Electronic Supplementary Material (ESI) for Dalton Transactions.

ELECTRONIC SUPPLEMENTARY INFORMATION

A dipyrromethane-based diphosphane–germylene as precursor to tetrahedral copper(I) and T-shaped silver(I) and gold(I) PGeP pincer complexes

Javier A. Cabeza,*[a] Israel Fernández,[b] Pablo García-Álvarez,[a] and Carlos J. Laglera-Gándara[a]

[a]*Centro de Innovación en Química Avanzada (ORFEO-CINQA Network), Departamento de Química Orgánica e Inorgánica, Universidad de Oviedo, 33071 Oviedo, Spain*

[b]*Centro de Innovación en Química Avanzada (ORFEO-CINQA Network), Departamento de Química Orgánica, Facultad de Ciencias Químicas, Universidad Complutense de Madrid, 28040 Madrid, Spain*

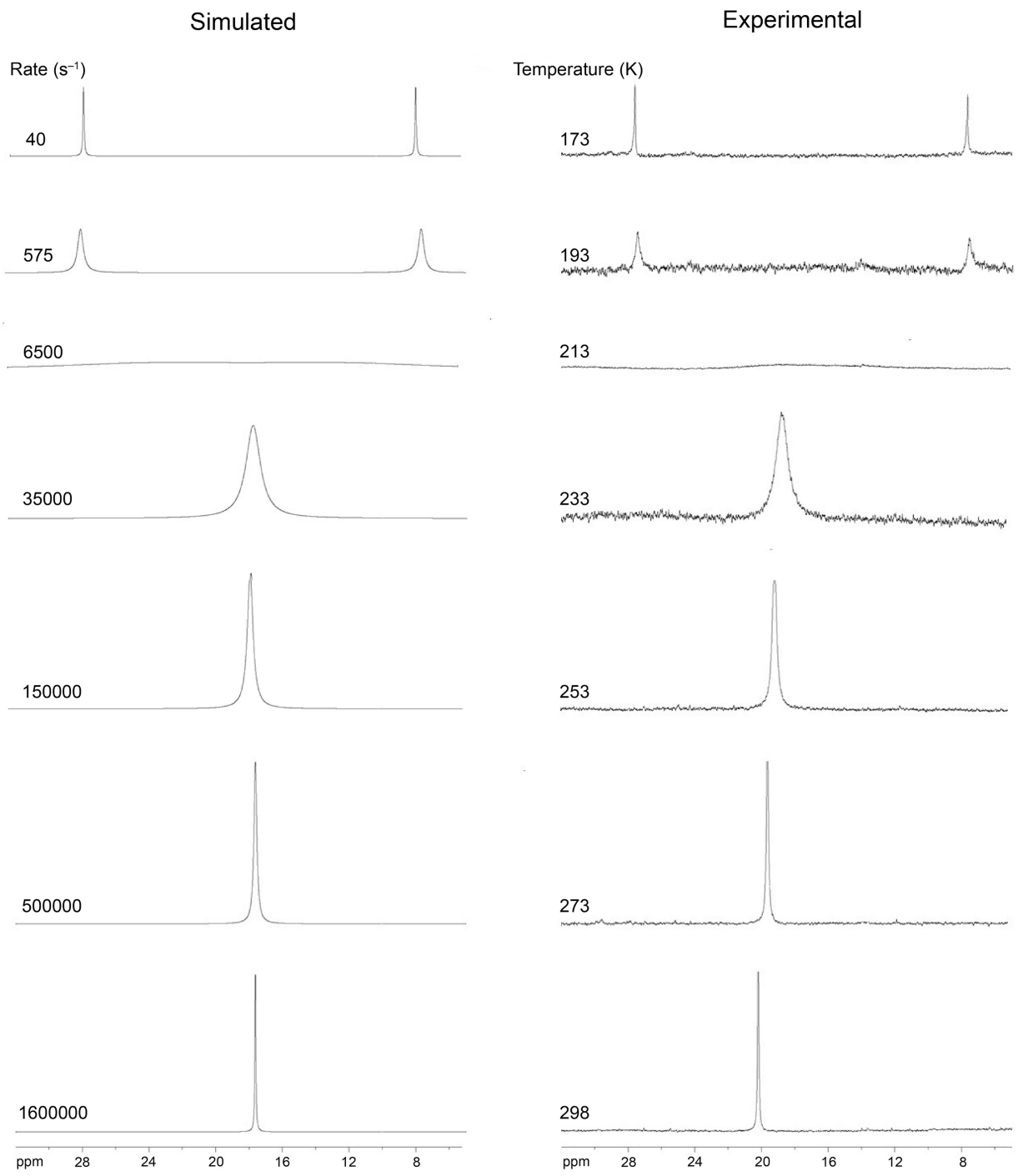
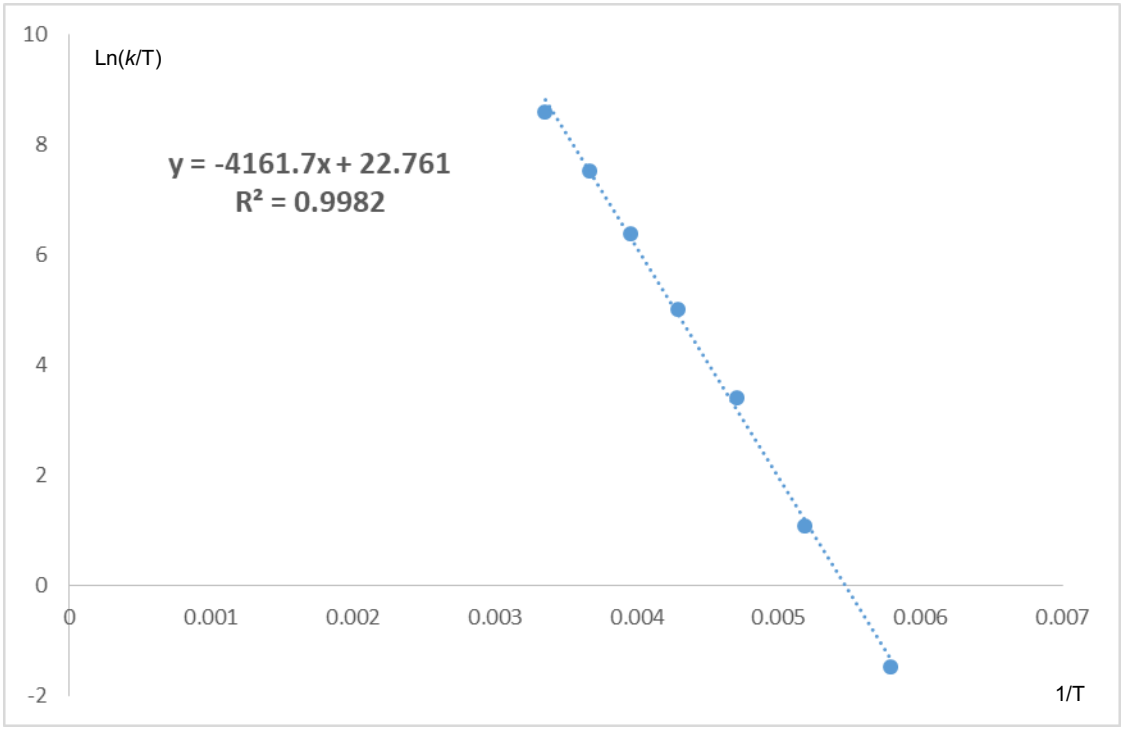


Figure S1. Simulated (left) and experimental (right) variable temperature $^{31}P\{^{1}H\}$ NMR (162.0 MHz) spectra of germylene **1** in 1/1 toluene/dichloromethane-D_2 solution.



T (K)	1/T	k (s^{-1})	k/T	Ln(k/T)	Lnk
298	0.00335458	1600000	5367.3264	8.58808519	14.2855142
273	0.00366435	500000	1832.17296	7.51325795	13.1223634
253	0.00395413	150000	593.11981	6.38539642	11.9183906
233	0.00429185	35000	150.214592	5.01206489	10.4631033
213	0.00470146	6500	30.5594734	3.41967473	8.77955746
193	0.00518672	575	2.98236515	1.09271666	6.35437004
173	0.00579039	40	0.23161552	-1.46267653	3.68887945

$$\Delta H^{\neq} = 8.27\ \frac{\text{kcal}}{\text{mol}} \quad \Delta S^{\neq} = -1.98\ \frac{\text{cal}}{\text{K mol}} \quad \Delta G^{\neq}(298.15) = 8.86\ \frac{\text{kcal}}{\text{mol}}$$

Figure S2. Eyring plot (data obtained from Figure S1) and activation parameters for the intramolecular exchange process occurring in solution in germylene **1**.

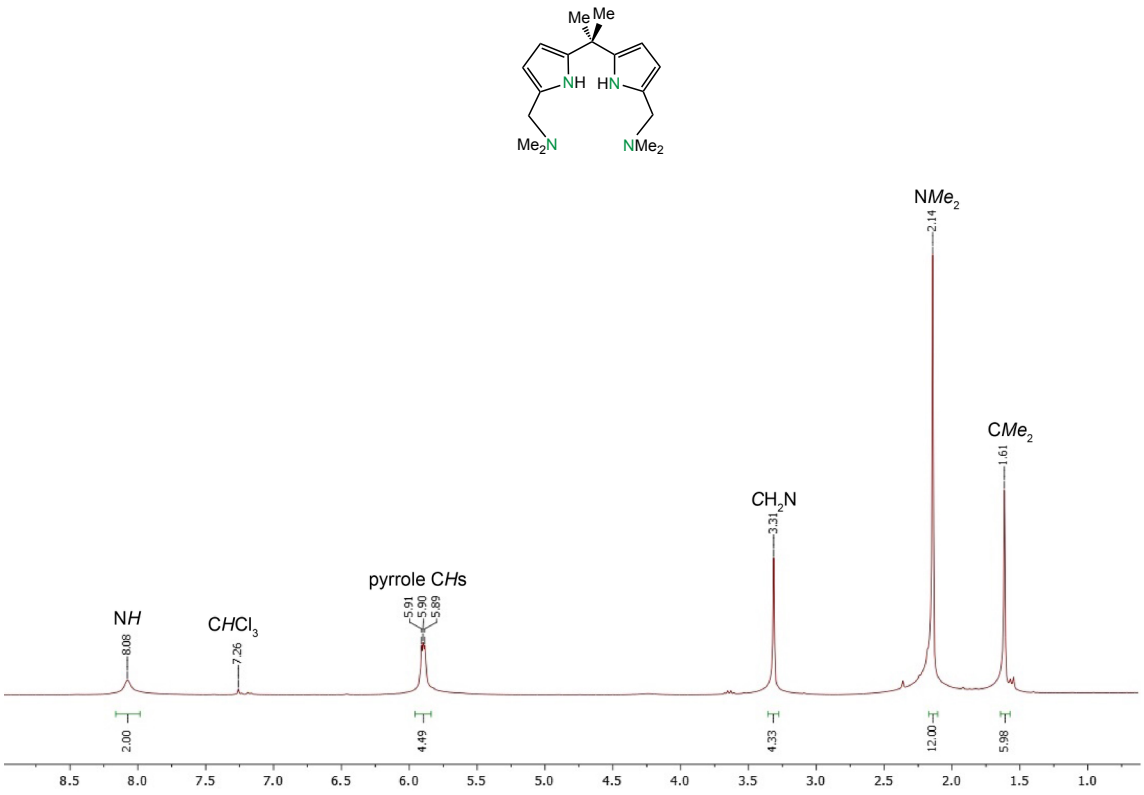


Figure S3. ^{1}H NMR spectrum (300.1 MHz, $CDCl_3$, 298 K) of $(HpyrmNMe_2)_2CMe_2$.

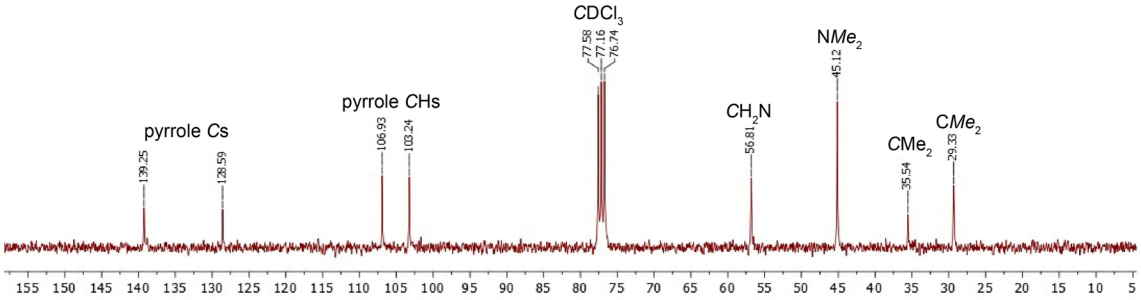


Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum (75.5 MHz, $CDCl_3$, 298 K) of $(HpyrmNMe_2)_2CMe_2$.

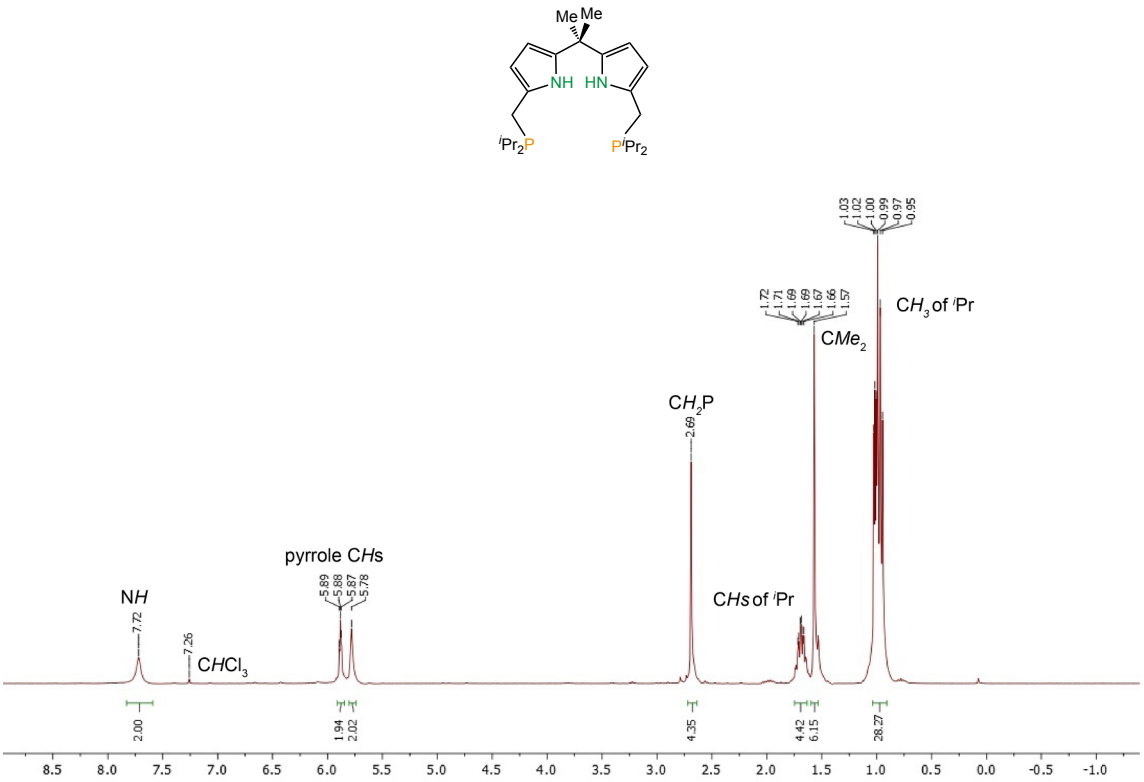


Figure S5. ^{1}H NMR spectrum (300.1 MHz, $CDCl_3$, 298 K) of $(HpyrmP^{i}Pr_2)_2CMe_2$.

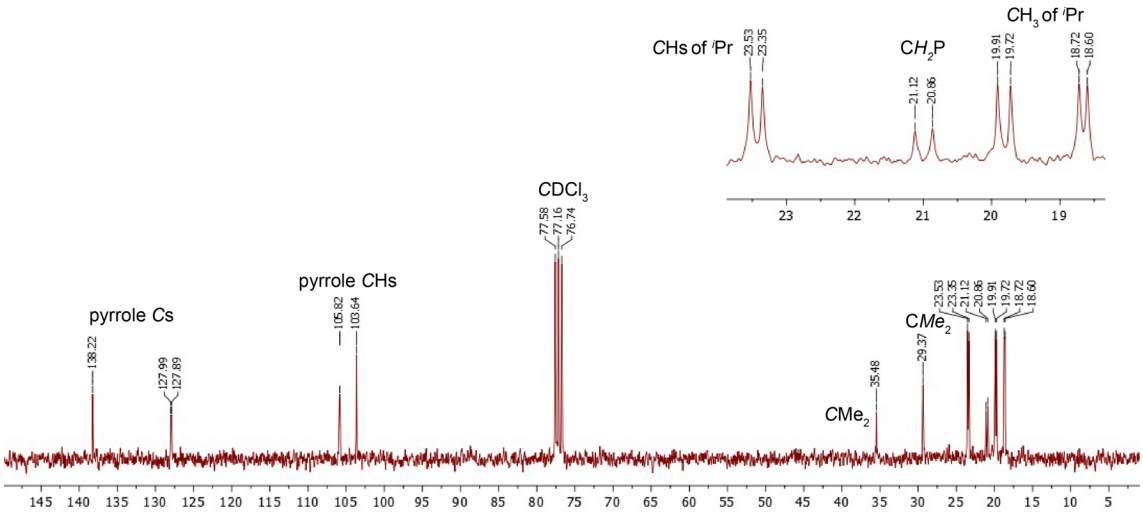
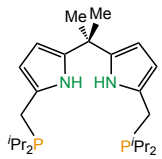


Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum (75.5 MHz, $CDCl_3$, 298 K) of $(HpyrmP^{i}Pr_2)_2CMe_2$.



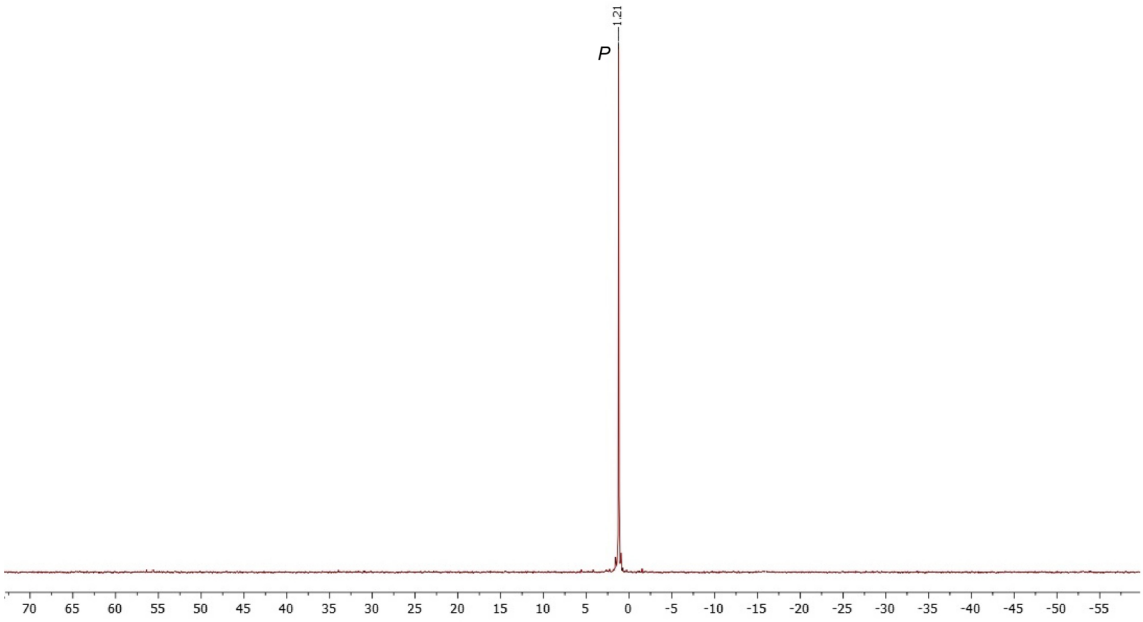


Figure S7. $^{31}P\{^{1}H\}$ NMR spectrum (121.5 MHz, $CDCl_3$, 298 K) of $(HpyrmP^{i}Pr_2)_2CMe_2$.

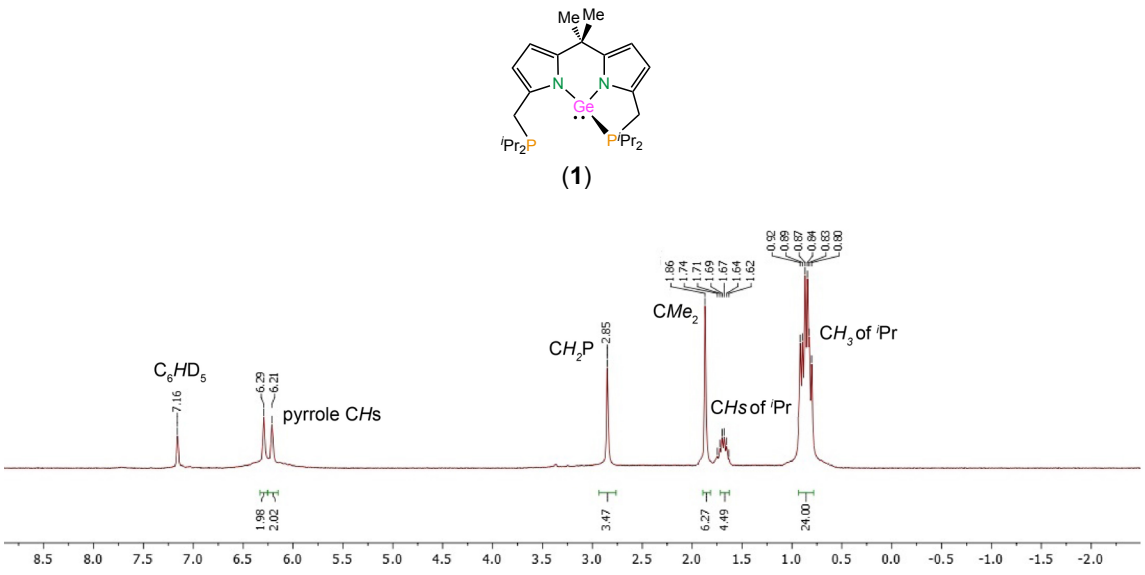


Figure S8. ^{1}H NMR spectrum (300.1 MHz, C_6D_6, 298 K) of Ge(pyrmP^{i}Pr$_2$)$_2$CMe$_2$ (**1**).

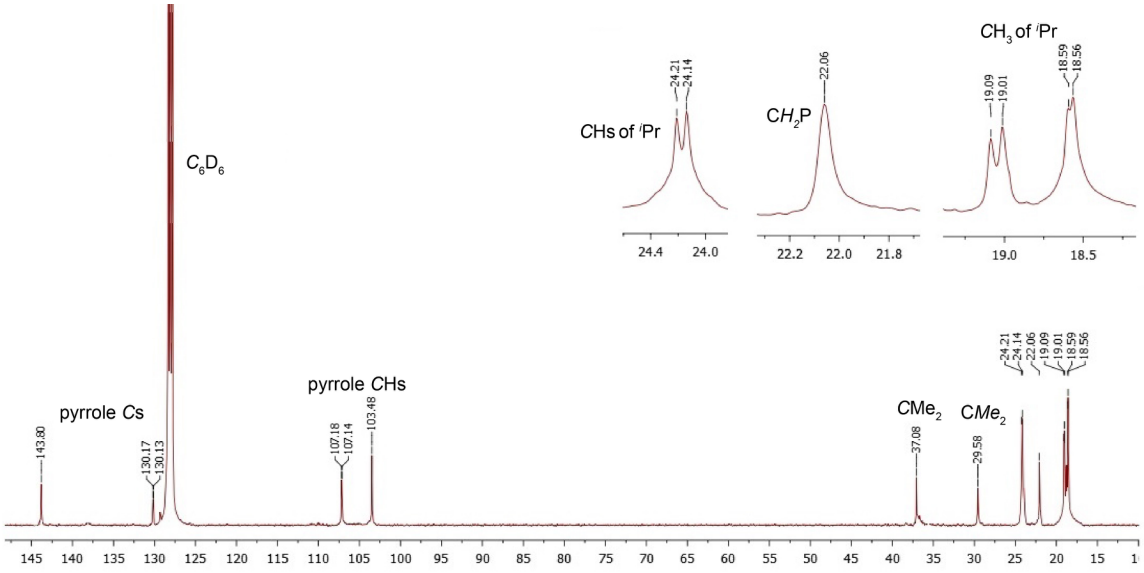
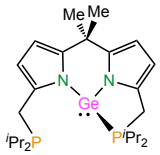


Figure S9. ^{13}C{^{1}H} NMR spectrum (100.6 MHz, C_6D_6, 298 K) of Ge(pyrmP^{i}Pr$_2$)$_2$CMe$_2$ (**1**).



(**1**)

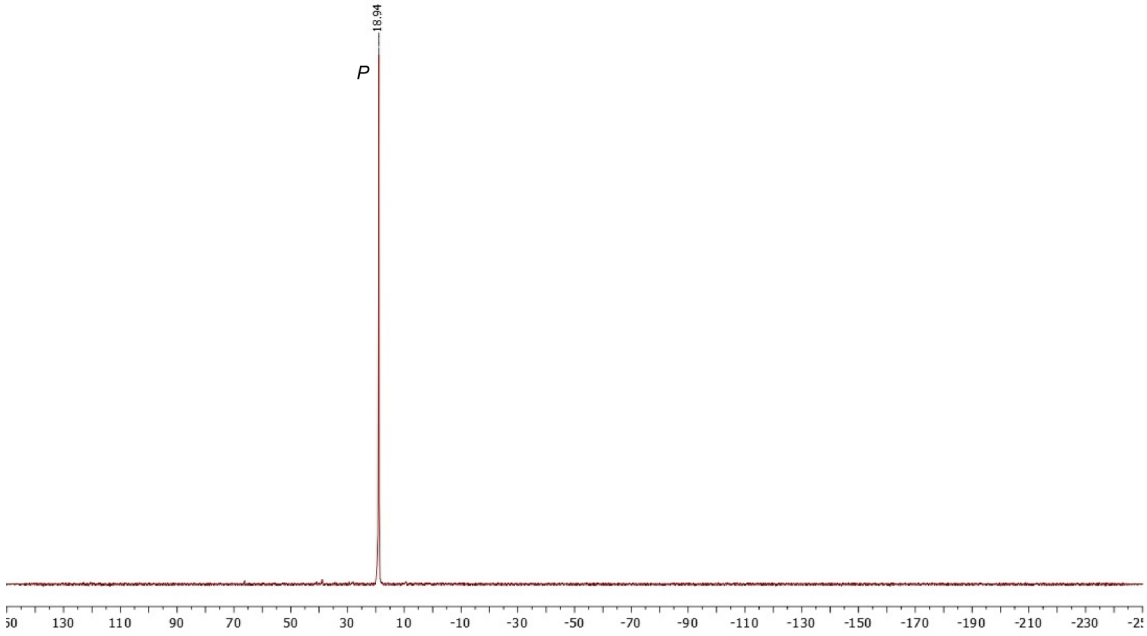


Figure S10. $^{31}P\{^{1}H\}$ NMR spectrum (121.5 MHz, C_6D_6, 298 K) of Ge(pyrmP^{i}Pr$_2$)$_2$CMe$_2$ (**1**).

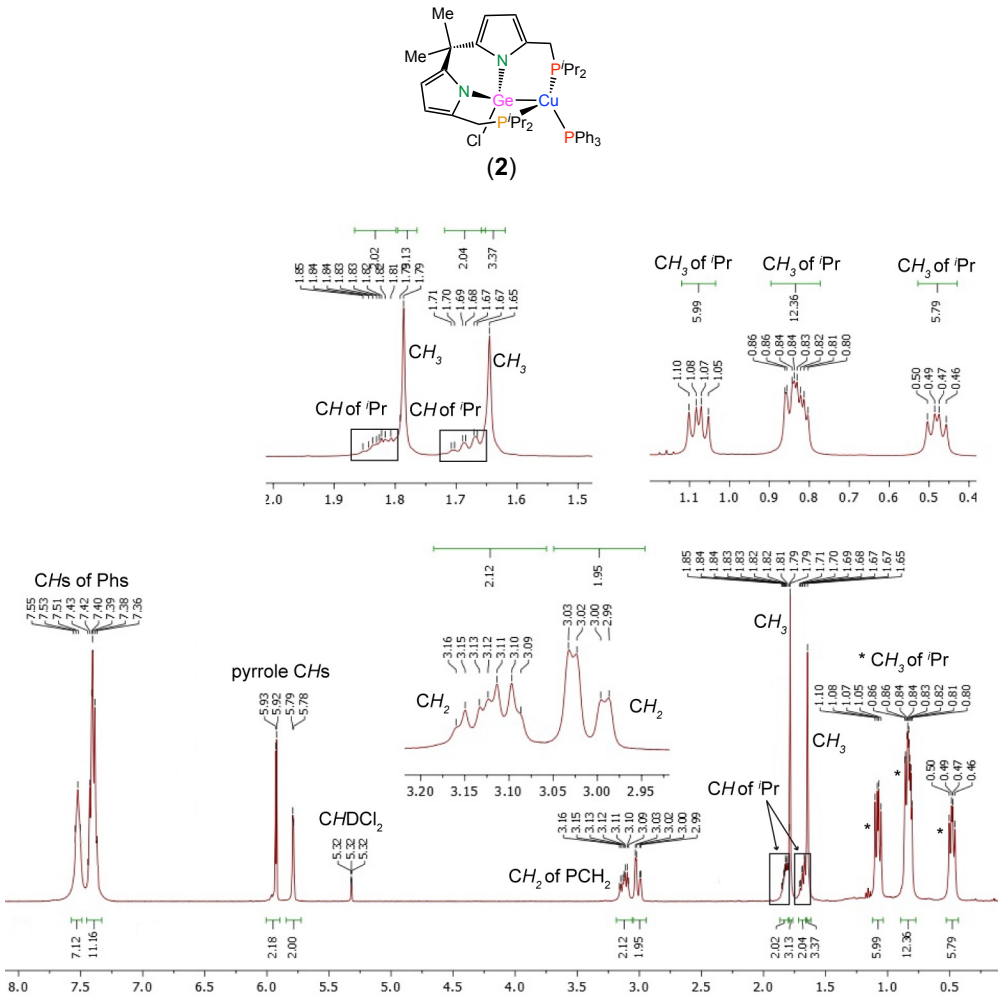


Figure S11. ^{1}H NMR spectrum (400.5 MHz, CD_2Cl_2, 298 K) of [Cu{κ^3*P*,*Ge*,*P*-GeCl(pyrmP^{i}Pr$_2$)$_2$CMe$_2$}(PPh$_3$)] (**2**).

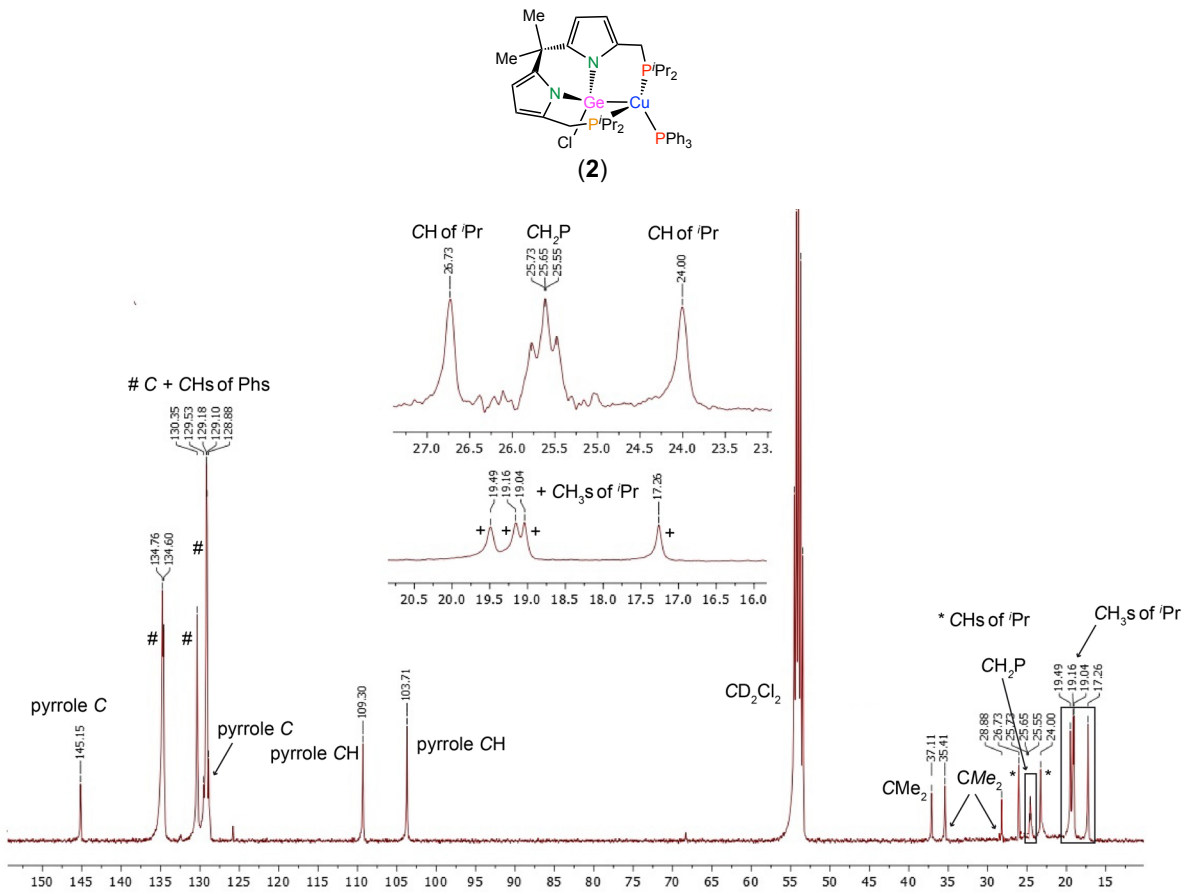


Figure S12. $^{13}C\{^1H\}$ NMR spectrum (100.6 MHz, CD_2Cl_2, 298 K) of [Cu{κ^3*P*,*Ge*,*P*-GeCl(pyrmP^{i}Pr$_2$)$_2$CMe$_2$}(PPh$_3$)] (**2**).

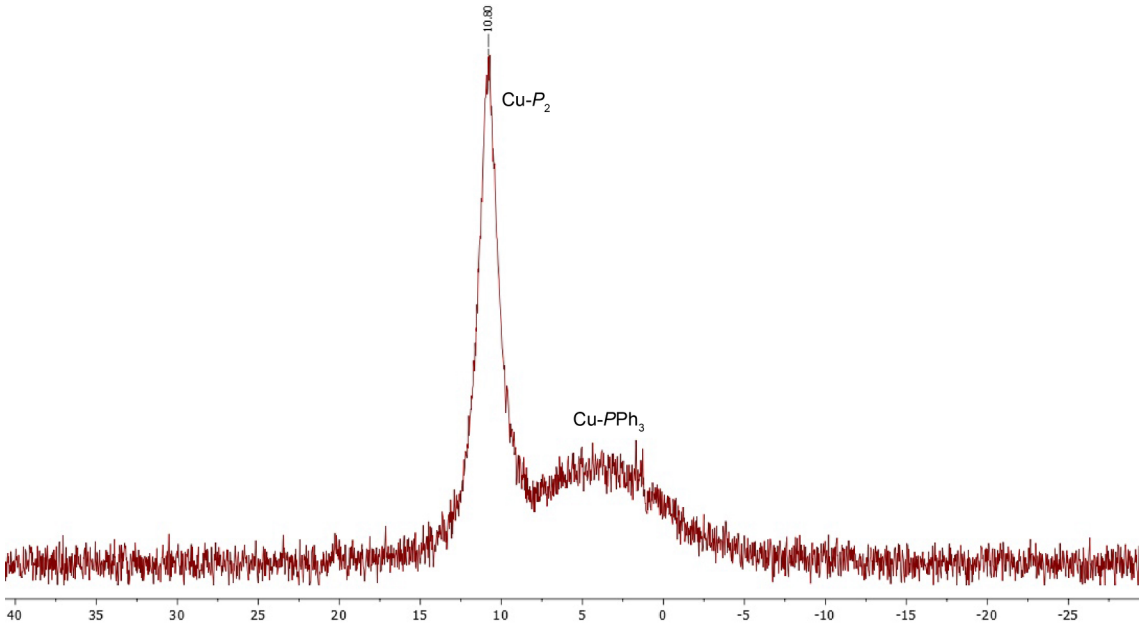


Figure S13. $^{31}P\{^1H\}$ NMR spectrum (162.1 MHz, CD_2Cl_2, 298 K) of [Cu{κ^3*P*,*Ge*,*P*-GeCl(pyrmP^{i}Pr$_2$)$_2$CMe$_2$}(PPh$_3$)] (**2**).

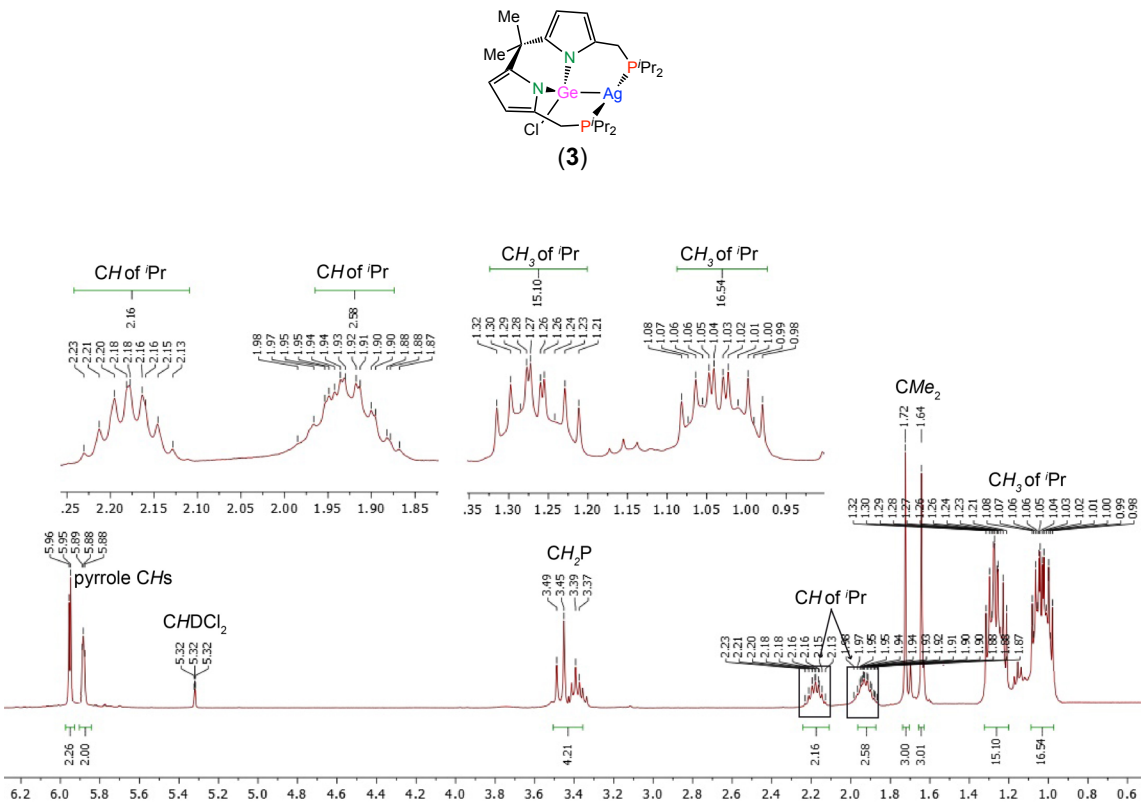


Figure S14. ^{1}H NMR spectrum (400.5 MHz, CD_2Cl_2, 298 K) of [Ag{κ^3*P*,*Ge*,*P*-GeCl(pyrmP^{i}Pr$_2$)$_2$CMe$_2$}] (**3**).

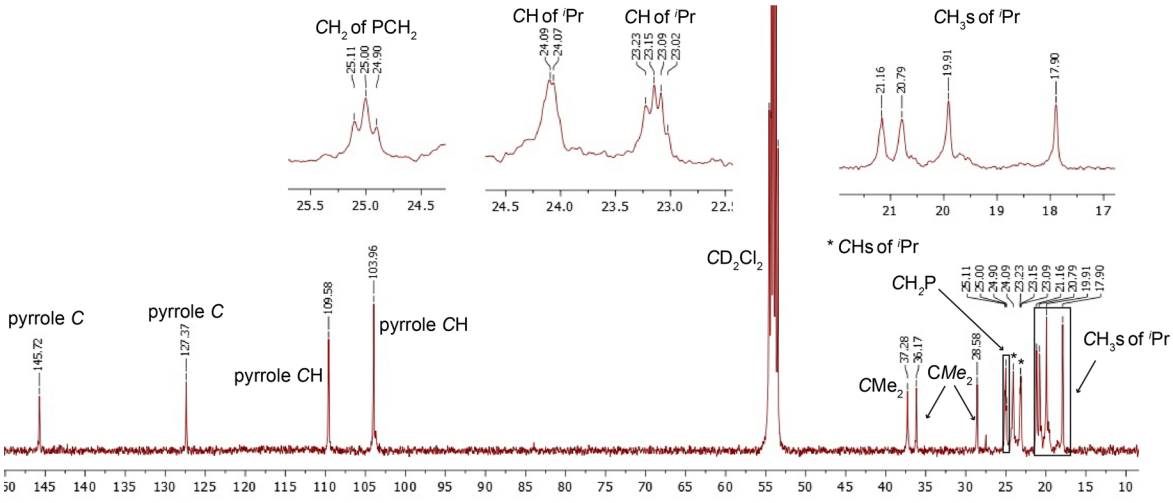


Figure S15. ^{13}C{^{1}H} NMR spectrum (100.6 MHz, CD_2Cl_2, 298 K) of [Ag{κ^3*P*,*Ge*,*P*-GeCl(pyrmP^{i}Pr$_2$)$_2$CMe$_2$}] (**3**).

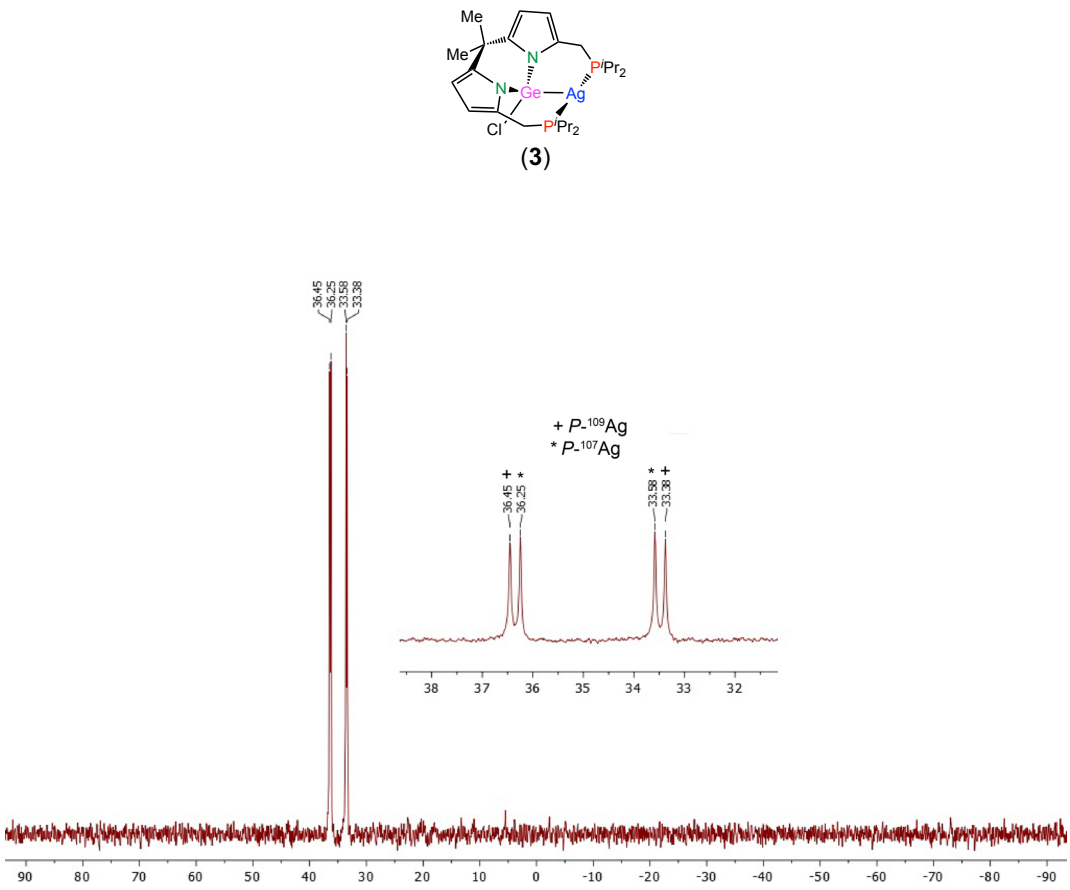
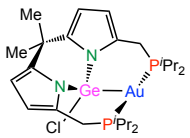


Figure S16. $^{31}P\{^{1}H\}$ NMR spectrum (162.1 MHz, CD_2Cl_2, 298 K) of [Ag{κ^3*P*,*Ge*,*P*-GeCl(pyrmP^{i}Pr$_2$)$_2$CMe$_2$}] (**3**).



(**4**)

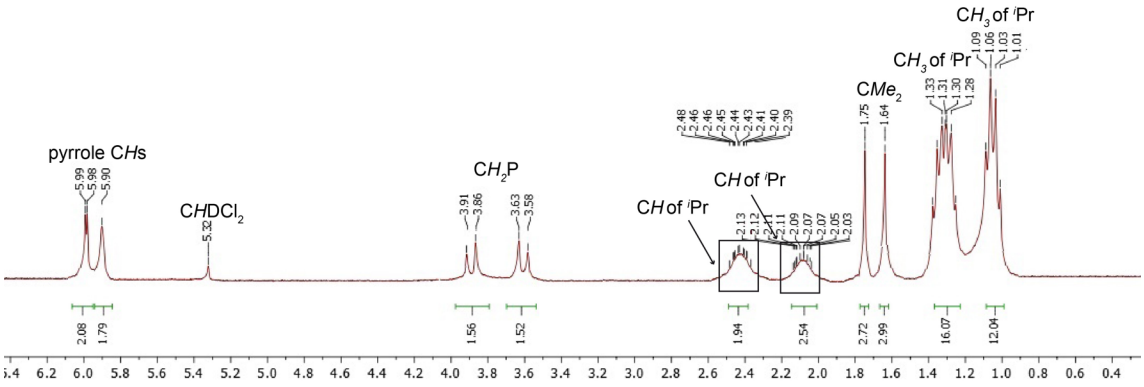


Figure S17. ^{1}H NMR spectrum (300.1 MHz, CD_2Cl_2, 298 K) of [Au{κ^3*P*,*Ge*,*P*-GeCl(pyrmP^{i}Pr$_2$)$_2$CMe$_2$}] (**4**).

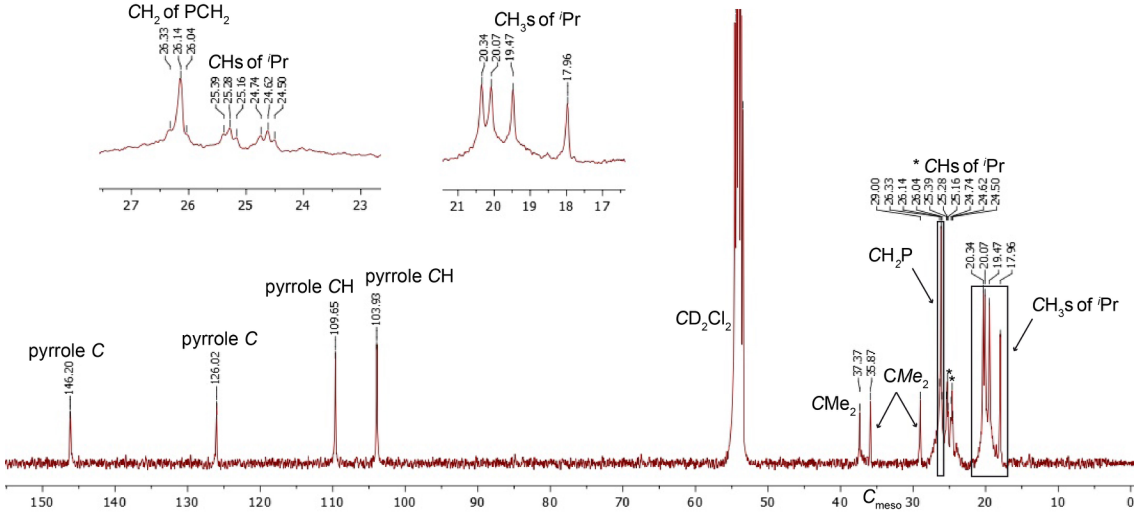
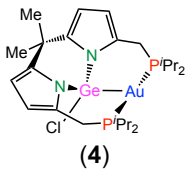


Figure S18. ^{13}C{^{1}H} NMR spectrum (100.6 MHz, CD_2Cl_2, 298 K) of [Au{κ^3*P*,*Ge*,*P*-GeCl(pyrmP^{i}Pr$_2$)$_2$CMe$_2$}] (**4**).



(**4**)

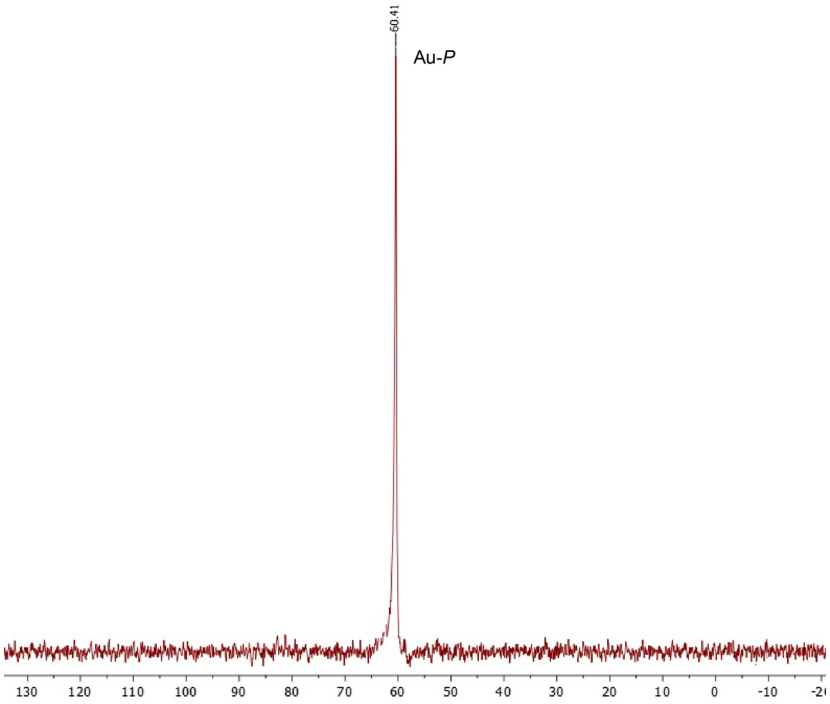


Figure S19. $^{31}P\{^{1}H\}$ NMR spectrum (121.5MHz, CD_2Cl_2, 298 K) of [Au{κ^3*P*,*Ge*,*P*-GeCl(pyrmP^{i}Pr$_2$)$_2$CMe$_2$}] (**4**)

.

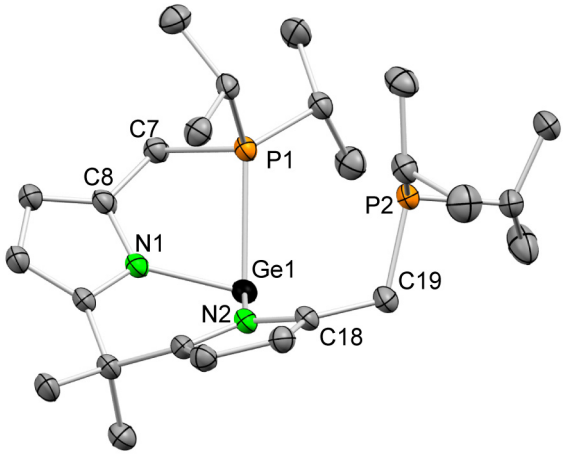


Figure S20. XRD molecular structure of germylene **1** (30% displacement ellipsoids, H atoms have been omitted for clarity). Selected bond lengths (Å) and angles (°): Ge1−N1 1.950(3), Ge1−N2 1.939(3), Ge1−P1 2.515(1), Ge1···P2 3.936(1), C7−P1 1.852(4), C7−C8 1.500(5), C8−N1 1.377(5), C18−N2 1.389(5), C18−C19 1.497(5), C19−P2 1.860(4), N1−Ge1−N2 88.5(1), N1−Ge1−P1 77.31(9), N2−Ge1−P2 65.6(1).

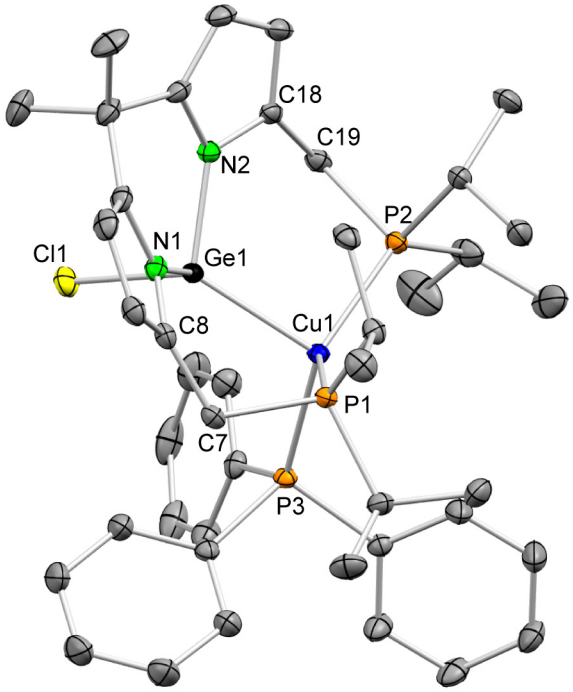


Figure S21. XRD molecular structure of complex **2** (30 % displacement ellipsoids, H atoms have been omitted for clarity). Selected bond lengths (Å) and angles (°): Cu1−P1 2.3267(5), Cu1−P2 2.3128(5), Cu1−P3 2.3089(5), Cu1−Ge1 2.3580(3), Ge1−Cl1 2.2631(5), Ge1−N1 1.903(2), Ge1−N2 1.903(2), C7−P1 1.863(2), C7−C8 1.502(3), C8−N1 1.389(3), C18−N2 1.388(3), C18−C19 1.492(3), C19−P2 1.864(2), N1−Ge1−N2 91.92(7), N1−Ge1−Cu1 114.70(5), N2−Ge1−Cu1 114.40(5), N1−Ge1−Cl1 101.91(5), N2−Ge1−Cl1 99.36(5), Cl1−Ge1−Cu1 127.87(2), P1−Cu1−P2 125.60(2), P1−Cu1−Ge1 92.87(2), P2−Cu1−Ge1 95.80(2), P1−Cu1−P3 103.78(2), P2−Cu1−P3 122.83(2), P3−Cu1−Ge1 109.83(2).

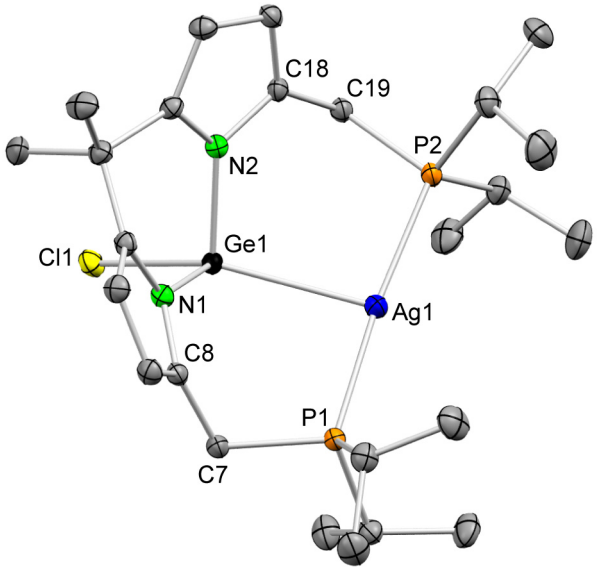


Figure S22. XRD molecular structure of complex **3** (30 % displacement ellipsoids, H atoms have been omitted for clarity). Selected bond lengths (Å) and angles (°): Ag1−P1 2.408(1), Ag1−P2 2.405(1), Ag1−Ge1 2.716(1), Ge1−Cl1 2.323(1), Ge1−N1 1.932(3), Ge1−N2 1.921(2), C7−P1 1.848(3), C7−C8 1.501(4), C8−N1 1.385(4), C18−N2 1.388(4), C18−C19 1.499(4), C19−P2 1.848(3), N1−Ge1−N2 90.9(1), N1−Ge1−Ag1 98.99(8), N2−Ge1−Ag1 98.85(8), N1−Ge1−Cl1 99.61(8), N2−Ge1−Cl1 101.49(8), Cl1−Ge1−Ag1 152.09(3), P1−Ag1−P2 173.49(3), P1−Ag1−Ge1 92.30(2), P2−Ag1−Ge1 93.54(2).

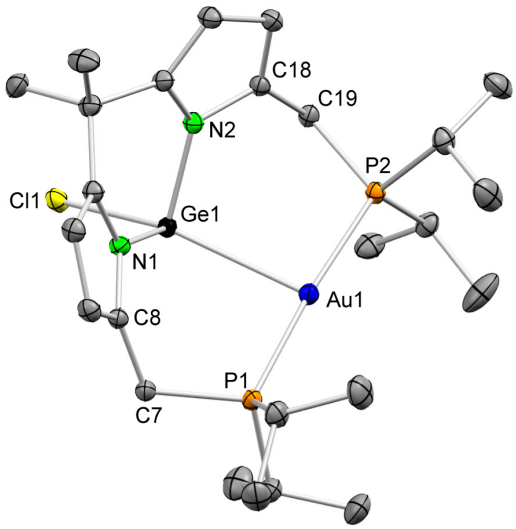
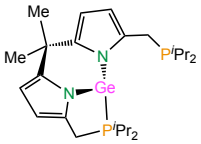
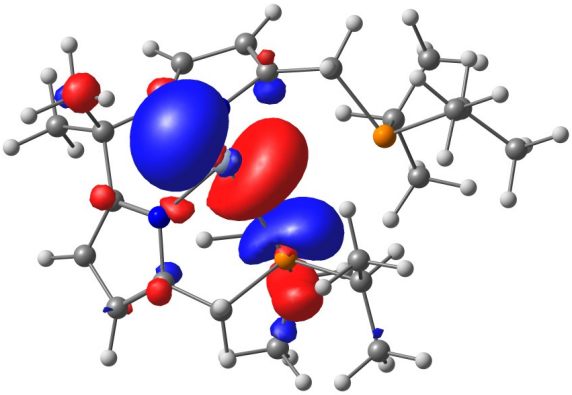


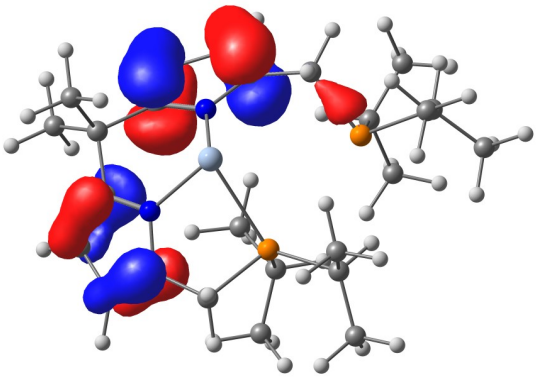
Figure S23. XRD molecular structure of complex **4** (45 % displacement ellipsoids, H atoms have been omitted for clarity). Selected bond lengths (Å) and angles (°): Au1−P1 2.325(1), Au1−P2 2.3254(9), Au1−Ge1 2.7604(4), Ge1−Cl1 2.3534(9), Ge1−N1 1.929(3), Ge1−N2 1.935(3), C7−P1 1.840(4), C7−C8 1.498(5), C8−N1 1.391(5), C18−N2 1.389(5), C18−C19 1.497(5), C19−P2 1.840(4), N1−Ge1−N2 89.8(1), N1−Ge1−Au1 97.05(9), N2−Ge1−Au1 97.11(9), N1−Ge1−Cl1 100.74(9), N2−Ge1−Cl1 99.44(9), Cl1−Ge1−Au1 155.66(3), P1−Au1−P2 175.30(3), P1−Au1−Ge1 92.75(2), P2−Au1−Ge1 91.95(2).



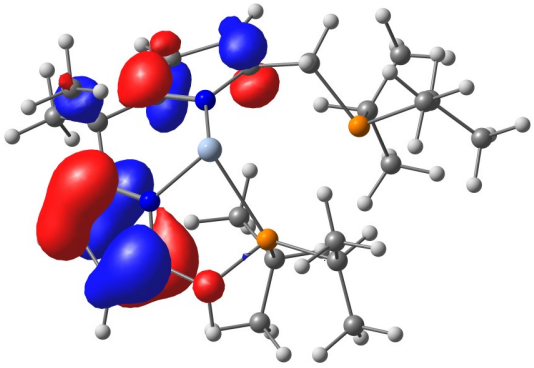
(**1**)



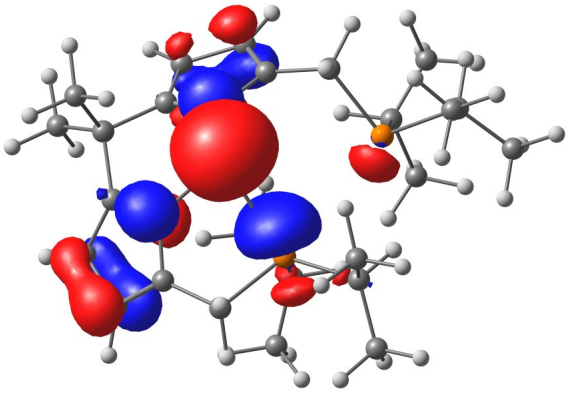
LUMO



HOMO

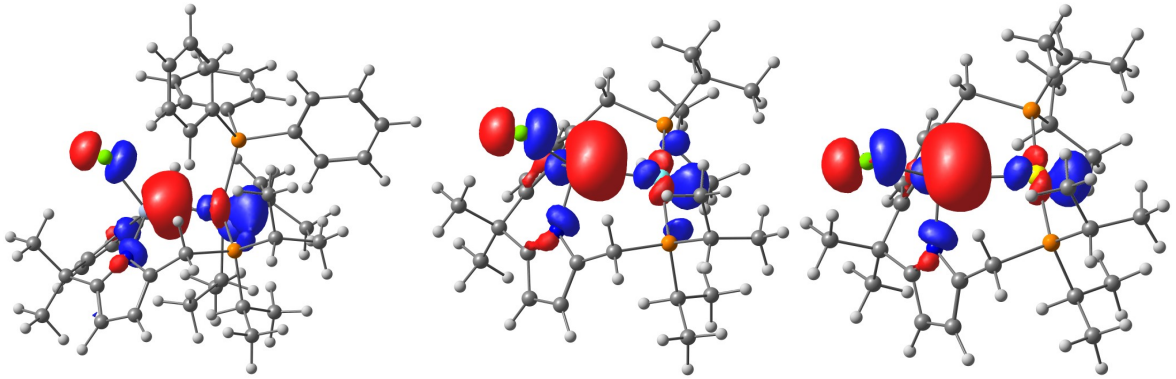


HOMO–1



HOMO–2

Figure S24. Selected NBO frontier molecular orbitals of germylene **1**.



(**2**) (**3**) (**4**)

Figure S25. NBO HOMO–2 orbitals of compounds **2**–**4**, showing the important contribution of the Ge lone pair (large red lobe) to each orbital.

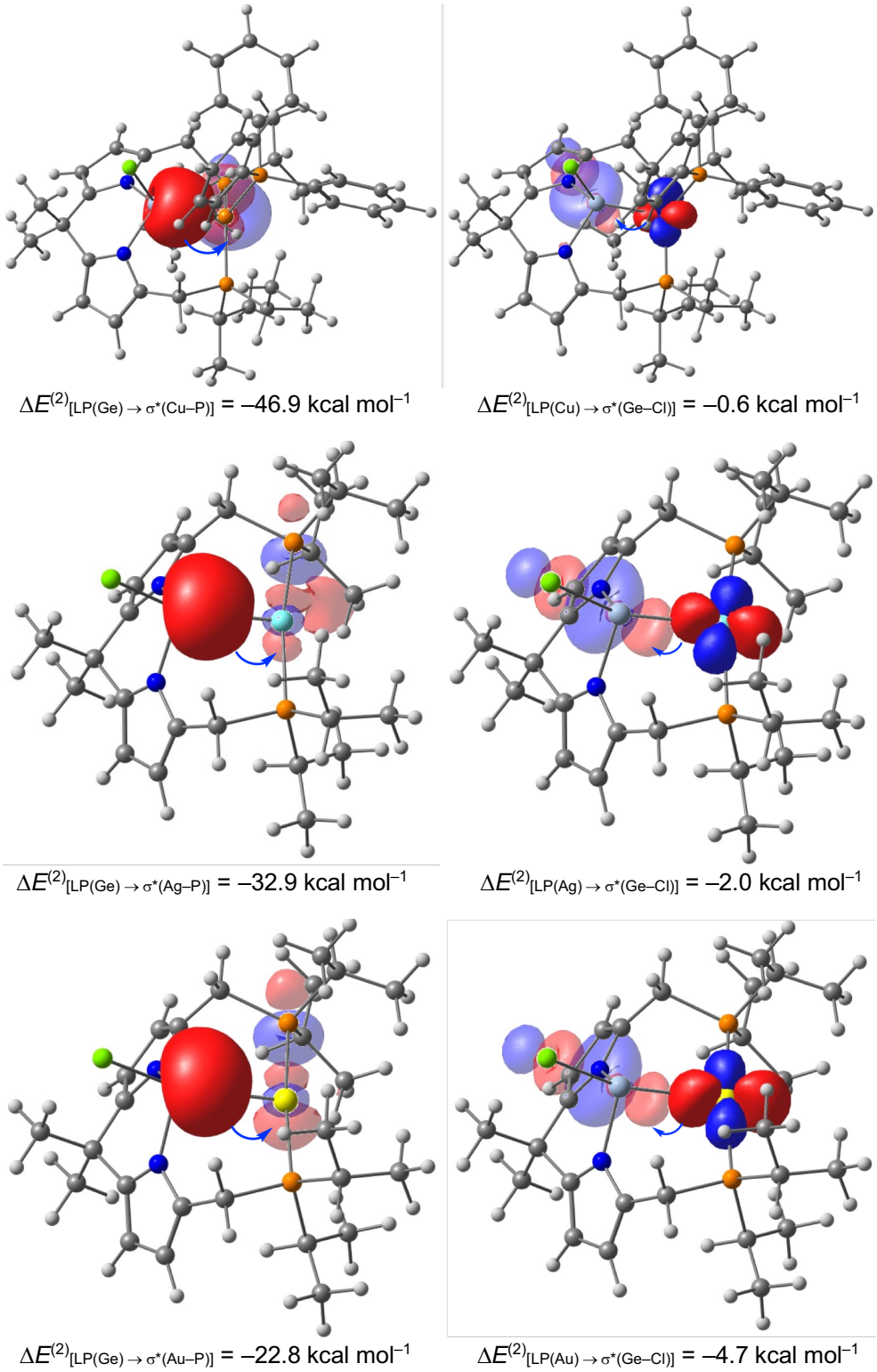
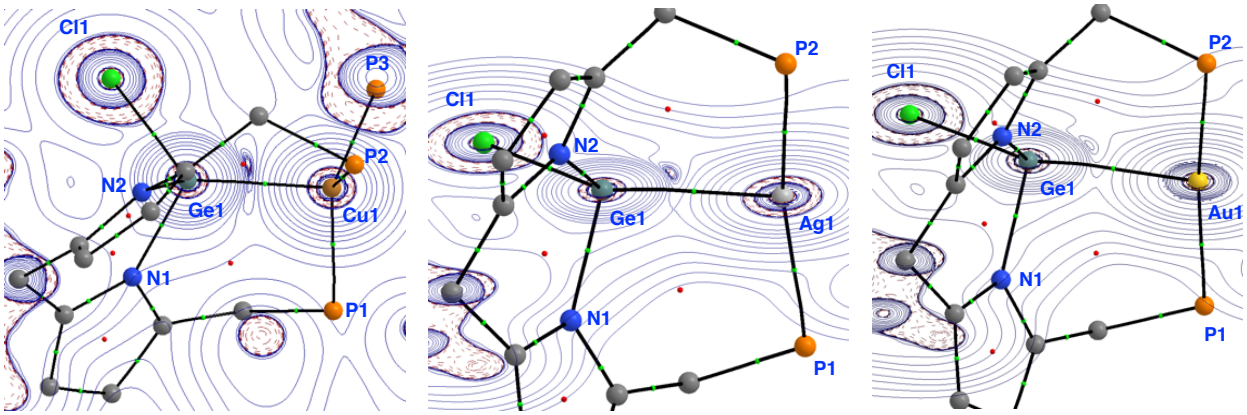


Figure S26. SOPT-NBO donor–acceptor interactions in complexes **2** (top)**, 3** (middle) and **4** (bottom). The donor and acceptor orbitals are represented with bright and faded colors, respectively.



(**2**) (**3**) (**4**)

Figure S27. QTAIM plots of selected portions of complexes **2**–**4**, showing the electron density Laplacian map on the planes Cl1–Ge1–Cu1–P3 (**2**), Cl1–Ge1–Ag1 (**3**) and Cl1–Ge1–Au1 (**4**), the bond paths (black lines) and the bond (small green circles) and ring (small red circles) critical points.

Table S1. Crystal, measurement, and refinement data for the compounds studied by X-ray diffraction.

	1	**2**	**3**·CD_2Cl_2	**4**·CH_2Cl_2
formula	$C_{25}H_{42}GeN_2P_2$	$C_{43}H_{57}ClCuGeN_2P_3$	$C_{25}H_{42}AgClGeN_2P_2 \cdot CD_2Cl_2$	$C_{25}H_{42}AuClGeN_2P_2 \cdot CH_2Cl_2$
fw	505.13	866.39	735.39	822.48
cryst syst	monoclinic	monoclinic	triclinic	triclinic
space group	*P*21/n	*P*21/c	*P*–1	*P*–1
a, Å	11.4095(6)	15.9072(2)	11.156(5)	11.1202(9)
b, Å	17.4206(7)	13.5272(2)	11.334(5)	11.3734(9)
c, Å	14.3260(6)	19.6745(2)	13.448(5)	13.369(1)
α, deg	90	90	91.841(5)	91.388(4)
β, deg	112.581(6)	92.328(1)	109.257(5)	109.574(4)
γ, deg	90	90	92.640(5)	92.995(4)
V, Å^3	2629.1(2)	4230.06(9)	1602(1)	1589.4(2)
Z	4	4	2	2
F(000)	1072	1808	748	812
D_{calcd}, g cm^{-3}	1.276	1.360	1.525	1.719
μ, mm^{-1}	2.825 (CuKα)	3.384 (CuKα)	5.115 (CuKα)	5.927 (MoKα)
cryst size, mm	0.15 x 0.06 x 0.01	0.10 x 0.10 x 0.10	0.24 x 0.14 x 0.11	0.08 x 0.06 x 0.03
T, K	150(2)	150(2)	152(2)	100(2)
θ range, deg	4.20 to 69.58	2.78 to 69.55	3.49 to 69.49	2.36 to 25.99
min./max. *h*	–13/11	–19/17	–13/11	–13/13
min./max. *k*	–21/20	–16/11	–12/13	–14/14
min./max. *l*	–16/17	–23/20	–13/15	–16/16
no. collected reflns	14749	19099	15491	203662
no. unique reflns	4880	7803	5943	6247
no. reflns with $I > 2\sigma(I)$	3594	6919	5570	6182
no. params/restraints	281/0	462/0	326/0	326/0
GOF (on F^2)	1.139	1.037	1.037	1.184
R_1 (on F, $I > 2\sigma(I)$)	0.043	0.028	0.035	0.024
wR_2 (on F^2, all data)	0.129	0.072	0.093	0.074
min./max. $\Delta\rho$, e Å^{-3}	–0.630/0.403	–0.407/0.386	–1.616/1.212	–2.223/1.784
CCDC dep. no.	1937808	1937809	1937810	1937811

Table S2. Total energies (in a. u., noncorrected zero-point vibrational energies included) and cartesian coordinates (in Å) for all the stationary points described in this manuscript (BP86-D3/def2-SVP level).

1: E= -3845.785180

C	-0.284737000	2.509963000	2.835532000
H	-1.389452000	2.597362000	2.781928000
H	0.158377000	3.505261000	2.635753000
H	-0.026037000	2.231077000	3.879516000
C	-0.461278000	0.065630000	2.192528000
H	-0.257655000	-0.210980000	3.249067000
H	-0.095410000	-0.757081000	1.548461000
H	-1.561426000	0.126289000	2.062847000
C	0.216064000	1.412341000	1.881321000
H	1.318881000	1.295775000	1.984977000
C	1.538005000	3.150683000	-1.936233000
H	0.706721000	3.835249000	-2.209015000
H	1.422414000	2.222501000	-2.532667000
H	2.483971000	3.641367000	-2.250473000
C	1.778958000	4.133035000	0.411177000
H	2.682002000	4.674744000	0.055120000
H	1.932563000	3.907013000	1.485212000
H	0.919719000	4.831683000	0.323979000
C	1.570176000	2.861811000	-0.425165000
H	2.395396000	2.143105000	-0.219878000
C	-1.449553000	2.967352000	-0.066351000
H	-1.422360000	3.786785000	0.678544000
H	-1.453935000	3.432464000	-1.079149000
C	-2.586161000	2.017427000	0.184983000
C	-3.605745000	1.987892000	1.139980000
H	-3.907425000	2.821486000	1.787462000
C	-4.152456000	0.663215000	1.125713000
H	-4.966838000	0.286381000	1.755330000
C	-3.438445000	-0.075353000	0.173139000
C	-3.459581000	-1.548584000	-0.201805000
C	-4.393064000	-2.316853000	0.751660000
H	-4.040689000	-2.244617000	1.800099000
H	-4.442862000	-3.388164000	0.471152000
H	-5.421647000	-1.906097000	0.697882000
C	-3.985999000	-1.715427000	-1.658623000
H	-5.017932000	-1.316013000	-1.746640000
H	-3.980847000	-2.785686000	-1.951978000
H	-3.351572000	-1.165786000	-2.387255000
C	-2.039761000	-2.112486000	-0.111519000
C	-1.586384000	-3.308694000	0.451043000
H	-2.198233000	-4.034593000	0.998957000
C	-0.194203000	-3.428252000	0.145825000
H	0.478007000	-4.252560000	0.418871000
C	0.164660000	-2.304426000	-0.604437000
C	1.506239000	-1.921396000	-1.146626000
H	1.406598000	-1.408849000	-2.128575000
H	2.112729000	-2.834951000	-1.325952000
C	2.758025000	-1.898804000	1.459367000
H	1.722069000	-2.277233000	1.620706000
C	3.169855000	-1.120191000	2.721141000
H	3.181388000	-1.793680000	3.605539000
H	2.463336000	-0.293629000	2.939645000
H	4.185161000	-0.679958000	2.630844000
C	3.668127000	-3.109775000	1.205603000
H	4.729467000	-2.812144000	1.070178000
H	3.360940000	-3.690859000	0.311347000
H	3.634341000	-3.805602000	2.072212000
C	4.139205000	-0.714039000	-0.933510000
H	4.440479000	-1.767974000	-1.132694000
C	5.222328000	-0.034757000	-0.078240000
H	6.176510000	0.040714000	-0.644170000
H	5.435545000	-0.590577000	0.856734000
H	4.921475000	0.997660000	0.205716000
C	3.976193000	0.015326000	-2.280027000
H	3.630358000	1.060868000	-2.131106000
H	3.252899000	-0.484799000	-2.955818000
H	4.948612000	0.061110000	-2.816820000
Ge	-1.026827000	0.263172000	-1.633771000

P	0.063607000	1.854274000	0.053646000
P	2.479678000	-0.743763000	-0.019083000
N	-2.508826000	0.762631000	-0.410559000
N	-0.959637000	-1.495498000	-0.742656000

2: E= -6982.141448

C	2.685322000	-0.579674000	-2.629386000
H	2.355762000	0.275513000	-2.006924000
H	3.404746000	-1.166943000	-2.026039000
H	3.228851000	-0.175368000	-3.509510000
C	1.937436000	-2.772434000	-3.703423000
H	1.097558000	-3.332465000	-4.161495000
H	2.690265000	-2.591016000	-4.501051000
H	2.417414000	-3.415711000	-2.939511000
C	1.490682000	-1.435943000	-3.092656000
H	0.944194000	-0.857899000	-3.869893000
C	-1.347873000	-3.924842000	-2.571254000
H	-1.319876000	-4.364078000	-1.553850000
H	-2.294719000	-4.266297000	-3.043826000
H	-0.510130000	-4.350041000	-3.160794000
C	-1.622241000	-1.750919000	-3.891851000
H	-1.551188000	-0.641767000	-3.862107000
H	-0.924959000	-2.107962000	-4.678155000
H	-2.652286000	-2.010705000	-4.217449000
C	-1.318583000	-2.390473000	-2.526313000
H	-2.119235000	-2.075549000	-1.825096000
C	0.876989000	-2.874598000	-0.543769000
H	0.145772000	-2.910286000	0.291754000
H	0.852351000	-3.865350000	-1.038404000
C	2.286319000	-2.612461000	-0.101594000
C	3.427289000	-3.358917000	-0.404321000
H	3.436197000	-4.331373000	-0.914173000
C	4.559887000	-2.608825000	0.039312000
H	5.611931000	-2.900301000	-0.056036000
C	4.082809000	-1.422841000	0.606034000
C	4.853067000	-0.243785000	1.194291000
C	4.865872000	-0.326446000	2.750546000
H	5.347666000	-1.273621000	3.072140000
H	5.435831000	0.528576000	3.171051000
H	3.843479000	-0.303116000	3.172124000
C	6.314235000	-0.300326000	0.699886000
H	6.801499000	-1.236740000	1.037818000
H	6.368949000	-0.253992000	-0.406300000
H	6.897379000	0.543516000	1.120595000
C	4.223941000	1.072660000	0.746424000
C	4.822150000	2.211606000	0.200145000
H	5.888886000	2.339728000	-0.015247000
C	3.793128000	3.182146000	-0.005718000
H	3.910430000	4.199016000	-0.402959000
C	2.591606000	2.613010000	0.421325000
C	1.217766000	3.208071000	0.380250000
H	1.299005000	4.305830000	0.239920000
H	0.674702000	3.044634000	1.335875000
C	1.164231000	2.799354000	-2.506273000
H	2.116550000	2.329816000	-2.167651000
C	1.457203000	4.269166000	-2.834693000
H	1.871401000	4.819408000	-1.965791000
H	2.209597000	4.332178000	-3.649953000
H	0.549980000	4.804985000	-3.185492000
C	0.638796000	2.010202000	-3.715062000
H	0.249889000	1.023554000	-3.391807000
H	-0.186882000	2.541025000	-4.231911000
H	1.445693000	1.840343000	-4.458658000
C	-1.269165000	3.799659000	-1.069398000
H	-0.752725000	4.781558000	-1.167448000
C	-2.101213000	3.810001000	0.222580000
H	-2.894058000	4.585619000	0.158038000
H	-1.494982000	4.031188000	1.123559000
H	-2.605676000	2.835377000	0.382830000
C	-2.163969000	3.571472000	-2.297657000
H	-2.591555000	2.548322000	-2.289865000
H	-1.619217000	3.710699000	-3.251996000
H	-3.015002000	4.286072000	-2.292264000

C	-2.405328000	0.543295000	2.367872000
C	-1.521832000	1.562605000	2.767504000
H	-0.762743000	1.906610000	2.051354000
C	-1.586427000	2.098093000	4.062925000
H	-0.874333000	2.880913000	4.366656000
C	-2.535877000	1.607085000	4.974525000
H	-2.583505000	2.016951000	5.995917000
C	-3.409962000	0.571592000	4.591546000
H	-4.140065000	0.170580000	5.312503000
C	-3.341867000	0.033907000	3.296292000
H	-4.000756000	-0.801935000	3.010516000
C	-3.778577000	0.364677000	-0.230821000
C	-3.708183000	0.319087000	-1.640709000
H	-2.748210000	0.046823000	-2.108008000
C	-4.822800000	0.652694000	-2.425963000
H	-4.751948000	0.608104000	-3.524310000
C	-6.014584000	1.069214000	-1.805482000
H	-6.888171000	1.346974000	-2.416335000
C	-6.083276000	1.145300000	-0.402365000
H	-7.010376000	1.486056000	0.085626000
C	-4.974342000	0.788925000	0.385691000
H	-5.038113000	0.856034000	1.482676000
C	-2.492332000	-1.937960000	0.976942000
C	-1.620184000	-2.561831000	1.901569000
H	-0.882847000	-1.960060000	2.461523000
C	-1.687694000	-3.949655000	2.103822000
H	-1.002136000	-4.424584000	2.823151000
C	-2.610890000	-4.729259000	1.381362000
H	-2.653660000	-5.819150000	1.534717000
C	-3.483573000	-4.110543000	0.469603000
H	-4.216228000	-4.712782000	-0.090833000
C	-3.431682000	-2.718623000	0.271529000
H	-4.127530000	-2.239509000	-0.435324000
Cl	1.256025000	-0.366007000	3.283432000
Cu	-0.310048000	0.313671000	-0.485751000
Ge	1.476504000	-0.026908000	1.035481000
N	2.693289000	-1.442629000	0.539098000
N	2.860740000	1.322092000	0.884707000
P	0.196560000	-1.570153000	-1.729013000
P	0.101804000	2.506405000	-0.982122000
P	-2.238889000	-0.134101000	0.662664000

3: E= -4453.083912

C	-2.474725000	-1.982268000	-2.784649000
H	-2.320641000	-2.307852000	-3.835452000
H	-2.147912000	-0.925259000	-2.702263000
H	-3.565786000	-2.010550000	-2.584030000
C	-2.094181000	-4.366919000	-1.931770000
H	-3.164884000	-4.518856000	-1.678914000
H	-1.488580000	-5.020899000	-1.270842000
H	-1.948869000	-4.729266000	-2.971810000
C	-1.682498000	-2.889739000	-1.829904000
H	-0.600792000	-2.809250000	-2.090657000
C	-4.445425000	-2.442054000	0.218070000
H	-5.310921000	-2.790609000	0.821386000
H	-4.582174000	-2.825364000	-0.812679000
H	-4.486940000	-1.331910000	0.175095000
C	-3.041429000	-2.498605000	2.333128000
H	-3.054497000	-1.391375000	2.435582000
H	-2.124923000	-2.871512000	2.832858000
H	-3.912815000	-2.898033000	2.894344000
C	-3.127930000	-2.916372000	0.853293000
H	-3.058155000	-4.025388000	0.782238000
C	-0.165083000	-3.126410000	0.670291000
H	-0.137824000	-2.842717000	1.743797000
H	-0.355989000	-4.218788000	0.618522000
C	1.113533000	-2.795313000	-0.035511000
C	1.743738000	-3.512538000	-1.056975000
H	1.429569000	-4.494851000	-1.434968000
C	2.862394000	-2.737420000	-1.488775000
H	3.581848000	-3.011424000	-2.268631000
C	2.884909000	-1.567125000	-0.722117000
C	3.895520000	-0.423674000	-0.731594000

C	4.867144000	-0.570900000	0.479631000
H	5.617621000	0.247044000	0.461990000
H	5.394390000	-1.546375000	0.423580000
H	4.328316000	-0.524231000	1.444480000
C	4.732422000	-0.496117000	-2.026755000
H	4.095402000	-0.397754000	-2.928664000
H	5.277597000	-1.459612000	-2.081569000
H	5.493597000	0.309393000	-2.041534000
C	3.187256000	0.926442000	-0.664903000
C	3.455724000	2.105969000	-1.368032000
H	4.237730000	2.243748000	-2.123042000
C	2.534500000	3.097273000	-0.912307000
H	2.460602000	4.141010000	-1.246177000
C	1.729146000	2.496785000	0.059969000
C	0.529110000	3.070409000	0.747123000
H	0.575756000	4.179377000	0.733771000
H	0.460057000	2.753549000	1.809680000
C	-0.890105000	3.161184000	-1.823258000
H	0.156515000	2.836357000	-2.031926000
C	-1.821083000	2.445548000	-2.814989000
H	-2.887942000	2.707094000	-2.656900000
H	-1.730965000	1.342859000	-2.730870000
H	-1.558539000	2.731135000	-3.855942000
C	-0.950880000	4.691743000	-1.943774000
H	-0.678698000	5.001519000	-2.975326000
H	-0.243047000	5.196303000	-1.254422000
H	-1.969693000	5.084977000	-1.741744000
C	-2.405977000	3.548915000	0.795495000
H	-2.084189000	4.612427000	0.722340000
C	-2.469684000	3.140079000	2.278525000
H	-3.255892000	3.723207000	2.803548000
H	-1.514271000	3.313581000	2.813093000
H	-2.724023000	2.062374000	2.381754000
C	-3.770997000	3.376430000	0.109569000
H	-4.064155000	2.304506000	0.076262000
H	-3.773817000	3.760668000	-0.929962000
H	-4.556513000	3.925865000	0.671433000
Ag	-1.252400000	0.136371000	0.212651000
Cl	2.401895000	-0.314784000	3.159234000
Ge	1.140204000	-0.139781000	1.279656000
N	1.816975000	-1.606815000	0.167152000
N	2.135086000	1.170344000	0.210570000
P	-1.650573000	-2.228179000	-0.074704000
P	-1.089315000	2.530386000	-0.068676000

4: E= -4441.910630

C	2.012059000	2.249415000	-2.790454000
H	1.834267000	2.634337000	-3.817122000
H	1.724026000	1.178811000	-2.769294000
H	3.102591000	2.306201000	-2.595014000
C	1.515454000	4.569129000	-1.819941000
H	2.581187000	4.771504000	-1.582413000
H	0.888008000	5.154773000	-1.116992000
H	1.324083000	4.967892000	-2.838652000
C	1.192881000	3.066814000	-1.779567000
H	0.111149000	2.929887000	-2.015962000
C	4.030347000	2.691669000	0.188870000
H	4.889268000	3.061164000	0.788879000
H	4.120371000	3.126945000	-0.826257000
H	4.127587000	1.588305000	0.096251000
C	2.677376000	2.572986000	2.335130000
H	2.764864000	1.465702000	2.379957000
H	1.749162000	2.858675000	2.869209000
H	3.532907000	3.003611000	2.897408000
C	2.706074000	3.064818000	0.875828000
H	2.573349000	4.170302000	0.857130000
C	-0.288948000	3.087602000	0.761507000
H	-0.265584000	2.755885000	1.821198000
H	-0.194589000	4.193522000	0.749889000
C	-1.535391000	2.661913000	0.051055000
C	-2.232806000	3.344938000	-0.951067000
H	-2.032440000	4.372484000	-1.283794000
C	-3.237574000	2.457075000	-1.439827000

H	-3.973286000	2.675219000	-2.222116000
C	-3.123082000	1.257289000	-0.726303000
C	-3.981539000	-0.000773000	-0.818827000
C	-5.041561000	-0.001126000	0.325843000
H	-4.562559000	-0.001055000	1.322806000
H	-5.681835000	-0.904931000	0.247169000
H	-5.682338000	0.902333000	0.247280000
C	-4.735292000	-0.000878000	-2.167010000
H	-5.390529000	0.889655000	-2.245015000
H	-5.390035000	-0.891761000	-2.245151000
H	-4.033091000	-0.000618000	-3.024867000
C	-3.122456000	-1.258421000	-0.726451000
C	-3.236366000	-2.458172000	-1.440134000
H	-3.971924000	-2.676542000	-2.222505000
C	-2.231244000	-3.345651000	-0.951406000
H	-2.030403000	-4.373068000	-1.284241000
C	-1.534204000	-2.662440000	0.050853000
C	-0.287656000	-3.087694000	0.761393000
H	-0.192906000	-4.193581000	0.749799000
H	-0.264507000	-2.755945000	1.821076000
C	1.194377000	-3.066313000	-1.779569000
H	0.112620000	-2.929734000	-2.016046000
C	1.517473000	-4.568514000	-1.819953000
H	1.326295000	-4.967324000	-2.838682000
H	0.890214000	-5.154409000	-1.117045000
H	2.583274000	-4.770499000	-1.582386000
C	2.013360000	-2.248651000	-2.790403000
H	3.103914000	-2.305333000	-2.595058000
H	1.725194000	-1.178087000	-2.769071000
H	1.835543000	-2.633460000	-3.817109000
C	2.707415000	-3.063756000	0.875895000
H	2.575191000	-4.169297000	0.857110000
C	2.678419000	-2.572011000	2.335213000
H	3.534162000	-3.002208000	2.897499000
H	1.750342000	-2.858222000	2.869249000
H	2.765316000	-1.464685000	2.380088000
C	4.031545000	-2.689987000	0.188993000
H	4.128283000	-1.586579000	0.096370000
H	4.121793000	-3.125221000	-0.826133000
H	4.890616000	-3.059093000	0.789029000
Au	1.156531000	0.000217000	0.064491000
Cl	-2.764208000	-0.000715000	3.114746000
Ge	-1.301741000	-0.000245000	1.352659000
N	-2.084065000	1.388688000	0.185829000
N	-2.083449000	-1.389470000	0.185739000
P	1.243531000	2.353569000	-0.050542000
P	1.244630000	-2.353087000	-0.050525000