

***In Situ* Surface Structures of Pd-Ag Catalyst and Their Influence on Acetylene Semihydrogenation Revealed by Machine Learning Simulation and Experiment**

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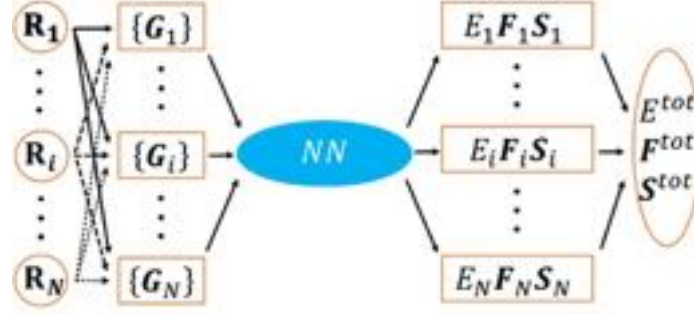
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1. Theoretical methodology and construction of the quaternary Pd-Ag-C-H G-NN potential

1.1 Architecture of neural network potential



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

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

$$E^{tot} = \sum_i E_i \quad (1)$$

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

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

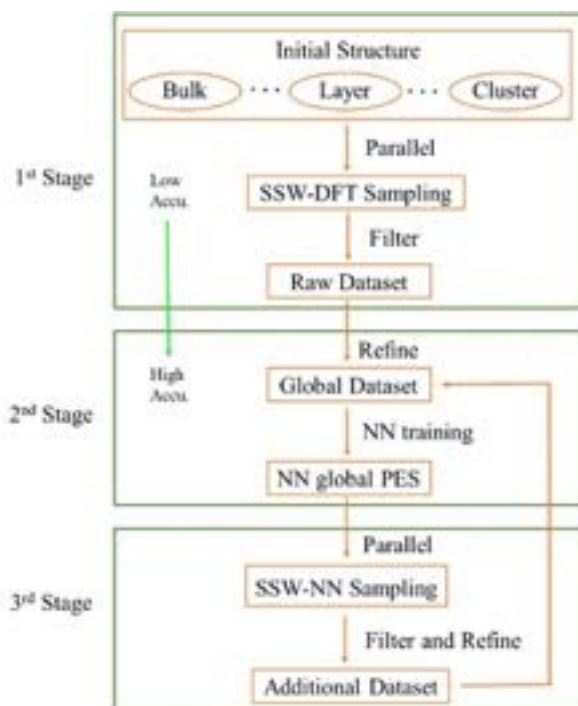
Similarly, the element $\sigma_{\alpha\beta}$ of static stress tensor matrix can be analytically derived as

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

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

1.2 Generation of global dataset using SSW-NN

Undoubtedly, the quality of the potential energy surface (PES) of G-NN is largely determined by its training dataset. Here we utilized the stochastic surface walking (SSW) global optimization⁴⁻⁶ to generate a global dataset, which is fully automated and does not need a priori knowledge on the system, such as the structural motif, e.g. bonding patterns and symmetry. The final obtained Pd-Ag-C-H global dataset contains a variety of structural patterns on the global PES, as summarized in Table S1.



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

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

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

(ii) **The second stage** trains a NN global PES. This is done by refining the dataset using DFT calculations with high accuracy setups, followed by NN training on the accurate global dataset (see our previous work⁷ for details). The NN architecture applied in this stage utilizes a small set of structural descriptors and a small network size.

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

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

Chem. Formula	N_{atm}	N_{cls}	N_{lay}	N_{bul}	N_{tot}
Ag14	14	0	3	30	33
Ag15	15	85	5	726	816
Ag16	16	0	1	6554	6555
Ag17	17	0	0	19	19
Ag28	28	0	0	34	34
Ag29	29	0	15	0	15
Ag30	30	0	31	32	63
Ag31	31	0	0	74	74
Ag32	32	0	2	93	95
Ag64	64	0	94	0	94
Pd1-Ag1	2	0	0	77	77
Pd1-Ag3	4	0	0	1	1
Pd1-Ag15	16	0	0	19	19
Pd2-Ag2	4	0	0	1	1
Pd2-Ag6	8	0	0	36	36
Pd2-Ag14	16	1	0	5	6
Pd2-Ag33	35	0	8	0	8
Pd2-Ag34	36	0	53	0	53
Pd3-Ag1	4	0	0	3	3
Pd3-Ag3	6	0	31	4	35
Pd3-Ag13	16	1	0	10	11
Pd4	4	2	2	23	27

Pd4-Ag4	8	0	3	0	3
Pd4-Ag12	16	5	0	10	15
Pd4-Ag44	48	0	7	0	7
Pd5-Ag11	16	1	0	84	85
Pd5-Ag43	48	0	9	0	9
Pd6-Ag10	16	2	0	85	87
Pd7-Ag9	16	2	0	8	10
Pd8	8	0	4	41	45
Pd8-Ag8	16	2	0	70	72
Pd8-Ag24	32	0	7	0	7
Pd8-Ag40	48	0	6	0	6
Pd8-Ag56	64	0	5	0	5
Pd9-Ag7	16	0	0	29	29
Pd10-Ag6	16	3	0	74	77
Pd10-Ag54	64	0	22	0	22
Pd11-Ag5	16	2	0	10	12
Pd11-Ag25	36	107	72	0	179
Pd12-Ag4	16	2	0	85	87
Pd12-Ag12	24	0	11	2	13
Pd12-Ag20	32	0	0	1	1
Pd12-Ag52	64	0	28	1	29
Pd13-Ag3	16	3	0	11	14
Pd14-Ag2	16	1	1	33	35
Pd14-Ag50	64	0	12	0	12
Pd15	15	0	0	36	36
Pd15-Ag1	16	3	0	26	29
Pd16	16	213	1	1342	1556
Pd16-Ag16	32	0	0	1	1
Pd16-Ag32	48	0	13	0	13
Pd16-Ag48	64	0	41	1	42
Pd18-Ag14	32	0	0	1	1
Pd18-Ag46	64	0	25	0	25
Pd19-Ag13	32	0	0	1	1
Pd20-Ag44	64	0	30	0	30
Pd21-Ag14	35	0	10	0	10
Pd22-Ag14	36	0	229	0	229
Pd22-Ag42	64	0	28	0	28
Pd23-Ag9	32	0	0	1	1
Pd24-Ag24	48	0	21	1	22
Pd24-Ag40	64	0	33	0	33
Pd26-Ag38	64	0	34	2	36
Pd28-Ag4	32	0	0	1	1
Pd28-Ag36	64	0	35	0	35
Pd29	29	0	22	34	56

Pd30-Ag34	64	0	25	0	25
Pd31	31	0	0	4	4
Pd32	32	0	74	156	230
Pd32-Ag16	48	0	8	0	8
Pd32-Ag32	64	0	94	12	106
Pd33-Ag2	35	0	4	0	4
Pd34-Ag2	36	0	21	0	21
Pd34-Ag30	64	0	35	0	35
Pd36-Ag28	64	0	29	0	29
Pd38-Ag26	64	0	22	1	23
Pd40-Ag24	64	0	29	0	29
Pd42-Ag22	64	0	16	2	18
Pd44-Ag20	64	0	8	0	8
Pd46-Ag18	64	0	5	0	5
Pd48	48	0	9	0	9
Pd48-Ag16	64	0	9	0	9
Pd52-Ag12	64	0	3	0	3
Pd54	54	0	10	6	16
Pd56-Ag8	64	0	8	1	9
Pd58	58	0	69	38	107
Pd60	60	0	88	28	116
Pd60-Ag4	64	0	11	0	11
Pd64	64	0	909	618	1527
C1-Ag12	13	0	4	0	4
C1-Pd1-Ag11	13	0	3	0	3
C1-Pd2-Ag10	13	0	4	0	4
C1-Pd3-Ag9	13	0	2	0	2
C1-Pd4-Ag8	13	0	5	1	6
C1-Pd6-Ag6	13	0	4	0	4
C1-Pd7-Ag5	13	0	7	0	7
C1-Pd8-Ag4	13	0	9	0	9
C1-Pd9-Ag3	13	0	6	0	6
C1-Pd10-Ag2	13	0	4	0	4
C1-Pd11-Ag1	13	0	14	1	15
C1-Pd12	13	0	150	0	150
C2-Ag10	12	0	2	0	2
C2-Ag25	27	0	0	2	2
C2-Pd1-Ag9	12	0	5	0	5
C2-Pd1-Ag28	31	0	0	1	1
C2-Pd2-Ag8	12	0	5	0	5
C2-Pd2-Ag23	27	0	0	1	1
C2-Pd2-Ag27	31	0	0	1	1
C2-Pd3-Ag7	12	0	23	1	24
C2-Pd3-Ag26	31	0	0	1	1

C2-Pd4-Ag6	12	0	3	0	3
C2-Pd4-Ag21	27	0	0	1	1
C2-Pd4-Ag25	31	0	0	1	1
C2-Pd5-Ag5	12	0	1	0	1
C2-Pd5-Ag24	31	0	0	1	1
C2-Pd6-Ag4	12	0	8	0	8
C2-Pd7-Ag3	12	0	4	0	4
C2-Pd8-Ag2	12	0	7	0	7
C2-Pd9-Ag1	12	0	8	0	8
C2-Pd9-Ag16	27	0	0	1	1
C2-Pd10	12	0	178	0	178
C2-Pd10-Ag19	31	0	0	1	1
C2-Pd11-Ag18	31	0	0	1	1
C2-Pd12-Ag13	27	0	0	1	1
C2-Pd12-Ag17	31	0	0	1	1
C2-Pd13-Ag16	31	0	0	1	1
C2-Pd14-Ag15	31	0	3	0	3
C2-Pd15-Ag14	31	0	0	1	1
C2-Pd16-Ag9	27	0	0	2	2
C2-Pd18-Ag11	31	0	1	1	2
C2-Pd19-Ag6	27	0	6	3	9
C2-Pd19-Ag10	31	0	0	4	4
C2-Pd20-Ag9	31	0	2	3	5
C2-Pd21-Ag4	27	0	0	1	1
C2-Pd21-Ag8	31	0	4	3	7
C2-Pd22-Ag3	27	0	0	1	1
C2-Pd23-Ag2	27	0	0	1	1
C2-Pd24-Ag5	31	0	0	1	1
C2-Pd25	27	0	0	51	51
C2-Pd25-Ag4	31	0	0	2	2
C2-Pd27-Ag2	31	0	15	2	17
C2-Pd28-Ag1	31	0	0	2	2
C2-Pd29	31	0	5	86	91
C3-Pd2-Ag14	19	1	0	0	1
C3-Pd7-Ag9	19	1	0	0	1
C3-Pd16	19	14	0	0	14
C4-Ag8	12	0	0	20	20
C4-Pd1-Ag7	12	0	6	15	21
C4-Pd1-Ag24	29	0	0	1	1
C4-Pd2-Ag6	12	0	35	15	50
C4-Pd2-Ag23	29	0	0	1	1
C4-Pd3-Ag5	12	0	0	8	8
C4-Pd3-Ag22	29	0	0	1	1
C4-Pd4-Ag4	12	0	0	19	19

C4-Pd4-Ag21	29	0	0	1	1
C4-Pd5-Ag3	12	0	3	16	19
C4-Pd5-Ag20	29	0	0	1	1
C4-Pd6-Ag2	12	0	4	23	27
C4-Pd7-Ag1	12	0	18	20	38
C4-Pd7-Ag18	29	0	0	1	1
C4-Pd8	12	0	0	504	504
C4-Pd11-Ag14	29	0	0	1	1
C4-Pd14-Ag11	29	0	0	2	2
C4-Pd15-Ag10	29	0	0	4	4
C4-Pd16-Ag9	29	0	0	1	1
C4-Pd17-Ag8	29	0	0	1	1
C4-Pd18-Ag7	29	0	4	2	6
C4-Pd20-Ag5	29	0	0	1	1
C4-Pd22-Ag3	29	0	0	1	1
C4-Pd23-Ag2	29	0	0	1	1
C4-Pd24-Ag1	29	0	0	1	1
C4-Pd25	29	0	3	49	52
C6-Pd1-Ag24	31	0	2	2	4
C6-Pd2-Ag23	31	0	9	1	10
C6-Pd3-Ag22	31	0	1	1	2
C6-Pd4-Ag21	31	0	6	1	7
C6-Pd5-Ag20	31	0	1	1	2
C6-Pd6-Ag19	31	0	2	0	2
C6-Pd7-Ag18	31	0	1	1	2
C6-Pd8-Ag17	31	0	4	2	6
C6-Pd9-Ag16	31	0	1	3	4
C6-Pd11-Ag14	31	0	1	2	3
C6-Pd12-Ag13	31	0	7	1	8
C6-Pd13-Ag12	31	0	3	0	3
C6-Pd15-Ag10	31	0	3	2	5
C6-Pd16-Ag9	31	0	18	3	21
C6-Pd17-Ag8	31	0	1	1	2
C6-Pd18-Ag7	31	0	3	1	4
C6-Pd19-Ag6	31	0	6	2	8
C6-Pd20-Ag5	31	0	5	3	8
C6-Pd21-Ag4	31	0	5	3	8
C6-Pd22-Ag3	31	0	16	3	19
C6-Pd23-Ag2	31	0	1	1	2
C6-Pd24-Ag1	31	0	4	0	4
C6-Pd25	31	0	175	114	289
C8-Pd2-Ag14	24	1	0	0	1
C8-Pd10-Ag6	24	1	0	0	1
C8-Pd11-Ag5	24	2	0	0	2

C8-Pd13-Ag3	24	1	0	0	1
C8-Pd14-Ag2	24	2	0	0	2
C8-Pd16	24	8	0	0	8
C10-Pd33-Ag16	59	0	2	0	2
C10-Pd36-Ag13	59	0	1	0	1
C10-Pd49	59	0	16	0	16
C12-Pd4-Ag46	62	0	1	0	1
C12-Pd5-Ag45	62	0	1	0	1
C12-Pd6-Ag44	62	0	2	0	2
C12-Pd9-Ag41	62	0	1	0	1
C12-Pd11-Ag39	62	0	1	0	1
C12-Pd12-Ag38	62	0	1	0	1
C12-Pd22-Ag28	62	0	1	0	1
C12-Pd27-Ag23	62	0	1	0	1
C12-Pd28-Ag22	62	0	2	0	2
C12-Pd30-Ag20	62	0	1	0	1
C12-Pd32-Ag18	62	0	1	0	1
C12-Pd35-Ag15	62	0	1	0	1
C12-Pd39-Ag11	62	0	1	0	1
C12-Pd41-Ag9	62	0	2	0	2
C12-Pd50	62	0	29	2	31
H1-Ag16	17	0	9	16	25
H1-Pd1-Ag15	17	0	16	0	16
H1-Pd2-Ag13	16	0	0	1	1
H1-Pd3-Ag12	16	0	0	1	1
H1-Pd4-Ag11	16	0	0	4	4
H1-Pd5-Ag10	16	0	0	2	2
H1-Pd5-Ag18	24	0	1	1	2
H1-Pd6-Ag9	16	0	0	2	2
H1-Pd6-Ag20	27	0	1	0	1
H1-Pd7-Ag8	16	0	0	3	3
H1-Pd7-Ag20	28	0	1	0	1
H1-Pd8-Ag7	16	0	0	2	2
H1-Pd9-Ag6	16	0	0	3	3
H1-Pd10-Ag13	24	0	1	0	1
H1-Pd10-Ag25	36	10	0	0	10
H1-Pd11-Ag4	16	0	0	6	6
H1-Pd11-Ag12	24	0	0	1	1
H1-Pd12-Ag3	16	0	0	7	7
H1-Pd13-Ag2	16	0	0	3	3
H1-Pd13-Ag13	27	0	1	0	1
H1-Pd14-Ag1	16	0	0	1	1
H1-Pd14-Ag2	17	0	19	0	19
H1-Pd15	16	0	0	365	365

H1-Pd16-Ag11	28	0	1	0	1
H1-Pd19-Ag7	27	0	1	0	1
H1-Pd21-Ag5	27	0	1	0	1
H1-Pd22-Ag4	27	0	1	0	1
H1-Pd23	24	0	33	17	50
H1-Pd24-Ag3	28	0	1	0	1
H1-Pd26	27	0	81	0	81
H1-Pd27	28	0	32	0	32
H1-Pd28-Ag3	32	0	0	1	1
H1-Pd31	32	1	0	16	17
H2-Ag16	18	0	3	240	243
H2-Pd1-Ag15	18	0	67	0	67
H2-Pd2-Ag12	16	0	0	2	2
H2-Pd2-Ag14	18	0	0	19	19
H2-Pd3-Ag11	16	0	2	6	8
H2-Pd4-Ag10	16	0	0	4	4
H2-Pd4-Ag23	29	0	0	1	1
H2-Pd5-Ag9	16	0	1	3	4
H2-Pd5-Ag17	24	0	1	0	1
H2-Pd6-Ag8	16	0	0	6	6
H2-Pd6-Ag21	29	0	1	0	1
H2-Pd6-Ag42	50	0	4	1	5
H2-Pd7-Ag7	16	0	0	5	5
H2-Pd7-Ag20	29	0	0	1	1
H2-Pd8-Ag6	16	0	1	9	10
H2-Pd8-Ag14	24	0	1	0	1
H2-Pd8-Ag19	29	0	0	1	1
H2-Pd9-Ag5	16	0	2	7	9
H2-Pd9-Ag19	30	0	1	0	1
H2-Pd10-Ag4	16	0	0	6	6
H2-Pd11-Ag3	16	0	1	5	6
H2-Pd12-Ag2	16	0	0	13	13
H2-Pd13-Ag1	16	0	0	7	7
H2-Pd13-Ag17	32	0	0	1	1
H2-Pd14	16	0	69	626	695
H2-Pd14-Ag2	18	0	36	102	138
H2-Pd14-Ag13	29	0	2	1	3
H2-Pd14-Ag14	30	0	1	0	1
H2-Pd15-Ag1	18	0	0	154	154
H2-Pd15-Ag12	29	0	0	2	2
H2-Pd15-Ag13	30	0	1	0	1
H2-Pd19-Ag9	30	0	1	0	1
H2-Pd20-Ag8	30	0	1	0	1
H2-Pd21-Ag6	29	0	0	1	1

H2-Pd22	24	0	29	0	29
H2-Pd22-Ag5	29	0	1	0	1
H2-Pd23-Ag4	29	0	1	0	1
H2-Pd23-Ag5	30	0	1	0	1
H2-Pd24-Ag4	30	0	1	0	1
H2-Pd25-Ag2	29	0	0	1	1
H2-Pd26-Ag1	29	0	1	0	1
H2-Pd26-Ag2	30	0	1	0	1
H2-Pd27	29	3	51	74	128
H2-Pd28	30	0	64	0	64
H2-Pd29-Ag1	32	0	0	1	1
H2-Pd30	32	2	0	16	18
H2-C2	4	2	0	0	2
H2-C4-Ag23	29	0	0	2	2
H2-C4-Pd1-Ag22	29	0	0	1	1
H2-C4-Pd2-Ag21	29	0	0	1	1
H2-C4-Pd3-Ag20	29	0	0	3	3
H2-C4-Pd7-Ag16	29	0	0	3	3
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H2-C4-Pd12-Ag11	29	0	7	1	8
H2-C4-Pd13-Ag10	29	0	0	2	2
H2-C4-Pd14-Ag9	29	0	0	2	2
H2-C4-Pd15-Ag8	29	0	0	4	4
H2-C4-Pd16-Ag7	29	0	0	4	4
H2-C4-Pd17-Ag6	29	0	0	1	1
H2-C4-Pd18-Ag5	29	0	0	4	4
H2-C4-Pd19-Ag4	29	0	0	3	3
H2-C4-Pd20-Ag3	29	0	0	2	2
H2-C4-Pd21-Ag2	29	0	0	2	2
H2-C4-Pd22-Ag1	29	0	0	2	2
H2-C4-Pd23	29	0	0	122	122
H3-Ag16	19	0	74	174	248
H3-Pd4-Ag12	19	0	13	0	13
H3-Pd4-Ag25	32	0	0	1	1
H3-Pd5-Ag21	29	0	1	0	1
H3-Pd6-Ag20	29	0	1	0	1
H3-Pd6-Ag23	32	0	0	1	1
H3-Pd7-Ag19	29	0	1	0	1
H3-Pd10-Ag16	29	0	2	0	2
H3-Pd12-Ag14	29	0	1	0	1
H3-Pd12-Ag17	32	1	0	0	1
H3-Pd16-Ag48	67	0	1	0	1
H3-Pd18-Ag8	29	0	1	0	1
H3-Pd19-Ag7	29	0	1	0	1

H3-Pd20-Ag6	29	0	1	0	1
H3-Pd21-Ag5	29	0	3	0	3
H3-Pd22-Ag4	29	0	2	0	2
H3-Pd23-Ag3	29	0	1	0	1
H3-Pd26	29	0	120	0	120
H3-Pd26-Ag3	32	0	0	1	1
H3-Pd27-Ag2	32	0	0	1	1
H3-Pd28	31	1	0	11	12
H3-Pd29	32	2	0	23	25
H3-Pd32-Ag7	42	0	141	0	141
H3-C2-Ag22	27	0	0	2	2
H3-C2-Pd1-Ag21	27	0	0	4	4
H3-C2-Pd2-Ag20	27	0	4	1	5
H3-C2-Pd3-Ag19	27	0	0	2	2
H3-C2-Pd5-Ag17	27	0	0	1	1
H3-C2-Pd6-Ag16	27	0	0	1	1
H3-C2-Pd7-Ag15	27	0	0	1	1
H3-C2-Pd8-Ag14	27	0	0	5	5
H3-C2-Pd9-Ag13	27	0	0	2	2
H3-C2-Pd10-Ag12	27	0	0	3	3
H3-C2-Pd11-Ag11	27	0	0	1	1
H3-C2-Pd12-Ag10	27	0	0	4	4
H3-C2-Pd13-Ag9	27	0	5	2	7
H3-C2-Pd14-Ag8	27	0	0	1	1
H3-C2-Pd15-Ag7	27	0	0	4	4
H3-C2-Pd16-Ag6	27	0	0	4	4
H3-C2-Pd17-Ag5	27	0	0	4	4
H3-C2-Pd18-Ag4	27	0	0	2	2
H3-C2-Pd19-Ag3	27	0	0	4	4
H3-C2-Pd20-Ag2	27	0	0	2	2
H3-C2-Pd21-Ag1	27	0	0	1	1
H3-C2-Pd22	27	0	0	150	150
H3-C6-Ag22	31	0	0	2	2
H3-C6-Pd5-Ag17	31	0	0	1	1
H3-C6-Pd7-Ag15	31	0	0	1	1
H3-C6-Pd10-Ag12	31	0	0	1	1
H3-C6-Pd13-Ag9	31	0	0	2	2
H3-C6-Pd17-Ag5	31	0	0	2	2
H3-C6-Pd18-Ag4	31	0	0	2	2
H3-C6-Pd19-Ag3	31	0	0	2	2
H3-C6-Pd20-Ag2	31	0	0	2	2
H3-C6-Pd21-Ag1	31	0	0	2	2
H3-C6-Pd22	31	0	0	81	81
H4-Ag12	16	1	0	0	1

H4-Pd1-Ag11	16	2	0	2	4
H4-Pd1-Ag15	20	0	3	203	206
H4-Pd2-Ag10	16	13	0	2	15
H4-Pd2-Ag15	21	0	0	1	1
H4-Pd2-Ag22	28	0	1	0	1
H4-Pd3-Ag9	16	16	0	2	18
H4-Pd3-Ag14	21	0	0	1	1
H4-Pd4-Ag8	16	27	0	3	30
H4-Pd4-Ag20	28	0	1	0	1
H4-Pd5-Ag7	16	14	0	4	18
H4-Pd6-Ag6	16	18	0	5	23
H4-Pd6-Ag11	21	0	0	2	2
H4-Pd7-Ag5	16	20	0	1	21
H4-Pd7-Ag10	21	0	0	1	1
H4-Pd8-Ag4	16	18	0	0	18
H4-Pd8-Ag8	20	0	0	16	16
H4-Pd8-Ag12	24	0	1	0	1
H4-Pd8-Ag40	52	0	7	0	7
H4-Pd9-Ag3	16	16	0	1	17
H4-Pd9-Ag8	21	0	0	2	2
H4-Pd10-Ag2	16	29	0	1	30
H4-Pd11-Ag1	16	35	0	2	37
H4-Pd11-Ag6	21	0	0	1	1
H4-Pd11-Ag13	28	0	1	0	1
H4-Pd12	16	2122	0	256	2378
H4-Pd12-Ag4	20	0	10	0	10
H4-Pd13-Ag4	21	0	0	2	2
H4-Pd13-Ag7	24	0	1	0	1
H4-Pd13-Ag11	28	0	1	0	1
H4-Pd14-Ag2	20	0	14	0	14
H4-Pd15-Ag2	21	0	0	2	2
H4-Pd16-Ag1	21	0	0	4	4
H4-Pd16-Ag48	68	0	1	0	1
H4-Pd17	21	0	0	170	170
H4-Pd17-Ag7	28	0	1	0	1
H4-Pd18-Ag2	24	0	1	0	1
H4-Pd18-Ag6	28	0	1	0	1
H4-Pd19-Ag5	28	0	1	0	1
H4-Pd20	24	0	24	0	24
H4-Pd22-Ag2	28	0	1	0	1
H4-Pd24	28	0	45	0	45
H4-Pd26-Ag10	40	0	319	0	319
H4-Pd31-Ag5	40	0	168	0	168
H4-Pd31-Ag7	42	0	3	0	3

H4-Pd35-Ag2	41	0	11	0	11
H4-Pd36-Ag2	42	0	149	0	149
H4-C1-Pd2-Ag34	41	0	1	0	1
H4-C1-Pd3-Ag33	41	0	1	0	1
H4-C1-Pd4-Ag32	41	0	4	0	4
H4-C1-Pd5-Ag31	41	0	2	0	2
H4-C1-Pd6-Ag30	41	0	1	0	1
H4-C1-Pd8-Ag28	41	0	1	0	1
H4-C1-Pd9-Ag27	41	0	1	0	1
H4-C1-Pd10-Ag26	41	0	1	0	1
H4-C1-Pd11-Ag25	41	0	5	0	5
H4-C1-Pd12-Ag24	41	0	2	0	2
H4-C1-Pd14-Ag22	41	0	1	0	1
H4-C1-Pd15-Ag21	41	0	2	0	2
H4-C1-Pd16-Ag20	41	0	7	0	7
H4-C1-Pd17-Ag19	41	0	10	1	11
H4-C1-Pd18-Ag18	41	0	1	0	1
H4-C1-Pd19-Ag17	41	0	4	0	4
H4-C1-Pd20-Ag16	41	0	5	0	5
H4-C1-Pd21-Ag15	41	0	7	1	8
H4-C1-Pd22-Ag14	41	0	2	0	2
H4-C1-Pd23-Ag13	41	0	2	0	2
H4-C1-Pd24-Ag12	41	0	5	0	5
H4-C1-Pd25-Ag11	41	0	2	0	2
H4-C1-Pd26-Ag10	41	0	4	0	4
H4-C1-Pd27-Ag9	41	0	6	0	6
H4-C1-Pd29-Ag7	41	0	9	1	10
H4-C1-Pd30-Ag6	41	0	12	0	12
H4-C1-Pd31-Ag5	41	0	7	0	7
H4-C1-Pd32-Ag4	41	0	2	0	2
H4-C1-Pd33-Ag3	41	0	4	0	4
H4-C1-Pd34-Ag2	41	0	5	0	5
H4-C1-Pd36	41	0	331	0	331
H4-C4	8	1109	752	0	1861
H4-C7-Pd45	56	0	0	10	10
H4-C8-Pd1-Ag45	58	0	0	1	1
H4-C8-Pd7-Ag39	58	0	0	1	1
H4-C8-Pd11-Ag35	58	0	0	2	2
H4-C8-Pd14-Ag32	58	0	0	1	1
H4-C8-Pd25-Ag21	58	0	0	1	1
H4-C8-Pd27-Ag19	58	0	0	2	2
H4-C8-Pd31-Ag15	58	0	0	1	1
H4-C8-Pd36-Ag10	58	0	0	1	1
H4-C8-Pd37-Ag9	58	0	0	1	1

H4-C8-Pd46	58	0	0	29	29
H5-Pd3-Ag13	21	0	1	0	1
H5-Pd4-Ag12	21	0	76	154	230
H5-Pd5-Ag11	21	0	1	1	2
H5-Pd5-Ag30	40	9	0	0	9
H5-Pd6-Ag10	21	0	1	2	3
H5-Pd8-Ag8	21	0	1	0	1
H5-Pd9-Ag7	21	0	2	0	2
H5-Pd10-Ag6	21	0	1	0	1
H5-Pd11-Ag5	21	0	4	1	5
H5-Pd12-Ag4	21	0	1	0	1
H5-Pd13-Ag3	21	0	4	1	5
H5-Pd14-Ag2	21	0	2	1	3
H5-Pd15-Ag1	21	0	1	0	1
H5-Pd16	21	0	182	38	220
H5-Pd25-Ag10	40	0	4	0	4
H5-C2-Pd1-Ag35	43	0	3	0	3
H5-C2-Pd2-Ag34	43	0	6	0	6
H5-C2-Pd3-Ag33	43	0	2	0	2
H5-C2-Pd4-Ag32	43	0	1	0	1
H5-C2-Pd5-Ag31	43	0	4	0	4
H5-C2-Pd6-Ag30	43	0	1	0	1
H5-C2-Pd7-Ag29	43	0	1	0	1
H5-C2-Pd8-Ag28	43	0	3	0	3
H5-C2-Pd11-Ag25	43	0	2	0	2
H5-C2-Pd12-Ag24	43	0	2	0	2
H5-C2-Pd13-Ag23	43	0	3	0	3
H5-C2-Pd14-Ag22	43	0	4	0	4
H5-C2-Pd15-Ag21	43	0	2	0	2
H5-C2-Pd16-Ag20	43	0	2	0	2
H5-C2-Pd16-Ag48	71	0	22	0	22
H5-C2-Pd18-Ag18	43	0	3	0	3
H5-C2-Pd19-Ag17	43	0	4	0	4
H5-C2-Pd20-Ag16	43	0	7	0	7
H5-C2-Pd21-Ag15	43	0	1	0	1
H5-C2-Pd23-Ag13	43	0	2	0	2
H5-C2-Pd24-Ag12	43	0	2	0	2
H5-C2-Pd25-Ag11	43	0	8	0	8
H5-C2-Pd26-Ag10	43	0	3	0	3
H5-C2-Pd27-Ag9	43	0	4	0	4
H5-C2-Pd28-Ag8	43	0	12	0	12
H5-C2-Pd29-Ag7	43	0	5	0	5
H5-C2-Pd30-Ag6	43	0	4	0	4
H5-C2-Pd31-Ag5	43	0	6	0	6

H5-C2-Pd32-Ag4	43	0	3	0	3
H5-C2-Pd33-Ag3	43	0	3	0	3
H5-C2-Pd34-Ag2	43	0	2	0	2
H5-C2-Pd35-Ag1	43	0	4	0	4
H5-C2-Pd36	43	0	310	0	310
H5-C6-Pd1-Ag19	31	0	0	1	1
H5-C6-Pd2-Ag18	31	0	0	1	1
H5-C6-Pd9-Ag11	31	0	0	3	3
H5-C6-Pd11-Ag9	31	0	0	2	2
H5-C6-Pd13-Ag7	31	0	0	1	1
H5-C6-Pd15-Ag5	31	0	0	5	5
H5-C6-Pd16-Ag4	31	0	0	3	3
H5-C6-Pd17-Ag3	31	0	0	2	2
H5-C6-Pd19-Ag1	31	0	0	1	1
H5-C6-Pd20	31	0	0	78	78
H6-Pd1-Ag9	16	0	0	1	1
H6-Pd1-Ag14	21	0	1	0	1
H6-Pd2-Ag8	16	0	0	3	3
H6-Pd2-Ag13	21	0	1	0	1
H6-Pd3-Ag7	16	0	0	5	5
H6-Pd3-Ag12	21	0	2	0	2
H6-Pd3-Ag23	32	1	0	0	1
H6-Pd4-Ag6	16	0	0	6	6
H6-Pd4-Ag22	32	0	0	1	1
H6-Pd5-Ag5	16	0	0	8	8
H6-Pd5-Ag10	21	0	4	0	4
H6-Pd5-Ag20	31	0	1	0	1
H6-Pd5-Ag31	42	38	0	0	38
H6-Pd6-Ag4	16	0	0	3	3
H6-Pd6-Ag9	21	0	5	0	5
H6-Pd7-Ag3	16	0	0	9	9
H6-Pd7-Ag8	21	0	2	0	2
H6-Pd7-Ag19	32	0	0	1	1
H6-Pd8-Ag2	16	0	0	7	7
H6-Pd8-Ag7	21	0	4	0	4
H6-Pd8-Ag18	32	0	1	0	1
H6-Pd8-Ag28	42	0	155	0	155
H6-Pd9-Ag1	16	0	0	5	5
H6-Pd9-Ag17	32	0	0	1	1
H6-Pd10	16	0	0	360	360
H6-Pd10-Ag5	21	0	1	0	1
H6-Pd10-Ag16	32	0	1	1	2
H6-Pd10-Ag38	54	0	16	0	16
H6-Pd11-Ag4	21	0	4	0	4

H6-Pd11-Ag15	32	0	0	1	1
H6-Pd11-Ag37	54	0	6	0	6
H6-Pd12-Ag3	21	0	3	0	3
H6-Pd12-Ag13	31	0	1	0	1
H6-Pd12-Ag14	32	0	1	1	2
H6-Pd12-Ag36	54	0	17	0	17
H6-Pd13-Ag2	21	0	1	0	1
H6-Pd14-Ag1	21	0	3	0	3
H6-Pd14-Ag11	31	0	1	0	1
H6-Pd14-Ag12	32	0	0	1	1
H6-Pd15	21	0	286	5	291
H6-Pd15-Ag10	31	0	3	0	3
H6-Pd15-Ag19	40	5	0	0	5
H6-Pd15-Ag21	42	85	0	0	85
H6-Pd16-Ag9	31	0	1	0	1
H6-Pd16-Ag10	32	0	1	0	1
H6-Pd16-Ag20	42	0	79	0	79
H6-Pd17-Ag9	32	1	0	0	1
H6-Pd18-Ag7	31	0	2	0	2
H6-Pd19-Ag7	32	1	1	0	2
H6-Pd20-Ag6	32	1	2	2	5
H6-Pd21-Ag4	31	0	1	0	1
H6-Pd21-Ag5	32	0	1	1	2
H6-Pd22-Ag3	31	0	1	0	1
H6-Pd22-Ag4	32	0	0	2	2
H6-Pd23-Ag3	32	1	0	0	1
H6-Pd24-Ag2	32	2	1	0	3
H6-Pd25	31	0	80	0	80
H6-Pd25-Ag1	32	1	1	1	3
H6-Pd26	32	108	77	106	291
H6-Pd27-Ag9	42	90	0	0	90
H6-Pd32-Ag4	42	0	56	0	56
H6-Pd35-Ag1	42	96	70	0	166
H6-C2-Ag36	44	0	2	0	2
H6-C2-Pd1-Ag35	44	0	1	0	1
H6-C2-Pd2-Ag34	44	0	4	0	4
H6-C2-Pd3-Ag33	44	0	2	0	2
H6-C2-Pd4-Ag32	44	0	4	0	4
H6-C2-Pd5-Ag31	44	0	2	0	2
H6-C2-Pd6-Ag30	44	0	1	0	1
H6-C2-Pd7-Ag29	44	0	1	0	1
H6-C2-Pd8-Ag28	44	0	4	0	4
H6-C2-Pd9-Ag27	44	0	4	0	4
H6-C2-Pd10-Ag26	44	0	1	0	1

H6-C2-Pd11-Ag25	44	0	1	0	1
H6-C2-Pd12-Ag24	44	0	1	0	1
H6-C2-Pd13-Ag23	44	0	6	0	6
H6-C2-Pd14-Ag22	44	0	3	0	3
H6-C2-Pd15-Ag21	44	0	1	0	1
H6-C2-Pd16-Ag20	44	0	5	0	5
H6-C2-Pd16-Ag48	72	0	24	0	24
H6-C2-Pd17-Ag19	44	0	2	0	2
H6-C2-Pd18-Ag18	44	0	5	0	5
H6-C2-Pd19-Ag17	44	0	3	0	3
H6-C2-Pd20-Ag16	44	0	5	0	5
H6-C2-Pd21-Ag15	44	0	3	0	3
H6-C2-Pd22-Ag14	44	0	4	0	4
H6-C2-Pd23-Ag13	44	0	3	0	3
H6-C2-Pd24-Ag12	44	0	7	0	7
H6-C2-Pd25-Ag11	44	0	2	0	2
H6-C2-Pd26-Ag10	44	0	3	0	3
H6-C2-Pd27-Ag9	44	0	5	0	5
H6-C2-Pd28-Ag8	44	0	2	0	2
H6-C2-Pd29-Ag7	44	0	5	0	5
H6-C2-Pd30-Ag6	44	0	6	0	6
H6-C2-Pd31-Ag5	44	0	5	0	5
H6-C2-Pd32-Ag4	44	0	4	0	4
H6-C2-Pd33-Ag3	44	0	11	0	11
H6-C2-Pd34-Ag2	44	0	2	0	2
H6-C2-Pd36	44	0	339	0	339
H6-C4	10	329	18	0	347
H6-C4-Pd4-Ag40	54	0	0	1	1
H6-C4-Pd12-Ag31	53	0	0	1	1
H6-C4-Pd13-Ag31	54	0	0	1	1
H6-C4-Pd18-Ag26	54	0	0	1	1
H6-C4-Pd21-Ag22	53	0	0	1	1
H6-C4-Pd25-Ag19	54	0	0	1	1
H6-C4-Pd30-Ag13	53	0	0	2	2
H6-C4-Pd31-Ag12	53	0	0	1	1
H6-C4-Pd31-Ag13	54	0	0	1	1
H6-C4-Pd37-Ag7	54	0	0	1	1
H6-C4-Pd38-Ag6	54	0	0	1	1
H6-C4-Pd39-Ag5	54	0	0	1	1
H6-C4-Pd41-Ag3	54	0	0	1	1
H6-C4-Pd42-Ag1	53	0	0	1	1
H6-C4-Pd42-Ag2	54	0	0	1	1
H6-C4-Pd43	53	0	0	14	14
H6-C4-Pd44	54	0	0	39	39

H7-Pd5-Ag20	32	0	0	1	1
H7-Pd8-Ag17	32	0	0	1	1
H7-Pd8-Ag27	42	0	4	0	4
H7-Pd12-Ag13	32	0	0	1	1
H7-Pd13-Ag12	32	0	0	1	1
H7-Pd17-Ag8	32	0	0	1	1
H7-Pd22-Ag3	32	0	0	2	2
H7-Pd23-Ag2	32	0	0	2	2
H7-Pd24-Ag1	32	0	0	3	3
H7-Pd25	32	0	0	68	68
H7-C2-Pd1-Ag34	44	0	1	0	1
H7-C2-Pd1-Ag35	45	0	3	0	3
H7-C2-Pd2-Ag33	44	0	1	0	1
H7-C2-Pd2-Ag34	45	0	4	0	4
H7-C2-Pd3-Ag32	44	0	1	0	1
H7-C2-Pd3-Ag33	45	0	17	0	17
H7-C2-Pd4-Ag31	44	0	2	0	2
H7-C2-Pd4-Ag32	45	0	14	0	14
H7-C2-Pd5-Ag31	45	0	5	0	5
H7-C2-Pd6-Ag29	44	0	1	0	1
H7-C2-Pd6-Ag30	45	0	3	0	3
H7-C2-Pd7-Ag29	45	0	1	0	1
H7-C2-Pd8-Ag27	44	0	1	0	1
H7-C2-Pd8-Ag28	45	0	5	0	5
H7-C2-Pd9-Ag26	44	0	1	0	1
H7-C2-Pd9-Ag27	45	0	5	0	5
H7-C2-Pd10-Ag25	44	0	1	0	1
H7-C2-Pd10-Ag26	45	0	15	0	15
H7-C2-Pd11-Ag24	44	0	1	0	1
H7-C2-Pd11-Ag25	45	0	3	0	3
H7-C2-Pd12-Ag23	44	0	1	0	1
H7-C2-Pd12-Ag24	45	0	8	0	8
H7-C2-Pd13-Ag22	44	0	3	0	3
H7-C2-Pd13-Ag23	45	0	3	0	3
H7-C2-Pd14-Ag21	44	0	1	0	1
H7-C2-Pd14-Ag22	45	0	3	0	3
H7-C2-Pd15-Ag21	45	0	2	0	2
H7-C2-Pd16-Ag20	45	0	4	0	4
H7-C2-Pd16-Ag48	73	0	23	0	23
H7-C2-Pd17-Ag18	44	0	2	0	2
H7-C2-Pd17-Ag19	45	0	2	0	2
H7-C2-Pd18-Ag17	44	0	1	0	1
H7-C2-Pd18-Ag18	45	0	11	0	11
H7-C2-Pd19-Ag16	44	0	3	0	3

H7-C2-Pd19-Ag17	45	0	3	0	3
H7-C2-Pd20-Ag15	44	0	3	0	3
H7-C2-Pd20-Ag16	45	0	2	0	2
H7-C2-Pd21-Ag14	44	0	3	0	3
H7-C2-Pd21-Ag15	45	0	7	0	7
H7-C2-Pd22-Ag13	44	0	4	0	4
H7-C2-Pd22-Ag14	45	0	6	0	6
H7-C2-Pd23-Ag13	45	0	7	0	7
H7-C2-Pd24-Ag11	44	0	3	0	3
H7-C2-Pd24-Ag12	45	0	9	0	9
H7-C2-Pd25-Ag10	44	0	3	0	3
H7-C2-Pd25-Ag11	45	0	5	0	5
H7-C2-Pd26-Ag9	44	0	4	0	4
H7-C2-Pd26-Ag10	45	0	5	0	5
H7-C2-Pd27-Ag8	44	0	3	0	3
H7-C2-Pd27-Ag9	45	0	11	0	11
H7-C2-Pd28-Ag7	44	0	3	0	3
H7-C2-Pd28-Ag8	45	0	10	0	10
H7-C2-Pd29-Ag6	44	0	2	0	2
H7-C2-Pd29-Ag7	45	0	18	0	18
H7-C2-Pd30-Ag5	44	0	3	0	3
H7-C2-Pd30-Ag6	45	0	5	0	5
H7-C2-Pd31-Ag4	44	0	4	0	4
H7-C2-Pd31-Ag5	45	0	10	0	10
H7-C2-Pd32-Ag3	44	0	1	0	1
H7-C2-Pd32-Ag4	45	0	10	0	10
H7-C2-Pd33-Ag2	44	0	5	0	5
H7-C2-Pd33-Ag3	45	0	12	0	12
H7-C2-Pd34-Ag1	44	0	2	0	2
H7-C2-Pd34-Ag2	45	0	9	1	10
H7-C2-Pd35	44	0	200	0	200
H7-C2-Pd35-Ag1	45	0	2	0	2
H7-C2-Pd36	45	0	641	0	641
H8-Ag8	16	9	0	7	16
H8-Pd1-Ag7	16	33	0	8	41
H8-Pd2-Ag6	16	31	0	19	50
H8-Pd2-Ag14	24	0	2	189	191
H8-Pd3-Ag5	16	37	0	21	58
H8-Pd3-Ag13	24	0	1	0	1
H8-Pd4-Ag4	16	43	0	17	60
H8-Pd4-Ag28	40	0	3	0	3
H8-Pd5-Ag3	16	37	0	17	54
H8-Pd5-Ag11	24	0	2	0	2
H8-Pd5-Ag27	40	0	11	0	11

H8-Pd6-Ag2	16	61	0	21	82
H8-Pd6-Ag26	40	0	31	1	32
H8-Pd7-Ag1	16	57	0	30	87
H8-Pd7-Ag9	24	0	1	0	1
H8-Pd7-Ag25	40	0	14	1	15
H8-Pd8	16	2986	0	1462	4448
H8-Pd8-Ag8	24	0	0	199	199
H8-Pd8-Ag12	28	0	1	0	1
H8-Pd8-Ag24	40	0	17	0	17
H8-Pd8-Ag56	72	0	10	0	10
H8-Pd9-Ag23	40	0	24	1	25
H8-Pd10-Ag6	24	0	1	0	1
H8-Pd10-Ag22	40	0	30	0	30
H8-Pd10-Ag54	72	0	26	0	26
H8-Pd11-Ag9	28	0	1	0	1
H8-Pd11-Ag21	40	0	34	1	35
H8-Pd12-Ag4	24	0	60	169	229
H8-Pd12-Ag8	28	0	1	0	1
H8-Pd12-Ag20	40	0	33	1	34
H8-Pd12-Ag36	56	0	8	0	8
H8-Pd12-Ag52	72	0	6	0	6
H8-Pd13-Ag7	28	0	1	0	1
H8-Pd13-Ag19	40	0	16	0	16
H8-Pd13-Ag35	56	0	17	0	17
H8-Pd14-Ag2	24	0	65	155	220
H8-Pd14-Ag18	40	0	38	1	39
H8-Pd14-Ag50	72	0	19	0	19
H8-Pd15-Ag1	24	0	2	0	2
H8-Pd15-Ag17	40	0	33	2	35
H8-Pd16	24	0	53	0	53
H8-Pd16-Ag4	28	0	1	0	1
H8-Pd16-Ag16	40	0	8	0	8
H8-Pd16-Ag32	56	0	15	0	15
H8-Pd16-Ag48	72	0	20	1	21
H8-Pd17-Ag3	28	0	1	0	1
H8-Pd17-Ag15	40	0	22	0	22
H8-Pd18-Ag14	40	0	16	0	16
H8-Pd18-Ag46	72	0	36	1	37
H8-Pd19-Ag13	40	0	27	0	27
H8-Pd20	28	0	28	0	28
H8-Pd20-Ag12	40	0	25	0	25
H8-Pd20-Ag44	72	0	44	0	44
H8-Pd21-Ag11	40	0	17	0	17
H8-Pd22-Ag10	40	0	18	0	18

H8-Pd22-Ag42	72	0	22	1	23
H8-Pd24-Ag8	40	0	2	0	2
H8-Pd24-Ag40	72	0	16	0	16
H8-Pd26-Ag38	72	0	12	0	12
H8-Pd28-Ag36	72	0	57	0	57
H8-Pd30-Ag34	72	0	23	0	23
H8-Pd32-Ag32	72	0	40	0	40
H8-Pd34-Ag30	72	0	37	0	37
H8-Pd36-Ag28	72	0	23	1	24
H8-Pd38-Ag26	72	0	23	0	23
H8-Pd40-Ag24	72	0	20	1	21
H8-Pd42-Ag22	72	0	31	1	32
H8-Pd44-Ag20	72	0	16	0	16
H8-Pd48-Ag16	72	0	2	0	2
H8-C2-Pd2-Ag14	26	0	1	0	1
H8-C2-Pd15-Ag1	26	0	1	0	1
H8-C2-Pd16	26	0	10	0	10
H8-C2-Pd16-Ag48	74	0	30	0	30
H8-C2-Pd20-Ag17	47	0	1	0	1
H8-C2-Pd37	47	0	10	0	10
H8-C7-Ag21	36	0	2	0	2
H8-C7-Pd1-Ag20	36	0	1	0	1
H8-C7-Pd3-Ag18	36	0	1	0	1
H8-C7-Pd5-Ag16	36	0	1	0	1
H8-C7-Pd6-Ag15	36	0	2	0	2
H8-C7-Pd7-Ag14	36	0	2	0	2
H8-C7-Pd9-Ag12	36	0	2	0	2
H8-C7-Pd10-Ag11	36	0	1	0	1
H8-C7-Pd11-Ag10	36	0	1	0	1
H8-C7-Pd12-Ag9	36	0	4	0	4
H8-C7-Pd13-Ag8	36	0	3	0	3
H8-C7-Pd14-Ag7	36	0	4	0	4
H8-C7-Pd17-Ag4	36	0	8	0	8
H8-C7-Pd18-Ag3	36	0	1	0	1
H8-C7-Pd19-Ag2	36	0	4	0	4
H8-C7-Pd20-Ag1	36	0	5	0	5
H8-C7-Pd21	36	0	94	1	95
H9-Pd5-Ag18	32	1	0	0	1
H9-Pd7-Ag16	32	1	0	0	1
H9-Pd9-Ag14	32	1	0	0	1
H9-Pd10-Ag13	32	1	0	0	1
H9-Pd13-Ag10	32	1	0	0	1
H9-Pd14-Ag9	32	2	0	0	2
H9-Pd21-Ag2	32	1	0	0	1

H9-Pd22-Ag1	32	1	0	0	1
H9-Pd23	32	96	0	0	96
H9-Pd27-Ag4	40	0	6	0	6
H9-C2-Pd1-Ag19	31	0	1	0	1
H9-C2-Pd2-Ag14	27	0	1	0	1
H9-C2-Pd2-Ag18	31	0	1	0	1
H9-C2-Pd3-Ag13	27	0	1	0	1
H9-C2-Pd5-Ag11	27	0	5	0	5
H9-C2-Pd5-Ag15	31	0	1	0	1
H9-C2-Pd9-Ag7	27	0	1	0	1
H9-C2-Pd11-Ag9	31	0	1	0	1
H9-C2-Pd12-Ag4	27	0	7	0	7
H9-C2-Pd12-Ag20	43	0	21	1	22
H9-C2-Pd13-Ag19	43	0	20	1	21
H9-C2-Pd16	27	0	23	0	23
H9-C2-Pd20	31	0	11	0	11
H10-Pd3-Ag19	32	0	2	0	2
H10-Pd4-Ag18	32	0	1	0	1
H10-Pd5-Ag17	32	0	0	2	2
H10-Pd6-Ag15	31	0	2	0	2
H10-Pd6-Ag16	32	0	0	2	2
H10-Pd7-Ag14	31	0	1	0	1
H10-Pd7-Ag15	32	0	1	2	3
H10-Pd8-Ag14	32	0	1	2	3
H10-Pd9-Ag12	31	0	1	0	1
H10-Pd10-Ag11	31	0	2	0	2
H10-Pd10-Ag12	32	0	0	3	3
H10-Pd12-Ag10	32	0	0	1	1
H10-Pd12-Ag36	58	0	11	0	11
H10-Pd13-Ag35	58	0	13	0	13
H10-Pd14-Ag7	31	0	1	0	1
H10-Pd16-Ag5	31	0	1	0	1
H10-Pd16-Ag6	32	0	0	2	2
H10-Pd17-Ag5	32	0	2	1	3
H10-Pd19-Ag3	32	0	0	3	3
H10-Pd20-Ag1	31	0	1	0	1
H10-Pd20-Ag2	32	0	0	3	3
H10-Pd21	31	0	92	0	92
H10-Pd21-Ag1	32	0	1	1	2
H10-Pd22	32	0	64	207	271
H10-C2-Pd12-Ag20	44	0	43	1	44
H10-C2-Pd13-Ag19	44	0	23	0	23
H10-C4	14	2	0	0	2
H10-C6-Pd3-Ag37	56	0	0	1	1

H10-C6-Pd6-Ag34	56	0	0	1	1
H10-C6-Pd13-Ag27	56	0	0	1	1
H10-C6-Pd27-Ag13	56	0	0	1	1
H10-C6-Pd29-Ag11	56	0	0	1	1
H10-C6-Pd30-Ag10	56	0	0	2	2
H10-C6-Pd40	56	0	0	16	16
H10-C8-Pd2-Ag40	60	0	1	0	1
H10-C8-Pd19-Ag23	60	0	1	0	1
H10-C8-Pd28-Ag14	60	0	1	0	1
H10-C8-Pd33-Ag9	60	0	2	0	2
H10-C8-Pd42	60	0	19	0	19
H10-C12-Pd6-Ag34	62	0	0	1	1
H10-C12-Pd12-Ag28	62	0	0	1	1
H10-C12-Pd13-Ag27	62	0	0	2	2
H10-C12-Pd19-Ag21	62	0	0	1	1
H10-C12-Pd20-Ag20	62	0	0	2	2
H10-C12-Pd21-Ag19	62	0	0	1	1
H10-C12-Pd25-Ag15	62	0	0	1	1
H10-C12-Pd30-Ag10	62	0	0	1	1
H10-C12-Pd32-Ag8	62	0	0	1	1
H10-C12-Pd33-Ag7	62	0	0	2	2
H10-C12-Pd36-Ag4	62	0	0	2	2
H10-C12-Pd40	62	0	0	26	26
H11-Ag5	16	0	0	10	10
H11-Pd1-Ag4	16	0	2	25	27
H11-Pd2-Ag3	16	0	2	26	28
H11-Pd3-Ag2	16	0	2	23	25
H11-Pd3-Ag18	32	0	0	3	3
H11-Pd4-Ag1	16	0	2	40	42
H11-Pd4-Ag17	32	0	0	1	1
H11-Pd5	16	0	41	1334	1375
H11-Pd6-Ag15	32	0	0	1	1
H11-Pd9-Ag12	32	0	0	2	2
H11-Pd10-Ag11	32	0	0	1	1
H11-Pd11-Ag10	32	0	0	1	1
H11-Pd12-Ag9	32	0	0	1	1
H11-Pd14-Ag7	32	0	0	1	1
H11-Pd15-Ag6	32	0	0	4	4
H11-Pd16-Ag5	32	0	0	1	1
H11-Pd18-Ag3	32	0	0	1	1
H11-Pd19-Ag2	32	0	0	1	1
H11-Pd20-Ag1	32	0	0	2	2
H11-Pd21	32	0	0	176	176
H11-C2-Pd12-Ag20	45	0	17	0	17

H11-C2-Pd13-Ag19	45	0	23	0	23
H12-Pd4-Ag28	44	0	7	0	7
H12-Pd5-Ag27	44	0	21	0	21
H12-Pd6-Ag26	44	0	17	0	17
H12-Pd7-Ag25	44	0	28	0	28
H12-Pd8-Ag24	44	0	22	0	22
H12-Pd9-Ag23	44	0	7	0	7
H12-Pd10-Ag22	44	0	31	0	31
H12-Pd11-Ag21	44	0	45	0	45
H12-Pd12-Ag20	44	0	22	0	22
H12-Pd13-Ag19	44	0	35	0	35
H12-Pd14-Ag18	44	0	22	0	22
H12-Pd15-Ag17	44	0	36	2	38
H12-Pd16-Ag16	44	0	31	0	31
H12-Pd16-Ag32	60	0	3	0	3
H12-Pd17-Ag15	44	0	12	0	12
H12-Pd18-Ag14	44	0	23	1	24
H12-Pd19-Ag13	44	0	21	1	22
H12-Pd20-Ag12	44	0	28	0	28
H12-Pd21-Ag11	44	0	8	0	8
H12-Pd22-Ag10	44	0	20	1	21
H12-Pd23-Ag9	44	0	3	0	3
H12-Pd24-Ag8	44	0	2	0	2
H12-C2-Pd12-Ag20	46	0	10	0	10
H12-C2-Pd13-Ag19	46	0	17	0	17
H13-Pd6-Ag13	32	0	0	1	1
H13-Pd9-Ag10	32	0	0	1	1
H13-Pd17-Ag2	32	0	0	1	1
H13-Pd19	32	0	0	53	53
H13-C2-Pd1-Ag15	31	0	1	0	1
H13-C2-Pd2-Ag14	31	0	1	0	1
H13-C2-Pd3-Ag13	31	0	12	0	12
H13-C2-Pd4-Ag12	31	0	11	0	11
H13-C2-Pd6-Ag10	31	0	1	0	1
H13-C2-Pd7-Ag9	31	0	11	0	11
H13-C2-Pd8-Ag8	31	0	1	0	1
H13-C2-Pd9-Ag7	31	0	1	0	1
H13-C2-Pd10-Ag6	31	0	2	0	2
H13-C2-Pd11-Ag5	31	0	1	0	1
H13-C2-Pd12-Ag4	31	0	1	0	1
H13-C2-Pd13-Ag3	31	0	1	0	1
H13-C2-Pd14-Ag2	31	0	1	0	1
H13-C2-Pd16	31	0	86	0	86
H13-C5-Pd2-Ag20	40	0	1	0	1

H13-C5-Pd7-Ag15	40	0	1	0	1
H13-C5-Pd9-Ag13	40	0	1	0	1
H13-C5-Pd11-Ag11	40	0	2	0	2
H13-C5-Pd12-Ag10	40	0	2	0	2
H13-C5-Pd17-Ag5	40	0	3	0	3
H13-C5-Pd18-Ag4	40	0	1	0	1
H13-C5-Pd19-Ag3	40	0	6	0	6
H13-C5-Pd20-Ag2	40	0	1	0	1
H13-C5-Pd21-Ag1	40	0	1	0	1
H13-C5-Pd22	40	0	29	0	29
H14-Pd2-Ag15	31	0	0	2	2
H14-Pd4-Ag13	31	0	0	3	3
H14-Pd5-Ag12	31	0	0	2	2
H14-Pd5-Ag13	32	0	0	2	2
H14-Pd7-Ag10	31	0	0	1	1
H14-Pd8-Ag9	31	0	0	1	1
H14-Pd9-Ag8	31	0	0	1	1
H14-Pd10-Ag7	31	0	0	1	1
H14-Pd10-Ag8	32	0	0	1	1
H14-Pd11-Ag6	31	0	0	1	1
H14-Pd11-Ag7	32	0	0	1	1
H14-Pd12-Ag5	31	0	0	1	1
H14-Pd12-Ag6	32	0	0	1	1
H14-Pd13-Ag4	31	0	0	1	1
H14-Pd14-Ag3	31	0	0	2	2
H14-Pd14-Ag4	32	0	0	1	1
H14-Pd15-Ag3	32	0	0	2	2
H14-Pd16-Ag1	31	0	0	1	1
H14-Pd17	31	0	0	126	126
H14-Pd17-Ag1	32	0	0	1	1
H14-Pd17-Ag31	62	0	2	0	2
H14-Pd18	32	0	0	84	84
H14-C2-Pd3-Ag37	56	0	1	0	1
H14-C2-Pd7-Ag33	56	0	1	0	1
H14-C2-Pd38-Ag2	56	0	1	0	1
H14-C2-Pd40	56	0	14	0	14
H15-Ag6	21	0	1	0	1
H15-Pd1-Ag5	21	0	8	0	8
H15-Pd1-Ag16	32	0	0	1	1
H15-Pd2-Ag4	21	0	10	0	10
H15-Pd2-Ag14	31	0	0	1	1
H15-Pd2-Ag15	32	0	0	1	1
H15-Pd3-Ag3	21	0	5	0	5
H15-Pd3-Ag14	32	0	0	1	1

H15-Pd4-Ag2	21	0	17	0	17
H15-Pd4-Ag12	31	0	0	2	2
H15-Pd4-Ag13	32	0	0	1	1
H15-Pd5-Ag1	21	0	16	0	16
H15-Pd5-Ag11	31	0	0	2	2
H15-Pd5-Ag12	32	0	0	1	1
H15-Pd6	21	0	650	0	650
H15-Pd6-Ag11	32	0	0	1	1
H15-Pd7-Ag9	31	0	0	1	1
H15-Pd7-Ag10	32	0	0	1	1
H15-Pd8-Ag8	31	0	0	1	1
H15-Pd9-Ag8	32	0	0	1	1
H15-Pd10-Ag6	31	0	0	1	1
H15-Pd10-Ag7	32	0	0	2	2
H15-Pd11-Ag6	32	0	0	3	3
H15-Pd12-Ag5	32	0	0	2	2
H15-Pd13-Ag4	32	0	0	1	1
H15-Pd14-Ag2	31	0	0	1	1
H15-Pd14-Ag3	32	0	0	8	8
H15-Pd15-Ag1	31	0	0	2	2
H15-Pd15-Ag2	32	0	0	5	5
H15-Pd16	31	0	0	165	165
H15-Pd16-Ag1	32	0	0	2	2
H15-Pd17	32	0	0	259	259
H15-C1-Pd2-Ag14	32	0	0	1	1
H15-C1-Pd3-Ag13	32	0	0	2	2
H15-C1-Pd4-Ag12	32	0	0	1	1
H15-C1-Pd5-Ag11	32	0	0	2	2
H15-C1-Pd6-Ag10	32	0	0	3	3
H15-C1-Pd7-Ag9	32	0	0	3	3
H15-C1-Pd8-Ag8	32	0	9	3	12
H15-C1-Pd9-Ag7	32	0	0	2	2
H15-C1-Pd10-Ag6	32	0	0	2	2
H15-C1-Pd12-Ag4	32	0	7	4	11
H15-C1-Pd13-Ag3	32	0	2	6	8
H15-C1-Pd14-Ag2	32	0	0	3	3
H15-C1-Pd15-Ag1	32	0	0	5	5
H15-C1-Pd16	32	0	0	100	100
H16-Ag5	21	0	4	0	4
H16-Pd1-Ag4	21	0	17	3	20
H16-Pd2-Ag3	21	0	21	2	23
H16-Pd3-Ag2	21	0	27	0	27
H16-Pd3-Ag13	32	0	0	1	1
H16-Pd4-Ag1	21	0	24	1	25

H16-Pd4-Ag12	32	0	0	5	5
H16-Pd4-Ag28	48	0	5	0	5
H16-Pd5	21	0	950	58	1008
H16-Pd5-Ag11	32	0	0	2	2
H16-Pd5-Ag27	48	0	12	0	12
H16-Pd6-Ag10	32	0	0	2	2
H16-Pd6-Ag26	48	0	9	0	9
H16-Pd7-Ag9	32	0	0	3	3
H16-Pd7-Ag25	48	0	19	0	19
H16-Pd8-Ag8	32	0	0	2	2
H16-Pd8-Ag24	48	0	22	0	22
H16-Pd9-Ag7	32	0	0	5	5
H16-Pd9-Ag23	48	0	25	0	25
H16-Pd10-Ag6	32	0	0	6	6
H16-Pd10-Ag22	48	0	20	0	20
H16-Pd11-Ag5	32	0	0	5	5
H16-Pd11-Ag21	48	0	20	0	20
H16-Pd12-Ag4	32	0	0	10	10
H16-Pd12-Ag20	48	0	28	0	28
H16-Pd13-Ag3	32	0	0	8	8
H16-Pd13-Ag19	48	0	13	0	13
H16-Pd14-Ag2	32	0	0	6	6
H16-Pd14-Ag18	48	0	19	0	19
H16-Pd15-Ag17	48	0	37	0	37
H16-Pd16	32	0	1	459	460
H16-Pd16-Ag16	48	0	20	0	20
H16-Pd17-Ag15	48	0	29	0	29
H16-Pd18-Ag14	48	0	33	0	33
H16-Pd18-Ag30	64	0	1	0	1
H16-Pd19-Ag13	48	0	14	0	14
H16-Pd20-Ag12	48	0	24	0	24
H16-Pd20-Ag28	64	0	2	0	2
H16-Pd21-Ag11	48	0	31	0	31
H16-Pd22-Ag10	48	0	28	0	28
H16-Pd24-Ag8	48	0	10	0	10
H16-C2-Ag16	34	0	22	0	22
H16-C2-Pd1-Ag15	34	0	6	0	6
H16-C2-Pd1-Ag19	38	0	7	0	7
H16-C2-Pd2-Ag14	34	0	6	0	6
H16-C2-Pd2-Ag18	38	0	11	0	11
H16-C2-Pd3-Ag13	34	0	2	0	2
H16-C2-Pd3-Ag17	38	0	8	0	8
H16-C2-Pd4-Ag12	34	0	7	0	7
H16-C2-Pd4-Ag16	38	0	2	0	2

H16-C2-Pd5-Ag11	34	0	3	0	3
H16-C2-Pd5-Ag15	38	0	21	0	21
H16-C2-Pd6-Ag10	34	0	2	0	2
H16-C2-Pd6-Ag14	38	0	16	0	16
H16-C2-Pd7-Ag9	34	0	2	0	2
H16-C2-Pd7-Ag13	38	0	21	0	21
H16-C2-Pd8-Ag8	34	0	5	0	5
H16-C2-Pd8-Ag12	38	0	13	0	13
H16-C2-Pd9-Ag7	34	0	1	0	1
H16-C2-Pd9-Ag11	38	0	5	0	5
H16-C2-Pd10-Ag6	34	0	3	0	3
H16-C2-Pd10-Ag10	38	0	8	0	8
H16-C2-Pd11-Ag5	34	0	4	0	4
H16-C2-Pd11-Ag9	38	0	14	0	14
H16-C2-Pd12-Ag4	34	0	4	0	4
H16-C2-Pd12-Ag8	38	0	7	0	7
H16-C2-Pd13-Ag3	34	0	7	0	7
H16-C2-Pd13-Ag7	38	0	13	0	13
H16-C2-Pd14-Ag2	34	0	3	0	3
H16-C2-Pd14-Ag6	38	0	9	0	9
H16-C2-Pd15-Ag1	34	0	3	0	3
H16-C2-Pd15-Ag5	38	0	15	0	15
H16-C2-Pd16	34	0	158	0	158
H16-C2-Pd16-Ag4	38	0	21	0	21
H16-C2-Pd17-Ag3	38	0	13	0	13
H16-C2-Pd18-Ag2	38	0	10	0	10
H16-C2-Pd19-Ag1	38	0	5	0	5
H16-C2-Pd20	38	0	465	1	466
H16-C4-Pd1-Ag19	40	0	1	0	1
H16-C4-Pd2-Ag18	40	0	0	1	1
H16-C4-Pd3-Ag17	40	0	23	0	23
H16-C4-Pd4-Ag16	40	0	5	0	5
H16-C4-Pd5-Ag15	40	0	4	0	4
H16-C4-Pd6-Ag14	40	0	1	0	1
H16-C4-Pd7-Ag13	40	0	2	0	2
H16-C4-Pd8-Ag12	40	0	1	0	1
H16-C4-Pd9-Ag11	40	0	3	0	3
H16-C4-Pd11-Ag9	40	0	10	0	10
H16-C4-Pd12-Ag8	40	0	4	0	4
H16-C4-Pd13-Ag7	40	0	1	0	1
H16-C4-Pd14-Ag6	40	0	3	0	3
H16-C4-Pd15-Ag5	40	0	16	0	16
H16-C4-Pd16-Ag4	40	0	4	0	4
H16-C4-Pd17-Ag3	40	0	13	1	14

H16-C4-Pd18-Ag2	40	0	3	0	3
H16-C4-Pd19-Ag1	40	0	3	0	3
H16-C4-Pd20	40	0	184	1	185
H16-C14-Pd4-Ag38	72	0	2	0	2
H16-C14-Pd18-Ag24	72	0	2	0	2
H16-C14-Pd22-Ag20	72	0	2	0	2
H16-C14-Pd23-Ag19	72	0	2	0	2
H16-C14-Pd26-Ag16	72	0	1	0	1
H16-C14-Pd29-Ag13	72	0	1	0	1
H16-C14-Pd30-Ag12	72	0	1	0	1
H16-C14-Pd32-Ag10	72	0	2	0	2
H16-C14-Pd33-Ag9	72	0	1	0	1
H16-C14-Pd34-Ag8	72	0	1	0	1
H16-C14-Pd35-Ag7	72	0	1	0	1
H16-C14-Pd38-Ag4	72	0	1	0	1
H16-C14-Pd42	72	0	42	0	42
H17-Pd3-Ag12	32	0	0	2	2
H17-Pd4-Ag11	32	0	0	2	2
H17-Pd5-Ag10	32	0	0	1	1
H17-Pd6-Ag9	32	0	0	2	2
H17-Pd7-Ag8	32	0	0	2	2
H17-Pd8-Ag7	32	0	0	3	3
H17-Pd9-Ag6	32	0	0	1	1
H17-Pd10-Ag5	32	0	0	2	2
H17-Pd13-Ag2	32	0	0	2	2
H17-Pd14-Ag1	32	0	0	3	3
H17-Pd15	32	0	0	103	103
H17-C2-Ag16	35	0	4	0	4
H17-C2-Pd1-Ag15	35	0	6	0	6
H17-C2-Pd2-Ag14	35	0	2	0	2
H17-C2-Pd3-Ag13	35	0	2	0	2
H17-C2-Pd4-Ag12	35	0	2	0	2
H17-C2-Pd5-Ag11	35	0	2	0	2
H17-C2-Pd6-Ag10	35	0	3	0	3
H17-C2-Pd8-Ag8	35	0	2	0	2
H17-C2-Pd9-Ag7	35	0	30	0	30
H17-C2-Pd10-Ag6	35	0	7	0	7
H17-C2-Pd11-Ag5	35	0	14	0	14
H17-C2-Pd13-Ag3	35	0	6	0	6
H17-C2-Pd14-Ag2	35	0	11	0	11
H17-C2-Pd15-Ag1	35	0	2	0	2
H17-C2-Pd16	35	0	191	0	191
H17-C2-Pd18-Ag14	51	0	39	0	39
H17-C2-Pd20-Ag12	51	0	41	0	41

H17-C2-Pd64	83	0	118	0	118
H17-C3-Ag20	40	0	2	0	2
H17-C3-Pd1-Ag19	40	0	3	0	3
H17-C3-Pd2-Ag18	40	0	1	0	1
H17-C3-Pd3-Ag17	40	0	4	0	4
H17-C3-Pd4-Ag16	40	0	3	0	3
H17-C3-Pd5-Ag15	40	0	2	0	2
H17-C3-Pd6-Ag14	40	0	2	0	2
H17-C3-Pd7-Ag13	40	0	23	0	23
H17-C3-Pd8-Ag12	40	0	6	0	6
H17-C3-Pd9-Ag11	40	0	4	0	4
H17-C3-Pd10-Ag10	40	0	3	0	3
H17-C3-Pd11-Ag9	40	0	3	0	3
H17-C3-Pd12-Ag8	40	0	6	0	6
H17-C3-Pd13-Ag7	40	0	4	0	4
H17-C3-Pd14-Ag6	40	0	9	0	9
H17-C3-Pd15-Ag5	40	0	11	0	11
H17-C3-Pd16-Ag4	40	0	5	0	5
H17-C3-Pd17-Ag3	40	0	2	0	2
H17-C3-Pd18-Ag2	40	0	7	0	7
H17-C3-Pd19-Ag1	40	0	6	0	6
H17-C3-Pd20	40	0	223	0	223
H17-C5-Pd1-Ag23	46	0	2	0	2
H17-C5-Pd2-Ag22	46	0	1	0	1
H17-C5-Pd3-Ag21	46	0	1	0	1
H17-C5-Pd4-Ag20	46	0	1	0	1
H17-C5-Pd6-Ag18	46	0	2	0	2
H17-C5-Pd9-Ag15	46	0	2	0	2
H17-C5-Pd10-Ag14	46	0	17	0	17
H17-C5-Pd11-Ag13	46	0	14	0	14
H17-C5-Pd12-Ag12	46	0	1	0	1
H17-C5-Pd13-Ag11	46	0	1	0	1
H17-C5-Pd14-Ag10	46	0	2	0	2
H17-C5-Pd15-Ag9	46	0	5	0	5
H17-C5-Pd16-Ag8	46	0	2	0	2
H17-C5-Pd17-Ag7	46	0	3	0	3
H17-C5-Pd18-Ag6	46	0	2	0	2
H17-C5-Pd19-Ag5	46	0	1	0	1
H17-C5-Pd20-Ag4	46	0	2	0	2
H17-C5-Pd21-Ag3	46	0	1	0	1
H17-C5-Pd24	46	0	100	0	100
H18-Pd6-Ag7	31	0	0	3	3
H18-Pd7-Ag6	31	0	0	1	1
H18-Pd11-Ag2	31	0	0	1	1

H18-Pd12-Ag1	31	0	0	1	1
H18-Pd13	31	0	0	50	50
H18-C2-Ag16	36	0	16	0	16
H18-C2-Ag20	40	0	6	0	6
H18-C2-Pd1-Ag15	36	0	2	0	2
H18-C2-Pd1-Ag19	40	0	2	0	2
H18-C2-Pd2-Ag14	36	0	6	0	6
H18-C2-Pd2-Ag18	40	0	1	0	1
H18-C2-Pd2-Ag24	46	0	1	0	1
H18-C2-Pd3-Ag13	36	0	4	0	4
H18-C2-Pd3-Ag17	40	0	3	0	3
H18-C2-Pd4-Ag12	36	0	5	0	5
H18-C2-Pd4-Ag16	40	0	1	0	1
H18-C2-Pd5-Ag11	36	0	6	0	6
H18-C2-Pd5-Ag15	40	0	3	0	3
H18-C2-Pd5-Ag21	46	0	1	0	1
H18-C2-Pd6-Ag10	36	0	11	0	11
H18-C2-Pd6-Ag14	40	0	3	0	3
H18-C2-Pd6-Ag20	46	0	1	0	1
H18-C2-Pd7-Ag9	36	0	4	0	4
H18-C2-Pd7-Ag13	40	0	6	0	6
H18-C2-Pd7-Ag19	46	0	2	0	2
H18-C2-Pd8-Ag8	36	0	11	0	11
H18-C2-Pd8-Ag12	40	0	7	0	7
H18-C2-Pd8-Ag18	46	0	1	0	1
H18-C2-Pd9-Ag7	36	0	6	0	6
H18-C2-Pd9-Ag11	40	0	2	0	2
H18-C2-Pd10-Ag6	36	0	9	0	9
H18-C2-Pd10-Ag10	40	0	4	0	4
H18-C2-Pd10-Ag16	46	0	15	0	15
H18-C2-Pd11-Ag5	36	0	5	0	5
H18-C2-Pd11-Ag9	40	0	7	0	7
H18-C2-Pd12-Ag4	36	0	5	0	5
H18-C2-Pd12-Ag8	40	0	6	0	6
H18-C2-Pd12-Ag14	46	0	1	0	1
H18-C2-Pd13-Ag3	36	0	7	0	7
H18-C2-Pd13-Ag7	40	0	8	0	8
H18-C2-Pd14-Ag2	36	0	6	0	6
H18-C2-Pd14-Ag6	40	0	7	0	7
H18-C2-Pd14-Ag12	46	0	1	0	1
H18-C2-Pd15-Ag1	36	0	9	0	9
H18-C2-Pd15-Ag5	40	0	4	0	4
H18-C2-Pd15-Ag11	46	0	2	0	2
H18-C2-Pd16	36	0	300	1	301

H18-C2-Pd16-Ag4	40	0	4	0	4
H18-C2-Pd16-Ag10	46	0	3	0	3
H18-C2-Pd17-Ag3	40	0	13	0	13
H18-C2-Pd17-Ag9	46	0	1	0	1
H18-C2-Pd18-Ag2	40	0	9	0	9
H18-C2-Pd18-Ag8	46	0	1	0	1
H18-C2-Pd18-Ag14	52	0	16	0	16
H18-C2-Pd19-Ag1	40	0	3	0	3
H18-C2-Pd19-Ag7	46	0	1	0	1
H18-C2-Pd20	40	0	282	0	282
H18-C2-Pd20-Ag6	46	0	2	0	2
H18-C2-Pd20-Ag12	52	0	12	0	12
H18-C2-Pd21-Ag5	46	0	2	0	2
H18-C2-Pd23-Ag3	46	0	1	0	1
H18-C2-Pd26	46	0	72	0	72
H18-C2-Pd64	84	0	119	0	119
H19-Pd3-Ag10	32	0	0	2	2
H19-Pd5-Ag8	32	0	0	1	1
H19-Pd10-Ag3	32	0	0	1	1
H19-Pd11-Ag2	32	0	0	1	1
H19-Pd13	32	0	0	64	64
H19-C2-Pd1-Ag19	41	0	2	0	2
H19-C2-Pd3-Ag17	41	0	1	0	1
H19-C2-Pd4-Ag16	41	0	2	0	2
H19-C2-Pd5-Ag15	41	0	1	0	1
H19-C2-Pd7-Ag13	41	0	3	0	3
H19-C2-Pd8-Ag12	41	0	1	0	1
H19-C2-Pd10-Ag10	41	0	2	0	2
H19-C2-Pd11-Ag9	41	0	1	0	1
H19-C2-Pd12-Ag8	41	0	2	0	2
H19-C2-Pd13-Ag7	41	0	3	0	3
H19-C2-Pd15-Ag5	41	0	2	0	2
H19-C2-Pd16-Ag4	41	0	1	0	1
H19-C2-Pd18-Ag14	53	0	27	0	27
H19-C2-Pd19-Ag1	41	0	1	0	1
H19-C2-Pd20	41	0	69	0	69
H20-C2-Pd3-Ag64	89	0	1	0	1
H20-C2-Pd8-Ag59	89	0	1	0	1
H20-C2-Pd9-Ag58	89	0	1	0	1
H20-C2-Pd18-Ag14	54	0	22	0	22
H20-C2-Pd20-Ag12	54	0	14	1	15
H20-C2-Pd22-Ag45	89	0	1	0	1
H20-C2-Pd25-Ag14	61	0	1	0	1
H20-C2-Pd33-Ag6	61	0	1	0	1

H20-C2-Pd39	61	0	14	0	14
H20-C2-Pd42-Ag25	89	0	1	0	1
H20-C2-Pd52-Ag15	89	0	1	0	1
H20-C2-Pd64	86	0	131	0	131
H20-C2-Pd67	89	0	12	0	12
H20-C8-Pd10-Ag34	72	0	1	0	1
H20-C8-Pd24-Ag20	72	0	1	0	1
H20-C8-Pd29-Ag15	72	0	1	0	1
H20-C8-Pd33-Ag11	72	0	1	0	1
H20-C8-Pd39-Ag5	72	0	1	0	1
H20-C8-Pd44	72	0	15	0	15
H21-C2-Pd20-Ag12	55	0	18	0	18
H21-C2-Pd64	87	0	145	0	145
H22-C2-Pd20-Ag11	55	0	0	1	1
H22-C2-Pd25-Ag6	55	0	0	2	2
H22-C2-Pd27-Ag4	55	0	0	1	1
H22-C2-Pd31	55	0	0	13	13
H22-C3-Pd3-Ag37	65	0	1	0	1
H22-C3-Pd4-Ag36	65	0	1	0	1
H22-C3-Pd5-Ag35	65	0	1	0	1
H22-C3-Pd6-Ag34	65	0	1	0	1
H22-C3-Pd7-Ag33	65	0	1	0	1
H22-C3-Pd9-Ag31	65	0	1	0	1
H22-C3-Pd23-Ag17	65	0	1	0	1
H22-C3-Pd29-Ag11	65	0	1	0	1
H22-C3-Pd31-Ag9	65	0	1	0	1
H22-C3-Pd32-Ag8	65	0	2	0	2
H22-C3-Pd35-Ag5	65	0	1	0	1
H22-C3-Pd40	65	0	25	0	25
H22-C4-Pd12-Ag36	74	0	1	0	1
H22-C4-Pd20-Ag28	74	0	1	0	1
H22-C4-Pd26-Ag22	74	0	1	0	1
H22-C4-Pd27-Ag21	74	0	1	0	1
H22-C4-Pd35-Ag13	74	0	1	0	1
H22-C4-Pd48	74	0	23	0	23
H23-Ag9	32	0	2	0	2
H23-Pd1-Ag7	31	0	1	0	1
H23-Pd1-Ag8	32	0	3	2	5
H23-Pd2-Ag6	31	0	4	0	4
H23-Pd2-Ag7	32	0	2	0	2
H23-Pd3-Ag5	31	0	1	0	1
H23-Pd3-Ag6	32	0	3	0	3
H23-Pd4-Ag4	31	0	1	0	1
H23-Pd4-Ag5	32	0	7	1	8

H23-Pd5-Ag3	31	0	2	1	3
H23-Pd5-Ag4	32	0	2	1	3
H23-Pd6-Ag2	31	0	4	1	5
H23-Pd6-Ag3	32	0	2	0	2
H23-Pd7-Ag1	31	0	1	2	3
H23-Pd7-Ag2	32	0	1	2	3
H23-Pd8	31	0	149	68	217
H23-Pd8-Ag1	32	0	1	2	3
H23-Pd9	32	0	235	139	374
H24-Pd1-Ag7	32	0	0	1	1
H24-Pd2-Ag6	32	0	0	3	3
H24-Pd3-Ag5	32	0	0	1	1
H24-Pd4-Ag4	32	0	3	0	3
H24-Pd7-Ag1	32	0	1	1	2
H24-Pd8	32	0	41	71	112
H24-C2-Ag20	46	0	8	0	8
H24-C2-Pd1-Ag19	46	0	4	0	4
H24-C2-Pd2-Ag18	46	0	5	0	5
H24-C2-Pd3-Ag17	46	0	4	0	4
H24-C2-Pd4-Ag16	46	0	4	0	4
H24-C2-Pd5-Ag15	46	0	2	0	2
H24-C2-Pd6-Ag14	46	0	2	0	2
H24-C2-Pd7-Ag13	46	0	15	0	15
H24-C2-Pd8-Ag12	46	0	10	0	10
H24-C2-Pd9-Ag11	46	0	9	0	9
H24-C2-Pd10-Ag10	46	0	22	0	22
H24-C2-Pd11-Ag9	46	0	12	0	12
H24-C2-Pd12-Ag8	46	0	11	0	11
H24-C2-Pd13-Ag7	46	0	14	0	14
H24-C2-Pd14-Ag6	46	0	13	0	13
H24-C2-Pd15-Ag5	46	0	10	0	10
H24-C2-Pd16-Ag4	46	0	14	0	14
H24-C2-Pd17-Ag3	46	0	13	0	13
H24-C2-Pd18-Ag2	46	0	22	0	22
H24-C2-Pd19-Ag1	46	0	10	0	10
H24-C2-Pd20	46	0	554	0	554
H25-C3-Pd4-Ag47	79	0	1	0	1
H25-C3-Pd19-Ag32	79	0	1	0	1
H25-C3-Pd26-Ag25	79	0	1	0	1
H25-C3-Pd27-Ag24	79	0	1	0	1
H25-C3-Pd35-Ag16	79	0	2	0	2
H25-C3-Pd36-Ag15	79	0	1	0	1
H25-C3-Pd51	79	0	13	0	13
H26-C2-Pd3-Ag37	68	0	2	0	2

H26-C2-Pd4-Ag36	68	0	1	0	1
H26-C2-Pd5-Ag35	68	0	1	0	1
H26-C2-Pd9-Ag31	68	0	5	0	5
H26-C2-Pd11-Ag29	68	0	2	0	2
H26-C2-Pd12-Ag28	68	0	2	0	2
H26-C2-Pd14-Ag26	68	0	1	0	1
H26-C2-Pd19-Ag21	68	0	3	0	3
H26-C2-Pd21-Ag19	68	0	1	0	1
H26-C2-Pd22-Ag18	68	0	1	0	1
H26-C2-Pd23-Ag17	68	0	1	0	1
H26-C2-Pd25-Ag15	68	0	1	0	1
H26-C2-Pd28-Ag12	68	0	1	0	1
H26-C2-Pd29-Ag11	68	0	1	0	1
H26-C2-Pd30-Ag10	68	0	3	0	3
H26-C2-Pd31-Ag9	68	0	1	0	1
H26-C2-Pd32-Ag8	68	0	2	0	2
H26-C2-Pd33-Ag7	68	0	1	0	1
H26-C2-Pd34-Ag6	68	0	1	0	1
H26-C2-Pd37-Ag3	68	0	2	0	2
H26-C2-Pd38-Ag2	68	0	2	0	2
H26-C2-Pd40	68	0	116	0	116
H26-C10-Pd2-Ag42	80	0	1	0	1
H26-C10-Pd5-Ag39	80	0	1	0	1
H26-C10-Pd9-Ag35	80	0	1	0	1
H26-C10-Pd21-Ag23	80	0	1	0	1
H26-C10-Pd24-Ag20	80	0	2	0	2
H26-C10-Pd26-Ag18	80	0	1	0	1
H26-C10-Pd28-Ag16	80	0	1	0	1
H26-C10-Pd34-Ag10	80	0	2	0	2
H26-C10-Pd35-Ag9	80	0	1	0	1
H26-C10-Pd36-Ag8	80	0	1	0	1
H26-C10-Pd38-Ag6	80	0	1	0	1
H26-C10-Pd44	80	0	37	0	37
H27-C2-Pd2-Ag33	64	0	2	0	2
H27-C2-Pd2-Ag34	65	0	3	0	3
H27-C2-Pd3-Ag33	65	0	4	0	4
H27-C2-Pd4-Ag31	64	0	7	0	7
H27-C2-Pd4-Ag32	65	0	4	0	4
H27-C2-Pd5-Ag30	64	0	1	0	1
H27-C2-Pd5-Ag31	65	0	1	0	1
H27-C2-Pd6-Ag29	64	0	3	0	3
H27-C2-Pd6-Ag30	65	0	2	0	2
H27-C2-Pd8-Ag27	64	0	2	0	2
H27-C2-Pd9-Ag27	65	0	3	0	3

H27-C2-Pd10-Ag25	64	0	1	0	1
H27-C2-Pd10-Ag26	65	0	1	0	1
H27-C2-Pd11-Ag24	64	0	3	0	3
H27-C2-Pd11-Ag25	65	0	1	0	1
H27-C2-Pd12-Ag24	65	0	4	0	4
H27-C2-Pd13-Ag22	64	0	4	0	4
H27-C2-Pd13-Ag23	65	0	7	0	7
H27-C2-Pd14-Ag21	64	0	5	0	5
H27-C2-Pd14-Ag22	65	0	5	0	5
H27-C2-Pd15-Ag20	64	0	1	0	1
H27-C2-Pd15-Ag21	65	0	1	0	1
H27-C2-Pd16-Ag19	64	0	2	0	2
H27-C2-Pd16-Ag20	65	0	2	0	2
H27-C2-Pd17-Ag18	64	0	2	0	2
H27-C2-Pd17-Ag19	65	0	2	0	2
H27-C2-Pd18-Ag17	64	0	4	0	4
H27-C2-Pd18-Ag18	65	0	4	0	4
H27-C2-Pd19-Ag16	64	0	3	0	3
H27-C2-Pd19-Ag17	65	0	3	0	3
H27-C2-Pd20-Ag15	64	0	2	0	2
H27-C2-Pd20-Ag16	65	0	2	0	2
H27-C2-Pd20-Ag38	87	0	1	0	1
H27-C2-Pd21-Ag14	64	0	5	0	5
H27-C2-Pd21-Ag15	65	0	1	0	1
H27-C2-Pd22-Ag13	64	0	2	0	2
H27-C2-Pd22-Ag14	65	0	5	0	5
H27-C2-Pd23-Ag12	64	0	2	0	2
H27-C2-Pd23-Ag13	65	0	4	0	4
H27-C2-Pd24-Ag11	64	0	3	0	3
H27-C2-Pd24-Ag12	65	0	4	0	4
H27-C2-Pd25-Ag10	64	0	3	0	3
H27-C2-Pd25-Ag11	65	0	1	0	1
H27-C2-Pd26-Ag9	64	0	3	0	3
H27-C2-Pd26-Ag10	65	0	2	0	2
H27-C2-Pd27-Ag8	64	0	2	0	2
H27-C2-Pd27-Ag9	65	0	3	0	3
H27-C2-Pd28-Ag7	64	0	2	0	2
H27-C2-Pd28-Ag8	65	0	2	0	2
H27-C2-Pd29-Ag7	65	0	5	0	5
H27-C2-Pd30-Ag5	64	0	2	0	2
H27-C2-Pd30-Ag6	65	0	4	0	4
H27-C2-Pd31-Ag4	64	0	2	0	2
H27-C2-Pd31-Ag5	65	0	2	0	2
H27-C2-Pd32-Ag3	64	0	1	0	1

H27-C2-Pd32-Ag4	65	0	3	0	3
H27-C2-Pd33-Ag2	64	0	3	0	3
H27-C2-Pd33-Ag3	65	0	3	0	3
H27-C2-Pd34-Ag1	64	0	1	0	1
H27-C2-Pd34-Ag2	65	0	4	0	4
H27-C2-Pd35	64	0	229	0	229
H27-C2-Pd35-Ag1	65	0	5	0	5
H27-C2-Pd36	65	0	369	0	369
H27-C2-Pd40-Ag18	87	0	0	1	1
H27-C2-Pd58	87	0	2	6	8
H27-C7-Pd11-Ag29	74	0	1	0	1
H27-C7-Pd18-Ag22	74	0	1	0	1
H27-C7-Pd21-Ag19	74	0	2	0	2
H27-C7-Pd22-Ag18	74	0	1	0	1
H27-C7-Pd25-Ag15	74	0	1	0	1
H27-C7-Pd37-Ag3	74	0	1	0	1
H27-C7-Pd40	74	0	33	0	33
H29-C2-Pd2-Ag37	70	0	1	0	1
H29-C2-Pd3-Ag36	70	0	2	0	2
H29-C2-Pd4-Ag35	70	0	1	0	1
H29-C2-Pd10-Ag29	70	0	1	0	1
H29-C2-Pd11-Ag28	70	0	2	0	2
H29-C2-Pd14-Ag25	70	0	1	0	1
H29-C2-Pd16-Ag23	70	0	1	0	1
H29-C2-Pd17-Ag22	70	0	1	0	1
H29-C2-Pd18-Ag21	70	0	1	0	1
H29-C2-Pd20-Ag19	70	0	2	0	2
H29-C2-Pd21-Ag18	70	0	1	0	1
H29-C2-Pd23-Ag16	70	0	1	0	1
H29-C2-Pd24-Ag15	70	0	1	0	1
H29-C2-Pd25-Ag14	70	0	2	0	2
H29-C2-Pd26-Ag13	70	0	1	0	1
H29-C2-Pd27-Ag12	70	0	1	0	1
H29-C2-Pd28-Ag11	70	0	1	0	1
H29-C2-Pd29-Ag10	70	0	2	0	2
H29-C2-Pd30-Ag9	70	0	3	0	3
H29-C2-Pd31-Ag8	70	0	1	0	1
H29-C2-Pd32-Ag7	70	0	1	0	1
H29-C2-Pd34-Ag5	70	0	1	0	1
H29-C2-Pd37-Ag2	70	0	1	0	1
H29-C2-Pd39	70	0	89	0	89
H30-C1-Pd6-Ag34	71	0	1	0	1
H30-C1-Pd16-Ag24	71	0	1	0	1
H30-C1-Pd22-Ag18	71	0	1	0	1

H30-C1-Pd40	71	0	17	0	17
H30-C2-Pd1-Ag31	64	0	0	1	1
H30-C2-Pd3-Ag29	64	0	0	1	1
H30-C2-Pd4-Ag28	64	0	0	1	1
H30-C2-Pd10-Ag22	64	0	0	1	1
H30-C2-Pd17-Ag15	64	0	0	1	1
H30-C2-Pd18-Ag14	64	0	0	1	1
H30-C2-Pd19-Ag13	64	0	0	2	2
H30-C2-Pd20-Ag12	64	0	0	3	3
H30-C2-Pd21-Ag11	64	0	0	2	2
H30-C2-Pd22-Ag10	64	0	0	1	1
H30-C2-Pd23-Ag9	64	0	0	1	1
H30-C2-Pd31-Ag1	64	0	0	1	1
H30-C2-Pd32	64	0	0	47	47
H32-Pd32	64	99	0	22	121
H32-C8-Pd3-Ag37	80	0	1	0	1
H32-C8-Pd4-Ag36	80	0	1	0	1
H32-C8-Pd6-Ag34	80	0	1	0	1
H32-C8-Pd7-Ag33	80	0	1	0	1
H32-C8-Pd11-Ag29	80	0	1	0	1
H32-C8-Pd12-Ag28	80	0	1	0	1
H32-C8-Pd14-Ag26	80	0	1	0	1
H32-C8-Pd19-Ag21	80	0	1	0	1
H32-C8-Pd21-Ag19	80	0	3	0	3
H32-C8-Pd23-Ag17	80	0	1	0	1
H32-C8-Pd24-Ag16	80	0	2	0	2
H32-C8-Pd25-Ag15	80	0	1	0	1
H32-C8-Pd27-Ag13	80	0	1	0	1
H32-C8-Pd30-Ag10	80	0	1	0	1
H32-C8-Pd33-Ag7	80	0	1	0	1
H32-C8-Pd34-Ag6	80	0	2	0	2
H32-C8-Pd36-Ag4	80	0	2	0	2
H32-C8-Pd37-Ag3	80	0	1	0	1
H32-C8-Pd38-Ag2	80	0	1	0	1
H32-C8-Pd39-Ag1	80	0	1	0	1
H32-C8-Pd40	80	0	51	0	51
H33-C2-Pd1-Ag39	75	0	1	0	1
H33-C2-Pd2-Ag38	75	0	1	0	1
H33-C2-Pd4-Ag36	75	0	2	0	2
H33-C2-Pd6-Ag34	75	0	2	0	2
H33-C2-Pd9-Ag31	75	0	1	0	1
H33-C2-Pd12-Ag28	75	0	1	0	1
H33-C2-Pd13-Ag27	75	0	1	0	1
H33-C2-Pd17-Ag23	75	0	2	0	2

H33-C2-Pd18-Ag22	75	0	1	0	1
H33-C2-Pd19-Ag21	75	0	1	0	1
H33-C2-Pd21-Ag19	75	0	1	0	1
H33-C2-Pd23-Ag17	75	0	1	0	1
H33-C2-Pd26-Ag14	75	0	2	0	2
H33-C2-Pd28-Ag12	75	0	1	0	1
H33-C2-Pd29-Ag11	75	0	2	0	2
H33-C2-Pd31-Ag9	75	0	2	0	2
H33-C2-Pd32-Ag8	75	0	1	0	1
H33-C2-Pd34-Ag6	75	0	2	0	2
H33-C2-Pd35-Ag5	75	0	3	0	3
H33-C2-Pd36-Ag4	75	0	2	0	2
H33-C2-Pd38-Ag2	75	0	1	0	1
H33-C2-Pd39-Ag1	75	0	1	0	1
H33-C2-Pd40	75	0	83	0	83
H34-C6-Pd15-Ag25	80	0	2	0	2
H34-C6-Pd20-Ag20	80	0	1	0	1
H34-C6-Pd22-Ag18	80	0	2	0	2
H34-C6-Pd26-Ag14	80	0	2	0	2
H34-C6-Pd30-Ag10	80	0	4	0	4
H34-C6-Pd35-Ag5	80	0	2	0	2
H34-C6-Pd36-Ag4	80	0	1	0	1
H34-C6-Pd38-Ag2	80	0	1	0	1
H34-C6-Pd40	80	0	41	0	41
H34-C10-Pd4-Ag44	92	0	1	0	1
H34-C10-Pd5-Ag43	92	0	1	0	1
H34-C10-Pd20-Ag28	92	0	2	0	2
H34-C10-Pd24-Ag24	92	0	1	0	1
H34-C10-Pd26-Ag22	92	0	1	0	1
H34-C10-Pd28-Ag20	92	0	1	0	1
H34-C10-Pd33-Ag15	92	0	1	0	1
H34-C10-Pd34-Ag14	92	0	1	0	1
H34-C10-Pd37-Ag11	92	0	1	0	1
H34-C10-Pd40-Ag8	92	0	1	0	1
H34-C10-Pd42-Ag6	92	0	1	0	1
H34-C10-Pd48	92	0	45	0	45
H35-C2-Pd12-Ag18	67	0	1	0	1
H35-C2-Pd19-Ag11	67	0	1	0	1
H35-C2-Pd22-Ag8	67	0	1	0	1
H35-C2-Pd23-Ag7	67	0	1	0	1
H35-C2-Pd27-Ag3	67	0	1	0	1
H35-C2-Pd30	67	0	30	0	30
H36-C4-Pd2-Ag50	92	0	1	0	1
H36-C4-Pd5-Ag47	92	0	2	0	2

H36-C4-Pd14-Ag38	92	0	1	0	1
H36-C4-Pd17-Ag35	92	0	1	0	1
H36-C4-Pd31-Ag21	92	0	1	0	1
H36-C4-Pd32-Ag20	92	0	1	0	1
H36-C4-Pd36-Ag16	92	0	1	0	1
H36-C4-Pd37-Ag15	92	0	1	0	1
H36-C4-Pd38-Ag14	92	0	1	0	1
H36-C4-Pd39-Ag13	92	0	1	0	1
H36-C4-Pd41-Ag11	92	0	1	0	1
H36-C4-Pd42-Ag10	92	0	1	0	1
H36-C4-Pd43-Ag9	92	0	2	0	2
H36-C4-Pd45-Ag7	92	0	1	0	1
H36-C4-Pd47-Ag5	92	0	1	0	1
H36-C4-Pd49-Ag3	92	0	1	0	1
H36-C4-Pd52	92	0	38	0	38
H37-C2-Pd2-Ag28	69	0	2	0	2
H37-C2-Pd3-Ag27	69	0	1	0	1
H37-C2-Pd4-Ag26	69	0	1	0	1
H37-C2-Pd5-Ag25	69	0	1	0	1
H37-C2-Pd15-Ag15	69	0	2	0	2
H37-C2-Pd16-Ag14	69	0	2	0	2
H37-C2-Pd24-Ag6	69	0	1	0	1
H37-C2-Pd25-Ag5	69	0	2	0	2
H37-C2-Pd30	69	0	34	0	34
H38-C2-Pd23-Ag22	85	0	1	0	1
H38-C2-Pd24-Ag21	85	0	1	0	1
H38-C2-Pd31-Ag14	85	0	1	0	1
H38-C2-Pd37-Ag8	85	0	1	0	1
H38-C2-Pd41-Ag4	85	0	1	0	1
H38-C2-Pd42-Ag3	85	0	1	0	1
H38-C2-Pd43-Ag2	85	0	1	0	1
H38-C2-Pd45	85	0	30	0	30
H40-C2-Pd1-Ag44	87	0	1	0	1
H40-C2-Pd6-Ag39	87	0	2	0	2
H40-C2-Pd11-Ag34	87	0	1	0	1
H40-C2-Pd18-Ag27	87	0	1	0	1
H40-C2-Pd19-Ag26	87	0	1	0	1
H40-C2-Pd24-Ag21	87	0	2	0	2
H40-C2-Pd28-Ag17	87	0	2	0	2
H40-C2-Pd29-Ag16	87	0	1	0	1
H40-C2-Pd32-Ag13	87	0	1	0	1
H40-C2-Pd36-Ag9	87	0	1	0	1
H40-C2-Pd37-Ag8	87	0	2	0	2
H40-C2-Pd38-Ag7	87	0	1	0	1

H40-C2-Pd41-Ag4	87	0	1	0	1
H40-C2-Pd45	87	0	32	0	32
H41-C2-Pd1-Ag38	82	0	2	0	2
H41-C2-Pd2-Ag37	82	0	4	0	4
H41-C2-Pd3-Ag36	82	0	5	0	5
H41-C2-Pd4-Ag35	82	0	3	0	3
H41-C2-Pd5-Ag34	82	0	1	0	1
H41-C2-Pd8-Ag31	82	0	1	0	1
H41-C2-Pd9-Ag30	82	0	1	0	1
H41-C2-Pd10-Ag29	82	0	1	0	1
H41-C2-Pd11-Ag28	82	0	2	0	2
H41-C2-Pd12-Ag27	82	0	2	0	2
H41-C2-Pd13-Ag26	82	0	4	0	4
H41-C2-Pd14-Ag25	82	0	3	0	3
H41-C2-Pd16-Ag23	82	0	1	0	1
H41-C2-Pd17-Ag22	82	0	5	0	5
H41-C2-Pd18-Ag21	82	0	4	0	4
H41-C2-Pd19-Ag20	82	0	3	0	3
H41-C2-Pd20-Ag19	82	0	4	0	4
H41-C2-Pd21-Ag18	82	0	4	0	4
H41-C2-Pd22-Ag17	82	0	1	0	1
H41-C2-Pd23-Ag16	82	0	3	0	3
H41-C2-Pd24-Ag15	82	0	4	0	4
H41-C2-Pd25-Ag14	82	0	3	0	3
H41-C2-Pd26-Ag13	82	0	4	0	4
H41-C2-Pd27-Ag12	82	0	1	0	1
H41-C2-Pd28-Ag11	82	0	4	0	4
H41-C2-Pd29-Ag10	82	0	5	0	5
H41-C2-Pd30-Ag9	82	0	3	0	3
H41-C2-Pd31-Ag8	82	0	9	0	9
H41-C2-Pd32-Ag7	82	0	3	0	3
H41-C2-Pd33-Ag6	82	0	3	0	3
H41-C2-Pd34-Ag5	82	0	3	0	3
H41-C2-Pd35-Ag4	82	0	1	0	1
H41-C2-Pd36-Ag3	82	0	4	0	4
H41-C2-Pd38-Ag1	82	0	1	0	1
H41-C2-Pd39	82	0	323	0	323
H41-C2-Pd64	107	0	52	0	52
H42-C2-Ag40	84	0	2	0	2
H42-C2-Pd1-Ag39	84	0	3	0	3
H42-C2-Pd2-Ag38	84	0	7	0	7
H42-C2-Pd3-Ag37	84	0	6	0	6
H42-C2-Pd4-Ag36	84	0	8	0	8
H42-C2-Pd5-Ag35	84	0	7	0	7

H42-C2-Pd6-Ag34	84	0	3	0	3
H42-C2-Pd7-Ag33	84	0	2	0	2
H42-C2-Pd9-Ag31	84	0	6	0	6
H42-C2-Pd10-Ag30	84	0	4	0	4
H42-C2-Pd11-Ag29	84	0	4	0	4
H42-C2-Pd12-Ag28	84	0	6	0	6
H42-C2-Pd13-Ag27	84	0	1	0	1
H42-C2-Pd14-Ag26	84	0	4	0	4
H42-C2-Pd15-Ag25	84	0	3	0	3
H42-C2-Pd16-Ag24	84	0	1	0	1
H42-C2-Pd17-Ag23	84	0	8	0	8
H42-C2-Pd18-Ag22	84	0	3	0	3
H42-C2-Pd19-Ag21	84	0	6	0	6
H42-C2-Pd20-Ag20	84	0	10	0	10
H42-C2-Pd21-Ag19	84	0	8	0	8
H42-C2-Pd22-Ag18	84	0	10	0	10
H42-C2-Pd23-Ag17	84	0	11	0	11
H42-C2-Pd24-Ag16	84	0	5	0	5
H42-C2-Pd25-Ag15	84	0	8	0	8
H42-C2-Pd26-Ag14	84	0	12	0	12
H42-C2-Pd27-Ag13	84	0	13	0	13
H42-C2-Pd28-Ag12	84	0	8	0	8
H42-C2-Pd29-Ag11	84	0	8	0	8
H42-C2-Pd30-Ag10	84	0	6	0	6
H42-C2-Pd31-Ag9	84	0	7	0	7
H42-C2-Pd32-Ag8	84	0	5	0	5
H42-C2-Pd33-Ag7	84	0	11	0	11
H42-C2-Pd34-Ag6	84	0	8	0	8
H42-C2-Pd35-Ag5	84	0	9	0	9
H42-C2-Pd36-Ag4	84	0	13	0	13
H42-C2-Pd37-Ag3	84	0	5	0	5
H42-C2-Pd38-Ag2	84	0	5	0	5
H42-C2-Pd39-Ag1	84	0	5	0	5
H42-C2-Pd40	84	0	773	0	773
H42-C2-Pd64	108	0	58	0	58
H44-C2-Pd2-Ag37	85	0	2	0	2
H44-C2-Pd3-Ag36	85	0	1	0	1
H44-C2-Pd9-Ag30	85	0	1	0	1
H44-C2-Pd11-Ag28	85	0	1	0	1
H44-C2-Pd12-Ag27	85	0	1	0	1
H44-C2-Pd18-Ag21	85	0	1	0	1
H44-C2-Pd20-Ag19	85	0	1	0	1
H44-C2-Pd23-Ag16	85	0	2	0	2
H44-C2-Pd24-Ag15	85	0	1	0	1

H44-C2-Pd25-Ag14	85	0	1	0	1
H44-C2-Pd26-Ag13	85	0	2	0	2
H44-C2-Pd34-Ag5	85	0	3	0	3
H44-C2-Pd35-Ag4	85	0	2	0	2
H44-C2-Pd38-Ag1	85	0	1	0	1
H44-C2-Pd39	85	0	62	0	62
H44-C2-Pd64	110	0	56	0	56
H45-C2-Pd1-Ag39	87	0	3	0	3
H45-C2-Pd2-Ag38	87	0	4	0	4
H45-C2-Pd3-Ag37	87	0	12	0	12
H45-C2-Pd4-Ag36	87	0	7	0	7
H45-C2-Pd5-Ag35	87	0	4	0	4
H45-C2-Pd6-Ag34	87	0	2	0	2
H45-C2-Pd7-Ag33	87	0	1	0	1
H45-C2-Pd8-Ag32	87	0	7	0	7
H45-C2-Pd9-Ag31	87	0	1	0	1
H45-C2-Pd10-Ag30	87	0	2	0	2
H45-C2-Pd11-Ag29	87	0	6	0	6
H45-C2-Pd12-Ag28	87	0	2	0	2
H45-C2-Pd13-Ag27	87	0	5	0	5
H45-C2-Pd14-Ag26	87	0	2	0	2
H45-C2-Pd15-Ag25	87	0	2	0	2
H45-C2-Pd16-Ag24	87	0	1	0	1
H45-C2-Pd17-Ag23	87	0	2	0	2
H45-C2-Pd18-Ag22	87	0	3	0	3
H45-C2-Pd19-Ag21	87	0	5	0	5
H45-C2-Pd20-Ag20	87	0	5	0	5
H45-C2-Pd21-Ag19	87	0	4	0	4
H45-C2-Pd22-Ag18	87	0	3	0	3
H45-C2-Pd23-Ag17	87	0	2	0	2
H45-C2-Pd24-Ag16	87	0	8	0	8
H45-C2-Pd25-Ag15	87	0	7	0	7
H45-C2-Pd26-Ag14	87	0	3	0	3
H45-C2-Pd27-Ag13	87	0	4	0	4
H45-C2-Pd28-Ag12	87	0	6	0	6
H45-C2-Pd29-Ag11	87	0	6	1	7
H45-C2-Pd30-Ag10	87	0	4	1	5
H45-C2-Pd31-Ag9	87	0	9	0	9
H45-C2-Pd32-Ag8	87	0	9	0	9
H45-C2-Pd33-Ag7	87	0	7	0	7
H45-C2-Pd34-Ag6	87	0	1	0	1
H45-C2-Pd35-Ag5	87	0	7	0	7
H45-C2-Pd36-Ag4	87	0	6	0	6
H45-C2-Pd37-Ag3	87	0	8	0	8

H45-C2-Pd38-Ag2	87	0	5	0	5
H45-C2-Pd40	87	0	536	9	545
H45-C2-Pd64	111	0	51	0	51
H46-C2-Pd3-Ag37	88	0	1	0	1
H46-C2-Pd5-Ag35	88	0	2	0	2
H46-C2-Pd13-Ag27	88	0	1	0	1
H46-C2-Pd20-Ag20	88	0	1	0	1
H46-C2-Pd22-Ag18	88	0	1	0	1
H46-C2-Pd23-Ag17	88	0	1	0	1
H46-C2-Pd25-Ag15	88	0	1	0	1
H46-C2-Pd27-Ag13	88	0	1	0	1
H46-C2-Pd28-Ag12	88	0	3	0	3
H46-C2-Pd31-Ag9	88	0	1	0	1
H46-C2-Pd32-Ag8	88	0	1	0	1
H46-C2-Pd33-Ag7	88	0	1	0	1
H46-C2-Pd36-Ag4	88	0	1	0	1
H46-C2-Pd37-Ag3	88	0	1	0	1
H46-C2-Pd40	88	0	75	0	75
H47-C2-Ag40	89	0	2	0	2
H47-C2-Pd1-Ag39	89	0	1	0	1
H47-C2-Pd2-Ag38	89	0	1	0	1
H47-C2-Pd3-Ag37	89	0	2	0	2
H47-C2-Pd4-Ag36	89	0	4	0	4
H47-C2-Pd5-Ag35	89	0	8	0	8
H47-C2-Pd6-Ag34	89	0	4	0	4
H47-C2-Pd7-Ag33	89	0	4	0	4
H47-C2-Pd8-Ag32	89	0	9	0	9
H47-C2-Pd9-Ag31	89	0	2	0	2
H47-C2-Pd10-Ag30	89	0	4	0	4
H47-C2-Pd11-Ag29	89	0	3	0	3
H47-C2-Pd12-Ag28	89	0	1	0	1
H47-C2-Pd13-Ag27	89	0	3	0	3
H47-C2-Pd14-Ag26	89	0	4	0	4
H47-C2-Pd15-Ag25	89	0	3	0	3
H47-C2-Pd16-Ag24	89	0	4	0	4
H47-C2-Pd17-Ag23	89	0	2	0	2
H47-C2-Pd18-Ag22	89	0	4	0	4
H47-C2-Pd19-Ag21	89	0	1	0	1
H47-C2-Pd20-Ag20	89	0	2	0	2
H47-C2-Pd21-Ag19	89	0	4	0	4
H47-C2-Pd22-Ag18	89	0	9	0	9
H47-C2-Pd23-Ag17	89	0	6	0	6
H47-C2-Pd24-Ag16	89	0	7	0	7
H47-C2-Pd25-Ag15	89	0	7	0	7

H47-C2-Pd26-Ag14	89	0	8	0	8
H47-C2-Pd27-Ag13	89	0	13	0	13
H47-C2-Pd28-Ag12	89	0	9	0	9
H47-C2-Pd29-Ag11	89	0	2	0	2
H47-C2-Pd30-Ag10	89	0	9	0	9
H47-C2-Pd31-Ag9	89	0	8	0	8
H47-C2-Pd32-Ag8	89	0	5	0	5
H47-C2-Pd33-Ag7	89	0	5	0	5
H47-C2-Pd34-Ag6	89	0	3	0	3
H47-C2-Pd35-Ag5	89	0	6	0	6
H47-C2-Pd36-Ag4	89	0	9	0	9
H47-C2-Pd37-Ag3	89	0	6	0	6
H47-C2-Pd38-Ag2	89	0	3	0	3
H47-C2-Pd39-Ag1	89	0	1	0	1
H47-C2-Pd40	89	0	492	0	492
H48-C2-Pd2-Ag38	90	0	2	0	2
H48-C2-Pd6-Ag34	90	0	1	0	1
H48-C2-Pd12-Ag28	90	0	1	0	1
H48-C2-Pd13-Ag27	90	0	1	0	1
H48-C2-Pd14-Ag26	90	0	1	0	1
H48-C2-Pd15-Ag25	90	0	1	0	1
H48-C2-Pd17-Ag23	90	0	1	0	1
H48-C2-Pd18-Ag22	90	0	2	0	2
H48-C2-Pd19-Ag21	90	0	1	0	1
H48-C2-Pd24-Ag16	90	0	1	0	1
H48-C2-Pd25-Ag15	90	0	2	0	2
H48-C2-Pd28-Ag12	90	0	1	0	1
H48-C2-Pd30-Ag10	90	0	2	0	2
H48-C2-Pd31-Ag9	90	0	1	0	1
H48-C2-Pd33-Ag7	90	0	2	0	2
H48-C2-Pd34-Ag6	90	0	1	0	1
H48-C2-Pd36-Ag4	90	0	1	0	1
H48-C2-Pd37-Ag3	90	0	3	0	3
H48-C2-Pd38-Ag2	90	0	1	0	1
H48-C2-Pd39-Ag1	90	0	1	0	1
H48-C2-Pd40	90	0	69	0	69
H48-C4-Pd3-Ag37	92	0	1	0	1
H48-C4-Pd4-Ag36	92	0	1	0	1
H48-C4-Pd5-Ag35	92	0	1	0	1
H48-C4-Pd6-Ag34	92	0	2	0	2
H48-C4-Pd8-Ag32	92	0	1	1	2
H48-C4-Pd13-Ag27	92	0	1	0	1
H48-C4-Pd17-Ag23	92	0	1	0	1
H48-C4-Pd24-Ag16	92	0	1	0	1

H48-C4-Pd26-Ag14	92	0	3	0	3
H48-C4-Pd34-Ag6	92	0	2	0	2
H48-C4-Pd35-Ag5	92	0	2	0	2
H48-C4-Pd38-Ag2	92	0	1	0	1
H48-C4-Pd40	92	0	37	1	38
H50-C2-Pd3-Ag45	100	0	1	0	1
H50-C2-Pd16-Ag32	100	0	1	0	1
H50-C2-Pd25-Ag23	100	0	1	0	1
H50-C2-Pd28-Ag20	100	0	1	0	1
H50-C2-Pd31-Ag17	100	0	2	0	2
H50-C2-Pd34-Ag14	100	0	1	0	1
H50-C2-Pd39-Ag9	100	0	1	0	1
H50-C2-Pd40-Ag8	100	0	1	0	1
H50-C2-Pd41-Ag7	100	0	1	0	1
H50-C2-Pd48	100	0	46	0	46
H51-C2-Pd64	117	0	87	0	87
H52-C2-Pd4-Ag44	102	0	1	0	1
H52-C2-Pd6-Ag42	102	0	1	0	1
H52-C2-Pd11-Ag37	102	0	1	0	1
H52-C2-Pd12-Ag36	102	0	1	0	1
H52-C2-Pd13-Ag35	102	0	2	0	2
H52-C2-Pd14-Ag34	102	0	1	0	1
H52-C2-Pd20-Ag28	102	0	1	0	1
H52-C2-Pd23-Ag25	102	0	2	0	2
H52-C2-Pd29-Ag19	102	0	1	0	1
H52-C2-Pd31-Ag17	102	0	1	0	1
H52-C2-Pd34-Ag14	102	0	1	0	1
H52-C2-Pd41-Ag7	102	0	1	0	1
H52-C2-Pd45-Ag3	102	0	1	0	1
H52-C2-Pd48	102	0	32	0	32
H52-C2-Pd64	118	0	83	0	83
H54-C2-Pd64	120	0	86	0	86
H55-C2-Pd64	121	0	76	0	76
Total	--	8196	24796	22221	55213

1.3 Benchmark of G-NN potential against DFT calculations

To examine the accuracy of the G-NN potential, we have calculated the total energy difference between G-NN and DFT for the representative surface structures of Pd-Ag-H/Pd₁Ag₃(111), Pd-Ag-H/Pd₁Ag₃(100), Pd-Ag-H/Pd₁Ag₁(111), and Pd-Ag-H/Pd₁Ag₁(100), which shows a low root mean square error (RMSE) of only 4.9 meV/atom, as seen in Figure S1.

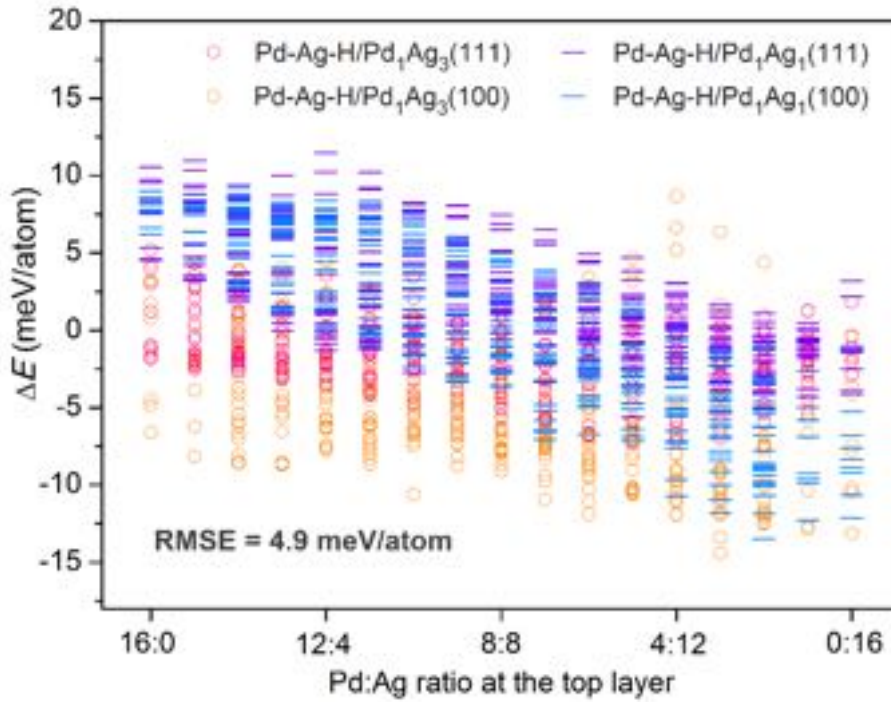


Figure S1. Total energy difference between G-NN potential and DFT calculations for the representative surface structures of Pd-Ag-H/Pd₁Ag₃(111), Pd-Ag-H/Pd₁Ag₃(100), Pd-Ag-H/Pd₁Ag₁(111), and Pd-Ag-H/Pd₁Ag₁(100), as distinguished by the Pd/Ag ratio at the top layer. The H coverage does not reflect in the figure.

One great advantage of the G-NN potential is the predictive power to chemical reactions, i.e., the PES near the transition states. For example, we have calculated the acetylene/ethene hydrogenation energetics (including the transition states and intermediate states) on Pd₁Ag₃/Pd₁Ag₃(111) by using G-NN and DFT (see Table S2), which show small energy differences (< 3 meV/atom) illustrating the high accuracy of G-NN for the hydrogenation reactions.

Table S2. Comparison of the energetics for acetylene/ethene hydrogenation on Pd₁Ag₃/Pd₁Ag₃(111) from G-NN and DFT single point calculation.

State	G-NN (eV)	VASP (eV)	Diff (meV/atom)
IS	-219.866	-219.846	0.29
H _v	-216.103	-216.099	0.05
C ₂ H ₂ *	-239.824	-239.807	0.24
TS1	-239.345	-239.239	1.49
C ₂ H ₃ *	-243.936	-243.996	0.83
TS2	-243.476	-243.650	2.42
C ₂ H ₄ *	-248.316	-248.357	0.55
TS3	-247.912	-247.916	0.05
C ₂ H ₅ *	-252.025	-252.009	0.22
TS4	-251.801	-251.828	0.35
FS	-252.901	-252.950	0.66

2. Surface structures of Pd₁Ag₁

In the main text, we have revealed the Pd-Ag-H surface PES for Pd₁Ag₃(111) and Pd₁Ag₃(100) (see Figure 2), where Pd₁Ag₃(111) has a set of energy-nearly-degenerate surface structures while Pd₁Ag₃(100) has only the mostly Ag-covered surfaces. Here we briefly discuss the surface PES for Pd₁Ag₁(111) and Pd₁Ag₁(100). As shown in Figure S2, both Pd₁Ag₁(111) and Pd₁Ag₁(100) have the major Pd exposure on surface, and therefore the most stable configurations, Pd/Pd₁Ag₁(111)-1 ML H and Pd₃Ag₁/Pd₁Ag₁(100)-1 ML H, both have the H coverage up to 1 ML with respect to the surface metal atom.

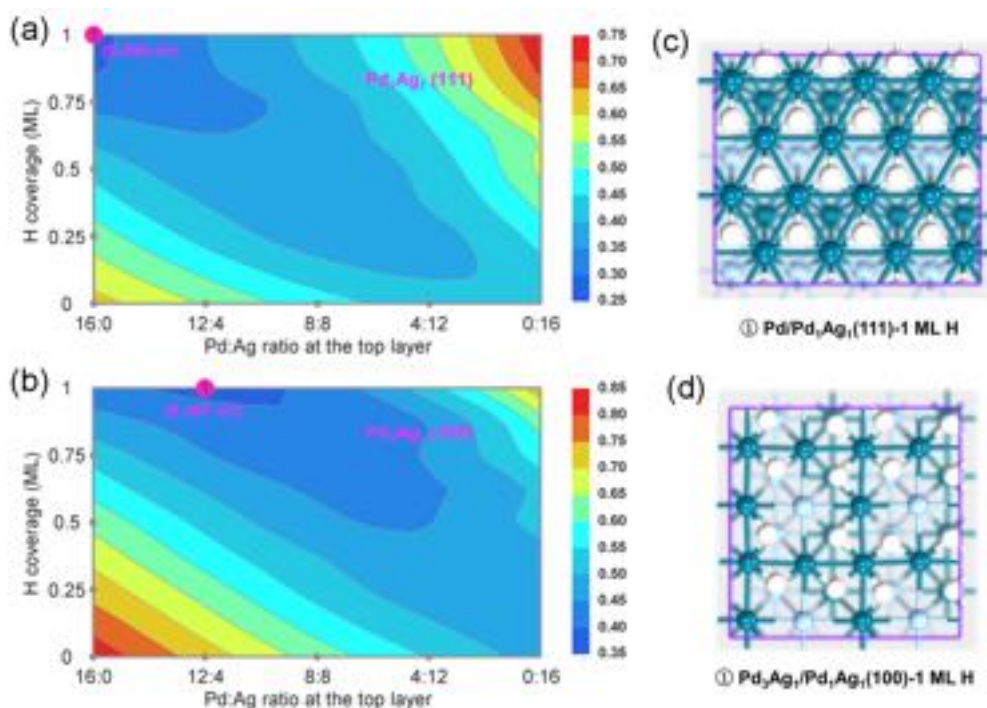


Figure S2. (a-b) DFT contour maps for the formation free energy of Pd-Ag-H/Pd₁Ag₁(111) and Pd-Ag-H/Pd₁Ag₁(100), at 25 °C, $p(\text{H}_2) = 0.05$ atm. The formation free energy here is averaged to each metal atom at the top layer. (c-d) Stable surface configurations of Pd₁Ag₁(111) and Pd₁Ag₁(100) at typical reaction conditions, as determined from the Pd-Ag-H surface contour maps.

3. Kinetic parameters utilized in microkinetic simulation

Table S3. Gibbs free energy barrier for the acetylene/ethene hydrogenation on Pd₁Ag₃/Pd₁Ag₃(111), Pd/Pd₁Ag₃(111), Pd₁Ag₇/Pd₁Ag₃(100), Pd/Pd₁Ag₁(111), and Pd₃Ag₁/Pd₁Ag₁(100). The data is with respect to the experiment reaction conditions, i.e. 60 °C, and 1 bar for all the gas phase molecules (e.g. hydrogen, acetylene, ethene, and ethane) since the effect of pressure change has been explicitly taken into account in the microkinetic simulation via standard thermodynamic equation.

Elementary step		Pd ₁ Ag ₃ /	Pd/	Pd ₁ Ag ₇ /	Pd/	Pd ₃ Ag ₁ /
		Pd ₁ Ag ₃ (111)	Pd ₁ Ag ₃ (111)	Pd ₁ Ag ₃ (100)	Pd ₁ Ag ₁ (111)	Pd ₁ Ag ₁ (100)
H ₂ + 2* ⇌ 2H*	Forward	0.35	0.35	0.34	0.35	0.34
	Reverse	0.78	0.78	0.97	0.78	0.97
C ₂ H ₂ + * ⇌ C ₂ H ₂ *	Forward	0.43	0.43	0.47	0.43	0.47
	Reverse	0.77	0.73	1.16	0.71	0.95
C ₂ H ₂ * + H* ⇌ C ₂ H ₃ * + *	Forward	0.66	0.74	0.67	0.56	0.78
	Reverse	0.75	0.52	0.57	0.46	0.48
C ₂ H ₃ * + H* ⇌ C ₂ H ₄ * + *	Forward	0.36	0.64	0.20	0.60	0.57
	Reverse	0.82	1.15	0.61	1.13	1.35
C ₂ H ₄ * ⇌ C ₂ H ₄ + *	Forward	0.19	0.00	0.48	0	0.44
	Reverse	0.45	0.56	0.43	0.44	0.43
C ₂ H ₄ * + H* ⇌ C ₂ H ₅ * + *	Forward	0.50	0.64	0.56	0.49	0.54
	Reverse	0.15	0.60	0.12	0.36	0.11
C ₂ H ₅ * + H* ⇌ C ₂ H ₆ * + *	Forward	0.24	0.49	0.26	0.37	0.40
	Reverse	1.05	1.29	0.60	1.14	0.77
C ₂ H ₆ * ⇌ C ₂ H ₆ + *	Forward	0.00	0.00	0.00	0	0
	Reverse	0.43	0.43	0.48	0.43	0.48

4. Synthesis and characterization of Pd-Ag catalysts

4.1 Materials

Palladium nitrate hydrate ($\text{Pd}(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$, 40% Pd basis) and Hydrotalcite (HT, $\text{Mg}_6\text{Al}_2(\text{CO}_3)(\text{OH})_{16} \cdot 4\text{H}_2\text{O}$) were obtained from Sigma-Aldrich. Silver nitrate (AgNO_3 , 63.5%), green silicon carbide (SiC, 99.0%, an average particle size of 60 mesh), quartz wool, $\alpha\text{-Al}_2\text{O}_3$, $\gamma\text{-Al}_2\text{O}_3$, SiO_2 , Y_2O_3 , CaCO_3 , rutile- TiO_2 (r- TiO_2), anatase- TiO_2 (a- TiO_2), P25, and Ti-MWW were purchased from Sinopharm Chemical Reagent Co.. Nitrogen (N_2 , 99.99%), hydrogen (5% H_2 and 95% Ar), helium (He, 99.99%), and the mixed gas (0.5% C_2H_2 , 50.0% C_2H_4 , 5.0% H_2 , 4.0% He and 40.5% N_2) were supplied by Shanghai Air Liquide Co., Ltd. All the chemicals were used directly without further purification and the deionized water with a resistivity of 18.2 $\text{M}\Omega \cdot \text{cm}$ was used in all the experiments.

The catalyst synthesis procedure has been introduced in method section in the main text.

4.2 Instruments for catalyst characterization

The transmission electron microscopy (TEM) images were taken by Tecnai G2 F20 S-Twin (FEI, USA); the powered X-ray diffraction (XRD) patterns were obtained by Bruker D8 Advance (Cu $\text{K}\alpha$ radiation, Bruker AXS, Germany); the Pd and Ag contents of the samples were analysed by inductively coupled plasma optical emission spectrometer (ICP-AES, iCAP7400, USA);

4.3 Catalyst characterization

To examine the hydrogenation activity and selectivity on Pd-Ag alloys, we have synthesized a series of HT supported Pd-Ag nanoparticle catalysts with different Pd/Ag ratios, including Pd, Pd₁Ag₁, Pd₁Ag₂, Pd₁Ag₃, Pd₁Ag₄, and Pd₁Ag₅, and have characterized them by XRD, TEM, and EDS-mapping, which show that: the Pd-Ag nanoparticles are uniformly dispersed on the HT support with an average particle size of 4.1 ~ 7.6 nm (see the TEM images in Figure S4); the ICP content analysis of Pd and Ag is consistent with the nominal loading, confirming the formation of Pd-Ag alloys (see Figure S5 and Table S4); importantly, new Pd-Ag crystal phases are found at Pd₁Ag₁ and Pd₁Ag₃ as indicated by the new peaks at 39.6° and 39.1° from the XRD, in line with our theoretical convex hull diagram (see Figure 1a).

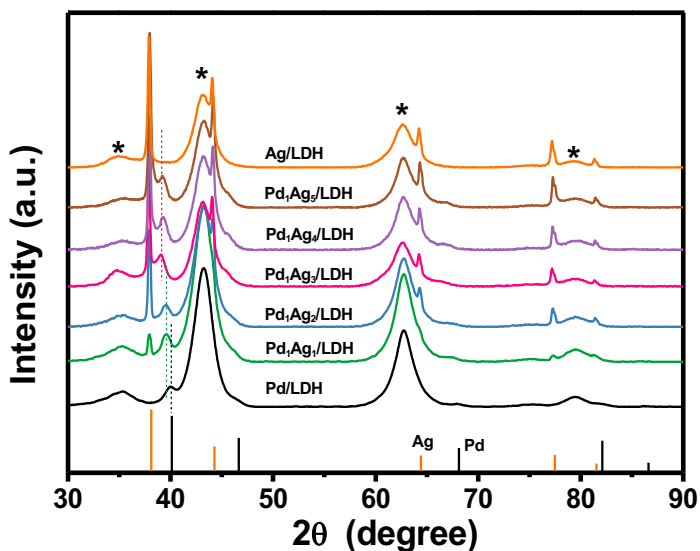


Figure S3. XRD of the Pd/HT, Pd₁Ag₁/HT, Pd₁Ag₂/HT, Pd₁Ag₃/HT, Pd₁Ag₄/HT, Pd₁Ag₅/HT, and Ag/HT catalysts. The reference peaks are Pd (JCPDS 46-1043) and Ag (JCPDS 04-0783), while the background peaks from the HT support are denoted by asterisks.

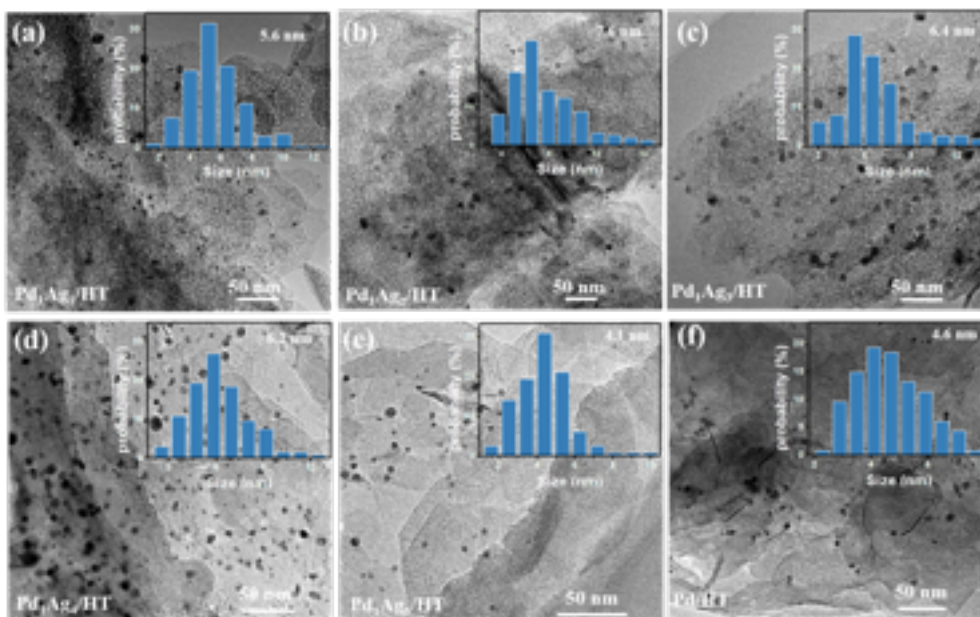


Figure S4. TEM and statistics of the nanoparticle size for (a) Pd₁Ag₁/HT, (b) Pd₁Ag₂/HT, (c) Pd₁Ag₃/HT, (d) Pd₁Ag₄/HT, (e) Pd₁Ag₅/HT, and (f) Pd/HT.

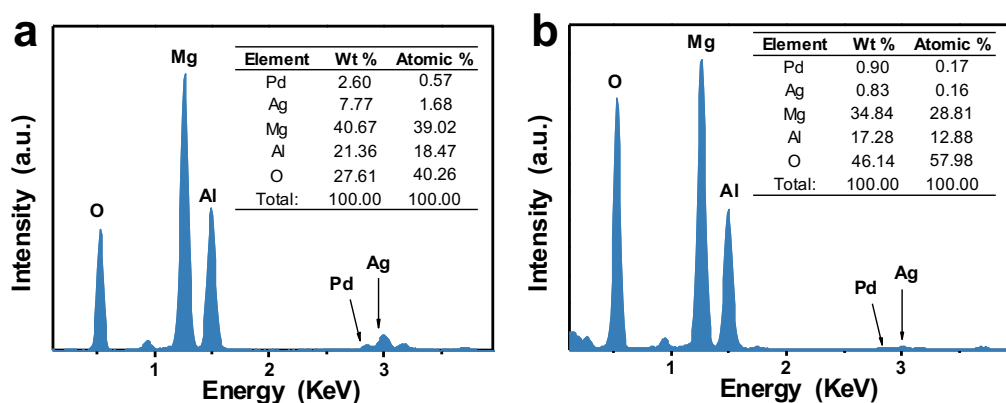


Figure S5. EDS patterns of (a) Pd₁Ag₃/HT and (b) Pd₁Ag₁/HT. The insets show the weight and atomic ratios for Pd and Ag.

Table S4. Content analysis of Pd and Ag for the Pd/HT, Pd₁Ag₁/HT, Pd₁Ag₂/HT, Pd₁Ag₃/HT, Pd₁Ag₄/HT, Pd₁Ag₅/HT, and Ag/HT catalysts.

Catalyst	Nominal loading		Actual loading ^a		Ag: Pd	Particle size (nm)
	Pd (wt%)	Ag (wt%)	Pd (wt%)	Ag (wt%)		
Pd/HT	1	-	0.93	-	-	4.6
Pd ₁ Ag ₁ /HT	1	1	0.98	1.01	1.0	5.6
Pd ₁ Ag ₂ /HT	1	2	0.89	1.91	2.1	7.6
Pd ₁ Ag ₃ /HT	1	3	0.86	2.82	3.3	6.4
Pd ₁ Ag ₄ /HT	1	4	1	3.94	3.9	6.2
Pd ₁ Ag ₅ /HT	1	5	1.08	5.74	5.3	4.3
Ag/HT	-	3	-	2.95	-	5.0

^aDetermined by ICP analysis.

We have performed a 200-hour catalysis test on the Pd₁Ag₃/HT catalyst, during which the activity gradually reduces but the selectivity remains (see Figure 4e). To reveal the structural evolution, we have analyzed the catalyst after the long-time test by HR-TEM and EDS elemental mapping (see Figure S6), which show nearly no change in particle size and no detectable deposition of carbon on the catalyst. This rules out the sintering of the nanoparticles and the formation of high-carbon weight overlayers that block the catalyst sites. With the help of microkinetic simulation, we deduce that the Pd atoms may slowly accumulate onto the surface layer forming the Pd₃ and Pd layer ensemble, which have high ethene hydrogenation barriers and thus reduce the activity.

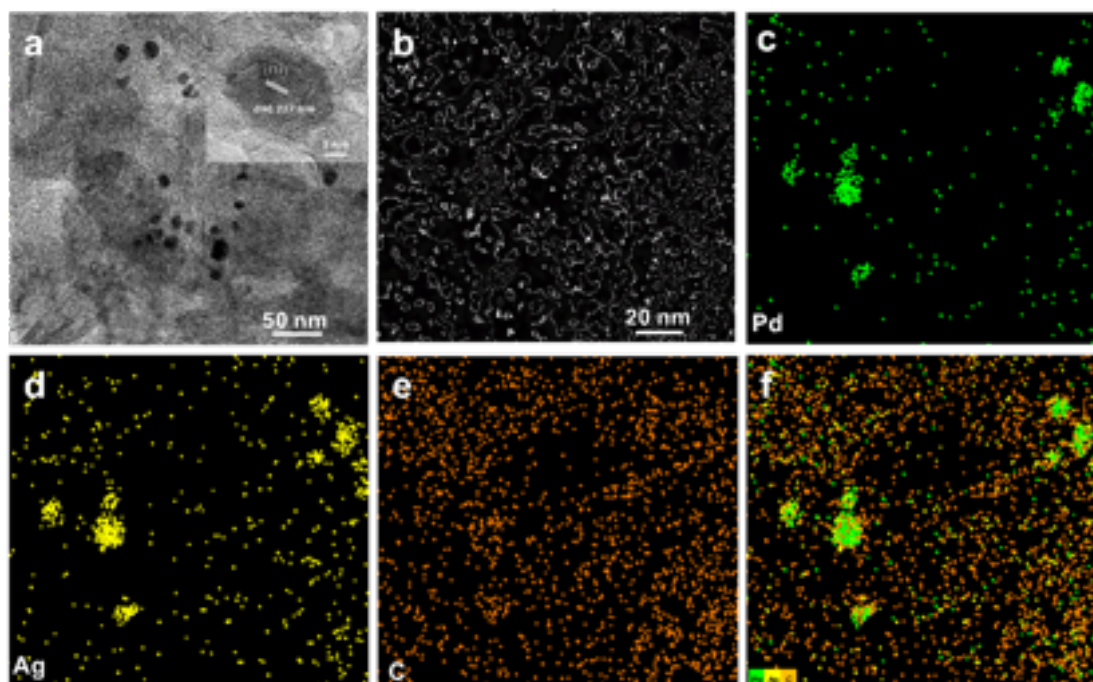


Figure S6. (a) TEM, HR-TEM (the inset) images and (b-f) the EDS elemental mapping images of the Pd₁Ag₃/HT catalyst, as taken after the 200-hour catalysis test.

Based on the atomic level understanding, we have performed the catalyst screening on the support material and the Pd₁Ag₃/TiO₂ rutile is found to have the best catalytic performance (conversion >96%, selectivity >85%, see Figure 6). We then analyzed the Pd₁Ag₃/TiO₂ rutile catalyst and found that there is no obvious peak for fcc crystal from XRD (see Figure S8), and the large Pd-Ag crystalline particles are scarce compared to that on HT support, with the average nanoparticle size below 4.9 nm as shown by TEM and HR-TEM (see Figure S7). These indicates that the rutile support can finely disperse the Pd₁Ag₃ nanoparticles and thus improve the selectivity.

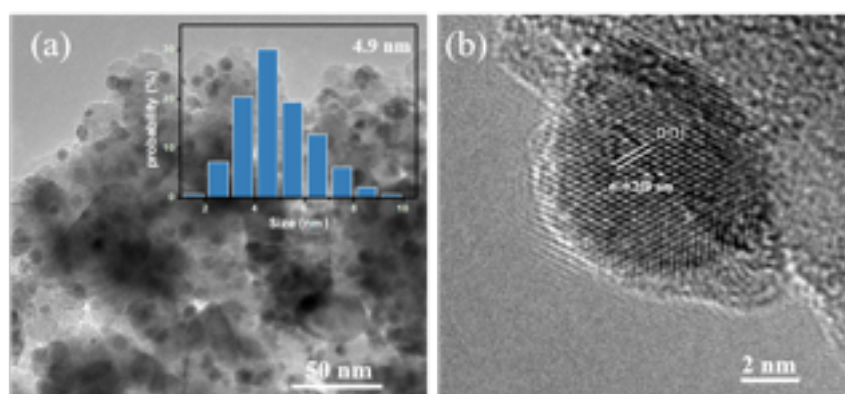


Figure S7. (a) TEM (the inset is the statistics of nanoparticle size) and (b) HR-TEM images of the Pd₁Ag₃/r-TiO₂ catalyst.

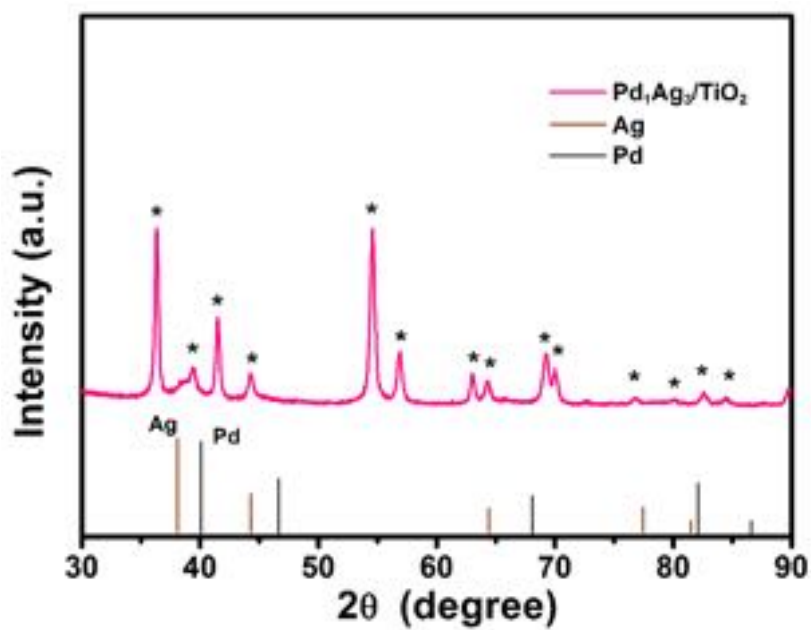


Figure S8. XRD of Pd₁Ag₃/r-TiO₂. The reference peaks are Pd (JCPDS 46-1043) and Ag (JCPDS 04-0783), while the background peaks from the rutile TiO₂ support are denoted by asterisks.

5. Acetylene hydrogenation catalysts reported in literatures

Table S5. Comparison of our Pd₁Ag₃/r-TiO₂ and Pd₁Ag₃/HT with the best acetylene hydrogenation catalysts reported previously.

Type	Catalyst	Conversion (%)	Selectivity (%)	C ₂ H ₂ /H ₂ /C ₂ H ₄	Temperature (°C)
	Pd ₁ Ag ₃ /r-TiO ₂	96	85	0.5 : 5 : 50	this work
	Pd ₁ Ag ₃ /HT	100	79	0.5 : 5 : 50	this work
	Pd ₁ Ag ₄	85	50	0.5 : 5 : 50	200 ⁸
	Pd ₁ Ag ₃ /MgAl ₂ O ₄	95	55	0.5 : 10 : 50	200 ⁹
	Pd ₂ Ga ₁ /Al ₂ O ₃	95	75	0.5 : 5 : 50	200 ¹⁰
	Pd ₂ Ga ₁ /CNT	90	60	0.5 : 5 : 50	200 ⁸
	Pd ₁ In ₁ /MgAl ₂ O ₄	96	92	0.5 : 5 : 50	90 ¹¹
Alloy & Intermetallics	Pd ₁ In ₁ /Al ₂ O ₃	99	77	0.87 : 3.1 : 73	120 ¹²
	Pd/ZnO	97	97	2 : 20 : 40	150 ¹³
	Pd ₁ Zn ₁ @ZIF-8C	70	80	0.65 : 5 : 50	115 ¹⁴
	Ni ₃ Ga ₁ /MgAl ₂ O ₄	90	77	0.5 : 10 : 50	200 ⁹
	Ni ₃ Sn ₂ /MgAl ₂ O ₄	80	80	0.5 : 10 : 50	200 ⁹
	Ni ₁ Ga ₁ /Mg/Al-LDHs	73	75	1 : 10 : 20	185 ¹⁵
	Ni ₃ Zn ₁ C _{0.7} /oCNT	99	94	0.5 : 4.5 : 20	200 ¹⁶
	Al ₁₃ Fe ₄	80	84	0.5 : 5 : 50	200 ¹⁷
	Co ₂ Mn _{0.5} Fe _{0.5} Ge ₁	100	90	0.1 : 40 : 10	250 ¹⁸
		Pd@H-Zn/Co-ZIF	80	80	0.5 : 5 : 50
Core-Shell	Pd/PPS	100	65	0.6 : 0.9 : 49.3	100 ²⁰
	Pd/CTS	100	74	1 : 2 : 20	100 ²¹
Single Atom	Pd ₁ /ND@G	100	90	1 : 10 : 20	180 ²²
	Pd ₁ /MPNC	83	82	0.5 : 5 : 50	110 ²³
	AgPd _{0.01} /SiO ₂	67	87	1 : 20 : 20	160 ²⁴
	CuPd _{0.006} /SiO ₂	100	85	1 : 20 : 20	160 ²⁵
	Na-Ni@CHA	100	90	0.5 : 8 : 50	180 ²⁶
	Cu ₁ /ND@G	95	98	1 : 10 : 20	200 ²⁷
Metallic Oxide	CeO ₂	86	81	1 : 30 : 0	250 ²⁸
	In ₂ O ₃	100	84	2.5 : 75 : 10	350 ²⁹
	Ni@CeO ₂	65	-	0.52 : 2 : 33.82	200 ³⁰

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6. XYZ coordinates for the configurations in Fig. 3

Initial Pd₁Ag₃/Pd₁Ag₃(111). The energy from VASP with high accuracy setups is -219.995711 eV.

PBC	11.56261009	10.01351407	25.00000000	90.00000000	90.00000000	90.00000000
Pd	0.722663130	0.625844629	8.959688149	CORE	1 Pd Pd	0.0000 1
Ag	3.613315652	0.625844629	8.959688149	CORE	2 Ag Ag	0.0000 2
Pd	6.503968173	0.625844629	8.959688149	CORE	3 Pd Pd	0.0000 3
Ag	9.394620695	0.625844629	8.959688149	CORE	4 Ag Ag	0.0000 4
Ag	2.167989391	3.129223146	8.959688149	CORE	5 Ag Ag	0.0000 5
Ag	5.058641913	3.129223146	8.959688149	CORE	6 Ag Ag	0.0000 6
Ag	7.949294434	3.129223146	8.959688149	CORE	7 Ag Ag	0.0000 7
Ag	10.839946956	3.129223146	8.959688149	CORE	8 Ag Ag	0.0000 8
Ag	0.722663130	5.632601664	8.959688149	CORE	9 Ag Ag	0.0000 9
Pd	3.613315652	5.632601664	8.959688149	CORE	10 Pd Pd	0.0000 10
Ag	6.503968173	5.632601664	8.959688149	CORE	11 Ag Ag	0.0000 11
Pd	9.394620695	5.632601664	8.959688149	CORE	12 Pd Pd	0.0000 12
Ag	2.167989391	8.135980181	8.959688149	CORE	13 Ag Ag	0.0000 13
Ag	5.058641913	8.135980181	8.959688149	CORE	14 Ag Ag	0.0000 14
Ag	7.949294434	8.135980181	8.959688149	CORE	15 Ag Ag	0.0000 15
Ag	10.839946956	8.135980181	8.959688149	CORE	16 Ag Ag	0.0000 16
Ag	2.167989391	1.460304135	11.319896050	CORE	17 Ag Ag	0.0000 17
Ag	5.058641913	1.460304135	11.319896050	CORE	18 Ag Ag	0.0000 18
Ag	7.949294434	1.460304135	11.319896050	CORE	19 Ag Ag	0.0000 19
Ag	10.839946956	1.460304135	11.319896050	CORE	20 Ag Ag	0.0000 20
Pd	0.722663130	3.963682652	11.319896050	CORE	21 Pd Pd	0.0000 21
Ag	3.613315652	3.963682652	11.319896050	CORE	22 Ag Ag	0.0000 22
Pd	6.503968173	3.963682652	11.319896050	CORE	23 Pd Pd	0.0000 23
Ag	9.394620695	3.963682652	11.319896050	CORE	24 Ag Ag	0.0000 24
Ag	2.167989391	6.467061169	11.319896050	CORE	25 Ag Ag	0.0000 25
Ag	5.058641913	6.467061169	11.319896050	CORE	26 Ag Ag	0.0000 26
Ag	7.949294434	6.467061169	11.319896050	CORE	27 Ag Ag	0.0000 27
Ag	10.839946956	6.467061169	11.319896050	CORE	28 Ag Ag	0.0000 28
Ag	0.722663130	8.970439686	11.319896050	CORE	29 Ag Ag	0.0000 29
Pd	3.613315652	8.970439686	11.319896050	CORE	30 Pd Pd	0.0000 30
Ag	6.503968173	8.970439686	11.319896050	CORE	31 Ag Ag	0.0000 31
Pd	9.394620695	8.970439686	11.319896050	CORE	32 Pd Pd	0.0000 32
Ag	0.728741607	2.299921440	13.660833994	CORE	33 Ag Ag	0.0000 33
Pd	3.616051626	2.297259355	13.685428033	CORE	34 Pd Pd	0.0000 34
Ag	6.510467073	2.300042563	13.661004839	CORE	35 Ag Ag	0.0000 35
Pd	9.396942608	2.297032984	13.685551642	CORE	36 Pd Pd	0.0000 36
Ag	2.156838434	4.786554772	13.652578176	CORE	37 Ag Ag	0.0000 37
Ag	5.065492199	4.785850682	13.652480550	CORE	38 Ag Ag	0.0000 38
Ag	7.937908715	4.786727469	13.652853717	CORE	39 Ag Ag	0.0000 39
Ag	10.846716001	4.785669719	13.652687019	CORE	40 Ag Ag	0.0000 40

Pd	0.722474075	7.285318952	13.706957936	CORE	41 Pd Pd	0.0000	41
Ag	3.615287306	7.296134749	13.680639711	CORE	42 Ag Ag	0.0000	42
Pd	6.503726135	7.285364508	13.706970660	CORE	43 Pd Pd	0.0000	43
Ag	9.396748879	7.295975959	13.680875371	CORE	44 Ag Ag	0.0000	44
Ag	2.175229275	9.795452279	13.671503121	CORE	45 Ag Ag	0.0000	45
Ag	5.045597993	9.796467012	13.669544896	CORE	46 Ag Ag	0.0000	46
Ag	7.956573506	9.795053871	13.671574570	CORE	47 Ag Ag	0.0000	47
Ag	10.827219886	9.796187364	13.669373798	CORE	48 Ag Ag	0.0000	48
Ag	3.613448736	0.653990127	16.043190078	CORE	49 Ag Ag	0.0000	49
Ag	0.723074179	5.605987535	16.058346013	CORE	50 Ag Ag	0.0000	50
Ag	6.504090063	5.605798586	16.058212730	CORE	51 Ag Ag	0.0000	51
Pd	10.848676619	3.108646630	15.985938624	CORE	52 Pd Pd	0.0000	52
Ag	0.723121682	0.648685021	16.047746448	CORE	53 Ag Ag	0.0000	53
Pd	7.944094317	3.110055138	15.987492224	CORE	54 Pd Pd	0.0000	54
Ag	2.162323739	8.126411873	16.037010364	CORE	55 Ag Ag	0.0000	55
Ag	6.504535210	0.648629308	16.048146545	CORE	56 Ag Ag	0.0000	56
Ag	7.943102820	8.125781898	16.037445733	CORE	57 Ag Ag	0.0000	57
Pd	5.067723415	3.108665401	15.986226378	CORE	58 Pd Pd	0.0000	58
Ag	10.842776370	8.125683991	16.035407599	CORE	59 Ag Ag	0.0000	59
Ag	5.061150886	8.125714701	16.035778730	CORE	60 Ag Ag	0.0000	60
Ag	3.613800901	5.596812225	16.060488354	CORE	61 Ag Ag	0.0000	61
Ag	9.394614140	0.653510367	16.043607128	CORE	62 Ag Ag	0.0000	62
Ag	9.395411785	5.596551732	16.060815732	CORE	63 Ag Ag	0.0000	63
Pd	2.162465918	3.110561050	15.987304425	CORE	64 Pd Pd	0.0000	64
H	0.723991309	3.631114089	16.876542864	CORE	65 H H	0.0000	65
H	3.615941315	3.581700618	16.831668309	CORE	66 H H	0.0000	66
H	6.505404348	3.630323157	16.876766323	CORE	67 H H	0.0000	67
H	9.397327785	3.580585423	16.832582360	CORE	68 H H	0.0000	68
end							
end							

Hv. The energy from VASP with high accuracy setups is -216.188418 eV.

PBC	11.56261009	10.01351407	25.00000000	90.00000000	90.00000000	90.00000000
Pd	0.722663130	0.625844629	8.959688149	CORE	1 Pd Pd	0.0000 1
Ag	3.613315652	0.625844629	8.959688149	CORE	2 Ag Ag	0.0000 2
Pd	6.503968173	0.625844629	8.959688149	CORE	3 Pd Pd	0.0000 3
Ag	9.394620695	0.625844629	8.959688149	CORE	4 Ag Ag	0.0000 4
Ag	2.167989391	3.129223146	8.959688149	CORE	5 Ag Ag	0.0000 5
Ag	5.058641913	3.129223146	8.959688149	CORE	6 Ag Ag	0.0000 6
Ag	7.949294434	3.129223146	8.959688149	CORE	7 Ag Ag	0.0000 7
Ag	10.839946956	3.129223146	8.959688149	CORE	8 Ag Ag	0.0000 8
Ag	0.722663130	5.632601664	8.959688149	CORE	9 Ag Ag	0.0000 9
Pd	3.613315652	5.632601664	8.959688149	CORE	10 Pd Pd	0.0000 10
Ag	6.503968173	5.632601664	8.959688149	CORE	11 Ag Ag	0.0000 11

Pd	9.394620695	5.632601664	8.959688149 CORE	12 Pd Pd	0.0000	12
Ag	2.167989391	8.135980181	8.959688149 CORE	13 Ag Ag	0.0000	13
Ag	5.058641913	8.135980181	8.959688149 CORE	14 Ag Ag	0.0000	14
Ag	7.949294434	8.135980181	8.959688149 CORE	15 Ag Ag	0.0000	15
Ag	10.839946956	8.135980181	8.959688149 CORE	16 Ag Ag	0.0000	16
Ag	2.167989391	1.460304135	11.319896050 CORE	17 Ag Ag	0.0000	17
Ag	5.058641913	1.460304135	11.319896050 CORE	18 Ag Ag	0.0000	18
Ag	7.949294434	1.460304135	11.319896050 CORE	19 Ag Ag	0.0000	19
Ag	10.839946956	1.460304135	11.319896050 CORE	20 Ag Ag	0.0000	20
Pd	0.722663130	3.963682652	11.319896050 CORE	21 Pd Pd	0.0000	21
Ag	3.613315652	3.963682652	11.319896050 CORE	22 Ag Ag	0.0000	22
Pd	6.503968173	3.963682652	11.319896050 CORE	23 Pd Pd	0.0000	23
Ag	9.394620695	3.963682652	11.319896050 CORE	24 Ag Ag	0.0000	24
Ag	2.167989391	6.467061169	11.319896050 CORE	25 Ag Ag	0.0000	25
Ag	5.058641913	6.467061169	11.319896050 CORE	26 Ag Ag	0.0000	26
Ag	7.949294434	6.467061169	11.319896050 CORE	27 Ag Ag	0.0000	27
Ag	10.839946956	6.467061169	11.319896050 CORE	28 Ag Ag	0.0000	28
Ag	0.722663130	8.970439686	11.319896050 CORE	29 Ag Ag	0.0000	29
Pd	3.613315652	8.970439686	11.319896050 CORE	30 Pd Pd	0.0000	30
Ag	6.503968173	8.970439686	11.319896050 CORE	31 Ag Ag	0.0000	31
Pd	9.394620695	8.970439686	11.319896050 CORE	32 Pd Pd	0.0000	32
Ag	0.729348203	2.292272771	13.662644370 CORE	33 Ag Ag	0.0000	33
Pd	3.620226876	2.286156290	13.676645208 CORE	34 Pd Pd	0.0000	34
Ag	6.509383025	2.292910649	13.648859909 CORE	35 Ag Ag	0.0000	35
Pd	9.393718430	2.287579001	13.677367535 CORE	36 Pd Pd	0.0000	36
Ag	2.154980743	4.777696380	13.654756362 CORE	37 Ag Ag	0.0000	37
Ag	5.066289421	4.779162113	13.649867581 CORE	38 Ag Ag	0.0000	38
Ag	7.936747538	4.779950711	13.652063733 CORE	39 Ag Ag	0.0000	39
Ag	10.847072525	4.777084513	13.654585657 CORE	40 Ag Ag	0.0000	40
Pd	0.723596492	7.272488309	13.712558825 CORE	41 Pd Pd	0.0000	41
Ag	3.610848838	7.287406225	13.679438844 CORE	42 Ag Ag	0.0000	42
Pd	6.504259520	7.285157852	13.690490893 CORE	43 Pd Pd	0.0000	43
Ag	9.402985490	7.287172384	13.678530966 CORE	44 Ag Ag	0.0000	44
Ag	2.174933180	9.788431954	13.672473807 CORE	45 Ag Ag	0.0000	45
Ag	5.042680502	9.786803111	13.668347967 CORE	46 Ag Ag	0.0000	46
Ag	7.959448772	9.787481501	13.668609799 CORE	47 Ag Ag	0.0000	47
Ag	10.828097075	9.789750109	13.670598635 CORE	48 Ag Ag	0.0000	48
Ag	3.619596890	0.645648129	16.048054368 CORE	49 Ag Ag	0.0000	49
Ag	0.725315764	5.589393810	16.060660246 CORE	50 Ag Ag	0.0000	50
Ag	6.506292286	5.583557572	16.021975550 CORE	51 Ag Ag	0.0000	51
Pd	10.846809947	3.096122282	15.992003230 CORE	52 Pd Pd	0.0000	52
Ag	0.723642098	0.638474368	16.048485869 CORE	53 Ag Ag	0.0000	53
Pd	7.935566986	3.096184492	15.940217475 CORE	54 Pd Pd	0.0000	54
Ag	2.163708919	8.109467840	16.040361838 CORE	55 Ag Ag	0.0000	55

Ag	6.504760753	0.636049249	16.032038552	CORE	56 Ag Ag	0.0000	56
Ag	7.943547003	8.109922415	16.029081153	CORE	57 Ag Ag	0.0000	57
Pd	5.081189081	3.096371549	15.939019585	CORE	58 Pd Pd	0.0000	58
Ag	10.843947479	8.109714059	16.040383373	CORE	59 Ag Ag	0.0000	59
Ag	5.062017212	8.110988755	16.031758568	CORE	60 Ag Ag	0.0000	60
Ag	3.627905928	5.575535945	16.058548129	CORE	61 Ag Ag	0.0000	61
Ag	9.391387590	0.645374761	16.046160083	CORE	62 Ag Ag	0.0000	62
Ag	9.384977496	5.576417510	16.062571118	CORE	63 Ag Ag	0.0000	63
Pd	2.172044934	3.096077355	15.993831779	CORE	64 Pd Pd	0.0000	64
H	0.727234333	3.613989897	16.872452662	CORE	65 H H	0.0000	65
H	3.663225699	3.542789591	16.822295183	CORE	66 H H	0.0000	66
H	9.356682699	3.540080928	16.820488707	CORE	67 H H	0.0000	67
end							
end							

C₂H₂*. The energy from VASP with high accuracy setups is -240.106852 eV.

PBC	11.56261009	10.01351407	25.00000000	90.00000000	90.00000000	90.00000000	90.00000000
Pd	0.722663130	0.625844629	8.959688149	CORE	1 Pd Pd	0.0000	1
Ag	3.613315652	0.625844629	8.959688149	CORE	2 Ag Ag	0.0000	2
Pd	6.503968173	0.625844629	8.959688149	CORE	3 Pd Pd	0.0000	3
Ag	9.394620695	0.625844629	8.959688149	CORE	4 Ag Ag	0.0000	4
Ag	2.167989391	3.129223146	8.959688149	CORE	5 Ag Ag	0.0000	5
Ag	5.058641913	3.129223146	8.959688149	CORE	6 Ag Ag	0.0000	6
Ag	7.949294434	3.129223146	8.959688149	CORE	7 Ag Ag	0.0000	7
Ag	10.839946956	3.129223146	8.959688149	CORE	8 Ag Ag	0.0000	8
Ag	0.722663130	5.632601664	8.959688149	CORE	9 Ag Ag	0.0000	9
Pd	3.613315652	5.632601664	8.959688149	CORE	10 Pd Pd	0.0000	10
Ag	6.503968173	5.632601664	8.959688149	CORE	11 Ag Ag	0.0000	11
Pd	9.394620695	5.632601664	8.959688149	CORE	12 Pd Pd	0.0000	12
Ag	2.167989391	8.135980181	8.959688149	CORE	13 Ag Ag	0.0000	13
Ag	5.058641913	8.135980181	8.959688149	CORE	14 Ag Ag	0.0000	14
Ag	7.949294434	8.135980181	8.959688149	CORE	15 Ag Ag	0.0000	15
Ag	10.839946956	8.135980181	8.959688149	CORE	16 Ag Ag	0.0000	16
Ag	2.167989391	1.460304135	11.319896050	CORE	17 Ag Ag	0.0000	17
Ag	5.058641913	1.460304135	11.319896050	CORE	18 Ag Ag	0.0000	18
Ag	7.949294434	1.460304135	11.319896050	CORE	19 Ag Ag	0.0000	19
Ag	10.839946956	1.460304135	11.319896050	CORE	20 Ag Ag	0.0000	20
Pd	0.722663130	3.963682652	11.319896050	CORE	21 Pd Pd	0.0000	21
Ag	3.613315652	3.963682652	11.319896050	CORE	22 Ag Ag	0.0000	22
Pd	6.503968173	3.963682652	11.319896050	CORE	23 Pd Pd	0.0000	23
Ag	9.394620695	3.963682652	11.319896050	CORE	24 Ag Ag	0.0000	24
Ag	2.167989391	6.467061169	11.319896050	CORE	25 Ag Ag	0.0000	25
Ag	5.058641913	6.467061169	11.319896050	CORE	26 Ag Ag	0.0000	26
Ag	7.949294434	6.467061169	11.319896050	CORE	27 Ag Ag	0.0000	27

Ag	10.839946956	6.467061169	11.319896050 CORE	28 Ag Ag	0.0000	28
Ag	0.722663130	8.970439686	11.319896050 CORE	29 Ag Ag	0.0000	29
Pd	3.613315652	8.970439686	11.319896050 CORE	30 Pd Pd	0.0000	30
Ag	6.503968173	8.970439686	11.319896050 CORE	31 Ag Ag	0.0000	31
Pd	9.394620695	8.970439686	11.319896050 CORE	32 Pd Pd	0.0000	32
Ag	0.731607162	2.287097282	13.655977500 CORE	33 Ag Ag	0.0000	33
Pd	3.633996939	2.298950096	13.677517909 CORE	34 Pd Pd	0.0000	34
Ag	6.513967278	2.285968701	13.668269870 CORE	35 Ag Ag	0.0000	35
Pd	9.385790147	2.300408456	13.675628127 CORE	36 Pd Pd	0.0000	36
Ag	2.157058363	4.773293812	13.648204847 CORE	37 Ag Ag	0.0000	37
Ag	5.073696149	4.763790953	13.661031646 CORE	38 Ag Ag	0.0000	38
Ag	7.935611053	4.765153403	13.661864773 CORE	39 Ag Ag	0.0000	39
Ag	10.851716164	4.773551815	13.643928610 CORE	40 Ag Ag	0.0000	40
Pd	0.725742559	7.273999411	13.700749472 CORE	41 Pd Pd	0.0000	41
Ag	3.617680817	7.286113000	13.667668782 CORE	42 Ag Ag	0.0000	42
Pd	6.507707250	7.277078132	13.692412540 CORE	43 Pd Pd	0.0000	43
Ag	9.404731036	7.287189214	13.668129897 CORE	44 Ag Ag	0.0000	44
Ag	2.178844494	9.790328848	13.660958219 CORE	45 Ag Ag	0.0000	45
Ag	5.054937814	9.794088835	13.674249072 CORE	46 Ag Ag	0.0000	46
Ag	7.953117670	9.791839218	13.674767048 CORE	47 Ag Ag	0.0000	47
Ag	10.830250865	9.790430061	13.661414109 CORE	48 Ag Ag	0.0000	48
Ag	3.603170110	0.625274170	16.025632775 CORE	49 Ag Ag	0.0000	49
Ag	0.729579414	5.585616916	16.051218793 CORE	50 Ag Ag	0.0000	50
Ag	6.512238409	5.606829032	16.029863726 CORE	51 Ag Ag	0.0000	51
Pd	10.863741030	3.094278725	15.967111302 CORE	52 Pd Pd	0.0000	52
Ag	0.728067917	0.634356805	16.045847078 CORE	53 Ag Ag	0.0000	53
Pd	7.934742317	3.077787743	16.064762095 CORE	54 Pd Pd	0.0000	54
Ag	2.163044849	8.107250063	16.027963705 CORE	55 Ag Ag	0.0000	55
Ag	6.508367308	0.596406499	16.092371211 CORE	56 Ag Ag	0.0000	56
Ag	7.953075693	8.103535690	16.022160769 CORE	57 Ag Ag	0.0000	57
Pd	5.088508512	3.079980083	16.060375659 CORE	58 Pd Pd	0.0000	58
Ag	10.850696663	8.108419687	16.031334049 CORE	59 Ag Ag	0.0000	59
Ag	5.059319711	8.102724428	16.022722496 CORE	60 Ag Ag	0.0000	60
Ag	3.617118901	5.586001581	16.040527635 CORE	61 Ag Ag	0.0000	61
Ag	9.416428703	0.625398606	16.020310581 CORE	62 Ag Ag	0.0000	62
Ag	9.405028839	5.585973285	16.039661273 CORE	63 Ag Ag	0.0000	63
Pd	2.158954306	3.093779890	15.972031936 CORE	64 Pd Pd	0.0000	64
H	0.728559638	3.509788699	16.907068315 CORE	65 H H	0.0000	65
H	3.578933821	3.653662151	16.803030552 CORE	66 H H	0.0000	66
H	9.446311579	3.650424317	16.805230406 CORE	67 H H	0.0000	67
C	7.165591544	2.510174521	17.872821925 CORE	68 C C	0.0000	68
C	5.854688142	2.504991718	17.869256306 CORE	69 C C	0.0000	69
H	7.897255697	2.354191081	18.667543002 CORE	70 H H	0.0000	70
H	5.120335036	2.342937396	18.660326761 CORE	71 H H	0.0000	71

end

end

TS1. The energy from VASP with high accuracy setups is -239.417522 eV.

PBC	11.56260000	10.01350000	25.00000000	90.00000000	90.00000000	90.00000000
Pd	0.722663130	0.625844629	8.959688149	CORE	1 Pd Pd	0.0000 1
Ag	3.613315652	0.625844629	8.959688149	CORE	2 Ag Ag	0.0000 2
Pd	6.503968173	0.625844629	8.959688149	CORE	3 Pd Pd	0.0000 3
Ag	9.394620695	0.625844629	8.959688149	CORE	4 Ag Ag	0.0000 4
Ag	2.167989391	3.129223146	8.959688149	CORE	5 Ag Ag	0.0000 5
Ag	5.058641913	3.129223146	8.959688149	CORE	6 Ag Ag	0.0000 6
Ag	7.949294434	3.129223146	8.959688149	CORE	7 Ag Ag	0.0000 7
Ag	10.839946956	3.129223146	8.959688149	CORE	8 Ag Ag	0.0000 8
Ag	0.722663130	5.632601664	8.959688149	CORE	9 Ag Ag	0.0000 9
Pd	3.613315652	5.632601664	8.959688149	CORE	10 Pd Pd	0.0000 10
Ag	6.503968173	5.632601664	8.959688149	CORE	11 Ag Ag	0.0000 11
Pd	9.394620695	5.632601664	8.959688149	CORE	12 Pd Pd	0.0000 12
Ag	2.167989391	8.135980181	8.959688149	CORE	13 Ag Ag	0.0000 13
Ag	5.058641913	8.135980181	8.959688149	CORE	14 Ag Ag	0.0000 14
Ag	7.949294434	8.135980181	8.959688149	CORE	15 Ag Ag	0.0000 15
Ag	10.839946956	8.135980181	8.959688149	CORE	16 Ag Ag	0.0000 16
Ag	2.167989391	1.460304135	11.319896050	CORE	17 Ag Ag	0.0000 17
Ag	5.058641913	1.460304135	11.319896050	CORE	18 Ag Ag	0.0000 18
Ag	7.949294434	1.460304135	11.319896050	CORE	19 Ag Ag	0.0000 19
Ag	10.839946956	1.460304135	11.319896050	CORE	20 Ag Ag	0.0000 20
Pd	0.722663130	3.963682652	11.319896050	CORE	21 Pd Pd	0.0000 21
Ag	3.613315652	3.963682652	11.319896050	CORE	22 Ag Ag	0.0000 22
Pd	6.503968173	3.963682652	11.319896050	CORE	23 Pd Pd	0.0000 23
Ag	9.394620695	3.963682652	11.319896050	CORE	24 Ag Ag	0.0000 24
Ag	2.167989391	6.467061169	11.319896050	CORE	25 Ag Ag	0.0000 25
Ag	5.058641913	6.467061169	11.319896050	CORE	26 Ag Ag	0.0000 26
Ag	7.949294434	6.467061169	11.319896050	CORE	27 Ag Ag	0.0000 27
Ag	10.839946956	6.467061169	11.319896050	CORE	28 Ag Ag	0.0000 28
Ag	0.722663130	8.970439686	11.319896050	CORE	29 Ag Ag	0.0000 29
Pd	3.613315652	8.970439686	11.319896050	CORE	30 Pd Pd	0.0000 30
Ag	6.503968173	8.970439686	11.319896050	CORE	31 Ag Ag	0.0000 31
Pd	9.394620695	8.970439686	11.319896050	CORE	32 Pd Pd	0.0000 32
Ag	0.731347458	2.305871113	13.661696886	CORE	33 Ag Ag	0.0000 33
Pd	3.630494969	2.315569074	13.685777081	CORE	34 Pd Pd	0.0000 34
Ag	6.513762160	2.313695511	13.678904599	CORE	35 Ag Ag	0.0000 35
Pd	9.380640004	2.309955501	13.693877643	CORE	36 Pd Pd	0.0000 36
Ag	2.161149751	4.787538255	13.656171517	CORE	37 Ag Ag	0.0000 37
Ag	5.074852664	4.781303718	13.669142952	CORE	38 Ag Ag	0.0000 38
Ag	7.942358343	4.787656113	13.653073142	CORE	39 Ag Ag	0.0000 39

Ag	10.845225219	4.785258530	13.658779715	CORE	40 Ag Ag	0.0000	40
Pd	0.729521352	7.282556330	13.700930918	CORE	41 Pd Pd	0.0000	41
Ag	3.616247634	7.303481784	13.670265077	CORE	42 Ag Ag	0.0000	42
Pd	6.506437042	7.298722199	13.689823798	CORE	43 Pd Pd	0.0000	43
Ag	9.406417643	7.306013306	13.669327450	CORE	44 Ag Ag	0.0000	44
Ag	2.179048925	9.807415730	13.666584018	CORE	45 Ag Ag	0.0000	45
Ag	5.053573456	9.814762277	13.674543493	CORE	46 Ag Ag	0.0000	46
Ag	7.959701523	9.816376634	13.677045271	CORE	47 Ag Ag	0.0000	47
Ag	10.833956648	9.803250194	13.663559457	CORE	48 Ag Ag	0.0000	48
Ag	3.601912467	0.645467270	16.035709557	CORE	49 Ag Ag	0.0000	49
Ag	0.720585359	5.609240933	16.061610761	CORE	50 Ag Ag	0.0000	50
Ag	6.514292144	5.648201881	16.027959448	CORE	51 Ag Ag	0.0000	51
Pd	10.858245831	3.118105575	15.960428610	CORE	52 Pd Pd	0.0000	52
Ag	0.726148434	0.656911473	16.059178300	CORE	53 Ag Ag	0.0000	53
Pd	8.021138317	3.121334914	16.031026886	CORE	54 Pd Pd	0.0000	54
Ag	2.166079351	8.134688990	16.029617105	CORE	55 Ag Ag	0.0000	55
Ag	6.522448745	0.647303423	16.063987546	CORE	56 Ag Ag	0.0000	56
Ag	7.959294530	8.145517626	16.024546176	CORE	57 Ag Ag	0.0000	57
Pd	5.041093780	3.094533620	16.075550115	CORE	58 Pd Pd	0.0000	58
Ag	10.855509239	8.129754388	16.031860843	CORE	59 Ag Ag	0.0000	59
Ag	5.066718929	8.138312426	16.023725972	CORE	60 Ag Ag	0.0000	60
Ag	3.618913465	5.614262640	16.047450421	CORE	61 Ag Ag	0.0000	61
Ag	9.428496796	0.647786465	16.032798750	CORE	62 Ag Ag	0.0000	62
Ag	9.408671650	5.610361061	16.055082639	CORE	63 Ag Ag	0.0000	63
Pd	2.150276652	3.127545593	16.005428024	CORE	64 Pd Pd	0.0000	64
H	0.691019771	3.581542720	16.900207398	CORE	65 H H	0.0000	65
H	3.571866393	3.597163523	16.880761281	CORE	66 H H	0.0000	66
H	7.919971307	4.219879863	17.221930625	CORE	67 H H	0.0000	67
C	7.223201185	2.804463339	17.917427849	CORE	68 C C	0.0000	68
C	5.907802771	2.632694929	17.850751485	CORE	69 C C	0.0000	69
H	7.890010546	2.654635726	18.770228231	CORE	70 H H	0.0000	70
H	5.267248108	2.259600814	18.655809169	CORE	71 H H	0.0000	71
end							
end							

C₂H₃*+H*. The energy from VASP with high accuracy setups is -244.169910 eV.

PBC	11.56260000	10.01350000	25.00000000	90.00000000	90.00000000	90.00000000
Pd	0.722663130	0.625844629	8.959688149	CORE	1 Pd Pd	0.0000 1
Ag	3.613315652	0.625844629	8.959688149	CORE	2 Ag Ag	0.0000 2
Pd	6.503968173	0.625844629	8.959688149	CORE	3 Pd Pd	0.0000 3
Ag	9.394620695	0.625844629	8.959688149	CORE	4 Ag Ag	0.0000 4
Ag	2.167989391	3.129223146	8.959688149	CORE	5 Ag Ag	0.0000 5
Ag	5.058641913	3.129223146	8.959688149	CORE	6 Ag Ag	0.0000 6
Ag	7.949294434	3.129223146	8.959688149	CORE	7 Ag Ag	0.0000 7

Ag	10.839946956	3.129223146	8.959688149 CORE	8 Ag Ag	0.0000	8
Ag	0.722663130	5.632601664	8.959688149 CORE	9 Ag Ag	0.0000	9
Pd	3.613315652	5.632601664	8.959688149 CORE	10 Pd Pd	0.0000	10
Ag	6.503968173	5.632601664	8.959688149 CORE	11 Ag Ag	0.0000	11
Pd	9.394620695	5.632601664	8.959688149 CORE	12 Pd Pd	0.0000	12
Ag	2.167989391	8.135980181	8.959688149 CORE	13 Ag Ag	0.0000	13
Ag	5.058641913	8.135980181	8.959688149 CORE	14 Ag Ag	0.0000	14
Ag	7.949294434	8.135980181	8.959688149 CORE	15 Ag Ag	0.0000	15
Ag	10.839946956	8.135980181	8.959688149 CORE	16 Ag Ag	0.0000	16
Ag	2.167989391	1.460304135	11.319896050 CORE	17 Ag Ag	0.0000	17
Ag	5.058641913	1.460304135	11.319896050 CORE	18 Ag Ag	0.0000	18
Ag	7.949294434	1.460304135	11.319896050 CORE	19 Ag Ag	0.0000	19
Ag	10.839946956	1.460304135	11.319896050 CORE	20 Ag Ag	0.0000	20
Pd	0.722663130	3.963682652	11.319896050 CORE	21 Pd Pd	0.0000	21
Ag	3.613315652	3.963682652	11.319896050 CORE	22 Ag Ag	0.0000	22
Pd	6.503968173	3.963682652	11.319896050 CORE	23 Pd Pd	0.0000	23
Ag	9.394620695	3.963682652	11.319896050 CORE	24 Ag Ag	0.0000	24
Ag	2.167989391	6.467061169	11.319896050 CORE	25 Ag Ag	0.0000	25
Ag	5.058641913	6.467061169	11.319896050 CORE	26 Ag Ag	0.0000	26
Ag	7.949294434	6.467061169	11.319896050 CORE	27 Ag Ag	0.0000	27
Ag	10.839946956	6.467061169	11.319896050 CORE	28 Ag Ag	0.0000	28
Ag	0.722663130	8.970439686	11.319896050 CORE	29 Ag Ag	0.0000	29
Pd	3.613315652	8.970439686	11.319896050 CORE	30 Pd Pd	0.0000	30
Ag	6.503968173	8.970439686	11.319896050 CORE	31 Ag Ag	0.0000	31
Pd	9.394620695	8.970439686	11.319896050 CORE	32 Pd Pd	0.0000	32
Ag	0.740351083	2.289717542	13.658759520 CORE	33 Ag Ag	0.0000	33
Pd	3.642844824	2.299138367	13.682424919 CORE	34 Pd Pd	0.0000	34
Ag	6.521840694	2.314470712	13.696525178 CORE	35 Ag Ag	0.0000	35
Pd	9.375781295	2.307684063	13.735473083 CORE	36 Pd Pd	0.0000	36
Ag	2.164404819	4.773572946	13.652382855 CORE	37 Ag Ag	0.0000	37
Ag	5.066253044	4.769845504	13.650154133 CORE	38 Ag Ag	0.0000	38
Ag	7.948908006	4.755437772	13.675707351 CORE	39 Ag Ag	0.0000	39
Ag	10.861422111	4.768729823	13.645577298 CORE	40 Ag Ag	0.0000	40
Pd	0.729380959	7.274136187	13.699597970 CORE	41 Pd Pd	0.0000	41
Ag	3.619516954	7.285536319	13.666814565 CORE	42 Ag Ag	0.0000	42
Pd	6.516998263	7.289323881	13.671466017 CORE	43 Pd Pd	0.0000	43
Ag	9.410000793	7.286511800	13.664895684 CORE	44 Ag Ag	0.0000	44
Ag	2.177489617	9.790702520	13.664234241 CORE	45 Ag Ag	0.0000	45
Ag	5.042978902	9.794652381	13.649047172 CORE	46 Ag Ag	0.0000	46
Ag	7.981967787	9.798609957	13.648318173 CORE	47 Ag Ag	0.0000	47
Ag	10.837056431	9.797233505	13.668393276 CORE	48 Ag Ag	0.0000	48
Ag	3.614891714	0.634110061	16.028041963 CORE	49 Ag Ag	0.0000	49
Ag	0.741439314	5.597159453	16.057198429 CORE	50 Ag Ag	0.0000	50
Ag	6.508013637	5.650102009	15.961188597 CORE	51 Ag Ag	0.0000	51

Pd	10.893902389	3.109688063	15.984247072	CORE	52 Pd Pd	0.0000	52
Ag	0.739416224	0.646772654	16.057357693	CORE	53 Ag Ag	0.0000	53
Pd	7.953353487	3.077308432	16.220546465	CORE	54 Pd Pd	0.0000	54
Ag	2.170502554	8.119348866	16.029882350	CORE	55 Ag Ag	0.0000	55
Ag	6.531224776	0.578584732	15.959030936	CORE	56 Ag Ag	0.0000	56
Ag	7.974354716	8.111417274	16.012501059	CORE	57 Ag Ag	0.0000	57
Pd	5.060570908	3.111455657	16.070461560	CORE	58 Pd Pd	0.0000	58
Ag	10.863996271	8.116497890	16.031146642	CORE	59 Ag Ag	0.0000	59
Ag	5.063068130	8.120704133	16.012664674	CORE	60 Ag Ag	0.0000	60
Ag	3.621856600	5.600065361	16.049621799	CORE	61 Ag Ag	0.0000	61
Ag	9.424141581	0.634898860	16.050142559	CORE	62 Ag Ag	0.0000	62
Ag	9.420939213	5.587931619	16.031321612	CORE	63 Ag Ag	0.0000	63
Pd	2.184468581	3.111879380	15.979412211	CORE	64 Pd Pd	0.0000	64
H	0.765020539	3.512346504	16.927729142	CORE	65 H H	0.0000	65
H	3.614255645	3.580396458	16.899995975	CORE	66 H H	0.0000	66
H	7.125981035	4.727042565	18.254831493	CORE	67 H H	0.0000	67
H	9.491834590	3.617191424	16.851873600	CORE	68 H H	0.0000	68
C	7.159450260	3.635646981	18.318475575	CORE	69 C C	0.0000	69
C	6.267165269	2.804385160	17.659078020	CORE	70 C C	0.0000	70
H	7.763675223	3.245948471	19.145669378	CORE	71 H H	0.0000	71
H	6.133935360	1.806330361	18.109664708	CORE	72 H H	0.0000	72

end
end

TS2. The energy from VASP with high accuracy setups is -243.783030 eV.

PBC	11.56260000	10.01350000	25.00000000	90.00000000	90.00000000	90.00000000
Pd	0.722663130	0.625844629	8.959688149	CORE	1 Pd Pd	0.0000 1
Ag	3.613315652	0.625844629	8.959688149	CORE	2 Ag Ag	0.0000 2
Pd	6.503968173	0.625844629	8.959688149	CORE	3 Pd Pd	0.0000 3
Ag	9.394620695	0.625844629	8.959688149	CORE	4 Ag Ag	0.0000 4
Ag	2.167989391	3.129223146	8.959688149	CORE	5 Ag Ag	0.0000 5
Ag	5.058641913	3.129223146	8.959688149	CORE	6 Ag Ag	0.0000 6
Ag	7.949294434	3.129223146	8.959688149	CORE	7 Ag Ag	0.0000 7
Ag	10.839946956	3.129223146	8.959688149	CORE	8 Ag Ag	0.0000 8
Ag	0.722663130	5.632601664	8.959688149	CORE	9 Ag Ag	0.0000 9
Pd	3.613315652	5.632601664	8.959688149	CORE	10 Pd Pd	0.0000 10
Ag	6.503968173	5.632601664	8.959688149	CORE	11 Ag Ag	0.0000 11
Pd	9.394620695	5.632601664	8.959688149	CORE	12 Pd Pd	0.0000 12
Ag	2.167989391	8.135980181	8.959688149	CORE	13 Ag Ag	0.0000 13
Ag	5.058641913	8.135980181	8.959688149	CORE	14 Ag Ag	0.0000 14
Ag	7.949294434	8.135980181	8.959688149	CORE	15 Ag Ag	0.0000 15
Ag	10.839946956	8.135980181	8.959688149	CORE	16 Ag Ag	0.0000 16
Ag	2.167989391	1.460304135	11.319896050	CORE	17 Ag Ag	0.0000 17
Ag	5.058641913	1.460304135	11.319896050	CORE	18 Ag Ag	0.0000 18

Ag	7.949294434	1.460304135	11.319896050 CORE	19 Ag Ag	0.0000	19
Ag	10.839946956	1.460304135	11.319896050 CORE	20 Ag Ag	0.0000	20
Pd	0.722663130	3.963682652	11.319896050 CORE	21 Pd Pd	0.0000	21
Ag	3.613315652	3.963682652	11.319896050 CORE	22 Ag Ag	0.0000	22
Pd	6.503968173	3.963682652	11.319896050 CORE	23 Pd Pd	0.0000	23
Ag	9.394620695	3.963682652	11.319896050 CORE	24 Ag Ag	0.0000	24
Ag	2.167989391	6.467061169	11.319896050 CORE	25 Ag Ag	0.0000	25
Ag	5.058641913	6.467061169	11.319896050 CORE	26 Ag Ag	0.0000	26
Ag	7.949294434	6.467061169	11.319896050 CORE	27 Ag Ag	0.0000	27
Ag	10.839946956	6.467061169	11.319896050 CORE	28 Ag Ag	0.0000	28
Ag	0.722663130	8.970439686	11.319896050 CORE	29 Ag Ag	0.0000	29
Pd	3.613315652	8.970439686	11.319896050 CORE	30 Pd Pd	0.0000	30
Ag	6.503968173	8.970439686	11.319896050 CORE	31 Ag Ag	0.0000	31
Pd	9.394620695	8.970439686	11.319896050 CORE	32 Pd Pd	0.0000	32
Ag	0.736465772	2.287810492	13.657503207 CORE	33 Ag Ag	0.0000	33
Pd	3.649825338	2.300873906	13.699962144 CORE	34 Pd Pd	0.0000	34
Ag	6.505857317	2.316125602	13.706834090 CORE	35 Ag Ag	0.0000	35
Pd	9.357243550	2.311270480	13.742226862 CORE	36 Pd Pd	0.0000	36
Ag	2.157699830	4.772520275	13.659729074 CORE	37 Ag Ag	0.0000	37
Ag	5.051905513	4.766831299	13.653708848 CORE	38 Ag Ag	0.0000	38
Ag	7.934543392	4.754806130	13.671169512 CORE	39 Ag Ag	0.0000	39
Ag	10.849814745	4.765624238	13.647334011 CORE	40 Ag Ag	0.0000	40
Pd	0.717802750	7.271871677	13.702314312 CORE	41 Pd Pd	0.0000	41
Ag	3.610934877	7.285524128	13.668354238 CORE	42 Ag Ag	0.0000	42
Pd	6.507608718	7.294560488	13.666369442 CORE	43 Pd Pd	0.0000	43
Ag	9.402610253	7.285322606	13.666606416 CORE	44 Ag Ag	0.0000	44
Ag	2.168839792	9.789660086	13.660761934 CORE	45 Ag Ag	0.0000	45
Ag	5.032599296	9.794721358	13.648882313 CORE	46 Ag Ag	0.0000	46
Ag	7.972770906	9.800198749	13.651394669 CORE	47 Ag Ag	0.0000	47
Ag	10.828077860	9.798409845	13.669595974 CORE	48 Ag Ag	0.0000	48
Ag	3.591246031	0.626881718	16.031723492 CORE	49 Ag Ag	0.0000	49
Ag	0.725663763	5.586697988	16.063652929 CORE	50 Ag Ag	0.0000	50
Ag	6.494481536	5.652328371	15.949296428 CORE	51 Ag Ag	0.0000	51
Pd	10.868339904	3.100373727	15.990943907 CORE	52 Pd Pd	0.0000	52
Ag	0.727529065	0.641513633	16.056000773 CORE	53 Ag Ag	0.0000	53
Pd	7.926838590	3.059097448	16.247831516 CORE	54 Pd Pd	0.0000	54
Ag	2.153924921	8.110371849	16.031380710 CORE	55 Ag Ag	0.0000	55
Ag	6.507610233	0.574317277	15.959553035 CORE	56 Ag Ag	0.0000	56
Ag	7.957691891	8.109317765	16.014344013 CORE	57 Ag Ag	0.0000	57
Pd	4.994825779	3.126484223	16.079049014 CORE	58 Pd Pd	0.0000	58
Ag	10.846339514	8.107834729	16.032579666 CORE	59 Ag Ag	0.0000	59
Ag	5.046452954	8.118640544	16.014320648 CORE	60 Ag Ag	0.0000	60
Ag	3.595613051	5.586425091	16.055101544 CORE	61 Ag Ag	0.0000	61
Ag	9.408249803	0.629523130	16.050824195 CORE	62 Ag Ag	0.0000	62

Ag	9.398677906	5.574522141	16.029176749	CORE	63 Ag Ag	0.0000	63
Pd	2.161484103	3.103588090	15.961306613	CORE	64 Pd Pd	0.0000	64
H	0.763041270	3.521407545	16.905331476	CORE	65 H H	0.0000	65
H	4.534948401	3.733488795	17.478981660	CORE	66 H H	0.0000	66
H	7.125056169	4.681982036	18.280789839	CORE	67 H H	0.0000	67
H	9.468317501	3.612163235	16.860326985	CORE	68 H H	0.0000	68
C	7.135517258	3.589534110	18.310078892	CORE	69 C C	0.0000	69
C	6.171181305	2.802447315	17.698894435	CORE	70 C C	0.0000	70
H	7.755214039	3.156757904	19.103900690	CORE	71 H H	0.0000	71
H	5.999756320	1.810966995	18.143330975	CORE	72 H H	0.0000	72
end							
end							

C₂H₄*+H*. The energy from VASP with high accuracy setups is -248.586137 eV.

PBC	11.56260000	10.01350000	25.00000000	90.00000000	90.00000000	90.00000000
Pd	0.722663130	0.625844629	8.959688149	CORE	1 Pd Pd	0.0000 1
Ag	3.613315652	0.625844629	8.959688149	CORE	2 Ag Ag	0.0000 2
Pd	6.503968173	0.625844629	8.959688149	CORE	3 Pd Pd	0.0000 3
Ag	9.394620695	0.625844629	8.959688149	CORE	4 Ag Ag	0.0000 4
Ag	2.167989391	3.129223146	8.959688149	CORE	5 Ag Ag	0.0000 5
Ag	5.058641913	3.129223146	8.959688149	CORE	6 Ag Ag	0.0000 6
Ag	7.949294434	3.129223146	8.959688149	CORE	7 Ag Ag	0.0000 7
Ag	10.839946956	3.129223146	8.959688149	CORE	8 Ag Ag	0.0000 8
Ag	0.722663130	5.632601664	8.959688149	CORE	9 Ag Ag	0.0000 9
Pd	3.613315652	5.632601664	8.959688149	CORE	10 Pd Pd	0.0000 10
Ag	6.503968173	5.632601664	8.959688149	CORE	11 Ag Ag	0.0000 11
Pd	9.394620695	5.632601664	8.959688149	CORE	12 Pd Pd	0.0000 12
Ag	2.167989391	8.135980181	8.959688149	CORE	13 Ag Ag	0.0000 13
Ag	5.058641913	8.135980181	8.959688149	CORE	14 Ag Ag	0.0000 14
Ag	7.949294434	8.135980181	8.959688149	CORE	15 Ag Ag	0.0000 15
Ag	10.839946956	8.135980181	8.959688149	CORE	16 Ag Ag	0.0000 16
Ag	2.167989391	1.460304135	11.319896050	CORE	17 Ag Ag	0.0000 17
Ag	5.058641913	1.460304135	11.319896050	CORE	18 Ag Ag	0.0000 18
Ag	7.949294434	1.460304135	11.319896050	CORE	19 Ag Ag	0.0000 19
Ag	10.839946956	1.460304135	11.319896050	CORE	20 Ag Ag	0.0000 20
Pd	0.722663130	3.963682652	11.319896050	CORE	21 Pd Pd	0.0000 21
Ag	3.613315652	3.963682652	11.319896050	CORE	22 Ag Ag	0.0000 22
Pd	6.503968173	3.963682652	11.319896050	CORE	23 Pd Pd	0.0000 23
Ag	9.394620695	3.963682652	11.319896050	CORE	24 Ag Ag	0.0000 24
Ag	2.167989391	6.467061169	11.319896050	CORE	25 Ag Ag	0.0000 25
Ag	5.058641913	6.467061169	11.319896050	CORE	26 Ag Ag	0.0000 26
Ag	7.949294434	6.467061169	11.319896050	CORE	27 Ag Ag	0.0000 27
Ag	10.839946956	6.467061169	11.319896050	CORE	28 Ag Ag	0.0000 28
Ag	0.722663130	8.970439686	11.319896050	CORE	29 Ag Ag	0.0000 29

Pd	3.613315652	8.970439686	11.319896050 CORE	30 Pd Pd	0.0000	30
Ag	6.503968173	8.970439686	11.319896050 CORE	31 Ag Ag	0.0000	31
Pd	9.394620695	8.970439686	11.319896050 CORE	32 Pd Pd	0.0000	32
Ag	0.729864934	2.289417404	13.650305553 CORE	33 Ag Ag	0.0000	33
Pd	3.645346380	2.304469868	13.702031817 CORE	34 Pd Pd	0.0000	34
Ag	6.509043256	2.303055316	13.676395973 CORE	35 Ag Ag	0.0000	35
Pd	9.370819299	2.299263755	13.697066263 CORE	36 Pd Pd	0.0000	36
Ag	2.152330237	4.777943830	13.647401451 CORE	37 Ag Ag	0.0000	37
Ag	5.068941088	4.764568598	13.666055583 CORE	38 Ag Ag	0.0000	38
Ag	7.934316972	4.763787832	13.662645510 CORE	39 Ag Ag	0.0000	39
Ag	10.849882789	4.774375155	13.642650221 CORE	40 Ag Ag	0.0000	40
Pd	0.722132112	7.277745059	13.703337907 CORE	41 Pd Pd	0.0000	41
Ag	3.611620421	7.289001872	13.666884375 CORE	42 Ag Ag	0.0000	42
Pd	6.504764769	7.286326535	13.681221003 CORE	43 Pd Pd	0.0000	43
Ag	9.402510015	7.287292195	13.665408907 CORE	44 Ag Ag	0.0000	44
Ag	2.175681162	9.793875278	13.667565309 CORE	45 Ag Ag	0.0000	45
Ag	5.039352729	9.794651927	13.652962733 CORE	46 Ag Ag	0.0000	46
Ag	7.965269914	9.793232583	13.650815764 CORE	47 Ag Ag	0.0000	47
Ag	10.828789053	9.793020438	13.665099724 CORE	48 Ag Ag	0.0000	48
Ag	3.611468417	0.646373150	16.034027365 CORE	49 Ag Ag	0.0000	49
Ag	0.724442744	5.598300327	16.053836308 CORE	50 Ag Ag	0.0000	50
Ag	6.510785524	5.635983860	15.999851157 CORE	51 Ag Ag	0.0000	51
Pd	10.856994578	3.101803533	15.958805555 CORE	52 Pd Pd	0.0000	52
Ag	0.723842061	0.644682556	16.046646761 CORE	53 Ag Ag	0.0000	53
Pd	7.883916433	3.092725096	16.123437863 CORE	54 Pd Pd	0.0000	54
Ag	2.160364183	8.117459685	16.026519375 CORE	55 Ag Ag	0.0000	55
Ag	6.508320241	0.594701444	15.987747227 CORE	56 Ag Ag	0.0000	56
Ag	7.954494323	8.118054511	16.014233528 CORE	57 Ag Ag	0.0000	57
Pd	5.131760689	3.092602187	16.126156551 CORE	58 Pd Pd	0.0000	58
Ag	10.845740099	8.118991447	16.026818976 CORE	59 Ag Ag	0.0000	59
Ag	5.052990701	8.116664397	16.015189814 CORE	60 Ag Ag	0.0000	60
Ag	3.615012705	5.590462389	16.030632656 CORE	61 Ag Ag	0.0000	61
Ag	9.399721437	0.647142281	16.030596530 CORE	62 Ag Ag	0.0000	62
Ag	9.399699309	5.590724140	16.028522652 CORE	63 Ag Ag	0.0000	63
Pd	2.157561610	3.101997385	15.964089772 CORE	64 Pd Pd	0.0000	64
H	0.724926175	3.558266608	16.880116055 CORE	65 H H	0.0000	65
H	5.284102789	3.970274777	18.566645806 CORE	66 H H	0.0000	66
H	7.721256153	3.966769452	18.562287208 CORE	67 H H	0.0000	67
H	9.436649810	3.654378259	16.772545804 CORE	68 H H	0.0000	68
H	3.580416849	3.656611469	16.775481938 CORE	69 H H	0.0000	69
C	7.209909278	3.058630782	18.232025891 CORE	70 C C	0.0000	70
C	5.791898800	3.060730300	18.234829440 CORE	71 C C	0.0000	71
H	7.724881350	2.126282405	18.485674519 CORE	72 H H	0.0000	72
H	5.274462159	2.130369354	18.491138563 CORE	73 H H	0.0000	73

end

end

TS3. The energy from VASP with high accuracy setups is -248.051566 eV.

PBC	11.56260000	10.01350000	25.00000000	90.00000000	90.00000000	90.00000000
Pd	0.722663130	0.625844629	8.959688149	CORE	1 Pd Pd	0.0000 1
Ag	3.613315652	0.625844629	8.959688149	CORE	2 Ag Ag	0.0000 2
Pd	6.503968173	0.625844629	8.959688149	CORE	3 Pd Pd	0.0000 3
Ag	9.394620695	0.625844629	8.959688149	CORE	4 Ag Ag	0.0000 4
Ag	2.167989391	3.129223146	8.959688149	CORE	5 Ag Ag	0.0000 5
Ag	5.058641913	3.129223146	8.959688149	CORE	6 Ag Ag	0.0000 6
Ag	7.949294434	3.129223146	8.959688149	CORE	7 Ag Ag	0.0000 7
Ag	10.839946956	3.129223146	8.959688149	CORE	8 Ag Ag	0.0000 8
Ag	0.722663130	5.632601664	8.959688149	CORE	9 Ag Ag	0.0000 9
Pd	3.613315652	5.632601664	8.959688149	CORE	10 Pd Pd	0.0000 10
Ag	6.503968173	5.632601664	8.959688149	CORE	11 Ag Ag	0.0000 11
Pd	9.394620695	5.632601664	8.959688149	CORE	12 Pd Pd	0.0000 12
Ag	2.167989391	8.135980181	8.959688149	CORE	13 Ag Ag	0.0000 13
Ag	5.058641913	8.135980181	8.959688149	CORE	14 Ag Ag	0.0000 14
Ag	7.949294434	8.135980181	8.959688149	CORE	15 Ag Ag	0.0000 15
Ag	10.839946956	8.135980181	8.959688149	CORE	16 Ag Ag	0.0000 16
Ag	2.167989391	1.460304135	11.319896050	CORE	17 Ag Ag	0.0000 17
Ag	5.058641913	1.460304135	11.319896050	CORE	18 Ag Ag	0.0000 18
Ag	7.949294434	1.460304135	11.319896050	CORE	19 Ag Ag	0.0000 19
Ag	10.839946956	1.460304135	11.319896050	CORE	20 Ag Ag	0.0000 20
Pd	0.722663130	3.963682652	11.319896050	CORE	21 Pd Pd	0.0000 21
Ag	3.613315652	3.963682652	11.319896050	CORE	22 Ag Ag	0.0000 22
Pd	6.503968173	3.963682652	11.319896050	CORE	23 Pd Pd	0.0000 23
Ag	9.394620695	3.963682652	11.319896050	CORE	24 Ag Ag	0.0000 24
Ag	2.167989391	6.467061169	11.319896050	CORE	25 Ag Ag	0.0000 25
Ag	5.058641913	6.467061169	11.319896050	CORE	26 Ag Ag	0.0000 26
Ag	7.949294434	6.467061169	11.319896050	CORE	27 Ag Ag	0.0000 27
Ag	10.839946956	6.467061169	11.319896050	CORE	28 Ag Ag	0.0000 28
Ag	0.722663130	8.970439686	11.319896050	CORE	29 Ag Ag	0.0000 29
Pd	3.613315652	8.970439686	11.319896050	CORE	30 Pd Pd	0.0000 30
Ag	6.503968173	8.970439686	11.319896050	CORE	31 Ag Ag	0.0000 31
Pd	9.394620695	8.970439686	11.319896050	CORE	32 Pd Pd	0.0000 32
Ag	0.719407087	2.296430518	13.659980986	CORE	33 Ag Ag	0.0000 33
Pd	3.622567224	2.300816552	13.692038681	CORE	34 Pd Pd	0.0000 34
Ag	6.535564426	2.315440540	13.705668759	CORE	35 Ag Ag	0.0000 35
Pd	9.380456821	2.308582651	13.710150185	CORE	36 Pd Pd	0.0000 36
Ag	2.154131945	4.782033662	13.653230030	CORE	37 Ag Ag	0.0000 37
Ag	5.064347229	4.782081883	13.653981348	CORE	38 Ag Ag	0.0000 38
Ag	7.938361878	4.754854299	13.693981759	CORE	39 Ag Ag	0.0000 39

Ag	10.843035105	4.774241104	13.654059274	CORE	40 Ag Ag	0.0000	40
Pd	0.726242489	7.281722578	13.705359199	CORE	41 Pd Pd	0.0000	41
Ag	3.611451352	7.296272466	13.672975863	CORE	42 Ag Ag	0.0000	42
Pd	6.504436936	7.288243828	13.687434698	CORE	43 Pd Pd	0.0000	43
Ag	9.397799429	7.297003913	13.656318263	CORE	44 Ag Ag	0.0000	44
Ag	2.175562977	9.799536548	13.672589443	CORE	45 Ag Ag	0.0000	45
Ag	5.042016406	9.800257977	13.662224578	CORE	46 Ag Ag	0.0000	46
Ag	7.957203132	9.797249729	13.655428485	CORE	47 Ag Ag	0.0000	47
Ag	10.831657904	9.797300423	13.658390527	CORE	48 Ag Ag	0.0000	48
Ag	3.618370317	0.669373844	16.048463429	CORE	49 Ag Ag	0.0000	49
Ag	0.722882719	5.606082108	16.064618992	CORE	50 Ag Ag	0.0000	50
Ag	6.502192138	5.618353333	16.016834970	CORE	51 Ag Ag	0.0000	51
Pd	10.848745159	3.122769955	16.001188122	CORE	52 Pd Pd	0.0000	52
Ag	0.726052496	0.656405909	16.057385028	CORE	53 Ag Ag	0.0000	53
Pd	7.932714106	3.109000767	16.255446581	CORE	54 Pd Pd	0.0000	54
Ag	2.165337383	8.131343103	16.031022341	CORE	55 Ag Ag	0.0000	55
Ag	6.501814004	0.630464817	16.023285443	CORE	56 Ag Ag	0.0000	56
Ag	7.943537287	8.126670641	16.021396401	CORE	57 Ag Ag	0.0000	57
Pd	5.094176246	3.122473383	15.976314560	CORE	58 Pd Pd	0.0000	58
Ag	10.852222853	8.130498975	16.027510121	CORE	59 Ag Ag	0.0000	59
Ag	5.057175529	8.132087304	16.022608455	CORE	60 Ag Ag	0.0000	60
Ag	3.617650990	5.598499041	16.051213101	CORE	61 Ag Ag	0.0000	61
Ag	9.409889203	0.625533848	16.001931711	CORE	62 Ag Ag	0.0000	62
Ag	9.407670054	5.618559180	15.998336063	CORE	63 Ag Ag	0.0000	63
Pd	2.156466471	3.122560262	15.988261604	CORE	64 Pd Pd	0.0000	64
H	0.713685413	3.583151612	16.919127173	CORE	65 H H	0.0000	65
H	6.705206766	4.092371866	18.544107448	CORE	66 H H	0.0000	66
H	9.142614161	3.933466451	18.891900242	CORE	67 H H	0.0000	67
H	9.471674269	3.140194484	17.225234572	CORE	68 H H	0.0000	68
H	3.637631013	3.536166560	16.801354829	CORE	69 H H	0.0000	69
C	8.626577536	3.067439282	18.468164245	CORE	70 C C	0.0000	70
C	7.200430367	3.150664484	18.308352174	CORE	71 C C	0.0000	71
H	9.047424166	2.110292139	18.789941206	CORE	72 H H	0.0000	72
H	6.598673809	2.262988988	18.507910964	CORE	73 H H	0.0000	73

end

end

C₂H₅*+H*. The energy from VASP with high accuracy setups is -252.183098 eV.

PBC	11.56260000	10.01350000	25.00000000	90.00000000	90.00000000	90.00000000
Pd	0.722663130	0.625844629	8.959688149	CORE	1 Pd Pd	0.0000 1
Ag	3.613315652	0.625844629	8.959688149	CORE	2 Ag Ag	0.0000 2
Pd	6.503968173	0.625844629	8.959688149	CORE	3 Pd Pd	0.0000 3
Ag	9.394620695	0.625844629	8.959688149	CORE	4 Ag Ag	0.0000 4
Ag	2.167989391	3.129223146	8.959688149	CORE	5 Ag Ag	0.0000 5

Ag	5.058641913	3.129223146	8.959688149 CORE	6 Ag Ag	0.0000	6
Ag	7.949294434	3.129223146	8.959688149 CORE	7 Ag Ag	0.0000	7
Ag	10.839946956	3.129223146	8.959688149 CORE	8 Ag Ag	0.0000	8
Ag	0.722663130	5.632601664	8.959688149 CORE	9 Ag Ag	0.0000	9
Pd	3.613315652	5.632601664	8.959688149 CORE	10 Pd Pd	0.0000	10
Ag	6.503968173	5.632601664	8.959688149 CORE	11 Ag Ag	0.0000	11
Pd	9.394620695	5.632601664	8.959688149 CORE	12 Pd Pd	0.0000	12
Ag	2.167989391	8.135980181	8.959688149 CORE	13 Ag Ag	0.0000	13
Ag	5.058641913	8.135980181	8.959688149 CORE	14 Ag Ag	0.0000	14
Ag	7.949294434	8.135980181	8.959688149 CORE	15 Ag Ag	0.0000	15
Ag	10.839946956	8.135980181	8.959688149 CORE	16 Ag Ag	0.0000	16
Ag	2.167989391	1.460304135	11.319896050 CORE	17 Ag Ag	0.0000	17
Ag	5.058641913	1.460304135	11.319896050 CORE	18 Ag Ag	0.0000	18
Ag	7.949294434	1.460304135	11.319896050 CORE	19 Ag Ag	0.0000	19
Ag	10.839946956	1.460304135	11.319896050 CORE	20 Ag Ag	0.0000	20
Pd	0.722663130	3.963682652	11.319896050 CORE	21 Pd Pd	0.0000	21
Ag	3.613315652	3.963682652	11.319896050 CORE	22 Ag Ag	0.0000	22
Pd	6.503968173	3.963682652	11.319896050 CORE	23 Pd Pd	0.0000	23
Ag	9.394620695	3.963682652	11.319896050 CORE	24 Ag Ag	0.0000	24
Ag	2.167989391	6.467061169	11.319896050 CORE	25 Ag Ag	0.0000	25
Ag	5.058641913	6.467061169	11.319896050 CORE	26 Ag Ag	0.0000	26
Ag	7.949294434	6.467061169	11.319896050 CORE	27 Ag Ag	0.0000	27
Ag	10.839946956	6.467061169	11.319896050 CORE	28 Ag Ag	0.0000	28
Ag	0.722663130	8.970439686	11.319896050 CORE	29 Ag Ag	0.0000	29
Pd	3.613315652	8.970439686	11.319896050 CORE	30 Pd Pd	0.0000	30
Ag	6.503968173	8.970439686	11.319896050 CORE	31 Ag Ag	0.0000	31
Pd	9.394620695	8.970439686	11.319896050 CORE	32 Pd Pd	0.0000	32
Ag	0.719438010	2.287567024	13.655979398 CORE	33 Ag Ag	0.0000	33
Pd	3.617362537	2.285205554	13.673699346 CORE	34 Pd Pd	0.0000	34
Ag	6.526806006	2.303549209	13.678149447 CORE	35 Ag Ag	0.0000	35
Pd	9.369681310	2.292349530	13.716120139 CORE	36 Pd Pd	0.0000	36
Ag	2.155458856	4.777324773	13.647874176 CORE	37 Ag Ag	0.0000	37
Ag	5.067339237	4.775046960	13.638789058 CORE	38 Ag Ag	0.0000	38
Ag	7.942134782	4.753251617	13.677645138 CORE	39 Ag Ag	0.0000	39
Ag	10.843937628	4.766845188	13.652926875 CORE	40 Ag Ag	0.0000	40
Pd	0.730169452	7.273843979	13.701406385 CORE	41 Pd Pd	0.0000	41
Ag	3.620079673	7.289896559	13.672718260 CORE	42 Ag Ag	0.0000	42
Pd	6.507896001	7.274012711	13.695188516 CORE	43 Pd Pd	0.0000	43
Ag	9.401605394	7.283281930	13.665360756 CORE	44 Ag Ag	0.0000	44
Ag	2.176129838	9.788073594	13.669476146 CORE	45 Ag Ag	0.0000	45
Ag	5.049024397	9.793721321	13.667719236 CORE	46 Ag Ag	0.0000	46
Ag	7.957069376	9.783820676	13.661534926 CORE	47 Ag Ag	0.0000	47
Ag	10.827703418	9.786161070	13.662208002 CORE	48 Ag Ag	0.0000	48
Ag	3.614100458	0.636761208	16.040547878 CORE	49 Ag Ag	0.0000	49

Ag	0.720843771	5.583465577	16.052943811	CORE	50 Ag Ag	0.0000	50
Ag	6.510382221	5.593356296	16.026837366	CORE	51 Ag Ag	0.0000	51
Pd	10.834312051	3.085635252	15.952341729	CORE	52 Pd Pd	0.0000	52
Ag	0.726382334	0.634165648	16.043838183	CORE	53 Ag Ag	0.0000	53
Pd	8.029105185	3.081189775	16.251535140	CORE	54 Pd Pd	0.0000	54
Ag	2.165650876	8.106303666	16.031015291	CORE	55 Ag Ag	0.0000	55
Ag	6.515749458	0.633189804	16.027872856	CORE	56 Ag Ag	0.0000	56
Ag	7.948250022	8.102994000	16.027737328	CORE	57 Ag Ag	0.0000	57
Pd	5.044098416	3.092636440	15.957395426	CORE	58 Pd Pd	0.0000	58
Ag	10.850755351	8.104624303	16.029434505	CORE	59 Ag Ag	0.0000	59
Ag	5.067977709	8.113959228	16.026784853	CORE	60 Ag Ag	0.0000	60
Ag	3.616960694	5.586895960	16.042948082	CORE	61 Ag Ag	0.0000	61
Ag	9.410793541	0.612388983	16.027075576	CORE	62 Ag Ag	0.0000	62
Ag	9.409231075	5.573914725	16.023915173	CORE	63 Ag Ag	0.0000	63
Pd	2.163645508	3.096242716	15.976269801	CORE	64 Pd Pd	0.0000	64
H	0.704959623	3.616795947	16.832998527	CORE	65 H H	0.0000	65
H	7.692352334	3.945686251	18.701593878	CORE	66 H H	0.0000	66
H	9.496696237	2.837761117	20.044721126	CORE	67 H H	0.0000	67
H	10.225119889	3.722537929	18.689592794	CORE	68 H H	0.0000	68
H	3.614412246	3.559416581	16.827662159	CORE	69 H H	0.0000	69
H	6.471867012	3.635941633	16.793082074	CORE	70 H H	0.0000	70
C	9.569354095	2.876491640	18.939370845	CORE	71 C C	0.0000	71
C	8.178779503	3.022272036	18.364857365	CORE	72 C C	0.0000	72
H	10.074533051	1.954874251	18.616128551	CORE	73 H H	0.0000	73
H	7.529013528	2.171954943	18.612794965	CORE	74 H H	0.0000	74
end							
end							

TS4. The energy from VASP with high accuracy setups is -251.907295 eV.

PBC	11.56260000	10.01350000	25.00000000	90.00000000	90.00000000	90.00000000
Pd	0.722663130	0.625844629	8.959688149	CORE	1 Pd Pd	0.0000 1
Ag	3.613315652	0.625844629	8.959688149	CORE	2 Ag Ag	0.0000 2
Pd	6.503968173	0.625844629	8.959688149	CORE	3 Pd Pd	0.0000 3
Ag	9.394620695	0.625844629	8.959688149	CORE	4 Ag Ag	0.0000 4
Ag	2.167989391	3.129223146	8.959688149	CORE	5 Ag Ag	0.0000 5
Ag	5.058641913	3.129223146	8.959688149	CORE	6 Ag Ag	0.0000 6
Ag	7.949294434	3.129223146	8.959688149	CORE	7 Ag Ag	0.0000 7
Ag	10.839946956	3.129223146	8.959688149	CORE	8 Ag Ag	0.0000 8
Ag	0.722663130	5.632601664	8.959688149	CORE	9 Ag Ag	0.0000 9
Pd	3.613315652	5.632601664	8.959688149	CORE	10 Pd Pd	0.0000 10
Ag	6.503968173	5.632601664	8.959688149	CORE	11 Ag Ag	0.0000 11
Pd	9.394620695	5.632601664	8.959688149	CORE	12 Pd Pd	0.0000 12
Ag	2.167989391	8.135980181	8.959688149	CORE	13 Ag Ag	0.0000 13
Ag	5.058641913	8.135980181	8.959688149	CORE	14 Ag Ag	0.0000 14

Ag	7.949294434	8.135980181	8.959688149 CORE	15 Ag Ag	0.0000	15
Ag	10.839946956	8.135980181	8.959688149 CORE	16 Ag Ag	0.0000	16
Ag	2.167989391	1.460304135	11.319896050 CORE	17 Ag Ag	0.0000	17
Ag	5.058641913	1.460304135	11.319896050 CORE	18 Ag Ag	0.0000	18
Ag	7.949294434	1.460304135	11.319896050 CORE	19 Ag Ag	0.0000	19
Ag	10.839946956	1.460304135	11.319896050 CORE	20 Ag Ag	0.0000	20
Pd	0.722663130	3.963682652	11.319896050 CORE	21 Pd Pd	0.0000	21
Ag	3.613315652	3.963682652	11.319896050 CORE	22 Ag Ag	0.0000	22
Pd	6.503968173	3.963682652	11.319896050 CORE	23 Pd Pd	0.0000	23
Ag	9.394620695	3.963682652	11.319896050 CORE	24 Ag Ag	0.0000	24
Ag	2.167989391	6.467061169	11.319896050 CORE	25 Ag Ag	0.0000	25
Ag	5.058641913	6.467061169	11.319896050 CORE	26 Ag Ag	0.0000	26
Ag	7.949294434	6.467061169	11.319896050 CORE	27 Ag Ag	0.0000	27
Ag	10.839946956	6.467061169	11.319896050 CORE	28 Ag Ag	0.0000	28
Ag	0.722663130	8.970439686	11.319896050 CORE	29 Ag Ag	0.0000	29
Pd	3.613315652	8.970439686	11.319896050 CORE	30 Pd Pd	0.0000	30
Ag	6.503968173	8.970439686	11.319896050 CORE	31 Ag Ag	0.0000	31
Pd	9.394620695	8.970439686	11.319896050 CORE	32 Pd Pd	0.0000	32
Ag	0.736816279	2.301998701	13.661094278 CORE	33 Ag Ag	0.0000	33
Pd	3.641393159	2.306338511	13.690203240 CORE	34 Pd Pd	0.0000	34
Ag	6.526840816	2.310058961	13.681800563 CORE	35 Ag Ag	0.0000	35
Pd	9.362489117	2.314764437	13.742755444 CORE	36 Pd Pd	0.0000	36
Ag	2.164301417	4.786735662	13.654182945 CORE	37 Ag Ag	0.0000	37
Ag	5.077071727	4.784479988	13.658524460 CORE	38 Ag Ag	0.0000	38
Ag	7.949105453	4.761288757	13.690596211 CORE	39 Ag Ag	0.0000	39
Ag	10.853470248	4.780251232	13.654015407 CORE	40 Ag Ag	0.0000	40
Pd	0.739552196	7.285434904	13.705945401 CORE	41 Pd Pd	0.0000	41
Ag	3.622648513	7.298404816	13.677589092 CORE	42 Ag Ag	0.0000	42
Pd	6.516611611	7.286250776	13.692505985 CORE	43 Pd Pd	0.0000	43
Ag	9.410215365	7.298593617	13.667715722 CORE	44 Ag Ag	0.0000	44
Ag	2.186659563	9.804247860	13.675815502 CORE	45 Ag Ag	0.0000	45
Ag	5.053627410	9.799857707	13.667148470 CORE	46 Ag Ag	0.0000	46
Ag	7.970850951	9.795583258	13.660743588 CORE	47 Ag Ag	0.0000	47
Ag	10.839882209	9.806020324	13.664545801 CORE	48 Ag Ag	0.0000	48
Ag	3.637985326	0.667220290	16.045834159 CORE	49 Ag Ag	0.0000	49
Ag	0.737202766	5.597349859	16.055825881 CORE	50 Ag Ag	0.0000	50
Ag	6.527451467	5.624489131	16.029237488 CORE	51 Ag Ag	0.0000	51
Pd	10.858424620	3.106672907	15.949301339 CORE	52 Pd Pd	0.0000	52
Ag	0.741533942	0.659273229	16.058309119 CORE	53 Ag Ag	0.0000	53
Pd	7.961979864	3.085289935	16.199765353 CORE	54 Pd Pd	0.0000	54
Ag	2.181443692	8.131276508	16.035035449 CORE	55 Ag Ag	0.0000	55
Ag	6.524121617	0.621006217	16.017473014 CORE	56 Ag Ag	0.0000	56
Ag	7.968926226	8.120275822	16.031857455 CORE	57 Ag Ag	0.0000	57
Pd	5.105517156	3.128600444	16.021688655 CORE	58 Pd Pd	0.0000	58

Ag	10.870096729	8.127853026	16.033688729	CORE	59 Ag Ag	0.0000	59
Ag	5.077558878	8.125252330	16.031256498	CORE	60 Ag Ag	0.0000	60
Ag	3.635036324	5.601510203	16.066786127	CORE	61 Ag Ag	0.0000	61
Ag	9.424512492	0.634205908	16.034476399	CORE	62 Ag Ag	0.0000	62
Ag	9.424021952	5.585575068	16.020684820	CORE	63 Ag Ag	0.0000	63
Pd	2.197288214	3.120439763	16.001503622	CORE	64 Pd Pd	0.0000	64
H	0.713208034	3.558444017	16.866232631	CORE	65 H H	0.0000	65
H	6.914302652	3.774831274	18.910133736	CORE	66 H H	0.0000	66
H	8.972509310	3.053580509	20.063597135	CORE	67 H H	0.0000	67
H	9.422818508	4.164199776	18.754603633	CORE	68 H H	0.0000	68
H	3.655286173	3.553985482	16.862312438	CORE	69 H H	0.0000	69
H	6.630792671	3.431663191	17.149809912	CORE	70 H H	0.0000	70
C	8.990836309	3.176708198	18.963187587	CORE	71 C C	0.0000	71
C	7.571542034	3.031648807	18.439500208	CORE	72 C C	0.0000	72
H	9.677139831	2.418518733	18.557478733	CORE	73 H H	0.0000	73
H	7.145504711	2.040122400	18.634386937	CORE	74 H H	0.0000	74
end							
end							

C₂H₆*. The energy from VASP with high accuracy setups is -252.918720 eV.

PBC	11.56260000	10.01350000	25.00000000	90.00000000	90.00000000	90.00000000	
Pd	0.722663130	0.625844629	8.959688149	CORE	1 Pd Pd	0.0000	1
Ag	3.613315652	0.625844629	8.959688149	CORE	2 Ag Ag	0.0000	2
Pd	6.503968173	0.625844629	8.959688149	CORE	3 Pd Pd	0.0000	3
Ag	9.394620695	0.625844629	8.959688149	CORE	4 Ag Ag	0.0000	4
Ag	2.167989391	3.129223146	8.959688149	CORE	5 Ag Ag	0.0000	5
Ag	5.058641913	3.129223146	8.959688149	CORE	6 Ag Ag	0.0000	6
Ag	7.949294434	3.129223146	8.959688149	CORE	7 Ag Ag	0.0000	7
Ag	10.839946956	3.129223146	8.959688149	CORE	8 Ag Ag	0.0000	8
Ag	0.722663130	5.632601664	8.959688149	CORE	9 Ag Ag	0.0000	9
Pd	3.613315652	5.632601664	8.959688149	CORE	10 Pd Pd	0.0000	10
Ag	6.503968173	5.632601664	8.959688149	CORE	11 Ag Ag	0.0000	11
Pd	9.394620695	5.632601664	8.959688149	CORE	12 Pd Pd	0.0000	12
Ag	2.167989391	8.135980181	8.959688149	CORE	13 Ag Ag	0.0000	13
Ag	5.058641913	8.135980181	8.959688149	CORE	14 Ag Ag	0.0000	14
Ag	7.949294434	8.135980181	8.959688149	CORE	15 Ag Ag	0.0000	15
Ag	10.839946956	8.135980181	8.959688149	CORE	16 Ag Ag	0.0000	16
Ag	2.167989391	1.460304135	11.319896050	CORE	17 Ag Ag	0.0000	17
Ag	5.058641913	1.460304135	11.319896050	CORE	18 Ag Ag	0.0000	18
Ag	7.949294434	1.460304135	11.319896050	CORE	19 Ag Ag	0.0000	19
Ag	10.839946956	1.460304135	11.319896050	CORE	20 Ag Ag	0.0000	20
Pd	0.722663130	3.963682652	11.319896050	CORE	21 Pd Pd	0.0000	21
Ag	3.613315652	3.963682652	11.319896050	CORE	22 Ag Ag	0.0000	22

Pd	6.503968173	3.963682652	11.319896050 CORE	23 Pd Pd	0.0000	23
Ag	9.394620695	3.963682652	11.319896050 CORE	24 Ag Ag	0.0000	24
Ag	2.167989391	6.467061169	11.319896050 CORE	25 Ag Ag	0.0000	25
Ag	5.058641913	6.467061169	11.319896050 CORE	26 Ag Ag	0.0000	26
Ag	7.949294434	6.467061169	11.319896050 CORE	27 Ag Ag	0.0000	27
Ag	10.839946956	6.467061169	11.319896050 CORE	28 Ag Ag	0.0000	28
Ag	0.722663130	8.970439686	11.319896050 CORE	29 Ag Ag	0.0000	29
Pd	3.613315652	8.970439686	11.319896050 CORE	30 Pd Pd	0.0000	30
Ag	6.503968173	8.970439686	11.319896050 CORE	31 Ag Ag	0.0000	31
Pd	9.394620695	8.970439686	11.319896050 CORE	32 Pd Pd	0.0000	32
Ag	0.726532863	2.287040650	13.661434849 CORE	33 Ag Ag	0.0000	33
Pd	3.622331575	2.288470764	13.681581080 CORE	34 Pd Pd	0.0000	34
Ag	6.517069599	2.285940673	13.653290217 CORE	35 Ag Ag	0.0000	35
Pd	9.388758787	2.276711010	13.668791500 CORE	36 Pd Pd	0.0000	36
Ag	2.156776520	4.775930356	13.658880432 CORE	37 Ag Ag	0.0000	37
Ag	5.068355676	4.776831936	13.653320629 CORE	38 Ag Ag	0.0000	38
Ag	7.938147075	4.773512538	13.655779456 CORE	39 Ag Ag	0.0000	39
Ag	10.843279350	4.773630443	13.654878363 CORE	40 Ag Ag	0.0000	40
Pd	0.725054361	7.269467756	13.711787654 CORE	41 Pd Pd	0.0000	41
Ag	3.612819114	7.285677580	13.678216788 CORE	42 Ag Ag	0.0000	42
Pd	6.503862701	7.281228771	13.692404728 CORE	43 Pd Pd	0.0000	43
Ag	9.401262535	7.286962013	13.669822785 CORE	44 Ag Ag	0.0000	44
Ag	2.176496366	9.792330142	13.676472121 CORE	45 Ag Ag	0.0000	45
Ag	5.045794916	9.789259311	13.672636218 CORE	46 Ag Ag	0.0000	46
Ag	7.956727670	9.779483354	13.672635826 CORE	47 Ag Ag	0.0000	47
Ag	10.828949418	9.787414543	13.672193661 CORE	48 Ag Ag	0.0000	48
Ag	3.620972643	0.647795081	16.047724118 CORE	49 Ag Ag	0.0000	49
Ag	0.712687815	5.583078802	16.058021191 CORE	50 Ag Ag	0.0000	50
Ag	6.522454431	5.573149851	16.031346075 CORE	51 Ag Ag	0.0000	51
Pd	10.816689876	3.092438742	15.946696867 CORE	52 Pd Pd	0.0000	52
Ag	0.714455375	0.640477103	16.051799732 CORE	53 Ag Ag	0.0000	53
Pd	7.961871016	3.091131725	15.910175477 CORE	54 Pd Pd	0.0000	54
Ag	2.162292620	8.107492494	16.037637450 CORE	55 Ag Ag	0.0000	55
Ag	6.514066493	0.638051991	16.048551466 CORE	56 Ag Ag	0.0000	56
Ag	7.945592009	8.102580801	16.035185157 CORE	57 Ag Ag	0.0000	57
Pd	5.094250767	3.095825412	15.950498957 CORE	58 Pd Pd	0.0000	58
Ag	10.843673879	8.107667382	16.040481387 CORE	59 Ag Ag	0.0000	59
Ag	5.061898354	8.106416770	16.031349505 CORE	60 Ag Ag	0.0000	60
Ag	3.630347760	5.573723754	16.051432827 CORE	61 Ag Ag	0.0000	61
Ag	9.387534130	0.644726803	16.044985127 CORE	62 Ag Ag	0.0000	62
Ag	9.385238649	5.556652247	16.038244690 CORE	63 Ag Ag	0.0000	63
Pd	2.163351786	3.098405906	16.006092448 CORE	64 Pd Pd	0.0000	64
H	0.668302192	3.599764378	16.832492488 CORE	65 H H	0.0000	65
H	7.253841847	3.790497929	20.753747570 CORE	66 H H	0.0000	66

H	9.705583961	3.096829546	20.891612096	CORE	67	H	H	0.0000	67
H	9.394092911	3.969210401	19.378621320	CORE	68	H	H	0.0000	68
H	3.666484314	3.534703981	16.798320169	CORE	69	H	H	0.0000	69
H	7.090140030	2.900528617	19.228385291	CORE	70	H	H	0.0000	70
C	9.147668061	3.058480339	19.944686717	CORE	71	C	C	0.0000	71
C	7.643079334	2.936701039	20.180240404	CORE	72	C	C	0.0000	72
H	9.535341021	2.206495080	19.366403233	CORE	73	H	H	0.0000	73
H	7.395383163	2.023137923	20.740248395	CORE	74	H	H	0.0000	74
end									
end									