E+02
CO ^{\$} + \$ → C ^{\$} + O ^{\$}	2.44E-14	2.74E-19
CO ^{\$} + H ^{\$} → CHO ^{\$} + \$	9.90E-02	9.90E-02
CHO ^{\$} + \$ → CH ^{\$} + O ^{\$}	1.14E-08	1.28E-13
O ^{\$} + H ^{\$} → OH ^{\$} + \$	1.14E-08	1.33E-12
OH ^{\$} + H ^{\$} → H ₂ O + 2\$	1.14E-08	-
CH ^{\$} + H ^{\$} → CH ₂ ^{\$} + \$	3.12E-07	3.01E-07
CH ₂ ^{\$} + H ^{\$} → CH ₃ ^{\$} + \$	1.19E-07	1.08E-07
CH ₃ ^{\$} + H ^{\$} → CH ₄ + 2\$	1.13E-08	-
CH ^{\$} + CO ^{\$} → CHCO ^{\$} + \$	4.32E-09	4.31E-09
CH ^{\$} + \$ → C ^{\$} + H ^{\$}	7.86E-07	7.86E-07
C ^{\$} + CO ^{\$} → CCO ^{\$} + \$	1.00E-07	1.00E-07
CCO ^{\$} + H ^{\$} → CHCO ^{\$} + \$	3.18E-08	3.17E-08
CHCO ^{\$} + H ^{\$} → CH ₂ CO ^{\$} + \$	3.52E-07	3.51E-07
CH ₂ CO ^{\$} + H ^{\$} → CH ₂ CHO ^{\$} + \$	2.24E-10	1.38E-10
CH ₂ CHO ^{\$} + H ^{\$} → CH ₃ CHO ^{\$} + \$	8.56E-11	3.40E-20
CH ₃ CHO ^{\$} → CH ₃ CHO + \$	8.56E-11	-
CH ₃ CHO ^{\$} + H ^{\$} → CH ₃ CH ₂ O ^{\$} + \$	3.38E-23	1.01E-23
CH ₃ CH ₂ O [*] + H ^{\$} → CH ₃ CH ₂ OH [*] + 2\$	2.37E-23	-

Table S16. Rates and selectivities of products on different surfaces at 523 K. Pressures of H₂, CO, and H₂O are set at 13.33, 6.67, and 10⁻⁵ bar, respectively.

Product	MnRh(211) (Without increment)		MnRh(211) (With 0.05 eV increment)		Rh(211)	
	Rate (s ⁻¹)	Selectivity ^a	Rate (s ⁻¹)	Selectivity ^a	Rate (s ⁻¹)	Selectivity ^a
CH ₄	8.12E-03	0.48	1.89E-02	0.76	1.13E-08	0.01
CH ₃ CHO	4.43E-03	0.52	3.04E-03	0.24	8.56E-11	0.99
CH ₃ CH ₂ OH	3.66E-15	0.00	7.61E-15	0.00	2.37E-23	0.00
H ₂ O	1.25E-02	-	2.20E-02	-	1.14E-08	-

^aThe selectivity of product *A* is calculated by $\chi(A) = \frac{n_A r(A)}{\sum_A n_A r(A)}$, where $\chi(A)$ is the selectivity of *A*, n_A is the number of C atoms in one *A* molecule, and $r(A)$ is the production rate of *A*.

Table S17. Degrees of rate control (X_i , see Eq. S13) and enthalpies (H_i , calculated in a similar method as Eq. 3) of intermediates and TSs on 0.17-0.17 ML(b) MnRh(211). Only those with non-zero degrees of rate control values are shown.

Species	$X_{i,\text{acetaldehyde}}$	$X_{i,\text{methane}}$	H_i/eV
Intermediates			
CO ^{\$}	-0.222	-1.431	-1.72
CO*	-0.007	-0.002	-1.93
O*	-0.005	-0.002	-0.42
OH*	-1.756	-0.560	-1.46
CHCO*	-0.009	-0.003	-3.15
C ^{\$}	0.000	-0.001	-1.28
CO(g)	0.222	1.431	0
H ₂ (g)	0.331	-0.972	0
TSs			
CHO* + \$ → CH ^{\$} + O*	-0.347	0.196	-1.48
OH* + H ^{\$} → H ₂ O + * + \$	1.551	0.681	-0.90
CH ^{\$} + H ^{\$} → CH ₂ ^{\$} + \$	-0.063	0.035	-1.46
CH ₂ ^{\$} + H ^{\$} → CH ₃ ^{\$} + \$	-0.028	0.016	-1.84
CH ₃ ^{\$} + H ^{\$} → CH ₄ + 2\$	-0.686	0.383	-2.04
CH ^{\$} + CO* → CHCO* + \$	0.010	-0.006	-2.61
CHCO* + H ^{\$} → CH ₂ CO* + \$	0.485	-0.260	-2.78
CH ₂ CO* + H ^{\$} → CH ₃ CO* + \$	0.001	-0.001	-3.40
CH ₃ CO* + H ^{\$} → CH ₃ CHO* + \$	0.080	-0.043	-3.55

* Apparent activation energy calculated using Eq. S14 is 195 kJ/mol for acetaldehyde and 238 kJ/mol for methane.

Table S18. Degrees of rate control (X_i , see Eq. S13) and enthalpies (H_i , calculated in a similar method as Eq. 3) of key intermediates and TSs on Rh(211). Only those with non-zero degrees of rate control values are shown.

Species	$X_{i,\text{acetaldehyde}}$	$X_{i,\text{methane}}$	H_i/eV
Intermediates			
CO ^{\$}	-1.999	-1.999	-1.70
CO(g)	0.007	1.007	0.00
H ₂ (g)	-0.387	-0.501	0.00
TSs			
CHO ^{\$} + \$ → CH ^{\$} + O ^{\$}	1.000	1.000	-0.49
CH ^{\$} + H ^{\$} → CH ₂ ^{\$} + \$	-0.036	0.000	-1.48
CH ₂ ^{\$} + H ^{\$} → CH ₃ ^{\$} + \$	-0.091	0.001	-1.78
CH ₃ ^{\$} + H ^{\$} → CH ₄ + 2\$	-0.865	0.007	-2.02
C ^{\$} + CO ^{\$} → CCO ^{\$} + \$	0.001	0.000	-0.67
CCO ^{\$} + H ^{\$} → CHCO ^{\$} + \$	0.002	0.000	-2.12
CH ₂ CO ^{\$} + H ^{\$} → CH ₂ CHO ^{\$} + \$	0.379	-0.003	-2.58
CH ₂ CHO ^{\$} + H ^{\$} → CH ₃ CHO ^{\$} + \$	0.611	-0.005	-2.90

* Apparent activation energy calculated using Eq. S14 is 209 kJ/mol for acetaldehyde and 286 kJ/mol for methane.

Reference

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