

Supplementary Information for

## Enhanced Oxygen Reduction Activity of Size-Selected Platinum Subnanocluster Catalysts: Pt<sub>n</sub> (n = 3 – 9)

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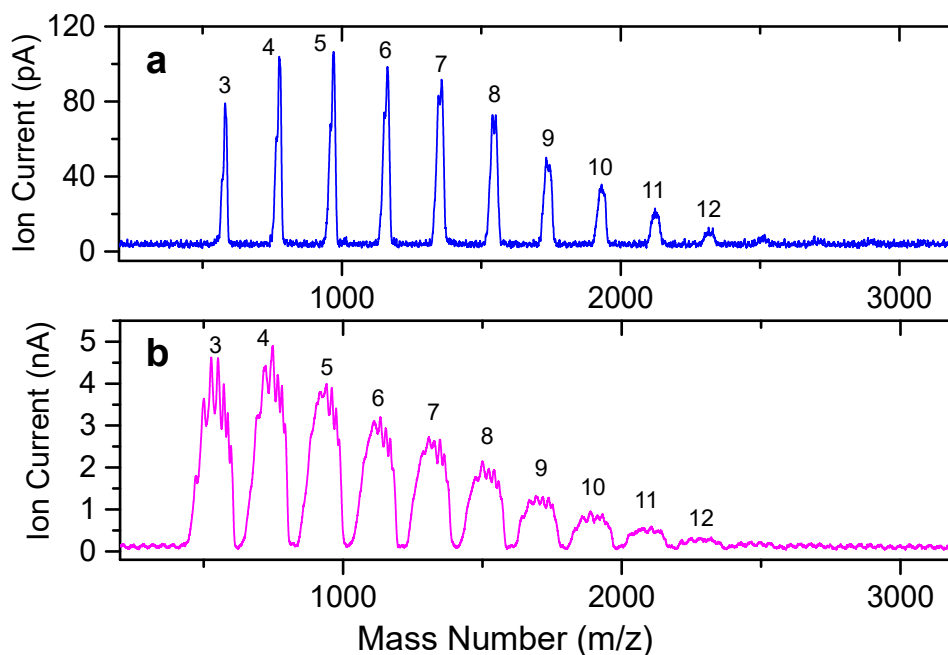
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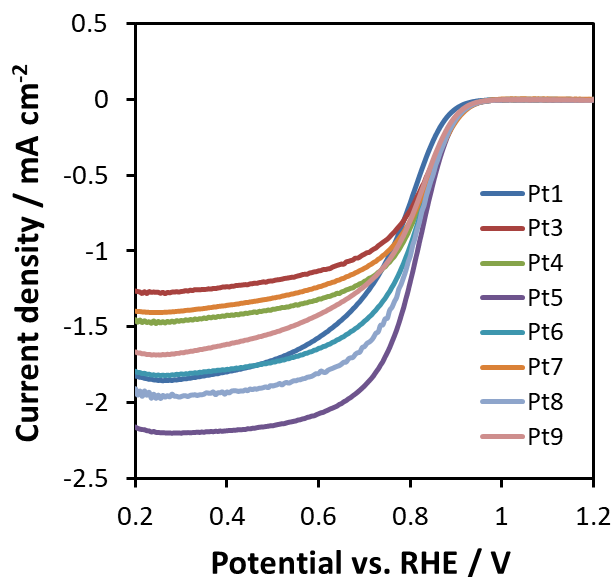
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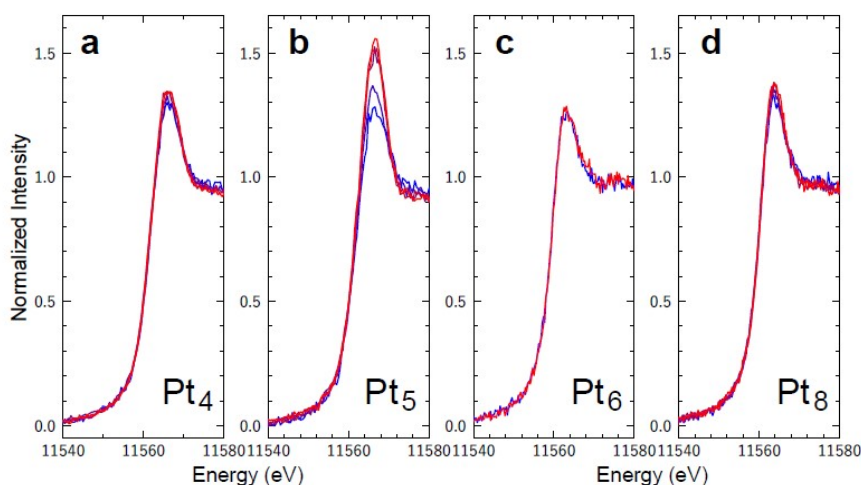
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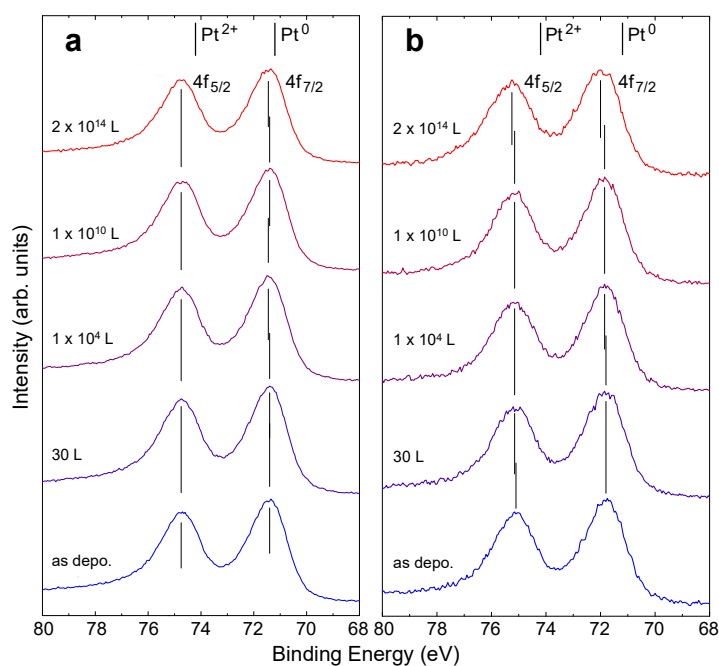
**Figure S1.** Mass spectra for anionic  $\text{Pt}_n$  NCs ( $n = 1 - 15$ ); (a) high mass resolution of  $m/\Delta m \sim 300$  for checking purity of  $\text{Pt}_n$  NCs and (b) low mass resolution of  $m/\Delta m \sim 15$  for size-selective deposition with high transmission efficiency of the Q-pole mass filter. After checking no contaminations, the mass resolution is lowered to the extent that adjacently different sizes of sub-NCs are not mixed with the targeted sub-NCs.



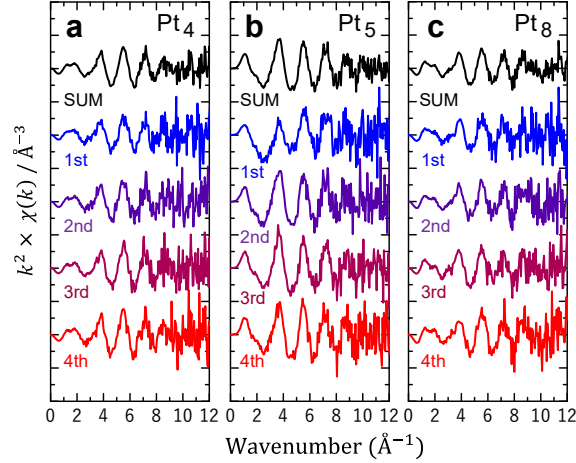
**Figure S2.** Hydrodynamic voltammograms under oxygen for Pt sub-NCs; Pt atom and  $\text{Pt}_n$  ( $n = 3 - 9$ ), wherein concentration of  $\text{HClO}_4$ , sweep rate, and rotation speed are 0.1 M,  $50 \text{ mV} \cdot \text{s}^{-1}$ , and 300 rpm, respectively.



**Figure S3.** Time evolutions of white lines for Pt  $L_3$  edge of  $Pt_n$  sub-NCs at  $n = 4, 5, 6,$  and  $8$  on a glassy carbon plate with the deposition amount of 0.5 monolayer equivalent. With measurement time, the intensity increases as shown from blue trace (initial) to red trace (final), while only the intensity at  $n = 5$  increases approximately by 20-25%. Details for  $Pt_6$  has been reported elsewhere [1].



**Figure S4.** X-ray photoelectron spectra for Pt 4f of (a)  $Pt_5$  and (b)  $Pt_6$  sub-NCs deposited on a glassy carbon plate against various  $O_2$  exposures, where the spectra have been offset vertically for clarity of presentation. The NC deposition amount is 0.5 monolayer equivalent, and the exposure amount of  $O_2$  is defined by the Langmuir (L) (Langmuir =  $1 \times 10^{-6}$  Torr-s); 0 –  $2 \times 10^{14}$  L). The energy positions for  $Pt^{2+}$  and  $Pt^0$  of Pt  $4f_{7/2}$  core level [2,3] are shown at top in the figure. No apparent oxidation is observed for either  $Pt_5$  or  $Pt_6$  NCs even under  $1.0 \times 10^5$  Pa (1 atm)  $O_2$  in 3 days ( $2 \times 10^{14}$  L).



**Figure S5.** Time evolution of the EXAFS oscillations in  $\chi(k)$  spectra; every scan from 1<sup>st</sup> (blue) to 4<sup>th</sup> (red) spectra together with their summation (black; top) for (a) Pt<sub>4</sub>, (b) Pt<sub>5</sub>, and (c) Pt<sub>8</sub> NCs deposited on a glassy carbon (GC) plate [4]. Although the intensity of white line at  $n = 5$  increases approximately by 20-25 % (Fig. S3), identical oscillations appear at each scan.

**Note S1. Computational model.**

The associative mechanism of ORR in the acid medium [ $\text{O}_2(\text{g}) + 4\text{H}^+ + 4\text{e}^- \rightarrow 2\text{H}_2\text{O}$ ] was considered in the present calculations. The four elementary steps involved in ORR are given as

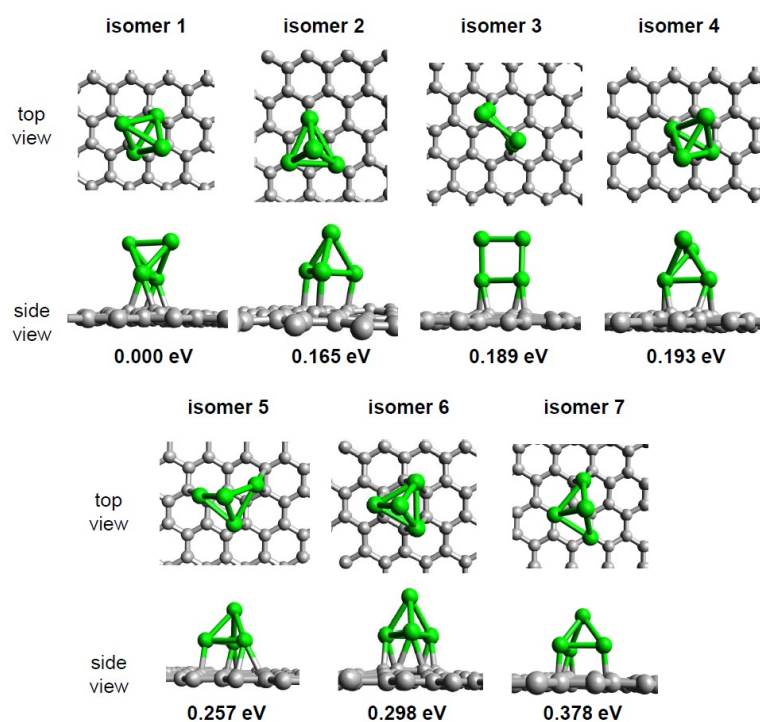


Based on the computational hydrogen electrode model introduced by Nørskov *et al.* [5], Gibbs free energy diagrams were constructed at 0 V (without any applied potential) and the ORR equilibrium potential of 1.23 V. The free energy change ( $\Delta G$ ) was determined as

$$\Delta G = \Delta E + \Delta ZPE - T\Delta S + \Delta G_U + \Delta G_{\text{pH}} \quad (5)$$

where  $\Delta E$  is the reaction energy obtained from the DFT calculations,  $\Delta ZPE$  is the change of zero-point energy,  $T$  is the temperature (298.15 K), and  $\Delta S$  is the change of entropy.  $\Delta G_U$  and  $\Delta G_{\text{pH}}$  are the contributions to the free energy due to the changes of the electrode potential ( $U$ ) and the pH value, respectively.  $\Delta G_U = -neU$ , in which  $n$  is the number of transferred electrons and  $U$  is the applied

potential.  $\Delta G_{\text{pH}} = k_{\text{B}}T \times \ln 10 \times \text{pH}$ , where  $k_{\text{B}}$  is the Boltzmann constant and the pH is 0 in the acid medium. The zero-point energies and entropies of the intermediates were obtained by calculating the vibrational frequencies. The overpotential is defined by  $\eta = U_0 - U_{\text{L}}$ , where  $U_0$  is the equilibrium potential, and  $U_{\text{L}}$  is the limiting potential defined as the maximum free energy change ( $\Delta G_{\text{max}}$ ) among all elementary steps using the relation  $U_{\text{L}} = -\Delta G_{\text{max}}/e$ .

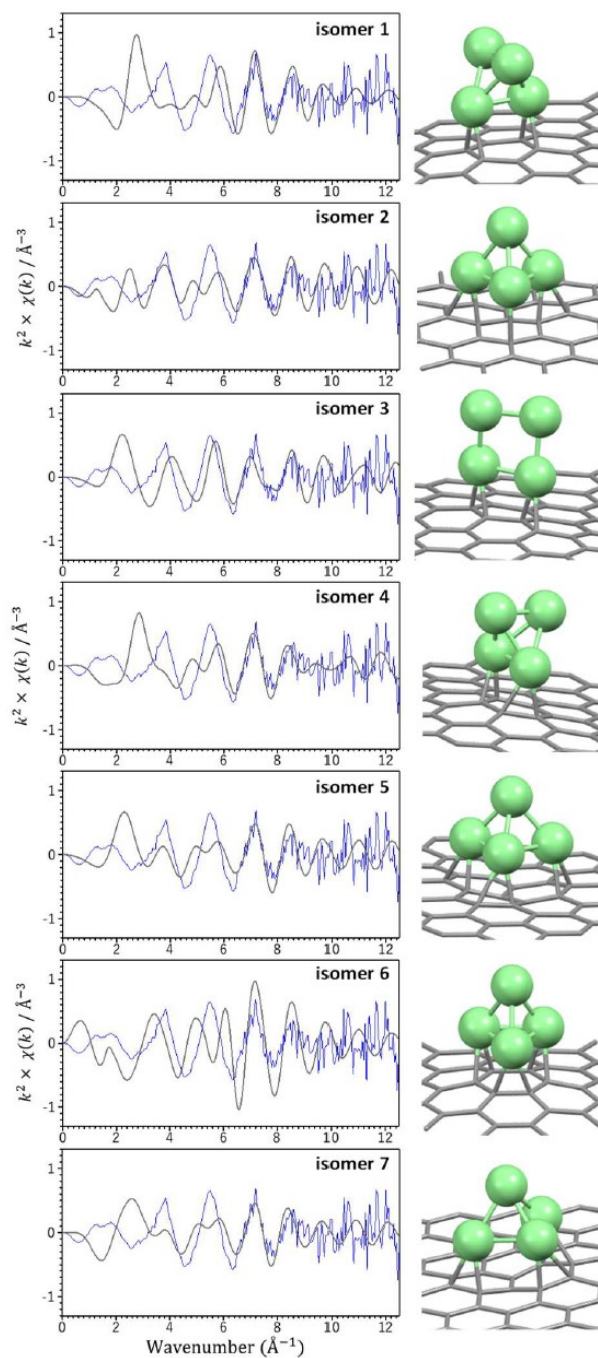


**Figure S6.** The lowest and higher energy isomers of Pt<sub>4</sub> supported on graphene (Pt<sub>4</sub>/Gr). Relative energies in eV are also indicated relative to the most stable isomer **1** (Pt<sub>4</sub>-1). The edge-standing tetrahedral structures given by isomer **4** (Pt<sub>4</sub>-4) including isomer **1** represent the most probable structures examined by FEFF simulations of  $\chi(k)$  spectra obtained by EXAFS shown in Fig. S7.

**Table S1. Relative energies, average Pt-C, and Pt-Pt distances for isomers of Pt<sub>4</sub>, Pt<sub>5</sub>, Pt<sub>6</sub>, and Pt<sub>8</sub> with PBE-D3.**

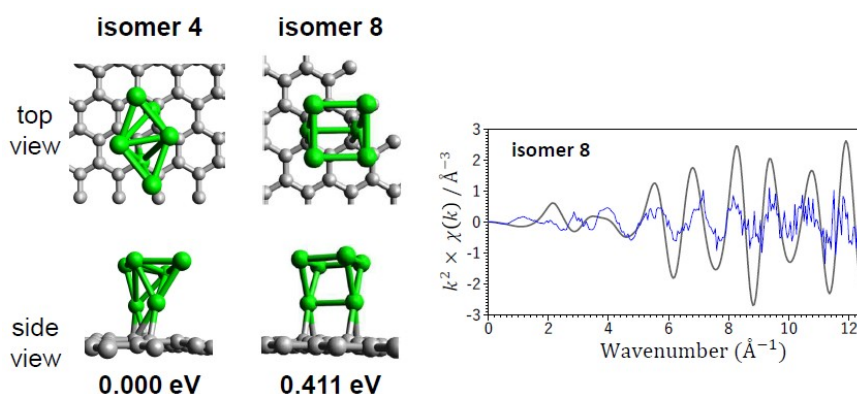
<b>Pt<sub>4</sub>/Gr</b>	Relative energy (eV)	d <sub>Pt-C</sub> (Å)	d <sub>Pt-Pt</sub> (Å)
<b>Pt<sub>4</sub> (1)</b>	<b>0.000</b>	<b>2.222</b>	<b>2.588</b>
Pt <sub>4</sub> (2)	0.165	2.204	2.618
Pt <sub>4</sub> (3)	0.189	2.215	2.479
Pt <sub>4</sub> (4)	0.193	2.224	2.594
Pt <sub>4</sub> (5)	0.257	2.301	2.580
Pt <sub>4</sub> (6)	0.298	2.263	2.640
Pt <sub>4</sub> (7)	0.378	2.250	2.579
<b>Pt<sub>5</sub>/Gr</b>	Relative energy (eV)	d <sub>Pt-C</sub> (Å)	d <sub>Pt-Pt</sub> (Å)
<b>Pt<sub>5</sub> (1)</b>	<b>0.000</b>	<b>2.193</b>	<b>2.475</b>
Pt <sub>5</sub> (2)	0.026	2.203	2.489
Pt <sub>5</sub> (3)	0.121	2.207	2.504
Pt <sub>5</sub> (4)	0.230	2.229	2.550
Pt <sub>5</sub> (5)	0.233	2.288	2.492
Pt <sub>5</sub> (6)	0.927	2.276	2.645
Pt <sub>5</sub> (7)	1.066	2.250	2.513
Pt <sub>5</sub> (8)	1.096	2.205	2.561
Pt <sub>5</sub> (9)	1.275	2.207	2.479
<b>Pt<sub>6</sub>/Gr<sup>a)</sup></b>	Relative energy (eV)	d <sub>Pt-C</sub> (Å)	d <sub>Pt-Pt</sub> (Å)
<b>Pt<sub>6</sub> (1)</b>	0.017	2.220	2.498
Pt <sub>6</sub> (3)	0.041	2.224	2.499
<b>Pt<sub>6</sub>(4)</b>	<b>0.000</b>	<b>2.251</b>	<b>2.649</b>
Pt <sub>6</sub> (5)	0.104	2.299	2.553
Pt <sub>6</sub> (6)	0.657	2.259	2.545
Pt <sub>6</sub> (7)	0.418	3.261	2.552
Pt <sub>6</sub> (8) <sup>a)</sup>	0.411	2.220	2.547
<b>Pt<sub>8</sub>/Gr</b>	Relative energy (eV)	d <sub>Pt-C</sub> (Å)	d <sub>Pt-Pt</sub> (Å)
<b>Pt<sub>8</sub>(1)</b>	<b>0.000</b>	<b>2.261</b>	<b>2.622</b>
Pt <sub>8</sub> (2)	0.147	2.258	2.603
Pt <sub>8</sub> (3)	0.242	2.267	2.652
Pt <sub>8</sub> (4)	0.519	2.224	2.669
Pt <sub>8</sub> (5)	0.520	2.223	2.692
Pt <sub>8</sub> (6)	0.644	2.233	2.628
Pt <sub>8</sub> (7)	1.112	2.275	2.576
Pt <sub>8</sub> (8)	1.152	2.279	2.596

a) With PBE-D3, **Pt<sub>6</sub>-4** is the most stable isomer which was identified as the most probable structure [1] and also a new isomer 8 (**Pt<sub>6</sub>-8**) is obtained, which is 0.411 eV above **Pt<sub>6</sub>-4** (see also Figure S8).

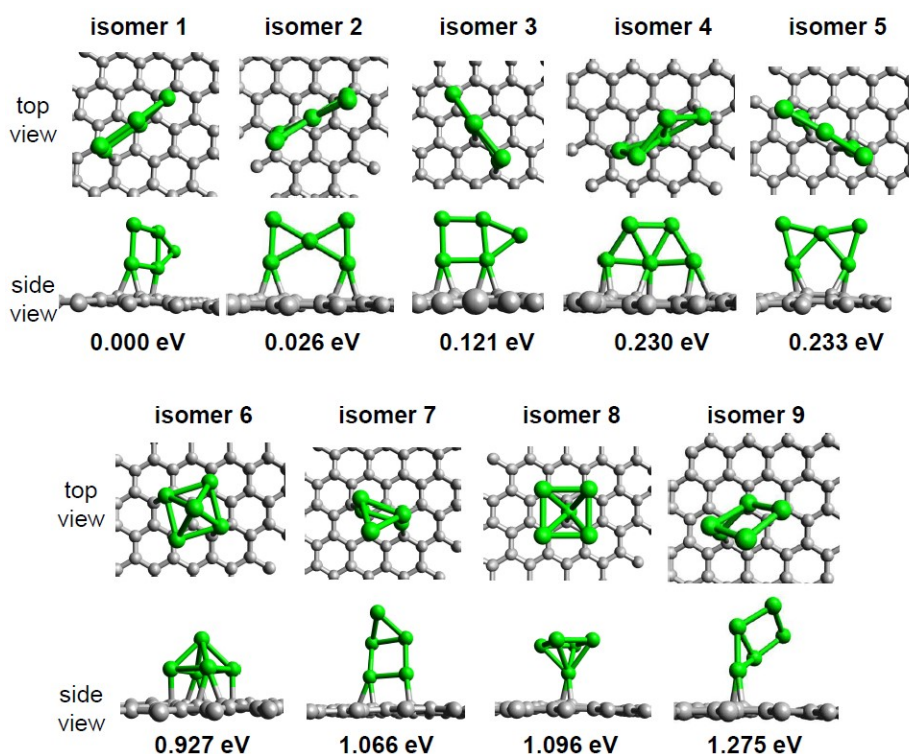


**Figure S7.** FEFF simulations of  $\chi(k)$  spectra for all isomers of Pt<sub>4</sub>/Gr shown in Fig. S6 including Figure 3 of the main text. Blue and black curves represent experimental and simulated  $\chi(k)$  spectra, respectively. Pt<sub>4</sub>/Gr coordinates were used without scaling of the geometry. The most probable structure for Pt<sub>4</sub>/GC seems to be an edge-standing tetrahedron isomer, which is given in isomer 4 (Pt<sub>4</sub>-4) (Figs. 3b), although the isomer 1 (Pt<sub>4</sub>-1) similarly has a tetrahedral structure.



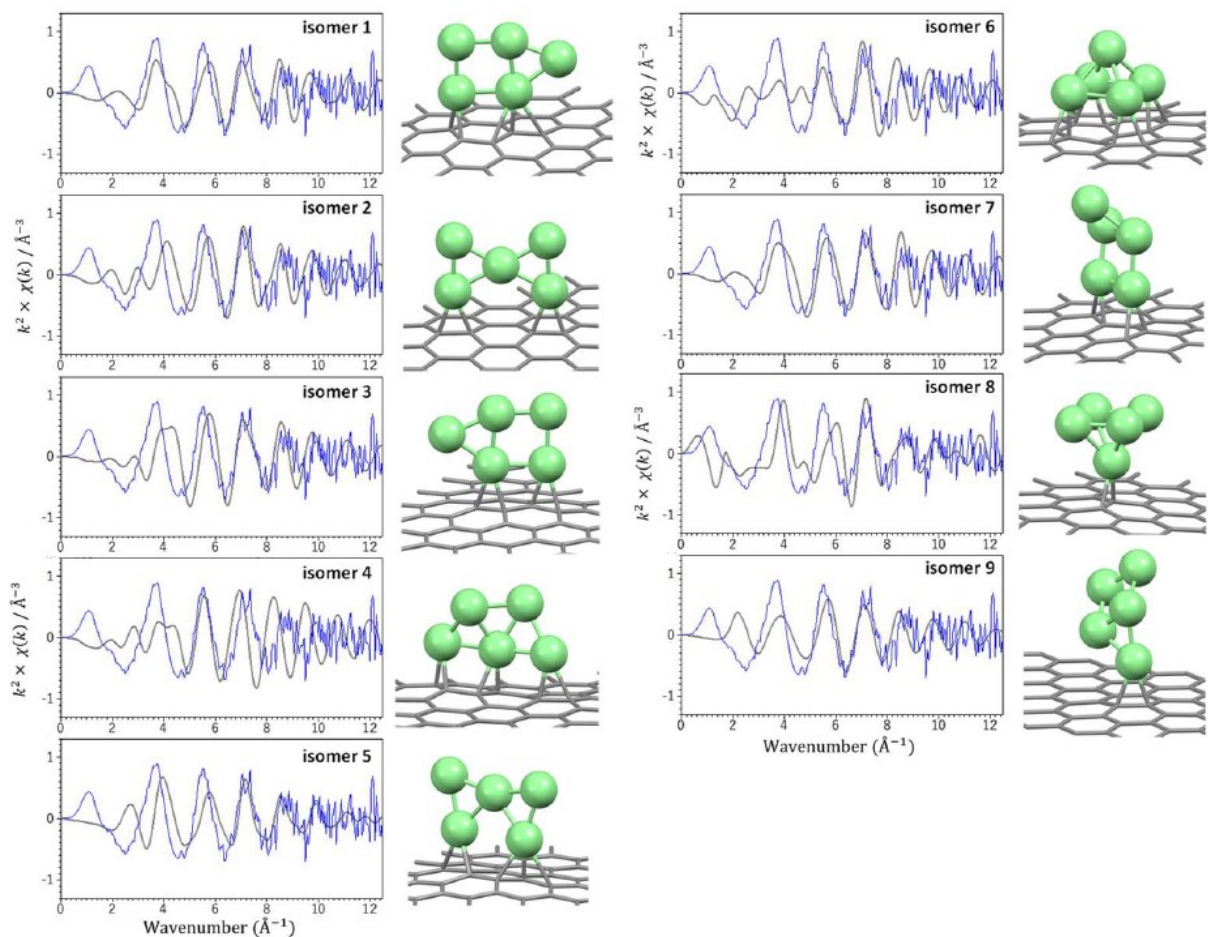


**Figure S8.** Two isomers among several  $\text{Pt}_6$  supported on graphene ( $\text{Pt}_6/\text{Gr}$ ) [1] and FEFF simulation of  $\chi(k)$  spectrum for a new isomer **8** ( $\text{Pt}_6\text{-8}$ ). The numbers below correspond to the relative energy to the most stable isomer **4** ( $\text{Pt}_6\text{-4}$ ) in eV. The  $\text{Pt}_6\text{-4}$  represents the most probable structure examined by FEFF simulations of  $\chi(k)$  spectra obtained by EXAFS reported previously [1]. With PBE-D3, the isomer **8** ( $\text{Pt}_6\text{-8}$ ), edge-standing triangle prism, is obtained, although the matching between  $\chi_{\text{obs}}(k)$  and  $\chi_{\text{sim}}(k)$  spectra is not good.

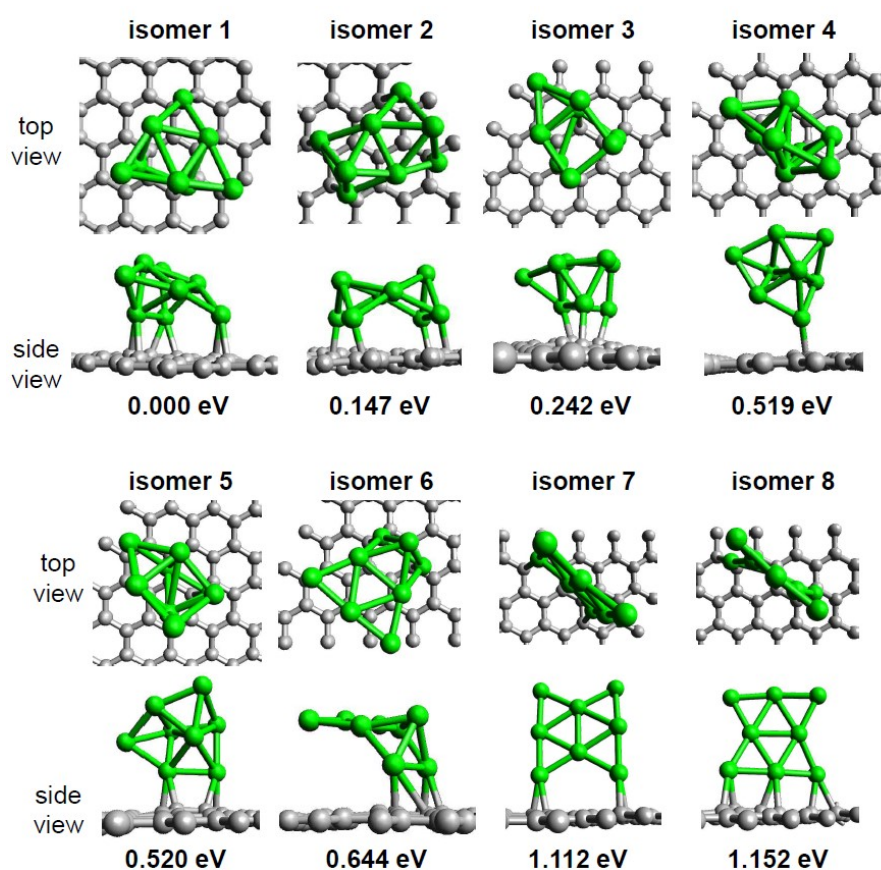


**Figure S9.** The lowest and higher energy isomers of  $\text{Pt}_5$  supported on graphene ( $\text{Pt}_5/\text{Gr}$ ). The number below correspond to the relative total energy of the clusters. Relative energies in eV are also indicated relative to the most stable isomer **1** ( $\text{Pt}_5\text{-1}$ ). Isomer **5** ( $\text{Pt}_5\text{-5}$ ), standing atom-sharing triangles, represents the most probable structure examined by FEFF simulations of  $\chi(k)$  spectra obtained by EXAFS shown in Fig. S10.

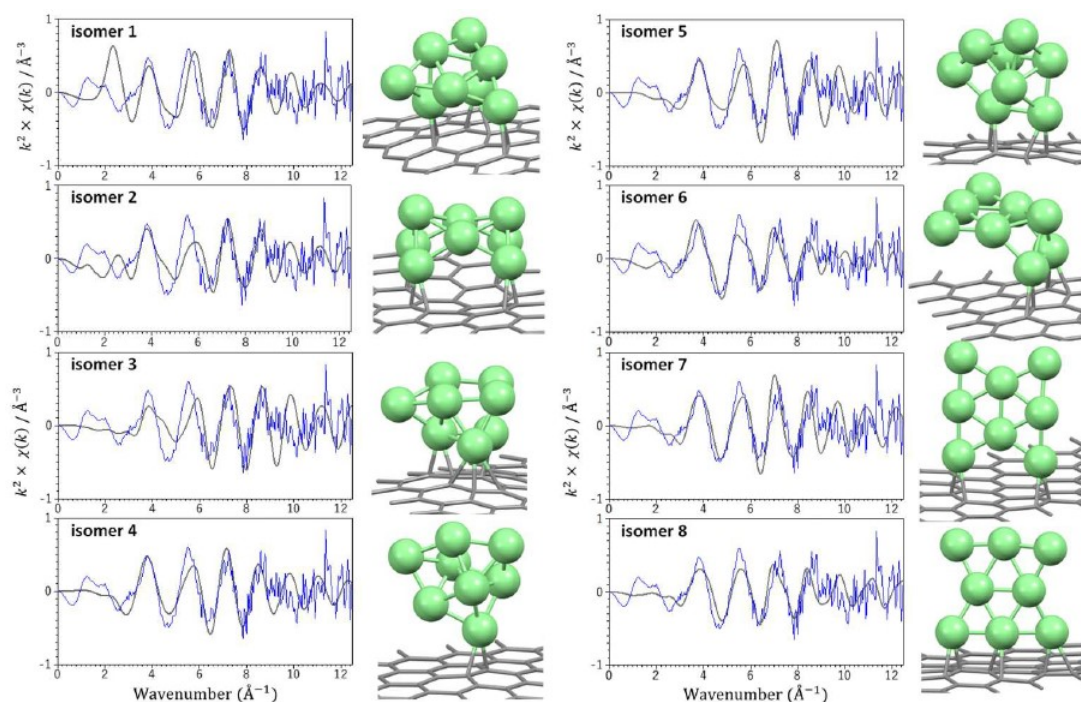




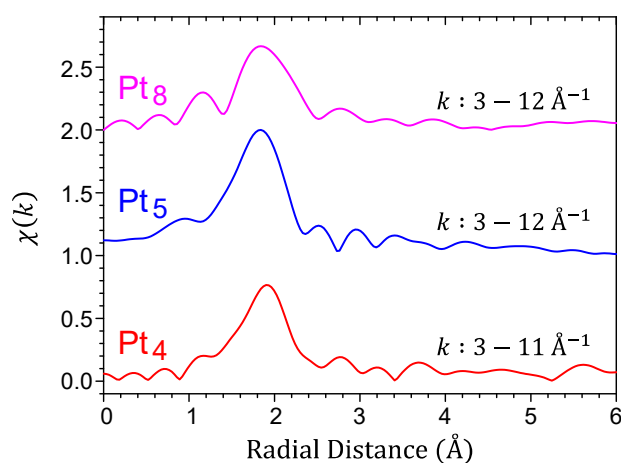
**Figure S10.** FEFF simulations of  $\chi(k)$  spectra for all isomers of  $\text{Pt}_5/\text{Gr}$  shown in Fig. S9 including Figure 4 of the main text. Blue and black curves represent experimental and simulated  $\chi(k)$  spectra, respectively.  $\text{Pt}_5/\text{Gr}$  coordinates were used without scaling of the geometry. The most probable structure for  $\text{Pt}_5/\text{GC}$  seems to be standing and atom-sharing triangles, isomer **5** ( $\text{Pt}_5\text{-5}$ ), or vertex-standing inverted pyramid, isomer **8** ( $\text{Pt}_5\text{-8}$ ), in Figs. 4b and 4d. The isomer  $\text{Pt}_5\text{-5}$  seems rather certain because  $\text{Pt}_5\text{-8}$  is by 0.86 eV less favorable than  $\text{Pt}_5\text{-5}$ .



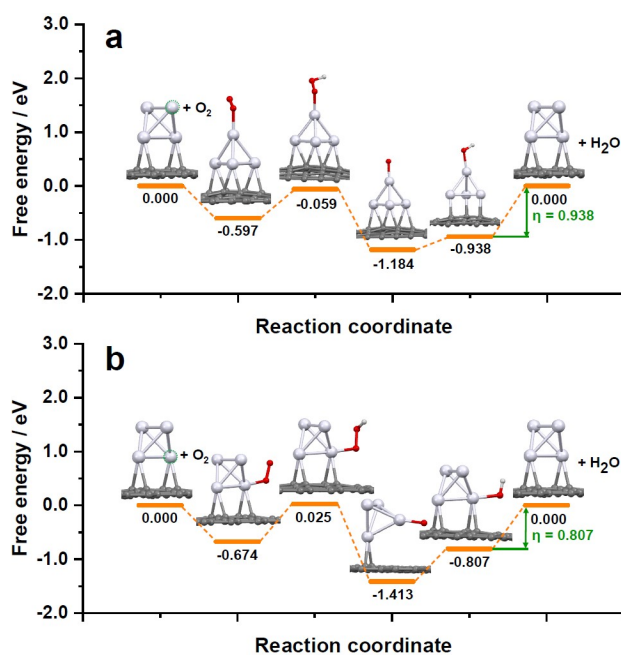
**Figure S11.** The lowest and higher energy isomers of Pt<sub>8</sub> supported on graphene (Pt<sub>8</sub>/Gr). The number below correspond to the relative total energy of the clusters. Relative energies in eV are also indicated relative to the most stable isomer **1** (Pt<sub>8</sub>-**1**). Isomer **6** (Pt<sub>8</sub>-**6**) represents the most probable structure examined by FEFF simulations of  $\chi(k)$  spectra obtained by EXAFS shown in Fig. S12.



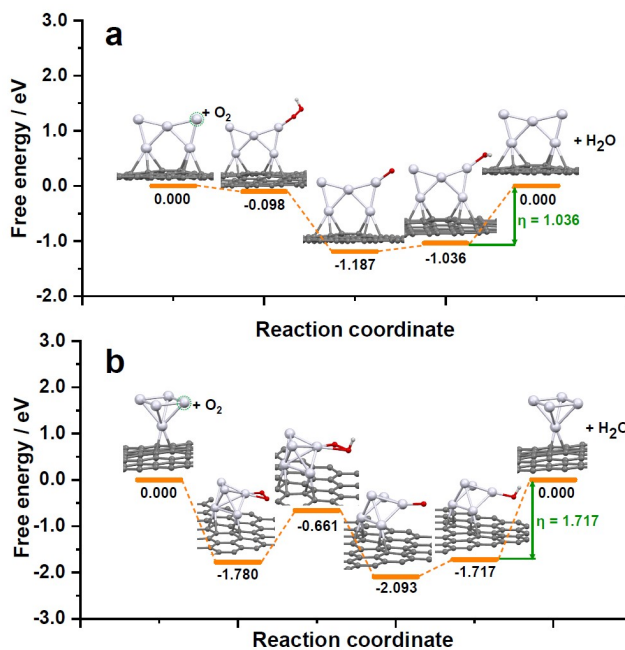
**Figure S12.** FEFF simulations of  $\chi(k)$  spectra for all isomers of  $\text{Pt}_8/\text{Gr}$  shown in Fig. S11 including Figure 5 of the main text. Blue and black curves represent experimental and simulated  $\chi(k)$  spectra, respectively.  $\text{Pt}_8/\text{Gr}$  coordinates were used without scaling of the geometry. The most probable structure for  $\text{Pt}_8/\text{GC}$  seems to be a triangular meshed hexamer fixed by two Pt atoms to Gr, which is given as eaves-like geometry of isomer 6 ( $\text{Pt}_8\text{-6}$ ).



**Figure S13.** Radial distributions analyzed by EXAFS spectra [4] that have been offset vertically for clarity of presentation;  $\text{Pt}_4/\text{GC}$ ,  $\text{Pt}_5/\text{GC}$ , and  $\text{Pt}_8/\text{GC}$ .

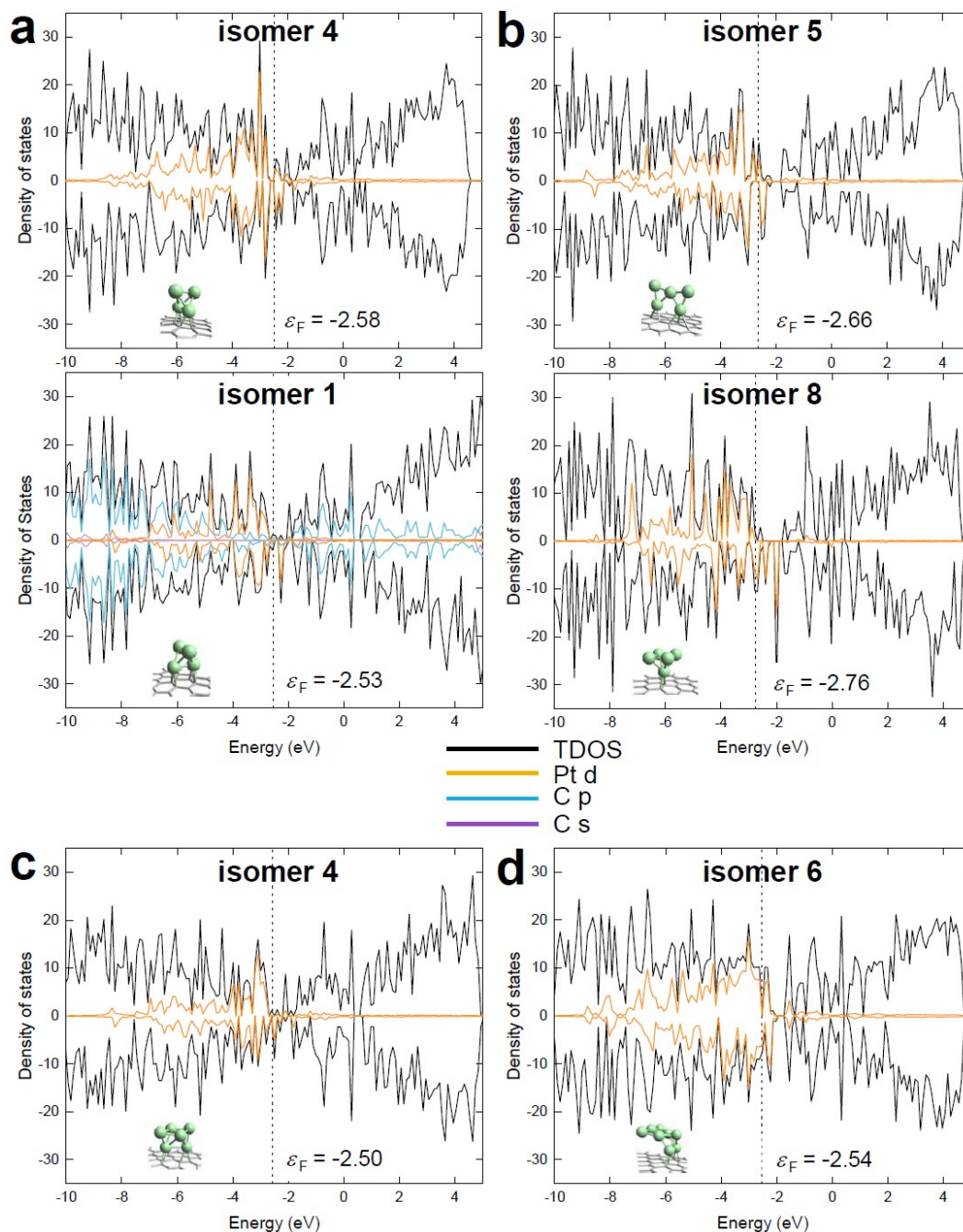


**Figure S14.** Oxygen reduction reaction (ORR) free energy diagrams in eV for sequential reactions of Pt<sub>4</sub>-4/Gr isomer between O<sub>2</sub> reactants and H<sub>2</sub>O products with applied potentials of 1.23 V: adsorbed O<sub>2</sub>, O<sub>2</sub>H, O, and OH starting from O<sub>2</sub> adsorption to (a) top Pt(3) and (b) bottom Pt(4) atoms. Overpotentials ( $\eta$ ) of (a) 0.938 V and (b) 0.807 V are obtained for the reaction of adsorbed OH into H<sub>2</sub>O products.



**Figure S15.** Oxygen reduction reaction (ORR) free energy diagrams in eV for sequential reactions of two isomers of (a) Pt<sub>5</sub>-5/Gr and (b) Pt<sub>5</sub>-8/Gr between O<sub>2</sub> reactants and H<sub>2</sub>O products with applied potentials of 1.23 V: adsorbed O<sub>2</sub>, O<sub>2</sub>H, O, and OH starting from O<sub>2</sub> adsorption to (a) top Pt(2) and (b) top Pt(2) atoms. Overpotentials ( $\eta$ ) of (a) 1.036 V and (b) 1.717 V are obtained for the reaction of adsorbed OH into H<sub>2</sub>O products. Note that a free O<sub>2</sub> does not adsorb to Pt atoms in Pt<sub>5</sub>-5/Gr.





**Table S2. Bader charge and *d*-band center (eV) of Pt atoms in Pt<sub>*n*</sub>/Gr at *n* = 4, 5, 6, and 8.**

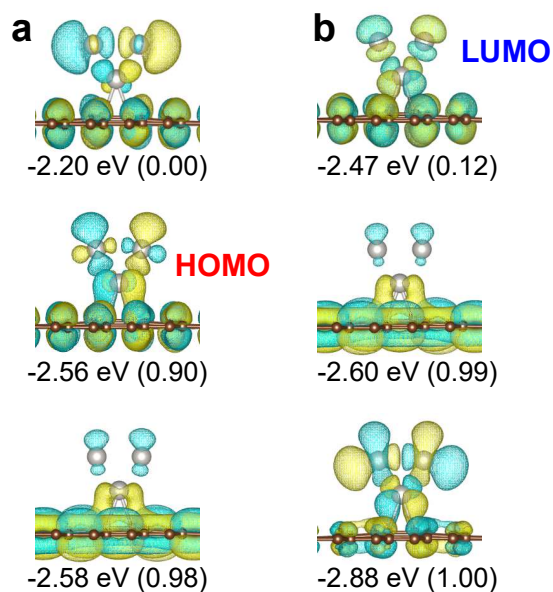
<b>Pt<sub>4</sub>-1</b>			<b>Pt<sub>4</sub>-4</b>	
Pt	charge	<i>d</i> -band center	charge	<i>d</i> -band center
1	-0.064	-3.75	-0.080	-4.01
2	0.118	-4.53	0.140	-4.72
3	-0.091	-3.75	-0.104	-3.73
4	0.125	-4.14	0.109	-4.73

<b>Pt<sub>5</sub>-5</b>			<b>Pt<sub>5</sub>-8</b>	
Pt	charge	<i>d</i> -band center	charge	<i>d</i> -band center
1	0.102	-4.50	0.153	-4.59
2	-0.197	-4.05	-0.115	-4.34
3	0.108	-4.53	-0.109	-4.38
4	-0.195	-4.06	-0.018	-4.39
5	0.116	-4.80	-0.041	-4.33

<b>Pt<sub>6</sub>-4</b> <sup>a)</sup>		
Pt	charge	<i>d</i> -band center
1	0.125	-4.40
2	0.086	-4.26
3	0.043	-4.35
4	0.043	-4.42
5	-0.148	-4.11
6	-0.151	-4.12

<b>Pt<sub>8</sub>-6</b>		
Pt	charge	<i>d</i> -band center
1	0.071	-4.41
2	0.074	-4.33
3	0.069	-4.28
4	0.058	-4.22
5	0.053	-4.30
6	-0.076	-4.42
7	-0.186	-4.01
8	-0.186	-4.03

a) Reference 1.



**Figure S17.** Frontier molecular orbitals for Pt<sub>4</sub>-4/Gr isomer at the  $\Gamma$  point with orbital energies in eV: (a) down- and (b) up-spin. Electron occupations for each orbital are shown in parentheses. Two top Pt atoms which are negatively charged possess relatively large amplitude in the frontier orbitals of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), while two bottom Pt atoms possess some amplitude in the HOMO and LUMO.

**Table S3.** Energies for *d*-band center and *d*-band top (eV) of the Pt<sub>*n*</sub> sub-NCs.

	Pt <sub>4</sub> -1	Pt <sub>5</sub> -5	Pt <sub>6</sub> -4	Pt <sub>8</sub> -6
d-band center	-3.75 (Pt(1)) <sup>a)</sup>	-4.05 (Pt(2)) <sup>a)</sup>	-4.11 (Pt(5)) <sup>a)</sup>	-4.01 (Pt(7)) <sup>a)</sup>
d-band top	-2.77	-2.82	-2.81	-2.62

a) See Figure 6 for the number labeled atom in each isomer.



**Table S4.** Cartesian coordinates of 7 isomers of Pt<sub>4</sub>.**Pt<sub>4</sub> Isomer 1**

C	-6.971196651	12.168397903	17.230991364	C	-0.822937965	5.776865959	17.075870514
C	1.638972282	0.094790913	17.235877991	C	0.389406681	6.476787090	16.957471848
C	-4.510962486	12.169235229	17.245540619	C	1.630735636	5.758845329	16.868583679
C	4.099505901	0.097174659	17.249689102	C	2.893638134	6.487955570	16.867668152
C	-2.050036430	12.172619820	17.237184525	C	4.121376038	5.766830444	17.032899857
C	6.559642792	0.100078166	17.237028122	C	5.339736938	6.485297680	17.110752106
C	0.410932541	12.174260139	17.198589325	C	6.567892551	5.776008606	17.181261063
C	9.022157669	0.102375738	17.205677032	C	7.793773174	6.488508224	17.207876205
C	2.871758938	12.177933693	17.180078506	C	9.023900986	5.779333591	17.221754074
C	11.481778145	0.100792192	17.207176208	C	10.250833511	6.490923405	17.206829071
C	5.329676151	12.171371460	17.205736160	C	-4.511748314	7.910310745	17.207885742
C	13.939455032	0.095612824	17.221420288	C	-3.285866737	8.622844696	17.181270599
C	-0.819691181	1.515500426	17.208637238	C	-2.057698011	7.913508892	17.111747742
C	0.410359740	2.220915079	17.182447433	C	-0.839426041	8.632020950	17.033544540
C	1.639972448	1.513967872	17.207595825	C	0.388267040	7.910796642	16.868875504
C	2.871142626	2.224604368	17.200328827	C	1.651134491	8.639966011	16.867706299
C	4.102406025	1.516261697	17.238019943	C	2.892571449	7.922049999	16.955459595
C	5.332082748	2.226246834	17.237855911	C	4.105010033	8.621987343	17.073232651
C	6.562551975	1.519162774	17.249435425	C	5.336273670	7.906237602	17.121036530
C	7.793054104	2.229602337	17.245342255	C	6.559767723	8.616970062	17.180644989
C	9.023163795	1.521496534	17.235013962	C	7.791198730	7.907883644	17.205944061
C	10.253303528	2.230385303	17.231048584	C	9.018130302	8.619487762	17.220956802
C	11.482649803	1.520643711	17.221359253	C	-5.741800785	10.038994789	17.230514526
C	12.712412834	2.227415085	17.207080841	C	-4.512819290	10.749940872	17.235149384
C	-2.045973539	3.648446083	17.182643890	C	-3.283266068	10.041190147	17.206346512
C	-0.818681479	4.352654934	17.123397827	C	-2.052266598	10.752173424	17.199079514
C	0.410120487	3.639221430	17.112558365	C	-0.826491833	10.047405243	17.123596191
C	1.641497135	4.335039616	17.034126282	C	0.408350945	10.760344505	17.123161316
C	2.873653889	3.638561964	17.124635696	C	1.640520573	10.063834190	17.032232285
C	4.108506680	4.351496696	17.124202728	C	2.871954441	10.759666443	17.109863281
C	5.334285736	3.646724224	17.199838638	C	4.100774288	10.046176910	17.120622635
C	6.565318108	4.357635021	17.206932068	C	5.328096867	10.750364304	17.180419922
C	7.794886589	3.648898840	17.235734940	C	6.558978081	10.038765907	17.198337555
C	9.023869514	4.359797478	17.231491089	C	7.786887169	10.747713089	17.227117538
C	10.255216599	3.651084900	17.228258133	Pt	0.538489342	6.564381123	12.866962433
C	11.483111382	4.360013485	17.200239182	Pt	2.273940563	6.100038528	14.769669533
C	-3.277680874	5.781826496	17.182430267	Pt	2.723450661	7.827837944	12.856511116
C	-2.054190636	6.492603302	17.123067856	Pt	1.002914906	8.298941612	14.770136833

**Pt<sub>4</sub> Isomer 2**

C	-6.943318367	12.171335220	17.200019836	C	9.046647072	1.518908620	17.170713425
C	1.666719198	0.096439153	17.167242050	C	10.273289680	2.227082491	17.238594055
C	-4.485410690	12.170739174	17.112615585	C	11.503802299	1.516163468	17.264266968
C	4.125020027	0.099039868	17.067720413	C	12.734872818	2.226343632	17.296794891
C	-2.024023533	12.170597076	17.052970886	C	-2.025264740	3.648150206	17.315572739
C	6.583944321	0.097113155	17.064073563	C	-0.797672868	4.356883526	17.324705124
C	0.434724331	12.173197746	17.076229095	C	0.433751583	3.643975735	17.294666290
C	9.044363022	0.099655107	17.135559082	C	1.662121296	4.350769997	17.245143890
C	2.892498016	12.172919273	17.173007965	C	2.878736496	3.638024092	17.090343475
C	11.503625870	0.099335179	17.233829498	C	4.121804237	4.340598106	16.944248199
C	5.356244087	12.171788216	17.233394623	C	5.369256020	3.637509108	17.014984131
C	13.965541840	0.097374640	17.240249634	C	6.587629318	4.349496365	17.117536545
C	-0.796549261	1.517169476	17.272665024	C	7.816123486	3.644700289	17.165401459
C	0.434387088	2.225790501	17.255338669	C	9.045868874	4.356387615	17.224317551
C	1.662993193	1.515378356	17.181644440	C	10.272994995	3.648117065	17.258344650
C	2.889182568	2.222538471	17.101932526	C	11.503392220	4.359124660	17.290416718
C	4.124009609	1.515118718	17.051242828	C	-3.256407499	5.777480602	17.261627197
C	5.359120369	2.223113775	17.036159515	C	-2.027279854	6.489145279	17.245206833
C	6.587574005	1.516200900	17.074741364	C	-0.799359322	5.779652119	17.289836884
C	7.816369534	2.226559639	17.132087708	C	0.426881313	6.490147591	17.242710114

C	1.658625126	5.775122643	17.268507004
C	2.872566938	6.475944996	17.156169891
C	4.122301102	5.775306225	17.006904602
C	5.378355026	6.482808590	17.086502075
C	6.591485977	5.775163651	17.150203705
C	7.821064949	6.489492416	17.184360504
C	9.047103882	5.778867245	17.221504211
C	10.275035858	6.489241600	17.226938248
C	-4.483069420	7.909660816	17.187841415
C	-3.255284071	8.620943069	17.155998230
C	-2.028236628	7.908321381	17.170578003
C	-0.802597046	8.616830826	17.095275879
C	0.418038845	7.900095940	17.087329865
C	1.648221493	8.625980377	16.946161270
C	2.890921593	7.908867359	17.009902954
C	4.131336212	8.642935753	17.092203140
C	5.368331432	7.917311668	17.034900665
C	6.604016781	8.630497932	17.092035294

#### Pt<sub>4</sub> Isomer 3

C	-6.952286720	12.158449173	17.226348877
C	1.656212687	0.083531052	17.249095917
C	-4.492796421	12.156047821	17.251567841
C	4.116915226	0.082974993	17.250406265
C	-2.033538818	12.155988693	17.236068726
C	6.576751232	0.082269594	17.223611832
C	0.426715374	12.156288147	17.181631088
C	9.035563469	0.083116472	17.181364059
C	2.886775970	12.156489372	17.134832382
C	11.495896339	0.084564790	17.177885056
C	5.346460819	12.158391953	17.174139023
C	13.956741333	0.084278792	17.222332001
C	-0.804807544	1.502511024	17.241315842
C	0.425132990	2.210861206	17.236425400
C	1.655360222	1.503486633	17.241699219
C	2.886034489	2.213492393	17.223199844
C	4.117634296	1.502984881	17.237112045
C	5.346910954	2.210711241	17.225019455
C	6.577894688	1.501600862	17.232683182
C	7.807260513	2.211338997	17.232694626
C	9.037049294	1.502515435	17.223360062
C	10.266059875	2.213593245	17.235553741
C	11.496212006	1.503829598	17.225286484
C	12.724675179	2.212929487	17.241434097
C	-2.035191774	3.633674860	17.242921829
C	-0.806341171	4.342772484	17.211479187
C	0.423136234	3.630530119	17.201103210
C	1.650619507	4.334796906	17.136108398
C	2.885165691	3.629156351	17.163982391
C	4.119142056	4.335815907	17.123819351
C	5.349133492	3.629551411	17.180372238
C	6.578871250	4.339534760	17.180393219
C	7.808769703	3.631900311	17.225166321
C	9.036248207	4.342634201	17.237329483
C	10.266431808	3.633155346	17.250202179
C	11.495616913	4.343482971	17.251415253
C	-3.263762474	5.764577866	17.249336243
C	-2.036744118	6.474729061	17.226583481

#### Pt<sub>4</sub> Isomer 4

C	-6.952286720	12.158449173	17.226348877
C	1.656212687	0.083531052	17.249095917
C	-4.492796421	12.156047821	17.251567841
C	4.116915226	0.082974993	17.250406265
C	-2.033538818	12.155988693	17.236068726

C	7.825819492	7.909024239	17.148303986
C	9.051860809	8.621000290	17.163661957
C	-5.710840225	10.041893959	17.149158478
C	-4.483461380	10.750502586	17.121919632
C	-3.254623890	10.038454056	17.106613159
C	-2.023829460	10.748974800	17.063991547
C	-0.797892094	10.040019035	17.047107697
C	0.432734489	10.755873680	17.036779404
C	1.662868023	10.057705879	17.018924713
C	2.888449669	10.756642342	17.125469208
C	4.125107765	10.047041893	17.159149170
C	5.358668804	10.754693985	17.194229126
C	6.590488434	10.049126625	17.154443741
C	7.820164680	10.754703522	17.170621872
Pt	3.649557114	6.930109024	12.793650627
Pt	3.931849241	5.425019741	14.884222031
Pt	5.089504242	7.756814003	14.732416153
Pt	2.490933418	7.925104141	14.887668610

C	-0.806805134	5.763484001	17.187864304
C	0.416435957	6.472868443	17.101957321
C	1.638417959	5.750842094	17.032440186
C	2.878758430	6.453771114	16.884729385
C	4.127988815	5.746010303	17.003152847
C	5.356215954	6.455091953	17.002622604
C	6.582337379	5.757669449	17.123855591
C	7.811107159	6.473011017	17.164928436
C	9.036723137	5.764477730	17.223924637
C	10.266908646	6.475319862	17.242338181
C	-4.490644932	7.894370079	17.237197876
C	-3.262300968	8.605459213	17.242126465
C	-2.034802675	7.894965649	17.223056793
C	-0.806169510	8.606303215	17.174966812
C	0.418719769	7.898426533	17.092163086
C	1.636131763	8.613352776	16.971139908
C	2.859608650	7.896928310	16.772029877
C	4.128139496	8.629107475	16.774688721
C	5.367673874	7.891376495	16.886610031
C	6.597002029	8.613759041	17.033433914
C	7.817259312	7.894995689	17.137092590
C	9.040812492	8.605949402	17.201908112
C	-5.721210003	10.026905060	17.212064743
C	-4.492712021	10.736649513	17.243396759
C	-3.262293339	10.026367188	17.242187500
C	-2.034025669	10.735796928	17.226108551
C	-0.804709911	10.026382446	17.178833008
C	0.425114632	10.735565186	17.135532379
C	1.650689602	10.027894974	17.035736084
C	2.886715889	10.741358757	17.035301208
C	4.119187355	10.046380997	16.971258163
C	5.347030163	10.743583679	17.091970444
C	6.582671165	10.033014297	17.102392197
C	7.808722496	10.737768173	17.188169479
Pt	3.182937622	8.829756737	12.998270988
Pt	2.816349745	6.914447308	14.744468689
Pt	4.408218384	6.667492390	12.644161224
Pt	5.014361382	8.155820847	14.743202209

C	6.576751232	0.082269594	17.223611832
C	0.426715374	12.156288147	17.181631088
C	9.035563469	0.083116472	17.181364059
C	2.886775970	12.156489372	17.134832382
C	11.495896339	0.084564790	17.177885056

C	5.346460819	12.158391953	17.174139023
C	13.956741333	0.084278792	17.222332001
C	-0.804807544	1.502511024	17.241315842
C	0.425132990	2.210861206	17.236425400
C	1.655360222	1.503486633	17.241699219
C	2.886034489	2.213492393	17.223199844
C	4.117634296	1.502984881	17.237112045
C	5.346910954	2.210711241	17.225019455
C	6.577894688	1.501600862	17.232683182
C	7.807260513	2.211338997	17.232694626
C	9.037049294	1.502515435	17.223360062
C	10.266059875	2.213593245	17.235553741
C	11.496212006	1.503829598	17.225286484
C	12.724675179	2.212929487	17.241434097
C	-2.035191774	3.633674860	17.242921829
C	-0.806341171	4.342772484	17.211479187
C	0.423136234	3.630530119	17.201103210
C	1.650619507	4.334796906	17.136108398
C	2.885165691	3.629156351	17.163982391
C	4.119142056	4.335815907	17.123819351
C	5.349133492	3.629551411	17.180372238
C	6.578871250	4.339534760	17.180393219
C	7.808769703	3.631900311	17.225166321
C	9.036248207	4.342634201	17.237329483
C	10.266431808	3.633155346	17.250202179
C	11.495616913	4.343482971	17.251415253
C	-3.263762474	5.764577866	17.249336243
C	-2.036744118	6.474729061	17.226583481
C	-0.806805134	5.763484001	17.187864304
C	0.416435957	6.472868443	17.101957321
C	1.638417959	5.750842094	17.032440186
C	2.878758430	6.453771114	16.884729385
C	4.127988815	5.746010303	17.003152847

#### Pt<sub>4</sub> Isomer 5

C	-6.948593616	12.229092598	17.179634094
C	1.661832094	0.153888896	17.146326065
C	-4.488308907	12.226959229	17.106935501
C	4.122798920	0.151575565	17.104976654
C	-2.026113033	12.227800369	17.100687027
C	6.581780434	0.155138493	17.130668640
C	0.433302879	12.228652954	17.170928955
C	9.042121887	0.158834413	17.218286514
C	2.891510487	12.235338211	17.275730133
C	11.502139091	0.161587521	17.264030457
C	5.352661610	12.234005928	17.259704590
C	13.961301804	0.157662556	17.217485428
C	-0.800944448	1.577445388	17.202388763
C	0.428765535	2.286005497	17.171909332
C	1.662271738	1.571268916	17.150777817
C	2.892248631	2.269659758	17.118394852
C	4.124283314	1.569968939	17.118583679
C	5.354167938	2.281999111	17.135158539
C	6.582012177	1.575490355	17.138732910
C	7.812478542	2.288407087	17.152000427
C	9.041411400	1.579447150	17.188240051
C	10.270017624	2.289068222	17.190551758
C	11.500282288	1.579071760	17.223541260
C	12.729326248	2.286776543	17.205265045
C	-2.033700705	3.707043409	17.175117493
C	-0.808913112	4.415085793	17.171638489
C	0.419483185	3.700275183	17.163499832
C	1.660316944	4.421052933	17.156847000
C	2.901086807	3.694948912	17.113080978
C	4.136407852	4.402523994	17.180425644

C	5.356215954	6.455091953	17.002622604
C	6.582337379	5.757669449	17.123855591
C	7.811107159	6.473011017	17.164928436
C	9.036723137	5.764477730	17.223924637
C	10.266908646	6.475319862	17.242338181
C	-4.490644932	7.894370079	17.237197876
C	-3.262300968	8.605459213	17.242126465
C	-2.034802675	7.894965649	17.223056793
C	-0.806169510	8.606303215	17.174966812
C	0.418719769	7.898426533	17.092163086
C	1.636131763	8.613352776	16.971139908
C	2.859608650	7.896928310	16.772029877
C	4.128139496	8.629107475	16.774688721
C	5.367673874	7.891376495	16.886610031
C	6.597002029	8.613759041	17.033433914
C	7.817259312	7.894995689	17.137092590
C	9.040812492	8.605949402	17.201908112
C	-5.721210003	10.026905060	17.212064743
C	-4.492712021	10.736649513	17.243396759
C	-3.262293339	10.026367188	17.242187500
C	-2.034025669	10.735796928	17.226108551
C	-0.804709911	10.026382446	17.178833008
C	0.425114632	10.735565186	17.135532379
C	1.650689602	10.027894974	17.035736084
C	2.886715889	10.741358757	17.035301208
C	4.119187355	10.046380997	16.971258163
C	5.347030163	10.743583679	17.091970444
C	6.582671165	10.033014297	17.102392197
C	7.808722496	10.737768173	17.188169479
Pt	3.182937622	8.829756737	12.998270988
Pt	2.816349745	6.914447308	14.744468689
Pt	4.408218384	6.667492390	12.644161224
Pt	5.014361382	8.155820847	14.743202209

C	5.357470512	3.704137802	17.154541016
C	6.586941719	4.419429302	17.112171173
C	7.813545227	3.707908869	17.121002197
C	9.042448997	4.418177128	17.100379944
C	10.269711494	3.708310366	17.140308380
C	11.498096466	4.419018269	17.135065079
C	-3.260239840	5.837498665	17.087026596
C	-2.029981375	6.546036243	17.079149246
C	-0.813199282	5.831909180	17.123149872
C	0.434450626	6.544865131	17.125888824
C	1.672107697	5.847388744	17.361206055
C	2.881558418	6.559474945	17.450868607
C	4.109015465	5.841714382	17.177961349
C	5.351112366	6.560070038	17.058748245
C	6.588024139	5.834490299	17.050762177
C	7.811837673	6.549290180	17.050474167
C	9.042736053	5.838473797	17.062957764
C	10.270207405	6.548419476	17.058834076
C	-4.489746094	7.968931675	17.046413422
C	-3.257668734	8.678777695	17.040521622
C	-2.026421785	7.972092152	17.041112900
C	-0.802739143	8.685763359	17.035520554
C	0.447431087	7.979683876	17.061922073
C	1.675721169	8.691618919	17.291246414
C	2.890771389	7.983432293	17.446319580
C	4.124763966	8.690182686	17.376457214
C	5.350572109	7.987921238	17.211177826
C	6.579098701	8.685075760	17.164447784
C	7.809369564	7.970179081	17.079103470
C	9.039384842	8.677962303	17.068656921

C	-5.718841076	10.100056648	17.100130081
C	-4.489939213	10.806890488	17.080408096
C	-3.257552624	10.098529816	17.051450729
C	-2.027831554	10.808012962	17.071239471
C	-0.796968460	10.101076126	17.080692291
C	0.434456825	10.811603546	17.165075302
C	1.666280270	10.107741356	17.268686295
C	2.893191338	10.817440033	17.323350906

#### Pt<sub>4</sub> Isomer 6

C	-6.971005440	12.169324875	17.297441483
C	1.638381004	0.095659465	17.316997528
C	-4.5111115551	12.167212486	17.327697754
C	4.098841667	0.095289655	17.323453903
C	-2.051895618	12.167768478	17.328239441
C	6.559148312	0.095477492	17.317874908
C	0.409204483	12.168757439	17.280529022
C	9.017720222	0.095800035	17.281581879
C	2.868815899	12.168575287	17.219427109
C	11.478748322	0.096441172	17.265869141
C	5.328808308	12.169285774	17.241981506
C	13.939940453	0.096713468	17.298671722
C	-0.820866644	1.515832186	17.316940308
C	0.409170866	2.225090504	17.279949188
C	1.637701750	1.515522242	17.281118393
C	2.868814468	2.225246191	17.219564438
C	4.098749638	1.514863014	17.266466141
C	5.328779697	2.224570036	17.243236542
C	6.559905052	1.514601827	17.300029755
C	7.788958549	2.224517584	17.298892975
C	9.018404007	1.515680671	17.317922592
C	10.248931885	2.226620913	17.328271866
C	11.478907585	1.516026378	17.323226929
C	12.708127975	2.226102829	17.327724457
C	-2.051546574	3.646325827	17.318490982
C	-0.821940422	4.356127739	17.258350372
C	0.408456326	3.646127224	17.215293884
C	1.631807566	4.350296974	17.074045181
C	2.867238998	3.636643648	17.077018738
C	4.100301743	4.328278542	16.953357697
C	5.330678463	3.636095047	17.109323502
C	6.566006660	4.349874496	17.104274750
C	7.789817810	3.645548344	17.238309860
C	9.019138336	4.356092930	17.258743286
C	10.248734474	3.646114349	17.318971634
C	11.478978157	4.356002808	17.322570801
C	-3.281655788	5.777066231	17.307601929
C	-2.053009510	6.487239361	17.287475586

#### Pt<sub>4</sub> Isomer 7

C	-6.982962132	12.233575821	17.475183487
C	1.628924370	0.161692426	17.453382492
C	-4.521462440	12.235550880	17.391416550
C	4.089505672	0.163156301	17.330873489
C	-2.061787128	12.236462593	17.250240326
C	6.546452045	0.163504958	17.212846756
C	0.396980762	12.240308762	17.182170868
C	9.006917000	0.166193679	17.226760864
C	2.855518341	12.238324165	17.283901215
C	11.464957237	0.164939970	17.374595642
C	5.314547062	12.236763954	17.439279556
C	13.924551964	0.162616432	17.475240707
C	-0.835945487	1.584773421	17.453535080
C	0.395683408	2.294281006	17.444715500
C	1.627566814	1.583056927	17.444532394

C	4.124144554	10.106755257	17.345947266
C	5.354381561	10.813842773	17.278562546
C	6.581663132	10.105359077	17.213275909
C	7.811981201	10.811547279	17.164049149
Pt	4.185673237	6.295480728	15.043390274
Pt	2.156719446	4.683618546	14.973383904
Pt	0.964737415	6.994403362	15.014610291
Pt	2.514946222	6.343334198	13.069218636

C	-0.822998047	5.775958538	17.231422424
C	0.399487734	6.483604431	17.099651337
C	1.614675522	5.764214039	16.949428558
C	2.828470945	6.471178055	16.652427673
C	4.105181217	5.731924057	16.651073456
C	5.362364769	6.458267689	16.639345169
C	6.582088470	5.761247158	16.943820953
C	7.797254562	6.483145714	17.064283371
C	9.019049644	5.776442528	17.208532333
C	10.249170303	6.487521648	17.270030975
C	-4.510884285	7.906332016	17.269842148
C	-3.281687737	8.616764069	17.307464600
C	-2.053005219	7.906628132	17.287460327
C	-0.822965622	8.617892265	17.231456757
C	0.399500370	7.910290718	17.099670410
C	1.614651203	8.629690170	16.949369431
C	2.828374863	7.922655582	16.652301788
C	4.105144978	8.661821365	16.650520325
C	5.362336159	7.935329914	16.638877869
C	6.582136631	8.632535934	16.942733765
C	7.797281265	7.910695076	17.063720703
C	9.019042969	8.617424011	17.207851410
C	-5.740865231	10.037750244	17.257694244
C	-4.511262894	10.747704506	17.318328857
C	-3.281005144	10.037817955	17.322364807
C	-2.051537037	10.747515678	17.318645477
C	-0.821929932	10.037699699	17.258571625
C	0.408458233	10.747710228	17.215616226
C	1.631805897	10.043574333	17.074090958
C	2.867267609	10.757159233	17.076694489
C	4.100313663	10.065532684	16.952459335
C	5.330701351	10.757741928	17.107948303
C	6.566013336	10.043939590	17.102682114
C	7.789825439	10.748302460	17.236764908
Pt	4.124005318	7.194551945	12.449436188
Pt	4.851464272	5.866607189	14.586361885
Pt	4.851598740	8.524389267	14.585224152
Pt	2.611153603	7.196646214	14.570082664

C	2.857430935	2.290740013	17.376480103
C	4.090201378	1.582121968	17.321647644
C	5.320361137	2.290150404	17.223608017
C	6.549224854	1.582486272	17.199026108
C	7.778323174	2.292411566	17.163478851
C	9.008259773	1.585574627	17.219497681
C	10.236908913	2.294847965	17.259206772
C	11.464651108	1.585264325	17.352760315
C	12.695530891	2.295293808	17.391674042
C	-2.064953566	3.716401339	17.331394196
C	-0.836431980	4.426506042	17.322547913
C	0.393643379	3.713213205	17.376960754
C	1.621272564	4.419835091	17.302385330
C	2.855564594	3.707195044	17.302017212
C	4.086198807	4.401455879	17.143413544

C	5.325395584	3.705212116	17.126392365	C	1.614799500	8.701192856	16.887111664
C	6.551471710	4.409179211	17.005418777	C	2.869207859	7.994881153	16.881597519
C	7.778243065	3.711325645	17.083890915	C	4.102173328	8.698737144	17.177509308
C	9.011659622	4.424266815	17.110267639	C	5.320743084	7.995223999	17.176931381
C	10.235504150	3.715989590	17.208072662	C	6.548804283	8.687933922	17.299741745
C	11.466472626	4.425882816	17.250616074	C	7.783644199	7.975882530	17.217735291
C	-3.293185234	5.844362736	17.213472366	C	9.009436607	8.685321808	17.283756256
C	-2.065673828	6.556258202	17.200290680	C	-5.751128197	10.104639053	17.374479294
C	-0.838364363	5.845888138	17.224924088	C	-4.520911694	10.814538002	17.352767944
C	0.384581327	6.557787418	17.127897263	C	-3.292527676	10.106058121	17.259555817
C	1.607149601	5.832757473	17.144258499	C	-2.061095715	10.815449715	17.208450317
C	2.836272955	6.528835297	16.952802658	C	-0.835810184	10.109691620	17.111133575
C	4.074398994	5.813963413	16.952384949	C	0.394908428	10.823755264	17.107032776
C	5.327528000	6.575543404	16.880428314	C	1.626358509	10.126290321	17.054262161
C	6.566473484	5.842428684	16.885629654	C	2.854022026	10.822201948	17.218381882
C	7.794887543	6.564869404	17.053277969	C	4.088085175	10.108601570	17.300334930
C	9.014629364	5.847137928	17.106369019	C	5.314677238	10.814354897	17.413698196
C	10.240366936	6.557160378	17.182285309	C	6.546689987	10.103055954	17.413526535
C	-4.521055222	7.976522446	17.226951599	C	7.778581619	10.814157486	17.439208984
C	-3.292505741	8.687375069	17.220191956	Pt	5.785645485	6.611990452	14.805561066
C	-2.065427780	7.975634098	17.164688110	Pt	3.336265087	5.968671799	14.806293488
C	-0.836575985	8.685032845	17.085344315	Pt	2.668124676	8.411471367	14.807429314
C	0.381111622	7.971541882	17.007114410	Pt	4.196371555	7.461104870	12.891751289

**Table S5.** Cartesian coordinates of 9 isomers of Pt<sub>5</sub>.

**Pt<sub>5</sub> Isomer 1**

C	-6.899875641	12.126688004	17.272327423	C	-1.982463717	6.443644524	17.184066772
C	1.709236145	0.054674063	17.283956528	C	-0.751795769	5.728579044	17.159353256
C	-4.440720558	12.127186775	17.277540207	C	0.475271940	6.422782898	17.035066605
C	4.170302391	0.055937812	17.275619507	C	1.695000410	5.719095230	17.036458969
C	-1.980591297	12.129023552	17.250274658	C	2.945920944	6.422550678	16.870658875
C	6.629539967	0.056290168	17.252687454	C	4.186238289	5.723830223	17.084449768
C	0.480696678	12.129789352	17.209131241	C	5.403771400	6.441944599	17.147956848
C	9.090688705	0.055987742	17.219985962	C	6.630696297	5.735014915	17.231479645
C	2.939666271	12.127466202	17.179456711	C	7.861112118	6.446212292	17.256727219
C	11.550403595	0.054445945	17.228958130	C	9.090366364	5.736601353	17.276088715
C	5.399672031	12.126776695	17.226726532	C	10.319687843	6.446894169	17.263156891
C	14.008841515	0.053055272	17.268043518	C	-4.442295551	7.865847111	17.255392075
C	-0.751262307	1.472496510	17.279838562	C	-3.213852167	8.577689171	17.219404221
C	0.479085207	2.182083845	17.271213531	C	-1.987472296	7.867133141	17.153894424
C	1.708804131	1.474824190	17.275426865	C	-0.768786907	8.583545685	17.052225113
C	2.939650297	2.187707901	17.258649826	C	0.460653305	7.857309818	16.876447678
C	4.171283245	1.475707889	17.274059296	C	1.694609642	8.601853371	16.761768341
C	5.400830269	2.184127569	17.272888184	C	2.967048645	7.866761684	16.746454239
C	6.630949020	1.474281907	17.274971008	C	4.192489147	8.585493088	16.977600098
C	7.861615658	2.185244560	17.278739929	C	5.405027866	7.869679451	17.113180161
C	9.090773582	1.475646377	17.266204834	C	6.631061077	8.577459335	17.199832916
C	10.320303917	2.185174227	17.278110504	C	7.860590935	7.866344929	17.248203278
C	11.549758911	1.473313689	17.269931793	C	9.088193893	8.576525688	17.263282776
C	12.779111862	2.182757378	17.279457092	C	-5.670909882	9.997552872	17.265129089
C	-1.981713414	3.602901459	17.267059326	C	-4.441282272	10.708395958	17.265449524
C	-0.751565576	4.310936928	17.225521088	C	-3.211491108	9.997822762	17.231004715
C	0.477534533	3.601391315	17.229064941	C	-1.982233524	10.708342552	17.207550049
C	1.705869198	4.310019016	17.167547226	C	-0.755540371	10.000146866	17.119619370
C	2.940126181	3.602710485	17.202833176	C	0.481575012	10.715673447	17.118141174
C	4.174692154	4.312505245	17.189542770	C	1.707972527	10.020901680	16.995117188
C	5.402993679	3.604208469	17.248331070	C	2.938694000	10.712586403	17.070997238
C	6.631539345	4.315204144	17.254692078	C	4.176456928	9.997361183	17.063558578
C	7.862160683	3.605262041	17.279760361	C	5.400549412	10.706119537	17.172246933
C	9.090658188	4.315091133	17.284515381	C	6.630635738	9.996765137	17.207918167
C	10.320643425	3.604824066	17.286554337	C	7.860146523	10.707119942	17.255672455
C	11.550716400	4.314169884	17.271339417	Pt	0.843953133	8.317543983	14.762861252
C	-3.207945824	5.736202240	17.246700287	Pt	3.027430534	7.011410713	14.746255875

Pt 2.931477547 7.045572281 12.267078400  
Pt 0.921859264 8.404910088 12.284221649

**Pt<sub>5</sub> Isomer 2**

C -6.921015263 12.182233810 17.260854721  
C 1.688935995 0.109102055 17.300100327  
C -4.460697174 12.182312012 17.320543289  
C 4.148892403 0.109669738 17.346179962  
C -2.000781536 12.182840347 17.341606140  
C 6.610305309 0.111099124 17.342285156  
C 0.459435463 12.185504913 17.310411453  
C 9.069448471 0.112628594 17.291831970  
C 2.919197559 12.185323715 17.246974945  
C 11.530113220 0.111658022 17.233928680  
C 5.379840851 12.185406685 17.215692520  
C 13.990387917 0.110460043 17.241266251  
C -0.770127058 1.529204845 17.235948563  
C 0.460718513 2.238128901 17.251976013  
C 1.690481186 1.528376579 17.298246384  
C 2.920442820 2.238039494 17.319250107  
C 4.149717808 1.529910445 17.347799301  
C 5.380847454 2.240700245 17.348114014  
C 6.611208439 1.531297803 17.346832275  
C 7.840795040 2.241211176 17.320821762  
C 9.071017265 1.531912684 17.296274185  
C 10.300968170 2.241289616 17.256654739  
C 11.529546738 1.530466676 17.237846375  
C 12.760137558 2.237982512 17.213699341  
C -2.000144720 3.656247616 17.164831161  
C -0.768270969 4.354085922 17.109170914  
C 0.461583853 3.653685808 17.196596146  
C 1.695095301 4.364766121 17.208457947  
C 2.921057940 3.658179522 17.282104492  
C 4.151939869 4.368824959 17.282888412  
C 5.382169247 3.659316063 17.320158005  
C 6.611778259 4.369657993 17.299131393  
C 7.841665745 3.661351919 17.299533844  
C 9.070959091 4.371805668 17.257999420  
C 10.302453995 3.662453175 17.233715057  
C 11.529558182 4.370879173 17.177364349  
C -3.234141827 5.793680191 17.162015915  
C -2.013909340 6.511420727 17.104057312  
C -0.777466059 5.786833286 16.995637894

**Pt<sub>5</sub> Isomer 3**

C -6.907557487 12.106749535 17.228391647  
C 1.702708721 0.035984140 17.210445404  
C -4.447143078 12.106517792 17.241373062  
C 4.163208961 0.033326093 17.237857819  
C -1.987729073 12.106046677 17.254264832  
C 6.622358322 0.032887124 17.252227783  
C 0.471683979 12.105436325 17.233119965  
C 9.081820488 0.031854097 17.233699799  
C 2.932223797 12.102183342 17.205461502  
C 11.542718887 0.031900357 17.222806931  
C 5.392533302 12.106571198 17.220783234  
C 14.002241135 0.032183267 17.217817307  
C -0.761158764 1.450314283 17.197359085  
C 0.467936516 2.156961441 17.141836166  
C 1.701909661 1.451736808 17.153472900  
C 2.937210083 2.162614107 17.138172150  
C 4.166424274 1.451996088 17.204517365  
C 5.394892693 2.161514759 17.230636597  
C 6.624240398 1.452094078 17.259796143  
C 7.853499413 2.161789656 17.280612946

Pt 4.756580353 5.811820507 13.309175491

C 0.471734524 6.507763386 16.967508316  
C 1.705558300 5.777803421 17.109466553  
C 2.923984289 6.481314182 17.110975266  
C 4.152922153 5.783913612 17.210674286  
C 5.385476112 6.496647358 17.200347900  
C 6.611906052 5.789576530 17.254032135  
C 7.841300964 6.501052856 17.236679077  
C 9.069684982 5.791190624 17.238437653  
C 10.297694206 6.503108501 17.210494995  
C -4.461245060 7.922505379 17.229967117  
C -3.231936455 8.634038925 17.241914749  
C -2.005642176 7.926913738 17.186042786  
C -0.773077488 8.639659882 17.195890427  
C 0.455963612 7.941960335 17.101482391  
C 1.674487591 8.645502090 17.103578568  
C 2.908792019 7.914914131 16.971141815  
C 4.157660961 8.636181831 17.001274109  
C 5.393786430 7.911933899 17.114723206  
C 6.614068031 8.629799843 17.170381546  
C 7.842288494 7.920444489 17.216165543  
C 9.070350647 8.632371902 17.237884521  
C -5.690928459 10.051733971 17.257968903  
C -4.461585045 10.762211800 17.295476913  
C -3.231720686 10.053936005 17.288709641  
C -2.002160072 10.764304161 17.308197021  
C -0.772088528 10.054810524 17.268335342  
C 0.458761215 10.765427589 17.270053864  
C 1.684805870 10.058679581 17.199798584  
C 2.918376923 10.769707680 17.192195892  
C 4.148375988 10.069140434 17.110872269  
C 5.380064011 10.767051697 17.168931961  
C 6.610371590 10.052541733 17.183519363  
C 7.837509155 10.761045456 17.237798691  
Pt -0.130088329 6.120355129 12.420996666  
Pt 3.604191780 8.308867455 14.905929565  
Pt 3.541715622 8.258344650 12.425025940  
Pt -0.213700771 6.098444939 14.901713371  
Pt 1.700871468 7.195830345 13.640213966

C 9.082814217 1.450922489 17.269216537  
C 10.312518120 2.162283421 17.276475906  
C 11.541488647 1.451609969 17.246397018  
C 12.770736694 2.161540270 17.227674484  
C -1.989974737 3.582695961 17.241994858  
C -0.762550473 4.291171074 17.173728943  
C 0.455922842 3.571738720 17.079223633  
C 1.699730396 4.274271965 16.930219650  
C 2.947966814 3.571749210 17.055458069  
C 4.170042038 4.289675713 17.126146317  
C 5.396837234 3.581431150 17.219860077  
C 6.624217510 4.292453289 17.272165298  
C 7.853698254 3.582398653 17.299785614  
C 9.082293510 4.293111324 17.321895599  
C 10.312591553 3.582503796 17.306371689  
C 11.541603088 4.293500423 17.296337128  
C -3.218762636 5.715007305 17.314037323  
C -1.989881396 6.425976753 17.277231216  
C -0.763715744 5.718490601 17.196517944  
C 0.453636408 6.430889606 17.084337234

C	1.677776337	5.711046219	16.884571075
C	2.955018282	6.427106857	16.862951279
C	4.182214737	5.707641125	17.076814651
C	5.395773888	6.421236515	17.196819305
C	6.623335361	5.713365555	17.276729584
C	7.852199554	6.424420357	17.318202972
C	9.081448555	5.714129925	17.335018158
C	10.311859131	6.425186157	17.335731506
C	-4.448451996	7.845867634	17.327816010
C	-3.219003201	8.556510925	17.305000305
C	-1.989710331	7.847351074	17.275621414
C	-0.761771679	8.557852745	17.220186234
C	0.465958118	7.850570679	17.125108719
C	1.688489914	8.566901207	17.051069260
C	2.938814640	7.868196011	16.917253494
C	4.180610657	8.567553520	17.105369568
C	5.395196438	7.849768639	17.197385788
C	6.623301983	8.556746483	17.262998581
C	7.852339745	7.846222878	17.308141708

#### Pt5 Isomer 4

C	-6.940713882	12.146049500	17.196561813
C	1.668501973	0.072596900	17.284070969
C	-4.482930183	12.146444321	17.339155197
C	4.126880169	0.073941976	17.385351181
C	-2.021297455	12.147800446	17.397161484
C	6.587132454	0.076950379	17.381097794
C	0.437659264	12.153041840	17.329315186
C	9.046760559	0.078811973	17.260324478
C	2.894545078	12.154419899	17.159158707
C	11.507894516	0.078500681	17.119676590
C	5.362089157	12.152151108	17.081769943
C	13.970400810	0.074497655	17.146923065
C	-0.792739987	1.493851542	17.163719177
C	0.437030911	2.202376366	17.224090576
C	1.668300509	1.492067575	17.295957565
C	2.897057772	2.200343370	17.346776962
C	4.127366543	1.492924571	17.381593704
C	5.358519077	2.205587626	17.377637863
C	6.588616848	1.497508287	17.369125366
C	7.817438602	2.207596779	17.314888000
C	9.048441887	1.498882890	17.262363434
C	10.276071548	2.205139637	17.192575455
C	11.506277084	1.492858410	17.146680832
C	12.738292694	2.200870752	17.131235123
C	-2.023703575	3.619433403	17.099248886
C	-0.793842196	4.317677498	17.076120377
C	0.434808969	3.616235495	17.194820404
C	1.669657946	4.325231552	17.265871048
C	2.897968769	3.621006489	17.326852798
C	4.128238201	4.333226681	17.314155579
C	5.360123634	3.623664618	17.338985443
C	6.587409019	4.334919930	17.297409058
C	7.817594528	3.626482964	17.286399841
C	9.047302246	4.335954666	17.226379395
C	10.277204514	3.626685619	17.179374695
C	11.504650116	4.335546970	17.119895935
C	-3.259349823	5.756598949	17.137378693
C	-2.037730217	6.473435402	17.110071182
C	-0.806673527	5.748942375	16.990556717

#### Pt5 Isomer 5

C	-6.931604862	12.177978516	17.281053543
C	1.678210735	0.105035909	17.299558640
C	-4.472851276	12.178693771	17.298353195

C	9.081401825	8.556407928	17.316820145
C	-5.677953243	9.976936340	17.288454056
C	-4.448247910	10.688055038	17.278129578
C	-3.218686581	9.977226257	17.286209106
C	-1.989690304	10.686596870	17.261949539
C	-0.760136127	9.977227211	17.229612350
C	0.468659401	10.686639786	17.201412201
C	1.697896957	9.976777077	17.136547089
C	2.933268070	10.686508179	17.155868530
C	4.167852402	9.979909897	17.164245605
C	5.396217823	10.688092232	17.215248108
C	6.623952866	9.977300644	17.246459961
C	7.853774071	10.687185287	17.259475708
Pt	1.593030214	4.988266945	12.339386940
Pt	3.023175716	6.940820694	12.324122429
Pt	2.994729042	7.116576195	14.806550980
Pt	1.565566778	4.981066227	14.822643280
Pt	4.155415058	8.839239120	13.341952324

C	0.440395832	6.462593079	17.040031433
C	1.680807590	5.734703064	17.205368042
C	2.900376558	6.438292027	17.167316437
C	4.129821777	5.746676922	17.222738266
C	5.362622261	6.465243340	17.166286469
C	6.587945938	5.756022930	17.233232498
C	7.816770077	6.466099739	17.212789536
C	9.046374321	5.755388260	17.215894699
C	10.272473335	6.466273785	17.199743271
C	-4.486364841	7.886377811	17.241830826
C	-3.257027149	8.595889091	17.292383194
C	-2.030604362	7.884406567	17.250547409
C	-0.801230431	8.599266052	17.296266556
C	0.417913437	7.899893761	17.192373276
C	1.652289391	8.609860420	17.076404572
C	2.881588936	7.857364655	16.926866531
C	4.144291878	8.589335442	16.803382874
C	5.375682831	7.873707294	17.034177780
C	6.591136456	8.591036797	17.096076965
C	7.818227768	7.884571075	17.185005188
C	9.047161102	8.596565247	17.227294922
C	-5.711535931	10.016123772	17.243175507
C	-4.483651638	10.724514008	17.319522858
C	-3.254286528	10.014622688	17.348340988
C	-2.021443367	10.726628304	17.382591248
C	-0.794126987	10.019792557	17.354053497
C	0.437865257	10.734081268	17.309602737
C	1.664965153	10.042671204	17.176092148
C	2.886379719	10.742156982	17.081640244
C	4.126286030	10.036573410	16.887580872
C	5.369665623	10.736521721	17.000215530
C	6.592877388	10.019154549	17.068210602
C	7.818389893	10.726947784	17.170045853
Pt	0.843509197	7.370632648	12.743373871
Pt	4.108437061	9.265180588	14.740961075
Pt	3.378047466	7.728715897	12.842554092
Pt	0.044221163	6.294658184	14.905494690
Pt	1.913835049	8.013988495	14.950198174

C	4.139050961	0.105136573	17.302202225
C	-2.011324406	12.179464340	17.267400742
C	6.596936226	0.106177755	17.269550323



C	0.448985100	12.179695129	17.221935272
C	9.056506157	0.108241573	17.252384186
C	2.905655861	12.181940079	17.234655380
C	11.518621445	0.108556062	17.257240295
C	5.368789673	12.181531906	17.244773865
C	13.977118492	0.106577829	17.270305634
C	-0.783391297	1.526326895	17.267410278
C	0.448464274	2.237239361	17.266881943
C	1.679657459	1.525760055	17.295886993
C	2.908527374	2.232133865	17.304460526
C	4.139893532	1.523766994	17.316219330
C	5.369462967	2.233688354	17.317996979
C	6.598437309	1.525134325	17.305633545
C	7.828366280	2.237543821	17.303503036
C	9.058357239	1.528544426	17.286718369
C	10.286715508	2.237076521	17.280029297
C	11.517919540	1.525058270	17.270252228
C	12.747999191	2.233766079	17.256481171
C	-2.012631655	3.654466391	17.217248917
C	-0.785344362	4.356663227	17.165199280
C	0.448543072	3.651594639	17.214591980
C	1.683529377	4.358566284	17.207830429
C	2.910654545	3.652003527	17.272218704
C	4.140955925	4.362302303	17.274925232
C	5.371704578	3.654242039	17.308429718
C	6.597942352	4.365240097	17.301946640
C	7.829074860	3.656239986	17.304607391
C	9.058572769	4.366479874	17.283752441
C	10.287123680	3.657227755	17.269151688
C	11.517292023	4.367726326	17.223505020
C	-3.244365454	5.786418438	17.193834305
C	-2.019280910	6.497981548	17.113281250
C	-0.793217421	5.776121616	17.061727524
C	0.457986116	6.480873108	16.943489075
C	1.699366093	5.769588947	17.099531174
C	2.912631035	6.470043659	17.105159760

### Pts Isomer 6

C	-6.931981564	12.159794807	17.237716675
C	1.674916863	0.083250538	17.198448181
C	-4.473652363	12.157292366	17.152660370
C	4.135163307	0.085774302	17.084568024
C	-2.016607761	12.159983635	17.052753448
C	6.593447208	0.086393483	17.019580841
C	0.444287300	12.161481857	17.004146576
C	9.053277969	0.087078720	17.051609039
C	2.907930851	12.162486076	17.106803894
C	11.517489433	0.088426702	17.184885025
C	5.365230083	12.162369728	17.228443146
C	13.976374626	0.087184042	17.247671127
C	-0.787660956	1.502923846	17.248050690
C	0.443476796	2.210332155	17.230163574
C	1.671221018	1.501691580	17.187454224
C	2.900835514	2.210200548	17.110534668
C	4.135457993	1.503051758	17.054944992
C	5.364408016	2.211153746	17.007884979
C	6.595238686	1.503703952	17.021013260
C	7.825260162	2.212658644	17.054084778
C	9.053521156	1.504316211	17.083454132
C	10.282336235	2.215319395	17.152130127
C	11.513807297	1.506849289	17.197078705
C	12.740690231	2.212853670	17.237623215
C	-2.022593260	3.632963896	17.229749680
C	-0.796062350	4.340610981	17.217983246
C	0.441043615	3.629151106	17.221891403

C	4.142486572	5.778405190	17.215034485
C	5.372418880	6.494373798	17.224695206
C	6.597472668	5.787198544	17.274379730
C	7.829143524	6.498594761	17.271663666
C	9.058565140	5.788356304	17.271278381
C	10.285473824	6.498300076	17.240465164
C	-4.473855972	7.918414116	17.250860214
C	-3.243272066	8.631468773	17.224206924
C	-2.018342257	7.928845406	17.135046005
C	-0.799377918	8.640532494	17.024480820
C	0.425134182	7.917093754	16.783779144
C	1.692368507	8.648535728	16.792089462
C	2.917486191	7.901119709	16.957584381
C	4.153478622	8.631853104	17.073856354
C	5.379339218	7.915195942	17.175987244
C	6.600761890	8.627207756	17.223943710
C	7.830922127	7.916350842	17.259504318
C	9.059740067	8.627275467	17.267791748
C	-5.701426983	10.049512863	17.276538849
C	-4.473714352	10.758955956	17.280590057
C	-3.242827415	10.050306320	17.243942261
C	-2.013256073	10.757950783	17.216320038
C	-0.788124084	10.050158501	17.113300323
C	0.449485302	10.764819145	17.117536545
C	1.676173687	10.070035934	17.034929276
C	2.901618004	10.770020485	17.147928238
C	4.141232014	10.055301666	17.124036789
C	5.370360851	10.760251999	17.200759888
C	6.597948074	10.049267769	17.227977753
C	7.828409195	10.759355545	17.268529892
Pt	-0.100590944	6.805757999	14.905022621
Pt	3.509950161	8.804229736	12.501526833
Pt	2.948858261	8.568510056	14.925208092
Pt	-0.553299904	6.449528694	12.473006248
Pt	1.530440807	7.529348850	13.089059830

C	1.666123867	4.325148582	17.168247223
C	2.891653061	3.619026184	17.087131500
C	4.130391121	4.335681438	16.956903458
C	5.371669292	3.630368233	16.988809586
C	6.597455502	4.338708878	17.073493958
C	7.825265884	3.632045984	17.093267441
C	9.051951408	4.343484879	17.146913528
C	10.279821396	3.632244825	17.170717239
C	11.509573936	4.343478680	17.201707840
C	-3.252824068	5.762956142	17.190275192
C	-2.026364803	6.472985268	17.168870926
C	-0.808620214	5.751563072	17.150810242
C	0.423226833	6.473661900	17.076278687
C	1.676055908	5.764593124	17.129138947
C	2.904566288	6.488721371	17.341815948
C	4.132237434	5.774837494	17.082859039
C	5.389429092	6.466883183	17.128311157
C	6.603543282	5.759844780	17.131135941
C	7.831347466	6.476765156	17.158079147
C	9.053201675	5.765659809	17.167539597
C	10.282176018	6.477281570	17.184307098
C	-4.473474503	7.895310879	17.183580399
C	-3.244536400	8.606927872	17.165195465
C	-2.022687435	7.895843506	17.155546188
C	-0.794898033	8.612775803	17.127300262
C	0.419239521	7.905757427	17.125392914
C	1.676484585	8.597870827	17.080381393

C	2.903838158	7.884243011	17.341474533
C	4.132564068	8.608080864	17.129293442
C	5.385424614	7.898900986	17.077848434
C	6.617304802	8.621029854	17.151424408
C	7.835081100	7.899605751	17.169721603
C	9.061546326	8.609654427	17.189729691
C	-5.700897694	10.029145241	17.200672150
C	-4.471154213	10.740349770	17.169439316
C	-3.243284464	10.029109955	17.144250870
C	-2.016608715	10.740540504	17.089914322
C	-0.788794994	10.033904076	17.068920135
C	0.436954498	10.742279053	16.984006882

### Pt5 Isomer 7

C	-6.965130329	12.135047913	17.138050079
C	1.644816041	0.061716095	17.175024033
C	-4.505606651	12.135591507	17.199666977
C	4.103623867	0.064337455	17.237136841
C	-2.045418739	12.135859489	17.245162964
C	6.564666748	0.063847817	17.251804352
C	0.414083004	12.136732101	17.243478775
C	9.025178909	0.064327240	17.224205017
C	2.874863148	12.137914658	17.197107315
C	11.484455109	0.062898666	17.163938522
C	5.335274220	12.133399963	17.131391525
C	13.945755005	0.061451517	17.132770538
C	-0.815562665	1.480642438	17.131668091
C	0.413604617	2.189035177	17.134273529
C	1.643110752	1.480208158	17.176570892
C	2.872406483	2.190381050	17.213209152
C	4.103723049	1.482667565	17.242712021
C	5.336860180	2.194812059	17.237316132
C	6.567251205	1.483750701	17.241014481
C	7.797111988	2.191975832	17.215427399
C	9.027353287	1.482565284	17.208639145
C	10.256633759	2.192122221	17.169944763
C	11.485926628	1.481945515	17.155048370
C	12.715681076	2.192320585	17.125192642
C	-2.043272495	3.612308264	17.101247787
C	-0.816020489	4.321794510	17.070726395
C	0.412910938	3.607823610	17.086921692
C	1.643722296	4.307949543	17.068950653
C	2.869109392	3.607520103	17.179683685
C	4.105380058	4.315830231	17.184713364
C	5.338994980	3.609771013	17.196409225
C	6.571771622	4.319484711	17.142995834
C	7.800381184	3.610141039	17.171262741
C	9.028183937	4.322110176	17.136543274
C	10.258446693	3.612318516	17.141141891
C	11.485224724	4.322927475	17.112167358
C	-3.276354790	5.743391991	17.108875275
C	-2.048254728	6.456195354	17.107707977
C	-0.819057703	5.745532990	17.069248199

### Pt5 Isomer 8

C	-6.944902420	12.174220085	17.159688950
C	1.664641261	0.102058813	17.162292480
C	-4.485692024	12.173856735	17.174800873
C	4.124363899	0.102229185	17.178924561
C	-2.026206017	12.174201965	17.192518234
C	6.583849907	0.101229884	17.193611145
C	0.433569908	12.174685478	17.192899704
C	9.044112206	0.099961609	17.181236267
C	2.894855499	12.170874596	17.161819458
C	11.505572319	0.100378007	17.157789230

C	1.678347588	10.036958694	16.952671051
C	2.917099476	10.753678322	17.083654404
C	4.142556190	10.047592163	17.166646957
C	5.367676258	10.743588448	17.220531464
C	6.604784966	10.032077789	17.217384338
C	7.831297874	10.739709854	17.229059219
Pt	2.906331539	7.186593056	13.101572037
Pt	3.859445572	5.499482155	14.903178215
Pt	1.331594229	6.294273853	14.987935066
Pt	1.951311111	8.874536514	14.901432037
Pt	4.479291916	8.079051018	14.988717079

C	0.400190592	6.461052418	17.047605515
C	1.635076523	5.737807751	16.958805084
C	2.878494024	6.456040382	17.027154922
C	4.107262611	5.719181061	17.093776703
C	5.339124680	6.435986519	16.930284500
C	6.584257126	5.730648994	17.041032791
C	7.799434662	6.448943615	17.053993225
C	9.028343201	5.741335392	17.101163864
C	10.256166458	6.453588963	17.106872559
C	-4.504781246	7.874719143	17.113452911
C	-3.277541161	8.585393906	17.149660110
C	-2.047848940	7.874349594	17.144701004
C	-0.817938328	8.585336685	17.178945541
C	0.407133102	7.876296520	17.145097733
C	1.639724731	8.591874123	17.172620773
C	2.869928837	7.895249844	17.114906311
C	4.092901230	8.599873543	17.069103241
C	5.332159519	7.885468960	16.900091171
C	6.576723099	8.592176437	16.987453461
C	7.797240734	7.87629965	17.034261703
C	9.025256157	8.585349083	17.088468552
C	-5.734208107	10.005367279	17.115629196
C	-4.505126953	10.715234756	17.169784546
C	-3.276697874	10.005557060	17.184638977
C	-2.046310425	10.716753960	17.224081039
C	-0.816817760	10.007053375	17.221611023
C	0.411524773	10.717592239	17.232736588
C	1.642308235	10.008621216	17.207408905
C	2.872541428	10.718702316	17.186950684
C	4.101604939	10.012187004	17.123010635
C	5.335577011	10.718398094	17.097402573
C	6.568004131	10.007535934	17.058444977
C	7.796410561	10.715799332	17.104703903
Pt	2.605985165	6.240029335	14.879306793
Pt	2.788325071	5.727296352	12.490842819
Pt	5.101039886	6.805755615	12.387708664
Pt	5.064128399	7.077943802	14.818621635
Pt	3.195585251	7.685448170	11.039928436

C	5.355765343	12.175084114	17.152215958
C	13.965542793	0.101696327	17.155879974
C	-0.795772254	1.520656109	17.160282135
C	0.434051394	2.230101347	17.158641815
C	1.663766742	1.521947980	17.155061722
C	2.894805193	2.234313726	17.152210236
C	4.125675678	1.521710753	17.169010162
C	5.356129646	2.229462862	17.181470871
C	6.585667610	1.520103931	17.191452026
C	7.815906525	2.229588032	17.195314407

C	9.045439720	1.519510508	17.187688828
C	10.275141716	2.230232954	17.184370041
C	11.504859924	1.519962192	17.169734955
C	12.734405518	2.230238676	17.169069290
C	-2.026413441	3.650683880	17.181758881
C	-0.796359420	4.360634804	17.177801132
C	0.431946754	3.649635553	17.162073135
C	1.660765648	4.359278202	17.139247894
C	2.894905090	3.650331020	17.136259079
C	4.130067348	4.358620167	17.145540237
C	5.359201431	3.648856163	17.178661346
C	6.587565422	4.358732700	17.195228577
C	7.817328453	3.649540901	17.201562881
C	9.046190262	4.359685421	17.207740784
C	10.275307655	3.649758577	17.198236465
C	11.505183220	4.360393047	17.198713303
C	-3.254273176	5.781358242	17.212909698
C	-2.025816917	6.491322517	17.216327667
C	-0.795645475	5.780676365	17.198663712
C	0.433159828	6.488632202	17.177604675
C	1.650390148	5.772910118	17.108133316
C	2.895493746	6.478786469	16.975383759
C	4.140810013	5.770941734	17.105289459
C	5.361271858	6.485129833	17.160614014
C	6.587540150	5.779382229	17.198345184
C	7.817946911	6.490981102	17.208522797
C	9.045933723	5.781274319	17.213979721
C	10.275585175	6.492066383	17.216741562
C	-4.484953880	7.911627293	17.214292526

**Pts Isomer 9**

C	7.717581749	12.162853241	17.129205704
C	1.566659212	0.091021985	17.124479294
C	-4.583013535	12.162282944	17.122838974
C	4.026581764	0.090966471	17.115690231
C	-2.123983383	12.162816048	17.108860016
C	6.485949039	0.090623006	17.104694366
C	0.335762024	12.163864136	17.089702606
C	8.945704460	0.089476272	17.094379425
C	2.796798706	12.159754753	17.086723328
C	11.407429695	0.088982694	17.109491348
C	5.257656574	12.163051605	17.117044449
C	13.867562294	0.090308726	17.127149582
C	13.866068840	1.508658767	17.125986099
C	0.335487247	2.218559265	17.117076874
C	1.565749884	1.510179043	17.114170074
C	2.796683311	2.222952127	17.101623535
C	4.027647972	1.510571837	17.110183716
C	5.257427216	2.218648911	17.113245010
C	6.487509727	1.508880615	17.113067627
C	7.717238903	2.219052076	17.116485596
C	8.946746826	1.508617640	17.112142563
C	10.176638603	2.219616890	17.121852875
C	11.406482697	1.508584380	17.121780396
C	12.635614395	2.218760014	17.126602173
C	12.634567261	3.638391733	17.124753952
C	-0.895626426	4.348678112	17.108343124
C	0.332917690	3.638050556	17.101039886
C	1.561661005	4.347737312	17.065002441
C	2.796387672	3.638139248	17.075601578
C	4.030452728	4.346372604	17.076471329
C	5.260076523	3.637275696	17.109874725
C	6.488185883	4.349458218	17.121074677
C	7.718263626	3.639292240	17.125274658
C	8.946456909	4.349469185	17.134441376

C	-3.255190134	8.622676849	17.216211319
C	-2.026863575	7.912684441	17.222183228
C	-0.797445297	8.623672485	17.217658997
C	0.430451870	7.915990353	17.193748474
C	1.645642281	8.634217262	17.139186859
C	2.886901379	7.927420616	16.987476349
C	4.138870716	8.631984711	17.077178955
C	5.360572338	7.913749695	17.138082504
C	6.586622238	8.622380257	17.169761658
C	7.817235947	7.911391735	17.197517395
C	9.045162201	8.622029305	17.201293945
C	-5.715060234	10.043530464	17.185520172
C	-4.485783577	10.754169464	17.188642502
C	-3.255835533	10.043643951	17.204471588
C	-2.027228832	10.753760338	17.202926636
C	-0.797436237	10.043967247	17.207387924
C	0.430966377	10.755540848	17.197063446
C	1.659179688	10.046765327	17.170984268
C	2.894449711	10.754357338	17.145923615
C	4.128268242	10.048080444	17.122266769
C	5.357686043	10.755563736	17.143795013
C	6.586331367	10.043731689	17.156324387
C	7.815770626	10.753572464	17.166625977
Pt	3.011729717	7.325347900	14.905977249
Pt	3.534682274	8.462854385	12.638907433
Pt	1.143215656	8.526096344	13.408913612
Pt	1.196401119	6.005516529	13.547462463
Pt	3.564003706	5.939088821	12.698055267

C	10.176530838	3.638362885	17.131738663
C	11.405958176	4.348889351	17.131248474
C	11.405954361	5.770032406	17.131038666
C	-2.126176357	6.480129719	17.113727570
C	-0.896340847	5.768195152	17.096317291
C	0.331399202	6.475219250	17.047302246
C	1.550820351	5.759561539	17.004947662
C	2.796009302	6.468482971	16.883335114
C	4.041877747	5.760675907	17.027893066
C	5.260341644	6.477854729	17.095302582
C	6.488741875	5.769026279	17.130331039
C	7.717975616	6.480290890	17.141607285
C	8.946269035	5.769918442	17.141721725
C	10.176169395	6.481057644	17.139102936
C	10.176298141	7.900010586	17.137094498
C	-3.354159832	8.611095428	17.122749329
C	-2.126097918	7.900497437	17.105772018
C	-0.896368027	8.612103462	17.074455261
C	0.330807209	7.902825832	17.029684067
C	1.551459789	8.620973587	16.980632782
C	2.799426079	7.913746834	16.896884918
C	4.042651176	8.621026993	17.023241043
C	5.261241436	7.903619289	17.091211319
C	6.488645077	8.612336159	17.125368118
C	7.718316078	7.901169300	17.139934540
C	8.946254730	8.611371994	17.140169144
C	8.946918488	10.031974792	17.135295868
C	-4.583351612	10.743309975	17.128000259
C	-3.353732109	10.032307625	17.118942261
C	-2.125200748	10.742764473	17.103904724
C	-0.895209789	10.032382965	17.079563141
C	0.333299160	10.744488716	17.067457199
C	1.562613487	10.036238670	17.030878067
C	2.797149181	10.743865967	17.054374695

C	4.031509399	10.035414696	17.064922333	Pt	4.541263580	5.730216026	13.773754120
C	5.259928226	10.744069099	17.106681824	Pt	2.892936230	6.974253654	12.305805206
C	6.488665581	10.032222748	17.121915817	Pt	4.863016605	7.576768875	10.960653305
C	7.718146801	10.742342949	17.131557465	Pt	2.811927795	7.251556396	14.806268692
Pt	6.378425121	6.169412613	12.270461082				

**Table S6.** Cartesian coordinates of 7 isomers of Pt<sub>6</sub>, 6 isomers of which were previously reported [1]. Isomer 2 is missing due to the same structure with isomer 1 in [1], while a new isomer 8 is added.

### Pt<sub>6</sub> Isomer 1

C	-6.898913383	12.162541389	17.285364151	C	0.459092855	6.487608433	16.881858826
C	1.711371541	0.088303678	17.262121201	C	1.698215723	5.753986359	16.824436188
C	-4.438794613	12.161600113	17.243446350	C	2.958275080	6.499007702	16.833126068
C	4.170933723	0.088135980	17.218212128	C	4.194389343	5.766082287	16.902498245
C	-1.979380131	12.162838936	17.204248428	C	5.420396328	6.491455078	17.090137482
C	6.630289078	0.089873441	17.200767517	C	6.636738300	5.774618149	17.145404816
C	0.480364799	12.164485931	17.202621460	C	7.864932060	6.484073639	17.193538666
C	9.089681625	0.091329843	17.225610733	C	9.090969086	5.771909714	17.193796158
C	2.939418316	12.164415359	17.246028900	C	10.319182396	6.482191086	17.186408997
C	11.549939156	0.090619728	17.271757126	C	-4.439178467	7.902046204	17.193809509
C	5.399782181	12.162970543	17.288873672	C	-3.207246304	8.611496925	17.166538239
C	14.011014938	0.090189807	17.289592743	C	-1.982094049	7.903349876	17.105827332
C	-0.749665976	1.510361671	17.263637543	C	-0.749677181	8.616496086	17.080226898
C	0.481141448	1.508554974	17.227163315	C	0.476893902	7.919486046	16.996932983
C	1.711212873	2.528711815	17.231348038	C	1.711577415	8.618980408	17.068431854
C	2.940813065	2.215761900	17.183032990	C	2.946052551	7.920899391	17.034334183
C	4.170844078	1.507848978	17.191810608	C	4.170692444	8.616933823	17.159854889
C	5.399887085	2.216388941	17.166633060	C	5.406387806	7.903024673	17.172819138
C	6.629378319	1.509978414	17.189807892	C	6.632969379	8.612496376	17.236429214
C	7.859178066	2.220649719	17.191120148	C	7.863001823	7.902896404	17.222572327
C	9.088088036	1.512327433	17.220012665	C	9.093011856	8.612389565	17.228347778
C	10.319091797	2.221436262	17.229478836	C	-5.668295860	10.032241821	17.251724243
C	11.549236298	1.511733890	17.256601334	C	-4.437619686	10.740998268	17.235601425
C	12.779606819	2.220402956	17.245822906	C	-3.208804846	10.032859802	17.194196701
C	-1.982185721	3.640487671	17.193902969	C	-1.979056835	10.742826462	17.184587479
C	-0.755487800	4.349679947	17.124120712	C	-0.749827385	10.036404610	17.145313263
C	0.482275724	3.636198759	17.143653870	C	0.480501175	10.744800568	17.169544220
C	1.707716465	4.330564022	17.039257050	C	1.710767746	10.036677361	17.160472870
C	2.940648794	3.633404016	17.091854095	C	2.940004349	10.744219780	17.218477249
C	4.174653530	4.333480358	17.028549194	C	4.170483589	10.033962250	17.232109070
C	5.398818493	3.637012720	17.110862732	C	5.400856495	10.742613792	17.276741028
C	6.631751060	4.351681709	17.131359100	C	6.631499290	10.032635689	17.273567200
C	7.857050896	3.642961979	17.172906876	C	7.861820698	10.741495132	17.279403687
C	9.089397430	4.352222443	17.190940857	Pt	5.752182484	5.842380524	13.413640976
C	10.317434311	3.641492367	17.206977844	Pt	3.635602474	6.149019718	14.756200790
C	11.547703743	4.351154804	17.187736511	Pt	1.067544699	6.076689720	14.766685486
C	-3.214803219	5.770270348	17.162233353	Pt	1.955837250	7.403719425	10.929788589
C	-1.987895131	6.480840206	17.102333069	Pt	1.146271706	5.592498302	12.352581978
C	-0.771053791	5.763808250	17.037429810	Pt	3.624668837	6.134196758	12.262310982

### Pt<sub>6</sub> Isomer 3

C	-6.958950043	12.200829506	17.361490250	C	0.421923876	2.256784678	17.279102325
C	1.651405811	0.124496788	17.336303711	C	1.651892900	1.543840766	17.269550323
C	-4.499289513	12.200244904	17.355140686	C	2.881119251	2.238994360	17.191749573
C	4.111675262	0.127685726	17.345031738	C	4.112061501	1.543678761	17.273832321
C	-2.036702633	12.202177048	17.375532150	C	5.348896027	2.256671906	17.274991989
C	6.572657585	0.129105091	17.374677658	C	6.574818611	1.549977422	17.344228745
C	0.423463821	12.203581810	17.384435654	C	7.805611610	2.261229038	17.356485367
C	9.034220695	0.132081866	17.383428574	C	9.036199570	1.552272677	17.380195618
C	2.883903027	12.206633568	17.376319885	C	10.264112473	2.262583017	17.380525589
C	11.493808746	0.133192211	17.376472473	C	11.496260643	1.553873062	17.375865936
C	5.343919754	12.205907822	17.370346069	C	12.724163055	2.262905836	17.351846695
C	13.952784538	0.130074173	17.358720779	C	-2.035319805	3.685549498	17.338109970
C	-0.804783046	1.552025318	17.335197449	C	-0.813188910	4.395155907	17.283107758

C	0.419775724	3.681098461	17.234115601
C	1.629852772	4.381032944	17.104858398
C	2.871894598	3.665277958	17.009784698
C	4.131287575	4.392040253	17.041740417
C	5.360766888	3.672224283	17.200597763
C	6.578914642	4.389095783	17.276260376
C	7.807929993	3.679251909	17.339931488
C	9.034709930	4.391702175	17.366041183
C	10.264865875	3.682861805	17.376621246
C	11.491874695	4.394376755	17.363979340
C	-3.270251989	5.813078403	17.365591049
C	-2.043531895	6.525432587	17.341264725
C	-0.814514637	5.816910744	17.279594421
C	0.401797295	6.533706188	17.202407837
C	1.630267859	5.813946247	17.006742477
C	2.890900850	6.541137695	17.011161804
C	4.131633759	5.822819710	17.106575012
C	5.346000671	6.524353027	17.232030869
C	6.576086044	5.810435772	17.283781052
C	7.800724030	6.520766735	17.339294434
C	9.032512665	5.811383724	17.364206314
C	10.258953094	6.522228241	17.375980377
C	-4.500740528	7.942361355	17.380310059
C	-3.271840096	8.653041840	17.379768372
C	-2.041121721	7.943898201	17.355834961
C	-0.811517239	8.653830528	17.345630646

#### Pt<sub>6</sub> Isomer 4

C	-6.962720394	12.222198486	17.179670334
C	1.646696210	0.150440499	17.207151413
C	-4.505735397	12.225414276	17.274339676
C	4.104827881	0.154724032	17.297386169
C	-2.044558525	12.227991104	17.316728592
C	6.564634323	0.156144172	17.297460556
C	0.412053585	12.232268333	17.241062164
C	9.031566620	0.155671850	17.166130066
C	2.875670433	12.238823891	17.049272537
C	11.486849785	0.156576157	17.062858582
C	5.339555264	12.224659920	17.084232330
C	13.945097923	0.149636030	17.114351273
C	-0.813259006	1.572189808	17.092193604
C	0.418204308	2.280395269	17.099523544
C	1.647742271	1.570950866	17.162841797
C	2.875507355	2.280739069	17.207626343
C	4.106150150	1.571725130	17.277532578
C	5.339682579	2.280211926	17.303609848
C	6.567723274	1.575447202	17.302185059
C	7.801205635	2.283939123	17.280780792
C	9.031579971	1.574824572	17.208700180
C	10.259185791	2.284686565	17.163824081
C	11.488816261	1.575396657	17.101203918
C	12.720201492	2.283739567	17.091058731
C	-2.038343906	3.706316233	17.106567383
C	-0.812520266	4.413575649	17.072059631
C	0.420332909	3.699111700	17.056282043
C	1.651928902	4.399502277	17.045209885
C	2.875775576	3.699894905	17.167716980
C	4.114982605	4.405612946	17.250158310
C	5.342576981	3.699404240	17.307207108
C	6.571774960	4.410072327	17.330701828
C	7.802499771	3.700953245	17.306228638
C	9.032931328	4.412921429	17.280040741
C	10.260208130	3.705416441	17.206848145
C	11.489473343	4.416215897	17.172611237
C	-3.272068024	5.833644867	17.218883514

C	0.415979385	7.944985390	17.278827667
C	1.652626514	8.659303665	17.276405334
C	2.882050514	7.965191364	17.197721481
C	4.111474991	8.660523415	17.273420334
C	5.342445850	7.947786808	17.278158188
C	6.568157673	8.652265549	17.334707260
C	7.800044537	7.941482067	17.352239609
C	9.028142929	8.650790215	17.376996994
C	-5.729775906	10.071754456	17.379362106
C	-4.500766754	10.779998779	17.380199432
C	-3.269939661	10.071784973	17.385318756
C	-2.038944721	10.782230377	17.385673523
C	-0.808906078	10.074227333	17.373851776
C	0.421715260	10.784505844	17.373477936
C	1.652883530	10.076117516	17.343423843
C	2.882386684	10.786179543	17.351848602
C	4.112146378	10.078832626	17.335010529
C	5.342509270	10.785446167	17.359378815
C	6.570296288	10.074163437	17.358934402
C	7.799839973	10.781188011	17.372932434
Pt	0.892274380	7.917709351	13.662343979
Pt	2.270060539	6.197689533	14.910076141
Pt	3.542315722	3.979627848	14.922063828
Pt	4.148235321	5.482512951	11.1321114006
Pt	2.996769428	3.841826677	12.516126633
Pt	2.168228388	6.255748749	12.424794197

C	-2.043512344	6.546022892	17.191467285
C	-0.816189051	5.836968422	17.104356766
C	0.403357983	6.553341866	17.057535172
C	1.647879362	5.830428123	16.955001831
C	2.900594950	6.527155399	17.090877533
C	4.133776665	5.815374374	17.236026764
C	5.349142075	6.537933350	17.303121567
C	6.574297905	5.830917835	17.338066101
C	7.803967476	6.543742180	17.335525513
C	9.032320976	5.83265305	17.308252335
C	10.259580612	6.543642998	17.285234451
C	-4.502241611	7.964282513	17.309553146
C	-3.274296284	8.676030159	17.304061890
C	-2.045324564	7.964395523	17.253692627
C	-0.818377972	8.674585342	17.232648849
C	0.395380974	7.962530136	17.111824036
C	1.633206844	8.683300972	16.989610672
C	2.895493507	7.954452515	16.996248245
C	4.132166862	8.675510406	17.133123398
C	5.345323086	7.963618279	17.258895874
C	6.572206974	8.673999786	17.277492523
C	7.801519394	7.962449551	17.320390701
C	9.029401779	8.674331665	17.315021515
C	-5.732586384	10.094886780	17.289011002
C	-4.505192757	10.805163383	17.302045822
C	-3.276734591	10.094669342	17.320186615
C	-2.047211170	10.807382584	17.318269730
C	-0.822309494	10.100181580	17.280124664
C	0.393154144	10.822590828	17.221672058
C	1.626697063	10.110226631	17.086320877
C	2.880577564	10.807188988	16.960762024
C	4.124540329	10.084413528	17.076160431
C	5.343372345	10.801493645	17.124092102
C	6.570376873	10.092426300	17.212062836
C	7.798899651	10.804982185	17.230514526
Pt	3.557885170	8.102275848	12.962679863
Pt	2.549470186	6.854741096	15.028591156

Pt 1.854924440 6.159603119 12.691759109  
Pt 2.770592690 10.526034355 17.21619606

**Pt<sub>6</sub> Isomer 5**

C -6.996704102 12.209305763 17.226423264  
C 1.615077853 0.135967791 17.208873749  
C -4.533390522 12.207891464 17.219720840  
C 4.075233936 0.132812947 17.211629868  
C -2.074259281 12.207835197 17.229171753  
C 6.534943104 0.136624679 17.231182098  
C 0.383460522 12.212352753 17.236572266  
C 8.993332863 0.139991522 17.239341736  
C 2.843470573 12.213859558 17.233783722  
C 11.452459335 0.138555914 17.234842300  
C 5.303442001 12.210139275 17.233026505  
C 13.914561272 0.135681003 17.225229263  
C -0.847995460 1.556530356 17.199781418  
C 0.378732443 2.262868166 17.147771835  
C 1.613866091 1.550807834 17.157995224  
C 2.846531391 2.254485846 17.112396240  
C 4.075839520 1.553233862 17.169244766  
C 5.305140495 2.263942719 17.178947449  
C 6.533814430 1.557853699 17.217178345  
C 7.762742996 2.268310547 17.223464966  
C 8.991820335 1.559363246 17.237405777  
C 10.222980499 2.268538237 17.232439041  
C 11.450942039 1.558926225 17.229330063  
C 12.681398392 2.267808914 17.205831528  
C -2.080833912 3.685803175 17.189168930  
C -0.851757288 4.396154881 17.136934280  
C 0.369117498 3.680002928 17.080299377  
C 1.601027966 4.398746014 16.946002960  
C 2.854877472 3.676531315 16.990709305  
C 4.088722229 4.384257793 17.030920029  
C 5.306843281 3.685062885 17.136383057  
C 6.538753033 4.398374557 17.163799286  
C 7.762031078 3.690485001 17.207317352  
C 8.994461060 4.400279045 17.220523834  
C 10.221953392 3.689329624 17.226253510  
C 11.451488495 4.398007870 17.212444305  
C -3.306531429 5.817874908 17.211311340  
C -2.074686289 6.527350426 17.192869186  
C -0.849832296 5.816571712 17.149049759

**Pt<sub>6</sub> Isomer 6**

C -6.932883739 12.159041405 17.224227905  
C 1.677883387 0.086125612 17.224042892  
C -4.471404552 12.157814980 17.221149445  
C 4.137733459 0.084133215 17.216972351  
C -2.011752605 12.157466888 17.213060379  
C 6.598046780 0.085330628 17.210905075  
C 0.447326183 12.160015106 17.209239960  
C 9.057153702 0.087862380 17.211971283  
C 2.907634735 12.161201477 17.213489532  
C 11.516760826 0.087572925 17.219085693  
C 5.367535591 12.159225464 17.221359253  
C 13.978158951 0.086379714 17.224092484  
C -0.782204151 1.507126331 17.217376709  
C 0.446860909 2.215888739 17.210214615  
C 1.677276850 1.504791260 17.216690063  
C 2.908177614 2.214003086 17.204095840  
C 4.138012409 1.504366398 17.208139420  
C 5.368076324 2.212743998 17.197671890  
C 6.598570824 1.505245566 17.204648972  
C 7.826637268 2.216553450 17.197935104

Pt 2.015945435 9.797179222 15.028691292  
Pt 1.062176704 8.580718994 12.920959473

C 0.381565094 6.530405045 17.112419128  
C 1.594803810 5.829174042 17.006952286  
C 2.834291458 6.544888020 16.882059097  
C 4.093077660 5.814345837 16.889316559  
C 5.323847294 6.533591270 17.071567535  
C 6.540097237 5.820951939 17.152746201  
C 7.769083500 6.531075478 17.199251175  
C 8.996358871 5.818897247 17.219240189  
C 10.226983070 6.528573513 17.223335266  
C -4.532608032 7.948918343 17.227943420  
C -3.302155495 8.657423019 17.227067947  
C -2.074093103 7.947770596 17.206476212  
C -0.842051029 8.659014702 17.193832397  
C 0.382887363 7.954521179 17.146430969  
C 1.613681316 8.666703224 17.140985489  
C 2.840945721 7.970775604 17.064174652  
C 4.070739746 8.666934013 17.122085571  
C 5.311609745 7.949856758 17.116926193  
C 6.540278912 8.661100388 17.186651230  
C 7.768393040 7.949648857 17.202808380  
C 8.998636246 8.659923553 17.225799561  
C -5.763376236 10.078138351 17.231775284  
C -4.532460690 10.787334442 17.233270645  
C -3.303872108 10.078738213 17.232475281  
C -2.073480606 10.788633347 17.231262207  
C -0.843802452 10.081111908 17.218517303  
C 0.383888245 10.791902542 17.222820282  
C 1.614041805 10.085223198 17.198211670  
C 2.843816757 10.793191910 17.209991455  
C 4.072944641 10.085276604 17.194488525  
C 5.304851532 10.792428970 17.220218658  
C 6.536327362 10.082147598 17.216064453  
C 7.765523434 10.789266586 17.230648041  
Pt 4.916722298 8.155345917 14.236869812  
Pt 3.455636263 6.178539753 14.760979652  
Pt 2.103474140 4.054264545 14.733062744  
Pt 3.313233614 5.738398552 10.346888542  
Pt 2.330660820 5.094400883 12.522174835  
Pt 4.198203564 6.889528751 12.307855606

C 9.056609154 1.507625341 17.207311630  
C 10.287313461 2.217334986 17.206171036  
C 11.516366005 1.507926702 17.213836670  
C 12.746871948 2.217605352 17.210351944  
C -2.013723135 3.636504650 17.196481705  
C -0.783722997 4.346802711 17.182628632  
C 0.446157217 3.636790991 17.186544418  
C 1.673880339 4.346601009 17.152746201  
C 2.909771681 3.631578445 17.165662766  
C 4.139096260 4.328884125 17.120357513  
C 5.368332386 3.631549120 17.163787842  
C 6.599172592 4.346124649 17.157136917  
C 7.825351715 3.638522863 17.181228638  
C 9.057668686 4.348381996 17.186676025  
C 10.286691666 3.637955904 17.196666718  
C 11.516583443 4.347435474 17.194297791  
C -3.243256569 5.767565250 17.190313339  
C -2.013651371 6.477926731 17.183069229  
C -0.785248280 5.766461372 17.171619415  
C 0.443380117 6.476409912 17.140895844

C	1.663783312	5.760999203	17.099416733
C	2.898697376	6.485822201	16.994132996
C	4.146901131	5.759096622	16.996026993
C	5.382217407	6.484449387	17.102714539
C	6.602224827	5.768975258	17.146156311
C	7.830718040	6.478985786	17.174667358
C	9.059251785	5.767479897	17.185464859
C	10.288609505	6.477808952	17.191228867
C	-4.471199036	7.897994995	17.195781708
C	-3.241307259	8.607457161	17.197174072
C	-2.012184143	7.896994114	17.184366226
C	-0.780100822	8.606886864	17.176481247
C	0.446249485	7.899171352	17.149688721
C	1.677184105	8.613704681	17.153573990
C	2.906410694	7.916024685	17.110748291
C	4.135640144	8.613828659	17.157091141
C	5.371649265	7.898743153	17.149738312
C	6.599301815	8.608692169	17.184452057
C	7.829052925	7.898581982	17.183607101

**Pt<sub>6</sub> Isomer 7**

C	-6.989686012	12.147485733	17.329433441
C	1.620342612	0.075735122	17.320158005
C	-4.529664040	12.148163795	17.316036224
C	4.080442905	0.076222934	17.315401077
C	-2.069362164	12.148151398	17.313875198
C	6.540674686	0.075749926	17.317064285
C	0.390787601	12.147459984	17.324821472
C	9.000829697	0.074949458	17.325012207
C	2.850555897	12.146291733	17.342281342
C	11.460443497	0.074610174	17.331602097
C	5.310482502	12.146357536	17.345426559
C	13.920201302	0.074945264	17.328659058
C	-0.839340210	1.495704889	17.318492889
C	0.390809536	2.206520796	17.325809479
C	1.620853901	1.496376395	17.326028824
C	2.850625992	2.207268000	17.338642120
C	4.080469608	1.496725440	17.328859329
C	5.310315609	2.207349539	17.338432312
C	6.540135860	1.496470213	17.324497223
C	7.770092487	2.206706524	17.324798584
C	9.000247955	1.495753050	17.316669464
C	10.230228424	2.205898285	17.312664032
C	11.460391998	1.495106101	17.314426422
C	12.690578461	2.205833673	17.313278198
C	-2.069071054	3.626631975	17.314222336
C	-0.838871002	4.336904526	17.329828262
C	0.391721249	3.627131939	17.340734482
C	1.621342897	4.337300777	17.372358322
C	2.850998402	3.627413273	17.368345261
C	4.080416203	4.337502003	17.390352249
C	5.309998512	3.627538204	17.369493484
C	6.539505005	4.337533951	17.375261307
C	7.769078255	3.627287149	17.341993332
C	8.999630928	4.336975574	17.331842422
C	10.229781151	3.626667738	17.314685822
C	11.460352898	4.336733818	17.313669205
C	-3.299589396	5.757060051	17.319196701
C	-2.068989038	6.467005730	17.326675415
C	-0.838266134	5.757515430	17.341392517

**Pt<sub>6</sub> Isomer 8**

C	7.739838123	12.136078835	17.276336670
C	1.588313699	0.062754683	17.309112549
C	-4.560579777	12.136561394	17.317085266

C	9.059214592	8.608861923	17.197994232
C	-5.701435566	10.027733803	17.210838318
C	-4.471014977	10.737441063	17.215541840
C	-3.241930246	10.028028488	17.206195831
C	-2.011190891	10.737707138	17.206474304
C	-0.781319618	10.028868675	17.193737030
C	0.446902752	10.740133286	17.199771881
C	1.677388668	10.032546043	17.189472198
C	2.907347679	10.741015434	17.201133728
C	4.137113571	10.031324387	17.196651459
C	5.368109703	10.740585327	17.212070465
C	6.598553181	10.029596329	17.206937790
C	7.827507019	10.738304138	17.216506958
Pt	5.311686039	7.742098331	10.572776794
Pt	4.460507870	7.032915592	12.770470619
Pt	3.539384127	6.108448982	14.854463577
Pt	2.010613918	4.191075802	10.597142220
Pt	2.725681543	5.057594776	12.786932945
Pt	3.665522337	5.962029934	10.467031479

C	0.391524315	6.467340469	17.373064041
C	1.622136593	5.757769585	17.395975113
C	2.851010084	6.467293739	17.432861328
C	4.080484390	5.757985115	17.427122116
C	5.310081959	6.467378616	17.436296463
C	6.538830757	5.757829666	17.401645660
C	7.769363403	6.467464447	17.379863739
C	8.999100685	5.757610321	17.345832825
C	10.229799271	6.467030048	17.329332352
C	-4.530069828	7.887336254	17.330047607
C	-3.299502373	8.597223228	17.320816040
C	-2.068946362	7.887316227	17.326940536
C	-0.838433743	8.596894264	17.339698792
C	0.391592026	7.887151718	17.369573593
C	1.621228695	8.596814156	17.391525269
C	2.851440907	7.886639118	17.428037643
C	4.080616951	8.596817017	17.436683655
C	5.309710026	7.886751175	17.432748795
C	6.539823532	8.596935272	17.398767471
C	7.769469738	7.887170792	17.377742767
C	8.999408722	8.596917152	17.345968246
C	-5.760129452	10.017301559	17.335296631
C	-4.529924393	10.727564812	17.318634033
C	-3.299500704	10.017484665	17.316381454
C	-2.069061756	10.727484703	17.315765381
C	-0.838833809	10.017244339	17.329589844
C	0.391507626	10.727019310	17.339155197
C	1.621227741	10.016669273	17.370563507
C	2.850844383	10.726370811	17.375970840
C	4.080529690	10.015676498	17.402309418
C	5.310319424	10.726446152	17.379848480
C	6.539920807	10.016768456	17.377532959
C	7.769551277	10.727083206	17.345600128
Pt	6.606214046	5.860049725	13.981509209
Pt	5.502315998	8.035037994	13.993450165
Pt	4.168986797	10.077918053	13.975888252
Pt	1.736797094	5.857966423	13.990930557
Pt	2.838595867	8.034061432	13.998373032
Pt	4.171859741	5.727045536	14.000836372

C	4.048466206	0.064856835	17.328807831
C	-2.101622581	12.138118744	17.307079315
C	6.509539127	0.065714203	17.305986404



C	0.354932785	12.142524719	17.238006592	C	4.052937508	5.737418175	17.238594055
C	8.971419334	0.073792681	17.235372543	C	5.289306641	6.451220036	17.235284805
C	2.821932316	12.160056114	17.143056870	C	6.514680862	5.745507240	17.302238464
C	11.432377815	0.074243478	17.206054688	C	7.745916843	6.455563068	17.302043915
C	5.282176495	12.143309593	17.203273773	C	8.975829124	5.746293545	17.327255249
C	13.889277458	0.065214075	17.259361267	C	10.204847336	6.457103252	17.318407059
C	13.890703201	1.486321807	17.287693024	C	10.204820633	7.877023697	17.306982040
C	0.360353112	2.193247557	17.305198669	C	-3.328111649	8.588499069	17.293857574
C	1.590108514	1.483294725	17.316225052	C	-2.096579075	7.879148960	17.269792557
C	2.820188522	2.192356586	17.328344345	C	-0.872944832	8.589718819	17.216073990
C	4.049706936	1.483853102	17.340980530	C	0.357090473	7.873745441	17.169782639
C	5.281072617	2.194783449	17.349597931	C	1.571119785	8.574621201	17.055807114
C	6.511271477	1.487128019	17.340223312	C	2.811726093	7.857571125	16.982978821
C	7.741054535	2.197104931	17.339437485	C	4.073161125	8.585693359	16.977422714
C	8.972853661	1.487819791	17.303316116	C	5.301550388	7.865146637	17.143390656
C	10.203431129	2.199075937	17.303588867	C	6.520164013	8.582296371	17.205598831
C	11.432534218	1.492385030	17.273849487	C	7.748370171	7.873337746	17.272657394
C	12.663279533	2.198156595	17.293359756	C	8.975011826	8.586225510	17.293048859
C	12.663953781	3.617794514	17.307241440	C	8.972295761	10.005163193	17.288448334
C	-0.866378546	4.324732780	17.293521881	C	-4.560722828	10.716658592	17.306465149
C	0.361177444	3.612958908	17.296977997	C	-3.330830812	10.007490158	17.297927856
C	1.591875792	4.318781376	17.280014038	C	-2.104157448	10.720414162	17.280412674
C	2.820890427	3.612138748	17.306783676	C	-0.875964165	10.011440277	17.216182709
C	4.051443100	4.323335648	17.306138992	C	0.342484474	10.728525162	17.150354385
C	5.283271790	3.614022493	17.340045929	C	1.570375443	10.007596016	16.981420517
C	6.513037682	4.324078083	17.338844299	C	2.831655025	10.736023903	16.975824356
C	7.743299484	3.616348982	17.348344803	C	4.072830677	10.019031525	17.044960022
C	8.974683762	4.327271938	17.340255737	C	5.287328720	10.720133781	17.155401230
C	10.204175949	3.618829727	17.328226089	C	6.517221928	10.004040718	17.203422546
C	11.434261322	4.327796936	17.318979263	C	7.740900993	10.714565277	17.259889603
C	11.436012268	5.748390675	17.314073563	Pt	2.158023357	10.423393250	14.883765221
C	-2.095517397	6.457656384	17.285503387	Pt	3.237314701	11.004265785	12.621881485
C	-0.864976406	5.745975018	17.269886017	Pt	1.041333199	9.734814644	12.668757439
C	0.362234116	6.450488567	17.216417313	Pt	3.465749264	8.159995079	14.884352684
C	1.591924191	5.736967564	17.216642380	Pt	4.505011082	8.811964035	12.623620033
C	2.822138786	6.433709145	17.151428223	Pt	2.308772087	7.542638302	12.670230865

**Table S7.** Cartesian coordinates of 8 isomers of Pt<sub>8</sub>.

**Pt<sub>8</sub> Isomer 1**

C	7.905653954	11.763402939	17.262054443	C	12.824709892	3.240888834	17.297803879
C	-5.624683857	12.472827911	17.268400192	C	-0.706339478	3.948021650	17.275184631
C	-4.395562172	11.763387680	17.228466034	C	0.522140980	3.238684177	17.285470963
C	-3.166542530	12.472938538	17.223266602	C	1.753727198	3.946830273	17.247047424
C	-1.937468052	11.764334679	17.169448853	C	2.984613419	3.238642693	17.254875183
C	-0.707732677	12.475672722	17.184570313	C	4.214886665	3.945983410	17.217781067
C	0.517966747	11.770641327	17.121185303	C	5.445893764	3.239404678	17.235599518
C	1.754091740	12.480054855	17.186931610	C	6.675828934	3.949799538	17.220279694
C	2.984517097	11.784037590	17.158061981	C	7.905548096	3.241635323	17.251441956
C	4.213007927	12.477264404	17.256977081	C	9.136734009	3.950415134	17.250673294
C	5.445624352	11.760569572	17.253068924	C	10.365144730	3.242918491	17.279817581
C	6.672929287	12.470135689	17.282592773	C	11.594880104	3.951335430	17.274564743
C	14.053072929	1.109814405	17.308774948	C	11.594950676	5.371407986	17.224824905
C	0.522955537	1.818644047	17.304450989	C	-1.937105894	6.081298351	17.184101105
C	1.754566431	1.109679580	17.289264679	C	-0.707617998	5.368998051	17.210746765
C	2.984502792	1.818368316	17.275293350	C	0.514847279	6.072970867	17.136175156
C	4.213845730	1.109987855	17.254888535	C	1.754022837	5.362630844	17.163330078
C	5.444702148	1.819993019	17.250654221	C	2.985388994	6.060348988	17.083417892
C	6.673780918	1.113027930	17.238922119	C	4.216690540	5.363814354	17.136451721
C	7.903321743	1.822695136	17.255964279	C	5.449172974	6.067783833	17.082294464
C	9.134356499	1.113751292	17.256265640	C	6.676870823	5.368581295	17.155509949
C	10.364406586	1.821736217	17.286184311	C	7.912783146	6.077183723	17.155427933
C	11.593848228	1.112812281	17.298656464	C	9.137152672	5.370687962	17.208377838
C	12.825224876	1.820929527	17.313951492	C	10.367573738	6.080833912	17.197496414

C	10.369298935	7.500759602	17.166902542
C	-3.165399790	8.212806702	17.142856598
C	-1.938267231	7.500441074	17.120639801
C	-0.715246677	8.211662292	17.035558701
C	0.501553059	7.488539696	16.996139526
C	1.737416267	8.199213028	16.848056793
C	2.990625381	7.491535187	16.932060242
C	4.216231823	8.224356651	17.064102173
C	5.449143410	7.501106262	16.965982437
C	6.695278645	8.218426704	17.043260574
C	7.921392918	7.496634007	17.108928680
C	9.143696785	8.212409973	17.153081894
C	9.139503479	9.632473946	17.182237625
C	-4.393990517	10.342882156	17.189207077
C	-3.165975571	9.632930756	17.145486832
C	-1.937905788	10.345297813	17.116935730

### Pt8 Isomer 2

C	-6.901262283	12.160610199	17.127841949
C	1.706480026	0.084419169	17.114253998
C	-4.440203190	12.157853127	17.057798386
C	4.170634747	0.084888071	17.082155228
C	-1.980156898	12.160064697	17.074598312
C	6.632540226	0.090977699	17.158700943
C	0.485946655	12.176072121	17.256145477
C	9.089553833	0.097803675	17.395843506
C	2.933074474	12.168111801	17.496990204
C	11.549427032	0.095968172	17.399469376
C	5.398174763	12.177103996	17.272403717
C	14.008733749	0.092153981	17.215774536
C	-0.752354324	1.508828163	17.259172440
C	0.478799343	2.214263201	17.238405228
C	1.707199574	1.502651691	17.180135727
C	2.939446449	2.208498955	17.181573868
C	4.171263695	1.503357649	17.136020660
C	5.400516510	2.214961052	17.151355743
C	6.631985188	1.507250905	17.179347992
C	7.862586498	2.219778776	17.230474472
C	9.089472771	1.516657710	17.328336716
C	10.319133759	2.226069212	17.330379486
C	11.549045563	1.514143348	17.355731964
C	12.777901649	2.218076229	17.299640656
C	-1.982778668	3.638398170	17.264495850
C	-0.756671906	4.343794823	17.252681732
C	0.477340221	3.630848885	17.263168335
C	1.709250212	4.328104019	17.259429932
C	2.940483332	3.623618603	17.227193832
C	4.170011044	4.330632687	17.187173843
C	5.400527954	3.634397984	17.153436661
C	6.635922432	4.348938465	17.132251740
C	7.862713814	3.639680624	17.177961349
C	9.091640472	4.350028515	17.174186707
C	10.319816589	3.640372038	17.242263794
C	11.548792839	4.349353313	17.220367432
C	-3.211029291	5.766453743	17.145202637
C	-1.981724262	6.473612785	17.143791199
C	-0.763827801	5.758979797	17.193983078
C	0.472801924	6.484577656	17.214328766

### Pt8 Isomer 3

C	-6.937325478	12.233550072	17.306680679
C	1.671659231	0.159444839	17.250406265
C	-4.472283840	12.232729912	17.278604507
C	4.143110752	0.155223906	17.239070892
C	-2.008794785	12.231249809	17.297630310

C	-0.711560249	9.637115479	17.030851364
C	0.506268978	10.360421181	16.983802795
C	1.744303703	9.658349991	16.830549240
C	2.997103214	10.360416412	16.969226837
C	4.225925922	9.622376442	17.126199722
C	5.451456547	10.342085838	17.199739456
C	6.683502197	9.642143250	17.161415100
C	7.910097599	10.345745087	17.210094452
Pt	1.750463963	7.351687908	12.306567192
Pt	2.193674564	7.553250790	14.812906265
Pt	4.978803635	9.855025291	13.720640182
Pt	3.550130367	11.904497147	13.201208115
Pt	2.649536133	9.698689461	12.294360161
Pt	6.024699688	7.864746094	14.818216324
Pt	4.181490898	7.413561821	13.152194023
Pt	2.564033985	10.092700005	14.773199081

C	1.715927124	5.765850544	17.285919189
C	2.945834637	6.493688107	17.454517365
C	4.161894321	5.770670891	17.202323914
C	5.404036522	6.487613678	17.090501785
C	6.642644882	5.762778282	17.079641342
C	7.863688469	6.476776600	17.072927475
C	9.093584061	5.768245697	17.104043961
C	10.322664261	6.478863239	17.085067749
C	-4.433186531	7.898138523	17.019716263
C	-3.201334476	8.606798172	17.010210037
C	-1.971188307	7.896549702	17.085533142
C	-0.741999626	8.602175713	17.157314301
C	0.480464935	7.912578583	17.354021072
C	1.703786373	8.604927063	17.573297501
C	2.946259499	7.892107010	17.599306107
C	4.181665421	8.594322205	17.479402542
C	5.399028778	7.911896229	17.254821777
C	6.633197784	8.614548683	17.142227173
C	7.861470222	7.900962830	17.060806274
C	9.091250420	8.608395576	17.017608643
C	-5.667796612	10.029466629	17.027252197
C	-4.437557697	10.740722656	17.013925552
C	-3.203167439	10.032032013	16.993556976
C	-1.981193066	10.745742798	17.012311935
C	-0.738976479	10.028350830	17.034168243
C	0.505429268	10.738368034	17.221717834
C	1.715246677	10.020718575	17.547758102
C	2.928602219	10.749220848	17.569786072
C	4.161153316	10.023756981	17.380100250
C	5.398583889	10.743083000	17.178794861
C	6.640476704	10.026124001	17.127395630
C	7.862474918	10.739109039	17.082771301
Pt	4.226357460	6.205954075	15.062531471
Pt	3.843618870	8.469510078	13.942218781
Pt	2.482693195	10.654073715	13.344900131
Pt	1.410006046	6.109179974	15.161608696
Pt	1.344677925	8.340484619	13.931997299
Pt	2.738172770	6.332642555	12.946063995
Pt	0.598013401	10.462379456	15.093779564
Pt	4.222367287	10.598165512	15.227884293

C	6.600300312	0.157560140	17.282852173
C	0.450201988	12.233049393	17.317584991
C	9.057706833	0.161680788	17.312032700
C	2.906597137	12.235670090	17.320203781
C	11.516809464	0.162912846	17.318189621

C	5.364392281	12.235986710	17.320510864
C	13.975098610	0.162912652	17.298067093
C	-0.786090136	1.581904531	17.257888794
C	0.441227198	2.289849281	17.159065247
C	1.659696102	1.566229820	17.124950409
C	2.905326128	2.259592295	16.920198441
C	4.158681870	1.562446833	17.093246460
C	5.377826691	2.267184019	17.081659317
C	6.602070808	1.575135708	17.208631516
C	7.832959652	2.290628672	17.229835510
C	9.056957245	1.583661318	17.288467407
C	10.288811684	2.294576645	17.301431656
C	11.516908646	1.584098339	17.308307648
C	12.745730400	2.293454409	17.280345917
C	-2.013492346	3.714377403	17.270168304
C	-0.786451817	4.424411774	17.197969437
C	0.431294918	3.711596966	17.083980560
C	1.648644209	4.426380157	16.895603180
C	2.894540310	3.694458246	16.777492523
C	4.161895275	4.437629700	16.811843872
C	5.396258831	3.701564550	16.911590576
C	6.621552467	4.429855347	17.104387283
C	7.838268280	3.714125156	17.205776215
C	9.062963486	4.425473690	17.274572372
C	10.290956497	3.713508368	17.300439835
C	11.519014359	4.424827099	17.302835464
C	-3.243824482	5.845810413	17.315410614
C	-2.016343117	6.556608677	17.298257828
C	-0.790463924	5.848313332	17.219352722
C	0.426560163	6.568742275	17.154857635
C	1.657910109	5.861536980	16.977876663
C	2.915125132	6.572182178	17.008100510
C	4.148926735	5.862077713	17.019798279
C	5.367866993	6.559022427	17.162982941
C	6.605940819	5.844148636	17.182767868

**Pts Isomer 4**

C	-6.781276703	12.081474304	17.215579987
C	1.830720901	0.011132547	17.194316864
C	-4.318017006	12.081309319	17.200511932
C	4.290739059	0.005585489	17.188638687
C	-1.858098030	12.078866959	17.195270538
C	6.751298904	0.005846047	17.193933487
C	0.599959850	12.078992844	17.190450668
C	9.209884644	0.008120729	17.203056335
C	3.059845924	12.080572128	17.199119568
C	11.667921066	0.007460530	17.219587326
C	5.519357681	12.079203606	17.219223022
C	14.129401207	0.006153528	17.221542358
C	-0.632671833	1.427020431	17.206016541
C	0.594907165	2.134789944	17.149757385
C	1.830293655	1.425446391	17.146224976
C	3.063847303	2.132788420	17.099569321
C	4.292907715	1.425179243	17.146781921
C	5.522677898	2.134751081	17.136672974
C	6.753046513	1.426645398	17.179668427
C	7.979448318	2.137113094	17.188667297
C	9.209944725	1.427286386	17.211568832
C	10.439674377	2.137533426	17.221281052
C	11.667270660	1.427803755	17.225326538
C	12.898566246	2.138133049	17.211734772
C	-1.861263871	3.557669401	17.194561005
C	-0.634060502	4.265325069	17.122196198
C	0.582284451	3.546179295	17.057403564
C	1.819890261	4.245363712	16.826940536

C	7.830188751	6.554643154	17.275985718
C	9.059097290	5.845151424	17.294921875
C	10.287950516	6.556639194	17.329402924
C	-4.473537445	7.975352287	17.349874496
C	-3.243858576	8.685845375	17.354675293
C	-2.015538931	7.976561546	17.328460693
C	-0.785531998	8.686832428	17.317565918
C	0.441364765	7.981423855	17.247350693
C	1.675377846	8.689173698	17.238834381
C	2.906406879	7.988196373	17.156259537
C	4.135914326	8.689519882	17.230264664
C	5.365716934	7.976973534	17.240510941
C	6.595325470	8.685017586	17.304710388
C	7.826710224	7.975542545	17.318168640
C	9.055029869	8.685799599	17.350061417
C	-5.705598354	10.105976105	17.349397659
C	-4.473733902	10.818069458	17.337947845
C	-3.242712498	10.105810165	17.352212906
C	-2.012758732	10.812530518	17.342147827
C	-0.782871246	10.105121613	17.338987350
C	0.447772503	10.813888550	17.328182220
C	1.677206039	10.105153084	17.300794601
C	2.906872749	10.816720009	17.305685043
C	4.136148930	10.108435631	17.293439865
C	5.365324497	10.815939903	17.320590973
C	6.594559669	10.104039192	17.328388214
C	7.824812412	10.813952446	17.338617325
Pt	2.875151157	6.170722961	12.555209160
Pt	4.747449398	4.461009502	12.308677673
Pt	2.864141226	2.782128096	14.781282425
Pt	0.910045743	1.749081850	13.471874237
Pt	1.296268225	4.207737923	12.873116493
Pt	4.961338043	4.229501247	14.793245316
Pt	1.998061180	5.617269516	14.860872269
Pt	3.081106186	2.545411825	12.277345657

C	3.075252771	3.543050528	16.973087311
C	4.295538902	4.246986389	16.956670761
C	5.524069786	3.552238941	17.071512222
C	6.754431725	4.266558647	17.102993011
C	7.978741646	3.559614420	17.167581558
C	9.211043358	4.270864964	17.194707870
C	10.439992905	3.560074806	17.216293335
C	11.667873383	4.269552231	17.209524155
C	-3.090960741	5.689840794	17.199121475
C	-1.861015677	6.401366711	17.157527924
C	-0.635324955	5.693296909	17.087665558
C	0.577512980	6.408819675	16.959072113
C	1.803497076	5.692949772	16.737573624
C	3.071538925	6.422272682	16.741521835
C	4.311389446	5.684787273	16.805923462
C	5.541749954	6.407934189	16.986019135
C	6.759652138	5.690834045	17.083667755
C	7.984386921	6.401254654	17.153118134
C	9.213375092	5.689091206	17.190975189
C	10.442317963	6.399820805	17.204319000
C	-4.318226814	7.821642399	17.202402115
C	-3.090636253	8.530888557	17.191074371
C	-1.860630512	7.820439339	17.153795242
C	-0.631693363	8.530220985	17.118171692
C	0.592855930	7.822083473	17.026521683
C	1.830230713	8.535444260	17.024120331
C	3.062457561	7.840837002	16.953071594
C	4.290049553	8.537536621	17.060224533

C	5.527405739	7.823918819	17.060916901
C	6.753554344	8.531722069	17.147466660
C	7.982244015	7.821502686	17.167785645
C	9.212244987	8.532397270	17.200597763
C	-5.548522472	9.950510979	17.210811615
C	-4.318865776	10.660576820	17.210813522
C	-3.090194225	9.950958252	17.198982239
C	-1.859048843	10.660409927	17.189838409
C	-0.629724979	9.951514244	17.156629562
C	0.598709583	10.659956932	17.157196045
C	1.830393314	9.949947357	17.117265701
C	3.059685230	10.660122871	17.155107498

### Pt<sub>8</sub> Isomer 5

C	-6.814643383	12.064432144	17.295902252
C	-5.582674503	12.776748657	17.275068283
C	-4.351408482	12.064528465	17.279617310
C	-3.122704983	12.771233559	17.266786575
C	-1.891589642	12.061813354	17.272064209
C	-0.662028313	12.771376610	17.270040512
C	0.566672325	12.062125206	17.266719818
C	1.796570778	12.773573875	17.280532837
C	3.026473522	12.063543320	17.276256561
C	4.254549503	12.772856712	17.298522949
C	5.486031532	12.062056541	17.297580719
C	6.716094494	12.771678925	17.302978516
C	-0.666215479	1.410022020	17.289354324
C	0.561470628	2.117655754	17.233627319
C	1.797043920	1.408465505	17.228607178
C	3.030661583	2.115758657	17.179738998
C	4.259512424	1.408176422	17.224338531
C	5.489188194	2.117874384	17.211879730
C	6.719612598	1.409662962	17.255062103
C	7.946111202	2.119918823	17.264148712
C	9.176642418	1.409987450	17.288959503
C	10.406383514	2.120323896	17.300327301
C	11.633886337	1.410695195	17.306116104
C	12.865077019	2.121270657	17.293979645
C	-1.894608736	3.540822744	17.276683807
C	-0.667427659	4.248476028	17.203613281
C	0.548657894	3.529058456	17.140220642
C	1.786189556	4.227676868	16.906284332
C	3.041935444	3.525904417	17.051420212
C	4.262069702	4.229848385	17.029020309
C	5.490818024	3.535262346	17.144084930
C	6.721313477	4.249665737	17.174757004
C	7.945351601	3.542424202	17.241577148
C	9.177652359	4.253521919	17.270046234
C	10.406618118	3.542862654	17.294904709
C	11.634417534	4.252564430	17.289831161
C	-3.124504089	5.672914028	17.277910233
C	-1.894528151	6.384510517	17.235427856
C	-0.668764114	5.676531315	17.165672302
C	0.543759823	6.391609669	17.033161163

### Pt<sub>8</sub> Isomer 6

C	-6.799846649	12.178588867	17.202823639
C	1.809884310	0.103811696	17.224708557
C	-4.339429379	12.176934242	17.262151718
C	4.269656181	0.103703350	17.303056717
C	-1.881503582	12.177945137	17.360570908
C	6.727828026	0.106282435	17.379627228
C	0.577910423	12.179816246	17.404396057
C	9.189462662	0.108739048	17.365852356
C	3.041455269	12.180624962	17.338068008

C	4.289677620	9.952009201	17.146604538
C	5.520960808	10.661879539	17.192441940
C	6.751555443	9.953027725	17.190654755
C	7.979824066	10.661814690	17.213340759
Pt	1.835763931	7.434152126	10.860518456
Pt	3.789861679	6.048686028	12.096241951
Pt	1.735722542	4.819467545	14.700651169
Pt	-0.179754734	3.696912766	13.422571182
Pt	0.240432978	5.754363537	11.915842056
Pt	3.938211203	6.129522800	14.672469139
Pt	1.806115627	7.126670361	13.389615059
Pt	2.134125710	4.137467384	12.310171127

C	1.769346476	5.675055504	16.810501099
C	3.037603140	6.404811859	16.809917450
C	4.277689934	5.667608738	16.874042511
C	5.508337021	6.390923023	17.053607941
C	6.726303101	5.674037933	17.153430939
C	7.950985909	6.384152412	17.225269318
C	9.179828644	5.671772003	17.265771866
C	10.408699036	6.382803917	17.281356812
C	-4.351821423	7.804725170	17.279342651
C	-3.124131441	8.513924599	17.268329620
C	-1.894057512	7.803548813	17.230533600
C	-0.664920807	8.513265610	17.193508148
C	0.559379578	7.804996967	17.099458694
C	1.796706200	8.518271446	17.095142365
C	3.028929710	7.823617935	17.021404266
C	4.256542683	8.520390511	17.129447937
C	5.494104862	7.806792259	17.129613876
C	6.720227718	8.514662743	17.218965530
C	7.948845863	7.804387569	17.240446091
C	9.178649902	8.515460968	17.276361465
C	-5.582008362	9.933530807	17.287923813
C	-4.352228165	10.643738747	17.288864136
C	-3.123719692	9.933982849	17.276624680
C	-1.892568111	10.643376350	17.266494751
C	-0.663174152	9.934558868	17.232275009
C	0.565279961	10.643019676	17.232311249
C	1.796996117	9.932841301	17.190401077
C	3.026448250	10.643205643	17.229101181
C	4.256427765	9.934949875	17.218721390
C	5.487689018	10.644751549	17.267047882
C	6.718202114	9.935905457	17.265155792
C	7.946335316	10.644760132	17.290819168
Pt	1.788117409	7.348944664	10.909371376
Pt	3.746447802	5.986216068	12.163156509
Pt	1.699734688	4.790134907	14.779964447
Pt	-0.213665843	3.640933514	13.523131371
Pt	0.199009180	5.682792664	11.993990898
Pt	3.898099899	6.104002476	14.739346504
Pt	1.765292168	7.083996773	13.443239212
Pt	2.095966101	4.073813438	12.398979187

C	11.650244713	0.108644024	17.275667191
C	5.499930382	12.184174538	17.228013992
C	14.110438347	0.107933909	17.212591171
C	-0.652228475	1.525677681	17.215402603
C	0.578364372	2.233695269	17.201330185
C	1.809622526	1.523300052	17.216770172
C	3.040339470	2.230257988	17.231475830
C	4.270174980	1.522923946	17.278350830
C	5.499444962	2.234120607	17.291351318

C	6.729131699	1.525579691	17.333023071
C	7.958418846	2.236795664	17.315217972
C	9.189032555	1.528085470	17.326772690
C	10.418681145	2.237766504	17.284227371
C	11.648729324	1.528092623	17.265432358
C	12.877931595	2.236026049	17.230131149
C	-1.883074641	3.656594992	17.216053009
C	-0.656323433	4.364919662	17.180820465
C	0.576039791	3.649281502	17.175041199
C	1.808074236	4.346548080	17.145593643
C	3.040595770	3.649181843	17.200307846
C	4.271316051	4.360928535	17.223445892
C	5.499905586	3.654128790	17.257417679
C	6.730720520	4.365768433	17.251861572
C	7.958772182	3.656469345	17.272779465
C	9.189065933	4.366883755	17.249881744
C	10.418271065	3.656805038	17.253803253
C	11.647184372	4.366840839	17.226955414
C	-3.112743139	5.786188126	17.227552414
C	-1.884897113	6.496655941	17.228437424
C	-0.665117979	5.781681061	17.160623550
C	0.567611217	6.509328365	17.090436935
C	1.813287258	5.774535656	17.092342377
C	3.052991629	6.481736183	17.168285370
C	4.276062489	5.781186581	17.200731277
C	5.509290695	6.497234344	17.180250168
C	6.733877182	5.786556721	17.210765839
C	7.963371277	6.497478485	17.197105408
C	9.190663338	5.786401749	17.221258163
C	10.419558525	6.497458935	17.226848602
C	-4.337763786	7.917134762	17.234165192

**Pt<sub>8</sub> Isomer 7**

C	-6.847603798	12.115255356	17.201320648
C	1.761874795	0.043699522	17.232423782
C	-4.389195442	12.115477562	17.262832642
C	4.220698357	0.042196523	17.280799866
C	-1.930189610	12.114995003	17.286195755
C	6.682005405	0.040532570	17.270341873
C	0.529645443	12.113418579	17.245595932
C	9.140786171	0.045771729	17.206241608
C	2.989341259	12.130323410	17.148424149
C	11.599710464	0.047695000	17.149055481
C	5.455086708	12.116271973	17.144420624
C	14.063016891	0.043792423	17.169269562
C	-0.698397160	1.464345098	17.170026779
C	0.531801820	2.174855709	17.197557449
C	1.762651563	1.462481022	17.233873367
C	2.992926598	2.170362949	17.272323608
C	4.222080231	1.461099505	17.285449982
C	5.452986240	2.170551062	17.293111801
C	6.682311535	1.461544156	17.274427414
C	7.910979748	2.173070669	17.257268906
C	9.140924454	1.465009093	17.219964981
C	10.370041847	2.173991919	17.194591522
C	11.600211143	1.464512229	17.167371750
C	12.831214905	2.173122644	17.164445877
C	-1.930746555	3.591681719	17.168258667
C	-0.700366974	4.299107552	17.162040710
C	0.532134056	3.591860056	17.195739746
C	1.766661167	4.300178051	17.251018524
C	2.995291471	3.589294672	17.287895203
C	4.223372459	4.299267292	17.316511154
C	5.453704357	3.590116024	17.307737350
C	6.682235718	4.300595760	17.302091599

C	-3.107428312	8.626772881	17.284683228
C	-1.881699800	7.917923450	17.292364120
C	-0.654092312	8.632588387	17.363950729
C	0.574349880	7.936787128	17.310541153
C	1.793601513	8.641831398	17.347555161
C	3.029311180	7.926259995	17.121475220
C	4.279404163	8.641903877	17.068246841
C	5.515872002	7.913755894	17.113162994
C	6.737483501	8.628462791	17.139551163
C	7.965785027	7.916823387	17.173656464
C	9.194086075	8.627578735	17.202381134
C	-5.567867756	10.047798157	17.208229065
C	-4.338417530	10.756860733	17.260978699
C	-3.108393431	10.048422813	17.312128067
C	-1.882092476	10.758953094	17.372879028
C	-0.651334286	10.050604820	17.417074203
C	0.577989101	10.758903503	17.445045471
C	1.807587147	10.052021980	17.413032532
C	3.041662693	10.764579773	17.333551407
C	4.269661903	10.069495201	17.195255280
C	5.500703812	10.765616417	17.187065125
C	6.731833458	10.050332069	17.155820847
C	7.960660458	10.757868767	17.183956146
Pt	3.441875935	8.163842201	15.002323151
Pt	1.845924854	9.783771515	13.785549164
Pt	-0.690424442	10.511730194	13.852538109
Pt	1.343605995	6.450703621	15.000267982
Pt	-0.147957325	7.900624275	13.522087097
Pt	2.259047985	7.470337868	12.803829193
Pt	-2.422247410	8.779408455	13.778064728
Pt	1.137407780	12.069694519	14.311385155

C	7.911478996	3.591985226	17.271114349
C	9.140673637	4.302967548	17.249486923
C	10.369862556	3.593880177	17.209817886
C	11.599126816	4.303395271	17.191556931
C	-3.162953138	5.723097801	17.215984344
C	-1.934935212	6.433243275	17.204496384
C	-0.709696531	5.717408180	17.153829575
C	0.538773537	6.426895618	17.129899979
C	1.777696371	5.711918354	17.254144669
C	2.995515108	6.427254677	17.330905914
C	4.224433899	5.718645573	17.335674286
C	5.453948975	6.428678513	17.325540543
C	6.682699203	5.720641136	17.308383942
C	7.910270214	6.432765961	17.283748627
C	9.139926910	5.723274231	17.262685776
C	10.368090630	6.433738232	17.249349594
C	-4.392867565	7.854074955	17.262863159
C	-3.163197041	8.565134048	17.272184372
C	-1.937259912	7.857007980	17.253999710
C	-0.711822510	8.571599960	17.260765076
C	0.529806137	7.865149975	17.215545654
C	1.767532349	8.570119858	17.303060532
C	2.994983673	7.849830151	17.325952530
C	4.222787857	8.547004700	17.260389328
C	5.454068184	7.847617149	17.287055969
C	6.681553841	8.562123299	17.248952866
C	7.909025669	7.853475094	17.266029358
C	9.139820099	8.564377785	17.259292603
C	-5.618555546	9.984768867	17.249553680
C	-4.390232086	10.695399284	17.265703201
C	-3.162208557	9.985837936	17.281909943
C	-1.934006214	10.696613312	17.291492462

C	-0.705935955	9.987416267	17.290576935	Pt	0.649079084	6.821573734	10.058347702
C	0.525758743	10.693816185	17.268207550	Pt	2.252862453	8.317278862	11.146791458
C	1.749848843	9.980034828	17.247795105	Pt	3.510009766	10.174318314	12.427226067
C	2.982412815	10.697972298	17.091156006	Pt	0.433968544	7.146425724	15.007486343
C	4.229328632	9.972741127	17.101806641	Pt	2.066665649	8.558196068	13.777526855
C	5.464987755	10.698758125	17.145196915	Pt	0.787307262	6.704942226	12.555366516
C	6.685358047	9.984679222	17.202093124	Pt	3.548334599	10.165323257	14.955556870
C	7.913602829	10.695931435	17.217391968	Pt	4.010565281	9.606053352	10.034266472

### Pt<sub>8</sub> Isomer 8

C	-6.927095413	12.160392761	17.140819550	C	1.680263042	5.763473511	17.152336121
C	1.680910110	0.087186359	17.182445526	C	2.916898251	6.472609520	17.204242706
C	-4.468397141	12.160264015	17.192775726	C	4.142794609	5.765860558	17.288396835
C	4.138669968	0.088970795	17.247842789	C	5.374535084	6.475272655	17.310760498
C	-2.011147976	12.162961960	17.248809814	C	6.604915142	5.765703201	17.326932907
C	6.596889496	0.090243958	17.308338165	C	7.833710670	6.476036072	17.288364410
C	0.446396828	12.162892342	17.297494888	C	9.063224792	5.766264439	17.275461197
C	9.059421539	0.090356007	17.345411301	C	10.291696548	6.476349831	17.201551437
C	2.911346912	12.167117119	17.310855865	C	-4.469916821	7.896277905	17.160791397
C	11.525759697	0.092858128	17.266355515	C	-3.244045734	8.608499527	17.102802277
C	5.372681141	12.173227310	17.144699097	C	-2.020740032	7.893410683	17.029508591
C	13.983820915	0.091819264	17.159336090	C	-0.792638779	8.619540215	16.933938980
C	-0.776796937	1.510287046	17.205986023	C	0.451114178	7.884686470	16.833217621
C	0.452742815	2.217717648	17.209705353	C	1.713386059	8.613333702	16.943264008
C	1.681571960	1.507331371	17.216312408	C	2.930547714	7.884731293	17.162391663
C	2.910595894	2.217894554	17.262380600	C	4.151170254	8.589555740	17.211154938
C	4.140018463	1.508427739	17.288219452	C	5.378949642	7.891666889	17.269683838
C	5.369314194	2.217867613	17.334997177	C	6.609526157	8.604973793	17.215024948
C	6.599586964	1.508753181	17.349765778	C	7.834122658	7.896939754	17.233366013
C	7.830461502	2.217617273	17.366600037	C	9.062950134	8.607753754	17.179248810
C	9.060986519	1.507601976	17.363126755	C	-5.695438862	10.026481628	17.150981903
C	10.293272972	2.218277454	17.336475372	C	-4.466907978	10.739210129	17.159040451
C	11.523938179	1.509589672	17.293489456	C	-3.240758181	10.030254364	17.136228561
C	12.753457069	2.219737053	17.243797302	C	-2.012531281	10.745421410	17.167140961
C	-2.008026361	3.637705564	17.226142883	C	-0.784807682	10.045929909	17.098522186
C	-0.777226210	4.346197605	17.183097839	C	0.436588287	10.752986908	17.179815292
C	0.452390671	3.637171268	17.201789856	C	1.680258751	10.047085762	17.102750778
C	1.681759596	4.346468449	17.212932587	C	2.906584740	10.760140419	17.222959518
C	2.911846876	3.637061119	17.268640518	C	4.138585091	10.026831627	17.076610565
C	4.141929626	4.345728874	17.306421280	C	5.383755207	10.745825768	17.049198151
C	5.370924950	3.637226105	17.342330933	C	6.614447594	10.021818161	17.115142822
C	6.602766037	4.346663952	17.350093842	C	7.836713314	10.737588882	17.128215790
C	7.832554817	3.637520552	17.355497360	Pt	4.000832081	10.915475845	10.512435913
C	9.062351227	4.347326279	17.319835663	Pt	3.347388268	9.988699913	12.687679291
C	10.293417931	3.637254953	17.306430817	Pt	2.050094604	9.477734566	14.845972061
C	11.521993637	4.346756935	17.240108490	Pt	0.693697453	7.272125244	10.564862251
C	-3.238160849	5.766695976	17.175884247	Pt	1.227554321	8.397830009	12.676061630
C	-2.011878014	6.473654270	17.085903168	Pt	2.385289669	9.053764343	10.375522614
C	-0.775561333	5.762277126	17.104665756	Pt	-0.177758217	8.270997047	14.769086838
C	0.454242468	6.458557129	17.039928436	Pt	4.473077774	10.264040947	14.922187805

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