Supporting Information:
Understanding and Tackling the Activity and Selectivity Issues for Methane to Methanol Using Single Atom Alloys

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Contents of Supporting Information:

SI.1. Computational method

Density functional theory calculations were performed with the Perdew−Burke−Ernzerhof (PBE)[1] functional within the generalized gradient approximation (GGA) in the Vienna ab initio simulation package (VASP).[2-4] Spin-polarized calculations were performed when necessary (e.g. the host nickel surfaces). The projector-augmented wave (PAW) method was used to represent the core−valence electron interaction.[5,6] Structures were optimised until the forces on all atoms were below 0.05 eV/Å. Transition states were searched with the constrained minimization technique and verified with a vibrational frequency calculation, where no imaginary frequencies were identified as an initial state and one imaginary frequency as a transition state.[7,8]

For the DFT calculations of the metal surfaces, the cut-off energy of the plane wave basis set was 450 eV. The Brillouin zone was sampled using the Monkhorst−Pack scheme with a 6 × 6 × 1 k-point mesh.[9] A 15 Å vacuum layer was used. The metal (111) surfaces calculated were modelled as a *p*(3x3) 4 layer slab, with the bottom 2 layers fixed. The cut-off energy of the plane wave basis set was 450 eV. Methane adsorption was tested and found to be very weak across all surfaces. Therefore, methane dissociation was calculated with respect to methane in the gas phase. Single atom alloys were modelled as one single surface atom replaced in the unit cell with the defined dopant atom.

The zero-point energy and entropic contributions for surface species were calculated from frequency calculations within VASP. The translational and rotational entropies of the molecules in the gas phase were obtained from Gaussian 09 with the Becke, 3-parameter, Lee-Yang-Parr (B3LYP) hybrid functional with the 6-311++g(d p) basis set. All free energies were calculated at standard pressure and 353 K. Microkinetic modelling was performed at 353 K, with initial partial pressures of 0.9 atm and 0.1 atm for methane and oxygen, respectively, with the ratio of the partial pressures for methane and oxygen (9:1) to mirror the experimental condition.[10,11]

Microkinetic modelling was performed using CATKINAS[12,13] with the free energy changes and the activation free energies of elementary steps calculated from the VASP code. The final surface coverages of species are determined until a steady state is achieved, where the forward and reverse rates are equivalent. It should be mentioned that anharmonicity can have some contributions to the free energies, which are not considered in this work.

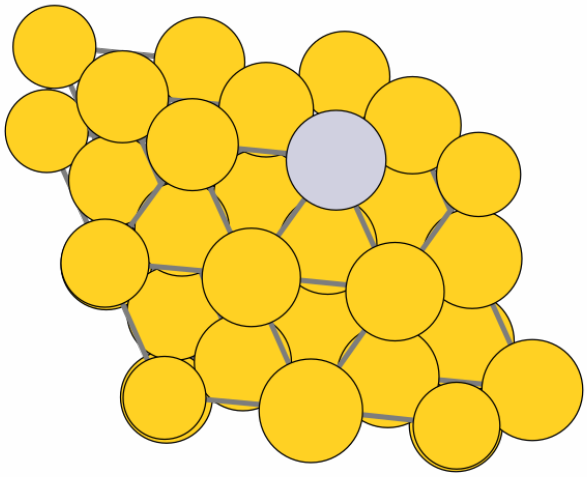
Pd-based catalysts are widely used in the field and Pd(111) is the most common Pd surface. Therefore, the properties of Pd(111) were used the benchmarks for the single atom alloys. This is to limit the number of single atom alloy candidates to a manageable number.

SI1.2. Model Information

The unit cell of the pure fcc metals were optimised and gave the following unit cell lengths:

Element	Unit cell length (Å)
Ag	4.14
Au	4.16
Cu	3.64
Ir	3.88
Ni	3.51
Pd	3.94
Pt	3.97
Rh	3.83

All pure metal surfaces and host single atom alloy surfaces were cleaved from the optimised pure metal unit cells. To make a single atom alloy, a single surface atom in the (111) *p*(3x3) host metal surface is replaced with the dopant metal as shown below:



SI2.1. Elementary steps of total methane combustion on Pd(111). Energies reported in eV.

Reactant	Product	ΔG	Ea^G
CH_4	CH_4*	0.56	0.66
CH_4*	CH_3*+H*	0.09	0.50
CH_3*	CH_2*+H*	-0.14	0.62
CH_2*	CH*+H*	-0.68	0.12
CH*	C*+H*	0.73	1.16
O_2	O_2*	-0.23	0.10
O_2*	O*+O*	-1.77	0.46
CH_3*+O*	CH_3O*	0.34	1.84
CH_2*+O*	CH_2O*	-0.26	1.05
CH*+O*	CHO*	-0.69	1.17
C*+O*	CO*	-2.43	1.34
CO*+O	CO_2*	0.25	1.31
CH_3*+OH*	CH_3OH*	-0.28	1.52
CH_2*+OH*	CH_2OH*	-0.26	0.97
CH*+OH*	CHOH*	0.10	0.97
C*+OH*	COH*	-1.26	0.90
CO*+OH*	COOH*	0.32	0.79
CH_3O*	CH_2O*+H*	-0.49	0.17
CH_2O*	CHO*+H*	-0.81	0.08
CHO*	CO*+H*	-1.21	0.47
CH_3OH*	CH_2OH*+H*	-0.53	0.40
CH_2OH*	CHOH*+H*	-0.36	0.63
CHOH*	COH*+H*	-1.04	0.70
CH_3OH*	CH_3O*+H*	0.09	0.68
CH_2OH*	CH_2O*+H*	0.09	0.61
CHOH*	CHO+H*	-0.50	0.31
COH*	CO*+H*	-0.70	0.69
COOH*	CO_2*+H*	-0.27	0.48
O*+H*	OH*	0.08	1.16
OH*+H*	H_2O*	-0.12	0.84
CH_3OH*	CH_3OH	-0.81	0.10
CH_2O*	CH_2O	-0.36	0.30
CO*	CO	1.52	2.10
CO_2*	CO_2	-0.75	0.10
H_2O*	H_2O	-0.40	0.16

SI2.2. Microkinetic model results. Rate reported in molecules per site per second.

Reactions	Forward	Backward	Overall
CH_4+#<->CH_4#	4.11E-11	4.11E-11	1.07E-30
CH_4#+#<->CH_3#+H#	1.07E-30	1.29E-35	1.07E-30
CH_3#+#<->CH_2#+H#	1.07E-30	3.14E-48	1.07E-30
CH_2#+#<->CH#+H#	2.74E-31	1.55E-47	2.74E-31
CH#+#<->C#+H#	6.46E-45	1.69E-53	6.46E-45
O_2+#<->O_2#	0.000452	0.000452	1.21E-30
O_2#+#<->O#+O#	1.03E-19	1.03E-19	1.21E-30
CH_3#+O#<->CH_3O#+#	2.57E-34	2.55E-53	2.57E-34
CH_2#+O#<->CH_2O#+#	7.96E-31	6.95E-62	7.96E-31
CH#+O#<->CHO#+#	2.74E-31	3.11E-51	2.74E-31
C#+O#<->CO#+#	6.45E-45	1.48E-97	6.45E-45
CO#+O#<->CO_2#+#	1.45E-48	4.29E-76	1.45E-48
CH_3#+OH#<->CH_3OH#+#	6.82E-39	5.1E-77	6.82E-39
CH_2#+OH#<->CH_2OH#+#	9.96E-39	8.7E-48	9.96E-39
CH#+OH#<->CHOH#+#	1.71E-37	1.6E-45	1.71E-37
C#+OH#<->COH#+#	1.01E-47	3.73E-64	1.01E-47
CO#+OH#<->COOH#+#	2.86E-50	1.64E-50	1.22E-50
CH_3O#+#<->CH_2O#+H#	2.57E-34	1.95E-60	2.57E-34
CH_2O#+#<->CHO#+H#	2.22E-44	2.74E-45	1.94E-44
CHO#+#<->CO#+H#	2.74E-31	2.17E-75	2.74E-31
CH_3OH#+#<->CH_2OH#+H#	6.88E-57	3.21E-51	-3.2E-51
CH_2OH#+#<->CHOH#+H#	2.9E-39	4.27E-55	2.9E-39

CHOH#+#<->COH#+H#	4.56E-43	5.28E-66	4.56E-43
CH_3OH#+#<->CH_3O#+H#	5.5E-61	2.84E-48	-2.8E-48
CH_2OH#+#<->CH_2O#+H#	7.06E-39	2.15E-58	7.06E-39
CHOH#+#<->CHO#+H#	1.74E-37	4.34E-44	1.74E-37
COH#+#<->CO#+H#	4.56E-43	2.3E-71	4.56E-43
COOH#+#<->CO_2#+H#	1.22E-50	1.63E-79	1.22E-50
O#+H#<->OH#+#	4.02E-26	4.02E-26	1.34E-30
OH#+H#<->H_2O#+#	1.34E-30	1.02E-56	1.34E-30
CH_3OH#<->CH_3OH+#	6.82E-39	0	6.82E-39
CH_2O#<->CH_2O+#	7.96E-31	0	7.96E-31
CO#<->CO+#	2.74E-31	0	2.74E-31
CO_2#<->CO_2+#	1.46E-48	0	1.46E-48
H_2O#<->H_2O+#	1.34E-30	0	1.34E-30

SI2.3. Streamlined microkinetic model results. Rate reported in molecules per site per second.

Reactions	Forward	Backward	Overall
CH_4+#<->CH_4#	4.11E-11	4.11E-11	1.07E-30
CH_4#+#<->CH_3#+H#	1.07E-30	1.15E-35	1.07E-30
CH_3#+#<->CH_2#+H#	1.07E-30	3.67E-53	1.07E-30
O_2+#<->O_2#	0.000452	0.000452	5.35E-31
O_2#+#<->O#+O#	1.03E-19	1.03E-19	5.35E-31
CH_3#+O#<->CH_3O#+#	2.57E-34	2.55E-53	2.57E-34
CH_3#+OH#<->CH_3OH#+#	6.08E-39	4.55E-77	6.08E-39
CH_3OH#+#<->CH_3O#+H#	4.91E-61	2.54E-48	-2.5E-48
CH_3O#+#<->CH_2O#+H#	2.57E-34	5.62E-64	2.57E-34
O#+H#<->OH#+#	3.59E-26	3.59E-26	1.07E-30
OH#+H#<->H_2O#+#	1.07E-30	8.13E-57	1.07E-30
CH_2#<->CH_2+#	1.07E-30	0	1.07E-30
CH_3OH#<->CH_3OH+#	6.08E-39	0	6.08E-39
CH_2O#<->CH_2O+#	2.57E-34	0	2.57E-34
H_2O#<->H_2O+#	1.07E-30	0	1.07E-30

SI3.1. Adsorption energies of SAA CH_3 and CH_2. All energies are in eV.

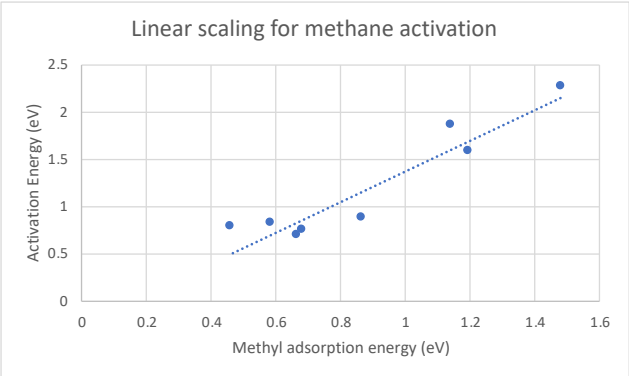
Metal	Dopant	CH_3#	CH_2#
Ag	Ag	1.483	2.953
Ag	Au	1.218	2.714
Ag	Cu	1.165	2.493
Ag	Ir	0.392	1.135
Ag	Ni	0.809	1.957
Ag	Pd	1.037	2.452
Ag	Pt	0.676	2.006
Ag	Rh	0.682	1.694
Au	Ag	1.594	2.798
Au	Au	1.146	2.454
Au	Cu	1.339	2.46
Au	Ir	0.374	1.188
Au	Ni	0.92	1.9
Au	Pd	0.981	2.167
Au	Pt	0.556	1.734
Au	Rh	0.688	1.58
Cu	Ag	1.418	2.533
Cu	Au	1.129	2.378
Cu	Cu	1.196	2.217
Cu	Ir	0.561	1.381
Cu	Ni	0.902	1.784
Cu	Pd	1.05	2.173
Cu	Pt	0.741	1.882
Cu	Rh	0.807	1.675
Ir	Ag	1.637	1.614
Ir	Au	1.185	1.556
Ir	Cu	1.521	1.582
Ir	Ir	0.588	1.057
Ir	Ni	1.045	1.285
Ir	Pd	0.932	1.275
Ir	Pt	0.63	1.146
Ir	Rh	0.817	1.154

Metal	Dopant	CH_3#	CH_2#
Ni	Ag	1.443	2.013
Ni	Au	1.084	1.882
Ni	Cu	1.248	1.411
Ni	Ir	0.52	1.132
Ni	Ni	0.869	1.371
Ni	Pd	0.867	1.556
Ni	Pt	0.607	1.375
Ni	Rh	0.731	1.301
Pd	Ag	1.493	2.02
Pd	Au	1.037	1.74
Pd	Cu	1.232	1.257
Pd	Ir	0.319	0.758
Pd	Ni	0.699	1.137
Pd	Pd	0.685	1.24
Pd	Pt	0.388	0.989
Pd	Rh	0.52	0.929
Pt	Ag	1.595	1.794
Pt	Au	1.079	1.61
Pt	Cu	1.417	1.711
Pt	Ir	0.405	0.893
Pt	Ni	0.907	1.256
Pt	Pd	0.822	1.268
Pt	Pt	0.464	1.057
Pt	Rh	0.636	1.05
Rh	Ag	1.483	1.729
Rh	Au	1.086	1.618
Rh	Cu	1.292	1.58
Rh	Ir	0.488	0.973
Rh	Ni	0.83	1.201
Rh	Pd	0.813	1.301
Rh	Pt	0.542	1.14
Rh	Rh	0.668	1.099

SI.3.2. BEP-like relationship on pure metals.

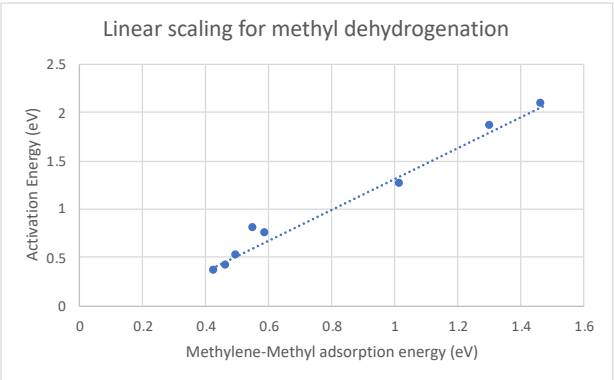
CH_3-H			
Metal	ΔU	E_a	CH_3#
Ag	1.74	2.251	1.483
Au	1.303	1.848	1.146
Cu	0.902	1.577	1.196
Ir	0.305	0.802	0.588
Ni	0.041	0.875	0.869
Pd	0.207	0.74	0.685
Pt	0.127	0.778	0.464
Rh	0.24	0.689	0.668

$y = 1.62x - 0.244$, $R^2=0.89$



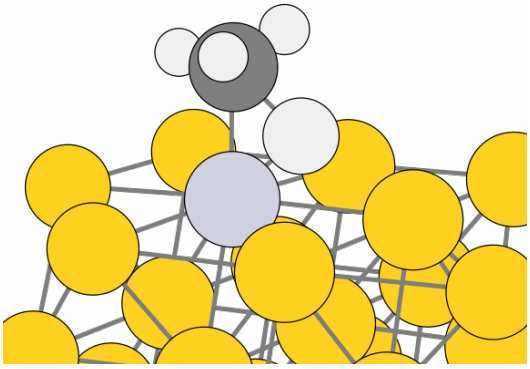
CH_2-H			
Metal	ΔU	E_a	CH_2-CH_3
Ag	1.663	2.072	1.47
Au	1.52	1.851	1.308
Cu	0.7	1.249	1.021
Ir	0.052	0.393	0.469
Ni	-0.26	0.502	0.502
Pd	0.062	0.784	0.555
Pt	0.265	0.728	0.593
Rh	-0.213	0.354	0.431

$y = 1.59 - 0.274$, $R^2=0.98$

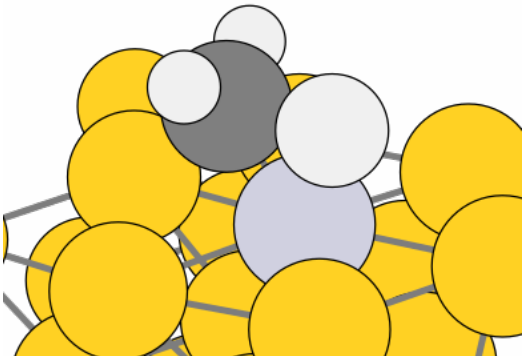


SI.3.3. Transition state structures.

Transition state of methane C-H activation on Pt-Au



Transition state of methyl C-H activation on Pt-Au



SI.4.1. Elementary steps for the streamlined microkinetic model for the SAAs. All energies reported in eV.

System:	AgIr		
Reactant	Product	ΔG	Ea^G
O_2+#	O_2#	-0.31	0.10
CH_4+#	CH_4#	0.45	0.55
CH_3OH#	CH_3OH+#	-0.18	0.10
H_2O#	H_2O+#	-0.27	0.10
CH_4#+#	CH_3#+H#	-0.13	0.10
CH_3#+#	CH_2#+H#	0.26	0.57
CH_3#+OH#	CH_3OH#+#	-0.01	1.73
CH_3#+O#	CH_3O#+#	-0.43	1.03
CH_3O#+#	CH_2O#+H#	-0.13	0.28
CH_3O#+H	CH_3OH#+#	0.11	0.64
O#+H#	OH#+#	-0.30	0.80
OH#+H#	H_2O#+#	0.13	0.94
O_2#+#	O#+O#	-1.56	0.16

System:	AgPt		
Reactant	Product	ΔG	Ea^G
O_2+#	O_2#	0.74	0.84
CH_4+#	CH_4#	0.45	0.55
CH_3OH#	CH_3OH+#	-0.38	0.10
H_2O#	H_2O+#	-0.45	0.10
CH_4#+#	CH_3#+H#	0.57	0.81
CH_3#+#	CH_2#+H#	1.07	1.20
CH_3#+OH#	CH_3OH#+#	-0.50	1.52
CH_3#+O#	CH_3O#+#	-0.78	0.84
CH_3O#+#	CH_2O#+H#	-0.23	0.05
CH_3O#+H	CH_3OH#+#	-0.51	0.53
O#+H#	OH#+#	-0.84	0.43
OH#+H#	H_2O#+#	-0.41	0.41
O_2#+#	O#+O#	-1.18	0.29

System:	AgRh		
Reactant	Product	ΔG	Ea^G
O_2+#	O_2#	-0.23	0.10
CH_4+#	CH_4#	0.45	0.55
CH_3OH#	CH_3OH+#	-0.16	0.10
H_2O#	H_2O+#	-0.23	0.10
CH_4#+#	CH_3#+H#	0.25	0.31
CH_3#+#	CH_2#+H#	0.46	0.64
CH_3#+OH#	CH_3OH#+#	-0.24	1.39
CH_3#+O#	CH_3O#+#	-0.61	0.73
CH_3O#+#	CH_2O#+H#	-0.22	0.06
CH_3O#+H	CH_3OH#+#	-0.13	0.58
O#+H#	OH#+#	-0.54	0.64
OH#+H#	H_2O#+#	-0.07	1.05
O_2#+#	O#+O#	-1.31	0.30

System:	AuIr		
Reactant	Product	ΔG	Ea^G
O_2+#	O_2#	-0.87	0.10
CH_4+#	CH_4#	0.45	0.55
CH_3OH#	CH_3OH+#	0.06	0.16
H_2O#	H_2O+#	0.82	0.92
CH_4#+#	CH_3#+H#	-0.03	0.28
CH_3#+#	CH_2#+H#	0.47	0.78
CH_3#+OH#	CH_3OH#+#	-0.75	1.30
CH_3#+O#	CH_3O#+#	-1.01	1.03
CH_3O#+#	CH_2O#+H#	0.33	0.75
CH_3O#+H	CH_3OH#+#	-0.44	0.35
O#+H#	OH#+#	-0.73	0.67
OH#+H#	H_2O#+#	-0.44	0.74
O_2#+#	O#+O#	-1.20	0.18

System:	AuPt		
Reactant	Product	ΔG	Ea^G
O_2+#	O_2#	0.47	0.57
CH_4+#	CH_4#	0.45	0.55
CH_3OH#	CH_3OH+#	-0.24	0.10
H_2O#	H_2O+#	-0.32	0.10
CH_4#+#	CH_3#+H#	0.34	0.59
CH_3#+#	CH_2#+H#	0.86	1.04
CH_3#+OH#	CH_3OH#+#	-0.84	1.33
CH_3#+O#	CH_3O#+#	-0.78	0.95
CH_3O#+#	CH_2O#+H#	-0.05	0.78
CH_3O#+H	CH_3OH#+#	-0.87	0.22
O#+H#	OH#+#	-1.05	0.34
OH#+H#	H_2O#+#	-0.86	0.19
O_2#+#	O#+O#	-0.59	0.79

System:	AuRh		
Reactant	Product	ΔG	Ea^G
O_2+#	O_2#	0.12	0.22
CH_4+#	CH_4#	0.45	0.55
CH_3OH#	CH_3OH+#	0.01	0.11
H_2O#	H_2O+#	-0.07	0.10
CH_4#+#	CH_3#+H#	0.28	0.31
CH_3#+#	CH_2#+H#	0.38	0.57
CH_3#+OH#	CH_3OH#+#	-0.83	1.08
CH_3#+O#	CH_3O#+#	-0.84	0.71
CH_3O#+#	CH_2O#+H#	-0.08	0.28
CH_3O#+H	CH_3OH#+#	-0.61	0.28
O#+H#	OH#+#	-0.78	0.59
OH#+H#	H_2O#+#	-0.66	0.79
O_2#+#	O#+O#	-1.05	0.36

System:	CuPt		
Reactant	Product	ΔG	Ea^G
O_2+#	O_2#	-0.05	0.10
CH_4+#	CH_4#	0.45	0.55
CH_3OH#	CH_3OH+#	-0.35	0.10
H_2O#	H_2O+#	-0.42	0.10
CH_4#+#	CH_3#+H#	0.51	0.85
CH_3#+#	CH_2#+H#	0.78	1.02
CH_3#+OH#	CH_3OH#+#	0.15	2.06
CH_3#+O#	CH_3O#+#	-0.16	1.08
CH_3O#+#	CH_2O#+H#	-0.43	0.65
CH_3O#+H	CH_3OH#+#	-0.21	0.92
O#+H#	OH#+#	-0.22	0.63
OH#+H#	H_2O#+#	-0.31	0.33
O_2#+#	O#+O#	-1.57	0.15

SI.4.2. Streamlined microkinetic results for SAAs. Rate reported in molecules per site per second.

Metal	Selectivity	Total rate	CH_2	CH_2O	MeOH
Pd	5.69E-09	1.07E-30	1.07E-30	2.57E-34	6.08E-39
AgIr	2.87E-12	4.82E-23	2.36E-29	4.82E-23	1.38E-34
AgPt	7.38E-12	2.58E-11	4.51E-19	2.58E-11	1.91E-22
AgRh	1.37E-09	3.57E-21	2.48E-30	3.57E-21	4.91E-30
AuIr	1.92E-06	5.47E-27	1.04E-37	5.47E-27	1.05E-32
AuPt	9.24E-06	1.61E-06	1.61E-06	3.61E-12	1.49E-11
AuRh	0.001532	5.36E-16	3.4E-20	5.35E-16	8.21E-19
CuPt	1.14E-18	1.90E-28	1.2E-38	1.90E-28	2.17E-46

SI.4.3. Surface coverage of intermediary species for the microkinetic models.

Pd	Percentage
Q_CH_2	1.43E-33
Q_CH_2O	9.35E-46
Q_CH_3	6.08E-21
Q_CH_3O	4.98E-31
Q_CH_3OH	2.21E-50
Q_CH_4	1.39E-22
Q_H	2.03E-22
Q_H_2O	3.89E-42
Q_O	1.00E+00
Q_O_2	3.37E-12
Q_OH	7.54E-10
Q_v	1.64E-14

AgIr	Percentage
Q_CH_2	4.41E-35
Q_CH_2O	1.75E-34
Q_CH_3	3.23E-21
Q_CH_3O	4.62E-19
Q_CH_3OH	5.04E-46
Q_CH_4	4.79E-20
Q_H	3.81E-20
Q_H_2O	1.75E-34
Q_O	9.95E-01
Q_O_2	4.01E-10
Q_OH	5.00E-03
Q_v	1.41E-13

AgPt	Percentage
Q_CH_2	8.43E-25
Q_CH_2O	9.40E-23
Q_CH_3	3.94E-12
Q_CH_3O	2.23E-19
Q_CH_3OH	6.94E-34
Q_CH_4	6.96E-10
Q_H	8.10E-17
Q_H_2O	9.40E-23
Q_O	9.66E-01
Q_O_2	5.92E-15
Q_OH	3.19E-02
Q_v	1.97E-03

AuIr	Percentage
Q_CH_2	1.94E-43
Q_CH_2O	1.99E-38
Q_CH_3	3.46E-25
Q_CH_3O	7.76E-15
Q_CH_3OH	2.74E-43
Q_CH_4	1.72E-21
Q_H	2.42E-27
Q_H_2O	1.99E-38
Q_O	9.87E-01
Q_O_2	1.37E-03
Q_OH	1.21E-02
Q_v	4.89E-15

AuPt	Percentage
Q_CH_2	3.01E-12
Q_CH_2O	1.32E-23
Q_CH_3	1.76E-04
Q_CH_3O	7.67E-14
Q_CH_3OH	5.41E-23
Q_CH_4	3.53E-07
Q_H	3.30E-08
Q_H_2O	5.85E-18
Q_O	4.58E-07
Q_O_2	2.29E-08
Q_OH	3.77E-09
Q_v	1.00E+00

AuRh	Percentage
Q_CH_2	6.37E-26
Q_CH_2O	1.95E-27
Q_CH_3	3.25E-16
Q_CH_3O	2.93E-16
Q_CH_3OH	2.99E-30
Q_CH_4	8.15E-16
Q_H	1.34E-17
Q_H_2O	1.95E-27
Q_O	2.97E-03
Q_O_2	4.18E-12
Q_OH	9.97E-01
Q_v	2.31E-09

CuPt	Percentage
Q_CH_2	2.24E-44
Q_CH_2O	3.56E-34
Q_CH_3	7.25E-26
Q_CH_3O	4.76E-21
Q_CH_3OH	7.91E-58
Q_CH_4	3.30E-18
Q_H	9.65E-26
Q_H_2O	6.92E-40
Q_O	1.00E+00
Q_O_2	4.84E-12
Q_OH	1.33E-11
Q_v	9.37E-12

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