Supporting Information

Designed Single-Source Precursors for Iron Germanide Nanoparticles: Colloidal Synthesis and Magnetic Properties

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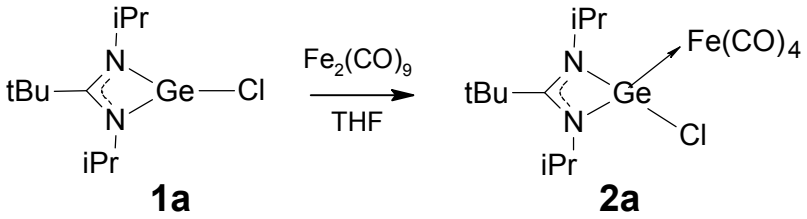


Scheme S1. Syntheses of [{iPrNC(tBu)NiPr}ClGe]$Fe(CO)_4$ (**2a**).

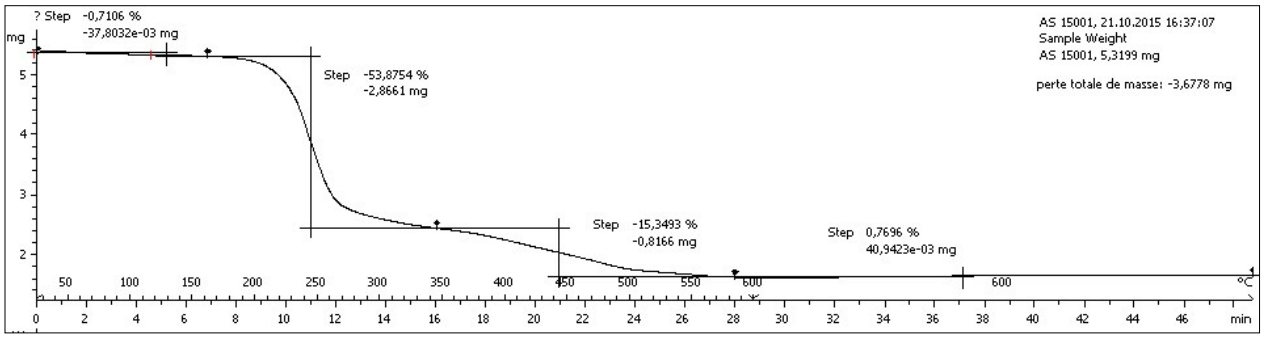


Figure S1. Thermal gravimetric analyses of complex **2a**.

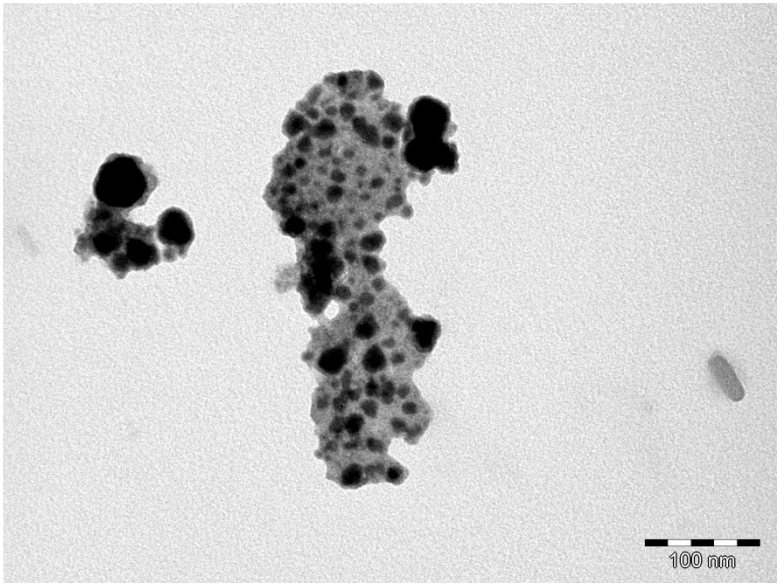
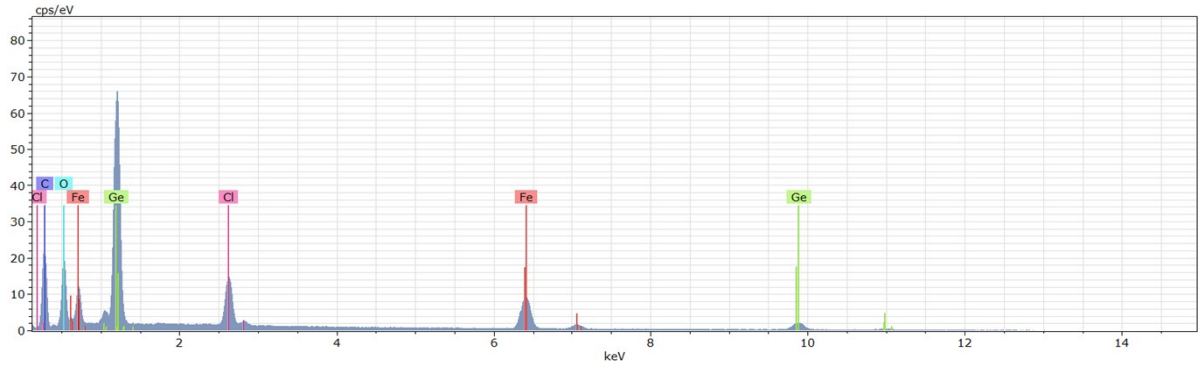


Figure S2. TEM pictures of the NPs prepared from **2a** in the presence of 0.5 equiv. HDA at 200°C.



El AN Series	unn. [wt.%]	C norm. [wt.%]	C Atom. [at.%]	C Error (1 Sigma) [wt.%]
Ge 32 L-series	43.13	58.21	48.84	2.43
Fe 26 K-series	24.40	32.93	35.93	0.75
Cl 17 K-series	6.56	8.86	15.22	0.25

Figure S3. EDX analysis of the NPs prepared from **2a** in the presence of 0.5 equiv. HDA at 200°C.

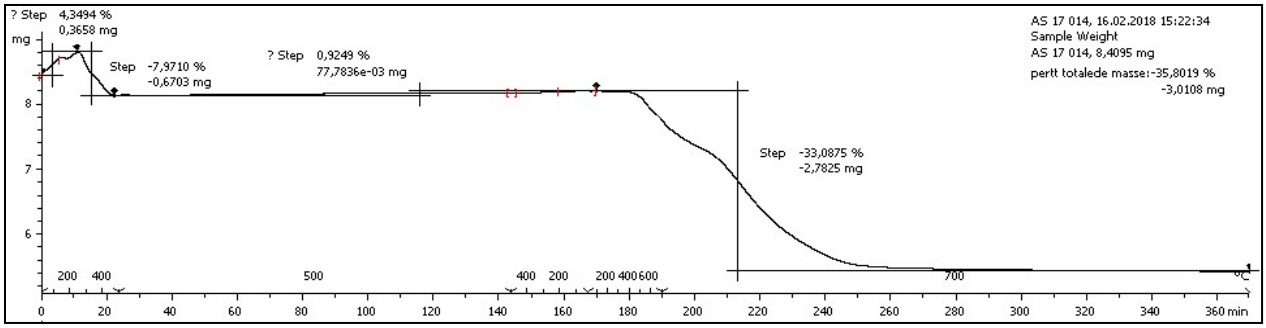


Figure S4. Thermal gravimetric analyses of the NPs prepared from **2a** in the presence of 0.5 equiv. HDA at 200°C.

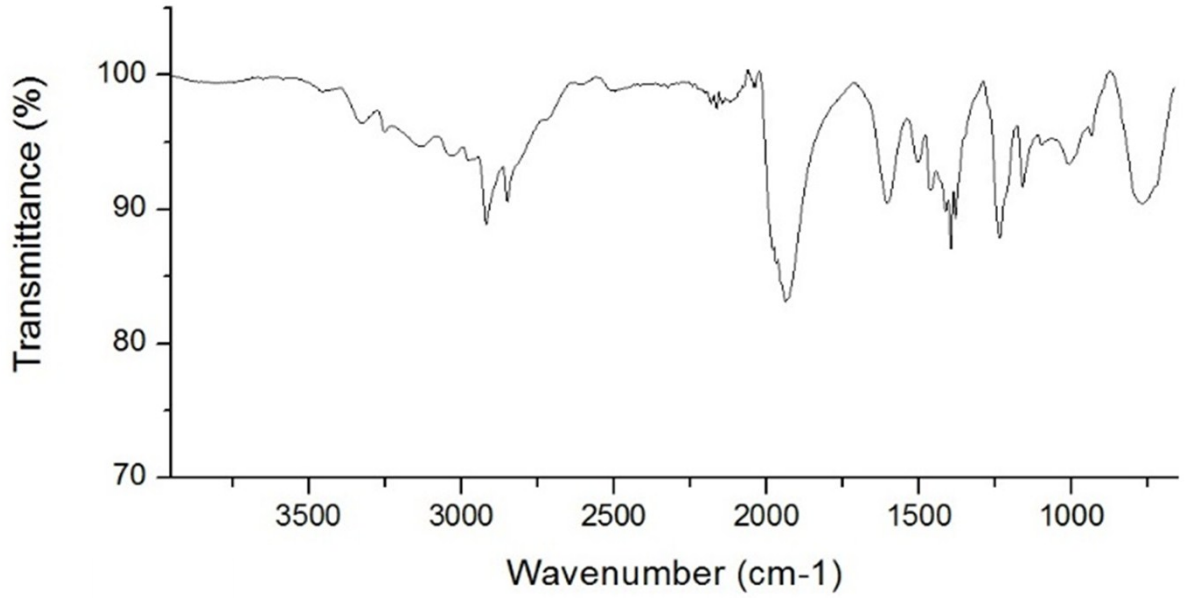


Figure S5. IR spectrum of the NPs prepared from **2a** in the presence of 0.5 equiv. HDA at 200°C.

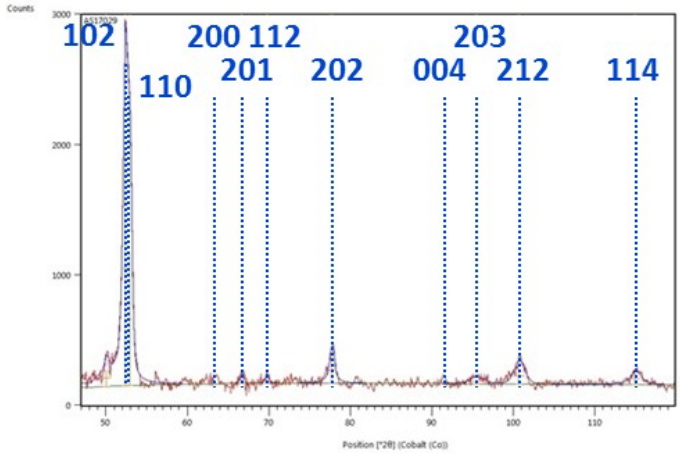


Figure S6. XRD diffractogram of the NPs prepared from **2a** in the presence of 0.5 equiv. HDA at 200°C.

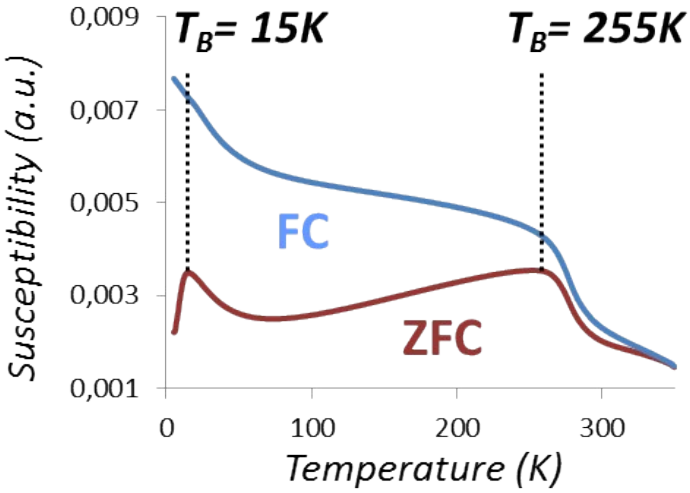


Figure S7. VSM of the NPs prepared from **2a** in the presence of 0.5 equiv. HDA at 200°C.

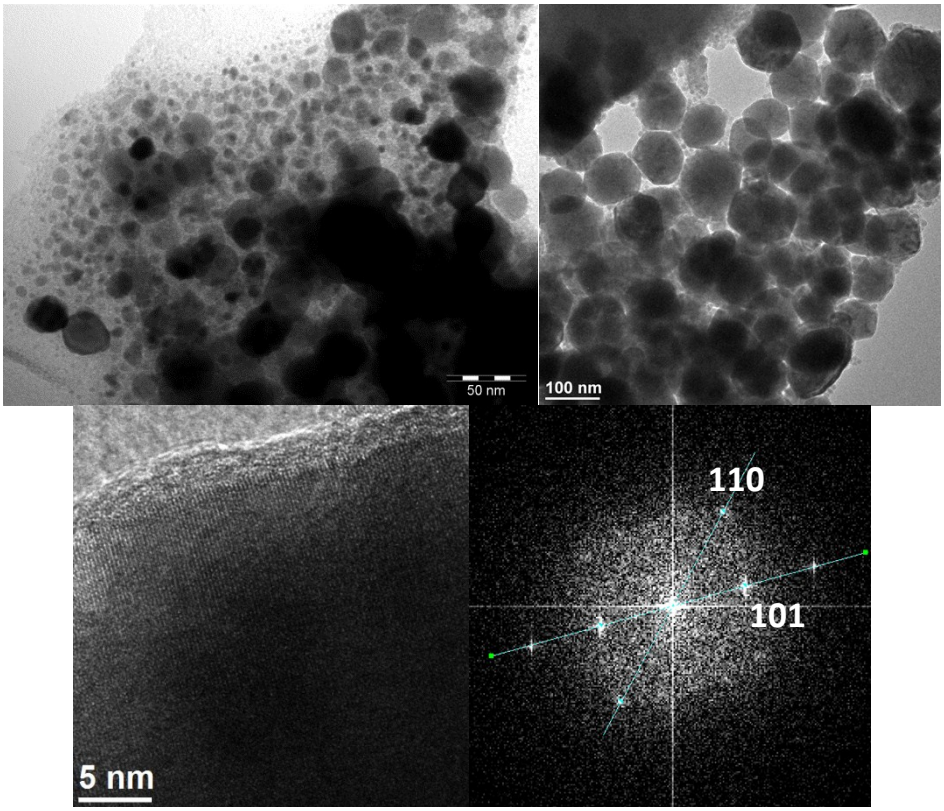


Figure S8. TEM, HRTEM pictures and SAED pattern for NPs of the NPs prepared from **2a** in the presence of 1 equiv. HDA and 1 equiv. PA at 200°C.

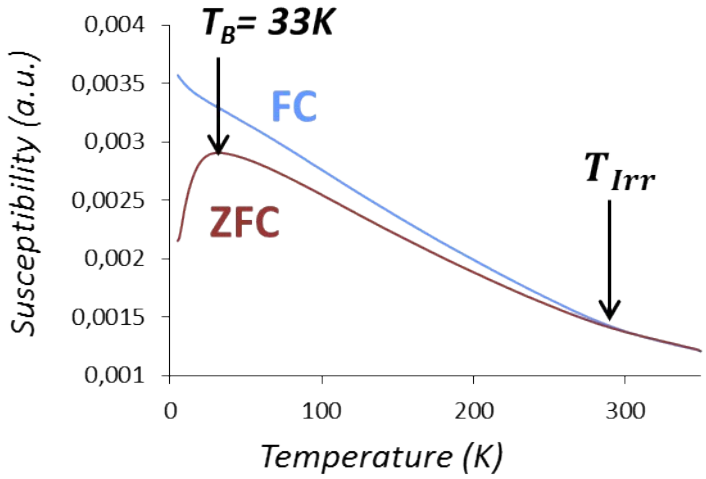


Figure S9. VSM of iron germanide NPs prepared from **2a** in the presence of 1 equiv. HDA and 1 equiv. of PA at 200°C.

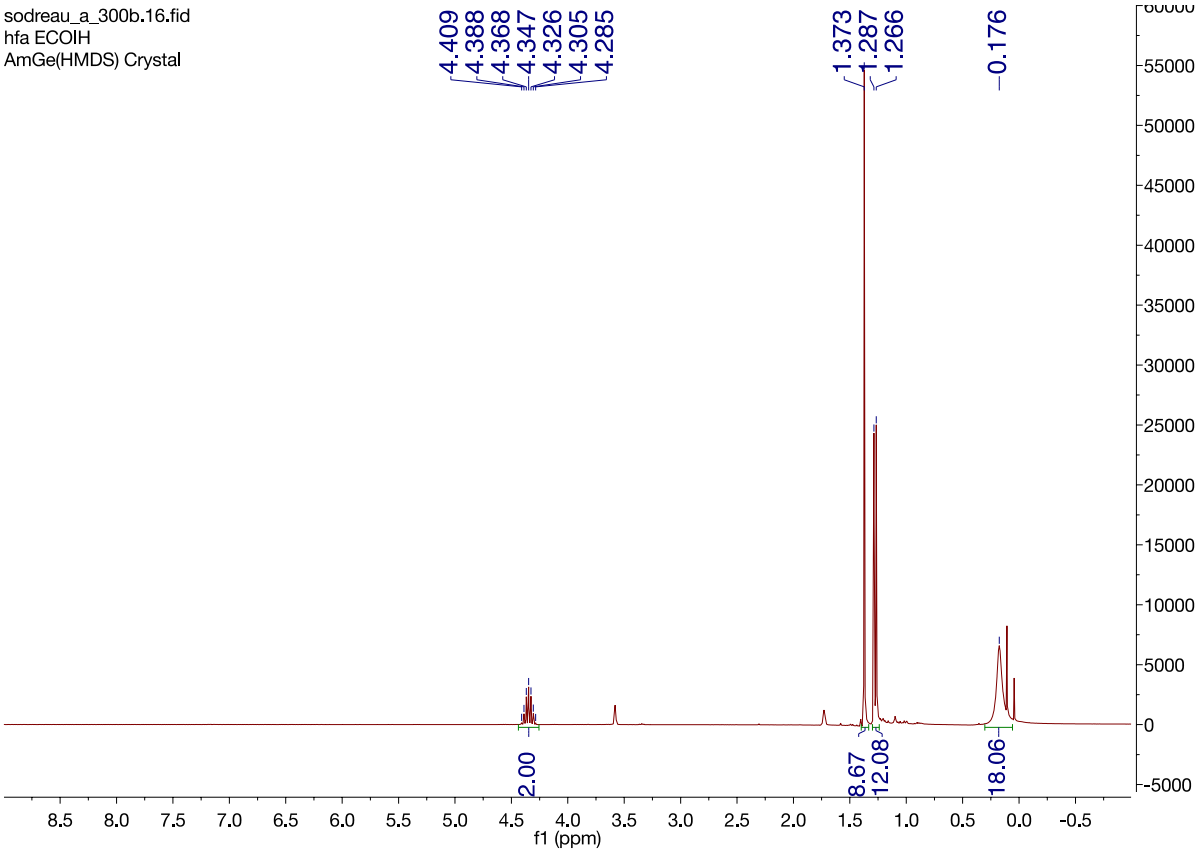


Figure S10. ^{1}H NMR spectrum of **1b** (THF-D_8).

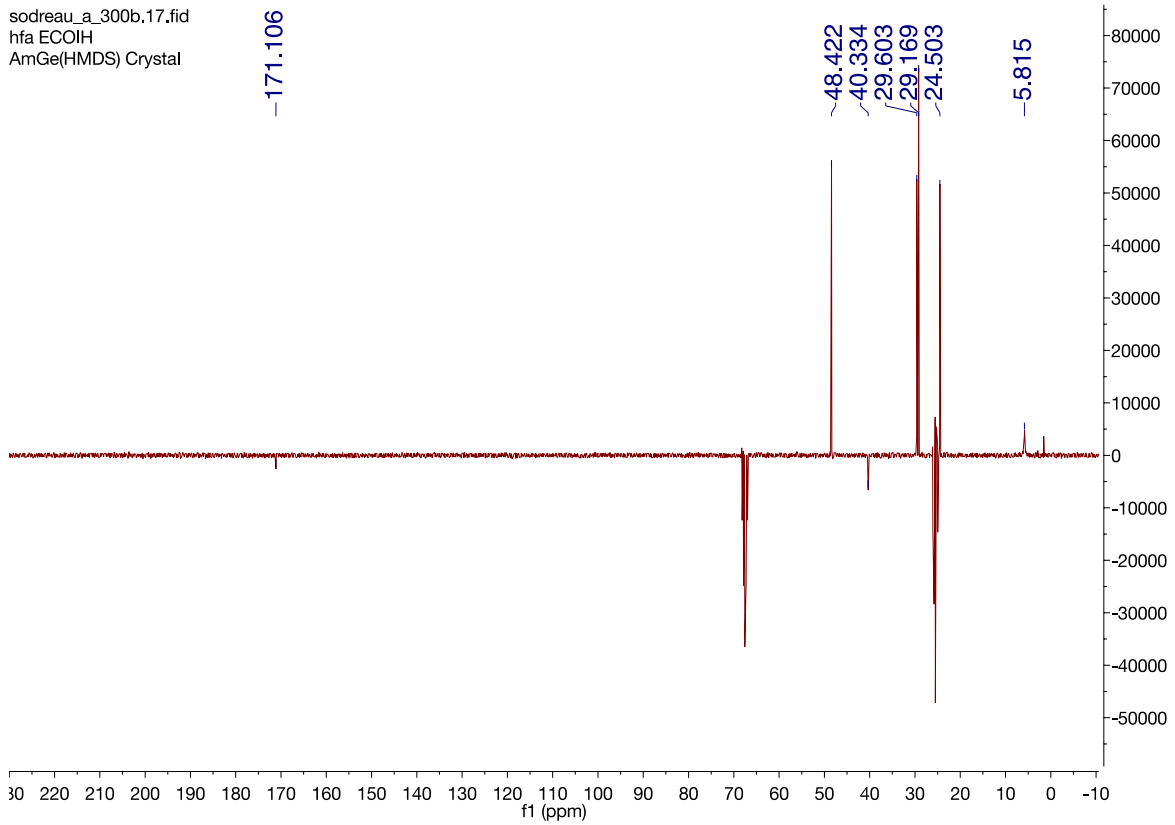


Figure S11. ^{13}C NMR spectrum of **1b** (THF-D_8).

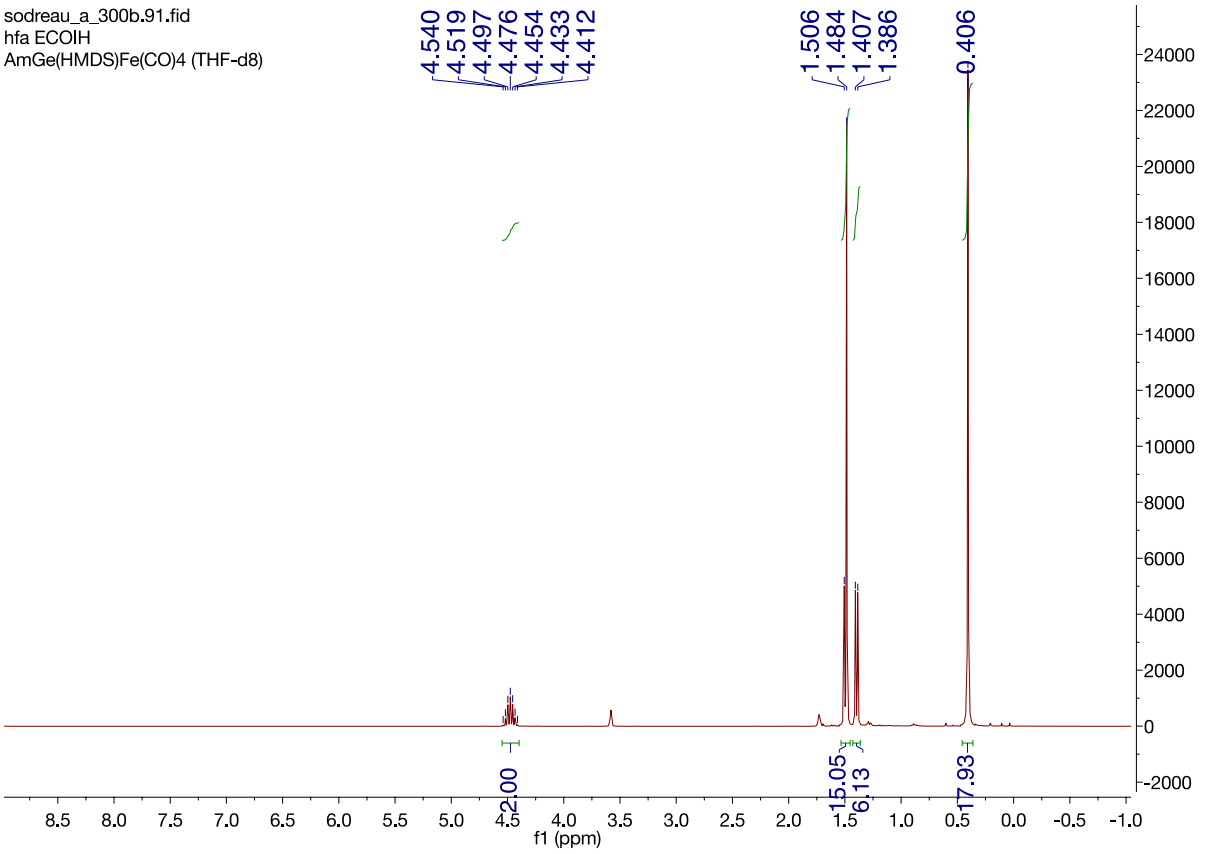


Figure S12. ^{1}H NMR spectrum of **2b** (THF-D_8).

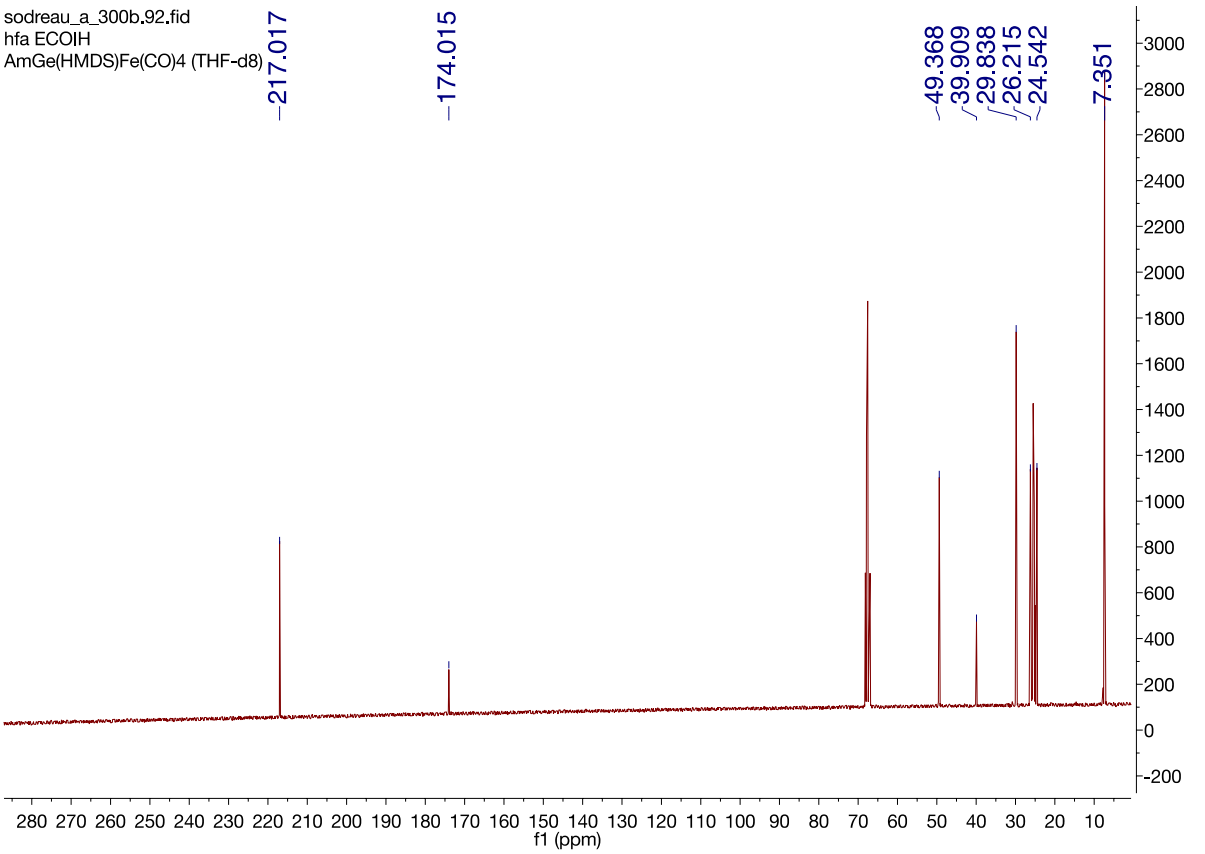


Figure S13. ^{13}C NMR spectrum of **2b** (THF-D_8).

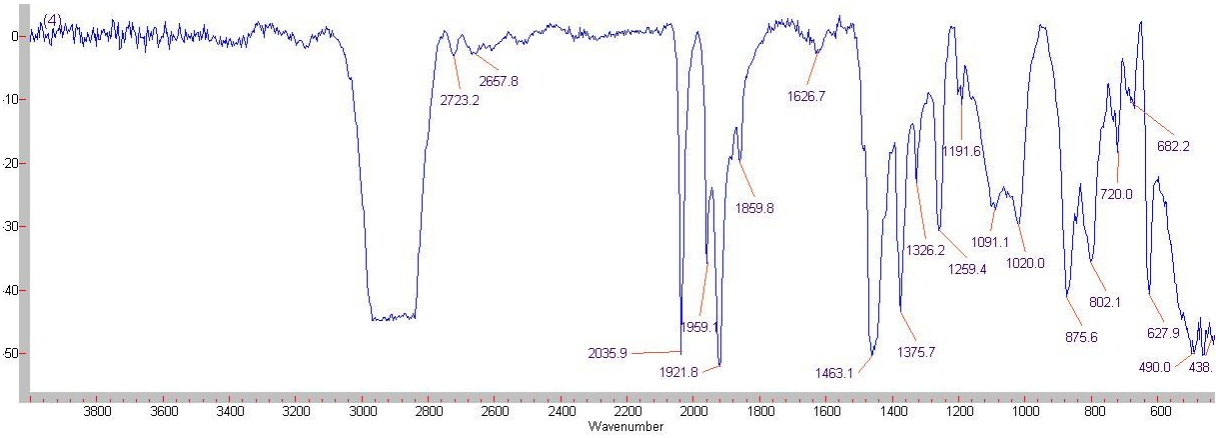


Figure S14. IR spectrum of **2b**.

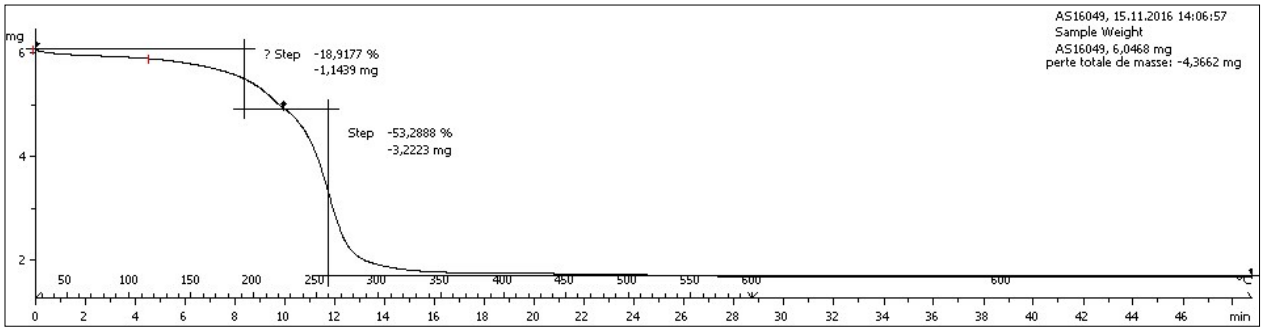


Figure S15. Thermal gravimetric analyses of complex **2b**.

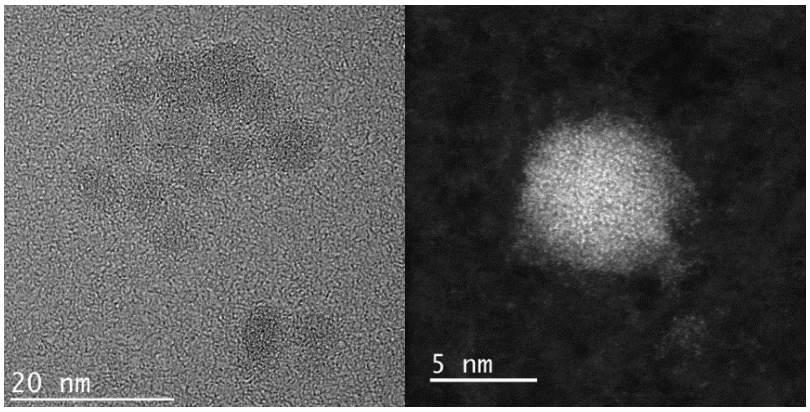


Figure S16. HRTEM pictures for NPs prepared from **2b** in the presence of 0.5 equiv. HDA at 200°C.

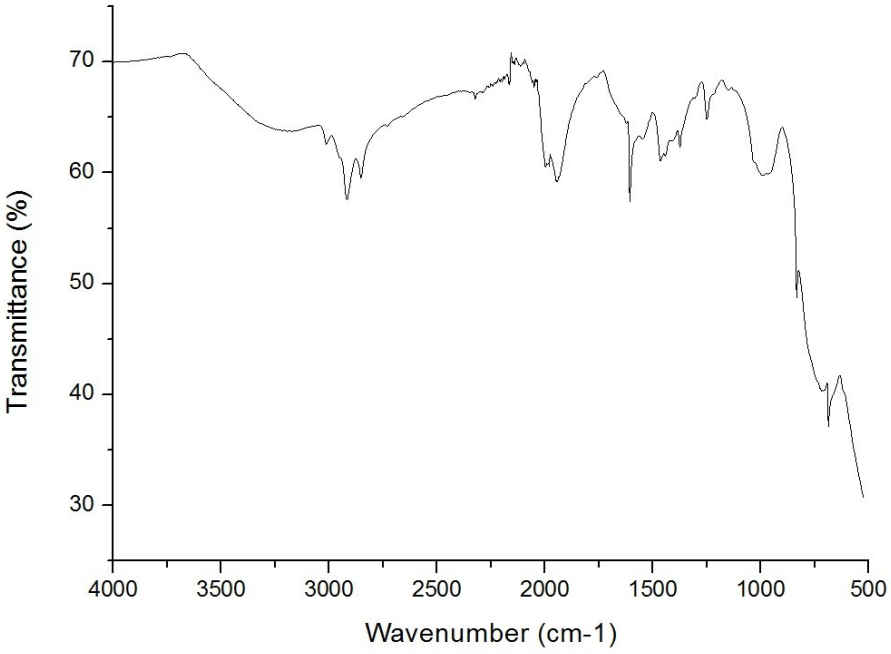


Figure S17. IR spectrum of the NPs prepared from **2b** in the presence of 0.5 equiv. HDA at 200°C.

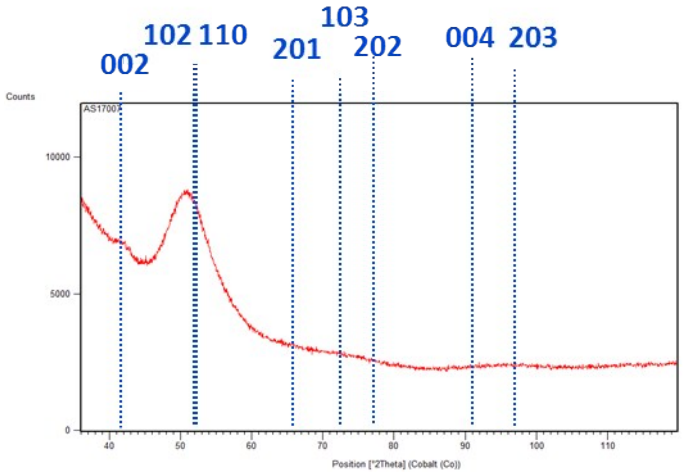


Figure S18. XRD diffractogram of the NPs prepared from **2b** in the presence of 0.5 equiv. HDA at 200°C.

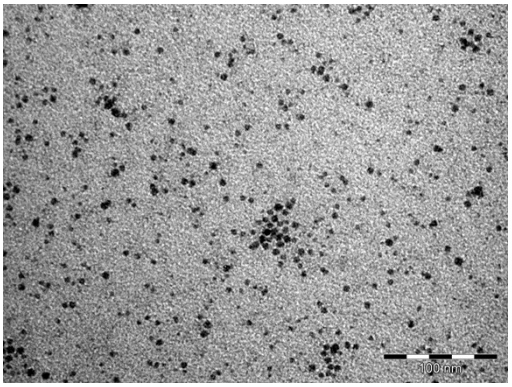


Figure S19. TEM pictures of the NPs prepared from **2b** in the presence of 1 equiv. PA at 200°C.

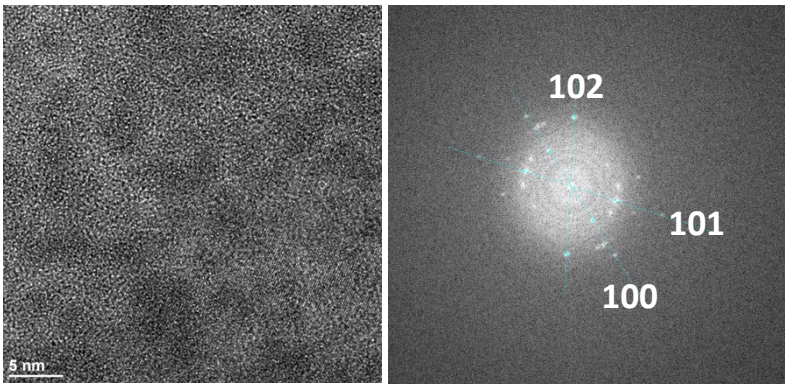


Figure S20. HRTEM and SAED pictures of the NPs prepared from **2b** in the presence of 1 equiv. PA at 200°C.

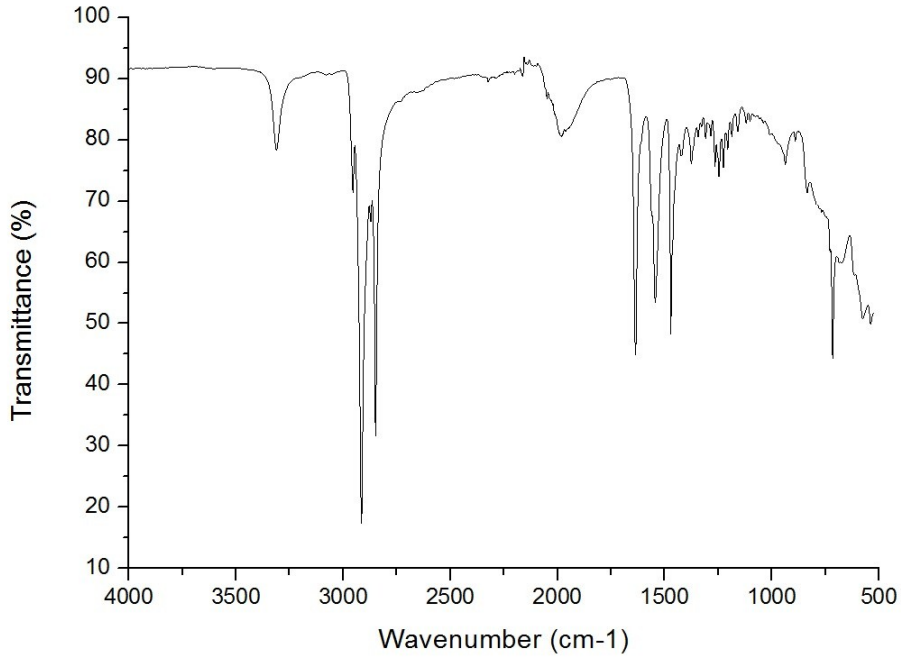


Figure S21. IR spectrum of the NPs prepared from **2b** in the presence of 1 equiv. HDA and 1 equiv. PA at 200°C.

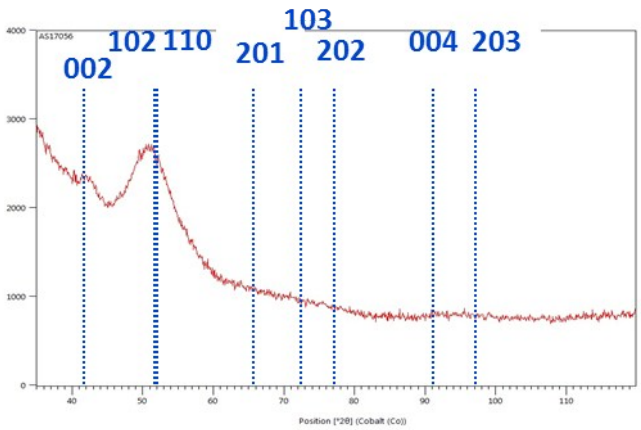


Figure S22. Powder XRD of iron germanide NPs prepared from **2b** in the presence of 1 equiv. HDA and 1 equiv. of PA at 200°C.

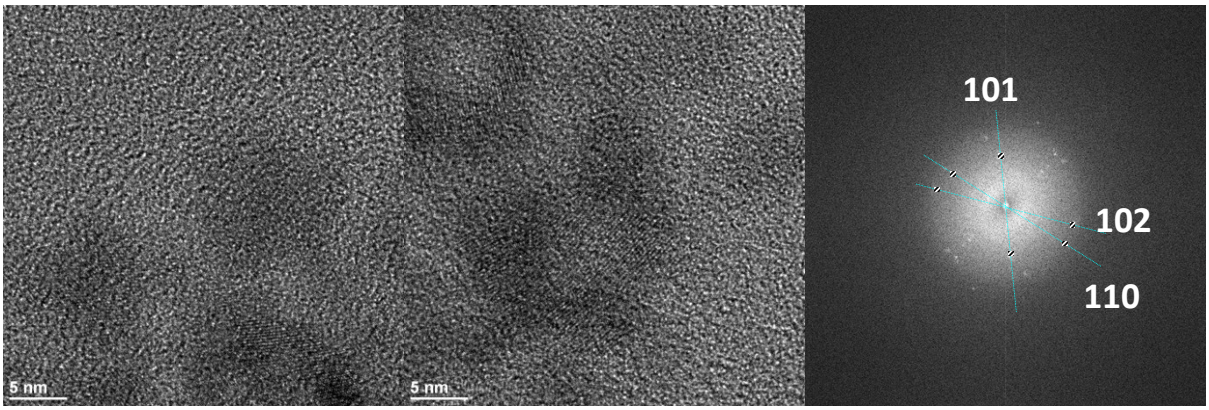


Figure S23 HRTEM and SAED of iron germanide NPs prepared from **2b** in the presence of 1 equiv. HDA and 1 equiv. of PA at 200°C.

Crystallographic data

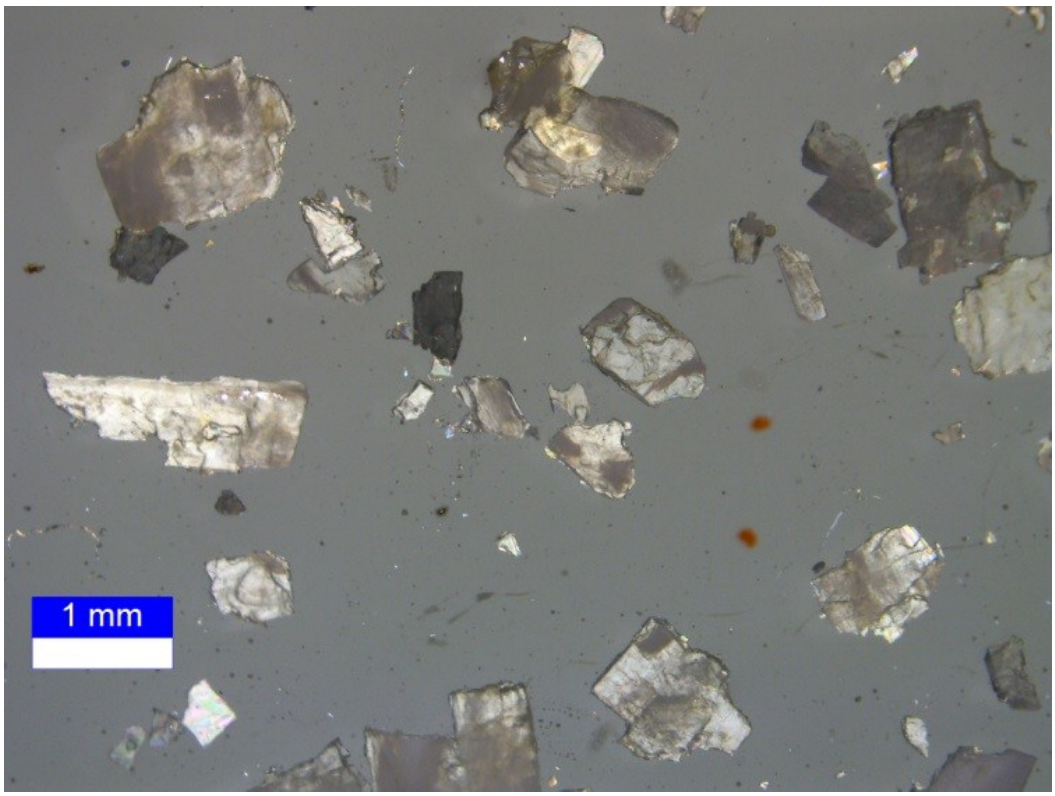


Figure S24 : Sample **1b**

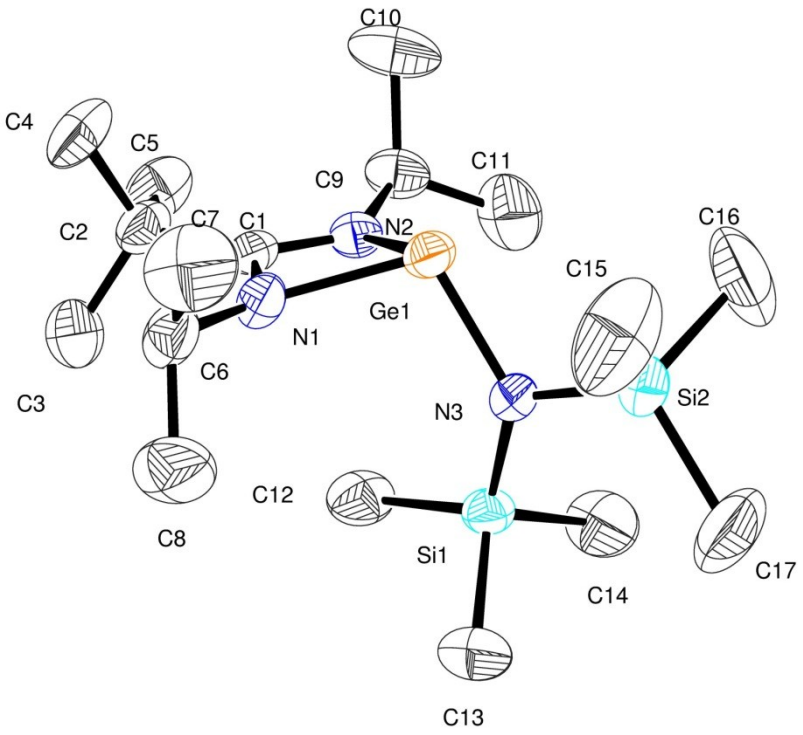


Figure S25 : Asymmetric Unit

Table S1. Crystal data and structure refinement for AS17040.

Identification code	AS17040
Empirical formula	C17 H41 Ge N3 Si2
Formula weight	416.32
Temperature	253(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 8.8800(19) A alpha = 90.873(4) deg.
	b = 11.262(3) A beta = 104.888(4) deg.
	c = 13.201(3) A gamma = 105.925(5) deg.
Volume	1221.7(5) A^3
Z, Calculated density	2, 1.132 Mg/m^3
Absorption coefficient	1.356 mm^-1

F(000)	448
Crystal size	0.260 x 0.220 x 0.200 mm
Theta range for data collection	5.126 to 30.507 deg.
Limiting indices	-12<=h<=12, -15<=k<=16, -18<=l<=18
Reflections collected / unique	25261 / 7415 [R(int) = 0.0281]
Completeness to theta = 25.242	99.1 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7415 / 0 / 221
Goodness-of-fit on F^2	1.038
Final R indices [I>2sigma(I)]	R1 = 0.0336, wR2 = 0.0860
R indices (all data)	R1 = 0.0497, wR2 = 0.0921
Largest diff. peak and hole	0.462 and -0.230 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for as17040_a. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	4550(2)	5403(1)	7448(1)	36(1)
C(2)	3427(2)	4180(2)	7647(2)	48(1)
C(3)	1878(3)	4425(2)	7817(2)	75(1)
C(4)	3027(3)	3239(2)	6687(2)	68(1)
C(5)	4148(3)	3603(2)	8626(2)	67(1)
C(6)	2595(2)	5941(2)	5857(2)	53(1)
C(7)	2965(4)	5957(3)	4800(2)	86(1)
C(8)	1831(3)	6949(3)	5995(2)	83(1)
C(9)	7351(3)	5572(2)	8705(2)	51(1)
C(10)	7994(4)	4684(3)	8164(2)	85(1)
C(11)	8695(3)	6727(3)	9233(2)	77(1)
C(12)	4606(3)	7922(2)	8862(2)	59(1)
C(13)	4633(3)	10256(2)	7848(2)	66(1)
C(15)	7636(3)	10036(3)	9463(2)	78(1)
C(16)	7309(5)	9462(3)	5308(2)	109(1)
C(17)	10040(3)	9612(4)	7247(4)	118(1)
C(18)	8045(5)	11397(2)	7013(3)	102(1)
N(1)	4097(2)	6112(1)	6694(1)	40(1)

N(2)	6103(2)	5967(1)	7949(1)	38(1)
N(4)	6623(2)	8713(1)	7331(1)	36(1)
Si(1)	5910(1)	9195(1)	8321(1)	40(1)
Si(2)	7944(1)	9744(1)	6766(1)	46(1)
Ge(1)	6402(1)	7075(1)	6788(1)	38(1)

Table S3. Bond lengths [A] and angles [deg] for as17040_a.

C(1)-N(2)	1.335(2)
C(1)-N(1)	1.336(2)
C(1)-C(2)	1.533(2)
C(2)-C(5)	1.528(3)
C(2)-C(4)	1.542(3)
C(2)-C(3)	1.544(3)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(3)-H(3C)	0.9700
C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700
C(4)-H(4C)	0.9700
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
C(5)-H(5C)	0.9700
C(6)-N(1)	1.461(2)
C(6)-C(8)	1.504(3)
C(6)-C(7)	1.512(4)
C(6)-H(6)	0.9900
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(7)-H(7C)	0.9700
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(8)-H(8C)	0.9700
C(9)-N(2)	1.462(2)
C(9)-C(11)	1.515(3)
C(9)-C(10)	1.530(3)
C(9)-H(9)	0.9900
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(10)-H(10C)	0.9700
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(11)-H(11C)	0.9700
C(12)-Si(1)	1.858(2)
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(12)-H(12C)	0.9700
C(13)-Si(1)	1.872(2)
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
C(13)-H(13C)	0.9700
C(15)-Si(1)	1.869(2)
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700

C(15)-H(15C)	0.9700
C(16)-Si(2)	1.857(3)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(16)-H(16C)	0.9700
C(17)-Si(2)	1.854(3)
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(17)-H(17C)	0.9700
C(18)-Si(2)	1.859(3)
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700
C(18)-H(18C)	0.9700
N(1)-Ge(1)	2.0066(15)
N(2)-Ge(1)	2.0146(14)
N(4)-Si(1)	1.7303(14)
N(4)-Si(2)	1.7350(14)
N(4)-Ge(1)	1.9086(13)

N(2)-C(1)-N(1)	106.79(14)
N(2)-C(1)-C(2)	129.22(16)
N(1)-C(1)-C(2)	123.98(15)
C(5)-C(2)-C(1)	114.70(17)
C(5)-C(2)-C(4)	107.78(18)
C(1)-C(2)-C(4)	108.07(15)
C(5)-C(2)-C(3)	105.90(19)
C(1)-C(2)-C(3)	108.75(16)
C(4)-C(2)-C(3)	111.7(2)
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2)-C(4)-H(4A)	109.5
C(2)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(2)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(2)-C(5)-H(5A)	109.5
C(2)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(2)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
N(1)-C(6)-C(8)	110.09(17)
N(1)-C(6)-C(7)	109.42(19)
C(8)-C(6)-C(7)	110.4(2)
N(1)-C(6)-H(6)	109.0
C(8)-C(6)-H(6)	109.0
C(7)-C(6)-H(6)	109.0
C(6)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5

C(6)-C(8)-H(8A)	109.5
C(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(6)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
N(2)-C(9)-C(11)	107.59(17)
N(2)-C(9)-C(10)	111.12(17)
C(11)-C(9)-C(10)	111.6(2)
N(2)-C(9)-H(9)	108.8
C(11)-C(9)-H(9)	108.8
C(10)-C(9)-H(9)	108.8
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(9)-C(11)-H(11A)	109.5
C(9)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(9)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
Si(1)-C(12)-H(12A)	109.5
Si(1)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
Si(1)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
Si(1)-C(13)-H(13A)	109.5
Si(1)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
Si(1)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
Si(1)-C(15)-H(15A)	109.5
Si(1)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
Si(1)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
Si(2)-C(16)-H(16A)	109.5
Si(2)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
Si(2)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
Si(2)-C(17)-H(17A)	109.5
Si(2)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
Si(2)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
Si(2)-C(18)-H(18A)	109.5
Si(2)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
Si(2)-C(18)-H(18C)	109.5

H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(1)-N(1)-C(6)	132.16(15)
C(1)-N(1)-Ge(1)	93.02(10)
C(6)-N(1)-Ge(1)	131.17(13)
C(1)-N(2)-C(9)	133.10(16)
C(1)-N(2)-Ge(1)	92.69(10)
C(9)-N(2)-Ge(1)	127.65(12)
Si(1)-N(4)-Si(2)	122.02(8)
Si(1)-N(4)-Ge(1)	129.75(8)
Si(2)-N(4)-Ge(1)	107.80(7)
N(4)-Si(1)-C(12)	114.64(8)
N(4)-Si(1)-C(15)	110.85(10)
C(12)-Si(1)-C(15)	106.05(13)
N(4)-Si(1)-C(13)	111.50(10)
C(12)-Si(1)-C(13)	105.27(12)
C(15)-Si(1)-C(13)	108.12(13)
N(4)-Si(2)-C(17)	110.84(12)
N(4)-Si(2)-C(16)	111.66(11)
C(17)-Si(2)-C(16)	108.2(2)
N(4)-Si(2)-C(18)	114.35(11)
C(17)-Si(2)-C(18)	107.53(18)
C(16)-Si(2)-C(18)	103.86(17)
N(4)-Ge(1)-N(1)	105.13(6)
N(4)-Ge(1)-N(2)	106.80(6)
N(1)-Ge(1)-N(2)	64.44(6)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for as17040_a.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	44(1)	29(1)	39(1)	1(1)	15(1)	12(1)
C(2)	59(1)	31(1)	56(1)	5(1)	25(1)	7(1)
C(3)	62(1)	58(1)	107(2)	10(1)	45(1)	2(1)
C(4)	94(2)	32(1)	67(1)	-4(1)	24(1)	0(1)
C(5)	99(2)	44(1)	62(1)	17(1)	35(1)	13(1)
C(6)	49(1)	40(1)	55(1)	-2(1)	-6(1)	9(1)
C(7)	98(2)	106(2)	44(1)	-5(1)	-10(1)	40(2)

C(8)	72(2)	84(2)	85(2)	-9(1)	-12(1)	44(1)
C(9)	57(1)	59(1)	46(1)	10(1)	12(1)	33(1)
C(10)	100(2)	109(2)	80(2)	21(2)	29(2)	81(2)
C(11)	52(1)	96(2)	68(2)	11(1)	-7(1)	21(1)
C(12)	77(1)	59(1)	56(1)	5(1)	36(1)	25(1)
C(13)	66(1)	63(1)	83(2)	8(1)	23(1)	36(1)
C(15)	68(1)	93(2)	60(1)	-34(1)	-2(1)	23(1)
C(16)	164(3)	78(2)	63(2)	17(1)	43(2)	-9(2)
C(17)	48(1)	124(3)	192(4)	66(3)	49(2)	22(2)
C(18)	131(3)	37(1)	142(3)	4(2)	73(2)	-2(1)
N(1)	41(1)	31(1)	41(1)	1(1)	4(1)	6(1)
N(2)	41(1)	35(1)	43(1)	7(1)	11(1)	17(1)
N(4)	37(1)	30(1)	42(1)	-2(1)	12(1)	7(1)
Si(1)	40(1)	40(1)	42(1)	-6(1)	9(1)	15(1)
Si(2)	44(1)	35(1)	57(1)	4(1)	18(1)	4(1)
Ge(1)	44(1)	30(1)	42(1)	1(1)	19(1)	11(1)

Crystallographic data of **2b**

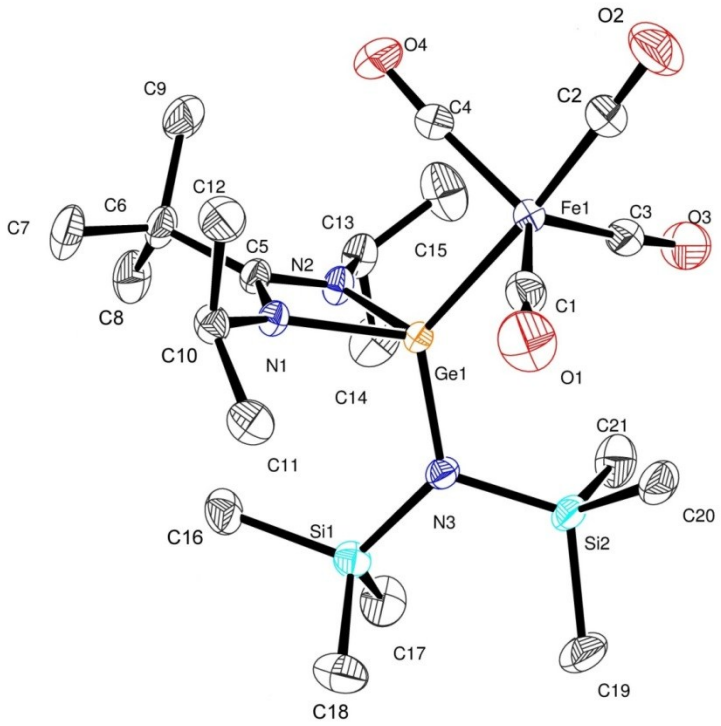


Figure S26 : Asymmetric Unit

Table S5. Crystal data and structure refinement for AS090616.

Identification code	AS090616
Empirical formula	C21 H41 Fe Ge N3 O4 Si2
Formula weight	584.21
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system, space group	monoclinic, P 21/c
Unit cell dimensions	a = 14.2986(10) A alpha = 90 deg. b = 12.8496(8) A beta = 96.027(2) deg. c = 15.7161(10) A gamma = 90 deg.
Volume	2871.6(3) A^3
Z, Calculated density	4, 1.351 Mg/m^3
Absorption coefficient	1.664 mm^-1
F(000)	1224
Crystal size	0.36 x 0.20 x 0.06 mm
Theta range for data collection	3.05 to 32.03 deg.

Limiting indices	-21<=h<=21, -19<=k<=19, -23<=l<=23
Reflections collected / unique	119176 / 9985 [R(int) = 0.0440]
Completeness to theta = 32.03	99.8 %
Max. and min. transmission	0.7465 and 0.6654
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9985 / 0 / 302
Goodness-of-fit on F^2	1.047
Final R indices [I>2sigma(I)]	R1 = 0.0256, wR2 = 0.0600
R indices (all data)	R1 = 0.0379, wR2 = 0.0662
Largest diff. peak and hole	0.474 and -0.465 e.A^-3

Table S6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for as. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	198(1)	131(1)	2315(1)	30(1)
C(2)	290(1)	701(1)	3836(1)	32(1)
C(3)	1847(1)	-294(1)	3718(1)	31(1)
C(4)	1408(1)	1936(1)	3208(1)	28(1)
C(5)	2697(1)	2271(1)	1550(1)	22(1)
C(6)	3053(1)	3378(1)	1393(1)	30(1)
C(7)	2458(1)	3985(1)	689(1)	42(1)
C(8)	4051(1)	3335(1)	1102(1)	43(1)
C(9)	3043(1)	4003(1)	2234(1)	43(1)
C(10)	1075(1)	2170(1)	655(1)	23(1)
C(11)	607(1)	1237(1)	192(1)	31(1)
C(12)	384(1)	2740(1)	1171(1)	35(1)
C(13)	4043(1)	1653(1)	2639(1)	31(1)
C(14)	4752(1)	900(2)	2332(1)	48(1)
C(15)	3888(1)	1442(2)	3564(1)	52(1)
C(16)	3216(1)	852(1)	-35(1)	36(1)
C(17)	4176(1)	-1103(2)	492(1)	43(1)
C(18)	2224(1)	-1126(2)	-533(1)	43(1)
C(19)	2564(2)	-2891(1)	1030(1)	52(1)
C(20)	1274(1)	-2149(1)	2203(1)	35(1)
C(21)	3410(1)	-1915(1)	2666(1)	43(1)

N(1)	1906(1)	1801(1)	1208(1)	19(1)
N(2)	3153(1)	1581(1)	2085(1)	23(1)
N(3)	2445(1)	-550(1)	1327(1)	21(1)
O(1)	-433(1)	-157(1)	1863(1)	48(1)
O(2)	-265(1)	786(1)	4307(1)	52(1)
O(3)	2287(1)	-847(1)	4170(1)	52(1)
O(4)	1572(1)	2800(1)	3337(1)	44(1)
Si(1)	2973(1)	-482(1)	362(1)	26(1)
Si(2)	2413(1)	-1804(1)	1798(1)	26(1)
Fe(1)	1118(1)	592(1)	3074(1)	20(1)
Ge(1)	2097(1)	584(1)	1961(1)	17(1)

Table S7. Bond lengths [A] and angles [deg] for as.

C(1)-O(1)	1.1490(18)
C(1)-Fe(1)	1.7816(15)
C(2)-O(2)	1.1451(19)
C(2)-Fe(1)	1.7770(15)
C(3)-O(3)	1.1457(18)
C(3)-Fe(1)	1.7842(15)
C(4)-O(4)	1.1478(17)
C(4)-Fe(1)	1.7838(14)
C(5)-N(2)	1.3435(16)
C(5)-N(1)	1.3436(15)
C(5)-C(6)	1.5395(18)
C(6)-C(7)	1.535(2)
C(6)-C(8)	1.545(2)
C(6)-C(9)	1.547(2)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-N(1)	1.4743(15)
C(10)-C(11)	1.5211(19)
C(10)-C(12)	1.5291(19)
C(10)-H(10)	1.0000
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-N(2)	1.4671(16)
C(13)-C(14)	1.517(2)
C(13)-C(15)	1.518(2)
C(13)-H(13)	1.0000
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800

C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-Si(1)	1.8689(16)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-Si(1)	1.8875(16)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-Si(1)	1.8693(17)
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-Si(2)	1.8734(17)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-Si(2)	1.8640(15)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-Si(2)	1.8716(17)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
N(1)-Ge(1)	1.9618(10)
N(2)-Ge(1)	1.9737(10)
N(3)-Si(1)	1.7658(11)
N(3)-Si(2)	1.7750(11)
N(3)-Ge(1)	1.8631(10)
Fe(1)-Ge(1)	2.3518(2)

O(1)-C(1)-Fe(1)	175.81(14)
O(2)-C(2)-Fe(1)	177.71(15)
O(3)-C(3)-Fe(1)	176.13(14)
O(4)-C(4)-Fe(1)	176.11(13)
N(2)-C(5)-N(1)	106.61(10)
N(2)-C(5)-C(6)	124.29(11)
N(1)-C(5)-C(6)	129.10(11)
C(7)-C(6)-C(5)	114.61(12)
C(7)-C(6)-C(8)	105.30(13)
C(5)-C(6)-C(8)	110.19(12)
C(7)-C(6)-C(9)	107.36(13)
C(5)-C(6)-C(9)	108.08(12)
C(8)-C(6)-C(9)	111.29(13)
C(6)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(6)-C(8)-H(8A)	109.5
C(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(6)-C(8)-H(8C)	109.5

H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(6)-C(9)-H(9A)	109.5
C(6)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(6)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
N(1)-C(10)-C(11)	108.36(10)
N(1)-C(10)-C(12)	111.50(11)
C(11)-C(10)-C(12)	110.75(12)
N(1)-C(10)-H(10)	108.7
C(11)-C(10)-H(10)	108.7
C(12)-C(10)-H(10)	108.7
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
N(2)-C(13)-C(14)	109.80(13)
N(2)-C(13)-C(15)	110.63(12)
C(14)-C(13)-C(15)	111.03(15)
N(2)-C(13)-H(13)	108.4
C(14)-C(13)-H(13)	108.4
C(15)-C(13)-H(13)	108.4
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
Si(1)-C(16)-H(16A)	109.5
Si(1)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
Si(1)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
Si(1)-C(17)-H(17A)	109.5
Si(1)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
Si(1)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
Si(1)-C(18)-H(18A)	109.5
Si(1)-C(18)-H(18B)	109.5

H(18A)-C(18)-H(18B)	109.5
Si(1)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
Si(2)-C(19)-H(19A)	109.5
Si(2)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
Si(2)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
Si(2)-C(20)-H(20A)	109.5
Si(2)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
Si(2)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
Si(2)-C(21)-H(21A)	109.5
Si(2)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
Si(2)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(5)-N(1)-C(10)	133.04(11)
C(5)-N(1)-Ge(1)	93.42(7)
C(10)-N(1)-Ge(1)	131.65(8)
C(5)-N(2)-C(13)	131.54(11)
C(5)-N(2)-Ge(1)	92.90(7)
C(13)-N(2)-Ge(1)	134.97(9)
Si(1)-N(3)-Si(2)	115.82(6)
Si(1)-N(3)-Ge(1)	125.66(6)
Si(2)-N(3)-Ge(1)	117.82(6)
N(3)-Si(1)-C(16)	116.29(6)
N(3)-Si(1)-C(18)	111.17(7)
C(16)-Si(1)-C(18)	105.46(8)
N(3)-Si(1)-C(17)	110.66(7)
C(16)-Si(1)-C(17)	103.03(8)
C(18)-Si(1)-C(17)	109.77(9)
N(3)-Si(2)-C(20)	114.87(6)
N(3)-Si(2)-C(21)	108.79(7)
C(20)-Si(2)-C(21)	111.02(8)
N(3)-Si(2)-C(19)	113.46(7)
C(20)-Si(2)-C(19)	101.94(8)
C(21)-Si(2)-C(19)	106.34(10)
C(2)-Fe(1)-C(1)	88.84(7)
C(2)-Fe(1)-C(4)	90.41(7)
C(1)-Fe(1)-C(4)	123.15(7)
C(2)-Fe(1)-C(3)	93.36(7)
C(1)-Fe(1)-C(3)	120.94(7)
C(4)-Fe(1)-C(3)	115.85(7)
C(2)-Fe(1)-Ge(1)	173.10(5)
C(1)-Fe(1)-Ge(1)	87.49(5)
C(4)-Fe(1)-Ge(1)	86.71(4)
C(3)-Fe(1)-Ge(1)	93.54(5)
N(3)-Ge(1)-N(1)	109.21(5)
N(3)-Ge(1)-N(2)	108.39(5)
N(1)-Ge(1)-N(2)	66.39(4)
N(3)-Ge(1)-Fe(1)	127.92(3)
N(1)-Ge(1)-Fe(1)	112.90(3)

N(2)-Ge(1)-Fe(1)	115.63(3)

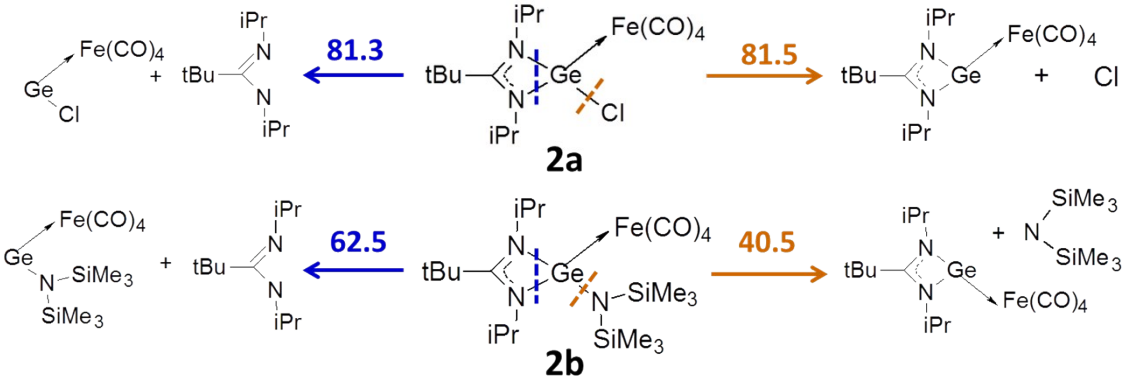
Symmetry transformations used to generate equivalent atoms:

Table S7. Anisotropic displacement parameters (A^2 x 10^3) for as. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	31(1)	31(1)	28(1)	2(1)	6(1)	-3(1)
C(2)	37(1)	32(1)	28(1)	1(1)	9(1)	1(1)
C(3)	42(1)	27(1)	24(1)	0(1)	4(1)	2(1)
C(4)	35(1)	26(1)	25(1)	-2(1)	8(1)	1(1)
C(5)	23(1)	18(1)	23(1)	2(1)	1(1)	-2(1)
C(6)	36(1)	19(1)	33(1)	5(1)	-2(1)	-8(1)
C(7)	52(1)	25(1)	46(1)	14(1)	-7(1)	-6(1)
C(8)	41(1)	37(1)	51(1)	11(1)	5(1)	-16(1)
C(9)	61(1)	24(1)	43(1)	-3(1)	0(1)	-13(1)
C(10)	22(1)	25(1)	21(1)	4(1)	0(1)	4(1)
C(11)	26(1)	37(1)	27(1)	-2(1)	-4(1)	-2(1)
C(12)	34(1)	38(1)	34(1)	4(1)	6(1)	16(1)
C(13)	24(1)	29(1)	36(1)	5(1)	-9(1)	-7(1)
C(14)	25(1)	47(1)	70(1)	2(1)	-8(1)	4(1)
C(15)	42(1)	77(1)	34(1)	11(1)	-14(1)	-12(1)
C(16)	36(1)	37(1)	37(1)	8(1)	18(1)	4(1)
C(17)	29(1)	46(1)	57(1)	5(1)	17(1)	9(1)
C(18)	49(1)	49(1)	33(1)	-11(1)	5(1)	5(1)
C(19)	78(1)	23(1)	60(1)	-11(1)	33(1)	-2(1)

C(20)	38(1)	24(1)	45(1)	-2(1)	14(1)	-9(1)
C(21)	38(1)	39(1)	51(1)	15(1)	1(1)	10(1)
N(1)	19(1)	18(1)	21(1)	2(1)	0(1)	0(1)
N(2)	21(1)	21(1)	25(1)	4(1)	-4(1)	-4(1)
N(3)	22(1)	17(1)	24(1)	-1(1)	6(1)	0(1)
O(1)	40(1)	59(1)	43(1)	-1(1)	-7(1)	-15(1)
O(2)	56(1)	64(1)	42(1)	3(1)	26(1)	7(1)
O(3)	78(1)	42(1)	34(1)	7(1)	-5(1)	22(1)
O(4)	60(1)	25(1)	49(1)	-8(1)	12(1)	-4(1)
Si(1)	23(1)	28(1)	27(1)	0(1)	9(1)	3(1)
Si(2)	30(1)	16(1)	32(1)	0(1)	8(1)	1(1)
Fe(1)	25(1)	19(1)	18(1)	0(1)	4(1)	0(1)
Ge(1)	18(1)	15(1)	18(1)	1(1)	1(1)	-1(1)

Computational results, coordinates



2a

Sum of electronic and thermal Enthalpies = -3661.497482
Sum of electronic and thermal Free Energies = -3661.591637

C	1.28649700	0.01746600	-1.89493200
C	2.60537000	-1.53870700	0.41888700
C	3.74220400	-0.04019100	-1.31525700
C	2.68096800	1.46131900	0.45790100
C	-2.07766000	0.07744000	-0.11370200
C	-3.50247000	0.06074800	-0.66480100
C	-3.49140400	-0.63307100	-2.03604900
H	-2.86406800	-0.08520100	-2.73981700
H	-4.50736000	-0.64910700	-2.43301900

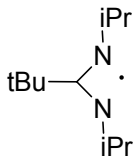
H	-3.13171300	-1.65692800	-1.99970300
C	-4.40603200	-0.67843300	0.33574700
H	-4.10247600	-1.70470100	0.52231600
H	-5.42427400	-0.69710600	-0.05525200
H	-4.42419500	-0.15706000	1.29328700
C	-4.12621700	1.44087200	-0.87459800
H	-4.28117400	1.97301400	0.06252900
H	-5.10906400	1.29430600	-1.32409900
H	-3.54984300	2.06639700	-1.55337700
C	-1.61569100	-2.44593000	-0.05673000
H	-2.65895500	-2.58045100	-0.33636200
C	-0.74893600	-3.02489800	-1.16803600
H	-0.92070300	-2.51604500	-2.11604700
H	-0.96816800	-4.08514500	-1.29862000
H	0.30930500	-2.92805500	-0.92398700
C	-1.38456300	-3.17402700	1.26004400
H	-0.34648100	-3.07681600	1.58123300
H	-1.59959400	-4.23646700	1.14293000
H	-2.01721600	-2.77344500	2.05121900
C	-1.46640600	2.56901500	0.16054100
H	-2.51826200	2.82780200	0.23786700
C	-0.91485300	3.10554700	-1.15445400
H	0.14876600	2.88040900	-1.24132200
H	-1.03801600	4.18823600	-1.20221400
H	-1.42032100	2.66468200	-2.01381600
C	-0.75530700	3.19610700	1.35021300
H	-1.15214700	2.81967800	2.29172400
H	-0.87956300	4.27868800	1.32632700
H	0.31619100	2.98998700	1.32573600
N	-1.35704400	-1.02481900	0.11328000
N	-1.32700300	1.12195100	0.23999800
O	0.67861500	0.03654200	-2.87208600
O	2.86655000	-2.52986500	0.93484900
O	4.71853700	-0.05553900	-1.90838000
O	2.99862800	2.42126700	1.00088700
Cl	0.06371700	-0.12541800	2.85501700
Fe	2.23407100	-0.01725600	-0.40585800
Ge	0.20959300	-0.00858200	0.67111600

2b

Sum of electronic and thermal Enthalpies = -4075.797114
Sum of electronic and thermal Free Energies = -4075.918164

C	-0.78709900	2.41577300	-1.64203000
C	-0.07242100	4.25507300	-0.08690300
C	-1.02963700	2.51439700	1.46201400
C	1.65991700	2.42532200	0.16244500
C	2.08675300	-0.95501400	0.06742900
C	3.51981300	-1.48952900	0.21006300
C	4.25283700	-1.74485300	-1.10927300
H	3.77318000	-2.52106200	-1.70374500
H	5.25386700	-2.10338300	-0.86491100
H	4.37120500	-0.84850500	-1.71316800
C	3.50691500	-2.84712600	0.93430300
H	3.04003400	-3.60990500	0.31231500
H	2.99323600	-2.83937600	1.89110200
H	4.53891500	-3.15105200	1.11522900
C	4.35602800	-0.46087900	0.98826600
H	5.37044700	-0.84719800	1.09890700
H	3.96912000	-0.25166500	1.98173700
H	4.40761800	0.48505600	0.45170900
C	1.79063400	-0.56571400	-2.44997900
H	2.47873500	-1.37757000	-2.67203800
C	0.55402600	-0.77937900	-3.30967500

H	0.10842400	-1.75706800	-3.13461000
H	0.82292600	-0.71412800	-4.36399800
H	-0.20035700	-0.01561000	-3.11733700
C	2.45958800	0.75765700	-2.80355600
H	1.76428900	1.58487700	-2.66578100
H	2.77759600	0.74765000	-3.84707200
H	3.33120800	0.95370900	-2.18044900
C	1.48049800	-0.83578300	2.53989400
H	2.46232800	-1.26725800	2.72193900
C	0.43799600	-1.77199100	3.13540100
H	-0.56791600	-1.40116100	2.93446500
H	0.56286700	-1.84144900	4.21638300
H	0.51824000	-2.77509700	2.71640800
C	1.44673700	0.52222000	3.22810900
H	2.18357300	1.20309700	2.80476800
H	1.65932800	0.39992500	4.29096600
H	0.46639500	0.98816600	3.13787800
C	0.22490900	-3.50238000	-0.50238800
H	0.80813100	-3.19802500	-1.36810600
H	0.06957900	-4.58245300	-0.56804900
H	0.80245900	-3.30794800	0.39722300
C	-2.31471300	-3.69079900	0.98051000
H	-1.71333300	-3.61284700	1.88781900
H	-2.36888900	-4.74918900	0.71400400
H	-3.32228900	-3.36153900	1.22352400
C	-2.29374200	-3.23149000	-2.07397100
H	-3.37396600	-3.34227200	-2.01069100
H	-1.88227600	-4.18969400	-2.39920200
H	-2.08204500	-2.49876100	-2.85350000
C	-4.56798100	-1.45910700	-0.53029200
H	-4.55899300	-1.41081100	-1.61929900
H	-5.50987700	-1.01560300	-0.19648100
H	-4.58161300	-2.50441000	-0.23261600
C	-3.62174200	1.30025700	-0.50986900
H	-3.06852700	2.12964600	-0.08110300
H	-4.68598100	1.46878800	-0.32603300
H	-3.46961900	1.31499300	-1.58936100
C	-3.46979300	-0.34883000	2.07724800
H	-3.32368000	-1.33765400	2.51410700
H	-4.48930100	-0.03182400	2.30782800
H	-2.79592600	0.34645400	2.57746500
N	1.41378600	-0.64214300	-1.04324000
N	1.27888600	-0.71623400	1.10364700
N	-1.57248600	-0.99367500	-0.16017900
O	-1.21950900	2.40240400	-2.70890500
O	-0.06339000	5.39802600	-0.12841900
O	-1.61525800	2.58189500	2.45087400
O	2.80467200	2.43333400	0.28808000
Si	-1.49471600	-2.74882300	-0.43375400
Si	-3.21223700	-0.37757700	0.21515100
Fe	-0.08667900	2.49974000	-0.02574900
Ge	-0.09995900	0.14095800	-0.03685700



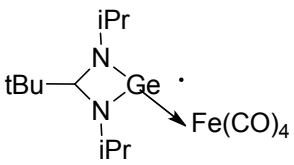
Sum of electronic and thermal Enthalpies = -544.173165
Sum of electronic and thermal Free Energies = -544.231920

C	0.04620400	-0.15067300	-0.04520000

C	-0.06689700	1.40043000	-0.10620500
C	-0.74916400	1.89628000	1.17958000
H	-1.71807100	1.44537700	1.37094900
H	-0.89056200	2.97775600	1.12344800
H	-0.11465600	1.69049500	2.04340800
C	-0.85051900	1.80721100	-1.36402800
H	-1.84976000	1.38681600	-1.41836400
H	-0.31168700	1.49514700	-2.26025900
H	-0.94567800	2.89469500	-1.39703600
C	1.25212500	2.17569000	-0.18238600
H	1.01517300	3.24103900	-0.13689700
H	1.78373400	2.00946000	-1.11811100
H	1.91823600	1.95968700	0.65109500
C	2.52594600	-0.55124800	-0.10975700
H	2.73859800	0.43393800	-0.52125100
C	3.08262600	-0.61030500	1.31453700
H	2.63298700	0.15163600	1.95208600
H	4.16234800	-0.45526100	1.30016500
H	2.87301100	-1.58584600	1.75386500
C	3.21804500	-1.58803600	-0.98982600
H	3.05542200	-2.58892700	-0.58981000
H	4.29081600	-1.39209600	-1.03733900
H	2.81937000	-1.56240100	-2.00402900
C	-2.42146100	-0.58525600	0.05720300
H	-2.63984000	0.48463500	0.02220700
C	-3.00362500	-1.14522500	1.35493200
H	-2.81652300	-2.21717900	1.41358600
H	-4.07981200	-0.96843700	1.39023500
H	-2.54789800	-0.67489600	2.22671400
C	-3.08928900	-1.24418700	-1.14963300
H	-2.69645900	-0.84353000	-2.08445300
H	-4.16623400	-1.07016300	-1.12470800
H	-2.90173500	-2.31766900	-1.13736900
N	1.13587500	-0.90348500	-0.04950300
N	-1.03226300	-0.94256800	0.02472800

Cl

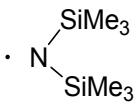
Sum of electronic and thermal Enthalpies = -460.490975
Sum of electronic and thermal Free Energies = -460.509012



Sum of electronic and thermal Enthalpies = -3200.860862
Sum of electronic and thermal Free Energies = -3200.952794

C	-1.16913900	0.00030100	1.53290800
C	-2.67732200	-1.58739700	-0.60398000
C	-3.69033400	-0.04671800	1.19931100
C	-2.75533100	1.46583200	-0.65962600
C	2.05849100	0.07274400	-0.06088800
C	3.49542700	0.05230700	0.45944600
C	3.51723500	-0.68636100	1.80691300

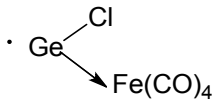
H	2.89208100	-0.17081900	2.53635500
H	4.53952300	-0.70251400	2.18787700
H	3.16946300	-1.71316400	1.74214400
C	4.39196400	-0.64333100	-0.57730900
H	4.09643700	-1.66711300	-0.79042600
H	5.41731700	-0.66329100	-0.20449600
H	4.38955600	-0.09183500	-1.51831100
C	4.10507200	1.43260400	0.70758500
H	4.25366100	1.99302200	-0.21401700
H	5.08966400	1.28602300	1.15370400
H	3.51995900	2.03225100	1.40222800
C	1.61292000	-2.44784200	-0.19821900
H	2.66250900	-2.59204900	0.05412400
C	0.76974300	-3.09391200	0.89421500
H	0.94650200	-2.62401100	1.86102900
H	1.00588300	-4.15574900	0.97422900
H	-0.29267900	-2.99978900	0.66761900
C	1.36267500	-3.10520900	-1.54930900
H	0.31998600	-2.98072600	-1.84877400
H	1.56746600	-4.17486300	-1.49770700
H	1.99228700	-2.66765600	-2.32423600
C	1.43984000	2.56197000	-0.32091800
H	2.49078400	2.82654400	-0.40174500
C	0.88912500	3.11037500	0.98989700
H	-0.17481400	2.88823800	1.07775900
H	1.01769900	4.19282400	1.03207700
H	1.39154400	2.67054300	1.85124300
C	0.72481200	3.18013300	-1.51397400
H	1.13137200	2.80627800	-2.45358700
H	0.83633400	4.26430900	-1.49754700
H	-0.34446600	2.96158500	-1.48917400
N	1.33298200	-1.02686100	-0.28975300
N	1.29550700	1.11759900	-0.38933900
O	-0.49368900	0.02132800	2.46812000
O	-2.95793800	-2.59577400	-1.07562700
O	-4.60973000	-0.05436400	1.87881900
O	-3.09482400	2.43810100	-1.16745500
Fe	-2.26258400	-0.03478800	0.15835400
Ge	-0.20912300	-0.01612500	-0.97284700



Sum of electronic and thermal Enthalpies = -874.836568
Sum of electronic and thermal Free Energies = -874.900867

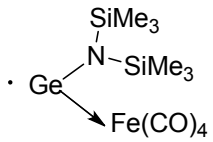
C	2.53967200	1.38094000	-0.95829200
H	2.43858600	1.26196700	-2.03718000
H	3.60267300	1.38463300	-0.70851300
H	2.13039500	2.35505500	-0.68686100
C	1.91954900	0.20464800	1.80235700
H	1.51741600	1.15610800	2.15531700
H	2.98332100	0.18476100	2.04938700
H	1.43150500	-0.59286100	2.36485300
C	2.31751500	-1.68189300	-0.58943400
H	1.79980700	-2.49602900	-0.08111000
H	3.37984600	-1.75600600	-0.34726000
H	2.19810800	-1.81957600	-1.66385800
C	-1.92272500	-0.39785900	1.77057900
H	-1.54096500	-1.39066200	2.01617400

H	-2.98591500	-0.38418500	2.02082900
H	-1.41887100	0.32212500	2.41736900
C	-2.55954000	-1.26121600	-1.09826500
H	-2.46059600	-1.02623000	-2.15816400
H	-3.62179900	-1.28092400	-0.84610800
H	-2.16035700	-2.26363000	-0.93688200
C	-2.29393800	1.74070400	-0.40737500
H	-1.76718100	2.48971600	0.18473700
H	-3.35583900	1.80188300	-0.15980100
H	-2.17082600	1.98957600	-1.46118900
N	-0.00014300	0.01831200	-0.55427500
Si	1.65304300	-0.00449500	-0.04911600
Si	-1.65315000	0.00622000	-0.04797300



Sum of electronic and thermal Enthalpies = -3117.171875
Sum of electronic and thermal Free Energies = -3117.230123

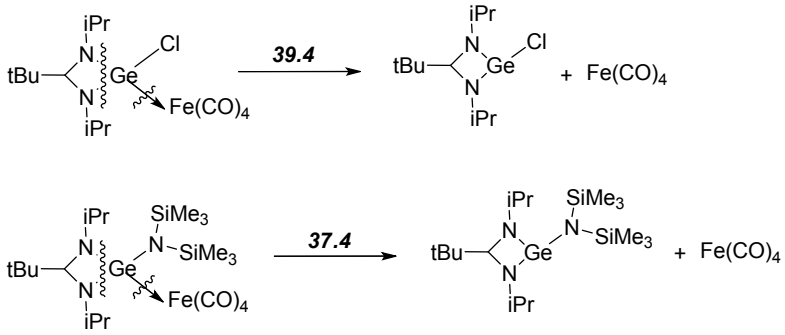
C	-1.63924100	0.59487100	1.48702000
C	-1.64001700	0.59541800	-1.48651500
C	0.18908200	1.61400000	0.00007400
C	-1.50190200	-1.54136200	0.00014900
O	-2.19636900	0.91257100	2.42903600
O	-2.19739700	0.91357600	-2.42823100
O	0.75059000	2.60621900	0.00022400
O	-1.96808700	-2.58047300	0.00050000
Fe	-0.78762500	0.11521700	-0.00005200
Ge	1.23289600	-0.88270600	-0.00076500
Cl	3.14518700	0.16813200	0.00054500

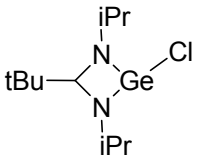


Sum of electronic and thermal Enthalpies = -3531.494677
Sum of electronic and thermal Free Energies = -3531.586660

C	-2.16412800	0.46274200	1.63800100
C	-3.82098200	0.71552000	-0.29657900
C	-1.60073300	0.60133900	-1.49252900
C	-2.99525200	-1.76910000	-0.16124000
C	2.25276600	-2.87179400	-0.63879300
H	1.61792600	-3.37952400	0.08771500
H	3.12208300	-3.51178300	-0.81294500
H	1.70581400	-2.80647100	-1.58123100
C	4.12678000	-0.60778900	-1.31904300
H	3.68147600	-0.53713300	-2.31222900
H	4.93587300	-1.33986500	-1.37078800
H	4.57366300	0.35594600	-1.07897200
C	3.67310600	-1.41111000	1.62524800
H	4.08901800	-0.48006700	2.00855000
H	4.48374900	-2.14047600	1.56686300
H	2.94833300	-1.77882900	2.35384800
C	3.30991800	2.11462500	1.08183400

H	3.15305000	1.83123500	2.12354500
H	3.47747800	3.19382800	1.05747900
H	4.22461000	1.63662400	0.73370000
C	0.37225500	2.66893300	0.79969700
H	-0.55117800	2.59483300	0.22880300
H	0.65748500	3.72316100	0.83907100
H	0.16495700	2.34934000	1.82154500
C	2.06214200	2.31657800	-1.72268300
H	2.93872900	1.86345400	-2.18492800
H	2.20644700	3.39934300	-1.72760800
H	1.19570100	2.09464200	-2.34599000
N	1.50612300	-0.04124300	0.04931400
O	-2.14524300	0.86376000	2.71323000
O	-4.80657800	1.26406400	-0.46839000
O	-1.23110500	1.10400100	-2.45893100
O	-3.47684700	-2.80113400	-0.25121500
Si	2.87071100	-1.19452300	-0.05495600
Si	1.79580100	1.72682900	0.03607400
Fe	-2.27372300	-0.12726900	-0.02865600
Ge	-0.10623400	-0.86525100	0.24677300

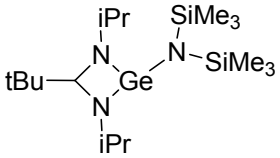




Sum of electronic and thermal Enthalpies = -3082.688849
Sum of electronic and thermal Free Energies = -3082.756551

C	-0.08574100	0.81043400	0.06596000
C	-0.37599400	2.25844200	0.45723500
C	-1.18670400	2.91920500	-0.66880700
H	-0.61730800	2.92885800	-1.59869800
H	-1.39811300	3.95327900	-0.39311500
H	-2.13405800	2.42661500	-0.86593000
C	-1.14825900	2.26120300	1.78671200
H	-2.09244400	1.72559600	1.74406700
H	-1.36204900	3.29315000	2.06853900
H	-0.54750100	1.81477700	2.57970400
C	0.86414300	3.12601200	0.67449300
H	1.45228500	2.80200000	1.53152200
H	0.52454600	4.14057200	0.88630200
H	1.50434500	3.17573300	-0.20408500
C	-2.48965700	-0.04760200	-0.19675800
H	-2.81067100	0.91856800	0.18815200
C	-3.02972400	-0.19622100	-1.61369500
H	-2.64611800	0.58254500	-2.27212400

H	-4.11871300	-0.13890100	-1.60617100
H	-2.74680900	-1.16048100	-2.03674800
C	-3.04459100	-1.12724700	0.72185700
H	-2.75712100	-2.12018600	0.37305900
H	-4.13380300	-1.08147500	0.73777700
H	-2.67393100	-1.01117600	1.73960600
C	2.48521200	0.61838800	-0.03456900
H	2.58348700	1.45570500	0.64996900
C	2.97363300	1.04075700	-1.41454700
H	2.90936500	0.20574600	-2.11322000
H	4.01452200	1.36284500	-1.36479200
H	2.37995400	1.86061500	-1.81919700
C	3.32533700	-0.52255900	0.51919500
H	2.98292400	-0.82202700	1.50848600
H	4.36821700	-0.21347400	0.58890400
H	3.28692000	-1.39657000	-0.13335500
N	-1.03597100	-0.09356900	-0.19021500
N	1.09158000	0.19885600	-0.07361500
Cl	0.32962500	-2.64898200	1.20607100
Ge	0.25978900	-1.47660900	-0.64460900



Sum of electronic and thermal Enthalpies = -3496.982652
Sum of electronic and thermal Free Energies = -3497.086141

C	2.06875100	0.06460700	-0.06019700
C	3.49059100	0.18838400	0.50792500
C	4.22101100	-1.13887700	0.72707700
H	3.72717100	-1.76328400	1.47018300
H	5.21421000	-0.90722400	1.11464500
H	4.35841600	-1.70778700	-0.18922100
C	3.44920600	0.85998100	1.89176200
H	2.96846200	0.20861000	2.62065100
H	2.93387800	1.81574200	1.91043700
H	4.47458400	1.03037800	2.22296400
C	4.34558100	1.00651000	-0.47321600
H	5.35188000	1.10349100	-0.06274400
H	3.96093900	2.00680200	-0.65187700
H	4.41707500	0.50670900	-1.43780700
C	1.78546400	-2.43637100	-0.55156600
H	2.45769600	-2.68857400	0.26476800
C	0.54656100	-3.30514900	-0.39577400
H	0.08122100	-3.16827500	0.57880800
H	0.81880800	-4.35586100	-0.49601200
H	-0.19283800	-3.08457100	-1.16653000
C	2.48135300	-2.73808600	-1.87388700
H	1.80239900	-2.56952400	-2.70894700
H	2.80117800	-3.78082700	-1.89754300
H	3.35546300	-2.10684600	-2.02844800
C	1.46006600	2.53908000	-0.09663900
H	2.43274100	2.70563900	0.36103300
C	0.39793500	3.09694500	0.84069200
H	-0.59998700	2.90915200	0.44240300
H	0.51924300	4.17461800	0.95402500
H	0.45901400	2.63986900	1.82839900
C	1.45199500	3.27885500	-1.42766100

H	2.20309200	2.88285700	-2.10940700
H	1.65998900	4.33649700	-1.26048200
H	0.48131200	3.20536700	-1.91622200
C	0.15766700	-0.60482100	2.42573400
H	0.74856000	-1.45750700	2.10012700
H	-0.01901900	-0.71206900	3.49917500
H	0.73718200	0.30229600	2.27751600
C	-2.38815500	0.86663700	2.62007800
H	-1.78715100	1.77700600	2.58900300
H	-2.46287500	0.55964900	3.66617800
H	-3.38945400	1.12087000	2.28030700
C	-2.35195100	-2.16794200	2.04451000
H	-3.43429100	-2.11028500	2.13602800
H	-1.95900900	-2.52919600	2.99757200
H	-2.12414500	-2.91852100	1.28681000
C	-4.59350000	-0.56018300	0.28752000
H	-4.58138200	-1.64652300	0.19769700
H	-5.52703700	-0.21075600	-0.16159400
H	-4.62854800	-0.30285300	1.34298600
C	-3.59251900	-0.43273200	-2.44957100
H	-3.02374600	0.02822100	-3.25069000
H	-4.65355300	-0.24387100	-2.63216400
H	-3.43798100	-1.51067600	-2.50264000
C	-3.47860900	2.08938600	-0.69980100
H	-3.35309600	2.48815900	0.30776700
H	-4.49205700	2.33070900	-1.02804400
H	-2.79202300	2.61674000	-1.36179000
N	1.40436600	-1.03406400	-0.42880600
N	1.26373800	1.10823200	-0.27517000
N	-1.59007100	-0.16880700	-0.10342500
Si	-1.54673800	-0.50943300	1.64114700
Si	-3.21796700	0.22787500	-0.73732600
Ge	-0.09548000	-0.00023200	-1.20284200

FeCO4

Sum of electronic and thermal Enthalpies = -578.724904
Sum of electronic and thermal Free Energies = -578.772365

C	-0.73151300	1.65014700	0.43109400
C	1.79514100	-0.19117500	0.43500600
C	-1.06496500	-1.45608500	0.43438800
C	0.00183900	-0.00291400	-1.35054600
O	-1.19519000	2.69279500	0.42232400
O	2.92976700	-0.31255700	0.42799800
O	-1.73942000	-2.37656400	0.42736800
O	0.00273300	-0.00482800	-2.49176700
Fe	0.00053300	0.00036200	0.38511400