Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information:

Fundamental peak disappears upon binding of noble gas: a case of vibrational spectrum of PtCO in argon matrix

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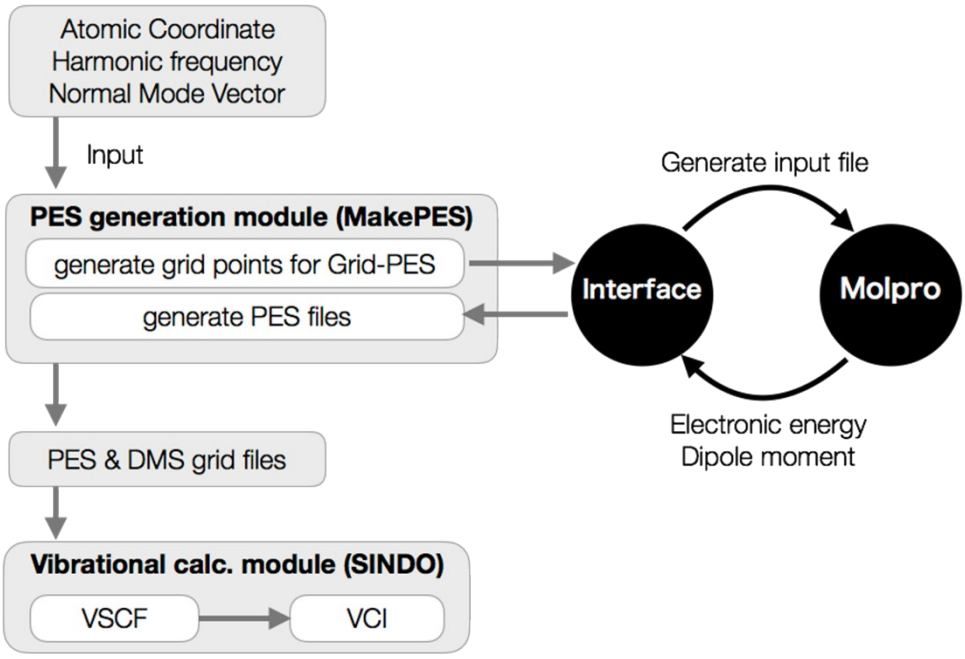

Fig. S1. The calculation flow of the SINDO program.

1. A part of the SINDO output for the VCI calculations on PtCO.

o ATOMIC MASS (amu)

12.0110 195.0800 15.9994

o REFERENCE GEOMETRY (bohr)

	X	Y	Z
Pt	0.000000	0.000000	-2.760502
C	0.000000	0.000000	0.575117
O	0.000000	0.000000	-4.940023

o NORMAL DISPLACEMENT VECTOR

0.000000 0.882429 0.000000
0.000000 -0.086530 0.000000
0.000000 -0.462420 0.000000

0.882429 0.000000 0.000000
-0.086530 0.000000 0.000000
-0.462420 0.000000 0.000000

0.000000 0.000000 0.554957
0.000000 0.000000 -0.353375
0.000000 0.000000 0.753093

0.000000 0.000000 0.798864
0.000000 0.000000 -0.026125
0.000000 0.000000 -0.600944

>> Harmonic Frequency (cm-1)

MODE :	1	2	3	4
FREQ :	416.30	416.30	595.28	2082.28

>> Energy Level (cm-1)

> STATE 00000: ZERO-POINT STATE

E(VCI) = 1747.28749

COEFF.	WEIGHT	CONFIG.
-0.999	0.998	0_0

> STATE 00001: 2_1

E(VCI) = 2158.67964
E(VCI)-E0= 411.39215

COEFF.	WEIGHT	CONFIG.	
-0.869	0.755	2_1	
-0.485	0.235	1_1	
-0.048	0.002	2_1	4_1
0.042	0.002	2_3	4_1
0.036	0.001	2_1	3_1

> STATE 00002: 1_1

E(VCI) = 2158.67964
E(VCI)-E0= 411.39215

COEFF.	WEIGHT	CONFIG.		
0.869	0.755	1_1		
-0.485	0.235	2_1		
0.048	0.002	1_1	4_1	
0.042	0.002	1_3	4_1	
-0.036	0.001	1_1	3_1	

> STATE 00003: 3_1

E(VCI) = 2332.43117
E(VCI)-E0= 585.14367

COEFF.	WEIGHT	CONFIG.		
-0.993	0.986	3_1		
-0.071	0.005	2_2		
-0.071	0.005	1_2		

> STATE 00004: 1_1 2_1

E(VCI) = 2570.03662
E(VCI)-E0= 822.74912

COEFF.	WEIGHT	CONFIG.		
-0.986	0.973	1_1	2_1	
-0.107	0.011	1_1	2_1	4_1
0.081	0.007	1_1	2_1	3_1
0.047	0.002	1_1	2_3	4_1
-0.047	0.002	1_3	2_1	4_1

> STATE 00005: 1_2

E(VCI) = 2570.09833
E(VCI)-E0= 822.81083

COEFF.	WEIGHT	CONFIG.	
0.697	0.486	1_2	
-0.697	0.486	2_2	
0.075	0.006	1_2	4_1
-0.075	0.006	2_2	4_1
-0.057	0.003	1_2	3_1
0.057	0.003	2_2	3_1
-0.049	0.002	1_4	4_1
-0.049	0.002	2_4	4_1
-0.038	0.001	1_4	
-0.038	0.001	2_4	

> STATE 00006: 2_2

E(VCI) = 2571.50449
E(VCI)-E0= 824.21700

COEFF.	WEIGHT	CONFIG.		
-0.689	0.475	2_2		
-0.689	0.475	1_2		
0.104	0.011	3_1		
0.090	0.008	4_1		
-0.074	0.005	2_2	4_1	
-0.074	0.005	1_2	4_1	
0.055	0.003	2_2	3_1	
0.055	0.003	1_2	3_1	
-0.048	0.002	2_4	4_1	
0.048	0.002	1_4	4_1	
-0.038	0.001	2_4		
0.038	0.001	1_4		
0.037	0.001	1_2	2_2	4_1

> STATE 00032: 4_1

E(VCI) = 3799.40337
E(VCI)-E0= 2052.11588

COEFF.	WEIGHT	CONFIG.	
-0.990	0.979	4_1	
-0.086	0.007	3_1	4_1
-0.066	0.004	1_2	
-0.066	0.004	2_2	
0.037	0.001	2_2	4_2
0.037	0.001	1_2	4_2

> STATE 00063: 3_1 4_1

E(VCI) = 4383.15899
E(VCI)-E0= 2635.87149

COEFF.	WEIGHT	CONFIG.		
0.975	0.951	3_1	4_1	
-0.119	0.014	3_2	4_1	
-0.082	0.007	4_1		
0.075	0.006	2_2	4_1	
0.075	0.006	1_2	4_1	
0.066	0.004	1_2	3_1	
0.066	0.004	2_2	3_1	
-0.037	0.001	1_2	3_1	4_2
-0.037	0.001	2_2	3_1	4_2
-0.033	0.001	3_3		

> STATE 00182: 4_2

E(VCI) = 5827.75838

E(VCI)-E0= 4080.47088

COEFF.	WEIGHT	CONFIG.	
-0.973	0.946	4_2	
-0.173	0.030	3_1	4_2
-0.091	0.008	1_2	4_1
-0.091	0.008	2_2	4_1
-0.042	0.002	1_2	4_3
-0.042	0.002	2_2	4_3

2. A part of the SINDO output for the VCI calculations on Ar-PtCO.

o ATOMIC MASS (amu)

39.9480 195.0800 12.0110 15.9994

o REFERENCE GEOMETRY (bohr)

	X	Y	Z
Ar	0.000000	0.000000	4.483616
Pt	0.000000	0.000000	-0.223921
C	0.000000	0.000000	-3.590682
O	0.000000	0.000000	-5.769052

o NORMAL DISPLACEMENT VECTOR

0.000000 0.557417 0.000000
0.000000 -0.485695 0.000000
0.000000 0.198059 0.000000
0.000000 0.643552 0.000000

0.557416 0.000000 0.000000
-0.485695 0.000000 0.000000
0.198059 0.000000 0.000000
0.643553 0.000000 0.000000

0.000000 0.000000 -0.920542
0.000000 0.000000 0.374623
0.000000 0.000000 0.070516
0.000000 0.000000 0.085368

0.000000 0.045936 0.000000
0.000000 -0.126265 0.000000
0.000000 0.901046 0.000000
0.000000 -0.412387 0.000000

0.045936 0.000000 0.000000
-0.126265 0.000000 0.000000
0.901046 0.000000 0.000000
-0.412387 0.000000 0.000000

0.000000 0.000000 -0.026685
0.000000 0.000000 -0.342756

```
      0.000000      0.000000      0.560108
      0.000000      0.000000      0.753714

      0.000000      0.000000     -0.004286
      0.000000      0.000000     -0.023156
      0.000000      0.000000      0.797273
      0.000000      0.000000     -0.603160
```

>> Harmonic Frequency (cm-1)

MODE :	1	2	3	4	5	6
FREQ :	69.27	69.27	171.91	460.77	460.77	585.68

MODE :	7
FREQ :	2083.48

>> Energy Level (cm-1)

> STATE 00000: ZERO-POINT STATE

E(VCI) = 1943.86367

COEFF.	WEIGHT	CONFIG.		
-0.995	0.990	0_0		
-0.041	0.002	2_2		
0.041	0.002	1_2		
0.033	0.001	2_1	5_1	7_1
0.033	0.001	1_1	4_1	7_1

> STATE 00001: 2_1

E(VCI) = 2012.28506
E(VCI)-E0= 68.42138

COEFF.	WEIGHT	CONFIG.		
0.723	0.523	2_1		
0.674	0.454	1_1		
-0.066	0.004	2_3		
-0.061	0.004	1_3		
-0.034	0.001	2_2	5_1	7_1
-0.033	0.001	1_2	2_1	

> STATE 00002: 1_1

E(VCI) = 2012.49887
E(VCI)-E0= 68.63520

COEFF.	WEIGHT	CONFIG.		
0.723	0.523	1_1		
-0.674	0.454	2_1		
-0.065	0.004	1_3		
0.061	0.004	2_3		
0.034	0.001	1_2	4_1	7_1

> STATE 00006: 3_1

E(VCI) = 2121.26965
E(VCI)-E0= 177.40598

COEFF.	WEIGHT	CONFIG.			
0.991	0.982	3_1			
0.047	0.002	2_2	3_1		
-0.047	0.002	1_2	3_1		
0.046	0.002	3_2			
-0.033	0.001	2_1	3_1	5_1	7_1
-0.033	0.001	1_1	3_1	4_1	7_1

> STATE 00036: 4_1

E(VCI) = 2397.61881
E(VCI)-E0= 453.75513

COEFF.	WEIGHT	CONFIG.			
0.893	0.797	4_1			
0.404	0.163	5_1			
-0.081	0.007	3_3			
-0.064	0.004	3_2			
0.056	0.003	1_1	2_1	5_1	
-0.049	0.002	1_1	7_1		
0.045	0.002	4_1	7_1		
0.044	0.002	2_2	4_1		
-0.041	0.002	1_2	4_1		
-0.041	0.002	1_1	4_2	7_1	
0.035	0.001	4_3	7_1		
-0.033	0.001	2_1	4_1	5_1	7_1
0.033	0.001	3_1	4_1		
-0.033	0.001	4_1	6_1		

> STATE 00037: 5_1

E(VCI) = 2397.84396
E(VCI)-E0= 453.98029

COEFF.	WEIGHT	CONFIG.			
0.899	0.808	5_1			
-0.402	0.162	4_1			
0.056	0.003	1_1	2_1	4_1	
-0.049	0.002	2_1	7_1		
0.045	0.002	5_1	7_1		
-0.045	0.002	1_2	5_1		
0.041	0.002	2_2	5_1		
-0.041	0.002	2_1	5_2	7_1	
0.036	0.001	5_3	7_1		
0.033	0.001	3_2			
-0.033	0.001	5_1	6_1		

-0.033 0.001 1_1 4_1 5_1 7_1

> STATE 00078: 6_1

E(VCI) = 2520.86454
E(VCI)-E0= 577.00087

COEFF.	WEIGHT	CONFIG.			
-0.983	0.966	6_1			
-0.060	0.004	3_1	4_1		
-0.054	0.003	1_6	2_1		
0.049	0.002	2_1	5_1		
0.049	0.002	1_1	4_1		
0.041	0.002	5_2			
0.041	0.002	4_2			
-0.038	0.001	2_2	6_1		
0.038	0.001	1_2	6_1		
0.034	0.001	3_3			
0.032	0.001	2_1	5_1	6_1	7_1
0.032	0.001	1_1	4_1	6_1	7_1

> STATE 00230: 4_2

E(VCI) = 2848.80138
E(VCI)-E0= 904.93771

COEFF.	WEIGHT	CONFIG.			
-0.767	0.588	4_2			
-0.534	0.285	5_2			
-0.211	0.044	4_1	5_1		
-0.117	0.014	1_1	2_1	4_1	5_1
-0.078	0.006	7_1			
-0.073	0.005	4_2	7_1		
0.060	0.004	1_1	4_1	7_1	
-0.058	0.003	6_1			
-0.056	0.003	3_1	4_2		
0.052	0.003	4_2	6_1		
-0.051	0.003	5_2	7_1		
-0.048	0.002	2_2	4_2		
0.044	0.002	2_1	5_1	7_1	
0.043	0.002	4_4	7_1		
0.040	0.002	1_1	4_3	7_1	
0.040	0.002	1_2	4_2		
0.038	0.001	1_2	5_2		
0.037	0.001	5_2	6_1		
0.035	0.001	4_4			
0.033	0.001	2_1	4_2	5_1	7_1
-0.032	0.001	2_2	5_2		

> STATE 00231: 4_1 5_1

E(VCI) = 2849.24913

E(VCI)-E0= 905.38546

COEFF.	WEIGHT	CONFIG.			
-0.935	0.874	4_1	5_1		
0.189	0.036	4_2			
0.100	0.010	5_2			
-0.090	0.008	4_1	5_1	7_1	
-0.083	0.007	1_1	2_1	4_2	
-0.082	0.007	1_1	2_1	5_2	
0.074	0.005	3_3	5_1		
0.073	0.005	3_2	5_1		
0.066	0.004	4_1	5_1	6_1	
0.059	0.003	1_2	4_1	5_1	
-0.059	0.003	2_2	4_1	5_1	
0.056	0.003	2_1	4_1	7_1	
0.056	0.003	1_1	5_1	7_1	
-0.049	0.002	3_1	4_1	5_1	
0.047	0.002	1_1	4_2	5_1	7_1
0.047	0.002	2_1	4_1	5_2	7_1
-0.037	0.001	4_3	5_1	7_1	
-0.037	0.001	4_1	5_3	7_1	

> STATE 00234: 5_2

E(VCI) = 2853.17042
E(VCI)-E0= 909.30675

COEFF.	WEIGHT	CONFIG.			
0.802	0.644	5_2			
-0.558	0.312	4_2			
0.076	0.006	5_2	7_1		
-0.056	0.003	5_2	6_1		
-0.056	0.003	2_1	5_1	7_1	
-0.053	0.003	4_2	7_1		
0.045	0.002	5_4	7_1		
-0.042	0.002	3_1	4_2		
-0.042	0.002	2_1	5_3	7_1	
0.038	0.001	3_1	5_2		
0.037	0.001	4_2	6_1		
-0.037	0.001	1_2	5_2		
0.037	0.001	5_4			
0.036	0.001	1_1	4_1	7_1	

> STATE 01448: 7_1

E(VCI) = 3998.83306
E(VCI)-E0= 2054.96939

COEFF.	WEIGHT	CONFIG.		
-0.981	0.962	7_1		
-0.081	0.007	6_1	7_1	
0.061	0.004	5_2		

```
 0.061   0.004          4_2
-0.057   0.003          1_1   4_1
-0.057   0.003          2_1   5_1
-0.044   0.002          1_1   4_1   7_2
-0.044   0.002          2_1   5_1   7_2
 0.043   0.002          3_4   5_3
-0.039   0.002          2_2   7_1
 0.039   0.002          1_2   7_1
```

> STATE 02199: 6_1 7_1

E(VCI) = 4574.78940
E(VCI)-E0= 2630.92572

```
COEFF.  WEIGHT     CONFIG.
 0.959  0.920      6_1  7_1
-0.112  0.012      6_2  7_1
-0.083  0.007      7_1
-0.063  0.004      1_1  4_1  7_1
-0.062  0.004      2_1  5_1  7_1
-0.061  0.004      5_2  6_1
-0.060  0.004      4_2  6_1
 0.058  0.003      3_1  4_1  7_1
 0.056  0.003      2_1  5_1  6_1
 0.055  0.003      1_1  4_1  6_1
-0.045  0.002      5_2  7_1
-0.045  0.002      4_2  7_1
 0.042  0.002      2_1  5_1  6_1  7_2
 0.041  0.002      1_1  4_1  6_1  7_2
 0.036  0.001      2_2  6_1  7_1
-0.035  0.001      1_2  6_1  7_1
```

> STATE 03969: 7_2

E(VCI) = 6030.69535
E(VCI)-E0= 4086.83168

```
COEFF.  WEIGHT     CONFIG.
-0.881  0.777      7_2
-0.152  0.023      6_1  7_2
 0.121  0.015      2_1  4_1  5_2  6_1  7_1
-0.121  0.015      2_1  4_3  6_1  7_1
-0.120  0.014      1_1  4_2  5_1  6_1  7_1
 0.113  0.013      1_1  5_3  6_1  7_1
 0.112  0.012      2_1  5_3  6_1  7_1
 0.104  0.011      1_1  4_1  5_2  6_1  7_1
 0.094  0.009      3_1  4_1  5_3  7_1
-0.092  0.008      2_1  4_2  5_1  6_1  7_1
-0.079  0.006      5_2  6_2  7_1
-0.076  0.006      5_2  7_1
-0.075  0.006      4_2  7_1
 0.071  0.005      2_1  5_1  7_1
```

0.071	0.005	1_1	4_1	7_1		
-0.063	0.004	1_1	4_3	6_1	7_1	
-0.060	0.004	3_1	4_3	5_1	7_1	
-0.057	0.003	1_1	3_3	4_2	5_1	7_1
0.057	0.003	2_1	3_3	5_3	7_1	
0.056	0.003	1_1	3_3	4_1	5_2	7_1
-0.045	0.002	1_1	4_1	7_3		
-0.045	0.002	2_1	5_1	7_3		
0.045	0.002	4_2	6_2	7_1		
0.039	0.002	2_1	3_3	4_1	5_2	7_1
0.037	0.001	2_1	3_3	4_2	5_1	7_1
-0.035	0.001	1_1	3_3	5_3	7_1	