Electronic Supplementary Information (ESI)

Palladium cluster complex $[Pd_{13}(\mu_4\text{-}C_7H_7)_6]^{2+}$ (C_7H_7 = Tropylium) with *fcc*-close-packed cuboctahedral Pd_{13} core and isomers: Theoretical insight into ligand-control of Pd_{13} core structure

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Table S1. Optimized Pd-Pd distances (in Å) in $[Pd_{13}(\mu_4\text{-}C_7H_7)_6]^{2+}$ cuboctahedral Pd_{13} core and their comparisons with experimental values.

Bonds	**$[Pd_{13}(C_7H_7)_6]^{2+}$**		
	Exp. [b]	**This work**	**|Δ|** [c]
Pd^C–$Pd^{T/B}$ [a]	2.769	2.742	0.027
Pd^C–Pd^E	2.766	2.738	0.028
$Pd^{T/B}$–Pd^E	2.766	2.740	0.026
Pd^E–Pd^E	2.766	2.738	0.028
$Pd^{T/B}$–$Pd^{T/B}$	2.764	2.746	0.018
	Exp. [b]	**This work**	**Previous work** [d]
Longest Pd–Pd	2.737	2.836	2.900
Shortest Pd–Pd	2.631	2.688	2.718
Average	2.716	2.767	2.808

[a] Pd^C, Pd^E, and $Pd^{T/B}$ represent Pd atoms at a center, equatorial, and top (or bottom) three-member ring, respectively. Mean value of Pd-Pd distances in each category is presented here because the unique comparison between the optimized geometry and the experimental one is difficult due to various orientations.
[b] Ref. S1.
[c] This is the absolute value of difference between the optimized Pd-Pd distance and the experimental one.
[d] Ref. S2.

Brief discussion: Generally, the DFT-optimized bond-distance of mono-nuclear transition metal complexes with a medium size does not deviate very much from experimental value (less than 0.3 Å to 0.5 Å in many cases). Here, the deviation of the longest Pd-Pd bond seems too large, whereas the average of Pd-Pd distances agree with experimental values. However, the flexibility and large size of this Pd_{13} cluster complex are the obstacle for geometry optimization. Nevertheless, the agreement with the experimental geometry is considerably better than that optimized previously (ref. S2). It is likely to state that the present DFT calculation overestimates Pd-Pd distances but the agreement is not bad, taking the large size and flexibility of the geometry of the Pd_{13} cluster complex.

Table S2. Atomic charge of $[Pd_{13}(C_7H_7)_6]^{2+}$ cuboctahedral and anticuboctahedral Pd_{13} core.

$[Pd_{13}(\mu_4\text{-}C_7H_7)_6]^{2+}$ (Cubo;μ4)				
	Pd^{C} [a]	**Pd^{E}** [a]	**$Pd^{T/B}$** [a]	**C_7H_7** [a]
NBO[a]	-0.517	0.085	0.085	0.249
Hirshfeld[a]	-0.064	0.081	0.081	0.181
Mulliken[b]	4.42	-0.498	-0.498	0.593
$[Pd_{13}(\mu_4\text{-}C_7H_7)_6]^{2+}$ (Anti;μ4)				
	Pd^{C}	**Pd^{E}**	**$Pd^{T/B}$**	**C_7H_7**
NBO[a]	-0.774	0.131	0.099	0.232
Hirshfeld[a]	-0.056	0.043	0.097	0.203
Mulliken[b]	4.761	-0.472	-0.547	0.559

[a] Pd^{C}, Pd^{E}, and $Pd^{T/B}$ represent Pd atoms at a center, equatorial, and top (or bottom) three-member ring, respectively.

[b] Because the Mulliken population analysis leads to unusual atomic charge when diffuse basis functions are involved, we here employed double-zeta quality basis sets for Pd and other atoms; LANL2DZ was used for Pd and 6-31G(d) were used for other atoms.

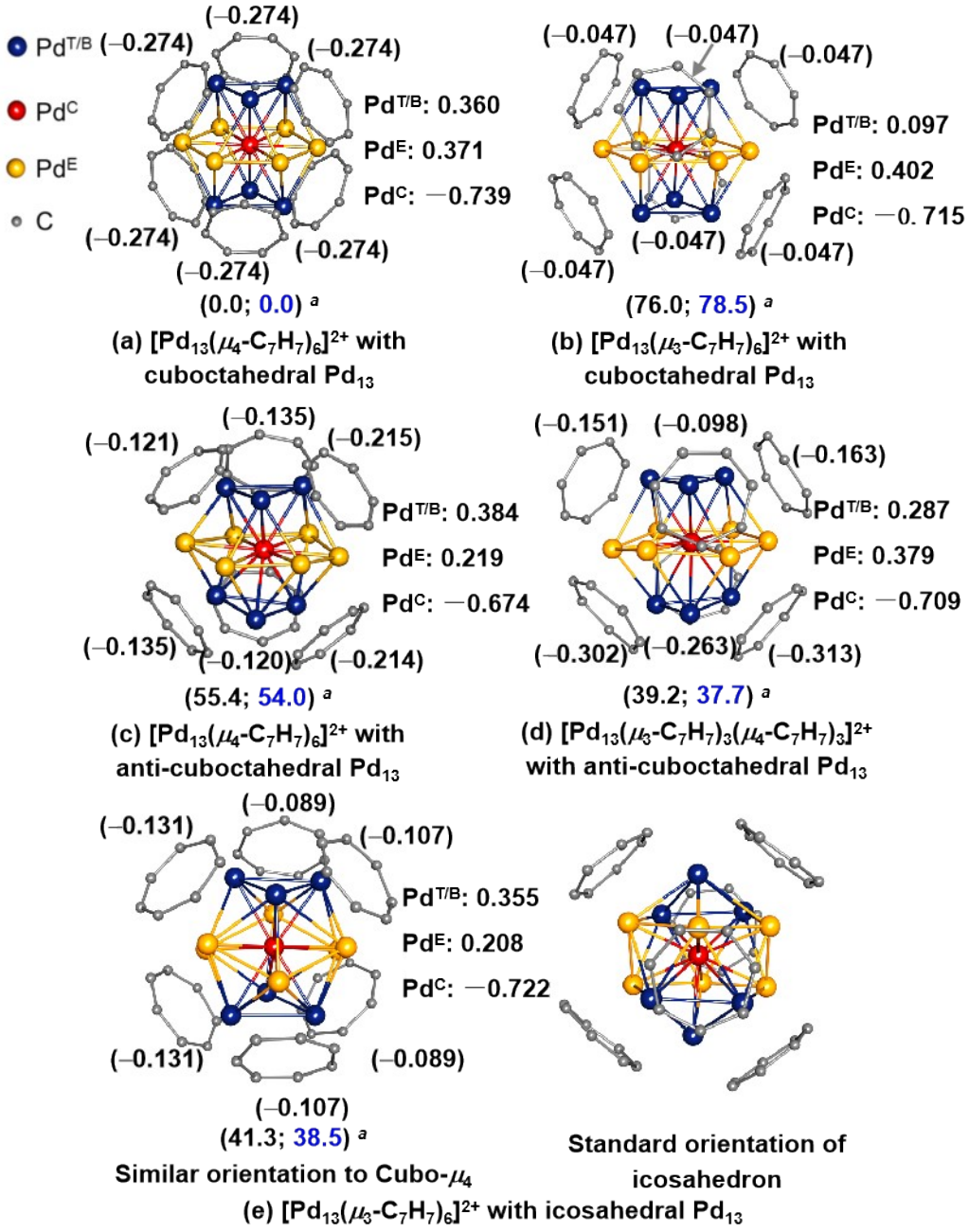
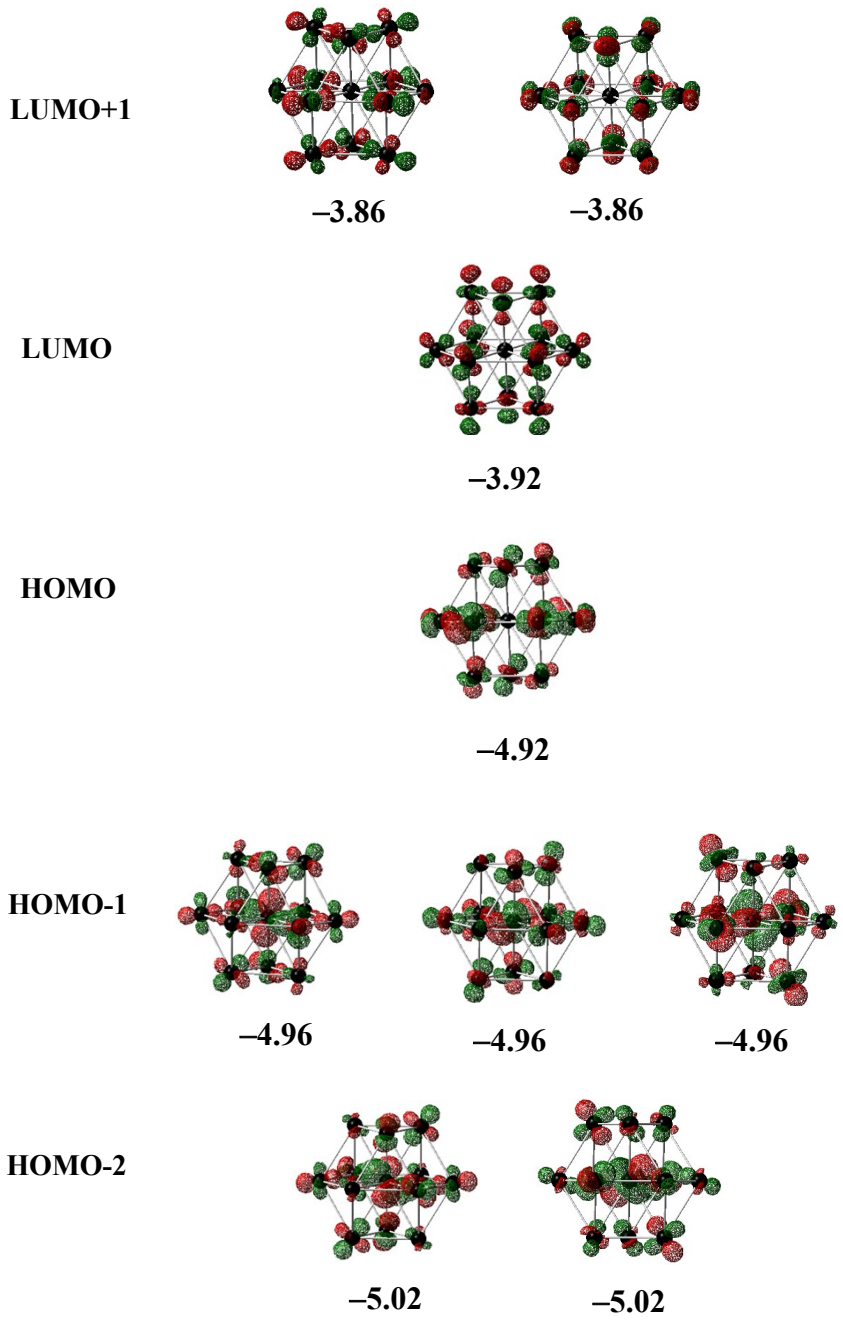
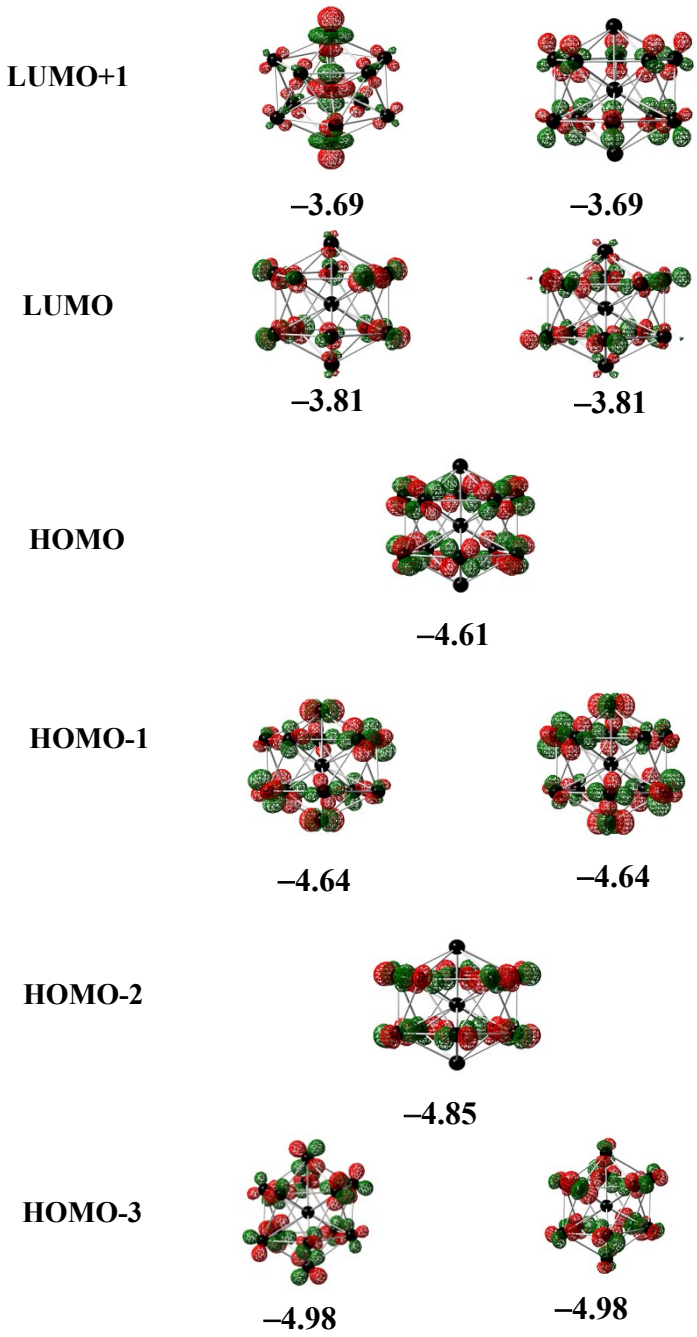


Figure S2. NBO charges (in *e* unit) of $[Pd_{13}(\mu_4\text{-}C_7H_7)_6]^{2+}$ with a cuboctaherdal Pd_{13} core **Cubo-μ4** (a), $[Pd_{13}(\mu_3\text{-}C_7H_7)_6]^{2+}$ with a cuboctaherdal Pd_{13} core **Cubo-μ3** (b), $[Pd_{13}(\mu_4\text{-}C_7H_7)_6]^{2+}$ with an anticuboctahedral Pd_{13} core **Anti-μ4** (c), $[Pd_{13}(\mu_3\text{-}C_7H_7)_3(\mu_4\text{-}C_7H_7)_3]^{2+}$ with an anticuboctahedral Pd_{13} core **Anti-μ3,4** (d) and $[Pd_{13}(\mu_3\text{-}C_7H_7)_6]^{2+}$ with an icosahedral Pd_{13} core **Ih-μ3** (e). [a]Relative potential energy and Gibbs energy (in kcal/mol) relative to those of $[Pd_{13}(\mu_4\text{-}C_7H_7)_6]^{2+}$ with a cuboctahedral Pd_{13} core.

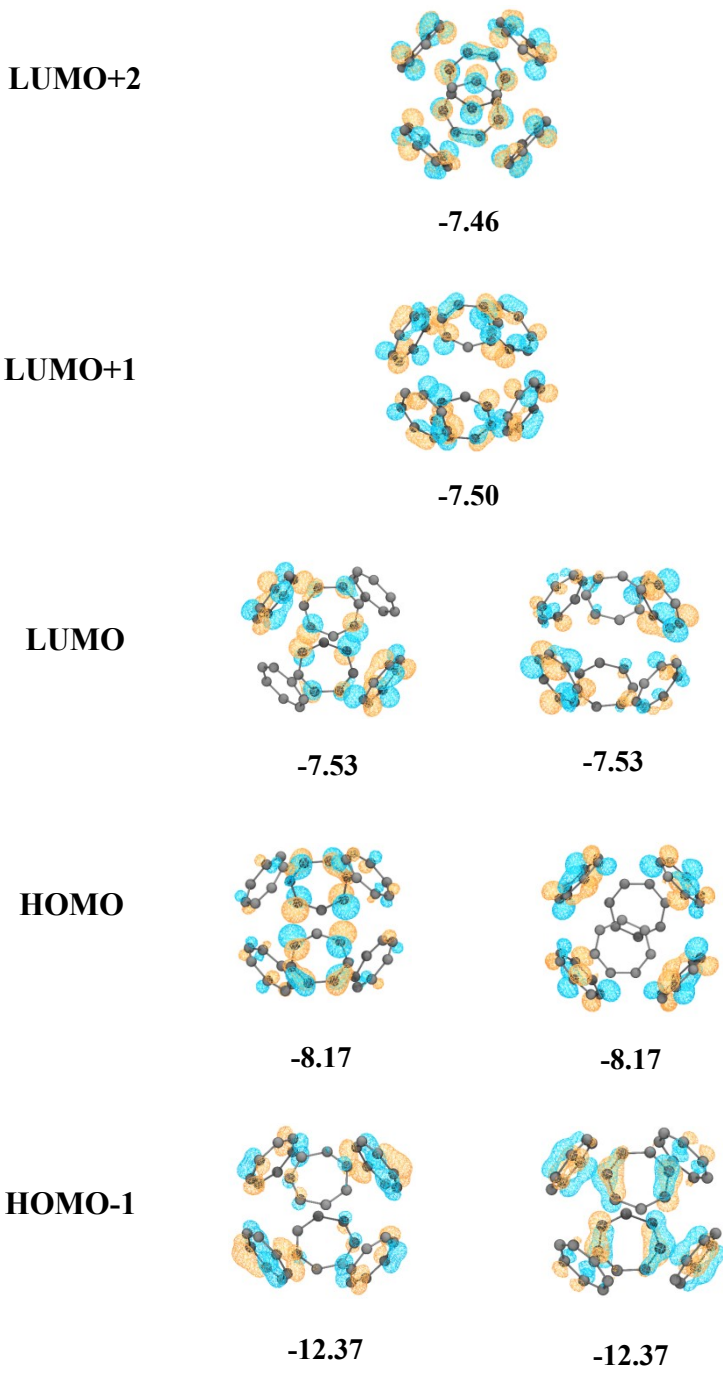


Scheme S1. Frontier orbitals of anticuboctahedral Pd_{13} cores, where the geometry was optimized. The number below each MO represents the Kohn-Sham orbital energy (in eV). B3PW91-D3(BJ)/BS-II was used here.[S3]

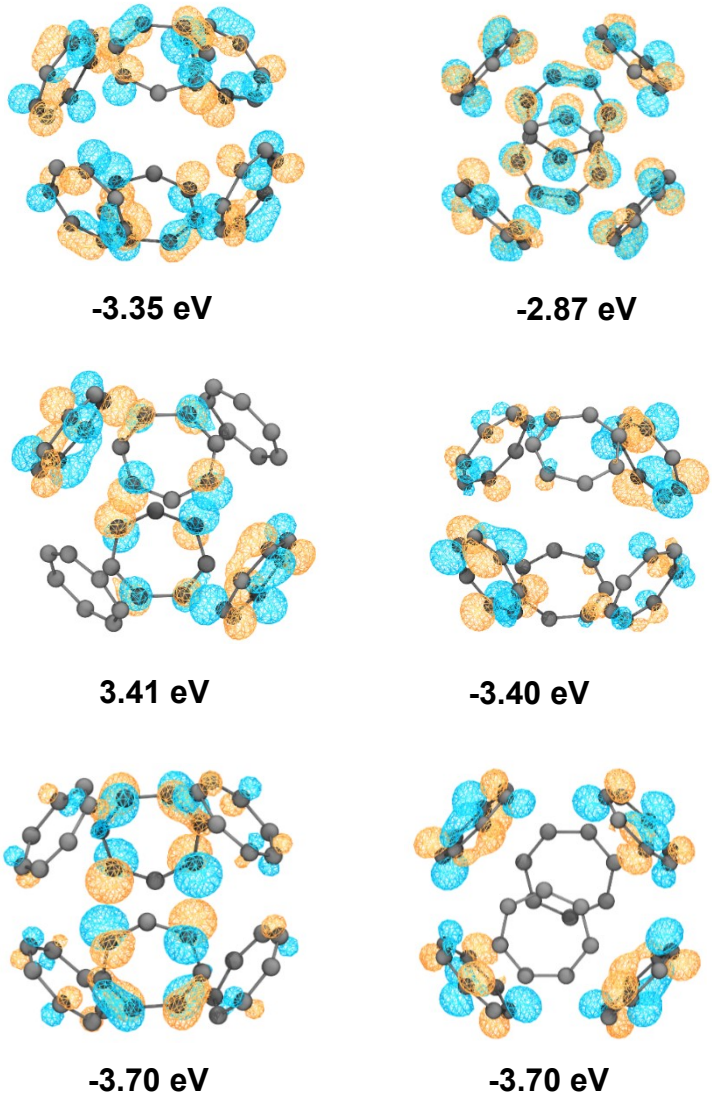


Scheme S2. Frontier orbitals of icosahedral Pd_{13} cores, where the geometry was optimized. The number below each MO represents the Kohn-Sham orbital energy (in eV). B3PW91-D3(BJ)/BS-II was used here.[S3]

Discussion: These Schemes 1 and 2 mean that both the neutral Pd_{13} and the $[Pd_{13}]^{2+}$ clusters can have anticuboctahedral and icosahedral structures at the closed shell singlet state; because both have non-degenerate HOMO, the $[Pd_{13}]^{2+}$ cluster does not induce the Jahn-Teller distortion.



Scheme S3. HOMO and LUMO of $[(C_7H_7)_6]^{2+}$ at the closed shell singlet, where the geometry is taken to be the same as that in $[Pd_{13}(\mu_4\text{-}C_7H_7)_6]^{2+}$ with cuboctahedral Pd_{13} core. The number below each MO represents the Kohn-Sham orbital energy (in eV). B3PW91-D3(BJ)/BS-I was used here, because BS-II presents overly diffuse features of MO.

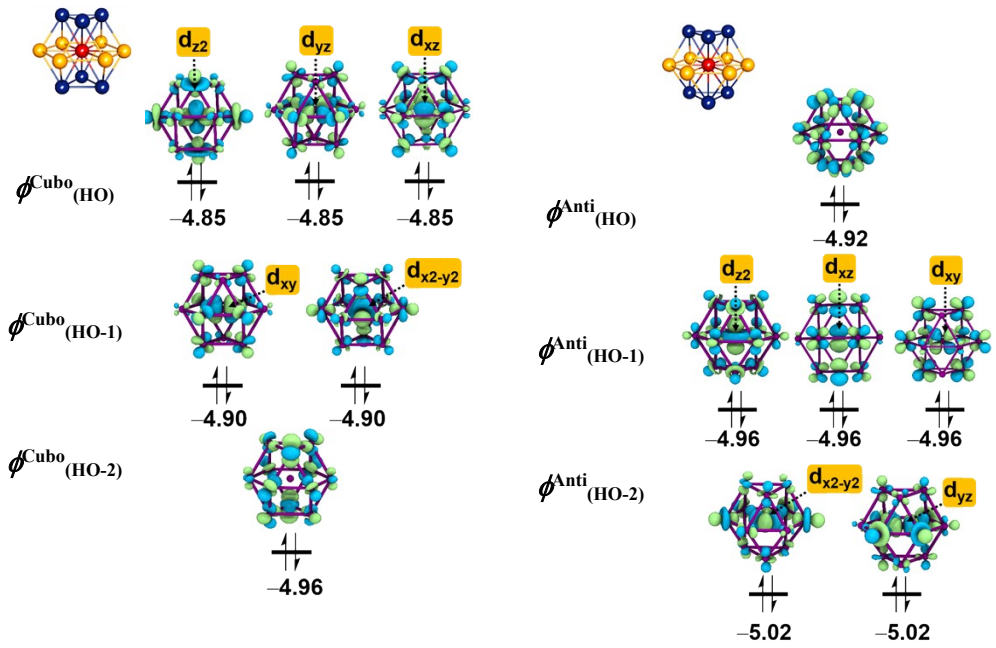


Scheme S4. Six singly occupied molecular orbitals (SOMOs) of $[(C_7H_7)_6]$ in the septet state, where geometries, positions, and orientations of six C_7H_7 molecules are taken to be the same as those in $[Pd_{13}(C_7H_7)]^{2+}$ with a cuboctahedral Pd_{13} core.
B3PW91-D3(BJ)/BS-I was used here, because BS-II presents overly diffuse features of MO.

Discussion: The two MOs at lower energy (-3.70 eV) than the other four MOs become doubly occupied HOMO in the $[(C_7H_7)_6]^{2+}$ at the closed shell singlet, as shown in Scheme S3.

Discussion of closed-shell singlet state of the $[(C_7H_7)_6]^{2+}$ ligand shell

When six neutral C_7H_7 molecules are separated well from each other, there exist six singly occupied molecular orbitals (SOMOs) at the same orbital energy in the septet spin state. When the $[(C_7H_7)_6]^{2+}$ system is calculated at the closed-shell singlet state, two of them are doubly occupied. Such an electronic structure may cause significantly large distortion in the $[(C_7H_7)_6]^{2+}$ moiety due to the Jahn-Teller effect and the six C_7H_7 molecules become non-equivalent. This is not suitable for the nearly octahedral $(C_7H_7)_6$ ligand shell. To check whether the closed shell singlet state of the $[(C_7H_7)_6]^{2+}$ ligand shell is reasonable or not, we calculated the neutral $[(C_7H_7)_6]$ ligand shell at the septet spin state, where the geometry was taken to be the same as that in **Cubo-μ4**. The neutral $[(C_7H_7)_6]$ system has six SOMOs at the septet state as expected, as shown in Scheme S4 of the Supporting Information. However, their orbital energies are not the same unexpectedly; two of them are calculated at lower energies than the other four SOMOs probably because six C_7H_7 molecules are not completely isolated but interact to some extent with each other in the ligand shell of **Cubo-μ4**. Consequently, those two MOs at a lower energy become a doubly-degenerated HOMO in the $[(C_7H_7)_6]^{2+}$ system at a closed shell singlet state, as shown in Scheme S3 of the Electronic Supplementary Information (ESI). Thus, there is no unreasonable feature in the $[(C_7H_7)_6]^{2+}$ ligand shell having the closed shell singlet state when the geometry is taken to be the same as that in **Cubo-μ4**.



Scheme S5. The HOMO, HOMO-1, HOMO-2 of cuboctahedral and anti-cuboctahedral Pd_{13} clusters[S3]
[a] The optimized geometries of cuboctahedral and anti-cuboctahedral Pd_{13} clusters were employed. B3PW91-D3(BJ)/BS-II was used.

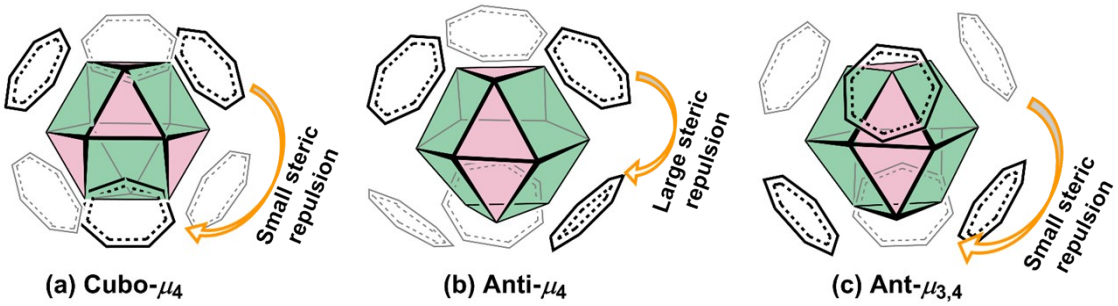
Discussion: The HOMO ϕ^{Anti}(HO) of the anti-cuboctahedral Pd_{13} corresponds to the HOMO-2 ϕ^{Cubo}(HO-2) of the cuboctahedral Pd_{13}, as shown in Scheme S5, but their energies do not differ very much. The HOMO-1 ϕ^{Anti}(HO-1) and HOMO-2 ϕ^{Anti}(HO-2) of the anti-cuboctahedral Pd_{13} correspond to the HOMO ϕ^{Cubo}(HO) and HOMO-1 ϕ^{Cubo}(HO-1) of the cuboctahedral Pd_{13}, respectively. However, the ϕ^{Anti}(HO-1) and ϕ^{Anti}(HO-2) exist at somewhat lower energies than the ϕ^{Cubo}(HO) and ϕ^{Cubo}(HO-1), respectively. As a result, ϕ^{Anti}(HO) becomes the HOMO of the anti-cuboctahedral Pd_{13} cluster despite that it resembles ϕ^{Cubo}(HO-2) of the cuboctahedral Pd_{13}. The orbital energy differences between ϕ^{Cubo}(HO)/ϕ^{Cubo}(HO-1) of the cuboctahedral Pd_{13} and ϕ^{Anti}(HO-1)/ϕ^{Anti}(HO-2) of the anti-cuboctahedral Pd_{13} may result from the extent of the d orbital participation of the Pd^{C} atom in these MOs but the details are not clear at the present stage. Further analysis is needed.

9. Comparisons between Anti-μ3,4 and Anti-μ4 and between Ih-μ3 and Cubo-μ3

9.1 Comparison between Anti-μ3,4 and Anti-μ4. As shown in Figure 2, **Anti-μ3,4** is more stable than **Anti-μ4**, which mainly results from the more negative E_{int} value in **Anti-μ3,4** than in **Anti-μ4** (Table 2). The larger stability of **Anti-μ3,4** than that of **Anti-μ4** is seemingly inconsistent with the conclusion above showing that the μ_4-coordination bond of C_7H_7 is stronger in **Cubo-μ4** than the μ_3-one in **Cubo-μ3**.

In **Anti-μ3,4**, the μ_4-C_7H_7 ligand is less positively charged (average value = +0.156 *e*) than the μ_3-C_7H_7 ligand (average value = +0.224 *e*), suggesting that the CT from the Pd_{13} core to the μ_4-C_7H_7 ligand is stronger than that to the μ_3-C_7H_7 ligand like in **Cubo-μ3** and **Cubo-μ4**. Consistent with this difference in CT, the $R(Pd^C–X)$ distance (1.976 Å; Table 1) of **Anti-μ3,4** is considerably shorter in the μ_4-coordination bond than in the μ_3-one (2.238 Å). In **Anti-μ4**, however, the $R(Pd^C–X)$ distance (2.230 Å) is considerably longer than that (1.976 Å) of the μ_4-coordiantion of **Anti-μ3,4** and the averaged charge (+0.203 *e*) of six μ_4-C_7H_7 ligands in **Anti-μ4** is larger than that (+0.156 *e*) of three μ_4-C_7H_7 ligands in **Anti-μ3,4**. These features suggest that the μ_4-coordination is much stronger and, therefore, the E_{int} is larger in **Anti-μ3,4** than in **Anti-μ4**. This is the reason why **Anti-μ3,4** is more stable than **Anti-μ4** despite that **Anti-μ3,4** has three μ_3- and three μ_4-coordiantion bonds of C_7H_7 but **Anti-μ4** has six μ_4-coordination bonds.

In the above explanation, we address a new open question why the μ_4-coordination bond is weaker in **Anti-μ4** than in **Anti-μ3,4**. We compared the positions of C_7H_7 ligands between **Anti-μ4** and **Anti-μ3,4**. In **Anti-μ4**, three μ_4-C_7H_7 ligands in the upper side of the Pd_{13} core are close to three μ_4-C_7H_7 ligands in the lower side (Figure 1c). Therefore, the steric repulsion between the upper μ_4-C_7H_7 and the lower μ_4-C_7H_7 is large (Scheme S6b), and the μ_4-C_7H_7 ligands are not located at the best position for interacting with the Pd_{13} core to decrease the E_{int} value. In the anticuboctahedral Pd_{13} core, the Pd_3 planes in the upper part of the Pd_{13} core is connected with the Pd_4 planes in the lower part. In **Anti-μ3,4**, therefore, three μ_3-C_7H_7 ligands in the upper side are distant from three μ_4-C_7H_7 ligands in the lower side and the steric repulsion between them is small (Scheme S6c). Therefore, the μ_4-C_7H_7 ligands are located at the best position to interact with the anticuboctahedral Pd_{13} core in **Anti-μ3,4** without any interference. Consistent with this understanding, the $R(Pd^C–X)$ distance of the μ_4-C_7H_7 in **Anti-μ4** is longer than in **Anti-μ3,4**, as mentioned above. Thus, it is likely concluded that the μ_4-coordination bond of the C_7H_7 ligand is weaker in **Anti-μ4** than in **Anti-μ3,4**.



Scheme S6. Schematical picture showing the positions of μ_3- and μ_4-C_7H_7 ligands.

9.2 Comparison between Ih-μ3 and Cubo-μ3

Ih-μ3 is more stable than **Cubo-μ3** despite that both have six μ_3-C_7H_7 ligands. All the C_7H_7 ligands have the moderately smaller positive charges (+0.211 *e* ~ +0.214 *e*) in **Ih-μ3** than those (+0.225 *e*) in **Cubo-μ3** (Figure 2). Also, the $R(Pd^C–X)$ distance (2.202 Å; Table 1) of **Ih-μ3** is moderately shorter than that (2.242 Å) of **Cubo-μ3** (Table 1). These features suggest that the μ_3-coordination bond of C_7H_7 is stronger in **Ih-μ3** than in **Cubo-μ3**. One factor is the interaction structure. The Type-A coordination bond of μ_3-C_7H_7 in **Ih-μ3** is stronger than in **Cubo-μ3** because three C=C double bonds interact with three Pd atoms in the Type A μ_3-coordination bond of **Ih-μ3** but one C=C double bond coordinates to one Pd atom and three C atoms coordinates to two Pd atoms through a π-allyl type interaction in the μ_3-coorination bond of **Cubo-μ3**. The other factor is the HOMO energy of the Pd_{13} core: The HOMO of the icosahedral Pd_{13} cluster exists at a higher energy (–4.61 eV; Scheme S2 in the ESI) than that (–4.85 eV; Scheme 3) of the cuboctahedral Pd_{13} cluster.[21] Consequently, the icosahedral Pd_{13} core forms the stronger CT to the μ_3-$(C_7H_7)_6$ ligand shell than does the cuboctahedral Pd_{13} core. Because of these two factors, the E_{int} value is larger (more negative) in **Ih-μ3** than in **Cubo-μ3**. In addition, the icosahedral Pd_{13} core and the $[(C_7H_7)_6]^{2+}$ shell in **Ih-μ3** are more stable than the cuboctahedral Pd_{13} core and the $[(C_7H_7)_6]^{2+}$ shell in **Cubo-μ3**, respectively (Table 2). Therefore, **Ih-μ3** is more stable than **Cubo-μ3**.

References

S1. M. Teramoto, K. Iwata, H. Yamaura, K. Kurashima, K. Miyazawa, Y. Kurashige, K. Yamamoto and T. Murahashi, *J. Am. Chem. Soc*., 2018, **140**, 12682–12686.

S2. J. Wei, S. Kahlal, J.-F. Halet and J.-Y. Saillard, *J. Cluster Science*, 2019, **30**, 1227-1233).

S3. Here, we compared HOMO energy using the optimized Pd_{13} bare cluster because the Pd_{13} cores in **Cubo-μ4** and **Anti-μ4** distort and the HOMO energy is influenced by the distortion. In other words, the discussion is presented on the intrinsic ability of HOMO of the Pd_{13} cluster for the CT from the Pd_{13} core to the $[(C_7H_7)_6]^{2+}$ ligand shell.

Cartesian coordinate

Cubo-μ4

Pd	**7.04727300**	**8.55225900**	**35.17618500**
Pd	**7.41182200**	**6.11795100**	**34.09106400**
Pd	**8.42256900**	**7.23592900**	**31.76405100**
Pd	**8.02436400**	**9.80280200**	**32.90126000**
Pd	**4.85422200**	**6.76944200**	**34.93665200**
Pd	**5.51319200**	**10.47297400**	**33.88367500**
C	**9.17192100**	**8.67761800**	**35.57866200**
H	**9.15635100**	**9.11552200**	**36.57579000**
C	**9.17844700**	**7.25167500**	**35.55477000**
H	**9.02118400**	**6.77608400**	**36.51883400**
C	**9.55490000**	**6.36762500**	**34.50213200**
H	**9.76767300**	**5.34848000**	**34.82141900**
C	**10.10286500**	**6.70452200**	**33.21563000**
H	**10.56866300**	**5.87025700**	**32.69672000**
C	**10.35316400**	**7.98709700**	**32.66890000**
H	**10.99946700**	**8.00518900**	**31.79431800**
C	**10.14245700**	**9.27863400**	**33.26774000**
H	**10.67189100**	**10.09079900**	**32.77367800**
C	**9.61466200**	**9.58110600**	**34.54812800**
H	**9.75639700**	**10.60465700**	**34.88545900**
C	**6.01363100**	**9.99784400**	**36.63379000**
H	**6.84425100**	**10.58374900**	**37.01882300**
C	**5.94452900**	**8.65748100**	**37.08997400**
H	**6.70482100**	**8.36658100**	**37.81201600**
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H	**4.94144500**	**6.85905100**	**37.62581700**
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H	**8.05038200**	**3.50752400**	**34.04359800**
C	**6.38230900**	**4.32828200**	**35.07204000**
H	**6.95118000**	**4.24215100**	**35.99463400**
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H	**4.66798100**	**4.58755800**	**36.30679200**
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Pd	**4.45283900**	**9.89431200**	**31.32138200**
Pd	**3.44209000**	**8.77633100**	**33.64839300**
Pd	**3.84029200**	**6.20945800**	**32.51118800**
Pd	**7.01044000**	**9.24282100**	**30.47579300**
Pd	**6.35146500**	**5.53928700**	**31.52877400**
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C	**2.68621500**	**8.76058700**	**29.85767600**
H	**2.84348100**	**9.23617800**	**28.89361100**
C	**2.30976100**	**9.64463800**	**30.91031400**
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C	**1.72220000**	**6.73362900**	**32.14470500**
H	**1.19276500**	**5.92146400**	**32.63876700**
C	**2.24999700**	**6.43115700**	**30.86431800**
H	**2.10826200**	**5.40760600**	**30.52698600**

C	**5.85102900**	**6.01441500**	**28.77866100**
H	**5.02040800**	**5.42850700**	**28.39363200**
C	**5.92012700**	**7.35477700**	**28.32247400**
H	**5.15983400**	**7.64567500**	**27.60043400**
C	**7.01643600**	**8.28118700**	**28.42989500**
H	**6.92320600**	**9.15320900**	**27.78662800**
C	**8.29771100**	**8.07763500**	**28.99846100**
H	**9.05025500**	**8.82092000**	**28.74654300**
C	**8.82289300**	**6.89646900**	**29.63028700**
H	**9.91024600**	**6.86729900**	**29.68153900**
C	**8.18789900**	**5.63081000**	**29.79037200**
H	**8.85027400**	**4.81748700**	**30.07343800**
C	**6.86173900**	**5.23460100**	**29.44597900**
H	**6.71585200**	**4.15822000**	**29.36599800**
C	**4.81891500**	**12.11467000**	**31.51536800**
H	**3.81427600**	**12.50473900**	**31.36885500**
C	**5.48234500**	**11.68398300**	**30.34040800**
H	**4.91347200**	**11.77011600**	**29.41781600**
C	**6.88097000**	**11.40855000**	**30.14774600**
H	**7.19666900**	**11.42470700**	**29.10565100**
C	**7.94111400**	**11.55114100**	**31.08994300**
H	**8.93994400**	**11.52299700**	**30.66344200**
C	**7.88417400**	**11.92127400**	**32.46579700**
H	**8.82827500**	**12.26951700**	**32.88241700**
C	**6.72679100**	**12.31026700**	**33.23019700**
H	**6.96050800**	**12.79235200**	**34.17601200**
C	**5.37589200**	**12.40365800**	**32.81082600**
H	**4.72138400**	**12.98387700**	**33.45804800**
Pd	**5.93233000**	**8.00613100**	**32.70622400**

Cubo-μ3

Pd	**-0.26152000**	**-1.50393600**	**2.27771000**
Pd	**-1.80323400**	**-2.14302700**	**0.03350200**
Pd	**-2.75729900**	**0.49021700**	**-0.03717800**
Pd	**-1.17344200**	**0.97539600**	**2.27766600**
Pd	**0.95424600**	**-2.63258400**	**-0.03654100**
Pd	**1.42940500**	**0.52507900**	**2.27919700**
C	**0.87366000**	**-3.64963200**	**3.25742500**
H	**1.57104000**	**-3.48125800**	**4.07407900**
C	**1.39651100**	**-4.25055000**	**2.11886800**
H	**2.45105300**	**-4.51131500**	**2.15720100**
C	**0.71873100**	**-4.65582300**	**0.93720900**
H	**1.27410200**	**-5.34121300**	**0.30260000**
C	**-0.63796800**	**-4.50115100**	**0.58787400**
H	**-0.95861400**	**-5.04632700**	**-0.29564500**
C	**-1.69212100**	**-3.85350800**	**1.31590500**
H	**-2.68281800**	**-4.25550400**	**1.11813400**
C	**-1.56599300**	**-3.24640400**	**2.62755200**
H	**-2.51597400**	**-2.95896800**	**3.07005400**
C	**-0.46625700**	**-3.26026200**	**3.51986400**
H	**-0.68092700**	**-2.95213500**	**4.54102100**
C	**3.05148400**	**1.22565500**	**3.52300800**
H	**2.89045100**	**0.88565900**	**4.54405500**
C	**3.58998700**	**0.26599200**	**2.63095900**
H	**3.81437600**	**-0.70149900**	**3.07365300**
C	**4.18018700**	**0.46046800**	**1.31967100**
H	**5.02325200**	**-0.19693300**	**1.12181900**
C	**4.21542300**	**1.69696400**	**0.59219100**
H	**4.84834900**	**1.69178700**	**-0.29134200**
C	**3.67144400**	**2.95041000**	**0.94310700**
H	**3.98916200**	**3.77427200**	**0.30981300**
C	**2.98040900**	**3.33551100**	**2.12362800**
H	**2.67788400**	**4.37834700**	**2.16554300**
C	**2.71999600**	**2.58042200**	**3.26106600**
H	**2.22465800**	**3.09895200**	**4.07789100**

C	**2.49159200**	**-3.38863900**	**-1.31670900**
H	**2.34357600**	**-4.44765000**	**-1.11901000**
C	**3.57818500**	**-2.80070200**	**-0.58832500**
H	**3.88834000**	**-3.35084900**	**0.29510700**
C	**4.39304700**	**-1.70420700**	**-0.93622700**
H	**5.26361900**	**-1.56706400**	**-0.30106300**
C	**4.38373400**	**-0.91316800**	**-2.11802600**
H	**5.13792700**	**-0.13201500**	**-2.15481700**
C	**3.60098700**	**-1.06503100**	**-3.25630400**
H	**3.80429600**	**-0.37724700**	**-4.07267300**
C	**2.59243300**	**-2.02980900**	**-3.51872200**
H	**2.21830500**	**-2.06061200**	**-4.53972600**
C	**2.03068400**	**-2.97535300**	**-2.62676200**
H	**1.30615500**	**-3.65391500**	**-3.06978900**
Pd	**0.26132700**	**1.50395700**	**-2.27774400**
Pd	**1.80322400**	**2.14304300**	**-0.03381200**
Pd	**2.75739900**	**-0.49013100**	**0.03677500**
Pd	**1.17347700**	**-0.97548000**	**-2.27772100**
Pd	**-0.95418800**	**2.63275200**	**0.03698000**
Pd	**-1.42945800**	**-0.52517800**	**-2.27941700**
C	**-0.87400100**	**3.64981900**	**-3.25703800**
H	**-1.57152400**	**3.48148700**	**-4.07357800**
C	**-1.39663900**	**4.25071400**	**-2.11838000**
H	**-2.45118200**	**4.51150000**	**-2.15652800**
C	**-0.71866400**	**4.65593800**	**-0.93681000**
H	**-1.27392200**	**5.34132600**	**-0.30210100**
C	**0.63810400**	**4.50125600**	**-0.58772400**
H	**0.95891900**	**5.04639200**	**0.29575900**
C	**1.69211900**	**3.85363200**	**-1.31597600**
H	**2.68287500**	**4.25554800**	**-1.11831800**
C	**1.56576000**	**3.24656000**	**-2.62761800**
H	**2.51567000**	**2.95913600**	**-3.07029100**
C	**0.46585800**	**3.26042200**	**-3.51972300**
H	**0.68035100**	**2.95234500**	**-4.54093400**
C	**-3.05168800**	**-1.22591000**	**-3.52295500**
H	**-2.89074500**	**-0.88592200**	**-4.54401900**

C	**-3.59019800**	**-0.26625400**	**-2.63089700**
H	**-3.81467500**	**0.70121500**	**-3.07360300**
C	**-4.18027600**	**-0.46069200**	**-1.31954700**
H	**-5.02332400**	**0.19672400**	**-1.12163200**
C	**-4.21543100**	**-1.69717800**	**-0.59202500**
H	**-4.84824200**	**-1.69197000**	**0.29159000**
C	**-3.67155800**	**-2.95064000**	**-0.94301800**
H	**-3.98920700**	**-3.77451100**	**-0.30970300**
C	**-2.98057400**	**-3.33574400**	**-2.12357100**
H	**-2.67806700**	**-4.37858800**	**-2.16548800**
C	**-2.72019700**	**-2.58067300**	**-3.26102800**
H	**-2.22490900**	**-3.09922200**	**-4.07787200**
C	**-2.49132400**	**3.38884400**	**1.31740300**
H	**-2.34322800**	**4.44787900**	**1.11989700**
C	**-3.57790100**	**2.80112300**	**0.58887700**
H	**-3.88807600**	**3.35151900**	**-0.29439100**
C	**-4.39264400**	**1.70440400**	**0.93636300**
H	**-5.26319300**	**1.56743000**	**0.30113000**
C	**-4.38328000**	**0.91303500**	**2.11792500**
H	**-5.13740200**	**0.13180400**	**2.15447800**
C	**-3.60061500**	**1.06466800**	**3.25631000**
H	**-3.80392600**	**0.37663900**	**4.07246900**
C	**-2.59218300**	**2.02947900**	**3.51909200**
H	**-2.21809000**	**2.06000400**	**4.54011400**
C	**-2.03041400**	**2.97523300**	**2.62736900**
H	**-1.30585400**	**3.65365900**	**3.07056800**
Pd	**-0.00000100**	**0.00001800**	**-0.00007400**

Anti-μ4

Pd	**-1.66035600**	**2.44814200**	**-0.21456600**
Pd	**-2.67997100**	**-0.10227600**	**-0.70003500**
Pd	**-1.53054000**	**-1.27995100**	**1.72647100**
Pd	**-1.19114200**	**1.33356900**	**2.19162600**
Pd	**-0.89426700**	**1.04806500**	**-2.44956000**
Pd	**0.98124300**	**2.47550100**	**-0.74291700**
C	**-4.30391200**	**1.74281800**	**0.66432700**
H	**-4.65656700**	**2.53659500**	**0.00990900**
C	**-4.58977000**	**0.41094800**	**0.20363900**
H	**-5.29185100**	**0.35464400**	**-0.62620200**
C	**-4.26374300**	**-0.80223000**	**0.82873600**
H	**-4.71808600**	**-1.69175500**	**0.40205700**
C	**-3.64419400**	**-1.02541900**	**2.12471400**
H	**-3.85822200**	**-2.01056600**	**2.53527900**
C	**-3.32259400**	**-0.04798300**	**3.10231900**
H	**-3.08845300**	**-0.43611600**	**4.09091600**
C	**-3.36761700**	**1.35954500**	**3.00240100**
H	**-3.23808000**	**1.89178500**	**3.94189100**
C	**-3.85899600**	**2.13463200**	**1.91454200**
H	**-3.89643000**	**3.20472500**	**2.09600800**
C	**0.82818000**	**2.48594600**	**-3.68249400**
H	**0.08078600**	**3.09900600**	**-4.18158600**
C	**1.00834800**	**1.21254300**	**-4.18958800**
H	**0.39257300**	**0.97291700**	**-5.05158800**
C	**1.97127600**	**0.18587100**	**-3.83470900**
H	**2.09168200**	**-0.58503600**	**-4.59844600**
C	**3.14058700**	**0.38176700**	**-3.03777400**
H	**3.91829200**	**-0.36404700**	**-3.18361700**
C	**3.49279500**	**1.47407600**	**-2.21018000**
H	**4.54733200**	**1.52676800**	**-1.94888300**
C	**2.78712500**	**2.73587100**	**-2.04727500**
H	**3.37799700**	**3.50584200**	**-1.55611200**
C	**1.62645800**	**3.18765900**	**-2.70332100**
H	**1.44368000**	**4.25948000**	**-2.66495500**

C	**-3.51084900**	**-1.47929600**	**-2.18324900**
H	**-4.56326300**	**-1.53295100**	**-1.91375200**
C	**-3.16579300**	**-0.38634900**	**-3.01278200**
H	**-3.94572900**	**0.35811600**	**-3.15362000**
C	**-2.00189400**	**-0.18824000**	**-3.81756900**
H	**-2.12946600**	**0.58200200**	**-4.58089400**
C	**-1.04094900**	**-1.21414200**	**-4.18025100**
H	**-0.43215900**	**-0.97367800**	**-5.04696200**
C	**-0.85631100**	**-2.48789700**	**-3.67571700**
H	**-0.11229800**	**-3.10007100**	**-4.18085600**
C	**-1.64623200**	**-3.19041100**	**-2.69052500**
H	**-1.46139300**	**-4.26189600**	**-2.65282200**
C	**-2.80230800**	**-2.74013800**	**-2.02528500**
H	**-3.38846200**	**-3.51088400**	**-1.52966900**
Pd	**1.65598900**	**-2.44929000**	**-0.22757500**
Pd	**1.54501000**	**1.28046200**	**1.71483000**
Pd	**2.67334800**	**0.10172000**	**-0.71732300**
Pd	**0.87320500**	**-1.04561500**	**-2.45432100**
Pd	**1.21135300**	**-1.33227800**	**2.18204800**
Pd	**-0.98837000**	**-2.47558500**	**-0.73489100**
C	**3.39181000**	**-1.36144000**	**2.97655100**
H	**3.26998400**	**-1.89493800**	**3.91635400**
C	**3.34712500**	**0.04572500**	**3.07877200**
H	**3.12048900**	**0.43253200**	**4.06962600**
C	**3.66025900**	**1.02480700**	**2.09978200**
H	**3.87750500**	**2.00935000**	**2.51013600**
C	**4.26916700**	**0.80356000**	**0.79852200**
H	**4.71830500**	**1.69413700**	**0.36844900**
C	**4.59171600**	**-0.40862400**	**0.16965200**
H	**5.28695900**	**-0.35053700**	**-0.66579300**
C	**4.31249400**	**-1.74136900**	**0.63179400**
H	**4.66078400**	**-2.53396800**	**-0.02635600**
C	**3.87600400**	**-2.13510300**	**1.88401300**
H	**3.91490500**	**-3.20541200**	**2.06380900**
C	**0.29386700**	**-4.50914100**	**0.24626800**
H	**0.58596000**	**-5.13819800**	**-0.59101300**

C	**1.34395200**	**-4.11543300**	**1.10818600**
H	**2.28782200**	**-4.63154300**	**0.92758000**
C	**1.21607300**	**-3.59165400**	**2.46505400**
H	**2.09414600**	**-3.74486200**	**3.08392200**
C	**0.07790500**	**-3.18496900**	**3.15663000**
H	**0.20917500**	**-2.98133600**	**4.21632800**
C	**-1.29757400**	**-3.23251000**	**2.71891200**
H	**-2.01977300**	**-3.11196600**	**3.52471600**
C	**-1.80597300**	**-3.78136700**	**1.52944900**
H	**-2.88507500**	**-3.90851100**	**1.49437600**
C	**-1.11412200**	**-4.31707600**	**0.39188900**
H	**-1.72710000**	**-4.95029000**	**-0.24686400**
C	**1.12155000**	**4.31743400**	**0.38339900**
H	**1.73066500**	**4.94963300**	**-0.26001000**
C	**1.82093700**	**3.78099700**	**1.51604800**
H	**2.89987200**	**3.90744300**	**1.47354400**
C	**1.32038600**	**3.23298100**	**2.70915500**
H	**2.04790000**	**3.11241500**	**3.51015300**
C	**-0.05224500**	**3.18502800**	**3.15589900**
H	**-0.17640300**	**2.98281300**	**4.21671400**
C	**-1.19496100**	**3.59151200**	**2.47141100**
H	**-2.06873900**	**3.74567100**	**3.09609600**
C	**-1.33187100**	**4.11504700**	**1.11523800**
H	**-2.27643000**	**4.63238500**	**0.94152100**
C	**-0.28702800**	**4.50937600**	**0.24687400**
H	**-0.58469000**	**5.13821100**	**-0.58860500**
Pd	**-0.00142800**	**0.00096900**	**-0.08816500**

Anti-μ3;4

Pd	**0.40541900**	**2.78979900**	**0.38219900**
Pd	**0.83770500**	**1.60137700**	**-2.04269500**
Pd	**-1.69607100**	**0.54709400**	**-2.27141500**
Pd	**-2.11971300**	**1.64314500**	**0.40513800**
Pd	**2.58539700**	**0.93251300**	**0.05688800**
Pd	**0.92448900**	**1.00546600**	**2.38505100**
C	**-0.78783100**	**4.40014200**	**-0.40795600**
H	**-0.51203500**	**5.24489300**	**0.22154600**
C	**0.08351500**	**4.15197300**	**-1.50441300**
H	**0.96748700**	**4.78194200**	**-1.54467400**
C	**-0.17427900**	**3.41988700**	**-2.71410200**
H	**0.47684100**	**3.67954400**	**-3.54722300**
C	**-1.37587000**	**2.75071000**	**-3.08412800**
H	**-1.44183500**	**2.49909600**	**-4.14036200**
C	**-2.57533300**	**2.55833100**	**-2.33465000**
H	**-3.44665700**	**2.28445300**	**-2.92839800**
C	**-2.90665200**	**3.08892000**	**-1.03350800**
H	**-3.97394000**	**3.08893000**	**-0.82135400**
C	**-2.11915700**	**3.91304600**	**-0.19030600**
H	**-2.64349300**	**4.38819600**	**0.63442700**
C	**1.43607500**	**3.80938400**	**2.33191100**
H	**0.77830400**	**4.67349800**	**2.38333500**
C	**2.28170400**	**3.74042300**	**1.18405800**
H	**2.30982400**	**4.64005600**	**0.57398400**
C	**3.41265000**	**2.86685200**	**0.99317400**
H	**4.12849200**	**3.21230300**	**0.25146500**
C	**3.78485600**	**1.73255100**	**1.73568300**
H	**4.77057900**	**1.31870300**	**1.53286800**
C	**3.14595100**	**1.22057500**	**2.93560100**
H	**3.60055800**	**0.31509100**	**3.32796300**
C	**2.26883500**	**1.88451400**	**3.81583600**
H	**2.15672900**	**1.47220700**	**4.81530700**
C	**1.42964000**	**2.99175900**	**3.48401300**
H	**0.73611600**	**3.29560800**	**4.26402400**

C	**2.18452300**	**0.85934300**	**-3.68964000**
H	**1.85967500**	**1.48144100**	**-4.52036100**
C	**2.95975700**	**1.50760100**	**-2.69544300**
H	**3.14892300**	**2.56426700**	**-2.87415800**
C	**3.86224500**	**0.92533800**	**-1.71082800**
H	**4.64589300**	**1.60645800**	**-1.38384500**
C	**4.14874100**	**-0.44004100**	**-1.50011600**
H	**5.02016900**	**-0.64893200**	**-0.88567000**
C	**3.51333200**	**-1.58587500**	**-2.07107400**
H	**4.08206200**	**-2.50898800**	**-1.97049600**
C	**2.56967700**	**-1.61681800**	**-3.16031000**
H	**2.44346100**	**-2.60315700**	**-3.60051600**
C	**1.99786800**	**-0.55320300**	**-3.89368600**
H	**1.54450700**	**-0.82056100**	**-4.84512800**
Pd	**-0.43584500**	**-2.64067500**	**-0.11666200**
Pd	**-1.50928900**	**-0.16581000**	**2.33471600**
Pd	**0.70815700**	**-1.61837500**	**2.09364200**
Pd	**2.21847700**	**-1.71573400**	**-0.35821700**
Pd	**-2.68824600**	**-0.93849000**	**-0.15401600**
Pd	**0.44399300**	**-1.12994600**	**-2.38705900**
C	**0.90495400**	**-4.17806800**	**0.69630600**
H	**0.34873400**	**-4.99577900**	**0.23818300**
C	**0.53677300**	**-3.89769800**	**2.06523900**
H	**-0.42956400**	**-4.29568800**	**2.36306700**
C	**1.32549700**	**-3.38474100**	**3.12816000**
H	**0.87238300**	**-3.45084900**	**4.11538400**
C	**2.67477600**	**-2.91288200**	**3.09500200**
H	**3.05645000**	**-2.54861100**	**4.04517700**
C	**3.55272100**	**-2.89840400**	**2.02518500**
H	**4.54682000**	**-2.50756200**	**2.22786300**
C	**3.35523300**	**-3.36419700**	**0.69704700**
H	**4.26643400**	**-3.46081200**	**0.11126500**
C	**2.19762700**	**-3.93272800**	**0.10612400**
H	**2.35036600**	**-4.42103300**	**-0.85353600**
C	**-0.86285500**	**-3.66182700**	**-2.07512400**
H	**-0.19728500**	**-4.52099000**	**-2.07702100**

C	**-1.99823700**	**-3.77352400**	**-1.23171900**
H	**-2.08173200**	**-4.69726800**	**-0.66241700**
C	**-3.15435100**	**-2.94103100**	**-1.18209900**
H	**-3.97133300**	**-3.34271500**	**-0.58929100**
C	**-3.47842000**	**-1.81344800**	**-1.99198700**
H	**-4.52369200**	**-1.51094400**	**-1.98032600**
C	**-2.71587200**	**-1.22176300**	**-3.05415100**
H	**-3.31649900**	**-0.61629600**	**-3.73549600**
C	**-1.49734700**	**-1.72027500**	**-3.64279500**
H	**-1.28668100**	**-1.33853200**	**-4.63803300**
C	**-0.67759800**	**-2.78855100**	**-3.21682200**
H	**0.00758100**	**-3.17646800**	**-3.96862800**
C	**-3.64286000**	**-1.36081600**	**3.38060000**
H	**-3.50537800**	**-2.12514200**	**4.14114600**
C	**-4.24568500**	**-1.76704700**	**2.20196800**
H	**-4.51422000**	**-2.81824700**	**2.13967600**
C	**-4.59499400**	**-0.99256900**	**1.06269000**
H	**-5.26539300**	**-1.49327400**	**0.36665200**
C	**-4.50989900**	**0.41482900**	**0.87425900**
H	**-5.09160300**	**0.81325300**	**0.04722600**
C	**-3.87402700**	**1.38504300**	**1.69922000**
H	**-4.22534400**	**2.40949300**	**1.57981100**
C	**-3.18002900**	**1.11744500**	**2.94587000**
H	**-2.84195800**	**2.01338000**	**3.46029000**
C	**-3.17117900**	**-0.06731300**	**3.73209500**
H	**-2.81934200**	**0.05151400**	**4.75455600**
Pd	**0.00950000**	**0.01295000**	**0.04505200**

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Pd	**0.00000000**	**0.00000000**	**0.04256900**
Pd	**1.47122600**	**2.34556800**	**0.15751000**
Pd	**-2.71537400**	**0.12305400**	**0.11268200**
Pd	**-0.99877100**	**2.06961400**	**-1.42608200**
Pd	**1.33614800**	**0.64157900**	**-2.14918800**
Pd	**-1.33614800**	**-0.64157900**	**-2.14918800**
Pd	**0.99877100**	**-2.06961400**	**-1.42608200**
Pd	**-1.47122600**	**-2.34556800**	**0.15751000**
Pd	**2.71537400**	**-0.12305400**	**0.11268200**
Pd	**1.15489300**	**-2.08696700**	**1.35956200**
Pd	**-1.27044900**	**-0.56131200**	**2.33536000**
Pd	**1.27044900**	**0.56131200**	**2.33536000**
Pd	**-1.15489300**	**2.08696700**	**1.35956200**
C	**-3.92342900**	**1.86690400**	**0.94891400**
C	**-3.02366600**	**2.96673700**	**0.68625500**
C	**-2.65976700**	**3.45891900**	**-0.62261900**
C	**-3.01631200**	**2.94967900**	**-1.89386900**
C	**-3.80467800**	**1.81526800**	**-2.21683400**
C	**-4.54258000**	**0.99833400**	**-1.36484600**
C	**-4.66926500**	**1.06951700**	**0.05024400**
H	**-5.15544000**	**0.23752600**	**-1.84201800**
H	**-5.44537600**	**0.45148600**	**0.49557100**
H	**-4.20512500**	**1.76459400**	**1.99373500**
H	**-3.02543400**	**3.72963300**	**1.46555600**
H	**-2.21742000**	**4.45205900**	**-0.62203400**
H	**-2.79910500**	**3.60116100**	**-2.73697700**
H	**-3.89811100**	**1.60729500**	**-3.27951400**
C	**-0.20597900**	**3.97188600**	**2.15665100**
C	**-0.69798200**	**3.23238100**	**3.25658500**
C	**0.00000000**	**2.31604900**	**4.08918000**
C	**1.34545500**	**1.92816000**	**4.03477200**
C	**2.32783600**	**2.25556000**	**3.03323900**
C	**2.26345700**	**3.30543000**	**2.04034500**
C	**1.14597400**	**4.06307400**	**1.65874600**

H	**3.23157100**	**3.65806900**	**1.69015300**
H	**1.34753000**	**4.94555100**	**1.05844700**
H	**-0.85717500**	**4.76800700**	**1.80289100**
H	**-1.68980900**	**3.50587000**	**3.61051400**
H	**-0.57563800**	**1.90877300**	**4.91603100**
H	**1.71212800**	**1.36225300**	**4.88902500**
H	**3.34140100**	**1.93583600**	**3.26616800**
C	**2.29558200**	**3.75478100**	**-1.39653100**
C	**0.98534100**	**4.10673700**	**-1.77766500**
C	**0.11916400**	**3.50028700**	**-2.72559700**
C	**0.48484800**	**2.52175000**	**-3.72040200**
C	**1.70909400**	**1.87971800**	**-3.92822200**
C	**2.86687100**	**1.90989600**	**-3.07036500**
C	**3.11804700**	**2.72953900**	**-1.95646100**
H	**3.71322700**	**1.32355600**	**-3.41949900**
H	**4.10745300**	**2.63572900**	**-1.51671600**
H	**2.81712000**	**4.47046600**	**-0.76501200**
H	**0.58240800**	**4.99273200**	**-1.29326400**
H	**-0.73417700**	**4.11429300**	**-3.00383900**
H	**-0.28040500**	**2.32176600**	**-4.46665700**
H	**1.80719000**	**1.30212300**	**-4.84359000**
C	**-0.98534100**	**-4.10673700**	**-1.77766500**
C	**-2.29558200**	**-3.75478100**	**-1.39653100**
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C	**-2.86687100**	**-1.90989600**	**-3.07036500**
C	**-1.70909400**	**-1.87971800**	**-3.92822200**
C	**-0.48484800**	**-2.52175000**	**-3.72040200**
C	**-0.11916400**	**-3.50028700**	**-2.72559700**
H	**0.28040500**	**-2.32176600**	**-4.46665700**
H	**0.73417700**	**-4.11429300**	**-3.00383900**
H	**-0.58240800**	**-4.99273200**	**-1.29326400**
H	**-2.81712000**	**-4.47046600**	**-0.76501200**
H	**-4.10745300**	**-2.63572900**	**-1.51671600**
H	**-3.71322700**	**-1.32355600**	**-3.41949900**
H	**-1.80719000**	**-1.30212300**	**-4.84359000**
C	**0.20597900**	**-3.97188600**	**2.15665100**

C	**0.69798200**	**-3.23238100**	**3.25658500**
C	**0.00000000**	**-2.31604900**	**4.08918000**
C	**-1.34545500**	**-1.92816000**	**4.03477200**
C	**-2.32783600**	**-2.25556000**	**3.03323900**
C	**-2.26345700**	**-3.30543000**	**2.04034500**
C	**-1.14597400**	**-4.06307400**	**1.65874600**
H	**-3.23157100**	**-3.65806900**	**1.69015300**
H	**-1.34753000**	**-4.94555100**	**1.05844700**
H	**0.85717500**	**-4.76800700**	**1.80289100**
H	**1.68980900**	**-3.50587000**	**3.61051400**
H	**0.57563800**	**-1.90877300**	**4.91603100**
H	**-1.71212800**	**-1.36225300**	**4.88902500**
H	**-3.34140100**	**-1.93583600**	**3.26616800**
C	**3.02366600**	**-2.96673700**	**0.68625500**
C	**2.65976700**	**-3.45891900**	**-0.62261900**
C	**3.01631200**	**-2.94967900**	**-1.89386900**
C	**3.80467800**	**-1.81526800**	**-2.21683400**
C	**4.54258000**	**-0.99833400**	**-1.36484600**
C	**4.66926500**	**-1.06951700**	**0.05024400**
C	**3.92342900**	**-1.86690400**	**0.94891400**
H	**5.44537600**	**-0.45148600**	**0.49557100**
H	**4.20512500**	**-1.76459400**	**1.99373500**
H	**3.02543400**	**-3.72963300**	**1.46555600**
H	**2.21742000**	**-4.45205900**	**-0.62203400**
H	**2.79910500**	**-3.60116100**	**-2.73697700**
H	**3.89811100**	**-1.60729500**	**-3.27951400**
H	**5.15544000**	**-0.23752600**	**-1.84201800**