

Supporting Information for

Discrete Palladium Clusters That Consist of Two Mutually Bisecting Perpendicular Planes

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General. Manipulation of air and moisture sensitive compounds was carried out under a dry nitrogen atmosphere using Schlenk tube techniques associated with a high-vacuum line or in the glove box which was filled with dry nitrogen. All solvents were purchased from Kanto Chemical Co. Inc., and was dried over activated molecular sieves. ^1H and ^{13}C NMR spectra were recorded on a JEOL Lambda 400 and JEOL ECZ600R spectrometer at ambient temperature unless otherwise noted. ^1H , ^{13}C NMR chemical shifts (δ values) were given in ppm relative to the solvent signal (^1H , ^{13}C). Elemental analyses were performed by a Thermo Scientific FLASH 2000 Organic Elemental Analyzer. IR spectra were recorded on a PerkinElmer Spectrum Two spectrometer. The starting compounds, $[\text{Pd}(\text{CN}'\text{Bu})_2]_3$ ¹ and Sn_3Me_8 (**4**)^{2,3}, $\text{Ge}_6\text{Me}_{12}$ (**5**)⁴ were synthesized by the method reported in the literature. All reagents were purchased from Tokyo Chemical Industries Co., Ltd. or Sigma-Aldrich, and were used without further purification.

Synthesis of $\text{Pd}_7(\text{SnMe}_2)_4(\text{CN}'\text{Bu})_{10}$ (2**).** In a 5 mL vial, Sn_3Me_8 (**4**) (9.7 mg, 0.020 mmol) was dissolved in toluene (0.5 mL). Subsequently, a toluene (1.5 mL) solution of $[\text{Pd}(\text{CN}'\text{Bu})_2]_3$ [19.4 mg, 0.023 mmol (7 equiv. of Pd relative to **4**)] was added to this solution at room temperature. The solution was stored at room temperature for 2 weeks, and dark red crystals of **2** were obtained in 74 % yield (16.0 mg, 7.4 μmol). ^1H NMR (400 MHz, r.t., C_6D_6): δ = 0.77 (s, 6H, SnMe_2) 1.04 (s, 6H, SnMe_2), 1.09 (s, 18H, ' Bu '), 1.25 (s, 6H, SnMe_2), 1.27 (s, 18H, ' Bu '), 1.31 (s, 6H, SnMe_2), 1.32 (s, 18H, ' Bu '), 1.41 (s, 18H, ' Bu '), 1.75 (s, 18H, ' Bu '). ^{13}C NMR (150 MHz, r.t., C_6D_6): δ = 29.82, 30.29, 30.35, 30.74, 31.01 ($\text{CNC}(\text{CH}_3)_3$), 54.07, 54.84, 55.04, 55.13, 56.63 ($\text{CNC}(\text{CH}_3)_3$), 63.13, 66.82, 67.10, 69.07 ($\text{Sn}(\text{CH}_3)_2$) (signals due to the $\text{CN}'\text{Bu}$ moieties were missing due to the low solubility of **2** toward C_6D_6). IR (ATR): ν_{CN} = 2093, 2058, 1829 cm^{-1} . Anal calcd for $\text{C}_{58}\text{H}_{114}\text{N}_{10}\text{Pd}_7\text{Sn}_4$; C 32.08, H 5.29, N 6.45; found: C 32.56, H 5.01, N 6.39.

<Note>

The ^{119}Sn NMR signals were not detectable, presumably due to the low solubility of **2** in C_6D_6 .

The ^1H -DOSY spectrum of a C_6D_6 solution of **2** indicates that all the ^1H NMR resonances have the same diffusion coefficient (3.7×10^{-10} (m^2/s))) (see Figure S2). This suggests that all the proton signals listed above were derived from cluster **2**.

The ^{13}C NMR signals were assigned based on the ^1H - ^{13}C HSQC and HMBC spectra. These spectra are shown in Figures S3–S8.

Synthesis of $\text{Pd}_8(\text{GeMe}_2)_6(\text{CN}'\text{Bu})_{10}$ (3**)** In a 5 mL vial, $\text{Ge}_6\text{Me}_{12}$ (6.8 mg, 0.011 mmol) was dissolved in cyclopentylmethylether (CPME, 0.5 mL). Subsequently, a CPME (1.5 mL) solution of $[\text{Pd}(\text{CN}'\text{Bu})_2]_3$ [24.1 mg, 0.029 mmol (8 equiv. of Pd relative to **5**)] was added to this solution at -20 °C. Upon adding the $[\text{Pd}(\text{CN}'\text{Bu})_2]_3$ solution, the resulting solution turned deep blue. The solution was stored at -20 °C for 3 days, and black crystals of **3** were obtained in 49 % yield (12.5 mg, 5.4 μmol). ^{13}C NMR measurements were unsuccessful due to the high instability of the Pd_8Ge_6 cluster at room temperature, as well as the low solubility of the Pd_8Ge_6 cluster in toluene-d₈ at -30 °C. ^1H NMR (400 MHz, -30°C, C_7D_8): δ = 0.99 (s, 36H, CNCMe_3), 1.32 (s, 36H, CNCMe_3), 1.38 (s, 12H, GeMe_2), 1.73 (s, 24H, GeMe_2), 1.87 (s, 18H, CNCMe_3). ^{13}C NMR measurement was unsuccessful due to the high instability of Pd_8Ge_6 cluster at room temperature as well as low solubility of Pd_8Ge_6 cluster in toluene-d₈ at -30°C. IR (ATR): ν_{CN} = 2136, 2119, 2065, 1825 cm^{-1} . Anal calcd for $\text{C}_{62}\text{H}_{126}\text{Ge}_6\text{N}_{10}\text{Pd}_8$; C 32.39, H 5.52, N 6.09; found: C 32.10, H 5.17, N 5.96.

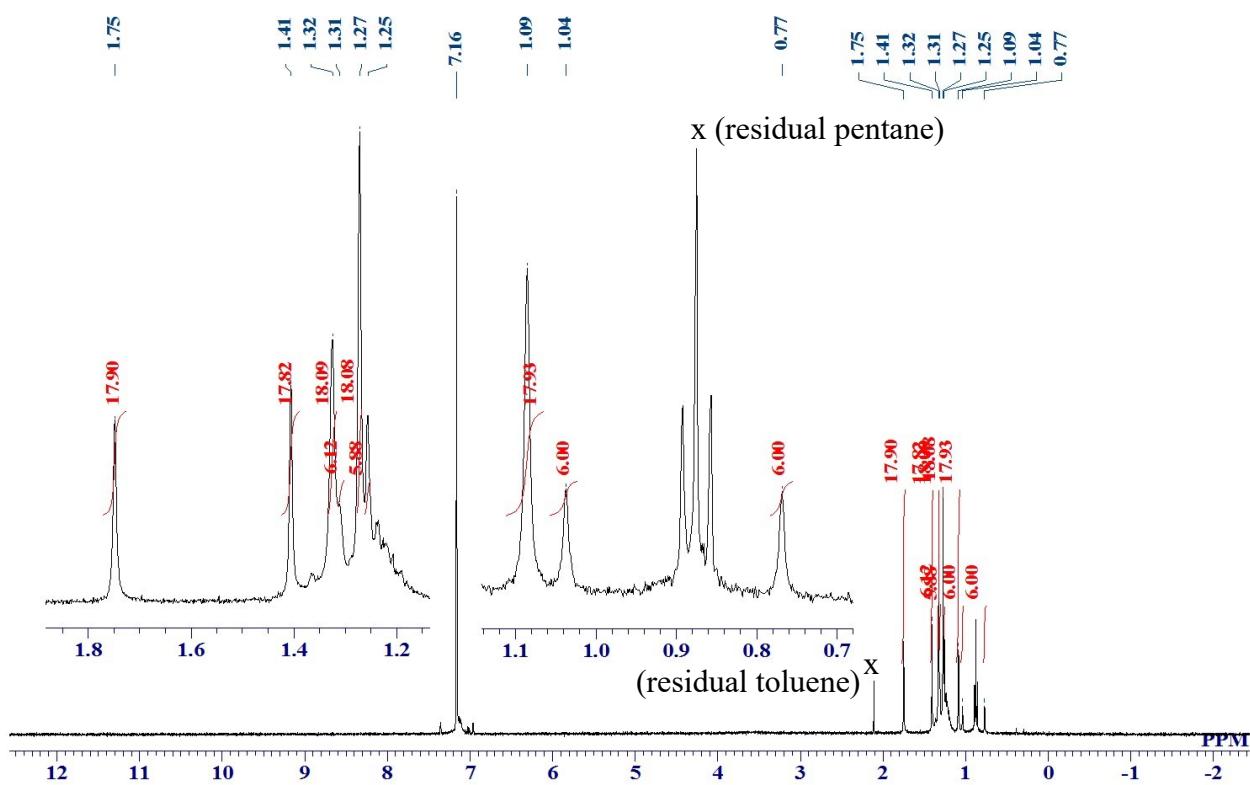


Figure S1. ¹H NMR spectrum of Pd₇Sn₄ cluster **2** in C₆D₆ at room temperature.

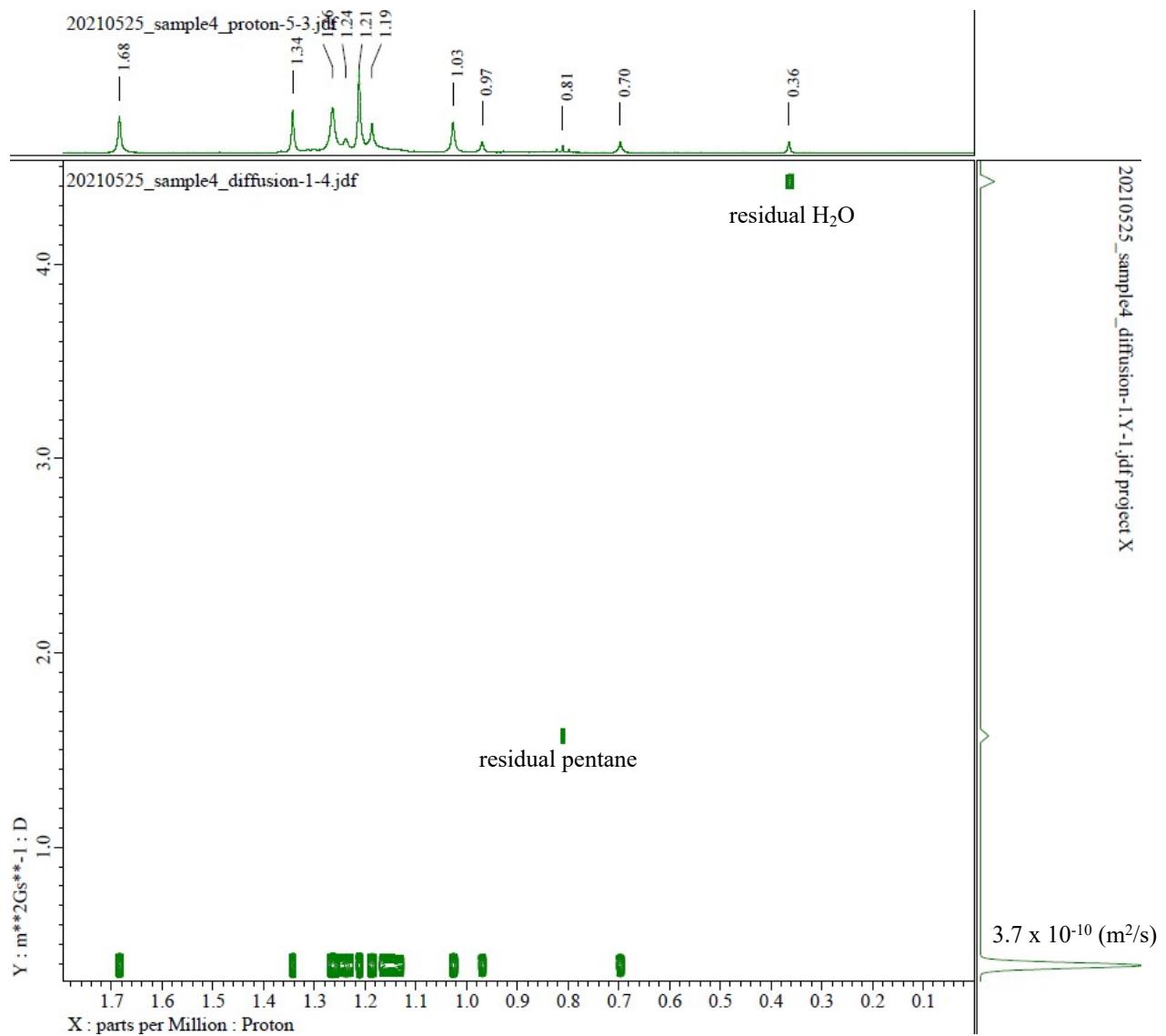


Figure S2. ^1H -DOSY spectrum of Pd_7Sn_4 cluster **2** in C_6D_6 at room temperature.

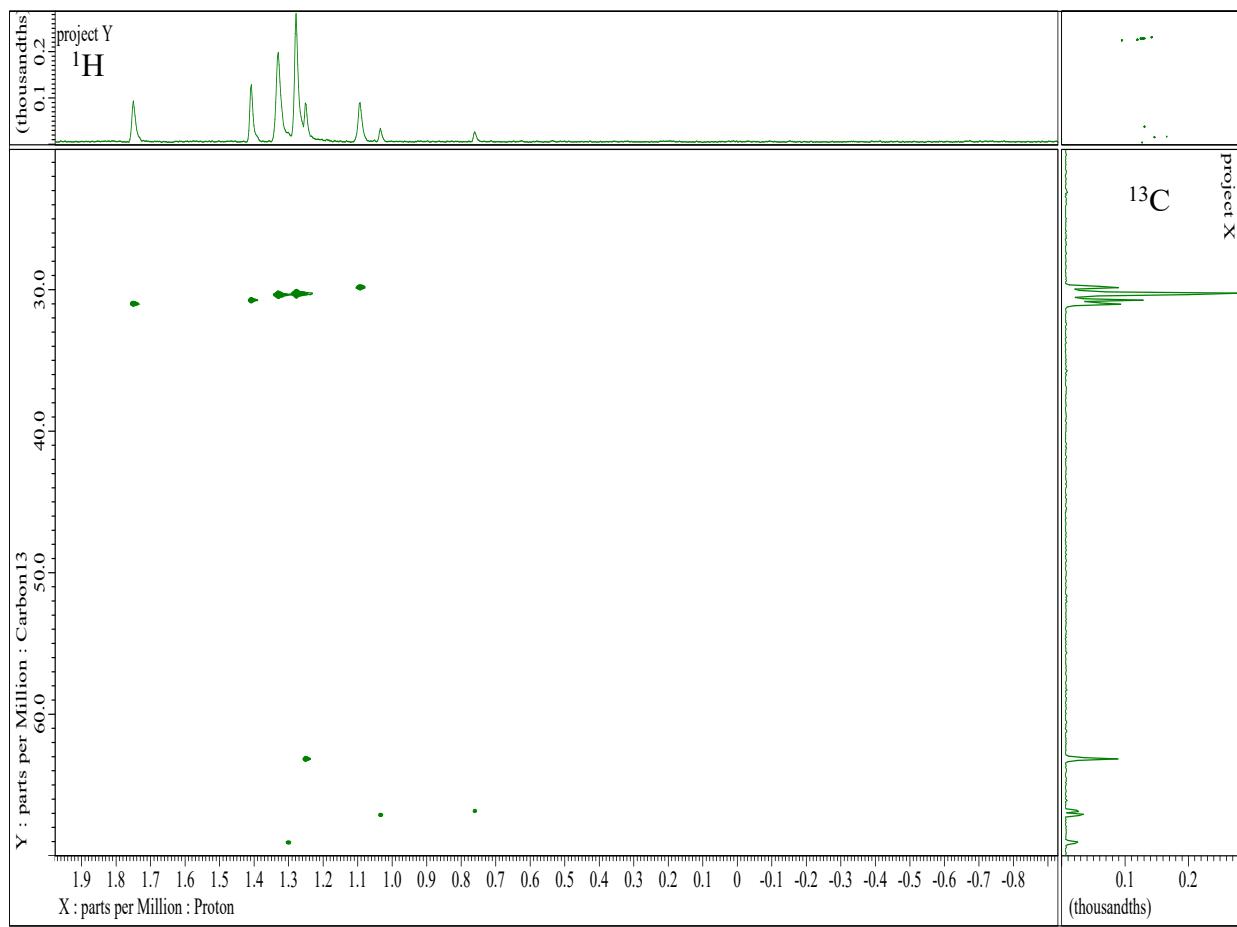


Figure S3. ^1H - ^{13}C HSQC spectrum of Pd_7Sn_4 cluster **2** in C_6D_6 at room temperature.

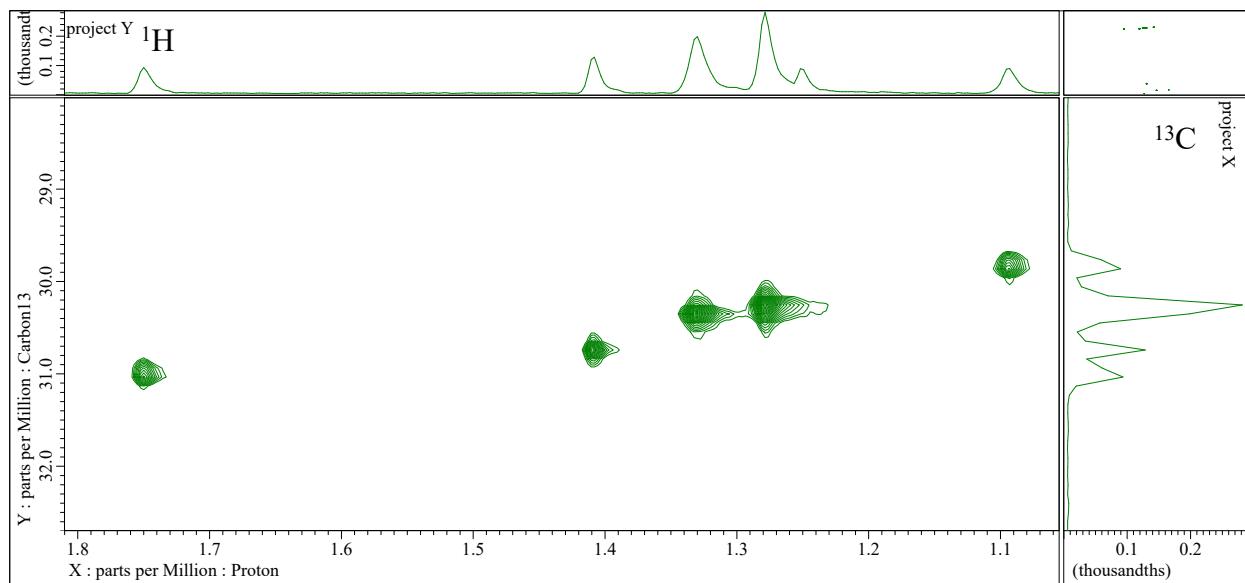


Figure S4. Enlarged view (28- 33 ppm) in ^1H - ^{13}C HSQC spectrum of Pd_7Sn_4 cluster **2** in C_6D_6 at room temperature.

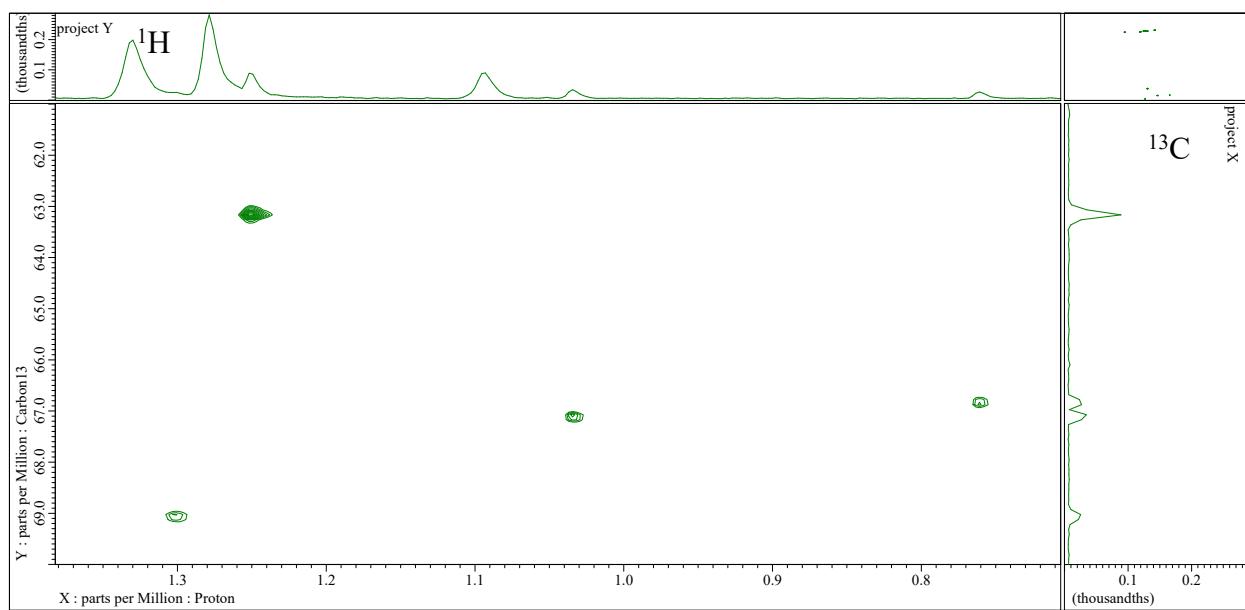


Figure S5. Enlarged view (60 - 70 ppm) in ^1H - ^{13}C HSQC spectrum of Pd_7Sn_4 cluster **2** in C_6D_6 at room temperature.

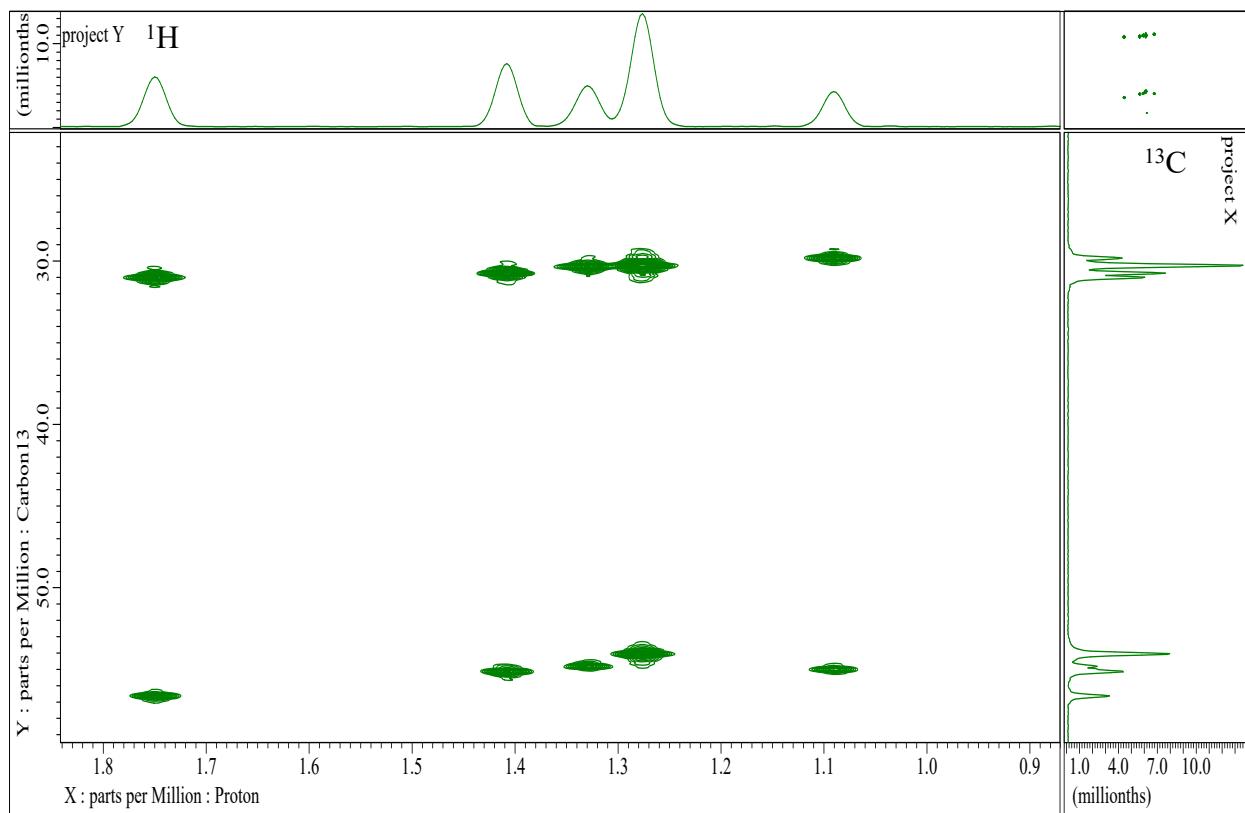


Figure S6. ^1H - ^{13}C HMBC spectrum of Pd_7Sn_4 cluster **2** in C_6D_6 at room temperature.

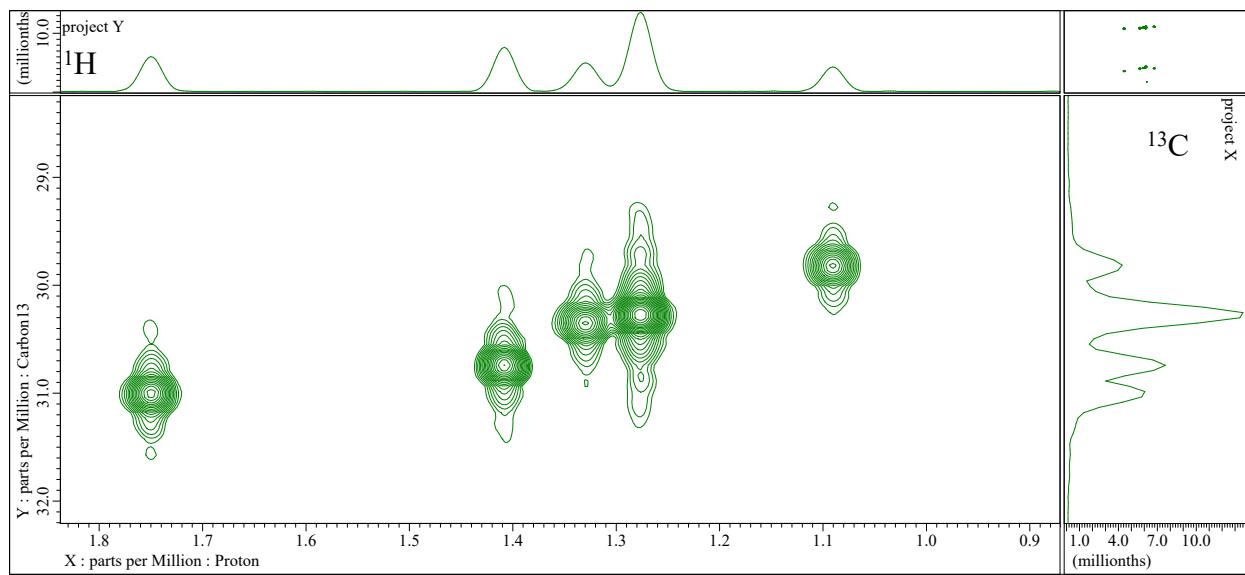


Figure S7. Enlarged view (28 - 32 ppm) in ¹H-¹³C HMBC spectrum of Pd₇Sn₄ cluster **2** in C₆D₆ at room temperature.

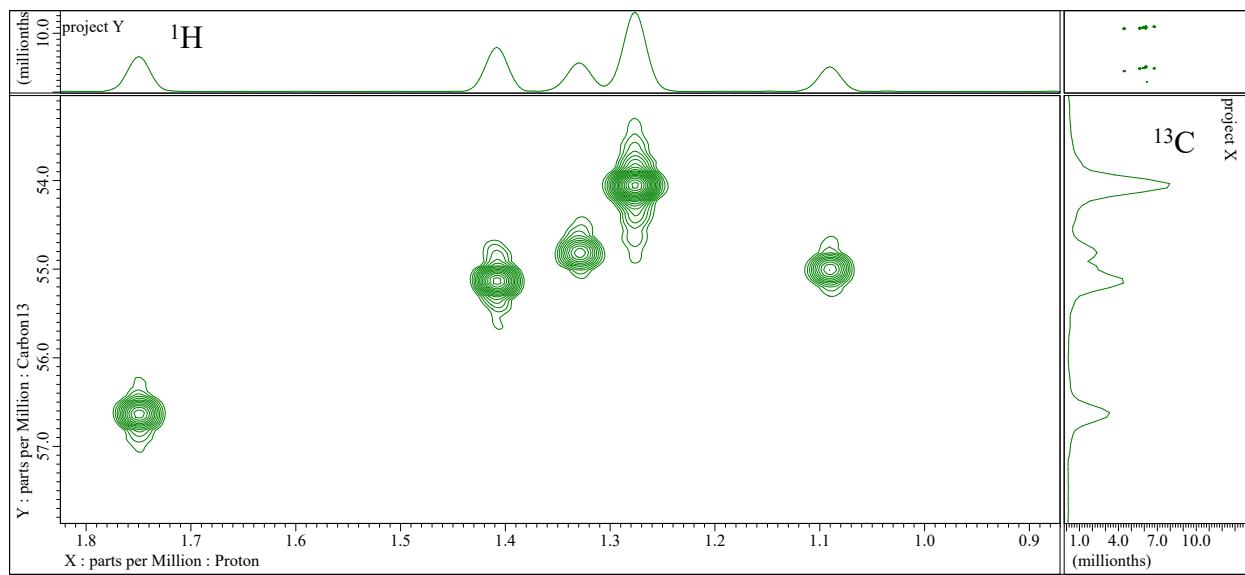


Figure S8. Enlarged view (53 - 58 ppm) in ^1H - ^{13}C HMBC spectrum of Pd_7Sn_4 cluster **2** in C_6D_6 at room temperature.

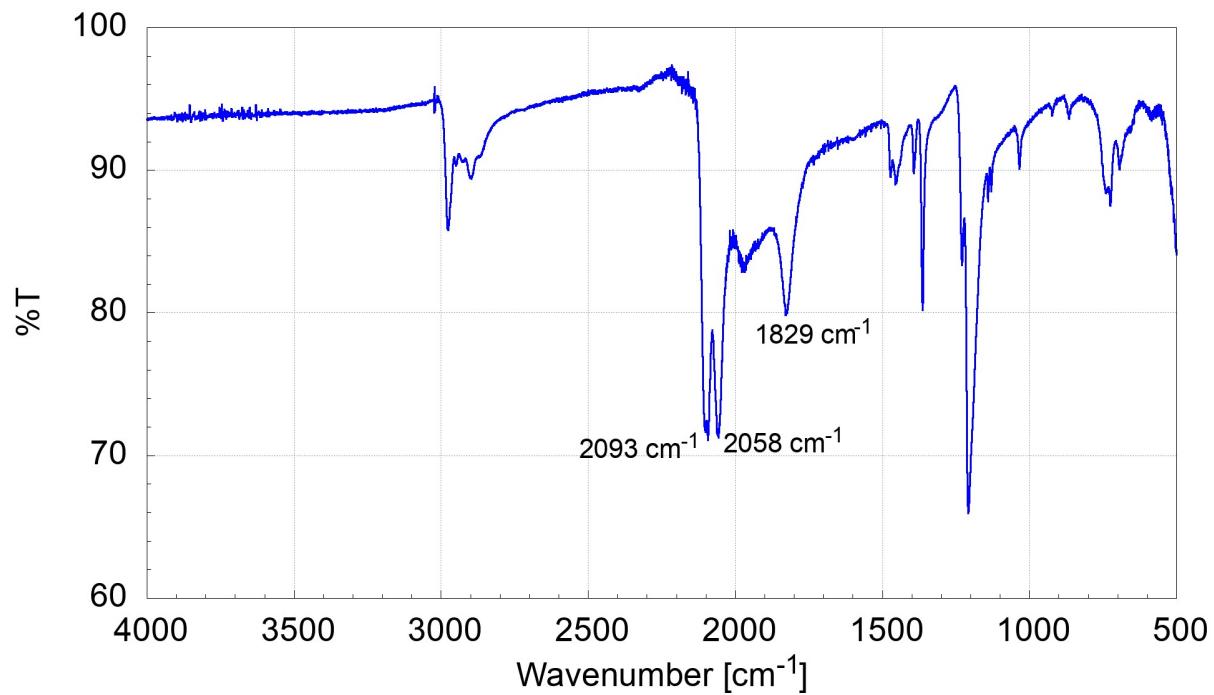


Figure S9. ATR-IR spectrum of Pd_7Sn_4 cluster **2** in the solid state.

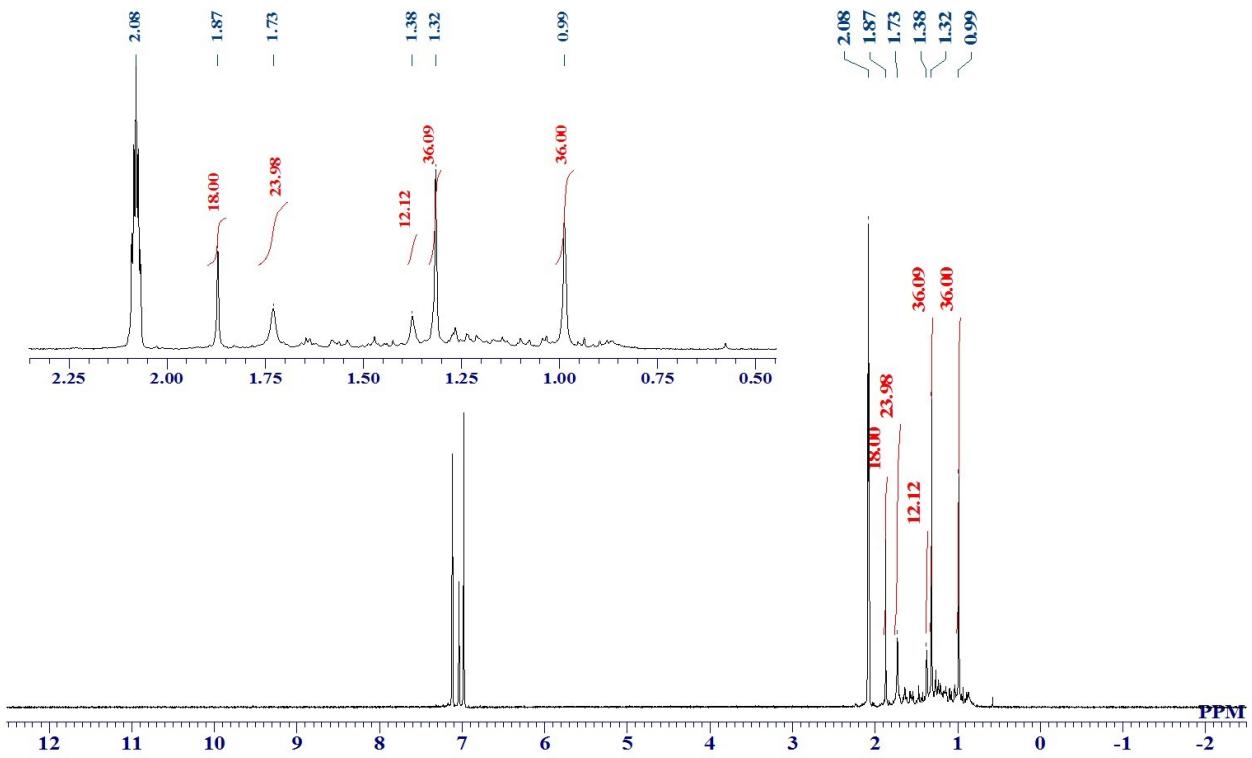


Figure S10. ¹H NMR spectrum of solution of Pd₈Ge₆ cluster **3** in C₇D₈ at -30 °C.

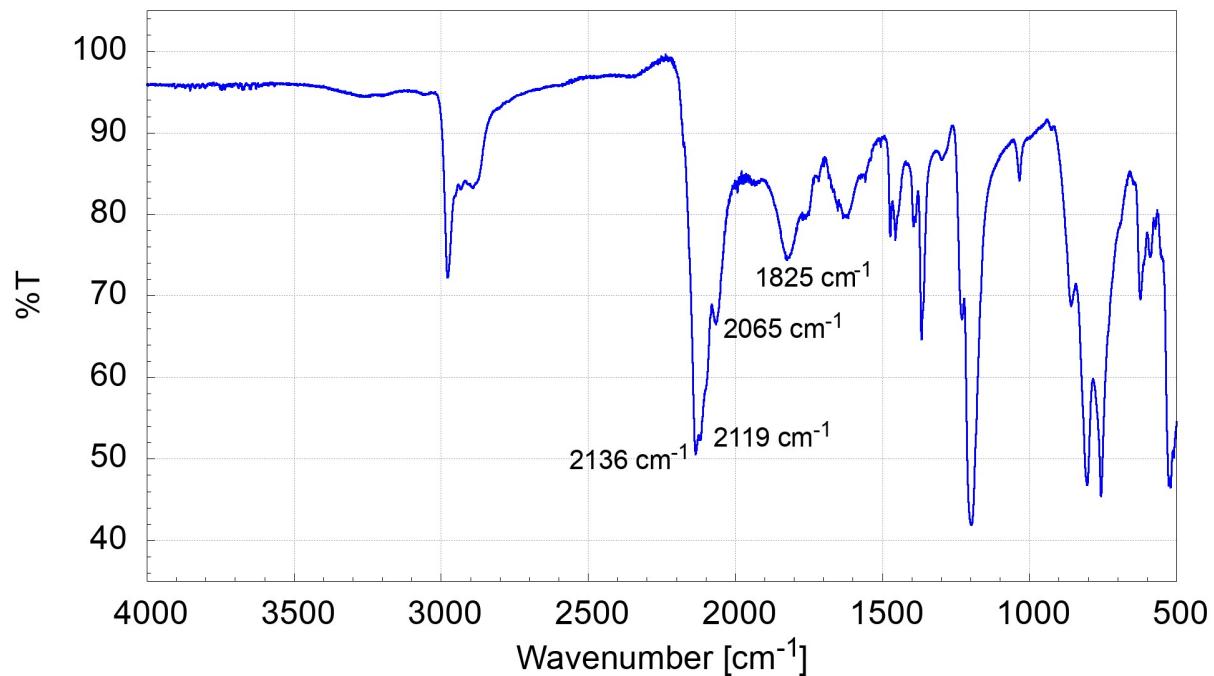
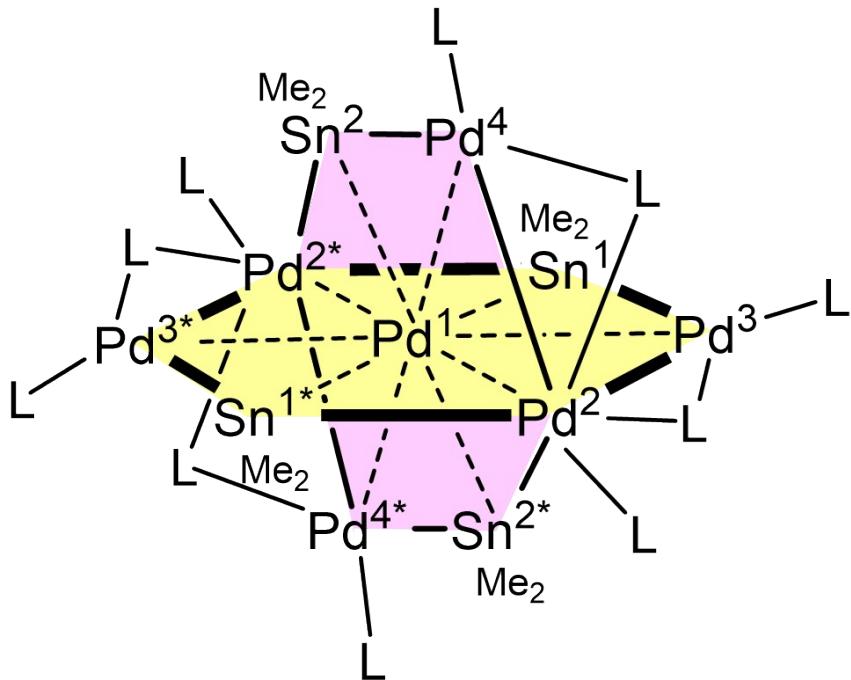


Figure S11. ATR-IR spectrum of Pd_8Ge_6 cluster **3** in the solid state.

Computational Details.

All of the calculations were performed using the Gaussian 16 program⁵. Geometry optimization for clusters **2** and **3** was carried out by using the DFT method with the PBE0^{6,7}, M06⁸, B3PW91⁹ or B3LYP¹⁰⁻¹³ functional, and the selected bond distances and the calculated values of bond distances and WBIs for cluster **2** (actual cluster **2** and optimized **2**_{opt}) and **3** (actual cluster **3** and optimized **3**_{opt}) were summarized in Tables S1 and S3. The optimized molecular structures for **2**_{opt} and **3**_{opt} were depicted in Figures S12 and S16. Natural Bond Orbital (NBO) analyses were performed using the NBO 3.1 program implemented in Gaussian 16. The effective core potentials and the basis set by the Stuttgart–Dresden–Bonn group¹⁴ and were used for Pd and Sn, and the 6-31G** basis sets¹⁵⁻¹⁹ were used for C, N, Ge and hydrogen atoms.

Table S1. Actual bond distances, calculated bond distances and Wiberg bond index for **2** and **2_{opt}**.



	Bond distance determined by XRD (Å)	Bond distances estimated by PBE0 (Å)	Wiberg bond index by PBE0
<i>intra-plane interaction -yellow plane (Sheet I)-</i>			
Pd(1)-Pd(2)	2.8005(3)	2.87297	0.2931
Pd(1)-Pd(3)	2.7650(3)	2.80738	0.2125
Pd(1)-Sn(1)	2.6216(4)	2.67129	0.5545
Pd(2)-Pd(3)	2.7121(5)	2.74106	0.2094
Pd(2)-Sn(1)*	2.830(3)	2.91389	0.2611
Pd(3)-Sn(1)	2.6586(5)	2.73397	0.3446
<i>intra-plane interaction –purple plane (Sheet II)-</i>			
Pd(1)-Pd(4)	2.7714(5)	2.82185	0.2205
Pd(1)-Sn(2)	2.6067(4)	2.65559	0.5701
Pd(2)-Pd(4)	2.6908(5)	2.71298	0.2112
Pd(4)-Sn(2)	2.7028(5)	2.78005	0.3151
Pd(2)*-Sn(2)	2.7979(5)	2.87150	0.2845
<i>inter-plane interaction</i>			
Pd(3)-Pd(4)	3.2925(7)	3.20761	0.0790
Pd(4)-Sn(1)*	3.1893(3)	3.21487	0.1011
Pd(3)*-Sn(2)	3.1830(3)	3.32599	0.0857
Sn(1)-Sn(2)	3.5403(7)	3.86968	0.0338

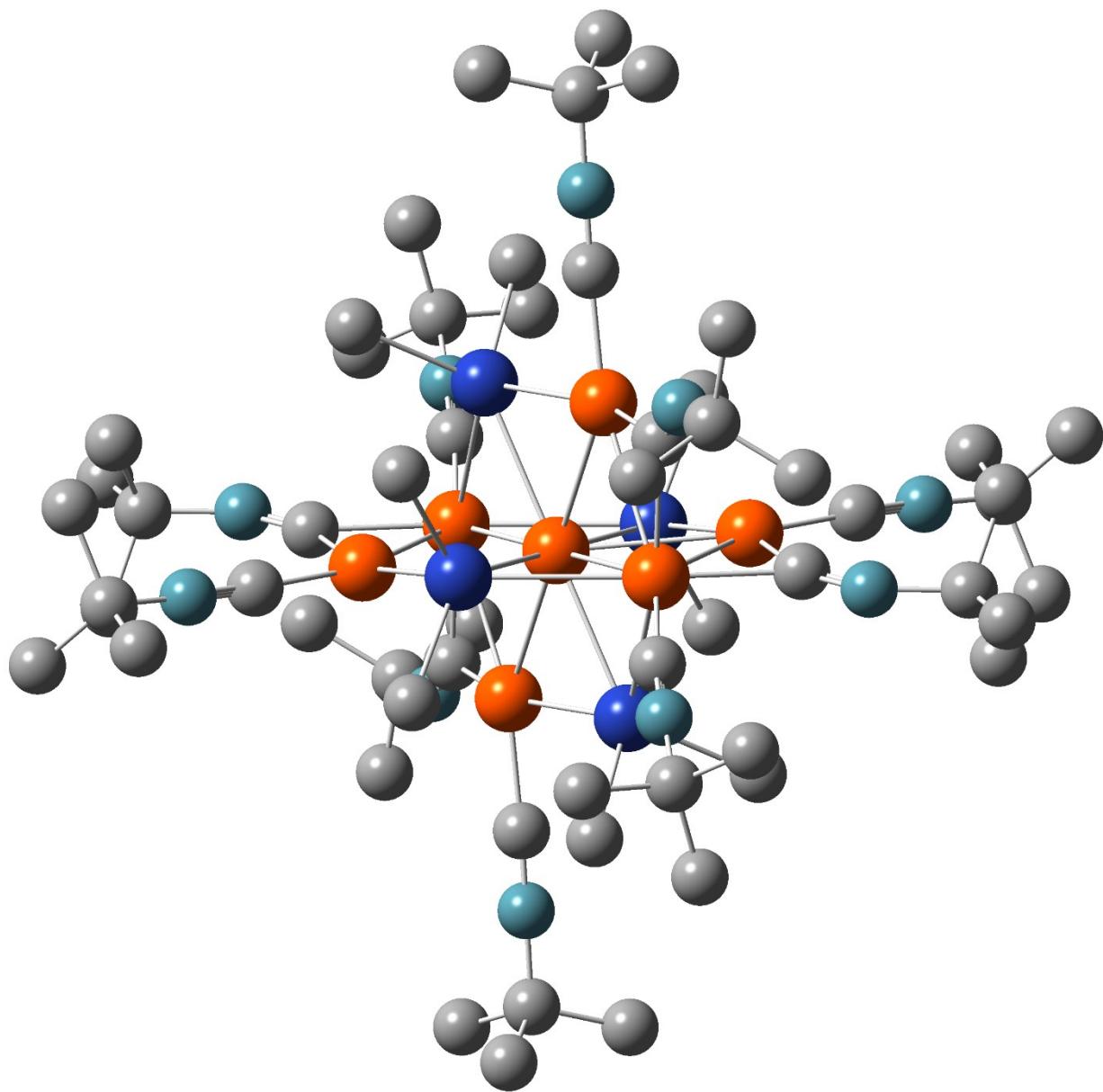


Figure S12. Optimized molecular structure of **2** (**2_{opt}**) with PBE0 functional. The orange balls are palladium atoms, the blue balls are tin atoms, the pale blue balls are nitrogen atoms, the grey ones are carbon atoms.

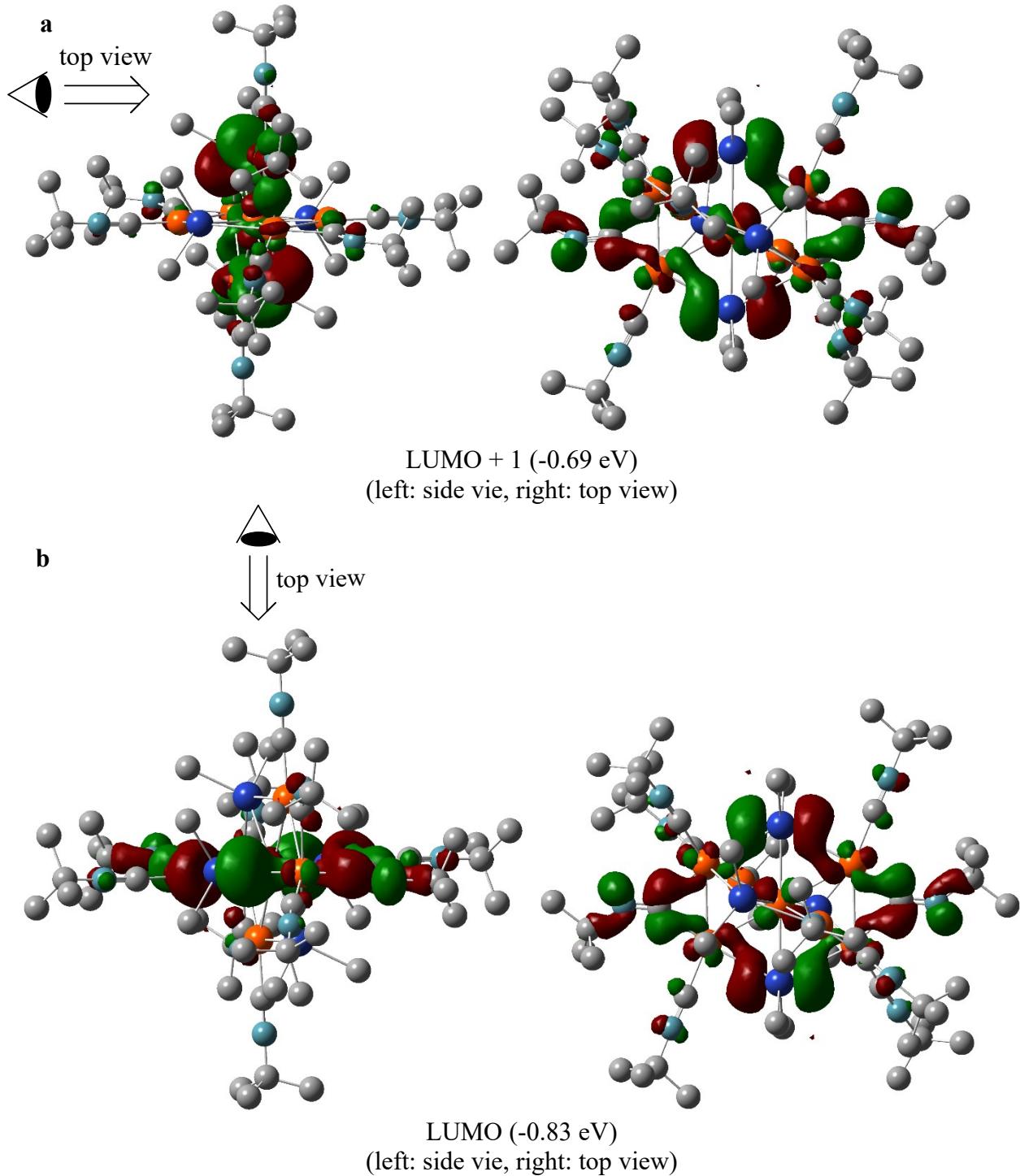
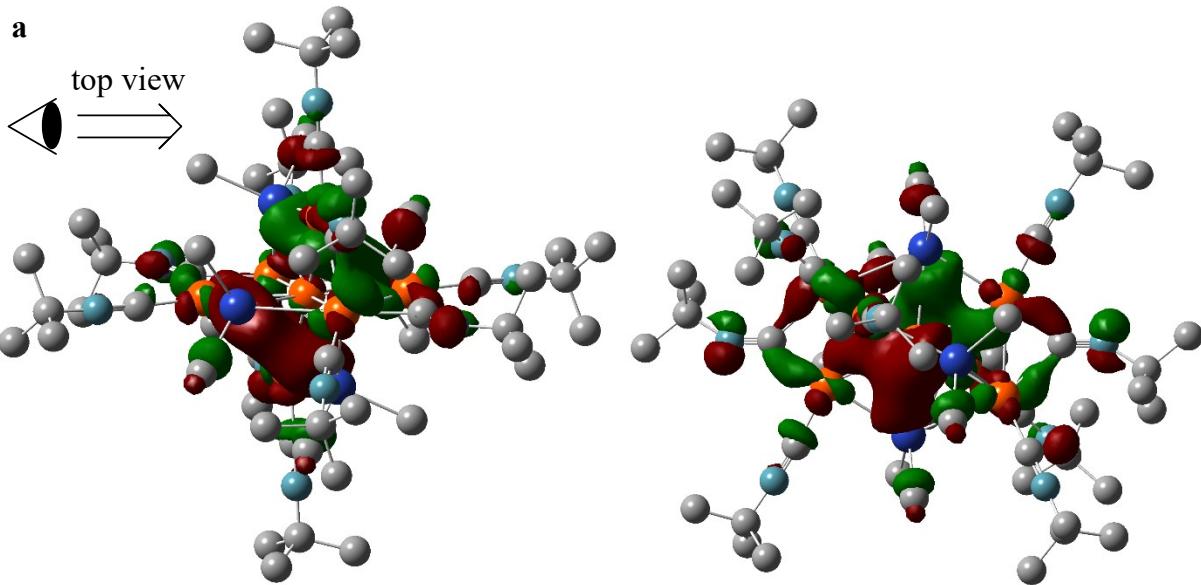
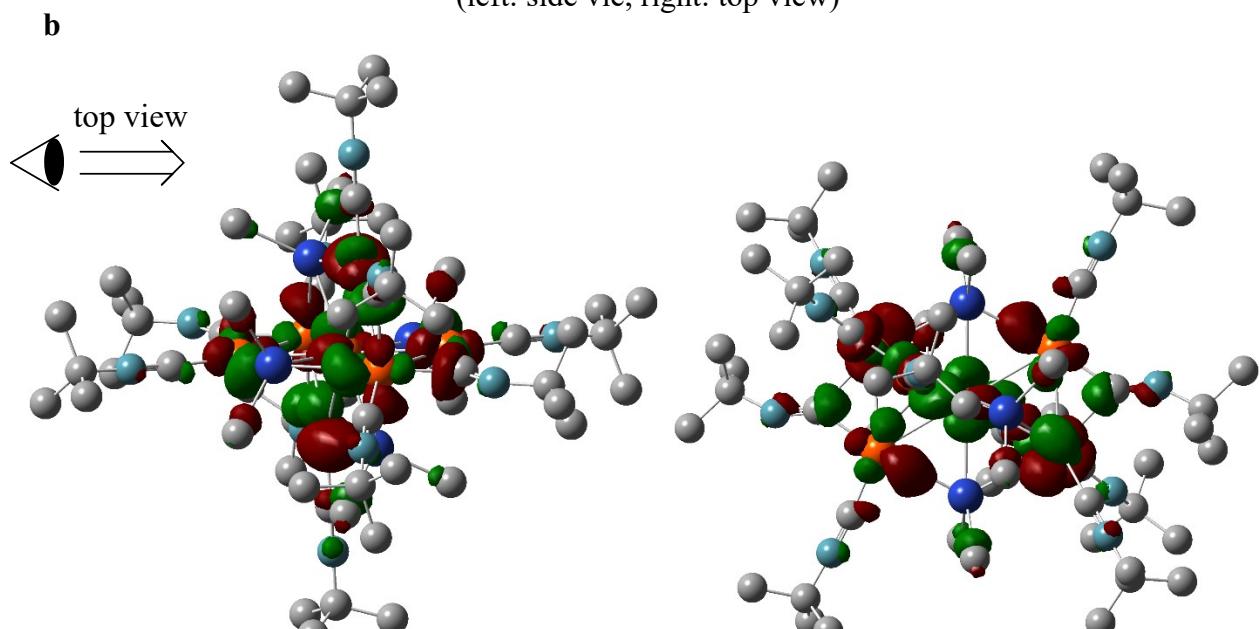


Figure S13. Orbital figures (LUMO+1 and LUMO) for $\mathbf{2}_{\text{opt}}$ depicted with the isovalue of 0.03 calculated by PBE0 functional. **a**, Orbital figures of LUMO+1. **b**, Orbital figures of LUMO.



HOMO (-3.78 eV)
(left: side vie, right: top view)



HOMO-1 (-3.99 eV)
(left: side vie, right: top view)

Figure S14. Orbital figures (HOMO and HOMO-1) for **2_{opt}** depicted with the isovalue of 0.03 calculated by PBE0 functional. **a**, Orbital figures of HOMO. **b**, Orbital figures of HOMO-1.

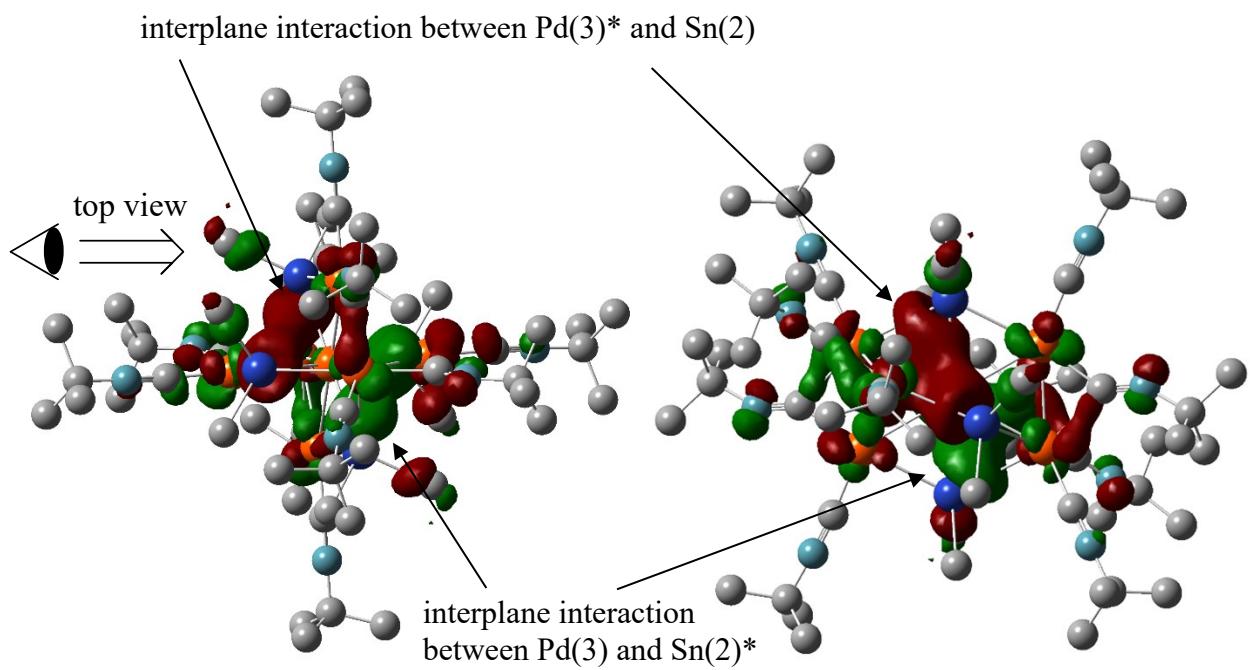


Figure S15. Orbital figures (HOMO-2) for 2_{opt} depicted with the isovalue of 0.03 calculated by PBE0 functional.

Table S2. The DFT-optimized Geometry for complex **2_{opt}** (in XYZ format)

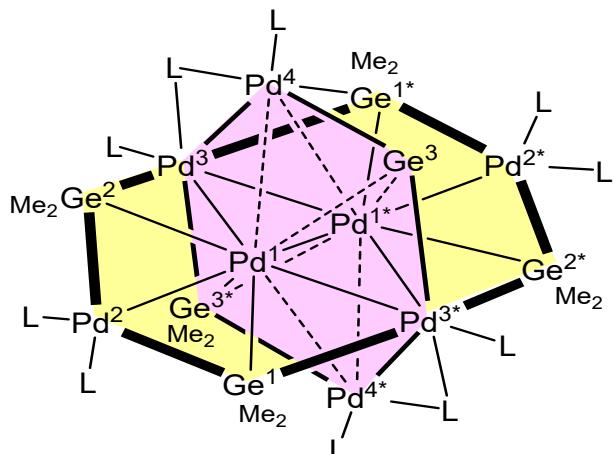
Sn	0.671800	-2.249700	-1.240900	Pd	-2.771400	0.380300	0.654800
Sn	0.912100	1.286800	-2.155700	N	5.014200	1.714800	-0.188100
Pd	0.000000	-0.000100	0.000100	N	2.444000	4.518300	2.229400
Pd	-2.034600	-1.776800	-0.816400	N	-2.061100	2.770500	-4.458400
Pd	1.790000	-1.285500	1.739400	N	-4.648900	2.257500	-1.197300
Pd	2.771500	-0.380500	-0.654500	N	-4.546400	1.107900	3.152200
N	-5.013800	-1.715600	0.189500	C	-1.204900	4.211500	0.382300
N	-2.444800	-4.517300	-2.231500	C	-0.935800	2.777100	3.373100
N	2.061400	-2.770100	4.458900	C	-1.565900	-3.391900	2.291000
N	4.648600	-2.258500	1.197200	C	-1.465800	-0.743700	4.224700
N	4.546600	-1.107100	-3.152100	C	3.878900	1.349800	0.002700
C	1.204300	-4.211800	-0.381900	C	5.930400	2.789700	0.144700
C	0.936500	-2.777400	-3.372800	C	5.370800	4.103100	-0.408900
C	1.566400	3.391600	-2.290900	C	7.283200	2.482700	-0.500000
C	1.465500	0.743300	-4.224500	C	6.073900	2.858300	1.667900
C	-3.878700	-1.350200	-0.001800	C	2.273400	3.467000	1.723700
C	-5.929900	-2.790600	-0.142900	C	2.595500	5.819700	2.805500
C	-5.369600	-4.103900	0.410300	C	3.847900	5.814400	3.687500
C	-7.282400	-2.484100	0.502800	C	2.743300	6.831400	1.664100
C	-6.074400	-2.859100	-1.665900	C	1.350900	6.132100	3.641200
C	-2.273900	-3.466500	-1.724700	C	-1.899600	2.197100	-3.443300
C	-2.596700	-5.817800	-2.809200	C	-2.301400	3.495900	-5.666000
C	-3.847300	-5.810100	-3.693800	C	-1.706200	4.898600	-5.505700
C	-2.748100	-6.830600	-1.669100	C	-1.624200	2.751400	-6.820700
C	-1.350800	-6.130900	-3.642700	C	-3.815600	3.572900	-5.886600
C	1.899800	-2.196900	3.443700	C	-3.640400	1.645300	-0.980100
C	2.301900	-3.495500	5.666500	C	-5.945600	2.696900	-0.748000
C	1.707100	-4.898300	5.506300	C	-5.744800	3.665400	0.421900
C	1.624500	-2.751100	6.821200	C	-6.639100	3.412500	-1.910200
C	3.816100	-3.572000	5.887200	C	-6.761300	1.476200	-0.313000
C	3.640400	-1.645900	0.980100	C	-3.854300	0.882500	2.227300
C	5.945100	-2.698300	0.747600	C	-5.382300	1.337200	4.291900
C	5.743700	-3.666200	-0.422800	C	-6.842300	1.302800	3.829400
C	6.638300	-3.414800	1.909300	C	-5.034200	2.709200	4.877500
C	6.761300	-1.477800	0.313100	C	-5.116400	0.230800	5.316700
C	3.854500	-0.882200	-2.227100	H	1.184300	-4.178100	0.710000
C	5.382600	-1.335700	-4.291900	H	0.508100	-4.980700	-0.736000
C	6.842500	-1.302700	-3.829100	H	2.216500	-4.476000	-0.707700
C	5.033800	-2.706800	-4.879000	H	0.280100	-2.179300	-4.009400
C	5.117500	-0.227900	-5.315500	H	1.975100	-2.625300	-3.680800
Sn	-0.671900	2.249500	1.241100	H	0.686000	-3.835900	-3.495700
Sn	-0.912000	-1.287000	2.156000	H	1.232600	3.970200	-1.427000
Pd	2.034600	1.776700	0.816400	H	2.660200	3.421600	-2.334400
Pd	-1.789900	1.285500	-1.739100	H	1.163500	3.838100	-3.207400

H	1.571000	-0.333100	-4.363100	H	4.067800	-0.226700	-5.619600
H	0.690700	1.116900	-4.902400	H	5.354800	0.751700	-4.891200
H	2.412500	1.237600	-4.463900	H	-1.184000	4.178000	-0.709600
H	-6.049500	-4.930600	0.175700	H	-0.509400	4.980600	0.737000
H	-4.387500	-4.312500	-0.021300	H	-2.217400	4.475000	0.707400
H	-5.258900	-4.045800	1.497200	H	-0.279200	2.178800	4.009400
H	-8.002500	-3.276400	0.273800	H	-1.974300	2.625000	3.681500
H	-7.179500	-2.412500	1.589900	H	-0.685100	3.835500	3.496000
H	-7.679800	-1.534700	0.131700	H	-1.232500	-3.970300	1.426800
H	-6.774000	-3.655700	-1.942500	H	-2.659700	-3.422100	2.335200
H	-6.457200	-1.911500	-2.056700	H	-1.162400	-3.838600	3.207100
H	-5.105500	-3.054100	-2.132700	H	-1.569700	0.332800	4.363800
H	-3.985300	-6.796900	-4.146000	H	-0.692000	-1.118900	4.902900
H	-4.736200	-5.568900	-3.104400	H	-2.413700	-1.236700	4.463300
H	-3.748800	-5.070400	-4.493200	H	6.050800	4.929500	-0.174100
H	-2.859300	-7.837300	-2.083200	H	4.388500	4.311900	0.022100
H	-1.868000	-6.813500	-1.020400	H	5.260700	4.044800	-1.495900
H	-3.629500	-6.602800	-1.063300	H	8.003400	3.274800	-0.270700
H	-1.452100	-7.120800	-4.098100	H	7.181000	2.411000	-1.587200
H	-1.220900	-5.390700	-4.436800	H	7.680100	1.533300	-0.128600
H	-0.455800	-6.124800	-3.014700	H	6.773600	3.654700	1.944800
H	1.876200	-5.477700	6.419000	H	6.456200	1.910600	2.059000
H	0.630900	-4.841100	5.321600	H	5.104800	3.053700	2.134000
H	2.174500	-5.420700	4.667200	H	3.985700	6.801800	4.138300
H	1.796900	-3.288400	7.758700	H	4.735900	5.573500	3.096500
H	2.029500	-1.740000	6.917700	H	3.752000	5.075500	4.487900
H	0.546700	-2.677600	6.652900	H	2.854100	7.838800	2.076800
H	4.029300	-4.130100	6.804100	H	1.862000	6.812600	1.017100
H	4.301300	-4.076700	5.047300	H	3.623800	6.604100	1.056600
H	4.241400	-2.568900	5.980300	H	1.452100	7.122500	4.095600
H	5.231200	-3.164400	-1.247400	H	1.223400	5.392400	4.436100
H	6.713800	-4.035000	-0.773600	H	0.454700	6.124500	3.015000
H	5.138200	-4.522400	-0.111100	H	-1.875200	5.478000	-6.418500
H	7.630000	-3.763000	1.602900	H	-0.630000	4.841100	-5.321100
H	6.754400	-2.738600	2.761500	H	-2.173500	5.421100	-4.666600
H	6.049900	-4.278800	2.232200	H	-1.796500	3.288700	-7.758200
H	6.244200	-0.929000	-0.477700	H	-2.029500	1.740400	-6.917100
H	6.903200	-0.797600	1.158300	H	-0.546400	2.677600	-6.652400
H	7.746000	-1.795500	-0.047400	H	-4.028600	4.131000	-6.803600
H	7.503700	-1.468000	-4.685200	H	-4.300600	4.077700	-5.046700
H	7.082500	-0.333500	-3.382900	H	-4.241200	2.569900	-5.979700
H	7.031200	-2.082800	-3.086500	H	-5.232100	3.164300	1.246800
H	5.663800	-2.904700	-5.751500	H	-6.715100	4.034000	0.772400
H	5.200900	-3.497100	-4.141700	H	-5.139700	4.521800	0.109800
H	3.986000	-2.738600	-5.189600	H	-7.630900	3.760400	-1.604000
H	5.742700	-0.387700	-6.199300	H	-6.754800	2.735800	-2.762000

H	-6.051000	4.276600	-2.233400
H	-6.244000	0.928100	0.478100
H	-6.902800	0.795500	-1.157800
H	-7.746200	1.793600	0.047200
H	-7.503500	1.468600	4.685400
H	-7.081800	0.333100	3.384200
H	-7.031600	2.082100	3.085900

H	-5.664200	2.907700	5.749800
H	-5.202000	3.498600	4.139300
H	-3.986400	2.742000	5.187800
H	-5.741600	0.391200	6.200500
H	-4.066600	0.230400	5.620500
H	-5.353200	-0.749500	4.893500

Table S3. Actual bond distances, calculated bond distances and Wiberg bond index for **3** and **3_{opt}**.



	Bond distance determined by XRD (Å)	Bond distances estimated by PBE0 (Å)	Wiberg bond index by PBE0
<i>intra-plane interaction -yellow plane (Sheet IV)-</i>			
Pd(1)-Pd(2)	2.7771(4)	2.83212	0.1898
Pd(1)-Pd(3)	2.8182(4)	2.89601	0.1699
Pd(1)-Pd(1)*	2.6920(3)	2.70101	0.1886
Pd(1)-Pd(3)*	2.7975(3)	2.89797	0.1690
Pd(1)-Ge(1)	2.4074(4)	2.41644	0.5880
Pd(1)-Ge(2)	2.3964(4)	2.41679	0.5868
Pd(2)-Ge(1)	2.5578(4)	2.57655	0.3892
Pd(2)-Ge(2)	2.5348(4)	2.57753	0.3875
Pd(3)-Ge(2)	2.7590(6)	2.79292	0.2414
Pd(3)*-Ge(1)	2.6783(4)	2.79863	0.2392
<i>intra-plane interaction -purple plane (Sheet III)-</i>			
Pd(3)-Pd(4)	2.5947(5)	2.59719	0.1920
Pd(3)-Ge(3)*	2.5100(3)	2.54784	0.3721
Pd(4)-Ge(3)	2.4486(4)	2.48721	0.3917
<i>inter-plane interaction</i>			
Pd(1)-Pd(4)	2.9317(4)	2.94026	0.1222
Pd(1)-Ge(3)	2.8531(6)	2.80030	0.3004
Pd(4)-Ge(1)*	3.2720(3)	3.10979	0.1143

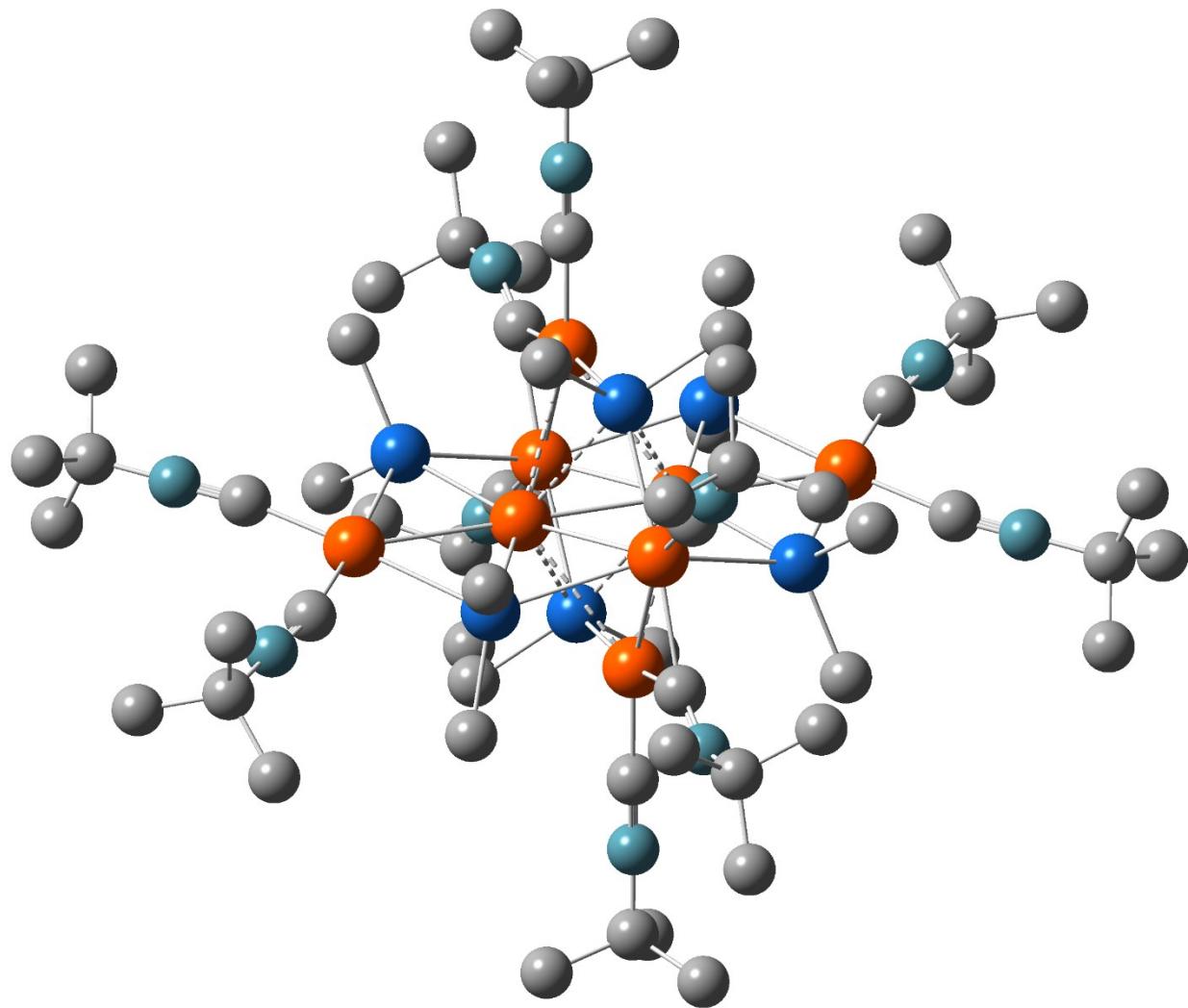


Figure S16. Optimized molecular structure of **3** ($\mathbf{3}_{\text{opt}}$) with PBE0 functional. The orange balls are palladium atoms, the blue balls are germanium atoms, the pale blue balls are nitrogen atoms, the grey ones are carbon atoms.

Table S4. The DFT-optimized Geometry for complex $\mathbf{3}_{\text{opt}}$ (in XYZ format).

Pd	1.350400	-0.023800	0.002800	C	1.531100	0.586100	3.701200
Pd	-0.038500	-2.407000	-0.879600	C	-1.527300	0.638800	3.695400
Pd	-4.181900	0.073300	-0.012300	C	5.510000	1.389600	0.000600
Pd	-0.039300	-1.994900	1.684700	C	7.185900	4.262800	-0.724500
Ge	2.588500	-2.099300	0.017500	C	8.771100	2.311900	-0.546300
Ge	-2.661000	-2.006200	0.012200	C	0.071200	3.845100	-0.724400
Ge	-0.000800	-0.380000	-2.422700	C	0.114300	6.364400	-0.461300
N	-6.446000	-2.098500	-0.014500	C	-1.156400	6.590300	0.361700
N	-0.095300	-5.021700	0.998800	C	1.355600	6.536900	0.417700
N	-0.098200	-2.912200	4.653400	C	0.161700	7.340900	-1.639100
C	3.219800	-3.276300	-1.474600	C	0.068200	2.523600	-3.542600
C	3.124700	-3.181200	1.607100	C	0.163000	3.405000	-5.991600
C	-3.323600	-3.171200	-1.475600	C	-0.507300	4.782100	-6.029100
C	-3.243800	-3.062400	1.602900	C	-0.573300	2.420400	-6.905400
C	-1.531400	-0.586500	-3.701300	C	1.638600	3.510900	-6.390800
C	1.527000	-0.638500	-3.695300	H	3.152200	-2.750600	-2.429700
C	-5.510000	-1.389700	-0.000500	H	4.255300	-3.592000	-1.304400
C	-7.186300	-4.262600	0.724600	H	2.585600	-4.165200	-1.517900
C	-8.771300	-2.311600	0.545500	H	3.074700	-2.565500	2.508600
C	-0.071100	-3.845200	0.724400	H	2.446800	-4.030300	1.729600
C	-0.113700	-6.364400	0.461100	H	4.146100	-3.556300	1.478300
C	1.157600	-6.590300	-0.360900	H	-3.239300	-2.652100	-2.433100
C	-1.354400	-6.536700	-0.418900	H	-2.716200	-4.078800	-1.513600
C	-0.162100	-7.341000	1.638800	H	-4.368200	-3.455100	-1.305100
C	-0.068500	-2.523600	3.542700	H	-3.167100	-2.449500	2.504300
C	-0.163000	-3.404900	5.991700	H	-4.280700	-3.392500	1.474000
C	0.507300	-4.782000	6.029100	H	-2.603600	-3.940500	1.724800
C	0.573400	-2.420300	6.905400	H	-2.472700	-0.340100	-3.202700
C	-1.638600	-3.510700	6.391200	H	-1.386200	0.090900	-4.550900
Pd	-1.350200	0.023800	-0.002800	H	-1.583500	-1.615000	-4.075500
Pd	0.038600	2.407000	0.879600	H	2.474200	-0.420800	-3.194600
Pd	4.182100	-0.073400	0.012300	H	1.546400	-1.668800	-4.066800
Pd	0.038700	1.994900	-1.684700	H	1.405500	0.040900	-4.547200
Ge	-2.588400	2.099300	-0.018000	H	-8.020300	-4.970300	0.695100
Ge	2.661100	2.006200	-0.011700	H	-6.302100	-4.743900	0.298300
Ge	0.000300	0.379900	2.422700	H	-6.974100	-4.013900	1.767900
N	6.446000	2.098500	0.014700	H	-9.633100	-2.985000	0.515300
N	0.095700	5.021700	-0.998900	H	-8.576300	-2.040700	1.586800
N	0.098000	2.912200	-4.653400	H	-9.019100	-1.403400	-0.011300
C	-3.219500	3.276500	1.474000	H	1.182500	-7.618000	-0.740300
C	-3.124800	3.181000	-1.607600	H	1.188500	-5.899200	-1.207200
C	3.323800	3.170900	1.476200	H	2.047900	-6.423900	0.252600
C	3.243700	3.062400	-1.602400	H	-1.405000	-7.562700	-0.800200

H	-2.264200	-6.332300	0.153300	H	1.059100	7.168500	-2.241000
H	-1.316600	-5.845300	-1.264600	H	-0.468200	5.186800	-7.045200
H	-0.175400	-8.375000	1.278600	H	0.003000	5.474700	-5.354100
H	0.712500	-7.205800	2.282200	H	-1.553700	4.707300	-5.720500
H	-1.059900	-7.168700	2.240000	H	-0.538200	2.776800	-7.939600
H	0.468300	-5.186700	7.045300	H	-1.619500	2.323400	-6.602600
H	-0.003200	-5.474600	5.354300	H	-0.107800	1.431900	-6.859000
H	1.553600	-4.707200	5.720300	H	1.719800	3.887400	-7.415300
H	0.538500	-2.776700	7.939500	H	2.121300	2.531200	-6.336900
H	1.619600	-2.323300	6.602300	H	2.168700	4.193800	-5.721300
H	0.108000	-1.431800	6.859000	C	-7.552200	-3.005400	-0.069300
H	-1.719600	-3.887300	7.415700	C	-7.807900	-3.349300	-1.540100
H	-2.121300	-2.531000	6.337300	H	-8.049700	-2.448600	-2.111100
H	-2.168800	-4.193700	5.721800	H	-6.924400	-3.814800	-1.985200
H	-3.151900	2.750800	2.429100	H	-8.647600	-4.046800	-1.613100
H	-4.255000	3.592200	1.303800	C	7.552200	3.005500	0.069200
H	-2.585200	4.165400	1.517200	C	7.808500	3.349200	1.539900
H	-3.075000	2.565400	-2.509100	H	6.925200	3.814600	1.985400
H	-2.446900	4.030100	-1.730200	H	8.050500	2.448400	2.110700
H	-4.146200	3.556300	-1.478600	H	8.648200	4.046700	1.612600
H	3.239400	2.651800	2.433700	C	0.062700	3.527200	2.482900
H	2.716600	4.078700	1.514200	C	0.136100	4.934900	4.677200
H	4.368500	3.454700	1.305900	C	-0.980400	5.983500	4.646600
H	3.166700	2.449500	-2.503800	H	-0.966800	6.566200	5.572800
H	4.280700	3.392400	-1.473800	H	-0.845400	6.666200	3.802900
H	2.603600	3.940600	-1.724200	H	-1.957000	5.501200	4.549300
H	2.472200	0.339200	3.202600	C	1.508900	5.609300	4.768800
H	1.385700	-0.091000	4.551000	H	1.660600	6.291200	3.927300
H	1.583600	1.614700	4.075000	H	1.578800	6.181500	5.699100
H	-2.474500	0.420800	3.194900	H	2.305700	4.860700	4.754700
H	-1.546800	1.669200	4.066600	C	-0.067000	3.967200	5.847000
H	-1.405700	-0.040300	4.547600	H	-1.037400	3.469000	5.771500
H	8.019800	4.970500	-0.695200	H	0.712600	3.200800	5.853200
H	6.301800	4.744000	-0.297700	H	-0.027100	4.518300	6.791800
H	6.973300	4.014100	-1.767700	C	-5.456200	1.583400	-0.035100
H	9.632800	2.985200	-0.516400	C	5.456500	-1.583400	0.035000
H	8.575600	2.041100	-1.587500	C	-7.437500	3.273600	0.023400
H	9.019100	1.403600	0.010300	C	-6.994800	4.543500	-0.709000
H	-1.181100	7.618100	0.740900	H	-6.108300	4.972800	-0.234700
H	-1.186600	5.899300	1.208000	H	-6.755400	4.325000	-1.753200
H	-2.047200	6.423700	-0.251200	H	-7.801200	5.282500	-0.681000
H	1.406500	7.562900	0.798900	C	-7.732600	3.573500	1.496400
H	2.265000	6.332500	-0.155200	H	-6.848400	3.986800	1.988900
H	1.318600	5.845500	1.263500	H	-8.546800	4.300900	1.566800
H	0.175300	8.374900	-1.279100	H	-8.029500	2.662900	2.024200
H	-0.713300	7.205600	-2.281900	C	-8.659400	2.652100	-0.659400

H	-8.437300	2.411600	-1.702700	N	-6.366000	2.325600	-0.027000
H	-8.962500	1.735000	-0.146300	C	-0.062600	-3.527200	-2.482800
H	-9.494800	3.358100	-0.634000	C	-0.136900	-4.934900	-4.677100
C	7.438000	-3.273400	-0.023500	C	-1.511700	-5.604700	-4.770700
C	8.659900	-2.651700	0.659100	H	-1.582100	-6.176800	-5.701100
H	9.495300	-3.357600	0.633700	H	-1.666900	-6.286100	-3.929300
H	8.962800	-1.734600	0.145900	H	-2.306000	-4.853600	-4.757800
H	8.437800	-2.411100	1.702400	C	0.071200	-3.967900	-5.846700
C	7.732900	-3.573400	-1.496500	H	-0.706000	-3.199000	-5.854200
H	6.848700	-3.986900	-1.988900	H	1.043000	-3.472800	-5.769700
H	8.029600	-2.662800	-2.024400	H	0.031000	-4.519100	-6.791400
H	8.547200	-4.300700	-1.567000	C	0.976200	-5.987000	-4.644700
C	6.995500	-4.543300	0.709100	H	0.837800	-6.669200	-3.800900
H	6.756200	-4.324700	1.753300	H	0.961900	-6.569900	-5.570800
H	6.109000	-4.972800	0.234900	H	1.954100	-5.507900	-4.546100
H	7.802000	-5.282200	0.681100	N	-0.084600	-4.187700	-3.458900
N	6.366400	-2.325600	0.026900	N	0.084400	4.187700	3.459000

X-ray data collection and reduction

X-ray crystallography for compounds **2** and **3** was performed on a Rigaku Saturn CCD area detector with graphite monochromated Mo-K α radiation ($\lambda=0.71075\text{ \AA}$). The data were collected at 113(2) K using ω scan in the θ range of $2.24 \leq \theta \leq 31.36\text{ deg}$ (**2**), $1.84 \leq \theta \leq 31.33\text{ deg}$ (**3**). The data obtained were processed using Crystal-Clear (Rigaku) on a Pentium computer, and were corrected for Lorentz and polarization effects. The structures were solved by direct methods²⁰, and expanded using Fourier techniques. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement on F^2 was based on 13,860 observed reflections and 414 variable parameters for **2**, 13,450 observed reflections and 409 variable parameters for **3**. Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C, Table 6.1.1.4²¹. Anomalous dispersion effects were included in F_{calc} ²²; the values for Δf and $\Delta f''$ were those of Creagh and McAuley²³. The values for the mass attenuation coefficients are those of Creagh and Hubbell²⁴. All calculations were performed using the CrystalStructure²⁵ crystallographic software package except for refinement, which was performed using SHELXL Version 2017/1²⁶. Details of final refinement as well as the bond lengths and angle are summarized in Tables S5 and S6, and the numbering scheme employed is also shown in Figures S17 - S20, which were drawn with ORTEP at 50% probability ellipsoids. CCDC 2087548 (**2**) and 2087549 (**3**) contain the supplementary crystallographic data for this paper.

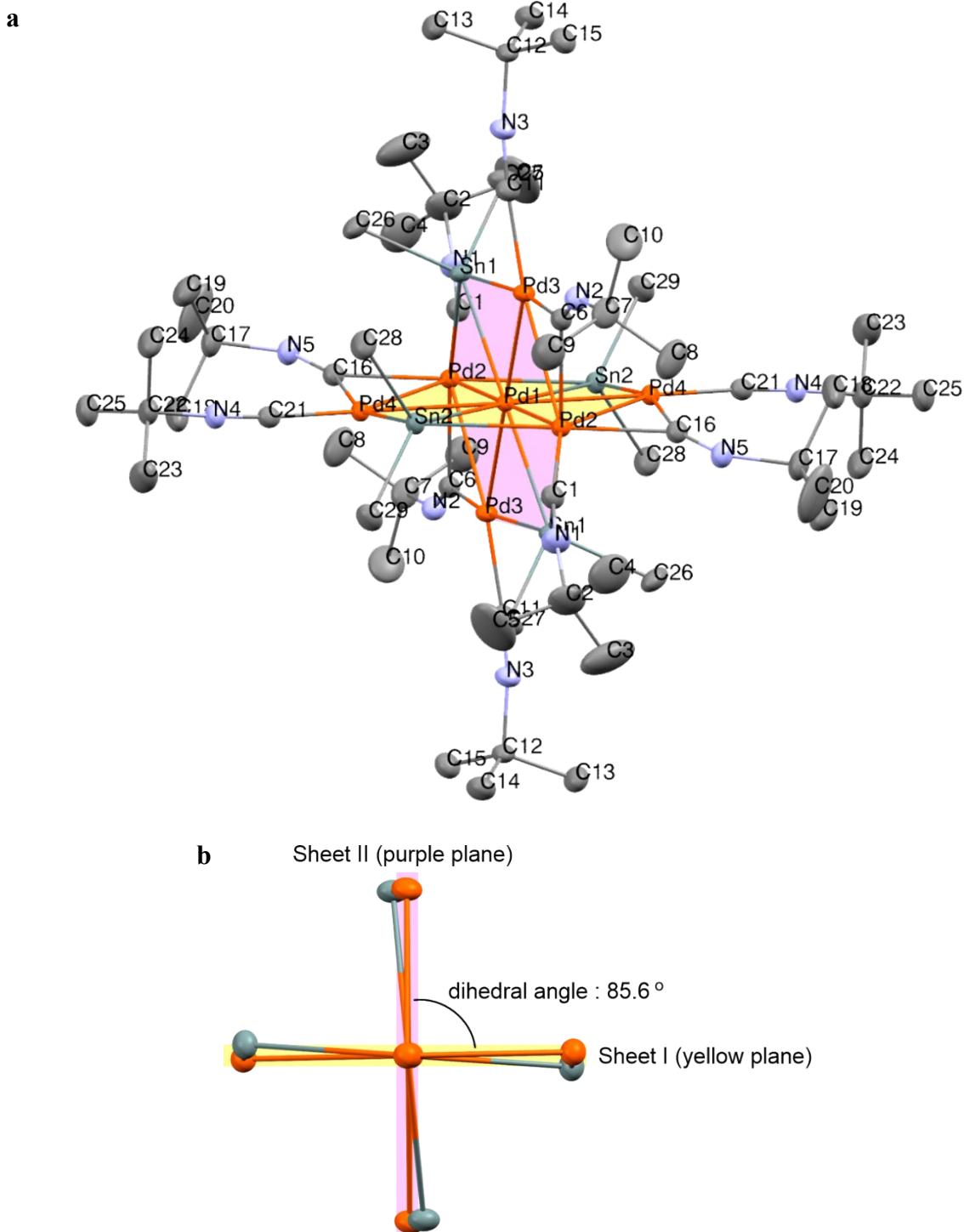


Figure S17. Molecular structure of **2** determined by a single crystal X-ray diffraction analysis. **a**, ORTEP drawing of **2** (50% probability of the thermal ellipsoids). Hydrogen atoms were omitted for clarity. One disordered toluene molecule is included in the unit cell, and the site occupancy factor for a methyl group was defined to be 0.5 (Solvated toluene molecule was omitted for clarity). **b**, Dihedral angle between Sheet I and Sheet II.

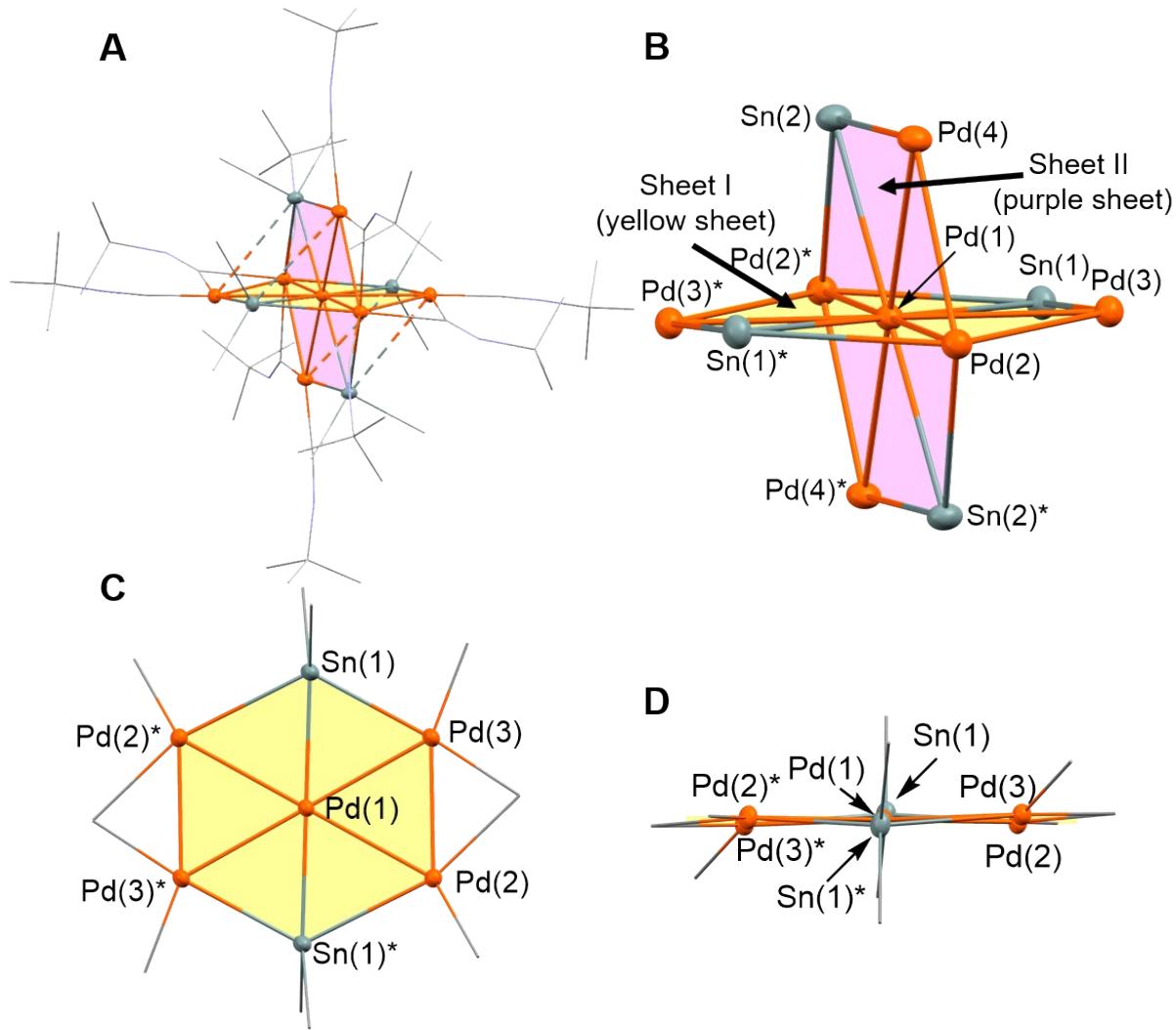


Figure S18. Molecular structure of **2** determined via single-crystal XRD analysis. **A)** ORTEP drawing of **2** with thermal ellipsoids at 50% probability. All carbon atoms and nitrogen atoms are shown in wireframe style; all hydrogen atoms are omitted for clarity. **B)** The core Pd_7Sn_4 structure of **2**. **C)** Front view of Sheet I. **D)** Side view of Sheet I.

Table S5. Crystal data and structure refinement for **2**.

Empirical Formula	C ₈₀ H ₁₃ N ₁₀ Pd ₇ Sn ₄
Formula Weight	2333.61
Crystal Color, Habit	red, block
Crystal Dimensions	0.200 X 0.160 X 0.100 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 14.2023(2) Å b = 26.2964(4) Å c = 12.15252(17) Å β = 94.3571(13) ° V = 4525.48(11) Å ³
Space Group	P2 ₁ /c (#14)
Z value	2
D _{calc}	1.712 g/cm ³
F ₀₀₀	2170.00
μ (MoK α)	24.796 cm ⁻¹
Diffractometer	Saturn724+
Radiation	MoK α (λ = 0.71073 Å) graphite monochromated
Voltage, Current	50kV, 24mA
Temperature	-160.0°C
Detector Aperture	72.8 x 72.8 mm
Data Images	1440 exposures
ω oscillation Range (χ =45.0, ϕ =0.0)	-70.0 - 110.0°
Exposure Rate	24.0 sec./°
Detector Swing Angle	20.00°
ω oscillation Range (χ =45.0, ϕ =90.0)	-70.0 - 110.0°
Exposure Rate	24.0 sec./°
Detector Swing Angle	20.00°
ω oscillation Range (χ =45.0, ϕ =180.0)	-70.0 - 110.0°
Exposure Rate	24.0 sec./°
Detector Swing Angle	20.00°
ω oscillation Range (χ =45.0, ϕ =270.0)	-70.0 - 110.0°
Exposure Rate	24.0 sec./°
Detector Swing Angle	20.00°
Detector Position	0.00 mm
Pixel Size	0.035 mm
2 θ _{max}	62.4°
No. of Reflections Measured	Total: 86268 Unique: 13860 (R _{int} = 0.0251)

Corrections	Lorentz-polarization Absorption (trans. factors: 0.662 - 0.780)
Structure Solution	Direct Methods (SHELXT Version 2014/5)
Refinement	Full-matrix least-squares on F ²
Function Minimized	$\Sigma w (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1 / [\sigma^2(Fo^2) + (0.0278 \cdot P)^2 + 5.0139 \cdot P]$ where $P = (\text{Max}(Fo^2, 0) + 2Fc^2)/3$
2θ _{max} cutoff	62.4°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	13860
No. Variables	414
Reflection/Parameter Ratio	33.48
Residuals: R1 (I>2.00σ(I))	0.0231
Residuals: R (All reflections)	0.0275
Residuals: wR2 (All reflections)	0.0571
Goodness of Fit Indicator	1.049
Max Shift/Error in Final Cycle	0.004
Maximum peak in Final Diff. Map	1.16 e ⁻ /Å ³
Minimum peak in Final Diff. Map	-0.65 e ⁻ /Å ³

< Atomic coordinates and B_{iso}/B_{eq} >

atom	x	y	z	B _{eq}	occ
Sn1	0.42776(2)	0.43350(2)	0.13049(2)	1.284(2)	1
Sn2	0.34261(2)	0.54971(2)	0.01436(2)	1.230(2)	1
Pd1	0.50000	0.50000	0.00000	0.955(3)	1/2
Pd2	0.66824(2)	0.54773(2)	0.07820(2)	1.116(2)	1
Pd3	0.57870(2)	0.48457(2)	0.21252(2)	1.223(2)	1
Pd4	0.50213(2)	0.59340(2)	0.10580(2)	1.172(2)	1
N1	0.86331(14)	0.58050(8)	-0.00202(17)	2.15(3)	1
N2	0.76471(13)	0.52566(7)	0.32589(15)	1.78(3)	1
N3	0.54555(14)	0.42527(7)	0.42696(15)	1.88(3)	1
N4	0.36966(13)	0.68442(7)	0.14430(15)	1.78(3)	1
N5	0.68254(13)	0.66170(7)	0.14760(16)	1.83(3)	1
C1	0.79448(15)	0.56450(8)	0.02876(17)	1.67(3)	1
C2	0.94255(19)	0.60569(12)	-0.0468(3)	3.18(5)	1
C3	0.9025(3)	0.64703(16)	-0.1241(3)	5.80(10)	1
C4	1.0035(2)	0.62828(14)	0.0482(3)	4.17(7)	1
C5	0.9947(3)	0.56598(19)	-0.1089(4)	6.55(12)	1
C6	0.70424(15)	0.51963(8)	0.25592(17)	1.56(3)	1
C7	0.85315(17)	0.55108(9)	0.3635(2)	2.23(4)	1

C8	0.8436(2)	0.60693(10)	0.3324(3)	3.25(5)	1
C9	0.93211(18)	0.52609(12)	0.3057(3)	3.17(5)	1
C10	0.8686(2)	0.54452(13)	0.4880(2)	3.62(6)	1
C11	0.55777(15)	0.44533(8)	0.34503(17)	1.65(3)	1
C12	0.53263(17)	0.40705(8)	0.53770(17)	1.75(3)	1
C13	0.56965(19)	0.35300(9)	0.5467(2)	2.39(4)	1
C14	0.42747(17)	0.40945(10)	0.5548(2)	2.37(4)	1
C15	0.58880(18)	0.44212(9)	0.61762(19)	2.27(4)	1
C16	0.63621(14)	0.62451(8)	0.13120(16)	1.49(3)	1
C17	0.67762(18)	0.71502(9)	0.1793(2)	2.31(4)	1
C18	0.6278(3)	0.71670(12)	0.2871(2)	4.60(8)	1
C19	0.6175(2)	0.74341(10)	0.0916(2)	3.02(5)	1
C20	0.7755(3)	0.73600(12)	0.1931(4)	5.80(11)	1
C21	0.41850(15)	0.64985(8)	0.13378(16)	1.53(3)	1
C22	0.30720(16)	0.72787(8)	0.15081(19)	1.90(3)	1
C23	0.22306(19)	0.71109(11)	0.2111(3)	3.01(5)	1
C24	0.2781(2)	0.74438(10)	0.0331(2)	2.67(4)	1
C25	0.3614(2)	0.76991(9)	0.2138(2)	2.63(4)	1
C26	0.4569(2)	0.35269(9)	0.1471(2)	2.49(4)	1
C27	0.31462(17)	0.43396(10)	0.24338(19)	2.32(4)	1
C28	0.27305(17)	0.60315(9)	-0.1020(2)	2.26(4)	1
C29	0.23442(16)	0.55146(9)	0.1328(2)	2.12(4)	1
C30	0.1693(4)	0.6072(2)	0.5874(6)	2.65(9)	1/2
C31	0.1198(4)	0.6420(2)	0.6434(5)	2.43(8)	1/2
C32	0.0616(5)	0.6780(3)	0.5928(6)	2.92(11)	1/2
C33	0.0544(5)	0.6789(3)	0.4731(7)	3.06(12)	1/2
C34	0.1001(5)	0.6439(3)	0.4128(6)	2.94(13)	1/2
C35	0.1572(5)	0.6083(3)	0.4703(7)	3.68(12)	1/2
C36	-0.0255(7)	0.7220(4)	0.4734(9)	5.65(18)	1/2
C37	-0.0058(7)	0.7230(4)	0.4214(9)	5.80(19)	1/2
C38	0.0849(5)	0.6563(3)	0.4210(5)	2.44(11)	1/2
C39	0.0458(5)	0.6799(3)	0.5067(6)	2.92(12)	1/2
C40	0.0761(7)	0.6621(4)	0.6084(9)	5.2(2)	1/2
C41	0.1428(6)	0.6230(4)	0.6239(7)	4.28(14)	1/2
C42	0.1788(5)	0.5989(3)	0.5353(7)	3.61(11)	1/2
C43	0.1507(5)	0.6157(3)	0.4285(6)	3.15(11)	1/2

$$B_{eq} = \frac{8}{3} \pi^2 (U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$$

< Anisotropic displacement parameters >

atom	U11	U22	U33	U12	U13	U23
Sn1	0.01847(6)	0.01721(6)	0.01289(6)	-0.00391(5)	-0.00020(5)	0.00262(4)
Sn2	0.01388(6)	0.01611(6)	0.01652(6)	0.00113(4)	-0.00035(5)	-0.00169(5)
Pd1	0.01312(9)	0.01252(9)	0.01051(8)	-0.00053(7)	-0.00008(6)	0.00025(6)
Pd2	0.01356(7)	0.01484(7)	0.01384(6)	-0.00133(5)	0.00002(5)	-0.00023(5)
Pd3	0.01684(7)	0.01836(7)	0.01103(6)	-0.00227(5)	-0.00052(5)	0.00115(5)

Pd4	0.01570(7)	0.01412(7)	0.01450(6)	0.00020(5)	-0.00028(5)	-0.00127(5)
N1	0.0202(9)	0.0315(10)	0.0304(10)	-0.0042(8)	0.0040(7)	0.0020(8)
N2	0.0233(9)	0.0233(9)	0.0200(8)	-0.0010(7)	-0.0038(7)	0.0005(7)
N3	0.0285(10)	0.0274(10)	0.0155(8)	0.0015(8)	0.0024(7)	0.0026(7)
N4	0.0254(9)	0.0195(9)	0.0227(9)	0.0029(7)	0.0016(7)	-0.0017(7)
N5	0.0237(9)	0.0198(9)	0.0253(9)	-0.0019(7)	-0.0022(7)	-0.0022(7)
C1	0.0195(9)	0.0230(10)	0.0208(9)	0.0001(8)	0.0001(7)	-0.0018(8)
C2	0.0279(12)	0.0489(17)	0.0453(15)	-0.0182(12)	0.0099(11)	0.0024(13)
C3	0.077(3)	0.073(3)	0.067(2)	-0.044(2)	-0.017(2)	0.033(2)
C4	0.0298(14)	0.056(2)	0.071(2)	-0.0189(13)	-0.0047(14)	0.0057(17)
C5	0.053(2)	0.103(4)	0.100(3)	-0.019(2)	0.052(2)	-0.034(3)
C6	0.0218(10)	0.0187(9)	0.0190(9)	0.0003(7)	0.0018(7)	-0.0005(7)
C7	0.0230(11)	0.0293(12)	0.0305(12)	-0.0026(9)	-0.0111(9)	-0.0011(9)
C8	0.0324(13)	0.0288(13)	0.0594(18)	-0.0062(11)	-0.0169(13)	0.0007(12)
C9	0.0242(12)	0.0434(16)	0.0523(17)	0.0011(11)	-0.0022(11)	0.0007(13)
C10	0.0486(17)	0.0530(18)	0.0319(14)	-0.0012(14)	-0.0232(13)	-0.0039(12)
C11	0.0222(10)	0.0232(10)	0.0171(9)	-0.0013(8)	-0.0002(7)	0.0007(8)
C12	0.0319(11)	0.0208(10)	0.0140(9)	0.0028(8)	0.0037(8)	0.0035(7)
C13	0.0405(13)	0.0230(11)	0.0273(11)	0.0056(10)	0.0029(10)	0.0039(9)
C14	0.0310(12)	0.0341(13)	0.0260(11)	0.0023(10)	0.0083(9)	0.0040(9)
C15	0.0367(13)	0.0289(12)	0.0204(10)	0.0010(10)	0.0012(9)	-0.0028(9)
C16	0.0190(9)	0.0191(9)	0.0181(9)	0.0009(7)	-0.0016(7)	0.0001(7)
C17	0.0365(13)	0.0170(10)	0.0333(12)	0.0004(9)	-0.0039(10)	-0.0038(9)
C18	0.116(3)	0.0283(14)	0.0304(14)	0.0205(17)	0.0063(17)	-0.0036(11)
C19	0.0522(17)	0.0236(12)	0.0378(14)	-0.0001(11)	-0.0050(12)	0.0060(10)
C20	0.051(2)	0.0274(15)	0.137(4)	-0.0150(14)	-0.029(2)	-0.007(2)
C21	0.0206(9)	0.0206(10)	0.0168(9)	-0.0019(8)	-0.0001(7)	-0.0005(7)
C22	0.0256(10)	0.0181(10)	0.0288(11)	0.0056(8)	0.0041(8)	-0.0010(8)
C23	0.0321(13)	0.0329(13)	0.0513(16)	0.0031(11)	0.0149(12)	-0.0004(12)
C24	0.0438(14)	0.0243(12)	0.0320(12)	0.0078(10)	-0.0050(11)	0.0027(9)
C25	0.0424(14)	0.0236(11)	0.0336(13)	0.0014(10)	0.0019(11)	-0.0075(10)
C26	0.0478(15)	0.0199(11)	0.0259(11)	-0.0052(10)	-0.0027(10)	0.0071(9)
C27	0.0242(11)	0.0431(14)	0.0215(10)	-0.0064(10)	0.0049(8)	0.0046(9)
C28	0.0284(11)	0.0270(11)	0.0294(11)	0.0076(9)	-0.0046(9)	0.0017(9)
C29	0.0216(10)	0.0319(12)	0.0277(11)	0.0011(9)	0.0058(8)	-0.0038(9)

The general temperature factor expression: $\exp(-2\pi^2(a^2U_{11}h^2 + b^2U_{22}k^2 + c^2U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

<Bond lengths (Å)>

atom	atom	distance	atom	atom	distance
Sn1	Pd1	2.6216(4)	Sn1	Pd2 ¹	2.8300(4)
Sn1	Pd3	2.6586(5)	Sn1	C26	2.171(2)
Sn1	C27	2.191(2)	Sn2	Pd1	2.6067(4)
Sn2	Pd2 ¹	2.7979(7)	Sn2	Pd4	2.7028(5)
Sn2	C28	2.177(2)	Sn2	C29	2.184(2)
Pd1	Pd2	2.8005(3)	Pd1	Pd2 ¹	2.8005(3)

Pd1	Pd3	2.7650(3)	Pd1	Pd3 ¹	2.7650(3)
Pd1	Pd4	2.7714(5)	Pd1	Pd4 ¹	2.7714(5)
Pd2	Pd3	2.7121(5)	Pd2	Pd4	2.6908(5)
Pd2	C1	1.983(2)	Pd2	C6	2.303(2)
Pd2	C16	2.178(2)	Pd3	C6	2.041(2)
Pd3	C11	1.954(2)	Pd4	C16	2.074(2)
Pd4	C21	1.947(2)	N1	C1	1.152(3)
N1	C2	1.447(4)	N2	C6	1.173(3)
N2	C7	1.465(3)	N3	C11	1.152(3)
N3	C12	1.453(3)	N4	C21	1.156(3)
N4	C22	1.452(3)	N5	C16	1.187(3)
N5	C17	1.457(3)	C2	C3	1.519(5)
C2	C4	1.511(4)	C2	C5	1.514(6)
C7	C8	1.520(4)	C7	C9	1.517(4)
C7	C10	1.521(4)	C12	C13	1.516(3)
C12	C14	1.525(3)	C12	C15	1.521(3)
C17	C18	1.536(4)	C17	C19	1.511(4)
C17	C20	1.494(4)	C22	C23	1.514(4)
C22	C24	1.521(3)	C22	C25	1.520(3)

Symmetry Operators:

(1) -X+1,-Y+1,-Z

<Bond angles (°)>

atom	atom	atom	angle	atom	atom	atom	angle
Pd1	Sn1	Pd2 ¹	61.681(11)	Pd1	Sn1	Pd3	63.153(12)
Pd1	Sn1	C26	128.94(7)	Pd1	Sn1	C27	135.60(7)
Pd2 ¹	Sn1	Pd3	124.59(2)	Pd2 ¹	Sn1	C26	109.24(7)
Pd2 ¹	Sn1	C27	103.53(6)	Pd3	Sn1	C26	108.47(7)
Pd3	Sn1	C27	111.80(6)	C26	Sn1	C27	95.21(10)
Pd1	Sn2	Pd2 ¹	62.300(12)	Pd1	Sn2	Pd4	62.897(11)
Pd1	Sn2	C28	129.00(7)	Pd1	Sn2	C29	134.79(6)
Pd2 ¹	Sn2	Pd4	124.989(18)	Pd2 ¹	Sn2	C28	108.76(6)
Pd2 ¹	Sn2	C29	105.32(6)	Pd4	Sn2	C28	108.52(7)
Pd4	Sn2	C29	109.27(6)	C28	Sn2	C29	96.15(9)
Sn1	Pd1	Sn1 ¹	180.000(16)	Sn1	Pd1	Sn2	85.240(12)
Sn1	Pd1	Sn2 ¹	94.760(12)	Sn1	Pd1	Pd2	117.176(9)
Sn1	Pd1	Pd2 ¹	62.824(9)	Sn1	Pd1	Pd3	59.077(11)
Sn1	Pd1	Pd3 ¹	120.923(11)	Sn1	Pd1	Pd4	107.548(11)
Sn1	Pd1	Pd4 ¹	72.452(11)	Sn1 ¹	Pd1	Sn2	94.760(12)
Sn1 ¹	Pd1	Sn2 ¹	85.240(12)	Sn1 ¹	Pd1	Pd2	62.824(9)
Sn1 ¹	Pd1	Pd2 ¹	117.176(9)	Sn1 ¹	Pd1	Pd3	120.923(11)
Sn1 ¹	Pd1	Pd3 ¹	59.077(11)	Sn1 ¹	Pd1	Pd4	72.452(11)
Sn1 ¹	Pd1	Pd4 ¹	107.548(11)	Sn2	Pd1	Sn2 ¹	180.000(17)
Sn2	Pd1	Pd2	117.801(13)	Sn2	Pd1	Pd2 ¹	62.199(13)
Sn2	Pd1	Pd3	107.391(9)	Sn2	Pd1	Pd3 ¹	72.609(9)
Sn2	Pd1	Pd4	60.245(11)	Sn2	Pd1	Pd4 ¹	119.755(11)

Sn2 ¹	Pd1	Pd2	62.199(13)	Sn2 ¹	Pd1	Pd2 ¹	117.801(13)
Sn2 ¹	Pd1	Pd3	72.609(9)	Sn2 ¹	Pd1	Pd3 ¹	107.391(9)
Sn2 ¹	Pd1	Pd4	119.755(11)	Sn2 ¹	Pd1	Pd4 ¹	60.245(11)
Pd2	Pd1	Pd2 ¹	180.000(16)	Pd2	Pd1	Pd3	58.323(11)
Pd2	Pd1	Pd3 ¹	121.677(11)	Pd2	Pd1	Pd4	57.752(11)
Pd2	Pd1	Pd4 ¹	122.248(11)	Pd2 ¹	Pd1	Pd3	121.677(11)
Pd2 ¹	Pd1	Pd3 ¹	58.323(11)	Pd2 ¹	Pd1	Pd4	122.248(11)
Pd2 ¹	Pd1	Pd4 ¹	57.752(11)	Pd3	Pd1	Pd3 ¹	180.000(17)
Pd3	Pd1	Pd4	72.982(12)	Pd3	Pd1	Pd4 ¹	107.018(12)
Pd3 ¹	Pd1	Pd4	107.018(12)	Pd3 ¹	Pd1	Pd4 ¹	72.982(12)
Pd4	Pd1	Pd4 ¹	180.000(13)	Sn1 ¹	Pd2	Sn2 ¹	77.958(15)
Sn1 ¹	Pd2	Pd1	55.495(10)	Sn1 ¹	Pd2	Pd3	115.478(15)
Sn1 ¹	Pd2	Pd4	70.525(11)	Sn1 ¹	Pd2	C1	94.29(6)
Sn1 ¹	Pd2	C6	162.53(6)	Sn1 ¹	Pd2	C16	90.35(5)
Sn2 ¹	Pd2	Pd1	55.501(10)	Sn2 ¹	Pd2	Pd3	70.556(16)
Sn2 ¹	Pd2	Pd4	115.901(17)	Sn2 ¹	Pd2	C1	96.04(6)
Sn2 ¹	Pd2	C6	94.86(6)	Sn2 ¹	Pd2	C16	164.07(5)
Pd1	Pd2	Pd3	60.185(10)	Pd1	Pd2	Pd4	60.581(11)
Pd1	Pd2	C1	139.86(6)	Pd1	Pd2	C6	107.30(5)
Pd1	Pd2	C16	108.90(5)	Pd3	Pd2	Pd4	75.089(15)
Pd3	Pd2	C1	142.61(6)	Pd3	Pd2	C6	47.15(5)
Pd3	Pd2	C16	105.77(6)	Pd4	Pd2	C1	139.45(7)
Pd4	Pd2	C6	99.24(5)	Pd4	Pd2	C16	49.05(5)
C1	Pd2	C6	102.36(8)	C1	Pd2	C16	95.59(8)
C6	Pd2	C16	93.24(7)	Sn1	Pd3	Pd1	57.770(9)
Sn1	Pd3	Pd2	119.029(13)	Sn1	Pd3	C6	171.46(6)
Sn1	Pd3	C11	82.73(6)	Pd1	Pd3	Pd2	61.492(9)
Pd1	Pd3	C6	117.28(6)	Pd1	Pd3	C11	140.46(6)
Pd2	Pd3	C6	55.84(6)	Pd2	Pd3	C11	157.96(6)
C6	Pd3	C11	102.13(8)	Sn2	Pd4	Pd1	56.857(13)
Sn2	Pd4	Pd2	118.33(2)	Sn2	Pd4	C16	163.81(6)
Sn2	Pd4	C21	83.83(6)	Pd1	Pd4	Pd2	61.667(13)
Pd1	Pd4	C16	113.34(6)	Pd1	Pd4	C21	140.48(6)
Pd2	Pd4	C16	52.47(6)	Pd2	Pd4	C21	156.10(7)
C16	Pd4	C21	103.81(9)	C1	N1	C2	172.8(2)
C6	N2	C7	148.4(2)	C11	N3	C12	171.8(2)
C21	N4	C22	176.8(2)	C16	N5	C17	143.1(2)
Pd2	C1	N1	171.16(19)	N1	C2	C3	107.1(2)
N1	C2	C4	108.0(2)	N1	C2	C5	107.2(3)
C3	C2	C4	110.9(3)	C3	C2	C5	111.1(3)
C4	C2	C5	112.2(3)	Pd2	C6	Pd3	77.01(7)
Pd2	C6	N2	137.30(18)	Pd3	C6	N2	145.69(18)
N2	C7	C8	107.76(19)	N2	C7	C9	107.7(2)
N2	C7	C10	108.3(2)	C8	C7	C9	111.0(2)
C8	C7	C10	111.1(2)	C9	C7	C10	110.8(2)
Pd3	C11	N3	175.37(19)	N3	C12	C13	107.94(18)

N3	C12	C14	107.84(18)	N3	C12	C15	107.13(18)
C13	C12	C14	111.5(2)	C13	C12	C15	111.12(19)
C14	C12	C15	111.08(19)	Pd2	C16	Pd4	78.48(7)
Pd2	C16	N5	133.46(17)	Pd4	C16	N5	147.24(17)
N5	C17	C18	106.7(2)	N5	C17	C19	109.0(2)
N5	C17	C20	108.8(2)	C18	C17	C19	108.3(2)
C18	C17	C20	112.3(3)	C19	C17	C20	111.6(3)
Pd4	C21	N4	176.00(18)	N4	C22	C23	107.75(19)
N4	C22	C24	107.26(19)	N4	C22	C25	108.14(19)
C23	C22	C24	111.7(2)	C23	C22	C25	110.9(2)
C24	C22	C25	110.89(19)				

Symmetry Operators:

(1) -X+1,-Y+1,-Z

< Torsion Angles($^{\circ}$) (Those having bond angles > 160 or < 20 degrees are excluded.) >

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Pd1	Sn1	Pd2 ¹	Sn2	-56.2	Pd1	Sn1	Pd2 ¹	Pd1	-0.0
Pd1	Sn1	Pd2 ¹	Pd3 ¹	5.189(14)	Pd1	Sn1	Pd2 ¹	Pd4 ¹	67.1
Pd1	Sn1	Pd2 ¹	C1 ¹	-151.49(2)	Pd1	Sn1	Pd2 ¹	C16 ¹	112.881(11)
Pd2 ¹	Sn1	Pd1	Sn2	61.096(11)	Pd2 ¹	Sn1	Pd1	Sn2 ¹	-118.904(11)
Pd2 ¹	Sn1	Pd1	Pd2	180.0	Pd2 ¹	Sn1	Pd1	Pd2 ¹	0.0
Pd2 ¹	Sn1	Pd1	Pd3	174.644(14)	Pd2 ¹	Sn1	Pd1	Pd3 ¹	-5.356(14)
Pd2 ¹	Sn1	Pd1	Pd4	117.822(11)	Pd2 ¹	Sn1	Pd1	Pd4 ¹	-62.178(11)
Pd1	Sn1	Pd3	Pd1	0.0	Pd1	Sn1	Pd3	Pd2	-5.628(16)
Pd1	Sn1	Pd3	C11	178.076(18)	Pd3	Sn1	Pd1	Sn2	-113.548(12)
Pd3	Sn1	Pd1	Sn2 ¹	66.452(12)	Pd3	Sn1	Pd1	Pd2	5.356(15)
Pd3	Sn1	Pd1	Pd2 ¹	-174.644(15)	Pd3	Sn1	Pd1	Pd3	0.000(10)
Pd3	Sn1	Pd1	Pd3 ¹	-180.000(10)	Pd3	Sn1	Pd1	Pd4	-56.822(12)
Pd3	Sn1	Pd1	Pd4 ¹	123.178(12)	C26	Sn1	Pd1	Sn2	153.73(9)
C26	Sn1	Pd1	Sn2 ¹	-26.27(9)	C26	Sn1	Pd1	Pd2	-87.37(9)
C26	Sn1	Pd1	Pd2 ¹	92.63(9)	C26	Sn1	Pd1	Pd3	-92.72(9)
C26	Sn1	Pd1	Pd3 ¹	87.28(9)	C26	Sn1	Pd1	Pd4	-149.55(9)
C26	Sn1	Pd1	Pd4 ¹	30.45(9)	C27	Sn1	Pd1	Sn2	-19.08(9)
C27	Sn1	Pd1	Sn2 ¹	160.92(9)	C27	Sn1	Pd1	Pd2	99.82(9)
C27	Sn1	Pd1	Pd2 ¹	-80.18(9)	C27	Sn1	Pd1	Pd3	94.47(9)
C27	Sn1	Pd1	Pd3 ¹	-85.53(9)	C27	Sn1	Pd1	Pd4	37.64(9)
C27	Sn1	Pd1	Pd4 ¹	-142.36(9)	Pd2 ¹	Sn1	Pd3	Pd1	-5.729(18)
Pd2 ¹	Sn1	Pd3	Pd2	-11.36(3)	Pd2 ¹	Sn1	Pd3	C11	172.35(2)
Pd3	Sn1	Pd2 ¹	Sn2	-50.40(2)	Pd3	Sn1	Pd2 ¹	Pd1	5.807(18)
Pd3	Sn1	Pd2 ¹	Pd3 ¹	11.00(3)	Pd3	Sn1	Pd2 ¹	Pd4 ¹	72.91(2)
Pd3	Sn1	Pd2 ¹	C1 ¹	-145.68(2)	Pd3	Sn1	Pd2 ¹	C16 ¹	118.69(2)
C26	Sn1	Pd2 ¹	Sn2	179.17(8)	C26	Sn1	Pd2 ¹	Pd1	-124.62(8)
C26	Sn1	Pd2 ¹	Pd3 ¹	-119.43(8)	C26	Sn1	Pd2 ¹	Pd4 ¹	-57.52(8)
C26	Sn1	Pd2 ¹	C1 ¹	83.90(8)	C26	Sn1	Pd2 ¹	C16 ¹	-11.74(8)
C27	Sn1	Pd2 ¹	Sn2	78.63(7)	C27	Sn1	Pd2 ¹	Pd1	134.84(7)
C27	Sn1	Pd2 ¹	Pd3 ¹	140.03(7)	C27	Sn1	Pd2 ¹	Pd4 ¹	-158.06(7)

C27	Sn1	Pd2 ¹	C1 ¹	-16.64(7)	C27	Sn1	Pd2 ¹	C16 ¹	-112.27(7)
C26	Sn1	Pd3	Pd1	125.00(7)	C26	Sn1	Pd3	Pd2	119.38(7)
C26	Sn1	Pd3	C11	-56.92(7)	C27	Sn1	Pd3	Pd1	-131.31(7)
C27	Sn1	Pd3	Pd2	-136.93(7)	C27	Sn1	Pd3	C11	46.77(7)
Pd1	Sn2	Pd2 ¹	Sn1	56.2	Pd1	Sn2	Pd2 ¹	Pd1	-0.0
Pd1	Sn2	Pd2 ¹	Pd3 ¹	-66.6	Pd1	Sn2	Pd2 ¹	Pd4 ¹	-4.943(10)
Pd1	Sn2	Pd2 ¹	C1 ¹	149.319(13)	Pd1	Sn2	Pd2 ¹	C6 ¹	-107.678(10)
Pd2 ¹	Sn2	Pd1	Sn1	-61.7	Pd2 ¹	Sn2	Pd1	Sn1 ¹	118.3
Pd2 ¹	Sn2	Pd1	Pd2	180.0	Pd2 ¹	Sn2	Pd1	Pd2 ¹	0.0
Pd2 ¹	Sn2	Pd1	Pd3	-117.2	Pd2 ¹	Sn2	Pd1	Pd3 ¹	62.8
Pd2 ¹	Sn2	Pd1	Pd4	-175.027(10)	Pd2 ¹	Sn2	Pd1	Pd4 ¹	4.973(10)
Pd1	Sn2	Pd4	Pd1	-0.0	Pd1	Sn2	Pd4	Pd2	5.201(12)
Pd1	Sn2	Pd4	C21	175.729(13)	Pd4	Sn2	Pd1	Sn1	113.3
Pd4	Sn2	Pd1	Sn1 ¹	-66.7	Pd4	Sn2	Pd1	Pd2	-4.973(11)
Pd4	Sn2	Pd1	Pd2 ¹	175.027(11)	Pd4	Sn2	Pd1	Pd3	57.837(10)
Pd4	Sn2	Pd1	Pd3 ¹	-122.163(10)	Pd4	Sn2	Pd1	Pd4	-0.0
Pd4	Sn2	Pd1	Pd4 ¹	180.0	C28	Sn2	Pd1	Sn1	-154.11(8)
C28	Sn2	Pd1	Sn1 ¹	25.89(8)	C28	Sn2	Pd1	Pd2	87.58(8)
C28	Sn2	Pd1	Pd2 ¹	-92.42(8)	C28	Sn2	Pd1	Pd3	150.39(8)
C28	Sn2	Pd1	Pd3 ¹	-29.61(8)	C28	Sn2	Pd1	Pd4	92.56(8)
C28	Sn2	Pd1	Pd4 ¹	-87.44(8)	C29	Sn2	Pd1	Sn1	22.52(9)
C29	Sn2	Pd1	Sn1 ¹	-157.48(9)	C29	Sn2	Pd1	Pd2	-95.79(9)
C29	Sn2	Pd1	Pd2 ¹	84.21(9)	C29	Sn2	Pd1	Pd3	-32.98(9)
C29	Sn2	Pd1	Pd3 ¹	147.02(9)	C29	Sn2	Pd1	Pd4	-90.81(9)
C29	Sn2	Pd1	Pd4 ¹	89.19(9)	Pd2 ¹	Sn2	Pd4	Pd1	5.375(14)
Pd2 ¹	Sn2	Pd4	Pd2	10.58(2)	Pd2 ¹	Sn2	Pd4	C21	-178.895(16)
Pd4	Sn2	Pd2 ¹	Sn1	50.800(16)	Pd4	Sn2	Pd2 ¹	Pd1	-5.405(14)
Pd4	Sn2	Pd2 ¹	Pd3 ¹	-72.002(16)	Pd4	Sn2	Pd2 ¹	Pd4 ¹	-10.35(2)
Pd4	Sn2	Pd2 ¹	C1 ¹	143.915(16)	Pd4	Sn2	Pd2 ¹	C6 ¹	-113.082(16)
C28	Sn2	Pd2 ¹	Sn1	-178.88(7)	C28	Sn2	Pd2 ¹	Pd1	124.92(7)
C28	Sn2	Pd2 ¹	Pd3 ¹	58.32(7)	C28	Sn2	Pd2 ¹	Pd4 ¹	119.98(7)
C28	Sn2	Pd2 ¹	C1 ¹	-85.76(7)	C28	Sn2	Pd2 ¹	C6 ¹	17.24(7)
C29	Sn2	Pd2 ¹	Sn1	-76.74(6)	C29	Sn2	Pd2 ¹	Pd1	-132.94(6)
C29	Sn2	Pd2 ¹	Pd3 ¹	160.46(6)	C29	Sn2	Pd2 ¹	Pd4 ¹	-137.88(6)
C29	Sn2	Pd2 ¹	C1 ¹	16.38(6)	C29	Sn2	Pd2 ¹	C6 ¹	119.38(6)
C28	Sn2	Pd4	Pd1	-125.04(7)	C28	Sn2	Pd4	Pd2	-119.84(7)
C28	Sn2	Pd4	C21	50.69(7)	C29	Sn2	Pd4	Pd1	131.26(7)
C29	Sn2	Pd4	Pd2	136.46(7)	C29	Sn2	Pd4	C21	-53.01(7)
Sn1	Pd1	Pd2	Sn1 ¹	180.000(11)	Sn1	Pd1	Pd2	Sn2 ¹	80.489(11)
Sn1	Pd1	Pd2	Pd3	-5.399(15)	Sn1	Pd1	Pd2	Pd4	-94.406(13)
Sn1	Pd1	Pd2	C1	132.40(3)	Sn1	Pd1	Pd2	C6	-3.40(2)
Sn1	Pd1	Pd2	C16	-103.149(16)	Sn1	Pd1	Pd2 ¹	Sn1	-0.000(11)
Sn1	Pd1	Pd2 ¹	Sn2	99.511(11)	Sn1	Pd1	Pd2 ¹	Pd3 ¹	-174.601(15)
Sn1	Pd1	Pd2 ¹	Pd4 ¹	-85.594(13)	Sn1	Pd1	Pd2 ¹	C1 ¹	47.60(3)
Sn1	Pd1	Pd2 ¹	C6 ¹	-176.60(2)	Sn1	Pd1	Pd2 ¹	C16 ¹	-76.851(16)
Sn1	Pd1	Pd3	Sn1	-0.000(11)	Sn1	Pd1	Pd3	Pd2	174.400(15)

Sn1	Pd1	Pd3	C6	171.98(3)	Sn1	Pd1	Pd3	C11	-3.00(3)
Sn1	Pd1	Pd3 ¹	Sn1 ¹	-180.000(11)	Sn1	Pd1	Pd3 ¹	Pd2 ¹	5.600(15)
Sn1	Pd1	Pd3 ¹	C6 ¹	8.02(3)	Sn1	Pd1	Pd3 ¹	C11 ¹	-177.00(3)
Sn1	Pd1	Pd4	Sn2	-73.7	Sn1	Pd1	Pd4	Pd2	111.5
Sn1	Pd1	Pd4	C16	120.989(13)	Sn1	Pd1	Pd4	C21	-80.36(2)
Sn1	Pd1	Pd4 ¹	Sn2 ¹	-106.3	Sn1	Pd1	Pd4 ¹	Pd2 ¹	68.5
Sn1	Pd1	Pd4 ¹	C16 ¹	59.011(13)	Sn1	Pd1	Pd4 ¹	C21 ¹	-99.64(2)
Sn1 ¹	Pd1	Pd2	Sn1 ¹	0.000(11)	Sn1 ¹	Pd1	Pd2	Sn2 ¹	-99.511(11)
Sn1 ¹	Pd1	Pd2	Pd3	174.601(15)	Sn1 ¹	Pd1	Pd2	Pd4	85.594(13)
Sn1 ¹	Pd1	Pd2	C1	-47.60(3)	Sn1 ¹	Pd1	Pd2	C6	176.60(2)
Sn1 ¹	Pd1	Pd2	C16	76.851(16)	Sn1 ¹	Pd1	Pd2 ¹	Sn1	180.000(11)
Sn1 ¹	Pd1	Pd2 ¹	Sn2	-80.489(11)	Sn1 ¹	Pd1	Pd2 ¹	Pd3 ¹	5.399(15)
Sn1 ¹	Pd1	Pd2 ¹	Pd4 ¹	94.406(13)	Sn1 ¹	Pd1	Pd2 ¹	C1 ¹	-132.40(3)
Sn1 ¹	Pd1	Pd2 ¹	C6 ¹	3.40(2)	Sn1 ¹	Pd1	Pd2 ¹	C16 ¹	103.149(16)
Sn1 ¹	Pd1	Pd3	Sn1	-180.000(11)	Sn1 ¹	Pd1	Pd3	Pd2	-5.600(15)
Sn1 ¹	Pd1	Pd3	C6	-8.02(3)	Sn1 ¹	Pd1	Pd3	C11	177.00(3)
Sn1 ¹	Pd1	Pd3 ¹	Sn1 ¹	0.000(11)	Sn1 ¹	Pd1	Pd3 ¹	Pd2 ¹	-174.400(15)
Sn1 ¹	Pd1	Pd3 ¹	C6 ¹	-171.98(3)	Sn1 ¹	Pd1	Pd3 ¹	C11 ¹	3.00(3)
Sn1 ¹	Pd1	Pd4	Sn2	106.3	Sn1 ¹	Pd1	Pd4	Pd2	-68.5
Sn1 ¹	Pd1	Pd4	C16	-59.011(13)	Sn1 ¹	Pd1	Pd4	C21	99.64(2)
Sn1 ¹	Pd1	Pd4 ¹	Sn2 ¹	73.7	Sn1 ¹	Pd1	Pd4 ¹	Pd2 ¹	-111.5
Sn1 ¹	Pd1	Pd4 ¹	C16 ¹	-120.989(13)	Sn1 ¹	Pd1	Pd4 ¹	C21 ¹	80.36(2)
Sn2	Pd1	Pd2	Sn1 ¹	-80.5	Sn2	Pd1	Pd2	Sn2 ¹	180.0
Sn2	Pd1	Pd2	Pd3	94.112(11)	Sn2	Pd1	Pd2	Pd4	5.105(11)
Sn2	Pd1	Pd2	C1	-128.08(3)	Sn2	Pd1	Pd2	C6	96.106(18)
Sn2	Pd1	Pd2	C16	-3.638(16)	Sn2	Pd1	Pd2 ¹	Sn1	-99.5
Sn2	Pd1	Pd2 ¹	Sn2	-0.0	Sn2	Pd1	Pd2 ¹	Pd3 ¹	85.888(11)
Sn2	Pd1	Pd2 ¹	Pd4 ¹	174.895(11)	Sn2	Pd1	Pd2 ¹	C1 ¹	-51.92(3)
Sn2	Pd1	Pd2 ¹	C6 ¹	83.894(18)	Sn2	Pd1	Pd2 ¹	C16 ¹	-176.362(16)
Sn2	Pd1	Pd3	Sn1	73.202(13)	Sn2	Pd1	Pd3	Pd2	-112.398(12)
Sn2	Pd1	Pd3	C6	-114.82(2)	Sn2	Pd1	Pd3	C11	70.20(4)
Sn2	Pd1	Pd3 ¹	Sn1 ¹	106.798(13)	Sn2	Pd1	Pd3 ¹	Pd2 ¹	-67.602(12)
Sn2	Pd1	Pd3 ¹	C6 ¹	-65.18(2)	Sn2	Pd1	Pd3 ¹	C11 ¹	109.80(4)
Sn2	Pd1	Pd4	Sn2	-0.0	Sn2	Pd1	Pd4	Pd2	-174.798(12)
Sn2	Pd1	Pd4	C16	-165.332(18)	Sn2	Pd1	Pd4	C21	-6.68(2)
Sn2	Pd1	Pd4 ¹	Sn2 ¹	-180.0	Sn2	Pd1	Pd4 ¹	Pd2 ¹	-5.202(12)
Sn2	Pd1	Pd4 ¹	C16 ¹	-14.668(18)	Sn2	Pd1	Pd4 ¹	C21 ¹	-173.32(2)
Sn2 ¹	Pd1	Pd2	Sn1 ¹	99.5	Sn2 ¹	Pd1	Pd2	Sn2 ¹	0.0
Sn2 ¹	Pd1	Pd2	Pd3	-85.888(11)	Sn2 ¹	Pd1	Pd2	Pd4	-174.895(11)
Sn2 ¹	Pd1	Pd2	C1	51.92(3)	Sn2 ¹	Pd1	Pd2	C6	-83.894(18)
Sn2 ¹	Pd1	Pd2	C16	176.362(16)	Sn2 ¹	Pd1	Pd2 ¹	Sn1	80.5
Sn2 ¹	Pd1	Pd2 ¹	Sn2	180.0	Sn2 ¹	Pd1	Pd2 ¹	Pd3 ¹	-94.112(11)
Sn2 ¹	Pd1	Pd2 ¹	Pd4 ¹	-5.105(11)	Sn2 ¹	Pd1	Pd2 ¹	C1 ¹	128.08(3)
Sn2 ¹	Pd1	Pd2 ¹	C6 ¹	-96.106(18)	Sn2 ¹	Pd1	Pd2 ¹	C16 ¹	3.638(16)
Sn2 ¹	Pd1	Pd3	Sn1	-106.798(13)	Sn2 ¹	Pd1	Pd3	Pd2	67.602(12)
Sn2 ¹	Pd1	Pd3	C6	65.18(2)	Sn2 ¹	Pd1	Pd3	C11	-109.80(4)

Sn2 ¹	Pd1	Pd3 ¹	Sn1 ¹	-73.202(13)	Sn2 ¹	Pd1	Pd3 ¹	Pd2 ¹	112.398(12)
Sn2 ¹	Pd1	Pd3 ¹	C6 ¹	114.82(2)	Sn2 ¹	Pd1	Pd3 ¹	C11 ¹	-70.20(4)
Sn2 ¹	Pd1	Pd4	Sn2	-180.0	Sn2 ¹	Pd1	Pd4	Pd2	5.202(12)
Sn2 ¹	Pd1	Pd4	C16	14.668(18)	Sn2 ¹	Pd1	Pd4	C21	173.32(2)
Sn2 ¹	Pd1	Pd4 ¹	Sn2 ¹	0.0	Sn2 ¹	Pd1	Pd4 ¹	Pd2 ¹	174.798(12)
Sn2 ¹	Pd1	Pd4 ¹	C16 ¹	165.332(18)	Sn2 ¹	Pd1	Pd4 ¹	C21 ¹	6.68(2)
Pd2	Pd1	Pd3	Sn1	-174.400(15)	Pd2	Pd1	Pd3	Pd2	-0.000(11)
Pd2	Pd1	Pd3	C6	-2.418(17)	Pd2	Pd1	Pd3	C11	-177.40(4)
Pd3	Pd1	Pd2	Sn1 ¹	-174.601(15)	Pd3	Pd1	Pd2	Sn2 ¹	85.888(13)
Pd3	Pd1	Pd2	Pd3	-0.000(11)	Pd3	Pd1	Pd2	Pd4	-89.007(12)
Pd3	Pd1	Pd2	C1	137.80(4)	Pd3	Pd1	Pd2	C6	1.994(14)
Pd3	Pd1	Pd2	C16	-97.750(15)	Pd2	Pd1	Pd3 ¹	Sn1 ¹	-5.600(15)
Pd2	Pd1	Pd3 ¹	Pd2 ¹	-180.000(11)	Pd2	Pd1	Pd3 ¹	C6 ¹	-177.582(17)
Pd2	Pd1	Pd3 ¹	C11 ¹	-2.60(4)	Pd3 ¹	Pd1	Pd2	Sn1 ¹	5.399(15)
Pd3 ¹	Pd1	Pd2	Sn2 ¹	-94.112(13)	Pd3 ¹	Pd1	Pd2	Pd3	180.000(11)
Pd3 ¹	Pd1	Pd2	Pd4	90.993(12)	Pd3 ¹	Pd1	Pd2	C1	-42.20(4)
Pd3 ¹	Pd1	Pd2	C6	-178.006(14)	Pd3 ¹	Pd1	Pd2	C16	82.250(15)
Pd2	Pd1	Pd4	Sn2	174.798(11)	Pd2	Pd1	Pd4	Pd2	0.0
Pd2	Pd1	Pd4	C16	9.466(12)	Pd2	Pd1	Pd4	C21	168.12(3)
Pd4	Pd1	Pd2	Sn1 ¹	-85.594(11)	Pd4	Pd1	Pd2	Sn2 ¹	174.895(11)
Pd4	Pd1	Pd2	Pd3	89.0	Pd4	Pd1	Pd2	Pd4	-0.0
Pd4	Pd1	Pd2	C1	-133.19(4)	Pd4	Pd1	Pd2	C6	91.001(15)
Pd4	Pd1	Pd2	C16	-8.743(10)	Pd2	Pd1	Pd4 ¹	Sn2 ¹	5.202(11)
Pd2	Pd1	Pd4 ¹	Pd2 ¹	180.0	Pd2	Pd1	Pd4 ¹	C16 ¹	170.534(12)
Pd2	Pd1	Pd4 ¹	C21 ¹	11.88(3)	Pd4 ¹	Pd1	Pd2	Sn1 ¹	94.406(11)
Pd4 ¹	Pd1	Pd2	Sn2 ¹	-5.105(11)	Pd4 ¹	Pd1	Pd2	Pd3	-91.0
Pd4 ¹	Pd1	Pd2	Pd4	180.0	Pd4 ¹	Pd1	Pd2	C1	46.81(4)
Pd4 ¹	Pd1	Pd2	C6	-88.999(15)	Pd4 ¹	Pd1	Pd2	C16	171.257(10)
Pd2 ¹	Pd1	Pd3	Sn1	5.600(15)	Pd2 ¹	Pd1	Pd3	Pd2	180.000(11)
Pd2 ¹	Pd1	Pd3	C6	177.582(17)	Pd2 ¹	Pd1	Pd3	C11	2.60(4)
Pd3	Pd1	Pd2 ¹	Sn1	-5.399(15)	Pd3	Pd1	Pd2 ¹	Sn2	94.112(13)
Pd3	Pd1	Pd2 ¹	Pd3 ¹	180.000(11)	Pd3	Pd1	Pd2 ¹	Pd4 ¹	-90.993(12)
Pd3	Pd1	Pd2 ¹	C1 ¹	42.20(4)	Pd3	Pd1	Pd2 ¹	C6 ¹	178.006(14)
Pd3	Pd1	Pd2 ¹	C16 ¹	-82.250(15)	Pd2 ¹	Pd1	Pd3 ¹	Sn1 ¹	174.400(15)
Pd2 ¹	Pd1	Pd3 ¹	Pd2 ¹	0.000(11)	Pd2 ¹	Pd1	Pd3 ¹	C6 ¹	2.418(17)
Pd2 ¹	Pd1	Pd3 ¹	C11 ¹	177.40(4)	Pd3 ¹	Pd1	Pd2 ¹	Sn1	174.601(15)
Pd3 ¹	Pd1	Pd2 ¹	Sn2	-85.888(13)	Pd3 ¹	Pd1	Pd2 ¹	Pd3 ¹	-0.000(11)
Pd3 ¹	Pd1	Pd2 ¹	Pd4 ¹	89.007(12)	Pd3 ¹	Pd1	Pd2 ¹	C1 ¹	-137.80(4)
Pd3 ¹	Pd1	Pd2 ¹	C6 ¹	-1.994(14)	Pd3 ¹	Pd1	Pd2 ¹	C16 ¹	97.750(15)
Pd2 ¹	Pd1	Pd4	Sn2	-5.202(11)	Pd2 ¹	Pd1	Pd4	Pd2	-180.0
Pd2 ¹	Pd1	Pd4	C16	-170.534(12)	Pd2 ¹	Pd1	Pd4	C21	-11.88(3)
Pd4	Pd1	Pd2 ¹	Sn1	-94.406(11)	Pd4	Pd1	Pd2 ¹	Sn2	5.105(11)
Pd4	Pd1	Pd2 ¹	Pd3 ¹	91.0	Pd4	Pd1	Pd2 ¹	Pd4 ¹	-180.0
Pd4	Pd1	Pd2 ¹	C1 ¹	-46.81(4)	Pd4	Pd1	Pd2 ¹	C6 ¹	88.999(15)
Pd4	Pd1	Pd2 ¹	C16 ¹	-171.257(10)	Pd2 ¹	Pd1	Pd4 ¹	Sn2 ¹	-174.798(11)
Pd2 ¹	Pd1	Pd4 ¹	Pd2 ¹	-0.0	Pd2 ¹	Pd1	Pd4 ¹	C16 ¹	-9.466(12)

Pd2 ¹	Pd1	Pd4 ¹	C21 ¹	-168.12(3)	Pd4 ¹	Pd1	Pd2 ¹	Sn1	85.594(11)
Pd4 ¹	Pd1	Pd2 ¹	Sn2	-174.895(11)	Pd4 ¹	Pd1	Pd2 ¹	Pd3 ¹	-89.0
Pd4 ¹	Pd1	Pd2 ¹	Pd4 ¹	0.0	Pd4 ¹	Pd1	Pd2 ¹	C1 ¹	133.19(4)
Pd4 ¹	Pd1	Pd2 ¹	C6 ¹	-91.001(15)	Pd4 ¹	Pd1	Pd2 ¹	C16 ¹	8.743(10)
Pd3	Pd1	Pd4	Sn2	-122.3	Pd3	Pd1	Pd4	Pd2	62.9
Pd3	Pd1	Pd4	C16	72.322(14)	Pd3	Pd1	Pd4	C21	-129.03(3)
Pd4	Pd1	Pd3	Sn1	123.4	Pd4	Pd1	Pd3	Pd2	-62.2
Pd4	Pd1	Pd3	C6	-64.59(2)	Pd4	Pd1	Pd3	C11	120.43(3)
Pd3	Pd1	Pd4 ¹	Sn2 ¹	-57.7	Pd3	Pd1	Pd4 ¹	Pd2 ¹	117.1
Pd3	Pd1	Pd4 ¹	C16 ¹	107.678(14)	Pd3	Pd1	Pd4 ¹	C21 ¹	-50.97(3)
Pd4 ¹	Pd1	Pd3	Sn1	-56.6	Pd4 ¹	Pd1	Pd3	Pd2	117.8
Pd4 ¹	Pd1	Pd3	C6	115.41(2)	Pd4 ¹	Pd1	Pd3	C11	-59.57(3)
Pd3 ¹	Pd1	Pd4	Sn2	57.7	Pd3 ¹	Pd1	Pd4	Pd2	-117.1
Pd3 ¹	Pd1	Pd4	C16	-107.678(14)	Pd3 ¹	Pd1	Pd4	C21	50.97(3)
Pd4	Pd1	Pd3 ¹	Sn1 ¹	56.6	Pd4	Pd1	Pd3 ¹	Pd2 ¹	-117.8
Pd4	Pd1	Pd3 ¹	C6 ¹	-115.41(2)	Pd4	Pd1	Pd3 ¹	C11 ¹	59.57(3)
Pd3 ¹	Pd1	Pd4 ¹	Sn2 ¹	122.3	Pd3 ¹	Pd1	Pd4 ¹	Pd2 ¹	-62.9
Pd3 ¹	Pd1	Pd4 ¹	C16 ¹	-72.322(14)	Pd3 ¹	Pd1	Pd4 ¹	C21 ¹	129.03(3)
Pd4 ¹	Pd1	Pd3 ¹	Sn1 ¹	-123.4	Pd4 ¹	Pd1	Pd3 ¹	Pd2 ¹	62.2
Pd4 ¹	Pd1	Pd3 ¹	C6 ¹	64.59(2)	Pd4 ¹	Pd1	Pd3 ¹	C11 ¹	-120.43(3)
Sn1 ¹	Pd2	Pd3	Sn1	10.34(3)	Sn1 ¹	Pd2	Pd3	Pd1	4.928(17)
Sn1 ¹	Pd2	Pd3	C6	-177.67(2)	Sn1 ¹	Pd2	Pd3	C11	-179.49(6)
Sn1 ¹	Pd2	Pd4	Sn2	55.686(18)	Sn1 ¹	Pd2	Pd4	Pd1	60.634(12)
Sn1 ¹	Pd2	Pd4	C16	-108.390(17)	Sn1 ¹	Pd2	Pd4	C21	-100.50(4)
Sn1 ¹	Pd2	C16	Pd4	63.46(5)	Sn1 ¹	Pd2	C16	N5	-108.12(18)
Sn2 ¹	Pd2	Pd3	Sn1	-55.244(18)	Sn2 ¹	Pd2	Pd3	Pd1	-60.7
Sn2 ¹	Pd2	Pd3	C6	116.741(15)	Sn2 ¹	Pd2	Pd3	C11	114.92(6)
Sn2 ¹	Pd2	Pd4	Sn2	-9.62(2)	Sn2 ¹	Pd2	Pd4	Pd1	-4.676(12)
Sn2 ¹	Pd2	Pd4	C16	-173.699(16)	Sn2 ¹	Pd2	Pd4	C21	-165.81(3)
Sn2 ¹	Pd2	C6	Pd3	-57.69(5)	Sn2 ¹	Pd2	C6	N2	123.0(2)
Pd1	Pd2	Pd3	Sn1	5.417(15)	Pd1	Pd2	Pd3	Pd1	0.0
Pd1	Pd2	Pd3	C6	177.402(18)	Pd1	Pd2	Pd3	C11	175.58(7)
Pd1	Pd2	Pd4	Sn2	-4.947(11)	Pd1	Pd2	Pd4	Pd1	-0.0
Pd1	Pd2	Pd4	C16	-169.023(12)	Pd1	Pd2	Pd4	C21	-161.13(4)
Pd1	Pd2	C6	Pd3	-2.36(7)	Pd1	Pd2	C6	N2	178.33(19)
Pd1	Pd2	C16	Pd4	10.10(6)	Pd1	Pd2	C16	N5	-161.49(16)
Pd3	Pd2	Pd4	Sn2	-68.809(16)	Pd3	Pd2	Pd4	Pd1	-63.861(11)
Pd3	Pd2	Pd4	C16	127.115(12)	Pd3	Pd2	Pd4	C21	135.01(3)
Pd4	Pd2	Pd3	Sn1	69.743(19)	Pd4	Pd2	Pd3	Pd1	64.3
Pd4	Pd2	Pd3	C6	-118.272(17)	Pd4	Pd2	Pd3	C11	-120.09(6)
C1	Pd2	Pd3	Sn1	-129.10(10)	C1	Pd2	Pd3	Pd1	-134.52(10)
C1	Pd2	Pd3	C6	42.88(10)	C1	Pd2	Pd3	C11	41.06(13)
Pd3	Pd2	C6	Pd3	-0.000(13)	Pd3	Pd2	C6	N2	-179.3(3)
C6	Pd2	Pd3	Sn1	-171.99(8)	C6	Pd2	Pd3	Pd1	-177.40(7)
C6	Pd2	Pd3	C6	-0.00(7)	C6	Pd2	Pd3	C11	-1.82(9)
Pd3	Pd2	C16	Pd4	-53.20(5)	Pd3	Pd2	C16	N5	135.22(17)

C16	Pd2	Pd3	Sn1	108.48(5)	C16	Pd2	Pd3	Pd1	103.07(5)
C16	Pd2	Pd3	C6	-79.53(5)	C16	Pd2	Pd3	C11	-81.35(8)
C1	Pd2	Pd4	Sn2	128.75(9)	C1	Pd2	Pd4	Pd1	133.70(9)
C1	Pd2	Pd4	C16	-35.32(9)	C1	Pd2	Pd4	C21	-27.43(10)
Pd4	Pd2	C6	Pd3	59.57(6)	Pd4	Pd2	C6	N2	-119.7(2)
C6	Pd2	Pd4	Sn2	-109.67(6)	C6	Pd2	Pd4	Pd1	-104.72(6)
C6	Pd2	Pd4	C16	86.26(5)	C6	Pd2	Pd4	C21	94.15(6)
Pd4	Pd2	C16	Pd4	0.0	Pd4	Pd2	C16	N5	-171.6(2)
C16	Pd2	Pd4	Sn2	164.08(7)	C16	Pd2	Pd4	Pd1	169.02(7)
C16	Pd2	Pd4	C16	0.00(7)	C16	Pd2	Pd4	C21	7.89(7)
C1	Pd2	C6	Pd3	-154.97(8)	C1	Pd2	C6	N2	25.7(2)
C1	Pd2	C16	Pd4	157.81(7)	C1	Pd2	C16	N5	-13.77(19)
C6	Pd2	C16	Pd4	-99.43(7)	C6	Pd2	C16	N5	88.99(19)
C16	Pd2	C6	Pd3	108.58(7)	C16	Pd2	C6	N2	-70.7(2)
Pd1	Pd3	C6	Pd2	2.57(7)	Pd1	Pd3	C6	N2	-178.3(2)
Pd2	Pd3	C6	Pd2	0.000(12)	Pd2	Pd3	C6	N2	179.2(3)
C11	Pd3	C6	Pd2	179.30(7)	C11	Pd3	C6	N2	-1.5(3)
Pd1	Pd4	C16	Pd2	-10.52(7)	Pd1	Pd4	C16	N5	158.2(2)
Pd2	Pd4	C16	Pd2	-0.0	Pd2	Pd4	C16	N5	168.7(3)
C21	Pd4	C16	Pd2	-176.72(7)	C21	Pd4	C16	N5	-8.0(3)
C6	N2	C7	C8	44.5(5)	C6	N2	C7	C9	-75.3(4)
C6	N2	C7	C10	164.8(3)	C7	N2	C6	Pd2	2.3(6)
C7	N2	C6	Pd3	-176.5(3)	C16	N5	C17	C18	52.7(4)
C16	N5	C17	C19	-64.1(4)	C16	N5	C17	C20	174.0(3)
C17	N5	C16	Pd2	178.1(2)	C17	N5	C16	Pd4	13.5(6)

Symmetry Operators:

(1) -X+1,-Y+1,-Z

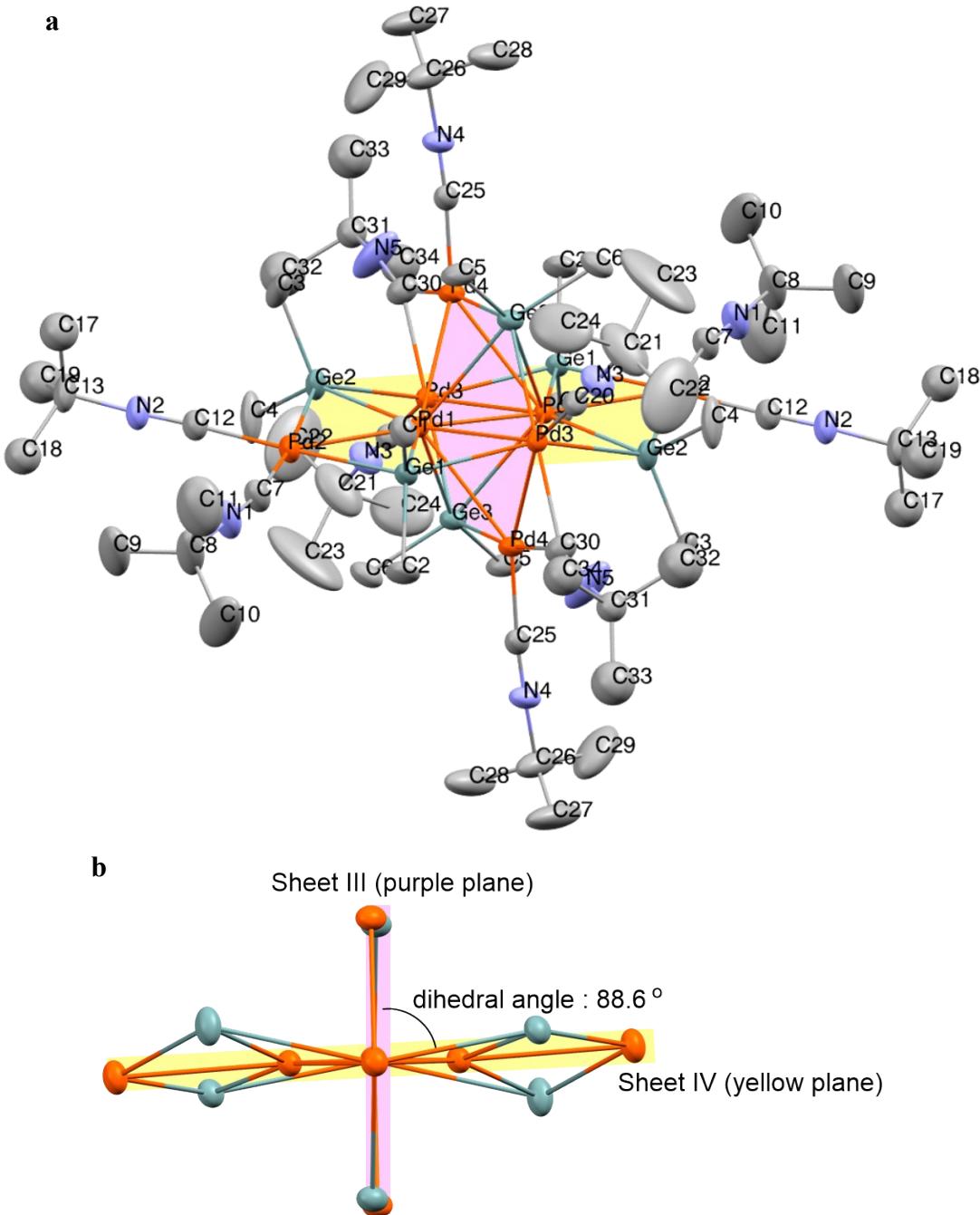


Figure S19. Molecular structure of **3** determined by a single crystal X-ray diffraction analysis. **a**, ORTEP drawing of **3** (50% probability of the thermal ellipsoids). Hydrogen atoms as well as a cyclopentylmethylether molecule included in a unit cell were omitted for clarity. Four ^tBu group was found to be disordered. The site occupancy factor for the carbons derived from the methyl groups on the disordered ^tBu group was defined as follows: 0.3 for C14, C15 and C16, 0.7 for C17, C18 and C19, 0.5 for C31, C32, C33, C34, C35, C36, C37 and C38 respectively. **b**, Dihedral angle between Sheet III and Sheet IV.

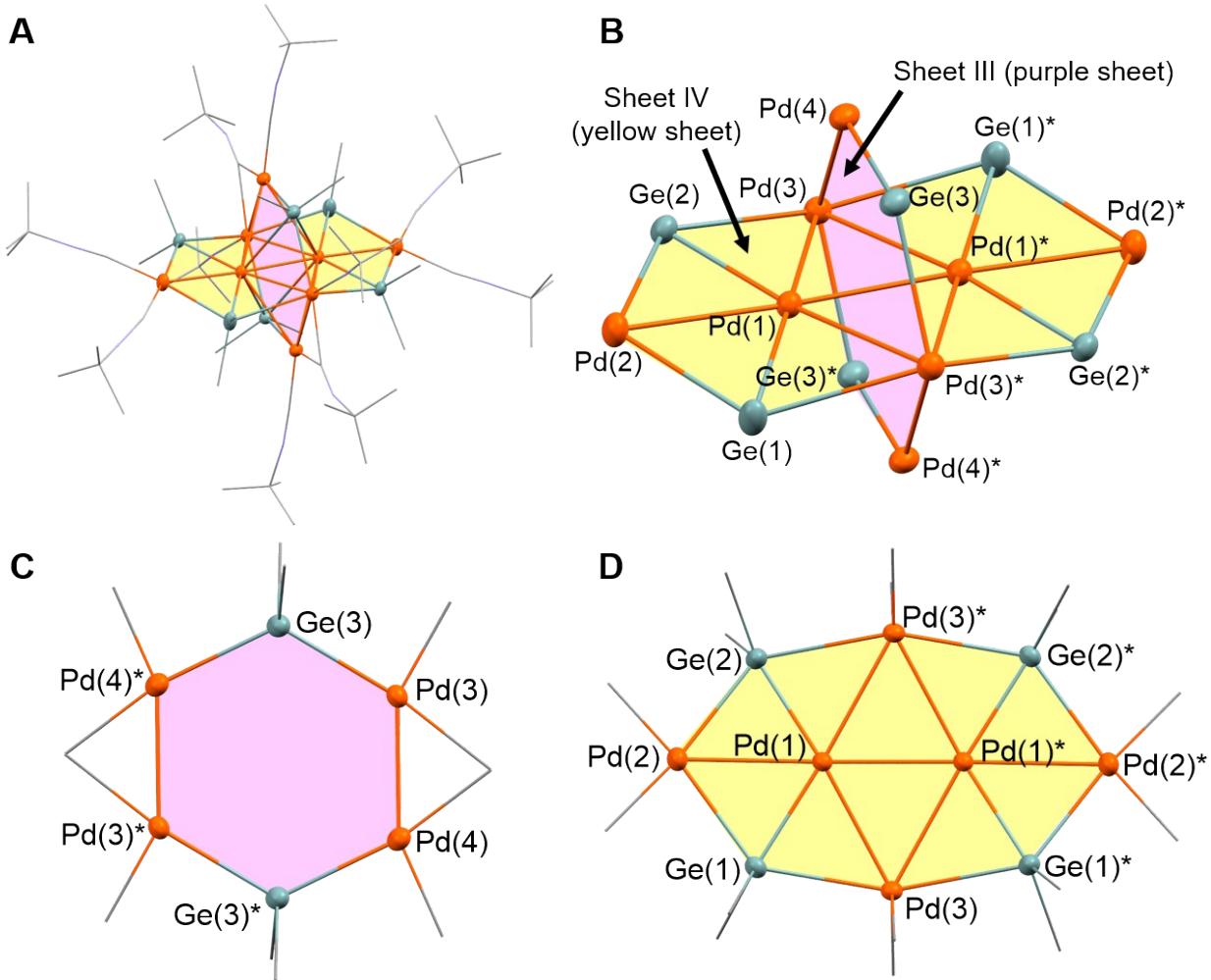


Figure S20. Molecular structure of **3** determined using single-crystal XRD analysis. **A)** ORTEP drawing of **3** with thermal ellipsoids at 50% probability. All carbon atoms and nitrogen atoms are shown in wireframe style; all hydrogen atoms are omitted for clarity. **B)** The core Pd_8Ge_6 structure of **3**. **C)** Front view of Sheet III. **D)** Side view of Sheet IV.

Table S6. Crystal data and structure refinement for **2**.

Empirical Formula	C ₇₄ H ₉₀ Ge ₆ N ₁₀ O ₂ Pd ₈
Formula Weight	2438.33
Crystal Color, Habit	black, plate
Crystal Dimensions	0.250 X 0.250 X 0.050 mm
Crystal System	triclinic
Lattice Type	Primitive
Lattice Parameters	a = 13.6964(4) Å b = 14.4844(4) Å c = 14.7143(5) Å α = 73.065(3) ° β = 62.695(3) ° γ = 82.678(2) ° V = 2481.29(15) Å ³
Space Group	P-1 (#2)
Z value	1
D _{calc}	1.632 g/cm ³
F ₀₀₀	1180.00
μ(MoKα)	32.377 cm ⁻¹
Diffractometer	Saturn724
Radiation	MoKα (λ = 0.71075 Å) graphite monochromated
Voltage, Current	50kV, 24mA
Temperature	-160.0°C
Detector Aperture	72.8 x 72.8 mm
Data Images	720 exposures
ω oscillation Range (χ =45.0, ϕ =0.0)	-70.0 - 110.0°
Exposure Rate	48.0 sec./°
Detector Swing Angle	20.00°
ω oscillation Range (χ =45.0, ϕ =90.0)	-70.0 - 110.0°
Exposure Rate	48.0 sec./°
Detector Swing Angle	20.00°
Detector Position	45.00 mm
Pixel Size	0.035 mm
2θ _{max}	62.4°
No. of Reflections Measured	Total: 23946 Unique: 13450 (R_{int} = 0.0250)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.749 - 0.851)

Structure Solution	Direct Methods (SHELXT Version 2014/5)
Refinement	Full-matrix least-squares on F ²
Function Minimized	$\Sigma w (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1 / [\sigma^2(Fo^2) + (0.0511 \cdot P)^2 + 3.2977 \cdot P]$ where $P = (\text{Max}(Fo^2, 0) + 2Fc^2)/3$
2θ _{max} cutoff	62.4°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	13450
No. Variables	409
Reflection/Parameter Ratio	32.89
Residuals: R1 (I>2.00σ(I))	0.0388
Residuals: R (All reflections)	0.0559
Residuals: wR2 (All reflections)	0.1020
Goodness of Fit Indicator	1.031
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	1.28 e ⁻ /Å ³
Minimum peak in Final Diff. Map	-0.92 e ⁻ /Å ³

<Atomic coordinates and B_{iso}/B_{eq}>

Pd1	0.53578(2)	0.90938(2)	0.49755(2)	1.328(6)	1
Pd2	0.61688(2)	0.72337(2)	0.49986(2)	1.891(6)	1
Pd3	0.37782(2)	0.94370(2)	0.69120(2)	1.458(6)	1
Pd4	0.30120(2)	0.94530(2)	0.55891(2)	1.746(6)	1
Ge1	0.69593(3)	0.87582(3)	0.34844(3)	1.615(7)	1
Ge2	0.43622(3)	0.77170(3)	0.63511(3)	2.075(8)	1
Ge3	0.42740(3)	1.00809(3)	0.37130(3)	1.755(7)	1
O1	1.1778(5)	0.4044(4)	0.2729(5)	7.22(13)	1
N1	0.8235(3)	0.6232(3)	0.3581(3)	3.40(8)	1
N2	0.5386(3)	0.5168(3)	0.6476(3)	2.67(7)	1
N3	0.3462(3)	0.8980(3)	0.9232(3)	3.03(8)	1
N4	0.1377(3)	0.8927(3)	0.4910(3)	2.49(7)	1
N5	0.1368(4)	0.8627(4)	0.7958(5)	5.66(14)	1
C1	0.7165(3)	0.8456(3)	0.2174(3)	2.40(7)	1
C2	0.8538(3)	0.8812(4)	0.3146(4)	2.97(9)	1
C3	0.3225(4)	0.7020(3)	0.6318(5)	3.89(12)	1
C4	0.4207(5)	0.7031(3)	0.7797(4)	4.23(12)	1
C5	0.4313(3)	0.9146(4)	0.2930(4)	2.73(8)	1
C6	0.3553(4)	1.1166(4)	0.3065(4)	2.79(8)	1
C7	0.7528(4)	0.6692(3)	0.4021(4)	2.71(8)	1
C8	0.9156(4)	0.5657(4)	0.3051(5)	4.31(13)	1
C9	0.9014(5)	0.4646(5)	0.3764(6)	5.90(17)	1
C10	1.0181(5)	0.6163(5)	0.2737(8)	7.9(3)	1

C11	0.9061(7)	0.5586(6)	0.2078(7)	7.4(2)	1
C12	0.5595(4)	0.5965(3)	0.6032(4)	2.45(7)	1
C13	0.5139(4)	0.4139(3)	0.6922(4)	3.10(9)	1
C14	0.543(2)	0.372(2)	0.777(2)	6.2(5)	0.300000
C15	0.3766(17)	0.4088(15)	0.7398(17)	4.5(4)	0.300000
C16	0.5543(14)	0.3679(13)	0.5972(14)	3.5(3)	0.300000
C17	0.4689(8)	0.3869(7)	0.6286(8)	4.73(18)	0.700000
C18	0.6256(7)	0.3602(6)	0.6790(7)	4.30(16)	0.700000
C19	0.4375(9)	0.3944(8)	0.8101(9)	5.8(2)	0.700000
C20	0.3581(3)	0.9151(3)	0.8378(3)	1.96(6)	1
C21	0.3386(7)	0.8786(6)	1.0280(5)	6.34(19)	1
C22	0.2486(11)	0.8155(9)	1.1021(6)	11.6(4)	1
C23	0.4528(10)	0.8388(10)	1.0174(8)	12.8(5)	1
C24	0.3291(8)	0.9775(8)	1.0511(7)	8.1(2)	1
C25	0.1978(3)	0.9161(3)	0.5144(3)	2.13(7)	1
C26	0.0767(5)	0.8593(5)	0.4472(4)	4.27(13)	1
C27	-0.0410(5)	0.8388(6)	0.5332(5)	6.8(2)	1
C28	0.0815(5)	0.9399(6)	0.3518(5)	5.82(19)	1
C29	0.1360(8)	0.7690(6)	0.4141(6)	7.1(2)	1
C30	0.2185(3)	0.8968(3)	0.7240(4)	2.54(8)	1
C31	0.0555(8)	0.8388(8)	0.8966(8)	2.93(16)	1/2
C32	0.1118(13)	0.7512(12)	0.9448(13)	6.5(3)	1/2
C33	-0.0564(13)	0.8267(12)	0.9080(14)	6.2(3)	1/2
C34	0.0488(11)	0.9221(10)	0.9479(11)	5.0(3)	1/2
C35	0.0398(8)	0.8055(7)	0.8678(8)	2.86(16)	1/2
C36	0.0519(9)	0.7004(8)	0.9126(9)	3.62(19)	1/2
C37	0.0007(11)	0.8139(10)	0.7794(11)	5.1(3)	1/2
C38	-0.0383(14)	0.8537(13)	0.9461(14)	6.5(4)	1/2
C39	1.2039(8)	0.3920(7)	0.3566(8)	8.1(2)	1
C40	1.2598(9)	0.3684(8)	0.1763(9)	8.8(2)	1
C41	1.3471(10)	0.4394(9)	0.1325(10)	10.8(3)	1
C42	1.3288(11)	0.5264(10)	0.0625(12)	12.0(4)	1
C43	1.2499(8)	0.5049(8)	0.0376(8)	8.3(2)	1
C44	1.2158(8)	0.4012(7)	0.0873(8)	8.0(2)	1

$$B_{eq} = \frac{8}{3} \pi^2 (U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$$

<Anisotropic displacement parameters>

atom	U11	U22	U33	U12	U13	U23
Pd1	0.01649(12)	0.01699(13)	0.01513(12)	0.00100(10)	-0.00589(9)	-0.00394(10)
Pd2	0.02470(14)	0.01883(14)	0.02366(14)	0.00451(11)	-0.00796(11)	-0.00561(11)
Pd3	0.01841(12)	0.01949(14)	0.01518(12)	-0.00045(10)	-0.00584(10)	-0.00380(10)
Pd4	0.01641(12)	0.02816(16)	0.02354(14)	0.00018(11)	-0.00838(11)	-0.01016(12)
Ge1	0.01621(17)	0.02188(19)	0.02027(18)	0.00245(14)	-0.00559(14)	-0.00659(15)
Ge2	0.0265(2)	0.01834(19)	0.0214(2)	0.00087(16)	-0.00244(16)	-0.00157(16)
Ge3	0.01796(17)	0.0296(2)	0.02061(19)	0.00054(15)	-0.00839(15)	-0.00920(16)

N1	0.037(2)	0.033(2)	0.041(2)	0.0129(17)	-0.0066(17)	-0.0072(18)
N2	0.043(2)	0.0219(17)	0.0317(19)	0.0026(15)	-0.0139(16)	-0.0060(15)
N3	0.044(2)	0.049(2)	0.0254(18)	0.0089(18)	-0.0193(17)	-0.0102(17)
N4	0.0237(16)	0.044(2)	0.0296(18)	-0.0032(15)	-0.0151(15)	-0.0060(16)
N5	0.046(3)	0.065(3)	0.071(4)	-0.028(2)	0.023(2)	-0.041(3)
C1	0.032(2)	0.031(2)	0.0225(19)	0.0074(17)	-0.0082(16)	-0.0096(17)
C2	0.0197(18)	0.047(3)	0.051(3)	0.0050(18)	-0.0161(19)	-0.020(2)
C3	0.032(2)	0.022(2)	0.075(4)	-0.0044(18)	-0.010(2)	-0.008(2)
C4	0.092(4)	0.022(2)	0.024(2)	0.008(2)	-0.013(3)	-0.0004(18)
C5	0.0244(19)	0.049(3)	0.037(2)	-0.0018(19)	-0.0119(18)	-0.024(2)
C6	0.031(2)	0.046(3)	0.036(2)	0.0113(19)	-0.0219(19)	-0.014(2)
C7	0.031(2)	0.030(2)	0.032(2)	0.0072(17)	-0.0091(18)	-0.0056(18)
C8	0.038(3)	0.034(3)	0.052(3)	0.013(2)	0.005(2)	-0.004(2)
C9	0.055(4)	0.043(3)	0.087(5)	0.019(3)	-0.010(3)	-0.006(3)
C10	0.042(3)	0.059(4)	0.157(9)	0.010(3)	-0.001(4)	-0.044(5)
C11	0.101(6)	0.087(6)	0.067(5)	0.026(5)	-0.010(4)	-0.040(5)
C12	0.035(2)	0.026(2)	0.031(2)	0.0039(17)	-0.0132(18)	-0.0096(17)
C13	0.058(3)	0.021(2)	0.035(2)	-0.002(2)	-0.018(2)	-0.0031(18)
C20	0.0267(18)	0.0254(19)	0.0230(18)	-0.0000(15)	-0.0108(15)	-0.0079(16)
C21	0.110(6)	0.104(6)	0.039(3)	0.047(5)	-0.046(4)	-0.033(4)
C22	0.233(13)	0.143(10)	0.030(4)	-0.065(9)	-0.032(6)	0.010(5)
C23	0.187(11)	0.253(15)	0.110(8)	0.128(11)	-0.127(9)	-0.088(9)
C24	0.113(7)	0.157(9)	0.073(5)	0.024(6)	-0.048(5)	-0.079(6)
C25	0.0228(18)	0.026(2)	0.0267(19)	-0.0011(15)	-0.0089(16)	-0.0029(16)
C26	0.053(3)	0.074(4)	0.037(3)	-0.034(3)	-0.026(2)	0.007(3)
C27	0.058(4)	0.137(7)	0.059(4)	-0.058(4)	-0.035(3)	0.019(4)
C28	0.047(3)	0.122(6)	0.045(3)	-0.034(4)	-0.030(3)	0.019(4)
C29	0.143(8)	0.075(5)	0.060(4)	-0.048(5)	-0.043(5)	-0.015(4)
C30	0.0261(19)	0.037(2)	0.031(2)	-0.0029(17)	-0.0053(17)	-0.0164(19)

The general temperature factor expression: $\exp(-2\pi^2(a^*2U_{11}h^2 + b^*2U_{22}k^2 + c^*2U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

<Bond lengths (Å)>

atom	atom	distance	atom	atom	distance
Pd1	Pd1 ¹	2.6920(4)	Pd1	Pd2	2.7771(4)
Pd1	Pd3	2.8182(4)	Pd1	Pd3 ¹	2.7975(4)
Pd1	Ge1	2.4074(4)	Pd1	Ge2	2.3964(4)
Pd1	Ge3	2.8531(6)	Pd1	Ge3 ¹	2.7925(7)
Pd2	Ge1	2.5578(4)	Pd2	Ge2	2.5348(4)
Pd2	C7	1.994(4)	Pd2	C12	1.988(4)
Pd3	Pd4	2.5947(5)	Pd3	Ge1 ¹	2.6783(5)
Pd3	Ge2	2.7590(6)	Pd3	Ge3 ¹	2.5100(5)
Pd3	C20	1.968(5)	Pd3	C30	2.162(5)
Pd4	Ge3	2.4486(4)	Pd4	C25	1.943(6)
Pd4	C30	2.088(4)	Ge1	C1	1.988(5)
Ge1	C2	1.990(5)	Ge2	C3	1.986(7)

Ge2	C4	1.992(6)	Ge3	C5	1.999(6)
Ge3	C6	1.988(5)	O1	C39	1.391(16)
O1	C40	1.540(13)	N1	C7	1.146(6)
N1	C8	1.450(6)	N2	C12	1.147(5)
N2	C13	1.457(6)	N3	C20	1.143(6)
N3	C21	1.441(9)	N4	C25	1.145(7)
N4	C26	1.458(10)	N5	C30	1.168(6)
N5	C31	1.359(10)	N5	C35	1.433(10)
C8	C9	1.508(8)	C8	C10	1.480(10)
C8	C11	1.528(14)	C13	C14	1.42(3)
C13	C15	1.68(2)	C13	C16	1.56(2)
C13	C17	1.486(15)	C13	C18	1.580(11)
C13	C19	1.520(11)	C14	C18	1.41(3)
C14	C19	1.32(3)	C15	C19	1.56(3)
C21	C22	1.421(14)	C21	C23	1.550(17)
C21	C24	1.543(15)	C26	C27	1.524(7)
C26	C28	1.523(9)	C26	C29	1.531(11)
C31	C32	1.56(2)	C31	C33	1.49(2)
C31	C34	1.57(2)	C32	C36	1.47(3)
C35	C36	1.494(15)	C35	C37	1.59(2)
C35	C38	1.45(2)	C40	C41	1.457(18)
C41	C42	1.454(19)	C42	C43	1.38(2)
C43	C44	1.496(14)			

Symmetry Operators:

(1) -X+1,-Y+2,-Z+1

<Bond angles (°)>

atom	atom	atom	angle	atom	atom	atom	angle
Pd1 ¹	Pd1	Pd2	176.251(18)	Pd1 ¹	Pd1	Pd3	60.969(10)
Pd1 ¹	Pd1	Pd3 ¹	61.743(10)	Pd1 ¹	Pd1	Ge1	121.835(14)
Pd1 ¹	Pd1	Ge2	121.901(14)	Pd1 ¹	Pd1	Ge3	60.392(14)
Pd1 ¹	Pd1	Ge3 ¹	62.663(13)	Pd2	Pd1	Pd3	117.761(11)
Pd2	Pd1	Pd3 ¹	119.406(12)	Pd2	Pd1	Ge1	58.604(12)
Pd2	Pd1	Ge2	58.120(12)	Pd2	Pd1	Ge3	123.296(18)
Pd2	Pd1	Ge3 ¹	113.646(16)	Pd3	Pd1	Pd3 ¹	122.713(13)
Pd3	Pd1	Ge1	168.25(2)	Pd3	Pd1	Ge2	63.281(13)
Pd3	Pd1	Ge3	97.419(13)	Pd3	Pd1	Ge3 ¹	53.148(11)
Pd3 ¹	Pd1	Ge1	61.398(12)	Pd3 ¹	Pd1	Ge2	164.04(2)
Pd3 ¹	Pd1	Ge3	52.734(11)	Pd3 ¹	Pd1	Ge3 ¹	99.339(14)
Ge1	Pd1	Ge2	116.107(18)	Ge1	Pd1	Ge3	93.418(16)
Ge1	Pd1	Ge3 ¹	116.590(19)	Ge2	Pd1	Ge3	113.740(18)
Ge2	Pd1	Ge3 ¹	95.630(18)	Ge3	Pd1	Ge3 ¹	123.055(16)
Pd1	Pd2	Ge1	53.457(11)	Pd1	Pd2	Ge2	53.396(11)
Pd1	Pd2	C7	133.31(12)	Pd1	Pd2	C12	131.97(12)
Ge1	Pd2	Ge2	106.338(16)	Ge1	Pd2	C7	80.17(12)
Ge1	Pd2	C12	172.65(16)	Ge2	Pd2	C7	173.20(12)

Ge2	Pd2	C12	78.63(12)	C7	Pd2	C12	94.71(17)
Pd1	Pd3	Pd1 ¹	57.287(9)	Pd1	Pd3	Pd4	65.435(11)
Pd1	Pd3	Ge1 ¹	108.395(13)	Pd1	Pd3	Ge2	50.881(10)
Pd1	Pd3	Ge3 ¹	62.901(14)	Pd1	Pd3	C20	137.65(12)
Pd1	Pd3	C30	108.99(14)	Pd1 ¹	Pd3	Pd4	65.696(11)
Pd1 ¹	Pd3	Ge1 ¹	52.107(10)	Pd1 ¹	Pd3	Ge2	106.445(13)
Pd1 ¹	Pd3	Ge3 ¹	64.771(13)	Pd1 ¹	Pd3	C20	138.78(13)
Pd1 ¹	Pd3	C30	111.03(12)	Pd4	Pd3	Ge1 ¹	76.690(16)
Pd4	Pd3	Ge2	72.648(15)	Pd4	Pd3	Ge3 ¹	121.680(15)
Pd4	Pd3	C20	149.93(13)	Pd4	Pd3	C30	51.10(13)
Ge1 ¹	Pd3	Ge2	148.33(2)	Ge1 ¹	Pd3	Ge3 ¹	95.468(16)
Ge1 ¹	Pd3	C20	104.48(12)	Ge1 ¹	Pd3	C30	86.52(12)
Ge2	Pd3	Ge3 ¹	93.897(16)	Ge2	Pd3	C20	105.98(12)
Ge2	Pd3	C30	80.47(13)	Ge3 ¹	Pd3	C20	88.32(13)
Ge3 ¹	Pd3	C30	171.87(14)	C20	Pd3	C30	98.83(18)
Pd3	Pd4	Ge3	115.302(17)	Pd3	Pd4	C25	156.31(10)
Pd3	Pd4	C30	53.67(16)	Ge3	Pd4	C25	88.10(10)
Ge3	Pd4	C30	168.97(16)	C25	Pd4	C30	102.89(19)
Pd1	Ge1	Pd2	67.939(12)	Pd1	Ge1	Pd3 ¹	66.495(13)
Pd1	Ge1	C1	132.78(13)	Pd1	Ge1	C2	129.22(18)
Pd2	Ge1	Pd3 ¹	133.616(15)	Pd2	Ge1	C1	106.58(12)
Pd2	Ge1	C2	106.13(14)	Pd3 ¹	Ge1	C1	97.88(12)
Pd3 ¹	Ge1	C2	108.82(15)	C1	Ge1	C2	97.8(2)
Pd1	Ge2	Pd2	68.484(12)	Pd1	Ge2	Pd3	65.839(14)
Pd1	Ge2	C3	123.49(18)	Pd1	Ge2	C4	136.4(2)
Pd2	Ge2	Pd3	129.561(18)	Pd2	Ge2	C3	104.58(16)
Pd2	Ge2	C4	108.57(17)	Pd3	Ge2	C3	117.74(14)
Pd3	Ge2	C4	90.76(15)	C3	Ge2	C4	99.8(3)
Pd1	Ge3	Pd1 ¹	56.945(13)	Pd1	Ge3	Pd3 ¹	62.495(14)
Pd1	Ge3	Pd4	66.635(13)	Pd1	Ge3	C5	104.04(15)
Pd1	Ge3	C6	157.82(19)	Pd1 ¹	Ge3	Pd3 ¹	63.952(15)
Pd1 ¹	Ge3	Pd4	67.605(15)	Pd1 ¹	Ge3	C5	160.90(15)
Pd1 ¹	Ge3	C6	100.93(19)	Pd3 ¹	Ge3	Pd4	122.87(2)
Pd3 ¹	Ge3	C5	107.43(12)	Pd3 ¹	Ge3	C6	108.46(14)
Pd4	Ge3	C5	108.48(11)	Pd4	Ge3	C6	108.75(11)
C5	Ge3	C6	98.0(2)	C39	O1	C40	118.3(8)
C7	N1	C8	177.3(7)	C12	N2	C13	173.1(6)
C20	N3	C21	176.2(6)	C25	N4	C26	170.9(4)
C30	N5	C31	159.1(10)	C30	N5	C35	165.9(9)
C31	N5	C35	34.5(8)	Pd2	C7	N1	168.2(4)
N1	C8	C9	108.6(4)	N1	C8	C10	108.1(6)
N1	C8	C11	106.4(6)	C9	C8	C10	115.9(6)
C9	C8	C11	106.5(6)	C10	C8	C11	111.1(6)
Pd2	C12	N2	167.7(4)	N2	C13	C14	112.7(14)
N2	C13	C15	103.5(8)	N2	C13	C16	107.3(7)
N2	C13	C17	106.2(5)	N2	C13	C18	107.2(5)

N2	C13	C19	109.3(6)	C14	C13	C15	109.1(13)
C14	C13	C16	120.5(14)	C14	C13	C17	141.1(14)
C14	C13	C18	55.6(11)	C14	C13	C19	53.3(11)
C15	C13	C16	101.9(13)	C15	C13	C17	61.8(10)
C15	C13	C18	149.1(8)	C15	C13	C19	58.0(10)
C16	C13	C17	41.2(9)	C16	C13	C18	71.7(9)
C16	C13	C19	141.5(8)	C17	C13	C18	111.0(6)
C17	C13	C19	115.0(7)	C18	C13	C19	107.8(7)
C13	C14	C18	67.8(15)	C13	C14	C19	67.1(16)
C18	C14	C19	133(3)	C13	C15	C17	53.2(8)
C13	C15	C19	55.8(10)	C17	C15	C19	105.0(14)
C13	C16	C17	65.6(12)	C13	C16	C18	54.6(9)
C17	C16	C18	117.8(17)	C13	C17	C15	65.0(11)
C13	C17	C16	73.2(15)	C15	C17	C16	135.7(19)
C13	C18	C14	56.6(14)	C13	C18	C16	53.7(7)
C14	C18	C16	105.1(16)	C13	C19	C14	59.6(14)
C13	C19	C15	66.2(9)	C14	C19	C15	123.0(19)
Pd3	C20	N3	179.6(4)	N3	C21	C22	110.0(9)
N3	C21	C23	105.0(6)	N3	C21	C24	106.4(6)
C22	C21	C23	115.1(9)	C22	C21	C24	113.7(7)
C23	C21	C24	105.9(10)	Pd4	C25	N4	175.6(4)
N4	C26	C27	107.7(6)	N4	C26	C28	107.2(6)
N4	C26	C29	106.1(6)	C27	C26	C28	111.3(6)
C27	C26	C29	112.8(6)	C28	C26	C29	111.4(6)
Pd3	C30	Pd4	75.23(12)	Pd3	C30	N5	140.1(6)
Pd4	C30	N5	144.6(6)	N5	C31	C32	98.7(8)
N5	C31	C33	116.0(12)	N5	C31	C34	107.3(8)
N5	C31	C35	77.6(10)	N5	C31	C36	97.3(7)
N5	C31	C38	140.5(14)	C32	C31	C33	119.5(11)
C32	C31	C34	107.2(13)	C32	C31	C35	91.3(14)
C32	C31	C36	47.7(10)	C32	C31	C38	119.4(12)
C33	C31	C34	107.3(11)	C33	C31	C35	54.2(12)
C33	C31	C36	78.5(9)	C33	C31	C38	37.0(15)
C34	C31	C35	159.4(15)	C34	C31	C36	148.0(9)
C34	C31	C38	72.6(14)	C35	C31	C36	45.5(10)
C35	C31	C38	90.8(17)	C36	C31	C38	100.9(11)
C31	C32	C35	27.7(7)	C31	C32	C36	80.3(13)
C35	C32	C36	53.6(9)	C31	C33	C35	33.8(10)
C31	C33	C37	90.3(10)	C31	C33	C38	52.2(15)
C35	C33	C37	62.0(11)	C35	C33	C38	86(2)
C37	C33	C38	138.1(17)	C31	C34	C38	42.7(8)
N5	C35	C31	67.9(9)	N5	C35	C32	86.4(8)
N5	C35	C33	132.1(11)	N5	C35	C36	118.7(8)
N5	C35	C37	93.9(8)	N5	C35	C38	111.9(11)
C31	C35	C32	61.0(12)	C31	C35	C33	91.9(15)
C31	C35	C36	111.2(14)	C31	C35	C37	142.0(13)

C31	C35	C38	54.3(12)	C32	C35	C33	122.2(13)
C32	C35	C36	52.2(9)	C32	C35	C37	154.4(11)
C32	C35	C38	93.8(12)	C33	C35	C36	109.0(10)
C33	C35	C37	75.7(13)	C33	C35	C38	38.1(15)
C36	C35	C37	106.8(11)	C36	C35	C38	113.6(9)
C37	C35	C38	109.6(12)	C31	C36	C32	52.0(9)
C31	C36	C35	23.4(7)	C32	C36	C35	74.2(10)
C33	C37	C35	42.3(8)	C31	C38	C33	90.7(19)
C31	C38	C34	64.7(13)	C31	C38	C35	34.9(10)
C33	C38	C34	147.9(17)	C33	C38	C35	56.3(15)
C34	C38	C35	98.9(12)	O1	C40	C41	99.0(10)
O1	C40	C44	108.0(8)	C41	C40	C44	100.2(9)
C40	C41	C42	111.7(13)	C41	C42	C43	107.5(12)
C42	C43	C44	111.0(11)	C40	C44	C43	103.2(10)

Symmetry Operators:

(1) -X+1,-Y+2,-Z+1

< Torsion Angles(^o) Those having bond angles > 160 or < 20 degrees are excluded. >

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Pd1 ¹	Pd1	Pd3	Pd1 ¹	-0.0	Pd1 ¹	Pd1	Pd3	Pd4	75.862(11)
Pd1 ¹	Pd1	Pd3	Ge1 ¹	10.620(12)	Pd1 ¹	Pd1	Pd3	Ge2	162.942(15)
Pd1 ¹	Pd1	Pd3	Ge3 ¹	-76.091(11)	Pd1 ¹	Pd1	Pd3	C20	-128.49(2)
Pd1 ¹	Pd1	Pd3	C30	103.304(15)	Pd3	Pd1	Pd1 ¹	Pd3 ¹	-180.000(14)
Pd3	Pd1	Pd1 ¹	Pd3	-0.0	Pd3	Pd1	Pd1 ¹	Ge1 ¹	-13.239(16)
Pd3	Pd1	Pd1 ¹	Ge2 ¹	162.02(2)	Pd3	Pd1	Pd1 ¹	Ge3 ¹	61.0
Pd3	Pd1	Pd1 ¹	Ge3	-119.029(11)	Pd1 ¹	Pd1	Pd3 ¹	Pd1 ¹	-0.0
Pd1 ¹	Pd1	Pd3 ¹	Pd4 ¹	75.399(11)	Pd1 ¹	Pd1	Pd3 ¹	Ge1	167.197(15)
Pd1 ¹	Pd1	Pd3 ¹	Ge2 ¹	13.726(12)	Pd1 ¹	Pd1	Pd3 ¹	Ge3	-72.791(10)
Pd1 ¹	Pd1	Pd3 ¹	C20 ¹	-126.85(2)	Pd1 ¹	Pd1	Pd3 ¹	C30 ¹	99.631(16)
Pd3 ¹	Pd1	Pd1 ¹	Pd3 ¹	-0.0	Pd3 ¹	Pd1	Pd1 ¹	Pd3	180.000(14)
Pd3 ¹	Pd1	Pd1 ¹	Ge1 ¹	166.76(2)	Pd3 ¹	Pd1	Pd1 ¹	Ge2 ¹	-17.976(16)
Pd3 ¹	Pd1	Pd1 ¹	Ge3 ¹	-119.029(11)	Pd3 ¹	Pd1	Pd1 ¹	Ge3	61.0
Pd1 ¹	Pd1	Ge1	Pd2	175.63(2)	Pd1 ¹	Pd1	Ge1	Pd3 ¹	-13.28(2)
Pd1 ¹	Pd1	Ge1	C1	-91.82(3)	Pd1 ¹	Pd1	Ge1	C2	82.41(3)
Ge1	Pd1	Pd1 ¹	Pd3 ¹	13.24(2)	Ge1	Pd1	Pd1 ¹	Pd3	-166.76(2)
Ge1	Pd1	Pd1 ¹	Ge1 ¹	180.00(2)	Ge1	Pd1	Pd1 ¹	Ge2 ¹	-4.74(3)
Ge1	Pd1	Pd1 ¹	Ge3 ¹	-105.79(2)	Ge1	Pd1	Pd1 ¹	Ge3	74.21(2)
Pd1 ¹	Pd1	Ge2	Pd2	-175.58(2)	Pd1 ¹	Pd1	Ge2	Pd3	-17.58(2)
Pd1 ¹	Pd1	Ge2	C3	90.77(3)	Pd1 ¹	Pd1	Ge2	C4	-80.85(3)
Ge2	Pd1	Pd1 ¹	Pd3 ¹	-162.02(2)	Ge2	Pd1	Pd1 ¹	Pd3	17.98(2)
Ge2	Pd1	Pd1 ¹	Ge1 ¹	4.74(3)	Ge2	Pd1	Pd1 ¹	Ge2 ¹	-180.00(2)
Ge2	Pd1	Pd1 ¹	Ge3 ¹	78.95(2)	Ge2	Pd1	Pd1 ¹	Ge3	-101.05(2)
Pd1 ¹	Pd1	Ge3	Pd1 ¹	-0.0	Pd1 ¹	Pd1	Ge3	Pd3 ¹	75.413(11)
Pd1 ¹	Pd1	Ge3	Pd4	-77.641(11)	Pd1 ¹	Pd1	Ge3	C5	178.001(16)
Pd1 ¹	Pd1	Ge3	C6	4.76(4)	Ge3	Pd1	Pd1 ¹	Pd3 ¹	-61.0
Ge3	Pd1	Pd1 ¹	Pd3	119.029(11)	Ge3	Pd1	Pd1 ¹	Ge1 ¹	105.790(18)

Ge3	Pd1	Pd1 ¹	Ge2 ¹	-78.947(17)	Ge3	Pd1	Pd1 ¹	Ge3 ¹	-180.000(11)
Ge3	Pd1	Pd1 ¹	Ge3	-0.0	Pd1 ¹	Pd1	Ge3 ¹	Pd1 ¹	0.0
Pd1 ¹	Pd1	Ge3 ¹	Pd3	72.8	Pd1 ¹	Pd1	Ge3 ¹	Pd4 ¹	-75.9
Pd1 ¹	Pd1	Ge3 ¹	C6 ¹	178.172(15)	Ge3 ¹	Pd1	Pd1 ¹	Pd3 ¹	119.029(11)
Ge3 ¹	Pd1	Pd1 ¹	Pd3	-61.0	Ge3 ¹	Pd1	Pd1 ¹	Ge1 ¹	-74.210(17)
Ge3 ¹	Pd1	Pd1 ¹	Ge2 ¹	101.053(18)	Ge3 ¹	Pd1	Pd1 ¹	Ge3 ¹	-0.0
Ge3 ¹	Pd1	Pd1 ¹	Ge3	180.000(10)	Pd2	Pd1	Pd3	Pd1 ¹	175.989(18)
Pd2	Pd1	Pd3	Pd4	-108.148(16)	Pd2	Pd1	Pd3	Ge1 ¹	-173.391(14)
Pd2	Pd1	Pd3	Ge2	-21.068(12)	Pd2	Pd1	Pd3	Ge3 ¹	99.898(16)
Pd2	Pd1	Pd3	C20	47.50(3)	Pd2	Pd1	Pd3	C30	-80.707(18)
Pd3	Pd1	Pd2	Ge1	-167.146(19)	Pd3	Pd1	Pd2	Ge2	22.218(13)
Pd3	Pd1	Pd2	C7	-159.26(2)	Pd3	Pd1	Pd2	C12	19.26(3)
Pd2	Pd1	Pd3 ¹	Pd1 ¹	-175.926(19)	Pd2	Pd1	Pd3 ¹	Pd4 ¹	-100.527(16)
Pd2	Pd1	Pd3 ¹	Ge1	-8.729(13)	Pd2	Pd1	Pd3 ¹	Ge2 ¹	-162.200(14)
Pd2	Pd1	Pd3 ¹	Ge3	111.283(17)	Pd2	Pd1	Pd3 ¹	C20 ¹	57.23(3)
Pd2	Pd1	Pd3 ¹	C30 ¹	-76.29(2)	Pd3 ¹	Pd1	Pd2	Ge1	8.980(14)
Pd3 ¹	Pd1	Pd2	Ge2	-161.655(19)	Pd3 ¹	Pd1	Pd2	C7	16.87(3)
Pd3 ¹	Pd1	Pd2	C12	-164.614(19)	Pd2	Pd1	Ge1	Pd2	0.0
Pd2	Pd1	Ge1	Pd3 ¹	171.090(18)	Pd2	Pd1	Ge1	C1	92.56(3)
Pd2	Pd1	Ge1	C2	-93.22(3)	Ge1	Pd1	Pd2	Ge1	0.000(15)
Ge1	Pd1	Pd2	Ge2	-170.64(2)	Ge1	Pd1	Pd2	C7	7.88(3)
Ge1	Pd1	Pd2	C12	-173.59(3)	Pd2	Pd1	Ge2	Pd2	-0.0
Pd2	Pd1	Ge2	Pd3	158.000(18)	Pd2	Pd1	Ge2	C3	-93.65(2)
Pd2	Pd1	Ge2	C4	94.73(3)	Ge2	Pd1	Pd2	Ge1	170.64(2)
Ge2	Pd1	Pd2	Ge2	-0.000(16)	Ge2	Pd1	Pd2	C7	178.52(3)
Ge2	Pd1	Pd2	C12	-2.96(2)	Pd2	Pd1	Ge3	Pd1 ¹	-179.206(12)
Pd2	Pd1	Ge3	Pd3 ¹	-103.793(13)	Pd2	Pd1	Ge3	Pd4	103.153(14)
Pd2	Pd1	Ge3	C5	-1.205(18)	Pd2	Pd1	Ge3	C6	-174.45(4)
Ge3	Pd1	Pd2	Ge1	71.502(13)	Ge3	Pd1	Pd2	Ge2	-99.133(14)
Ge3	Pd1	Pd2	C7	79.39(3)	Ge3	Pd1	Pd2	C12	-102.09(2)
Pd2	Pd1	Ge3 ¹	Pd1 ¹	179.275(11)	Pd2	Pd1	Ge3 ¹	Pd3	-107.896(11)
Pd2	Pd1	Ge3 ¹	Pd4 ¹	103.375(12)	Pd2	Pd1	Ge3 ¹	C6 ¹	-2.552(16)
Ge3 ¹	Pd1	Pd2	Ge1	-107.771(13)	Ge3 ¹	Pd1	Pd2	Ge2	81.593(12)
Ge3 ¹	Pd1	Pd2	C7	-99.89(2)	Ge3 ¹	Pd1	Pd2	C12	78.63(2)
Pd3	Pd1	Pd3 ¹	Pd1 ¹	0.000(15)	Pd3	Pd1	Pd3 ¹	Pd4 ¹	75.399(17)
Pd3	Pd1	Pd3 ¹	Ge1	167.20(2)	Pd3	Pd1	Pd3 ¹	Ge2 ¹	13.73(2)
Pd3	Pd1	Pd3 ¹	Ge3	-72.791(16)	Pd3	Pd1	Pd3 ¹	C20 ¹	-126.85(2)
Pd3	Pd1	Pd3 ¹	C30 ¹	99.631(17)	Pd3 ¹	Pd1	Pd3	Pd1 ¹	-0.000(15)
Pd3 ¹	Pd1	Pd3	Pd4	75.862(16)	Pd3 ¹	Pd1	Pd3	Ge1 ¹	10.62(2)
Pd3 ¹	Pd1	Pd3	Ge2	162.94(2)	Pd3 ¹	Pd1	Pd3	Ge3 ¹	-76.091(16)
Pd3 ¹	Pd1	Pd3	C20	-128.49(2)	Pd3 ¹	Pd1	Pd3	C30	103.304(18)
Pd3	Pd1	Ge2	Pd2	-158.000(17)	Pd3	Pd1	Ge2	Pd3	0.0
Pd3	Pd1	Ge2	C3	108.35(2)	Pd3	Pd1	Ge2	C4	-63.27(3)
Ge2	Pd1	Pd3	Pd1 ¹	-162.942(18)	Ge2	Pd1	Pd3	Pd4	-87.080(16)
Ge2	Pd1	Pd3	Ge1 ¹	-152.322(19)	Ge2	Pd1	Pd3	Ge2	-0.000(13)
Ge2	Pd1	Pd3	Ge3 ¹	120.967(17)	Ge2	Pd1	Pd3	C20	68.56(2)

Ge2	Pd1	Pd3	C30	-59.638(17)	Pd3	Pd1	Ge3	Pd1 ¹	50.4
Pd3	Pd1	Ge3	Pd3 ¹	125.854(13)	Pd3	Pd1	Ge3	Pd4	-27.200(12)
Pd3	Pd1	Ge3	C5	-131.558(14)	Pd3	Pd1	Ge3	C6	55.20(4)
Ge3	Pd1	Pd3	Pd1 ¹	-50.051(11)	Ge3	Pd1	Pd3	Pd4	25.811(11)
Ge3	Pd1	Pd3	Ge1 ¹	-39.431(17)	Ge3	Pd1	Pd3	Ge2	112.891(15)
Ge3	Pd1	Pd3	Ge3 ¹	-126.142(13)	Ge3	Pd1	Pd3	C20	-178.54(2)
Ge3	Pd1	Pd3	C30	53.253(16)	Pd3	Pd1	Ge3 ¹	Pd1 ¹	-72.829(10)
Pd3	Pd1	Ge3 ¹	Pd3	0.0	Pd3	Pd1	Ge3 ¹	Pd4 ¹	-148.729(15)
Pd3	Pd1	Ge3 ¹	C6 ¹	105.344(15)	Ge3 ¹	Pd1	Pd3	Pd1 ¹	76.091(12)
Ge3 ¹	Pd1	Pd3	Pd4	151.953(14)	Ge3 ¹	Pd1	Pd3	Ge1 ¹	86.711(15)
Ge3 ¹	Pd1	Pd3	Ge2	-120.967(14)	Ge3 ¹	Pd1	Pd3	Ge3 ¹	0.000(10)
Ge3 ¹	Pd1	Pd3	C20	-52.40(2)	Ge3 ¹	Pd1	Pd3	C30	179.395(17)
Pd3 ¹	Pd1	Ge1	Pd2	-171.090(18)	Pd3 ¹	Pd1	Ge1	Pd3 ¹	0.0
Pd3 ¹	Pd1	Ge1	C1	-78.53(3)	Pd3 ¹	Pd1	Ge1	C2	95.69(3)
Ge1	Pd1	Pd3 ¹	Pd1 ¹	-167.197(19)	Ge1	Pd1	Pd3 ¹	Pd4 ¹	-91.798(17)
Ge1	Pd1	Pd3 ¹	Ge1	0.000(14)	Ge1	Pd1	Pd3 ¹	Ge2 ¹	-153.47(2)
Ge1	Pd1	Pd3 ¹	Ge3	120.012(19)	Ge1	Pd1	Pd3 ¹	C20 ¹	65.96(2)
Ge1	Pd1	Pd3 ¹	C30 ¹	-67.566(19)	Pd3 ¹	Pd1	Ge3	Pd1 ¹	-75.413(12)
Pd3 ¹	Pd1	Ge3	Pd3 ¹	-0.0	Pd3 ¹	Pd1	Ge3	Pd4	-153.055(18)
Pd3 ¹	Pd1	Ge3	C5	102.588(16)	Pd3 ¹	Pd1	Ge3	C6	-70.66(4)
Ge3	Pd1	Pd3 ¹	Pd1 ¹	72.791(13)	Ge3	Pd1	Pd3 ¹	Pd4 ¹	148.190(15)
Ge3	Pd1	Pd3 ¹	Ge1	-120.012(17)	Ge3	Pd1	Pd3 ¹	Ge2 ¹	86.517(15)
Ge3	Pd1	Pd3 ¹	Ge3	0.000(12)	Ge3	Pd1	Pd3 ¹	C20 ¹	-54.06(2)
Ge3	Pd1	Pd3 ¹	C30 ¹	172.42(2)	Pd3 ¹	Pd1	Ge3 ¹	Pd1 ¹	51.3
Pd3 ¹	Pd1	Ge3 ¹	Pd3	124.138(11)	Pd3 ¹	Pd1	Ge3 ¹	Pd4 ¹	-24.592(11)
Pd3 ¹	Pd1	Ge3 ¹	C6 ¹	-130.519(13)	Ge3 ¹	Pd1	Pd3 ¹	Pd1 ¹	-51.920(11)
Ge3 ¹	Pd1	Pd3 ¹	Pd4 ¹	23.479(10)	Ge3 ¹	Pd1	Pd3 ¹	Ge1	115.276(13)
Ge3 ¹	Pd1	Pd3 ¹	Ge2 ¹	-38.194(15)	Ge3 ¹	Pd1	Pd3 ¹	Ge3	-124.711(12)
Ge3 ¹	Pd1	Pd3 ¹	C20 ¹	-178.768(18)	Ge3 ¹	Pd1	Pd3 ¹	C30 ¹	47.711(16)
Ge1	Pd1	Ge2	Pd2	8.90(2)	Ge1	Pd1	Ge2	Pd3	166.90(2)
Ge1	Pd1	Ge2	C3	-84.75(3)	Ge1	Pd1	Ge2	C4	103.63(3)
Ge2	Pd1	Ge1	Pd2	-8.85(2)	Ge2	Pd1	Ge1	Pd3 ¹	162.24(2)
Ge2	Pd1	Ge1	C1	83.70(3)	Ge2	Pd1	Ge1	C2	-102.07(3)
Ge1	Pd1	Ge3	Pd1 ¹	-125.019(15)	Ge1	Pd1	Ge3	Pd3 ¹	-49.606(15)
Ge1	Pd1	Ge3	Pd4	157.340(17)	Ge1	Pd1	Ge3	C5	52.982(18)
Ge1	Pd1	Ge3	C6	-120.26(4)	Ge3	Pd1	Ge1	Pd2	-127.432(15)
Ge3	Pd1	Ge1	Pd3 ¹	43.658(13)	Ge3	Pd1	Ge1	C1	-34.88(3)
Ge3	Pd1	Ge1	C2	139.35(2)	Ge1	Pd1	Ge3 ¹	Pd1 ¹	113.908(16)
Ge1	Pd1	Ge3 ¹	Pd3	-173.263(16)	Ge1	Pd1	Ge3 ¹	Pd4 ¹	38.007(17)
Ge1	Pd1	Ge3 ¹	C6 ¹	-67.920(19)	Ge3 ¹	Pd1	Ge1	Pd2	102.707(16)
Ge3 ¹	Pd1	Ge1	Pd3 ¹	-86.203(16)	Ge3 ¹	Pd1	Ge1	C1	-164.74(2)
Ge3 ¹	Pd1	Ge1	C2	9.49(3)	Ge2	Pd1	Ge3	Pd1 ¹	114.461(17)
Ge2	Pd1	Ge3	Pd3 ¹	-170.126(18)	Ge2	Pd1	Ge3	Pd4	36.820(18)
Ge2	Pd1	Ge3	C5	-67.54(2)	Ge2	Pd1	Ge3	C6	119.22(4)
Ge3	Pd1	Ge2	Pd2	115.639(17)	Ge3	Pd1	Ge2	Pd3	-86.362(16)
Ge3	Pd1	Ge2	C3	21.99(3)	Ge3	Pd1	Ge2	C4	-149.63(2)

Ge2	Pd1	Ge3 ¹	Pd1 ¹	-123.148(13)	Ge2	Pd1	Ge3 ¹	Pd3	-50.320(13)
Ge2	Pd1	Ge3 ¹	Pd4 ¹	160.951(14)	Ge2	Pd1	Ge3 ¹	C6 ¹	55.024(16)
Ge3 ¹	Pd1	Ge2	Pd2	-114.413(14)	Ge3 ¹	Pd1	Ge2	Pd3	43.587(11)
Ge3 ¹	Pd1	Ge2	C3	151.94(2)	Ge3 ¹	Pd1	Ge2	C4	-19.68(3)
Ge3	Pd1	Ge3 ¹	Pd1 ¹	0.000(12)	Ge3	Pd1	Ge3 ¹	Pd3	72.829(14)
Ge3	Pd1	Ge3 ¹	Pd4 ¹	-75.900(14)	Ge3	Pd1	Ge3 ¹	C6 ¹	178.172(12)
Ge3 ¹	Pd1	Ge3	Pd1 ¹	-0.000(12)	Ge3 ¹	Pd1	Ge3	Pd3 ¹	75.413(14)
Ge3 ¹	Pd1	Ge3	Pd4	-77.641(15)	Ge3 ¹	Pd1	Ge3	C5	178.001(12)
Ge3 ¹	Pd1	Ge3	C6	4.76(5)	Pd1	Pd2	Ge1	Pd1	-0.0
Pd1	Pd2	Ge1	Pd3 ¹	-11.31(2)	Pd1	Pd2	Ge1	C1	-130.09(2)
Pd1	Pd2	Ge1	C2	126.37(3)	Pd1	Pd2	Ge2	Pd1	-0.0
Pd1	Pd2	Ge2	Pd3	-26.317(19)	Pd1	Pd2	Ge2	C3	120.69(2)
Pd1	Pd2	Ge2	C4	-133.52(3)	Ge1	Pd2	Ge2	Pd1	-7.830(19)
Ge1	Pd2	Ge2	Pd3	-34.15(3)	Ge1	Pd2	Ge2	C3	112.86(2)
Ge1	Pd2	Ge2	C4	-141.35(2)	Ge2	Pd2	Ge1	Pd1	7.823(19)
Ge2	Pd2	Ge1	Pd3 ¹	-3.49(4)	Ge2	Pd2	Ge1	C1	-122.26(2)
Ge2	Pd2	Ge1	C2	134.19(2)	C7	Pd2	Ge1	Pd1	-174.19(18)
C7	Pd2	Ge1	Pd3 ¹	174.50(19)	C7	Pd2	Ge1	C1	55.73(18)
C7	Pd2	Ge1	C2	-47.82(18)	C12	Pd2	Ge2	Pd1	177.76(19)
C12	Pd2	Ge2	Pd3	151.44(19)	C12	Pd2	Ge2	C3	-61.56(19)
C12	Pd2	Ge2	C4	44.24(19)	Pd1	Pd3	Pd4	Ge3	-33.811(12)
Pd1	Pd3	Pd4	C25	136.55(4)	Pd1	Pd3	Pd4	C30	145.947(12)
Pd1	Pd3	Ge1 ¹	Pd1 ¹	-11.332(16)	Pd1	Pd3	Ge1 ¹	Pd2 ¹	-22.77(4)
Pd1	Pd3	Ge1 ¹	C1 ¹	-144.764(15)	Pd1	Pd3	Ge1 ¹	C2 ¹	114.128(18)
Pd1	Pd3	Ge2	Pd1	-0.0	Pd1	Pd3	Ge2	Pd2	26.875(19)
Pd1	Pd3	Ge2	C3	-116.58(2)	Pd1	Pd3	Ge2	C4	141.97(2)
Pd1	Pd3	Ge3 ¹	Pd1 ¹	64.5	Pd1	Pd3	Ge3 ¹	Pd1	0.0
Pd1	Pd3	Ge3 ¹	Pd4 ¹	34.847(18)	Pd1	Pd3	Ge3 ¹	C5 ¹	161.61(2)
Pd1	Pd3	Ge3 ¹	C6 ¹	-93.40(2)	Pd1	Pd3	C30	Pd4	-32.59(14)
Pd1	Pd3	C30	N5	146.2(5)	Pd1 ¹	Pd3	Pd4	Ge3	29.729(12)
Pd1 ¹	Pd3	Pd4	C25	-159.91(4)	Pd1 ¹	Pd3	Pd4	C30	-150.512(12)
Pd1 ¹	Pd3	Ge1 ¹	Pd1 ¹	0.0	Pd1 ¹	Pd3	Ge1 ¹	Pd2 ¹	-11.44(2)
Pd1 ¹	Pd3	Ge1 ¹	C1 ¹	-133.43(2)	Pd1 ¹	Pd3	Ge1 ¹	C2 ¹	125.46(3)
Pd1 ¹	Pd3	Ge2	Pd1	14.912(14)	Pd1 ¹	Pd3	Ge2	Pd2	41.79(3)
Pd1 ¹	Pd3	Ge2	C3	-101.666(19)	Pd1 ¹	Pd3	Ge2	C4	156.879(14)
Pd1 ¹	Pd3	Ge3 ¹	Pd1 ¹	-0.0	Pd1 ¹	Pd3	Ge3 ¹	Pd1	-64.5
Pd1 ¹	Pd3	Ge3 ¹	Pd4 ¹	-29.687(18)	Pd1 ¹	Pd3	Ge3 ¹	C5 ¹	97.076(18)
Pd1 ¹	Pd3	Ge3 ¹	C6 ¹	-157.94(2)	Pd1 ¹	Pd3	C30	Pd4	28.73(15)
Pd1 ¹	Pd3	C30	N5	-152.5(5)	Pd4	Pd3	Ge1 ¹	Pd1 ¹	-69.402(11)
Pd4	Pd3	Ge1 ¹	Pd2 ¹	-80.84(3)	Pd4	Pd3	Ge1 ¹	C1 ¹	157.166(15)
Pd4	Pd3	Ge1 ¹	C2 ¹	56.059(18)	Ge1 ¹	Pd3	Pd4	Ge3	83.879(14)
Ge1 ¹	Pd3	Pd4	C25	-105.76(4)	Ge1 ¹	Pd3	Pd4	C30	-96.362(11)
Pd4	Pd3	Ge2	Pd1	72.104(10)	Pd4	Pd3	Ge2	Pd2	98.98(2)
Pd4	Pd3	Ge2	C3	-44.474(17)	Pd4	Pd3	Ge2	C4	-145.929(15)
Ge2	Pd3	Pd4	Ge3	-88.081(13)	Ge2	Pd3	Pd4	C25	82.28(4)
Ge2	Pd3	Pd4	C30	91.678(11)	Pd4	Pd3	Ge3 ¹	Pd1 ¹	34.368(15)

Pd4	Pd3	Ge3 ¹	Pd1	-30.166(15)	Pd4	Pd3	Ge3 ¹	Pd4 ¹	4.68(3)
Pd4	Pd3	Ge3 ¹	C5 ¹	131.444(18)	Pd4	Pd3	Ge3 ¹	C6 ¹	-123.57(2)
Ge3 ¹	Pd3	Pd4	Ge3	-4.35(2)	Ge3 ¹	Pd3	Pd4	C25	166.01(3)
Ge3 ¹	Pd3	Pd4	C30	175.41(2)	C20	Pd3	Pd4	Ge3	179.9(2)
C20	Pd3	Pd4	C25	-9.8(2)	C20	Pd3	Pd4	C30	-0.4(2)
Pd4	Pd3	C30	Pd4	0.0	Pd4	Pd3	C30	N5	178.8(6)
C30	Pd3	Pd4	Ge3	-179.76(16)	C30	Pd3	Pd4	C25	-9.40(17)
C30	Pd3	Pd4	C30	0.00(16)	Ge1 ¹	Pd3	Ge2	Pd1	57.08(3)
Ge1 ¹	Pd3	Ge2	Pd2	83.95(4)	Ge1 ¹	Pd3	Ge2	C3	-59.50(3)
Ge1 ¹	Pd3	Ge2	C4	-160.95(2)	Ge2	Pd3	Ge1 ¹	Pd1 ¹	-54.67(3)
Ge2	Pd3	Ge1 ¹	Pd2 ¹	-66.11(5)	Ge2	Pd3	Ge1 ¹	C1 ¹	171.90(2)
Ge2	Pd3	Ge1 ¹	C2 ¹	70.79(3)	Ge1 ¹	Pd3	Ge3 ¹	Pd1 ¹	-43.352(13)
Ge1 ¹	Pd3	Ge3 ¹	Pd1	-107.886(14)	Ge1 ¹	Pd3	Ge3 ¹	Pd4 ¹	-73.04(2)
Ge1 ¹	Pd3	Ge3 ¹	C5 ¹	53.72(2)	Ge1 ¹	Pd3	Ge3 ¹	C6 ¹	158.71(2)
Ge3 ¹	Pd3	Ge1 ¹	Pd1 ¹	51.897(16)	Ge3 ¹	Pd3	Ge1 ¹	Pd2 ¹	40.46(3)
Ge3 ¹	Pd3	Ge1 ¹	C1 ¹	-81.535(18)	Ge3 ¹	Pd3	Ge1 ¹	C2 ¹	177.36(2)
C20	Pd3	Ge1 ¹	Pd1 ¹	141.57(13)	C20	Pd3	Ge1 ¹	Pd2 ¹	130.14(13)
C20	Pd3	Ge1 ¹	C1 ¹	8.14(13)	C20	Pd3	Ge1 ¹	C2 ¹	-92.97(13)
Ge1 ¹	Pd3	C30	Pd4	75.68(10)	Ge1 ¹	Pd3	C30	N5	-105.5(5)
C30	Pd3	Ge1 ¹	Pd1 ¹	-120.19(13)	C30	Pd3	Ge1 ¹	Pd2 ¹	-131.63(14)
C30	Pd3	Ge1 ¹	C1 ¹	106.37(13)	C30	Pd3	Ge1 ¹	C2 ¹	5.27(14)
Ge2	Pd3	Ge3 ¹	Pd1 ¹	106.354(13)	Ge2	Pd3	Ge3 ¹	Pd1	41.820(12)
Ge2	Pd3	Ge3 ¹	Pd4 ¹	76.67(2)	Ge2	Pd3	Ge3 ¹	C5 ¹	-156.570(17)
Ge2	Pd3	Ge3 ¹	C6 ¹	-51.58(2)	Ge3 ¹	Pd3	Ge2	Pd1	-49.916(14)
Ge3 ¹	Pd3	Ge2	Pd2	-23.04(3)	Ge3 ¹	Pd3	Ge2	C3	-166.494(19)
Ge3 ¹	Pd3	Ge2	C4	92.051(17)	C20	Pd3	Ge2	Pd1	-139.28(13)
C20	Pd3	Ge2	Pd2	-112.41(13)	C20	Pd3	Ge2	C3	104.14(13)
C20	Pd3	Ge2	C4	2.68(13)	Ge2	Pd3	C30	Pd4	-75.34(10)
Ge2	Pd3	C30	N5	103.5(5)	C30	Pd3	Ge2	Pd1	124.18(13)
C30	Pd3	Ge2	Pd2	151.05(13)	C30	Pd3	Ge2	C3	7.60(13)
C30	Pd3	Ge2	C4	-93.86(13)	C20	Pd3	Ge3 ¹	Pd1 ¹	-147.74(12)
C20	Pd3	Ge3 ¹	Pd1	147.72(12)	C20	Pd3	Ge3 ¹	Pd4 ¹	-177.43(12)
C20	Pd3	Ge3 ¹	C5 ¹	-50.67(12)	C20	Pd3	Ge3 ¹	C6 ¹	54.32(12)
C20	Pd3	C30	Pd4	179.81(15)	C20	Pd3	C30	N5	-1.4(6)
Pd3	Pd4	Ge3	Pd1	32.994(14)	Pd3	Pd4	Ge3	Pd1 ¹	-29.321(14)
Pd3	Pd4	Ge3	Pd3 ¹	4.41(3)	Pd3	Pd4	C5	130.708(19)	
Pd3	Pd4	Ge3	C6	-123.72(2)	Pd3	Pd4	C30	Pd3	0.0
Pd3	Pd4	C30	N5	-178.7(7)	C25	Pd4	Ge3	Pd1	-143.15(12)
C25	Pd4	Ge3	Pd1 ¹	154.54(12)	C25	Pd4	Ge3	Pd3 ¹	-171.73(12)
C25	Pd4	Ge3	C5	-45.43(12)	C25	Pd4	Ge3	C6	60.14(13)
C25	Pd4	C30	Pd3	176.14(14)	C25	Pd4	C30	N5	-2.5(6)
C39	O1	C40	C41	-70.4(9)	C39	O1	C40	C44	-174.3(7)
C30	N5	C31	C32	-82(2)	C30	N5	C31	C33	149.5(16)
C30	N5	C31	C34	30(2)	C30	N5	C31	C35	-171.1(16)
C30	N5	C31	C36	-129.8(17)	C30	N5	C31	C38	113(2)
C31	N5	C30	Pd3	26(2)	C31	N5	C30	Pd4	-156.4(16)

C31	N5	C35	C31	0.0(8)	C31	N5	C35	C32	-60.0(10)
C31	N5	C35	C33	71.5(15)	C31	N5	C35	C36	-102.8(15)
C31	N5	C35	C37	145.6(12)	C31	N5	C35	C38	32.7(9)
C35	N5	C31	C32	89.5(11)	C35	N5	C31	C33	-39.5(10)
C35	N5	C31	C34	-159.3(15)	C35	N5	C31	C35	-0.0(7)
C35	N5	C31	C36	41.3(9)	C35	N5	C31	C38	-76(2)
N2	C13	C14	C18	-95.9(10)	N2	C13	C14	C19	97.7(10)
N2	C13	C15	C17	101.3(6)	N2	C13	C15	C19	-104.5(6)
N2	C13	C16	C17	-95.0(8)	N2	C13	C16	C18	103.0(5)
N2	C13	C17	C15	-96.9(4)	N2	C13	C17	C16	97.9(5)
N2	C13	C18	C14	106.1(5)	N2	C13	C18	C16	-103.0(4)
N2	C13	C19	C14	-104.4(6)	N2	C13	C19	C15	94.2(5)
C14	C13	C15	C17	-138.5(14)	C14	C13	C15	C19	15.8(15)
C15	C13	C14	C18	149.7(11)	C15	C13	C14	C19	-16.7(16)
C14	C13	C16	C17	134.3(14)	C14	C13	C16	C18	-27.8(14)
C16	C13	C14	C18	32.4(16)	C16	C13	C14	C19	-133.9(10)
C14	C13	C17	C15	85.9(17)	C14	C13	C17	C16	-79.2(17)
C17	C13	C14	C18	81.1(16)	C17	C13	C14	C19	-85.3(18)
C14	C13	C18	C14	-0.0(15)	C14	C13	C18	C16	150.9(16)
C18	C13	C14	C18	-0.0(4)	C18	C13	C14	C19	-166.3(19)
C14	C13	C19	C14	0.0(16)	C14	C13	C19	C15	-161.3(17)
C19	C13	C14	C18	166.3(19)	C19	C13	C14	C19	-0.0(6)
C15	C13	C16	C17	13.4(11)	C15	C13	C16	C18	-148.6(8)
C16	C13	C15	C17	-9.9(8)	C16	C13	C15	C19	144.3(8)
C15	C13	C17	C15	0.0(8)	C15	C13	C17	C16	-165.1(10)
C17	C13	C15	C17	-0.0(4)	C17	C13	C15	C19	154.2(9)
C15	C13	C18	C14	-68(2)	C15	C13	C18	C16	83(2)
C18	C13	C15	C17	-84(2)	C18	C13	C15	C19	70(2)
C15	C13	C19	C14	161.3(11)	C15	C13	C19	C15	-0.0(9)
C19	C13	C15	C17	-154.2(10)	C19	C13	C15	C19	-0.0(5)
C16	C13	C17	C15	165.1(11)	C16	C13	C17	C16	0.0(9)
C17	C13	C16	C17	0.0(5)	C17	C13	C16	C18	-162.0(10)
C16	C13	C18	C14	-150.9(7)	C16	C13	C18	C16	0.0(6)
C18	C13	C16	C17	162.0(9)	C18	C13	C16	C18	0.0(3)
C16	C13	C19	C14	94.6(16)	C16	C13	C19	C15	-66.7(16)
C19	C13	C16	C17	66.1(17)	C19	C13	C16	C18	-95.9(14)
C17	C13	C18	C14	-138.3(5)	C17	C13	C18	C16	12.6(4)
C18	C13	C17	C15	146.8(4)	C18	C13	C17	C16	-18.3(6)
C17	C13	C19	C14	136.3(6)	C17	C13	C19	C15	-25.0(6)
C19	C13	C17	C15	24.0(6)	C19	C13	C17	C16	-141.1(6)
C18	C13	C19	C14	11.8(7)	C18	C13	C19	C15	-149.5(6)
C19	C13	C18	C14	-11.5(7)	C19	C13	C18	C16	139.5(7)
C13	C14	C18	C13	0.0(2)	C13	C14	C18	C16	-23.9(11)
C13	C14	C19	C13	-0.0(2)	C13	C14	C19	C15	20.4(17)
C18	C14	C19	C13	-17(2)	C18	C14	C19	C15	3(4)
C19	C14	C18	C13	17(2)	C19	C14	C18	C16	-7(3)

C13	C15	C17	C13	-0.00(18)	C13	C15	C17	C16	20.6(14)
C13	C15	C19	C13	-0.00(19)	C13	C15	C19	C14	-19.2(10)
C17	C15	C19	C13	21.1(8)	C17	C15	C19	C14	1.9(18)
C19	C15	C17	C13	-21.9(9)	C19	C15	C17	C16	-1(2)
C13	C16	C17	C13	-0.00(16)	C13	C16	C17	C15	-19.5(15)
C13	C16	C18	C13	0.00(19)	C13	C16	C18	C14	24.8(6)
C17	C16	C18	C13	-18.5(12)	C17	C16	C18	C14	6.3(17)
C18	C16	C17	C13	16.5(10)	C18	C16	C17	C15	-3(2)
N5	C31	C32	C35	-77.7(9)	N5	C31	C32	C36	-92.1(9)
N5	C31	C33	C35	49.9(10)	N5	C31	C33	C37	18.4(12)
N5	C31	C33	C38	-141.3(12)	N5	C31	C34	C38	138.6(11)
N5	C31	C35	N5	-0.0(2)	N5	C31	C35	C32	98.6(5)
N5	C31	C35	C33	-135.2(7)	N5	C31	C35	C36	113.5(8)
N5	C31	C35	C37	-66.3(15)	N5	C31	C35	C38	-141.9(8)
N5	C31	C36	C32	95.1(7)	N5	C31	C36	C35	-64.6(8)
N5	C31	C38	C33	62(3)	N5	C31	C38	C34	-96(2)
N5	C31	C38	C35	71(2)	C32	C31	C33	C35	-68.0(13)
C32	C31	C33	C37	-99.6(13)	C32	C31	C33	C38	100.8(15)
C33	C31	C32	C35	48.8(12)	C33	C31	C32	C36	34.4(14)
C32	C31	C34	C38	-116.2(9)	C34	C31	C32	C35	171.0(11)
C34	C31	C32	C36	156.6(7)	C32	C31	C35	N5	-98.6(7)
C32	C31	C35	C32	0.0(5)	C32	C31	C35	C33	126.2(7)
C32	C31	C35	C36	14.9(9)	C32	C31	C35	C37	-164.9(14)
C32	C31	C35	C38	119.5(8)	C35	C31	C32	C35	0.0(6)
C35	C31	C32	C36	-14.4(9)	C32	C31	C36	C32	0.0(7)
C32	C31	C36	C35	-159.6(11)	C36	C31	C32	C35	14.4(8)
C36	C31	C32	C36	0.0(4)	C32	C31	C38	C33	-101.0(18)
C32	C31	C38	C34	100.3(16)	C32	C31	C38	C35	-92.0(16)
C38	C31	C32	C35	91.6(19)	C38	C31	C32	C36	77.3(19)
C33	C31	C34	C38	13.3(7)	C34	C31	C33	C35	169.8(12)
C34	C31	C33	C37	138.3(8)	C34	C31	C33	C38	-21.4(11)
C33	C31	C35	N5	135.2(10)	C33	C31	C35	C32	-126.2(9)
C33	C31	C35	C33	-0.0(8)	C33	C31	C35	C36	-111.3(11)
C33	C31	C35	C37	68.9(17)	C33	C31	C35	C38	-6.7(10)
C35	C31	C33	C35	0.0(8)	C35	C31	C33	C37	-31.6(10)
C35	C31	C33	C38	168.8(17)	C33	C31	C36	C32	-149.8(10)
C33	C31	C36	C35	50.5(10)	C36	C31	C33	C35	-42.7(7)
C36	C31	C33	C37	-74.3(7)	C36	C31	C33	C38	126.1(11)
C33	C31	C38	C33	-0.0(10)	C33	C31	C38	C34	-158.6(17)
C33	C31	C38	C35	9.1(16)	C38	C31	C33	C35	-169(2)
C38	C31	C33	C37	159.6(19)	C38	C31	C33	C38	-0.0(13)
C34	C31	C35	N5	107(3)	C34	C31	C35	C32	-155(3)
C34	C31	C35	C33	-29(3)	C34	C31	C35	C36	-140(3)
C34	C31	C35	C37	40(4)	C34	C31	C35	C38	-35(3)
C35	C31	C34	C38	37(3)	C34	C31	C36	C32	-45.6(16)
C34	C31	C36	C35	155(2)	C36	C31	C34	C38	-82.6(15)

C34	C31	C38	C33	158.6(14)	C34	C31	C38	C34	0.0(6)
C34	C31	C38	C35	167.7(11)	C38	C31	C34	C38	0.0(9)
C35	C31	C36	C32	159.6(12)	C35	C31	C36	C35	-0.0(8)
C36	C31	C35	N5	-113.5(8)	C36	C31	C35	C32	-14.9(9)
C36	C31	C35	C33	111.3(9)	C36	C31	C35	C36	0.0(4)
C36	C31	C35	C37	-180(2)	C36	C31	C35	C38	104.5(9)
C35	C31	C38	C33	-9.1(14)	C35	C31	C38	C34	-167.7(12)
C35	C31	C38	C35	0.0(7)	C38	C31	C35	N5	141.9(11)
C38	C31	C35	C32	-119.5(11)	C38	C31	C35	C33	6.7(11)
C38	C31	C35	C36	-104.5(11)	C38	C31	C35	C37	75.7(17)
C38	C31	C35	C38	0.0(8)	C36	C31	C38	C33	-53.7(14)
C36	C31	C38	C34	147.7(9)	C36	C31	C38	C35	-44.7(7)
C38	C31	C36	C32	-120.1(14)	C38	C31	C36	C35	80.2(15)
C31	C32	C35	N5	66.6(9)	C31	C32	C35	C31	0.0(6)
C31	C32	C35	C33	-72.3(12)	C31	C32	C35	C36	-162.3(11)
C31	C32	C35	C37	158(2)	C31	C32	C35	C38	-45.1(8)
C31	C32	C36	C31	0.0(3)	C31	C32	C36	C35	8.2(5)
C35	C32	C36	C31	-8.2(5)	C35	C32	C36	C35	-0.0(3)
C36	C32	C35	N5	-131.1(8)	C36	C32	C35	C31	162.3(10)
C36	C32	C35	C33	90.0(11)	C36	C32	C35	C36	-0.0(5)
C36	C32	C35	C37	-39.6(18)	C36	C32	C35	C38	117.2(8)
C31	C33	C35	N5	-61.5(17)	C31	C33	C35	C31	0.0(7)
C31	C33	C35	C32	56.5(12)	C31	C33	C35	C36	113.2(14)
C31	C33	C35	C37	-143.6(11)	C31	C33	C35	C38	8.9(13)
C31	C33	C37	C35	19.3(5)	C31	C33	C38	C31	0.0(5)
C31	C33	C38	C34	38(3)	C31	C33	C38	C35	-6.2(11)
C35	C33	C37	C35	0.0(5)	C37	C33	C35	N5	82.1(17)
C37	C33	C35	C31	143.6(10)	C37	C33	C35	C32	-159.9(12)
C37	C33	C35	C36	-103.2(11)	C37	C33	C35	C37	-0.0(5)
C37	C33	C35	C38	152.5(12)	C35	C33	C38	C31	6.2(11)
C35	C33	C38	C34	45(4)	C35	C33	C38	C35	0.0(4)
C38	C33	C35	N5	-70(2)	C38	C33	C35	C31	-8.9(15)
C38	C33	C35	C32	47.6(18)	C38	C33	C35	C36	104.3(16)
C38	C33	C35	C37	-152.5(15)	C38	C33	C35	C38	-0.0(10)
C37	C33	C38	C31	-31(3)	C37	C33	C38	C34	7(6)
C37	C33	C38	C35	-38(2)	C38	C33	C37	C35	44(3)
C31	C34	C38	C31	0.0(6)	C31	C34	C38	C33	-43(3)
C31	C34	C38	C35	-7.1(7)	N5	C35	C36	C31	75.6(12)
N5	C35	C36	C32	59.1(11)	N5	C35	C37	C33	-132.5(8)
N5	C35	C38	C31	-38.0(10)	N5	C35	C38	C33	131.1(11)
N5	C35	C38	C34	-26.7(14)	C31	C35	C36	C31	0.0(6)
C31	C35	C36	C32	-16.6(10)	C31	C35	C37	C33	-74.3(17)
C31	C35	C38	C31	0.0(8)	C31	C35	C38	C33	169.1(17)
C31	C35	C38	C34	11.3(11)	C32	C35	C36	C31	16.6(10)
C32	C35	C36	C32	-0.0(6)	C32	C35	C37	C33	138(2)
C32	C35	C38	C31	49.7(9)	C32	C35	C38	C33	-141.2(11)

C32	C35	C38	C34	61.0(10)	C33	C35	C36	C31	-99.9(17)
C33	C35	C36	C32	-116.4(15)	C33	C35	C37	C33	0.0(8)
C33	C35	C38	C31	-169.1(19)	C33	C35	C38	C33	0.0(12)
C33	C35	C38	C34	-157.8(19)	C36	C35	C37	C33	105.9(7)
C37	C35	C36	C31	179.9(13)	C37	C35	C36	C32	163.3(7)
C36	C35	C38	C31	99.8(14)	C36	C35	C38	C33	-91.1(14)
C36	C35	C38	C34	111.1(11)	C38	C35	C36	C31	-59.1(13)
C38	C35	C36	C32	-75.7(14)	C37	C35	C38	C31	-140.7(11)
C37	C35	C38	C33	28.3(12)	C37	C35	C38	C34	-129.5(10)
C38	C35	C37	C33	-17.6(8)	O1	C40	C41	C42	-86.1(11)
O1	C40	C44	C43	79.5(7)	C41	C40	C44	C43	-23.5(9)
C44	C40	C41	C42	24.1(12)	C40	C41	C42	C43	-15.4(15)
C41	C42	C43	C44	-2.1(13)	C42	C43	C44	C40	16.5(11)

Symmetry Operators:

(1) -X+1,-Y+2,-Z+1

References

1. M. Suginome, H. Oike, S. -S. Park, Y. Ito, *Bull. Chem. Soc. Jpn.*, 1996, **69**, 289-299.
2. S. Harrypersad, L. Liao, A. Khan, R. S. Wylie, D. A. Foucher, *J. Inorg. Organomet. Polym.* 2015, **25**, 515–528.
3. R. Sommer, B. Schneider, W. P. Neumann, *Justus Liebigs Ann. Chem.* 1966, **692**, 12-21.
4. E. Carberry, B. D. Dombek, S. C. Cohen, *J. Organomet. Chem.* 1972, **36**, 61-70.
5. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Jr. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, Revision C.01; Gaussian, Inc., Wallingford, CT, 2010.
6. J. Perdew, M. Ernzerhof, K. Burke, *J. Chem. Phys.* 1996, **105**, 9982-9985.
7. C. Adamo, V. Barone, *J. Chem. Phys.* 1999, **110**, 6158-6170.
8. Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.* 2008, **120**, 215-241.
9. J. P. Perdew, J. A. Chevary, S. H. Vosko, K. A. Jackson, M. R. Pederson, D. J. Singh, C. Fiolhais, *Phys. Rev. B.* 1993, **48**, 4978.
10. C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B.* 1988, **37**, 785-789.
11. A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098–3100.
12. A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648-5652.
13. B. Miehlich, A. Savin, H. Stoll, H. Preuss, *Chem. Phys. Lett.* 1989, **157**, 200-206.
14. D. Andrae, U. Häußermann, M. Dolg, H. Stoll, H. Preuß, *Theor. Chim. Acta*, 1990, **77**, 123-14.
15. M. S. Gordon, *Chem. Phys. Lett.* 1980, **76**, 163–168.
16. P. C. Hariharan, J. A. Pople, *Mol. Phys.* 1974, **27**, 209–214.
17. P. C. Hariharan, J. A. Pople, *Theor. Chem. Acc.* 1973, **28**, 213–222.
18. W. J. Hehre, R. Ditchfield, J. A. Pople, *J. Chem. Phys.* 1972, **56**, 2257–2261.
19. R. Ditchfield, W. J. Hehre, J. A. Pople, *J. Chem. Phys.* 1971, **54**, 724–728.
20. SIR2008: M. C. Burla, R. Caliandro, M. Camalli, B. Carrozzini, G. L. Cascarano, L. De Caro, C. Giacovazzo, G. Polidori, D. Siliqi, R. Spagna, *J. Appl. Cryst.* 2007, **40**, 609-613.
21. International Tables for Crystallography, Vol. C; (Ed. A. J. C. Wilson) Kluwer Academic Publishers, Dordrecht, Netherlands, Table 6.1.1.4, 1992, pp. 572.

22. J. A. Ibers, W. C. Hamilton, *Acta Cryst.* 1964, **17**, 781-782.
23. J. A. Ibers, W. C. Hamilton, in International Tables for Crystallography, Vol C; (Ed. A. J. C. Wilson), Kluwer Academic Publishers, Dordrecht, Netherlands, Table 4.2.6.8, 1992, pages 219-222.
24. D. C. Creagh, J. H. Hubbell, in International Tables for Crystallography, Vol C; (Ed. A. J. C. Wilson), Kluwer Academic Publishers, Boston, Table 4.2.4.3, 1992, pages 200-206.
25. CrystalStructure 4.2.5: Crystal Structure Analysis Package, Rigaku Corporation (2000-2017). Tokyo 196-8666, Japan.
26. SHELXL Version 2017/1: G. M. Sheldrick, *Acta Cryst.* 2008, **A64**, 112-122.