Supplementary Information

The use of a germene for the synthesis of esters of α-germyl-substituted α-amino acid and α-aminophosphonic acid

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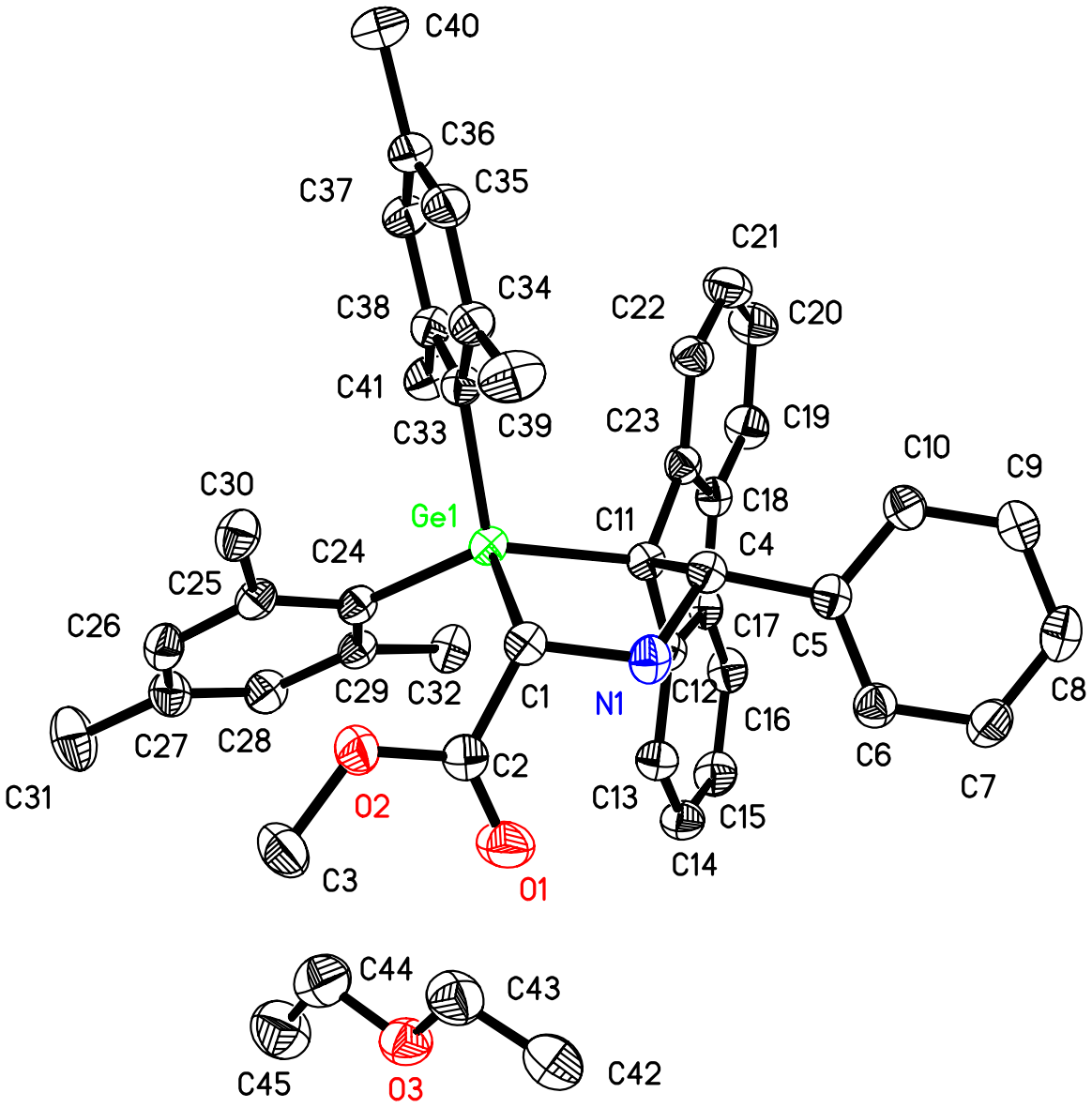
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C45
O3
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4

Table 1. Crystal data and structure refinement for **4**.

Identification code	**4**	
Empirical formula	C45 H51 Ge N O3	
Formula weight	726.46	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.9777(7) Å	α = 101.8250(10)°.
	b = 12.1155(7) Å	β = 95.7740(10)°.
	c = 14.5540(8) Å	γ = 108.6110(10)°.
Volume	1927.47(19) $Å^3$	
Z	2	
Density (calculated)	1.252 Mg/m^3	
Absorption coefficient	0.835 mm^{-1}	
F(000)	768	
Crystal size	0.5 x 0.7 x 0.7 mm^3	
Theta range for data collection	1.45 to 29.43°.	
Index ranges	-15<=h<=11, -15<=k<=16, -18<=l<=19	
Reflections collected	12972	
Independent reflections	9290 [R(int) = 0.0247]	
Completeness to theta = 29.43°	87.1 %	
Absorption correction	SEMI-EMPIRICAL	
Max. and min. transmission	1.000000 and 0.760492	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9290 / 0 / 463	
Goodness-of-fit on F^2	1.028	
Final R indices [I>2sigma(I)]	R1 = 0.0316, wR2 = 0.0830	
R indices (all data)	R1 = 0.0380, wR2 = 0.0864	
Largest diff. peak and hole	0.493 and -0.326 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ge(1)	8325(1)	7372(1)	2557(1)	20(1)
C(1)	9015(1)	9083(1)	3382(1)	23(1)
C(2)	8408(1)	9891(1)	3075(1)	27(1)
O(1)	7616(1)	10148(1)	3412(1)	44(1)
O(2)	8877(1)	10318(1)	2369(1)	34(1)
C(3)	8302(2)	11000(2)	1928(2)	47(1)
N(1)	8857(1)	8991(1)	4347(1)	26(1)
C(4)	8708(1)	7799(1)	4501(1)	23(1)
C(5)	8479(1)	7739(1)	5498(1)	24(1)
C(6)	7905(1)	8435(1)	6007(1)	29(1)
C(7)	7719(2)	8349(2)	6922(1)	34(1)
C(8)	8085(2)	7566(2)	7337(1)	36(1)
C(9)	8647(2)	6861(2)	6836(1)	36(1)
C(10)	8846(1)	6955(2)	5929(1)	31(1)
C(11)	7707(1)	6813(1)	3701(1)	21(1)
C(12)	6446(1)	6741(1)	3818(1)	22(1)
C(13)	5926(1)	7621(1)	3914(1)	26(1)
C(14)	4718(1)	7298(2)	3999(1)	31(1)
C(15)	4036(1)	6122(2)	3972(1)	33(1)
C(16)	4549(1)	5238(2)	3884(1)	30(1)
C(17)	5755(1)	5554(1)	3814(1)	23(1)
C(18)	6514(1)	4821(1)	3732(1)	24(1)
C(19)	6253(2)	3615(2)	3722(1)	32(1)
C(20)	7172(2)	3147(2)	3698(1)	37(1)
C(21)	8330(2)	3880(2)	3692(1)	35(1)
C(22)	8596(1)	5082(2)	3693(1)	28(1)
C(23)	7677(1)	5558(1)	3696(1)	23(1)
C(24)	7375(1)	7366(1)	1360(1)	23(1)
C(25)	8029(1)	7993(1)	752(1)	25(1)
C(26)	7415(2)	8116(2)	-67(1)	29(1)
C(27)	6179(2)	7603(2)	-332(1)	32(1)

C(28)	5558(1)	6934(2)	240(1)	30(1)
C(29)	6126(1)	6799(1)	1076(1)	24(1)
C(30)	9381(1)	8489(2)	907(1)	32(1)
C(31)	5535(2)	7717(2)	-1239(2)	50(1)
C(32)	5348(1)	6001(2)	1604(1)	30(1)
C(33)	9492(1)	6583(1)	2199(1)	24(1)
C(34)	10745(1)	7082(2)	2522(1)	28(1)
C(35)	11472(1)	6444(2)	2189(1)	31(1)
C(36)	11018(2)	5332(2)	1545(1)	32(1)
C(37)	9783(2)	4828(2)	1249(1)	31(1)
C(38)	9017(1)	5424(1)	1574(1)	26(1)
C(39)	11380(1)	8291(2)	3221(1)	39(1)
C(40)	11833(2)	4684(2)	1178(2)	47(1)
C(41)	7689(1)	4748(2)	1249(1)	32(1)
C(42)	4805(2)	10315(2)	3662(2)	47(1)
C(43)	4862(2)	9757(2)	2671(2)	51(1)
O(3)	3743(1)	9476(1)	2067(1)	43(1)
C(44)	3709(2)	8847(2)	1133(2)	58(1)
C(45)	2509(2)	8582(2)	546(2)	65(1)

Table 3. Bond lengths [Å] and angles [°] for **4**.

Ge(1)-C(24)	1.9800(14)
Ge(1)-C(33)	1.9841(15)
Ge(1)-C(1)	2.0274(14)
Ge(1)-C(11)	2.0410(14)
C(1)-N(1)	1.4581(19)
C(1)-C(2)	1.501(2)
C(2)-O(1)	1.207(2)
C(2)-O(2)	1.3361(19)
O(2)-C(3)	1.435(2)
N(1)-C(4)	1.464(2)
C(4)-C(5)	1.515(2)
C(4)-C(11)	1.5670(19)
C(5)-C(10)	1.396(2)
C(5)-C(6)	1.396(2)
C(6)-C(7)	1.391(2)
C(7)-C(8)	1.382(3)
C(8)-C(9)	1.387(3)
C(9)-C(10)	1.385(2)
C(11)-C(23)	1.509(2)
C(11)-C(12)	1.5130(19)
C(12)-C(13)	1.387(2)
C(12)-C(17)	1.410(2)
C(13)-C(14)	1.399(2)
C(14)-C(15)	1.388(2)
C(15)-C(16)	1.385(2)
C(16)-C(17)	1.392(2)
C(17)-C(18)	1.457(2)
C(18)-C(19)	1.390(2)
C(18)-C(23)	1.408(2)
C(19)-C(20)	1.390(2)
C(20)-C(21)	1.389(3)
C(21)-C(22)	1.387(2)
C(22)-C(23)	1.396(2)
C(24)-C(29)	1.4093(19)

C(24)-C(25)	1.417(2)
C(25)-C(26)	1.396(2)
C(25)-C(30)	1.511(2)
C(26)-C(27)	1.388(2)
C(27)-C(28)	1.386(2)
C(27)-C(31)	1.515(2)
C(28)-C(29)	1.398(2)
C(29)-C(32)	1.506(2)
C(33)-C(38)	1.409(2)
C(33)-C(34)	1.415(2)
C(34)-C(35)	1.397(2)
C(34)-C(39)	1.510(2)
C(35)-C(36)	1.379(3)
C(36)-C(37)	1.391(2)
C(36)-C(40)	1.509(2)
C(37)-C(38)	1.399(2)
C(38)-C(41)	1.511(2)
C(42)-C(43)	1.479(3)
C(43)-O(3)	1.426(2)
O(3)-C(44)	1.405(3)
C(44)-C(45)	1.498(3)

C(24)-Ge(1)-C(33)	107.39(6)
C(24)-Ge(1)-C(1)	108.42(6)
C(33)-Ge(1)-C(1)	116.49(6)
C(24)-Ge(1)-C(11)	127.84(6)
C(33)-Ge(1)-C(11)	107.23(6)
C(1)-Ge(1)-C(11)	89.16(6)
N(1)-C(1)-C(2)	110.46(12)
N(1)-C(1)-Ge(1)	105.46(9)
C(2)-C(1)-Ge(1)	112.95(10)
O(1)-C(2)-O(2)	123.36(15)
O(1)-C(2)-C(1)	126.03(15)
O(2)-C(2)-C(1)	110.61(13)
C(2)-O(2)-C(3)	117.07(14)
C(1)-N(1)-C(4)	113.97(12)

N(1)-C(4)-C(5)	111.46(12)
N(1)-C(4)-C(11)	109.66(12)
C(5)-C(4)-C(11)	112.97(11)
C(10)-C(5)-C(6)	118.13(14)
C(10)-C(5)-C(4)	119.16(14)
C(6)-C(5)-C(4)	122.71(13)
C(7)-C(6)-C(5)	120.45(15)
C(8)-C(7)-C(6)	120.65(16)
C(7)-C(8)-C(9)	119.51(16)
C(10)-C(9)-C(8)	119.93(16)
C(9)-C(10)-C(5)	121.32(16)
C(23)-C(11)-C(12)	102.54(11)
C(23)-C(11)-C(4)	112.41(12)
C(12)-C(11)-C(4)	114.21(11)
C(23)-C(11)-Ge(1)	112.95(9)
C(12)-C(11)-Ge(1)	117.63(9)
C(4)-C(11)-Ge(1)	97.63(9)
C(13)-C(12)-C(17)	119.64(13)
C(13)-C(12)-C(11)	130.55(13)
C(17)-C(12)-C(11)	109.81(12)
C(12)-C(13)-C(14)	118.61(14)
C(15)-C(14)-C(13)	121.37(15)
C(16)-C(15)-C(14)	120.48(15)
C(15)-C(16)-C(17)	118.54(15)
C(16)-C(17)-C(12)	121.33(14)
C(16)-C(17)-C(18)	129.86(14)
C(12)-C(17)-C(18)	108.81(12)
C(19)-C(18)-C(23)	121.16(14)
C(19)-C(18)-C(17)	130.36(14)
C(23)-C(18)-C(17)	108.44(13)
C(18)-C(19)-C(20)	118.77(15)
C(21)-C(20)-C(19)	120.25(16)
C(22)-C(21)-C(20)	121.40(16)
C(21)-C(22)-C(23)	119.01(15)
C(22)-C(23)-C(18)	119.35(14)
C(22)-C(23)-C(11)	130.37(13)

C(18)-C(23)-C(11)	110.24(12)
C(29)-C(24)-C(25)	118.52(13)
C(29)-C(24)-Ge(1)	125.51(11)
C(25)-C(24)-Ge(1)	115.97(10)
C(26)-C(25)-C(24)	119.45(14)
C(26)-C(25)-C(30)	116.94(14)
C(24)-C(25)-C(30)	123.53(14)
C(27)-C(26)-C(25)	122.32(15)
C(28)-C(27)-C(26)	117.55(14)
C(28)-C(27)-C(31)	121.00(16)
C(26)-C(27)-C(31)	121.38(16)
C(27)-C(28)-C(29)	122.47(14)
C(28)-C(29)-C(24)	119.49(14)
C(28)-C(29)-C(32)	116.79(13)
C(24)-C(29)-C(32)	123.69(13)
C(38)-C(33)-C(34)	118.02(14)
C(38)-C(33)-Ge(1)	116.42(10)
C(34)-C(33)-Ge(1)	125.55(12)
C(35)-C(34)-C(33)	119.71(15)
C(35)-C(34)-C(39)	116.13(14)
C(33)-C(34)-C(39)	124.16(14)
C(36)-C(35)-C(34)	122.53(15)
C(35)-C(36)-C(37)	117.62(14)
C(35)-C(36)-C(40)	121.11(16)
C(37)-C(36)-C(40)	121.27(17)
C(36)-C(37)-C(38)	121.93(16)
C(37)-C(38)-C(33)	120.08(14)
C(37)-C(38)-C(41)	116.78(14)
C(33)-C(38)-C(41)	123.12(13)
O(3)-C(43)-C(42)	109.79(17)
C(44)-O(3)-C(43)	112.28(16)
O(3)-C(44)-C(45)	109.09(19)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ge(1)	16(1)	21(1)	20(1)	2(1)	2(1)	4(1)
C(1)	19(1)	22(1)	23(1)	3(1)	2(1)	3(1)
C(2)	26(1)	21(1)	27(1)	3(1)	2(1)	3(1)
O(1)	42(1)	44(1)	60(1)	25(1)	23(1)	24(1)
O(2)	45(1)	31(1)	31(1)	12(1)	10(1)	15(1)
C(3)	68(1)	41(1)	41(1)	19(1)	8(1)	27(1)
N(1)	27(1)	21(1)	21(1)	1(1)	-1(1)	2(1)
C(4)	18(1)	23(1)	22(1)	4(1)	1(1)	4(1)
C(5)	19(1)	24(1)	22(1)	3(1)	-1(1)	3(1)
C(6)	31(1)	27(1)	27(1)	6(1)	5(1)	9(1)
C(7)	41(1)	32(1)	29(1)	5(1)	11(1)	13(1)
C(8)	41(1)	39(1)	25(1)	8(1)	9(1)	10(1)
C(9)	41(1)	42(1)	29(1)	13(1)	4(1)	18(1)
C(10)	30(1)	36(1)	26(1)	7(1)	1(1)	14(1)
C(11)	18(1)	21(1)	22(1)	4(1)	2(1)	5(1)
C(12)	19(1)	24(1)	19(1)	4(1)	2(1)	5(1)
C(13)	25(1)	24(1)	28(1)	6(1)	4(1)	8(1)
C(14)	28(1)	36(1)	33(1)	9(1)	6(1)	15(1)
C(15)	21(1)	42(1)	34(1)	11(1)	7(1)	9(1)
C(16)	23(1)	32(1)	31(1)	11(1)	6(1)	3(1)
C(17)	23(1)	25(1)	20(1)	6(1)	3(1)	5(1)
C(18)	25(1)	22(1)	22(1)	5(1)	3(1)	6(1)
C(19)	35(1)	24(1)	36(1)	9(1)	7(1)	6(1)
C(20)	46(1)	24(1)	45(1)	11(1)	8(1)	14(1)
C(21)	38(1)	33(1)	39(1)	8(1)	4(1)	18(1)
C(22)	26(1)	30(1)	28(1)	6(1)	3(1)	11(1)
C(23)	24(1)	22(1)	20(1)	3(1)	2(1)	7(1)
C(24)	20(1)	24(1)	21(1)	1(1)	2(1)	6(1)
C(25)	26(1)	24(1)	23(1)	2(1)	5(1)	7(1)
C(26)	33(1)	29(1)	24(1)	6(1)	6(1)	8(1)
C(27)	34(1)	35(1)	26(1)	6(1)	-1(1)	12(1)

C(28)	24(1)	34(1)	25(1)	2(1)	-1(1)	8(1)
C(29)	21(1)	25(1)	22(1)	1(1)	3(1)	7(1)
C(30)	25(1)	37(1)	31(1)	9(1)	8(1)	6(1)
C(31)	45(1)	62(1)	37(1)	21(1)	-7(1)	11(1)
C(32)	20(1)	37(1)	26(1)	5(1)	3(1)	2(1)
C(33)	20(1)	25(1)	25(1)	7(1)	5(1)	6(1)
C(34)	22(1)	30(1)	31(1)	9(1)	6(1)	8(1)
C(35)	21(1)	39(1)	37(1)	15(1)	8(1)	12(1)
C(36)	34(1)	41(1)	33(1)	15(1)	13(1)	22(1)
C(37)	35(1)	30(1)	30(1)	5(1)	8(1)	14(1)
C(38)	26(1)	28(1)	25(1)	6(1)	5(1)	8(1)
C(39)	19(1)	38(1)	50(1)	-1(1)	2(1)	5(1)
C(40)	48(1)	61(1)	49(1)	16(1)	20(1)	37(1)
C(41)	27(1)	28(1)	33(1)	-3(1)	2(1)	5(1)
C(42)	40(1)	39(1)	60(1)	17(1)	3(1)	8(1)
C(43)	39(1)	62(1)	58(1)	22(1)	10(1)	23(1)
O(3)	37(1)	47(1)	48(1)	12(1)	8(1)	19(1)
C(44)	61(1)	64(2)	54(1)	13(1)	14(1)	31(1)
C(45)	76(2)	58(2)	56(1)	8(1)	-5(1)	25(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **4.**

	x	y	z	U(eq)
H(1)	9890	9421	3366	27
H(3A)	7476	10490	1634	71
H(3B)	8738	11282	1438	71
H(3C)	8299	11693	2412	71
H(1N)	9300(18)	9427(19)	4686(15)	31
H(4)	9477	7654	4438	27
H(6)	7640	8971	5727	34
H(7)	7335	8834	7264	41
H(8)	7954	7510	7962	43
H(9)	8896	6314	7114	43
H(10)	9239	6475	5594	37
H(13)	6381	8426	3923	32
H(14)	4356	7896	4076	37
H(15)	3212	5922	4015	39
H(16)	4087	4434	3871	35
H(19)	5461	3119	3732	39
H(20)	7009	2323	3686	45
H(21)	8951	3551	3687	42
H(22)	9393	5573	3693	34
H(26)	7858	8567	-455	35
H(28)	4714	6553	58	35
H(30A)	9679	7841	660	48
H(30B)	9701	8822	1591	48
H(30C)	9639	9124	570	48
H(31A)	6004	8458	-1396	75
H(31B)	4745	7744	-1146	75
H(31C)	5441	7023	-1763	75
H(32A)	4992	6470	2034	45
H(32B)	5835	5675	1975	45
H(32C)	4710	5337	1145	45

H(35)	12312	6789	2414	37
H(37)	9450	4057	814	38
H(39A)	12187	8344	3482	59
H(39B)	10930	8381	3742	59
H(39C)	11433	8932	2894	59
H(40A)	12252	5072	720	71
H(40B)	11357	3842	862	71
H(40C)	12420	4717	1713	71
H(41A)	7558	3948	846	49
H(41B)	7343	5192	883	49
H(41C)	7304	4666	1807	49
H(42A)	4619	11049	3677	71
H(42B)	5580	10517	4072	71
H(42C)	4180	9749	3892	71
H(43A)	5506	10319	2442	61
H(43B)	5048	9014	2652	61
H(44A)	3847	8086	1143	69
H(44B)	4347	9338	851	69
H(45A)	1884	8071	815	97
H(45B)	2488	8164	-111	97
H(45C)	2371	9337	550	97