# Electronic Supporting Information For

## A diamidinatogermylene as a Z-type ligand in a nickel(0) complex

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## Content

## Experimental Section

### General information

All reactions were performed under a dry nitrogen atmosphere by using standard Schlenk-line and in a glovebox. Solvents were dried by the proper drying agents; NaK/benzophenone (diethyl ether, THF, toluene, hexane), $CaH_2$ (triethylamine, dichloromethane) and degassed before use. All NMR spectra were recorded on Bruker AVQ-400 or DRX 500 spectrometers referenced to residual solvent signals as internal standards for $^{1}H$ and $^{13}C\{^{1}H\}$ NMR or with an external standard ($H_3PO_4$ for $^{31}P\{1H\}$ NMR).. Element analyses were performed on an Elementar Vario EL III instrument at Shanghai Institute of Organic Chemistry, the Chinese Academy of Science. For the single crystal X-ray structure analyses the crystals were each mounted on a glass capillary in perfluorinated oil and measured in a cold $N_2$ flow. The data were collected on Bruker D8 CMOS detectors at 153 K. The structures were solved by direct methods and all refined on $F^2$ with the SHELX-2014/7 software package. $GeCl_2$(dioxane),[S1] *N*-mesitylpivalimidoyl chloride,[S2] and 2-(diphenylphosphino)benzenamine[S3] were synthesized according to the reported procedures.

### Synthesis of *N*-(2-(diphenylphosphino)phenyl)-*N*'-mesitylpivalamidine

Triethylamine (2.08 mL, 15.0 mmol) was added dropwise at room temperature to a solution of *N*-mesitylpivalimidoyl chloride (2.38 g, 10 mmol) and 2-(diphenylphosphino)benzenamine (2.77 g, 10 mmol) in 50 mL toluene. The mixture was heated to reflux and stirred overnight, and then the mixture was filtered to remove triethylamine hydrochloride in air. The filtrate was dried in vacuum, and the bright yellow solid was isolated after recrystallization from *n*-hexane. Yield: 98%. $^{1}H$ NMR (400 MHz, $CDCl_3$): $\delta$ 7.37-7.31 (m, 4H), 7.26 (d, $J$ = 5.0 Hz, 8H), 6.89 (d, $J$ = 12.8 Hz, 2H), 6.54 (d, $J$ = 20.5 Hz, 2H), 6.24 (s, 1H), 2.25 (s, 3H), 2.21–2.02 (m, 6H), 1.19 (s, 9H). $^{31}P$ NMR (162 MHz, $CDCl_3$, ppm): $\delta$ -11.9, -17.8.

**Synthesis of chlorogermylene 1**

*n*-BuLi (2.5 M, 1.26 mL, 3.15 mmol) was added dropwise to a cooled solution of N-(2-(diphenylphosphino)phenyl)-*N*'-mesitylpivalamidine (1.436 g, 3.0 mmol) in 30 mL THF at -78 °C, then the mixture was allowed to slowly warm up to room temperature. The mixture was stirred for 3 h, and a solution of $GeCl_2$(dioxane) (0.709 g, 3 mmol) in THF (20 mL) was added to the mixture at -78 °C. The mixture was left to warm up to room temperature and stirred for 12 h. After that, all the volatile was evaporated, and the remaining bright yellow solid was extracted with hot toluene and filtered through celite. The filtrate was concentrated to ca. 10 mL and left at -20 °C to afford bright yellow crystals of **1**. Yield: 84%. Anal. Calcd (%) for $C_{32}H_{34}ClGeN_2P$: C, 65.62; H, 5.85; N, 4.78. Found: C, 65.91; H, 6.03; N, 4.87. $^1$H NMR (400 MHz, $C_6D_6$, ppm): $\delta$ 7.54 (d, J = 7.0 Hz, 1H), 7.33 (d, *J* = 44.7 Hz, 4H, $C_6H_4$), 7.07-6.99 (d, *J* = 26.5 Hz, 8H, *o*-$C_6H_5$, *m*-$C_6H_5$), 6.83 (s, 1H), 6.69 (s, 1H, *m*-$C_6H_2$), 6.64 (s, 1H, *m*-$C_6H_2$), 2.58 (s, 3H, *p*-Ph$CH_3$), 2.38 (s, 3H, *o*-Ph$CH_3$), 2.08 (s, 3H, *o*-Ph$CH_3$), 0.99 (s, 9H, C$(CH_3)_3$). $^{31}$P NMR (162 MHz, $C_6D_6$, ppm): δ -15.64. $^{13}$C NMR (101 MHz, $C_6D_6$, ppm): $\delta$ 180.46 (N=*C*-N), 146.36 (*C*$_6H_4$), 139.04 (*p*-$C_6H_2$), 134.52 (*m*-$C_6H_2$), 134.37 (*p*-*C*$_6H_5$), 133.65 (*m*-$C_6H_2$), 133.53 (*m*-*C*$_6H_5$), 132.79 (*o*-*C*$_6H_2$), 129.53-128.81 (*C*$_6H_4$), 129.18 (*o*-$C_6H_5$), 128.73 (*o*-$C_6H_2$), 127.93 (*C*$_6H_4$), 127.69 (*C*$_6H_5$), 127.45 ($C_6H_5$), 41.46(*C*$(CH_3)_3$), 28.19 (C(*C*$H_3)_3$), 20.52 (Mes-*C*$H_3$), 19.66(Mes-*C*$H_3$).

**Preparation of chlorogermylene nickel(0) complex 2**

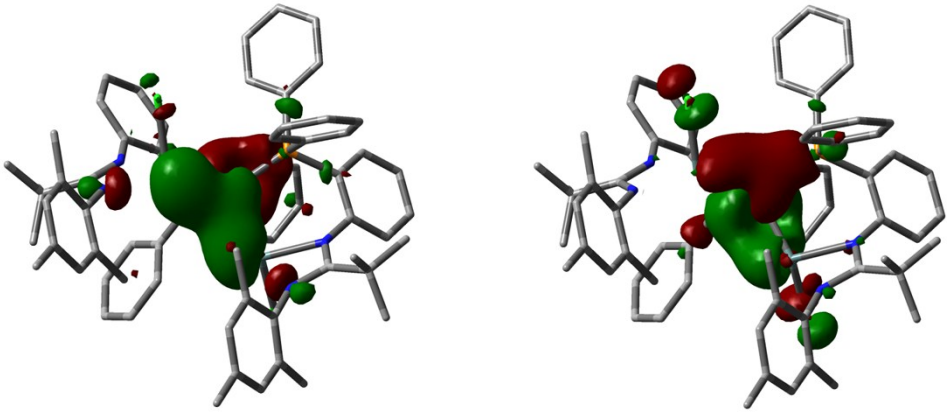
Toluene (20 mL) was added into a flask containing $Ni(COD)_2$ (55.0 mg, 0.20 mmol) and compound **1** (0.246 g, 0.42 mmol) at 0 °C. The mixture was stirring overnight at 0 °C and an orange suspension was formed. After cooling at -40 °C overnight, the suspension was filtered, and the obtained orange solid of **2** was obtained by drying in vacuum for 2 h. Yield: 69%. Anal. Calcd (%) for $C_{64}H_{68}Cl_2Ge_2N_4NiP_2$•$2C_7H_8$: C, 66.24; H, 5.99; N, 3.96. Found: C, 65.71; H, 5.98; N, 4.18. $^1$H NMR (500 MHz, $CD_2Cl_2$, ppm): $\delta$ 8.01 (br, 4 H, Ar-*H*), 6.80-7.37 (m, 28H, Ar-*H*), 2.30 (s, 6H, Mes-C*H*$_3$), 2.26 (s, 6H, Mes-C*H*$_3$), 2.21 (s, 6H, Mes-C*H*$_3$), 0.47 (s, 18H, C$(CH_3)_3$). $^{31}$P NMR (202 MHz, $CD_2Cl_2$, ppm): $\delta$ 24.7. $^{13}$C NMR (126 MHz, $CD_2Cl_2$, ppm $C_6D_6$, ppm): $\delta$ 176.9 (N*C*N), 143.6, 138.0, 136.2, 136.1, 136.0, 134.9, 134.8, 134.6,

134.5, 134.0, 133.8, 131.7, 129.6, 129.1, 129.0, 128.7, 128.4, 128.2, 128.1, 127.8, 127.7, 127.5, 127.4, 127.3, 124.3 (Ph-*C*), 39.4 ($C(CH_3)_3$), 28.1 ($C(CH_3)_3$), 21.2, 20.6, 20.4 (Mes-$CH_3$).

**Preparation of the germylene nickel(0) complex 3**

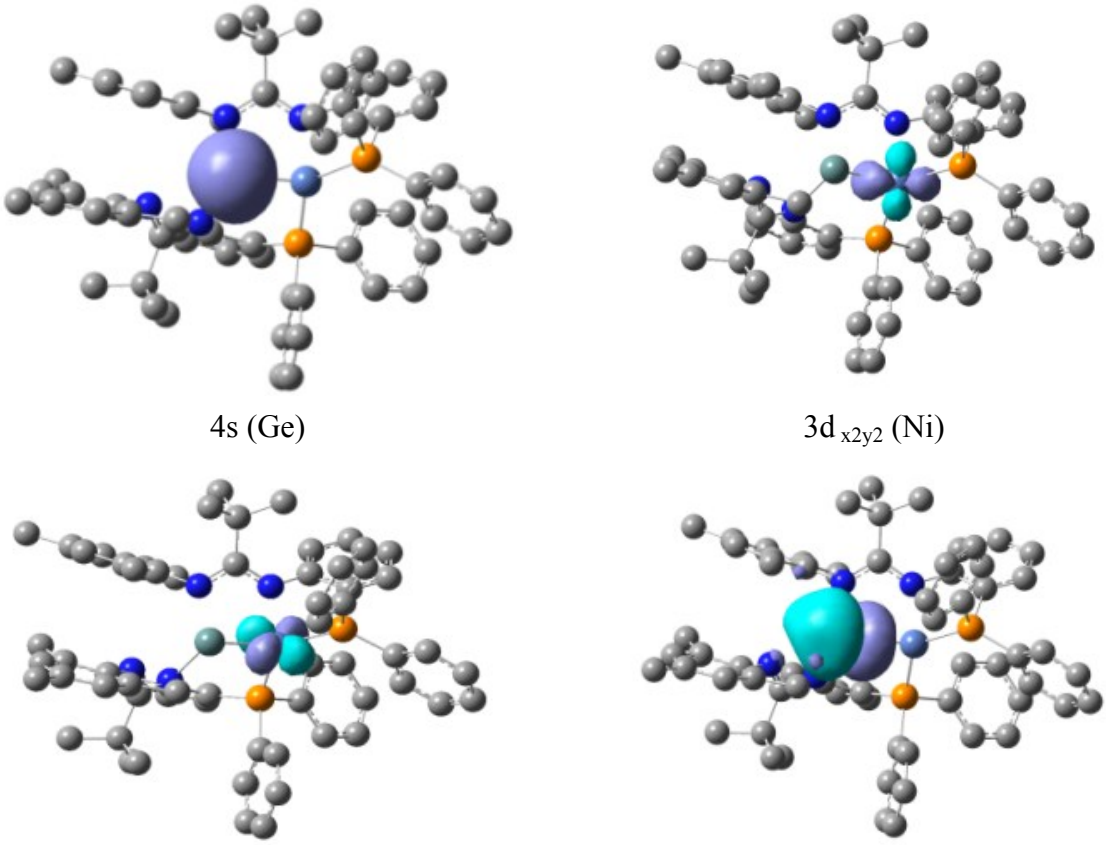
THF (20 mL) was added into a flask containing K (25.0 mg, 0.63 mmol) and **2** (0.369 g, 0.3 mmol) at room temperature. The mixture was stirred at room temperature for 3 days. Then all the volatiles were removed in vacuum. The residue was extracted with diethyl ether (20 mL) and filtered. The filtrate was concentrated to ca. 10 mL and left at room temperature for 24 h to afford the dark brown crystals of compound **3**. Yield: 20%. Anal.Calcd (%) for $C_{64}H_{68}GeN_4NiP_2$: C, 70.75; H, 6.31; N, 5.16. Found: C, 70.09; H, 6.63; N, 4.97. Due to the extremely low solubility of the crystals in THF-$d_8$ and $C_6D_6$, we could not get the NMR spectra of **3**.

## Selected Figures



**2**: HOMO　　**2**: HOMO-1

Fig. S1 Selected molecular orbitals of **2**.



4s (Ge)　　$3d_{x2y2}$ (Ni)

$3d_{xz}$(Ni)　　$4p_z$(Ge)

**Fig. S2** Natural Bond Orbitals (Isovalue=0.05) involved in the FMOs of **3**.

## NMR spectra for the new compounds

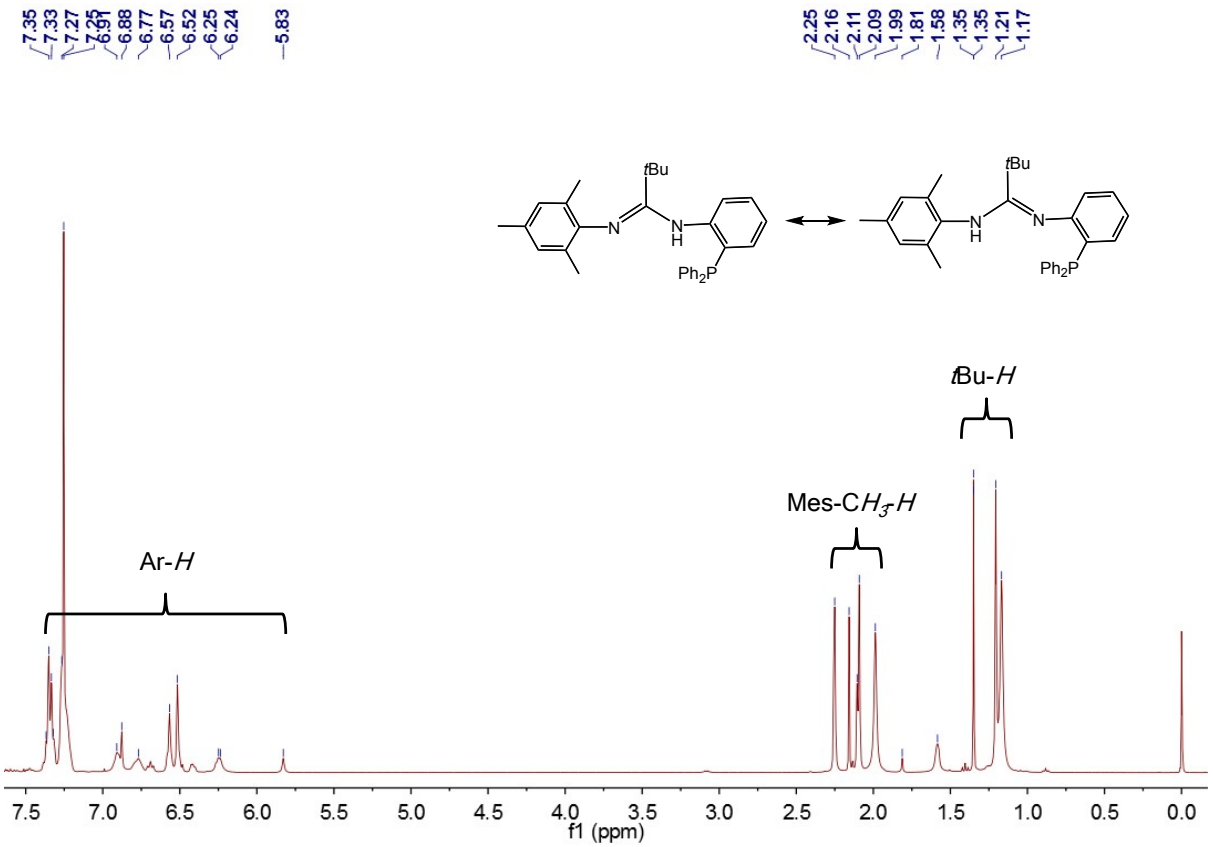



**Fig. S3** $^{1}$H NMR spectrum of N-(2-(diphenylphosphino)phenyl)-N'-mesitylpivalamidine in $CDCl_3$ at room temperature. Due to the presence of two possible NH groups, two sets NMR signals for two isomers were observed in the NMR spectrum.

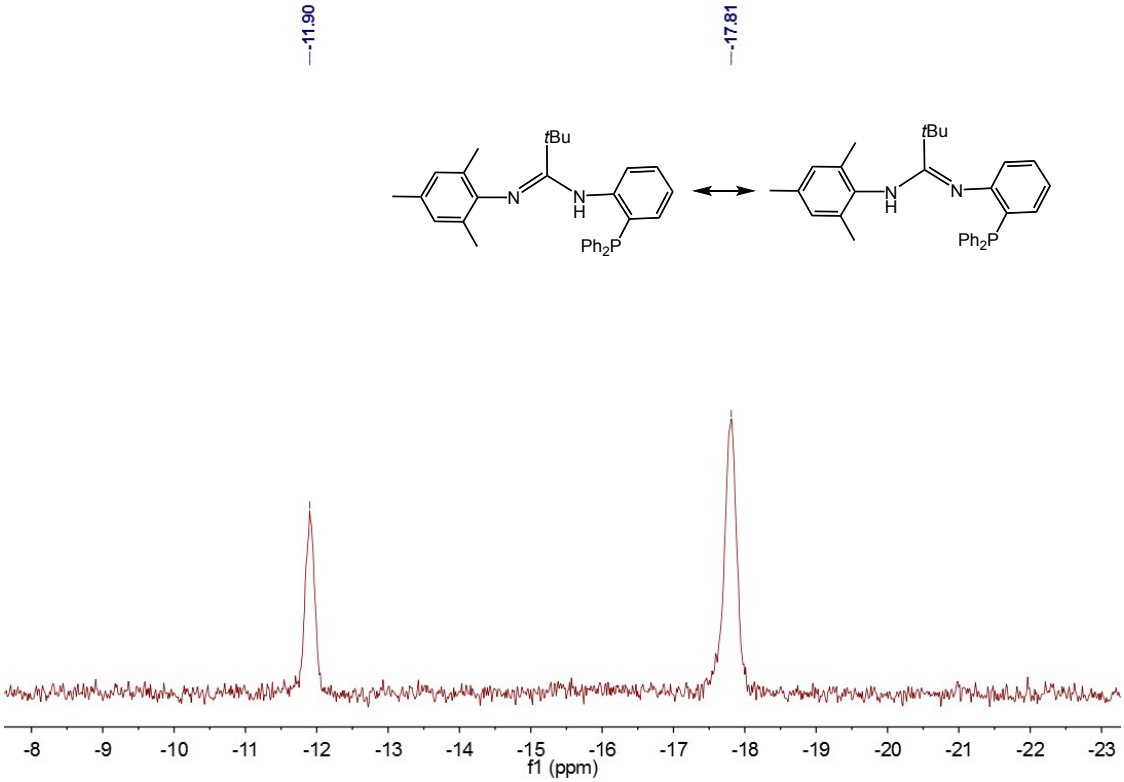



**Fig. S4** $^{31}$P NMR spectrum of N-(2-(diphenylphosphino)phenyl)-N'-mesitylpivalamidine in $CDCl_3$ at room temperature.

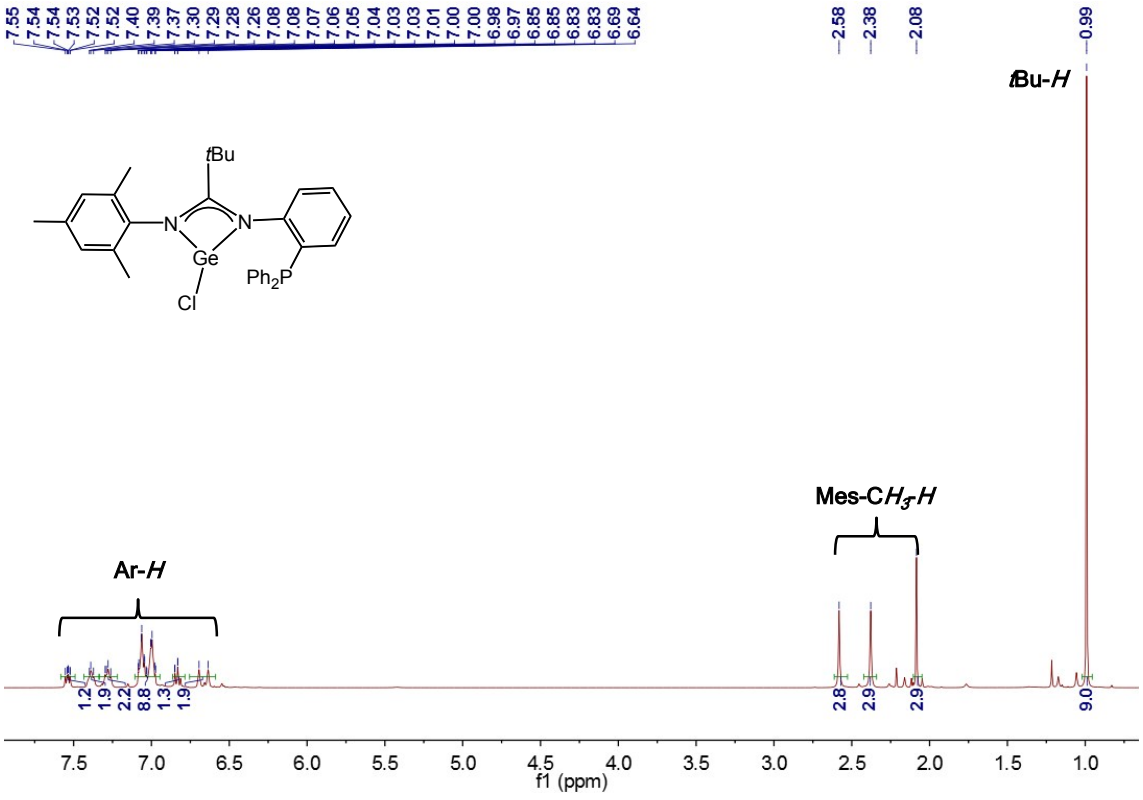



**Fig. S5** $^{1}$H NMR spectrum of **1** in $C_6D_6$ at room temperature.

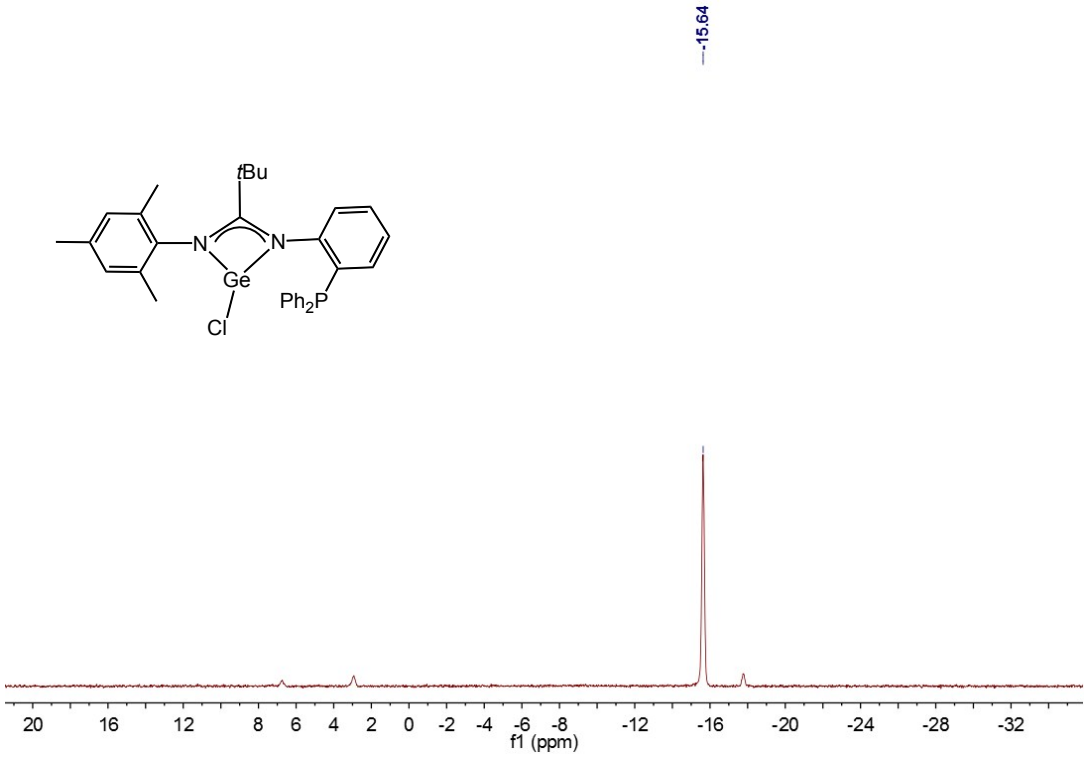



**Fig. S6** $^{31}P\{^{1}H\}$ NMR spectrum of **1** in $C_6D_6$ at room temperature.

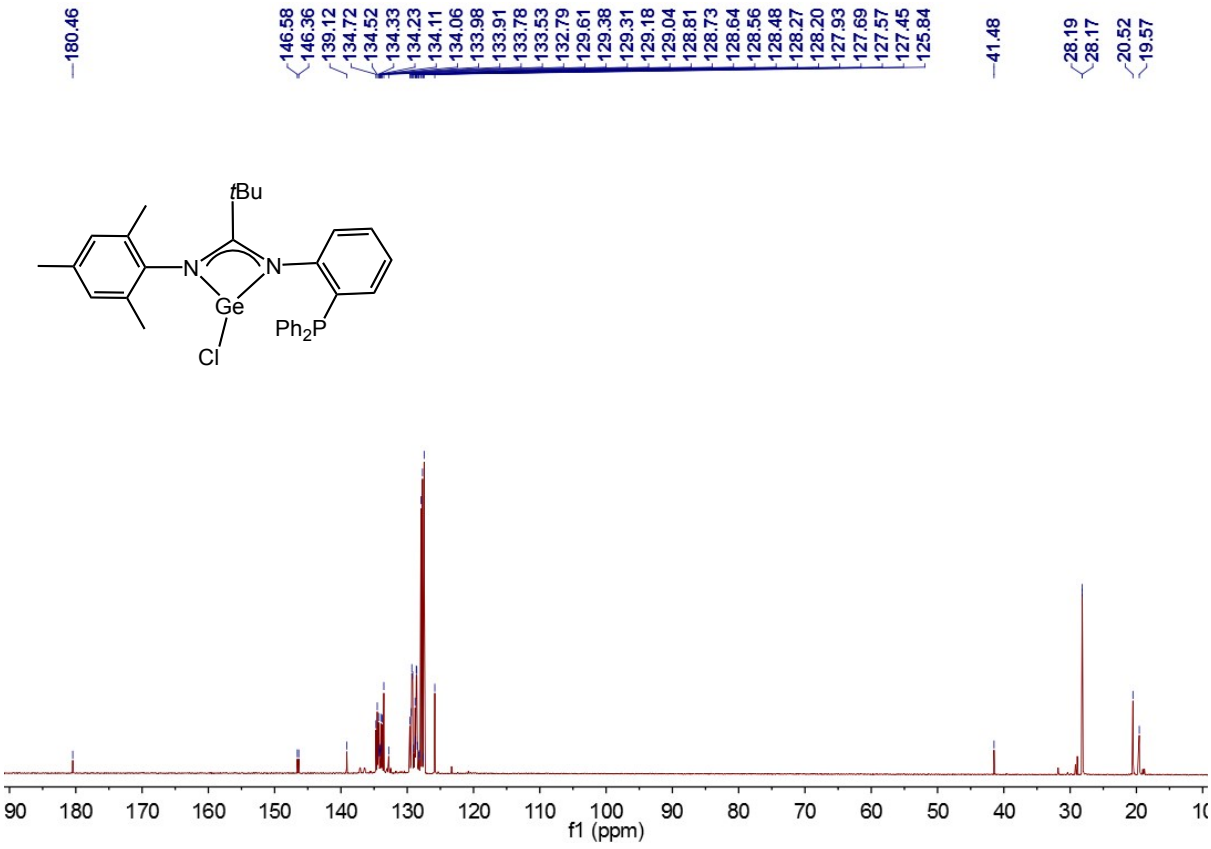



**Fig. S7** $^{13}C\{^{1}H\}$ NMR spectrum of **1** in $C_6D_6$ at room temperature.

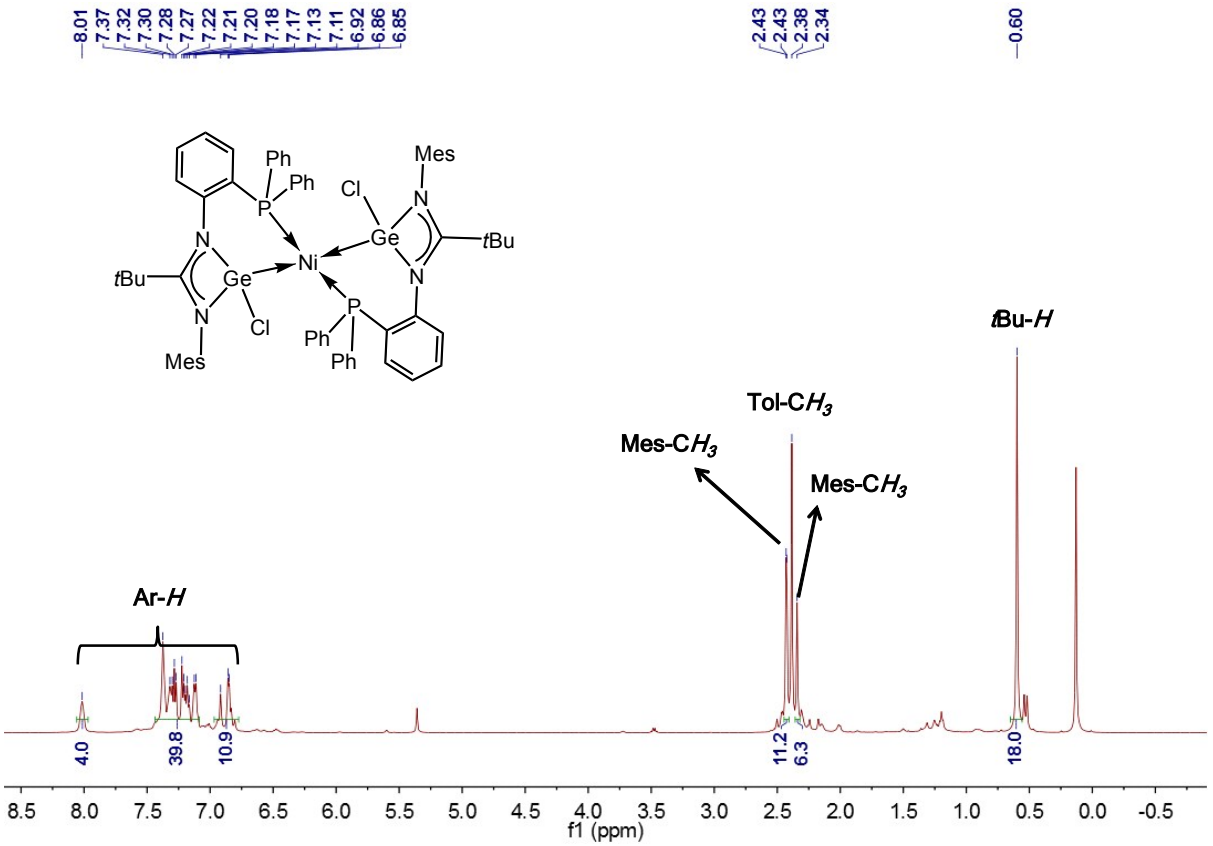



**Fig. S8** $^{1}H$ NMR spectrum of **2** in $CD_2Cl_2$ at room temperature.

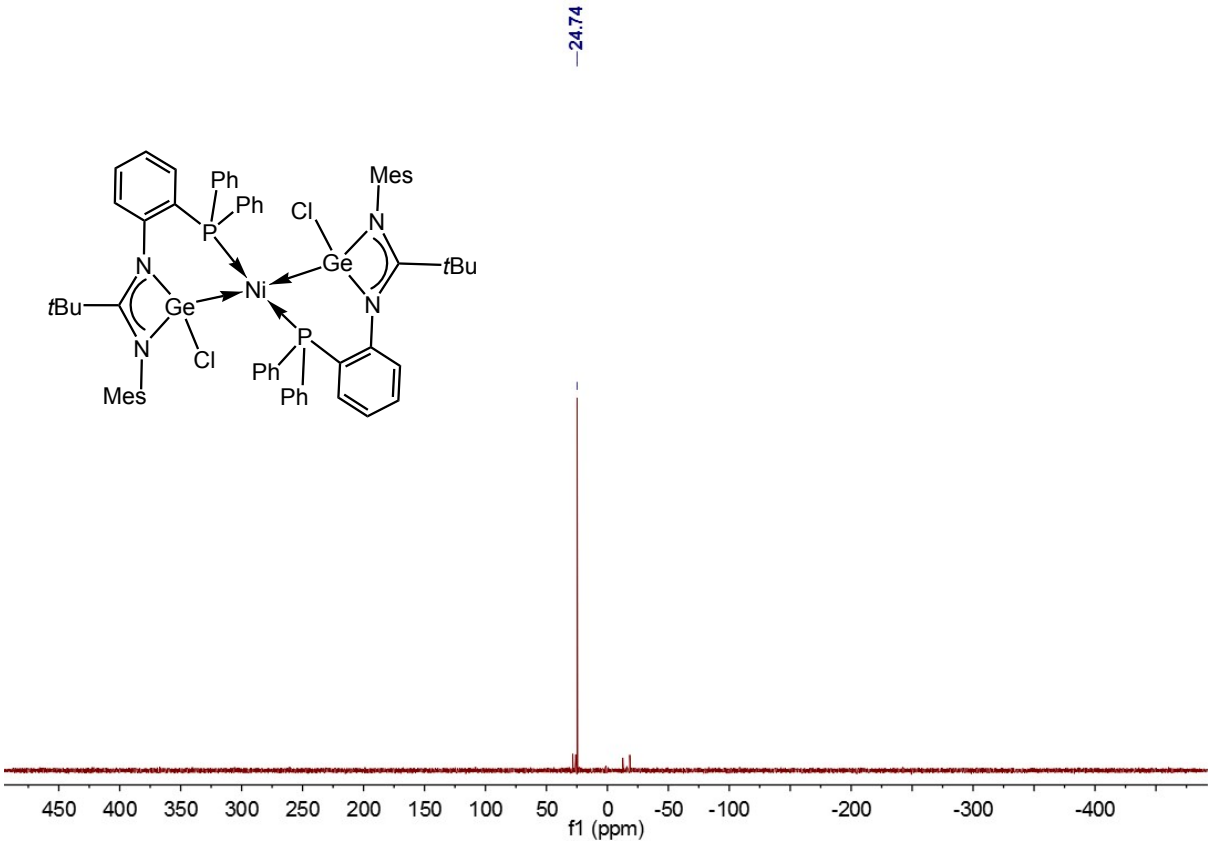



**Fig. S9** $^{31}P\{^{1}H\}$ NMR spectrum of **2** in $CD_2Cl_2$ at room temperature.

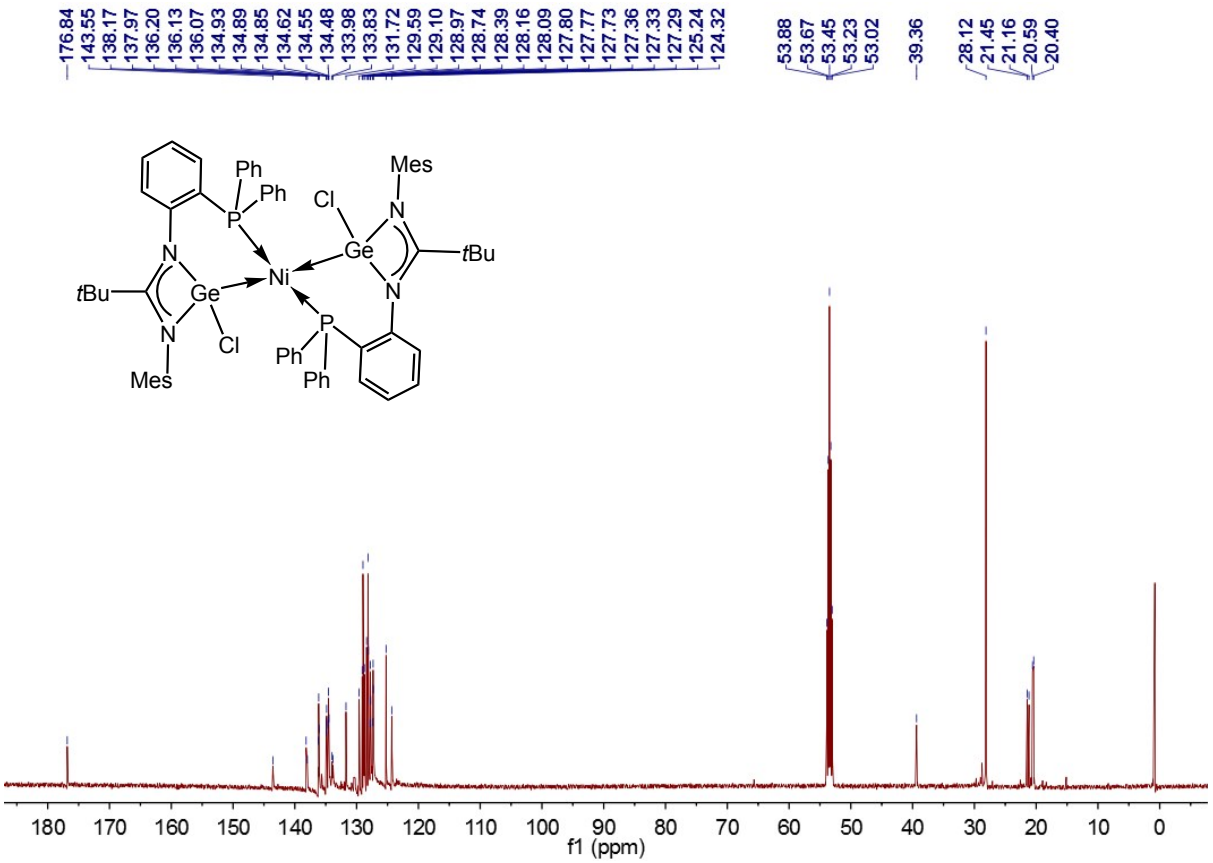



**Fig. S10** $^{13}C\{^{1}H\}$ NMR spectrum of **2** in $CD_2Cl_2$ at room temperature.

**Table S1. Crystal data and structure refinement for compounds 1-3**

| | **1** | **2** | **3** |
|---|---|---|---|
| Formula | $C_{32}H_{34}ClGeN_2P$ | $C_{78}H_{84}Cl_2Ge_2N_4NiP_2$ | $C_{64}H_{68}GeN_4NiP_2$ |
| Formula weight | 585.62 | 1414.22 | 1086.46 |
| Temp. (K) | 150(2) | 150(2) | 150(2) |
| Crystal system | Triclinic | Triclinic | Triclinic |
| Space group | *P*-1 | *P*-1 | *P*-1 |
| *a* (Å) | 8.2747(12) | 12.7731(14) | 11.2674(13) |
| *b* (Å) | 9.0970(11) | 13.8926(17) | 13.6982(15) |
| *c* (Å) | 20.186(3) | 21.428(3) | 19.294(2) |
| $\alpha$(°) | 86.729(4) | 101.727(4) | 89.501(2) |
| $\beta$(°) | 79.820(5) | 100.858(3) | 76.818(2) |
| $\gamma$(°) | 79.365(4) | 105.974(3) | 74.009(2) |
| *V* [Å$^3$] | 1469.4(3) | 3456.7(7) | 2782.5(5) |
| *Z* | 2 | 2 | 2 |
| $\rho_{calcd}$(g·cm$^{-3}$) | 1.324 | 1.361 | 1.297 |
| $\mu$(mm-1) | 1.211 | 1.304 | 0.979 |
| *F*(000) | 608 | 1476 | 1140 |
| Collected data | 12133 | 30832 | 25639 |
| Unique data | 6698 | 15875 | 12634 |
| GOF on $F^2$ | 1.052 | 1.011 | 1.006 |
| Final *R* indexes | R1 = 0.0567, | R1 = 0.0589, | R1 = 0.0402, |
| | ωR2 = 0.1416 | ωR2 = 0.1093 | ωR2 = 0.0992 |
| [I > 2σ(I)] | R1 = 0.0863, | R1 = 0.1244, | R1 = 0.0591, |
| *R* indexes (all data) | ωR2 = 0.1578 | ωR2 = 0.1297 | ωR2 = 0.1070 |
| Completeness | 0.991 | 0.994 | 0.983 |

**Table S2 The calculated main Ni and Ge atom orbital contributions of HOMOs**

| **Compound 2** | | | **Compound 3** | | |
|---|---|---|---|---|---|
| Ni | $4p_y$ | 10.8% | Ni | $3d_{xz}$ | 4.85% |
| | $3d_{xz}$ | 36.1% | | $3d_{yz}$ | 5.44% |
| Ge | 4s | 3.56% | | $3d_{x2y2}$ | 25.6% |
| | $4p_x$ | 2.21% | Ge | 4s | 8.85% |
| | $4p_y$ | 2.46% | | $4p_z$ | 11.6% |

## Theoretical Calculations

All the calculations were performed with Gaussian 09 program suite.[S4] The ground-state structures of the studied compounds were optimized at the B3LYP/Gen (6-31G* for C, H, N, P, Ge, (Cl) atoms and LANL2Dz for Ni atoms). In addition, the second-order perturbation energy due to the LP ($d_{Ni}$)→LP*($p_{Ge}$) orbital interaction ($E_{Ni\cdots Ge}$) obtained by NBO analysis[S5] at the same level. The calculated results show that there is a strong interaction between Ni and Ge in complex **3**, displaying the obvious Lewis acid character of the germanium moiety in compound **3**.

**Coordinates of the studied molecules**

**2**

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 28 | 0 | -1.157876 | -0.230702 | 0.104223 |
| 2 | 15 | 0 | -2.436010 | -1.911665 | -0.693060 |
| 3 | 15 | 0 | -1.853607 | 1.062167 | 1.834573 |
| 4 | 32 | 0 | 0.648362 | -1.542567 | 0.597002 |
| 5 | 32 | 0 | -1.073170 | 1.492317 | -1.394053 |
| 6 | 7 | 0 | 2.028999 | -2.705242 | -0.424917 |
| 7 | 7 | 0 | 0.064531 | -3.433949 | 0.107046 |
| 8 | 7 | 0 | -1.791300 | 3.116626 | -0.401493 |
| 9 | 7 | 0 | -0.054120 | 3.270035 | -1.676411 |
| 10 | 17 | 0 | 1.378102 | -2.106959 | 2.719385 |
| 11 | 17 | 0 | -2.429596 | 1.718545 | -3.239465 |
| 12 | 6 | 0 | 1.190261 | -3.749189 | -0.550557 |
| 13 | 6 | 0 | 1.458759 | -5.033837 | -1.370460 |

| | | | | | |
|---|---|---|---|---|---|
| 14 | 6 | 0 | 0.193043 | -5.893705 | -1.570078 |
| 15 | 1 | 0 | 0.431711 | -6.688440 | -2.286142 |
| 16 | 1 | 0 | -0.636081 | -5.312710 | -1.982791 |
| 17 | 1 | 0 | -0.145851 | -6.371876 | -0.650493 |
| 18 | 6 | 0 | 2.528548 | -5.889683 | -0.650752 |
| 19 | 1 | 0 | 3.500952 | -5.393777 | -0.630976 |
| 20 | 1 | 0 | 2.643174 | -6.838270 | -1.188293 |
| 21 | 1 | 0 | 2.236486 | -6.121513 | 0.379499 |
| 22 | 6 | 0 | 1.972743 | -4.663313 | -2.782105 |
| 23 | 1 | 0 | 2.893784 | -4.080096 | -2.754920 |
| 24 | 1 | 0 | 1.214243 | -4.106685 | -3.341812 |
| 25 | 1 | 0 | 2.178850 | -5.588934 | -3.331830 |
| 26 | 6 | 0 | 3.353495 | -2.464959 | -0.881088 |
| 27 | 6 | 0 | 4.465804 | -2.902522 | -0.129553 |
| 28 | 6 | 0 | 5.754129 | -2.615642 | -0.606268 |
| 29 | 1 | 0 | 6.606805 | -2.975074 | -0.032607 |
| 30 | 6 | 0 | 5.976633 | -1.876511 | -1.766650 |
| 31 | 6 | 0 | 4.856214 | -1.386224 | -2.449484 |
| 32 | 1 | 0 | 4.999750 | -0.774070 | -3.337799 |
| 33 | 6 | 0 | 3.553702 | -1.654342 | -2.028094 |
| 34 | 6 | 0 | 2.388020 | -1.076315 | -2.794144 |
| 35 | 1 | 0 | 2.741424 | -0.400146 | -3.578718 |
| 36 | 1 | 0 | 1.713144 | -0.511566 | -2.142015 |
| 37 | 1 | 0 | 1.782239 | -1.856188 | -3.268107 |
| 38 | 6 | 0 | 4.341658 | -3.609993 | 1.201526 |
| 39 | 1 | 0 | 4.664117 | -2.938663 | 2.006746 |
| 40 | 1 | 0 | 4.985157 | -4.497370 | 1.238897 |
| 41 | 1 | 0 | 3.319163 | -3.906403 | 1.430325 |
| 42 | 6 | 0 | 7.373881 | -1.613985 | -2.278959 |
| 43 | 1 | 0 | 8.124419 | -1.773722 | -1.497859 |

| | | | | | |
|---|---|---|---|---|---|
| 44 | 1 | 0 | 7.481261 | -0.586892 | -2.646402 |
| 45 | 1 | 0 | 7.623576 | -2.281728 | -3.114618 |
| 46 | 6 | 0 | -1.091193 | -4.092662 | 0.542124 |
| 47 | 6 | 0 | -1.005761 | -5.219126 | 1.376842 |
| 48 | 1 | 0 | -0.022216 | -5.593537 | 1.643957 |
| 49 | 6 | 0 | -2.153343 | -5.835074 | 1.868207 |
| 50 | 1 | 0 | -2.064537 | -6.712299 | 2.503442 |
| 51 | 6 | 0 | -3.407951 | -5.312096 | 1.553177 |
| 52 | 1 | 0 | -4.312144 | -5.788421 | 1.922203 |
| 53 | 6 | 0 | -3.501141 | -4.160044 | 0.770726 |
| 54 | 1 | 0 | -4.481900 | -3.752492 | 0.552298 |
| 55 | 6 | 0 | -2.361169 | -3.517053 | 0.263914 |
| 56 | 6 | 0 | -4.247373 | -1.512372 | -0.751807 |
| 57 | 6 | 0 | -4.924167 | -1.331163 | -1.967743 |
| 58 | 1 | 0 | -4.408469 | -1.490788 | -2.907610 |
| 59 | 6 | 0 | -6.262238 | -0.930409 | -1.986848 |
| 60 | 1 | 0 | -6.763283 | -0.790517 | -2.941141 |
| 61 | 6 | 0 | -6.950715 | -0.711242 | -0.794522 |
| 62 | 1 | 0 | -7.993373 | -0.404996 | -0.811209 |
| 63 | 6 | 0 | -6.285238 | -0.877776 | 0.422410 |
| 64 | 1 | 0 | -6.807023 | -0.701224 | 1.359452 |
| 65 | 6 | 0 | -4.944248 | -1.258712 | 0.443866 |
| 66 | 1 | 0 | -4.440181 | -1.361319 | 1.399985 |
| 67 | 6 | 0 | -2.134602 | -2.564400 | -2.411064 |
| 68 | 6 | 0 | -2.755212 | -3.742437 | -2.863672 |
| 69 | 1 | 0 | -3.409618 | -4.298909 | -2.198677 |
| 70 | 6 | 0 | -2.542422 | -4.206208 | -4.162012 |
| 71 | 1 | 0 | -3.031715 | -5.117568 | -4.496229 |
| 72 | 6 | 0 | -1.703438 | -3.500677 | -5.030032 |
| 73 | 1 | 0 | -1.539666 | -3.860349 | -6.042568 |

| | | | | | |
|---|---|---|---|---|---|
| 74 | 6 | 0 | -1.082280 | -2.331360 | -4.591102 |
| 75 | 1 | 0 | -0.436125 | -1.769903 | -5.260661 |
| 76 | 6 | 0 | -1.296262 | -1.868429 | -3.288829 |
| 77 | 1 | 0 | -0.818159 | -0.955646 | -2.952301 |
| 78 | 6 | 0 | -0.844181 | 3.961454 | -0.834838 |
| 79 | 6 | 0 | -0.635573 | 5.435130 | -0.416352 |
| 80 | 6 | 0 | 0.790494 | 5.613353 | 0.158910 |
| 81 | 1 | 0 | 0.930251 | 5.010851 | 1.062135 |
| 82 | 1 | 0 | 0.927013 | 6.665462 | 0.434649 |
| 83 | 1 | 0 | 1.565947 | 5.355452 | -0.563987 |
| 84 | 6 | 0 | -0.803734 | 6.351906 | -1.651062 |
| 85 | 1 | 0 | -0.017364 | 6.190192 | -2.390001 |
| 86 | 1 | 0 | -0.750138 | 7.397023 | -1.324317 |
| 87 | 1 | 0 | -1.774119 | 6.201948 | -2.137213 |
| 88 | 6 | 0 | -1.624879 | 5.905324 | 0.668394 |
| 89 | 1 | 0 | -2.650586 | 5.977636 | 0.303966 |
| 90 | 1 | 0 | -1.318747 | 6.905576 | 0.995591 |
| 91 | 1 | 0 | -1.613028 | 5.251835 | 1.542788 |
| 92 | 6 | 0 | 1.129980 | 3.593425 | -2.393790 |
| 93 | 6 | 0 | 2.386205 | 3.211025 | -1.855224 |
| 94 | 6 | 0 | 3.544137 | 3.470203 | -2.589100 |
| 95 | 1 | 0 | 4.504042 | 3.182181 | -2.164504 |
| 96 | 6 | 0 | 3.507259 | 4.076155 | -3.851292 |
| 97 | 6 | 0 | 2.257743 | 4.387234 | -4.383044 |
| 98 | 1 | 0 | 2.197810 | 4.821640 | -5.379711 |
| 99 | 6 | 0 | 1.061407 | 4.140377 | -3.693357 |
| 100 | 6 | 0 | -0.243069 | 4.431333 | -4.402390 |
| 101 | 1 | 0 | -1.113123 | 4.196976 | -3.790762 |
| 102 | 1 | 0 | -0.318150 | 3.823715 | -5.312124 |
| 103 | 1 | 0 | -0.301519 | 5.482283 | -4.712084 |

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|---|---|---|---|---|---|
| 104 | 6 | 0 | 2.490749 | 2.516917 | -0.518107 |
| 105 | 1 | 0 | 2.150210 | 3.149325 | 0.308088 |
| 106 | 1 | 0 | 3.528152 | 2.233053 | -0.314155 |
| 107 | 1 | 0 | 1.880044 | 1.608134 | -0.481977 |
| 108 | 6 | 0 | 4.781314 | 4.377680 | -4.605685 |
| 109 | 1 | 0 | 5.275662 | 5.275786 | -4.211385 |
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| 111 | 1 | 0 | 5.501059 | 3.554718 | -4.525029 |
| 112 | 6 | 0 | -3.006722 | 3.162676 | 0.293728 |
| 113 | 6 | 0 | -4.074046 | 3.947710 | -0.169726 |
| 114 | 1 | 0 | -3.916673 | 4.575967 | -1.040833 |
| 115 | 6 | 0 | -5.320679 | 3.896736 | 0.447090 |
| 116 | 1 | 0 | -6.131108 | 4.518812 | 0.076930 |
| 117 | 6 | 0 | -5.528597 | 3.023283 | 1.513839 |
| 118 | 1 | 0 | -6.500602 | 2.964985 | 1.995859 |
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| 121 | 6 | 0 | -3.213592 | 2.250337 | 1.366115 |
| 122 | 6 | 0 | -0.627647 | 2.188653 | 2.670468 |
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| 124 | 1 | 0 | -2.037307 | 3.710587 | 3.279911 |
| 125 | 6 | 0 | -0.061678 | 4.143487 | 4.007222 |
| 126 | 1 | 0 | -0.371388 | 5.062112 | 4.499571 |
| 127 | 6 | 0 | 1.271214 | 3.729285 | 4.068076 |
| 128 | 1 | 0 | 2.003123 | 4.323224 | 4.609424 |
| 129 | 6 | 0 | 1.656536 | 2.547166 | 3.432882 |
| 130 | 1 | 0 | 2.687239 | 2.205176 | 3.478336 |
| 131 | 6 | 0 | 0.713417 | 1.787083 | 2.736739 |
| 132 | 1 | 0 | 1.019669 | 0.868334 | 2.248777 |
| 133 | 6 | 0 | -2.511085 | 0.171067 | 3.332666 |

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|---|---|---|---|---|---|
| 134 | 6 | 0 | -2.491717 | -1.229542 | 3.318777 |
| 135 | 1 | 0 | -2.112812 | -1.740930 | 2.440887 |
| 136 | 6 | 0 | -2.924750 | -1.967865 | 4.423532 |
| 137 | 1 | 0 | -2.896129 | -3.053271 | 4.385320 |
| 138 | 6 | 0 | -3.378694 | -1.310603 | 5.565933 |
| 139 | 1 | 0 | -3.714155 | -1.879960 | 6.428939 |
| 140 | 6 | 0 | -3.386017 | 0.086952 | 5.602620 |
| 141 | 1 | 0 | -3.724435 | 0.607270 | 6.495097 |
| 142 | 6 | 0 | -2.950028 | 0.820743 | 4.499858 |
| 143 | 1 | 0 | -2.945997 | 1.904444 | 4.556298 |
| 144 | 6 | 0 | 6.430906 | 0.977800 | 2.497162 |
| 145 | 6 | 0 | 7.053591 | 1.424235 | 3.603922 |
| 146 | 1 | 0 | 7.994642 | 1.966045 | 3.522299 |
| 147 | 6 | 0 | 6.427688 | 1.272658 | 4.971928 |
| 148 | 1 | 0 | 5.815038 | 2.166910 | 5.182944 |
| 149 | 1 | 0 | 7.199130 | 1.246429 | 5.750884 |
| 150 | 6 | 0 | 5.543580 | 0.016719 | 5.064939 |
| 151 | 1 | 0 | 6.180555 | -0.876506 | 5.184683 |
| 152 | 1 | 0 | 4.915251 | 0.062069 | 5.962197 |
| 153 | 6 | 0 | 4.697980 | -0.162339 | 3.825261 |
| 154 | 1 | 0 | 3.761978 | -0.711769 | 3.895513 |
| 155 | 6 | 0 | 5.136974 | 0.283316 | 2.634690 |
| 156 | 1 | 0 | 4.554619 | 0.101964 | 1.732964 |
| 157 | 6 | 0 | 6.983036 | 1.168854 | 1.107842 |
| 158 | 1 | 0 | 7.956517 | 1.669821 | 1.125379 |
| 159 | 1 | 0 | 6.301530 | 1.773704 | 0.492661 |
| 160 | 1 | 0 | 7.097359 | 0.208113 | 0.588752 |

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**3**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 32 | 0 | 0.846058 | -0.235108 | 0.356803 |
| 2 | 7 | 0 | -1.354720 | -1.831564 | -0.723764 |
| 3 | 7 | 0 | 0.921382 | -1.878750 | -0.852566 |
| 4 | 7 | 0 | 1.794894 | 1.262671 | -0.615524 |
| 5 | 7 | 0 | 3.432492 | 0.568554 | 0.746566 |
| 6 | 15 | 0 | -3.156561 | -0.793413 | 1.303718 |
| 7 | 15 | 0 | -1.192397 | 1.984383 | -0.828006 |
| 8 | 6 | 0 | -3.713304 | -1.831110 | -0.110226 |
| 9 | 6 | 0 | -5.047343 | -2.107539 | -0.425562 |
| 10 | 1 | 0 | -5.825319 | -1.844318 | 0.285482 |
| 11 | 6 | 0 | -5.396003 | -2.675697 | -1.653350 |
| 12 | 1 | 0 | -6.437069 | -2.882014 | -1.884893 |
| 13 | 6 | 0 | -4.394889 | -2.929114 | -2.593458 |
| 14 | 1 | 0 | -4.652961 | -3.324792 | -3.572806 |
| 15 | 6 | 0 | -3.058635 | -2.666197 | -2.294215 |
| 16 | 1 | 0 | -2.289951 | -2.833545 | -3.040510 |
| 17 | 6 | 0 | -2.684228 | -2.170343 | -1.031080 |
| 18 | 6 | 0 | -2.733927 | -1.966543 | 2.664060 |
| 19 | 6 | 0 | -1.741665 | -1.588518 | 3.581819 |
| 20 | 1 | 0 | -1.234095 | -0.635783 | 3.457180 |
| 21 | 6 | 0 | -1.387716 | -2.434277 | 4.634432 |
| 22 | 1 | 0 | -0.616694 | -2.128323 | 5.336600 |
| 23 | 6 | 0 | -2.012341 | -3.675390 | 4.775424 |
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| 25 | 6 | 0 | -2.993111 | -4.066988 | 3.861335 |

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|---|---|---|---|---|---|
| 26 | 1 | 0 | -3.477237 | -5.035006 | 3.962200 |
| 27 | 6 | 0 | -3.353679 | -3.217700 | 2.812667 |
| 28 | 1 | 0 | -4.114147 | -3.531328 | 2.102667 |
| 29 | 6 | 0 | -4.709823 | 0.018641 | 1.891491 |
| 30 | 6 | 0 | -5.405170 | -0.357058 | 3.050792 |
| 31 | 1 | 0 | -5.049437 | -1.186333 | 3.653992 |
| 32 | 6 | 0 | -6.557925 | 0.330418 | 3.440669 |
| 33 | 1 | 0 | -7.082980 | 0.028253 | 4.343363 |
| 34 | 6 | 0 | -7.035307 | 1.395535 | 2.676303 |
| 35 | 1 | 0 | -7.932610 | 1.927719 | 2.981273 |
| 36 | 6 | 0 | -6.348943 | 1.778681 | 1.520721 |
| 37 | 1 | 0 | -6.707646 | 2.610476 | 0.920122 |
| 38 | 6 | 0 | -5.191134 | 1.103785 | 1.137526 |
| 39 | 1 | 0 | -4.656661 | 1.420655 | 0.246468 |
| 40 | 6 | 0 | -0.263064 | -2.567480 | -0.928417 |
| 41 | 6 | 0 | -0.277846 | -4.149599 | -1.002991 |
| 42 | 6 | 0 | -1.569407 | -4.768215 | -0.407541 |
| 43 | 1 | 0 | -2.445236 | -4.660164 | -1.044586 |
| 44 | 1 | 0 | -1.801841 | -4.347199 | 0.575543 |
| 45 | 1 | 0 | -1.397526 | -5.842438 | -0.275168 |
| 46 | 6 | 0 | -0.085750 | -4.701903 | -2.436097 |
| 47 | 1 | 0 | -0.081317 | -5.798177 | -2.392793 |
| 48 | 1 | 0 | 0.862316 | -4.383328 | -2.875455 |
| 49 | 1 | 0 | -0.898850 | -4.408182 | -3.106135 |
| 50 | 6 | 0 | 0.866093 | -4.715019 | -0.125703 |
| 51 | 1 | 0 | 0.822683 | -4.320357 | 0.894060 |
| 52 | 1 | 0 | 1.849130 | -4.508391 | -0.540975 |
| 53 | 1 | 0 | 0.757098 | -5.803827 | -0.067940 |
| 54 | 6 | 0 | 2.097708 | -2.225554 | -1.588911 |
| 55 | 6 | 0 | 2.083274 | -2.041751 | -2.996931 |

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| 56 | 6 | 0 | 3.230478 | -2.335986 | -3.736959 |
| 57 | 1 | 0 | 3.203364 | -2.196935 | -4.816492 |
| 58 | 6 | 0 | 4.408610 | -2.789690 | -3.134186 |
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| 60 | 1 | 0 | 5.318636 | -3.264595 | -1.249231 |
| 61 | 6 | 0 | 3.291981 | -2.634793 | -0.953830 |
| 62 | 6 | 0 | 0.857293 | -1.524765 | -3.714524 |
| 63 | 1 | 0 | 1.129475 | -1.126276 | -4.696574 |
| 64 | 1 | 0 | 0.365549 | -0.730747 | -3.147128 |
| 65 | 1 | 0 | 0.112869 | -2.314255 | -3.877223 |
| 66 | 6 | 0 | 5.643326 | -3.081644 | -3.955534 |
| 67 | 1 | 0 | 6.196280 | -2.161700 | -4.189926 |
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| 70 | 6 | 0 | 3.427890 | -2.803676 | 0.543753 |
| 71 | 1 | 0 | 2.503564 | -2.571008 | 1.072475 |
| 72 | 1 | 0 | 4.206604 | -2.144287 | 0.936820 |
| 73 | 1 | 0 | 3.713678 | -3.833194 | 0.794603 |
| 74 | 6 | 0 | 1.425225 | 1.715975 | -1.894010 |
| 75 | 6 | 0 | 2.355620 | 1.697147 | -2.948057 |
| 76 | 1 | 0 | 3.351034 | 1.309980 | -2.750368 |
| 77 | 6 | 0 | 2.018864 | 2.155516 | -4.220004 |
| 78 | 1 | 0 | 2.762844 | 2.137732 | -5.012521 |
| 79 | 6 | 0 | 0.728458 | 2.618733 | -4.473537 |
| 80 | 1 | 0 | 0.453088 | 2.979490 | -5.460666 |
| 81 | 6 | 0 | -0.220700 | 2.598324 | -3.448310 |
| 82 | 1 | 0 | -1.229690 | 2.937603 | -3.658898 |
| 83 | 6 | 0 | 0.096136 | 2.145166 | -2.160358 |
| 84 | 6 | 0 | -2.772140 | 2.307725 | -1.748458 |
| 85 | 6 | 0 | -3.265171 | 1.277163 | -2.570768 |

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| 86 | 1 | 0 | -2.700467 | 0.355006 | -2.673077 |
| 87 | 6 | 0 | -4.477160 | 1.418118 | -3.244469 |
| 88 | 1 | 0 | -4.838599 | 0.607447 | -3.871155 |
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| 90 | 1 | 0 | -6.179301 | 2.694173 | -3.617672 |
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| 92 | 1 | 0 | -5.336246 | 4.523539 | -2.156493 |
| 93 | 6 | 0 | -3.537400 | 3.475085 | -1.608960 |
| 94 | 1 | 0 | -3.189549 | 4.283085 | -0.974562 |
| 95 | 6 | 0 | -0.965494 | 3.502103 | 0.203771 |
| 96 | 6 | 0 | -0.697357 | 4.768854 | -0.340841 |
| 97 | 1 | 0 | -0.585193 | 4.882788 | -1.415850 |
| 98 | 6 | 0 | -0.567198 | 5.883763 | 0.488743 |
| 99 | 1 | 0 | -0.360496 | 6.858675 | 0.054837 |
| 100 | 6 | 0 | -0.694534 | 5.745580 | 1.873665 |
| 101 | 1 | 0 | -0.588032 | 6.613671 | 2.518907 |
| 102 | 6 | 0 | -0.953451 | 4.489858 | 2.425646 |
| 103 | 1 | 0 | -1.049158 | 4.376033 | 3.502288 |
| 104 | 6 | 0 | -1.089310 | 3.374675 | 1.594763 |
| 105 | 1 | 0 | -1.290340 | 2.393401 | 2.016654 |
| 106 | 6 | 0 | 2.983693 | 1.562320 | 0.036624 |
| 107 | 6 | 0 | 3.549604 | 3.030812 | 0.081079 |
| 108 | 6 | 0 | 2.854206 | 4.044141 | -0.851702 |
| 109 | 1 | 0 | 3.224765 | 5.043964 | -0.594490 |
| 110 | 1 | 0 | 1.771807 | 4.053937 | -0.721154 |
| 111 | 1 | 0 | 3.075692 | 3.873842 | -1.906431 |
| 112 | 6 | 0 | 5.055947 | 3.074178 | -0.251747 |
| 113 | 1 | 0 | 5.256645 | 2.664194 | -1.247765 |
| 114 | 1 | 0 | 5.659133 | 2.534093 | 0.478621 |
| 115 | 1 | 0 | 5.388958 | 4.119199 | -0.252091 |

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|---|---|---|---|---|---|
| 116 | 6 | 0 | 3.341055 | 3.556509 | 1.524483 |
| 117 | 1 | 0 | 3.892520 | 2.968655 | 2.259643 |
| 118 | 1 | 0 | 2.278607 | 3.559713 | 1.792420 |
| 119 | 1 | 0 | 3.702466 | 4.590226 | 1.583941 |
| 120 | 6 | 0 | 4.470987 | 0.483687 | 1.687689 |
| 121 | 6 | 0 | 5.782229 | 0.121196 | 1.286461 |
| 122 | 6 | 0 | 6.771057 | -0.057531 | 2.262531 |
| 123 | 1 | 0 | 7.774702 | -0.325468 | 1.935014 |
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| 125 | 6 | 0 | 5.195747 | 0.350458 | 4.005938 |
| 126 | 1 | 0 | 4.949340 | 0.405356 | 5.065242 |
| 127 | 6 | 0 | 4.169489 | 0.529437 | 3.076927 |
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| 130 | 1 | 0 | 6.893034 | -0.907529 | -0.244065 |
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| 132 | 6 | 0 | 7.609149 | -0.080656 | 4.656408 |
| 133 | 1 | 0 | 8.002191 | 0.892909 | 4.981181 |
| 134 | 1 | 0 | 8.453585 | -0.654216 | 4.258597 |
| 135 | 1 | 0 | 7.246814 | -0.595040 | 5.554295 |
| 136 | 6 | 0 | 2.749855 | 0.705991 | 3.561642 |
| 137 | 1 | 0 | 2.321307 | 1.674389 | 3.280312 |
| 138 | 1 | 0 | 2.703601 | 0.624020 | 4.652771 |
| 139 | 1 | 0 | 2.093822 | -0.057285 | 3.128418 |
| 140 | 28 | 0 | -1.396736 | 0.018824 | 0.047645 |

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