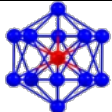
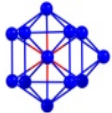
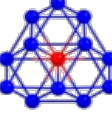
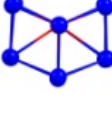
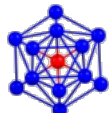
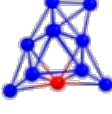
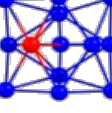

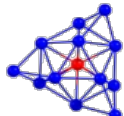
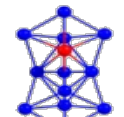
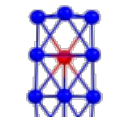
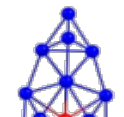
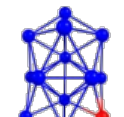
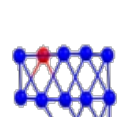
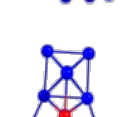
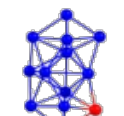
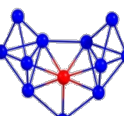


Supplementary Information

Table 1.- Representative structures characterizing the energy landscape of the PES of the $\text{Pd}_{12}\text{Pt}_1$ cluster. The Relative Abundance (RA) of the root pairs is also presented. E_{Bottom} is the Total Energy of the structures found in the search, E_{Top} indicates the energy lid value at which the transition occurs, and ΔE is the energy barrier value. All energies are eV/atom.

Type	E_{Bottom}	E_{Top}	ΔE	Structure	CNA indices	RA
Ih	-3.5385	-3.4400	0.0985		322	0.7142
					555	0.2857
Ih-Ino	-3.4309	-3.4000	0.0309		211	0.2500
					311	0.3333
					322	0.1666
					422	0.1666
					432	0.0833
BP	-3.4222	-3.3700	0.0522		211	0.1428
					311	0.7142
					421	0.1428
S1	-3.4181	-3.4000	0.0181		211	0.3157
					311	0.4210
					322	0.0526
					421	0.1052
					422	0.1052
S2	-3.3987	-3.3500	0.0487		211	0.2222
					322	0.4444
					422	0.1111
					432	0.1111
S3	-3.3976	-3.3800	0.0176		555	0.1111
					211	0.2666
					311	0.3666
					322	0.2000
S4	-3.3952	-3.3600	0.0352		422	0.1333
					432	0.0333
					211	0.2631
					322	0.3684
					432	0.2368
					555	0.1315

S5	-3.3803	-3.3600	0.0203		211	0.2857
					311	0.2380
					322	0.2380
					432	0.2380
MT-Ih ₁	-3.3786	-3.3300	0.0486		211	0.3333
					322	0.3333
					432	0.2500
					555	0.0833
S6	-3.3651	-3.3200	0.0451		211	0.3055
					322	0.3888
					432	0.2222
					555	0.0833
S7	-3.3638	-3.3400	0.0238		211	0.2222
					311	0.4444
					322	0.2222
					422	0.1111
S8	-3.3620	-3.3500	0.0120		211	0.3714
					322	0.3142
					432	0.2571
					555	0.0571
MT-Ih ₂	-3.3561	-3.3000	0.0561		211	0.2105
					322	0.4736
					432	0.1842
					555	0.1315
S9	-3.3488	-3.3100	0.0388		211	0.1428
					311	0.5714
					322	0.0714
					421	0.0714
S10	-3.3480	-3.3000	0.0480		211	0.1818
					311	0.7272
					421	0.0909
					S11	-3.3488
322	0.3714					
432	0.2285					
555	0.0571					
MT-Ih ₃	-3.3421	-3.2800	0.0621		211	0.2162
					322	0.5135
					432	0.1621
					555	0.1081
S12	-3.3365	-3.3000	0.0365		211	0.3823
					322	0.3529
					432	0.2352
					555	0.0294

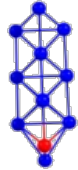
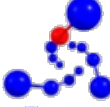


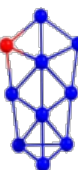
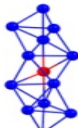
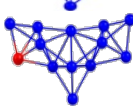
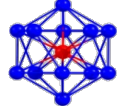
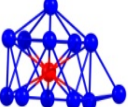
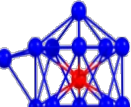

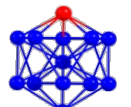
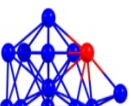
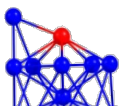

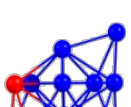

S13	-3.3113	-3.2900	0.0213		211	0.3461
					311	0.5000
					322	0.0769
					421	0.0384
					422	0.0384
HL	-3.3110	-3.2800	0.0310		211	0.4242
					322	0.3333
					432	0.2424
HR	-3.3110	-3.2800	0.0310		211	0.4242
					322	0.3333
					432	0.2424
S14	-3.3066	-3.2900	0.0166		211	0.3750
					311	0.3750
					322	0.1666
					422	0.0833
S15	-3.2989	-3.2800	0.0189		211	0.3846
					311	0.3076
					322	0.2307
					421	0.0384
					543	0.0384
S16	-3.2935	-3.2700	0.0235		211	0.4242
					322	0.3333
					432	0.2424
S17	-3.2651	-3.2400	0.0251		211	0.4545
					322	0.2727
					432	0.2727

Table 2.- Icosahedral-type structures found for Pd₁₂Pt₁ clusters.

Type	E _{Bottom}	E _{Top}	ΔE	Pd-Pd Bonds	Pt-Pd Bonds	Structure	CNA indices	RA
Ih ₁	-3.5385	-3.4400	0.0985	30	12		322	0.7142
							555	0.2857
Ih ₂	-3.4677	-3.4200	0.0477	28	11		211	0.1794
							322	0.4871
							432	0.1794
							555	0.1538
Ih ₃	-3.4661	-3.4200	0.0461	28	11		211	0.2051
							322	0.4358
							432	0.2051
							555	0.1538
Ih ₄	-3.4641	-3.4200	0.0441	28	11		211	0.2051
							322	0.4358
							432	0.2051
							555	0.1538
Ih ₅	-3.4158	-3.3800	0.0358	36	6		322	0.7142
							555	0.2857
Ih ₆	-3.3905	-3.3400	0.0505	32	7		211	0.1794
							322	0.4871
							432	0.1794
							555	0.1538
Ih ₇	-3.3797	-3.3300	0.0497	32	7		211	0.2051
							322	0.4358
							432	0.2051
							555	0.1538
Ih ₈	-3.3712	-3.3300	0.0412	33	6		211	0.2051
							322	0.4358
							432	0.2051
							555	0.1538
Ih ₉	-3.3648	-3.3200	0.0448	33	6		211	0.2051
							322	0.4358
							432	0.2051
							555	0.1538
Ih ₁₀	-3.3618	-3.3200	0.0418	33	6		211	0.2051
							322	0.4358
							432	0.2051
							555	0.1538

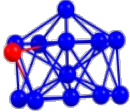
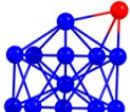









Ih ₁₁	-3.3309	-3.3000	0.0309	36	3		211	0.2051
							322	0.4358
							432	0.2051
							555	0.1538
Ih ₁₂	-3.3234	-3.2800	0.0434	36	3		211	0.2051
							322	0.4358
							432	0.2051
							555	0.1538

Table 3.- Helical (“Bernal spiral”) structures found for Pd₁₂Pt₁ clusters. The helical shape is obtained by face-sharing tetrahedra growing in a preferential direction (anisotropic growth). Helical structures are characterized by the CNA indices 211, 322 and 432, with relative abundances 0.4242, 0.3333 and 0.2424, respectively.

Type	E _{Bottom}	E _{Top}	ΔE	Pd-Pd Bonds	Pt-Pd Bonds	Structure
HR ₁	-3.3110	-3.2800	0.0310	27	6	
HL ₁	-3.3110	-3.2800	0.0310	27	6	
HR ₂	-3.3026	-3.2700	0.0326	27	6	
HL ₂	-3.3026	-3.2700	0.0326	27	6	
HR ₃	-3.2982	-3.2800	0.0182	27	6	
HL ₃	-3.2982	-3.2800	0.0182	27	6	
HR ₄	-3.2965	-3.2700	0.0265	28	5	
HL ₄	-3.2965	-3.2600	0.0365	28	5	
HR ₅	-3.2960	-3.2800	0.0160	27	6	

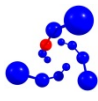


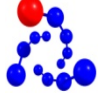
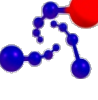
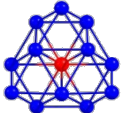

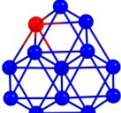
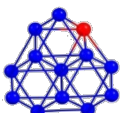
HL ₅	-3.2960	-3.2600	0.0360	27	6	
HR ₆	-3.2801	-3.2400	0.0401	29	4	
HL ₆	-3.2801	-3.2300	0.0501	29	4	
HR ₇	-3.2606	-3.2200	0.0406	30	3	
HL ₇	-3.2606	-3.2200	0.0406	30	3	

Table 4.- Homotops found for the biplanar topology of the Pd₁₂Pt₁ cluster. Biplanar structures are characterized by the CNA indices 211, 311 and 421, with relative abundances 0.1428, 0.7142 and 0.1428, respectively. Homotop BP₃ is chiral, existing as the enantiomers BP₃' and BP₃''.

Type	E _{Bottom}	E _{Top}	ΔE	Pd-Pd Bonds	Pt-Pd Bonds	Structure
BP ₁	-3.4222	-3.3700	0.0522	27	9	
BP ₂	-3.3963	-3.3600	0.0363	27	7	
BP ₃ '	-3.3661	-3.3200	0.0461	31	5	
BP ₃ ''	-3.3661	-3.3000	0.0661	31	5	
BP ₄	-3.3522	-3.2800	0.0722	32	4	