Z-matrix, total (ZPE correction) and repulsion energies for compounds **1** and **3**

1

z-matrix :
X
X,1,1.
X,2,1.,1,90.
C,1,1.,2,90.,3,180.,0
C,1,R1,2,90.,3,0.,0
C,4,R2,1,A1,2,0.,0
N,5,R3,1,A2,2,D1,0
N,6,R4,4,A3,1,D2,0
C,5,R5,1,A4,2,D3,0
H,4,R6,1,A5,2,D4,0
C,6,R7,4,A6,1,D5,0
H,9,1.12,5,A7,4,D6,0
H,9,1.12,5,A8,12,D7,0
H,9,1.12,5,A9,12,D8,0
H,11,1.12,6,A10,4,D9,0
H,11,1.12,6,A11,15,D10,0
H,11,1.12,6,A12,15,D11,0
C,7,R14,5,A13,1,D12,0
C,18,R15,7,A14,5,D13,0
C,19,R16,18,A15,7,180.,0
C,20,R17,19,A16,18,0.,0
C,21,R18,20,A17,19,0.,0
C,22,R19,21,A18,20,0.,0
H,23,1.1,18,A19,22,180.,0
H,22,1.1,21,A20,20,180.,0
H,21,1.1,20,A21,19,180.,0
H,20,1.1,21,A22,22,180.,0
H,19,1.1,20,A23,21,180.,0
C,8,R25,6,A24,4,180.,0
C,29,R26,8,A25,6,D14,0
C,30,R27,29,A26,8,180.,0
C,31,R28,30,A27,29,0.,0
C,32,R29,31,A28,30,0.,0
C,33,R30,32,A29,31,0.,0
H,34,1.1,33,A30,32,180.,0
H,33,1.1,32,A31,31,180.,0
H,32,1.1,31,A32,30,180.,0
H,31,1.1,30,A33,29,180.,0
H,30,1.1,31,A34,32,180.,0
Ge,8,R36,6,A35,4,D15,0
Cl,40,R37,8,A36,6,D16,0
Variables:
R1=0.40051626
R2=1.40073733
R3=1.33445754
R4=1.33423185
R5=1.50977717
R6=1.07967502
R7=1.50979652

R14=1.43618451
R15=1.3977306
R16=1.39292967
R17=1.39278168
R18=1.3933359
R19=1.39213598
R25=1.43652046
R26=1.39779447
R27=1.39286631
R28=1.39285147
R29=1.39322135
R30=1.39220499
R36=2.0276616
R37=2.35722679
A1=127.72070368
A2=123.29569136
A3=123.34313973
A4=117.41576979
A5=116.07539524
A6=117.37424595
A7=110.98017415
A8=111.2462125
A9=110.77594643
A10=110.84129317
A11=110.99405146
A12=111.18597518
A13=120.78566845
A14=120.12543297
A15=119.88099174
A16=120.37994403
A17=119.73873066
A18=120.18903901
A19=119.21145343
A20=120.12908389
A21=120.1585553
A22=120.11458145
A23=121.00368023
A24=120.74929238
A25=120.15059978
A26=119.8616655
A27=120.39089787
A28=119.74484676
A29=120.1735289
A30=120.69176726
A31=120.13387152
A32=120.15077522
A33=119.4977693
A34=120.99929988
A35=126.37187661
A36=94.86201401
D1=5.00991978
D2=-5.82118327
D3=185.53502194
D4=175.6778021

D5=174.11044557
D6=-1.91571824
D7=120.86834555
D8=-120.79056924
D9=120.8155433
D10=-120.80902479
D11=118.3196207
D12=182.81203657
D13=-92.89371231
D14=90.32965345
D15=-9.76874239
D16=-76.92860262

Energies :

Nuclear repulsion energy : 2262.4643167775 Hartrees

Sum of electronic and zero-point Energies : -3304.758368 ua

3

z-matrix :
X
X,1,1.
X,2,1.,1,90.
C,1,1.,2,90.,3,D17,0
C,1,R1,2,90.,3,D18,0
C,4,R2,1,A1,2,D19,0
N,5,R3,1,A2,2,D1,0
N,6,R4,4,A3,1,D2,0
C,5,R5,1,A4,2,D3,0
H,4,R6,1,A5,2,D4,0
C,6,R7,4,A6,1,D5,0
H,9,1.1,5,A7,4,D6,0
H,9,1.1,5,A8,12,D7,0
H,9,1.1,5,A9,12,D8,0
H,11,1.1,6,A10,4,D9,0
H,11,1.1,6,A11,15,D10,0
H,11,1.1,6,A12,15,D11,0
C,7,R14,5,A13,1,D12,0
C,18,R15,7,A14,5,D13,0
C,19,R16,18,A15,7,180.,0
C,20,R17,19,A16,18,0.,0
C,21,R18,20,A17,19,0.,0
C,22,R19,21,A18,20,0.,0
H,23,1.1,18,120.,22,180.,0
H,22,1.1,21,120.,20,180.,0
H,21,1.1,20,120.,19,180.,0
H,20,1.1,21,120.,22,180.,0
H,19,1.1,20,120.,21,180.,0
C,8,R25,6,A24,4,180.,0
C,29,R26,8,A25,6,D14,0
C,30,R27,29,A26,8,180.,0
C,31,R28,30,A27,29,0.,0
C,32,R29,31,A28,30,0.,0
C,33,R30,32,A29,31,0.,0
H,34,1.1,33,120.,32,180.,0
H,33,1.1,32,120.,31,180.,0
H,32,1.1,31,120.,30,180.,0
H,31,1.1,30,120.,29,180.,0
H,30,1.1,31,120.,32,180.,0
Ge,8,R36,6,A35,4,D15,0
C,40,R37,8,A36,6,D16,0
H,41,1.1,40,A37,7,D20,0
H,41,1.1,40,A38,42,D21,0
H,41,1.1,40,A39,42,-D21,0
Variables:
R1=0.40936512
R2=1.40552338
R3=1.32840914

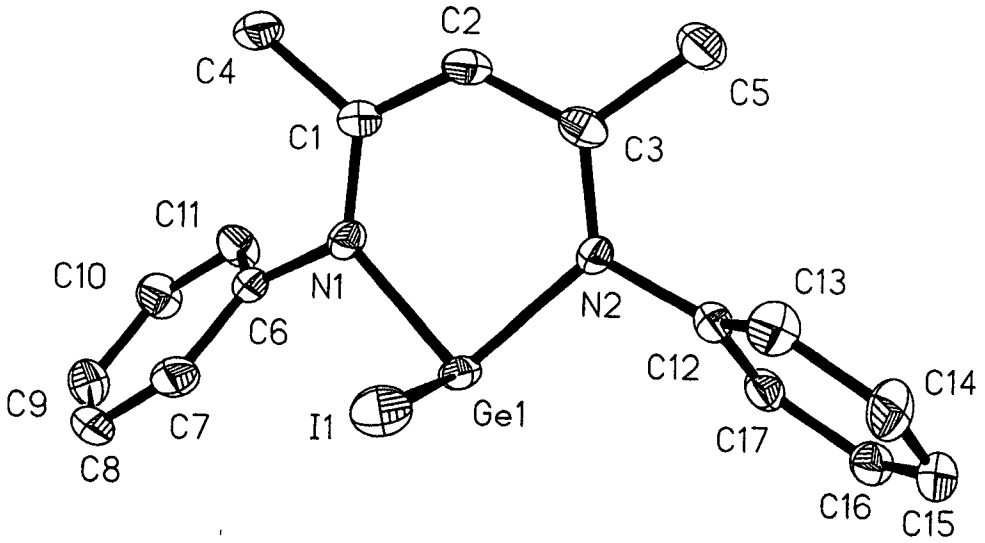
R4=1.32768897
R5=1.51449889
R6=1.07998683
R7=1.51465585
R14=1.43019408
R15=1.39805129
R16=1.39258684
R17=1.392766
R18=1.39304193
R19=1.39306951
R25=1.4293451
R26=1.39806541
R27=1.39226307
R28=1.39379803
R29=1.39279094
R30=1.39277904
R36=2.07203915
R37=2.04262738
A1=128.50336637
A2=124.99009152
A3=123.82237545
A4=114.96093391
A5=115.05395056
A6=116.77600958
A7=110.8704956
A8=110.74346326
A9=111.08539364
A10=110.81044173
A11=110.75442987
A12=111.17080307
A13=121.16694579
A14=120.68933352
A15=120.40740232
A16=120.17820557
A17=119.59060826
A18=120.44192559
A24=121.26363454
A25=120.06671815
A26=120.48738416
A27=120.15161515
A28=119.64482031
A29=120.27205016
A35=126.23876275
A36=93.8910523
A37=109.12063064
A38=110.41725393
A39=112.16786541
D1=7.6474909
D2=-11.48755305
D3=197.59186074
D4=166.19045429
D5=167.29372662
D6=1.77219715
D7=120.68497959

D8=-120.90623953
D9=-5.40252993
D10=-120.73812473
D11=120.76573353
D12=192.5956415
D13=-83.36064102
D14=259.27375302
D15=-6.81812187
D16=-78.93466296
D17=258.0148673
D18=87.9658991
D19=-3.26057738
D20=75.39314125
D21=119.17064483

Energies :

Nuclear repulsion energy : 2087.4333487249 Hartrees

Sum of electronic and zero-point Energies : -2884.357582 ua


C2
C4
C5
C1
C3
C11
C10
N1
N2
C13
C6
C12
C14
C9
C7
I1
Ge1
C17
C8
C16
C15

2

Table 1. Crystal data and structure refinement for 2.

Identification code	2	
Empirical formula	C17 H17 Ge I N2	
Formula weight	448.82	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 7.2834(7) Å	α= 90°.
	b = 8.8051(8) Å	β= 90°.
	c = 26.107(3) Å	γ = 90°.
Volume	1674.2(3) $Å^3$	
Z	4	
Density (calculated)	1.781 Mg/m^3	
Absorption coefficient	3.669 mm^{-1}	
F(000)	872	
Crystal size	0.1 x 0.2 x 0.5 mm^3	
Theta range for data collection	1.56 to 26.37°.	
Index ranges	-6<=h<=9, -11<=k<=9, -32<=l<=30	
Reflections collected	9788	
Independent reflections	3409 [R(int) = 0.0514]	
Completeness to theta = 26.37°	100.0 %	
Absorption correction	Semi-empirical	
Max. and min. transmission	1.000000 and 0.548861	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3409 / 0 / 192	
Goodness-of-fit on F^2	0.996	
Final R indices [I>2sigma(I)]	R1 = 0.0327, wR2 = 0.0745	
R indices (all data)	R1 = 0.0376, wR2 = 0.0763	
Absolute structure parameter	0.00(2)	
Largest diff. peak and hole	0.817 and -0.778 $e.Å^{-3}$	

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

	x	y	z	U(eq)
I(1)	3243(1)	883(1)	8882(1)	28(1)
Ge(1)	2524(1)	3649(1)	8411(1)	19(1)
N(1)	502(6)	2989(5)	7962(2)	19(1)
N(2)	806(5)	4280(5)	8948(1)	19(1)
C(1)	-1237(7)	2731(6)	8111(2)	21(1)
C(2)	-1882(8)	3094(6)	8598(2)	23(1)
C(3)	-989(7)	3906(6)	8983(2)	22(1)
C(4)	-2593(8)	2030(6)	7741(2)	28(1)
C(5)	-2082(7)	4415(6)	9444(2)	29(1)
C(6)	1112(7)	2803(6)	7441(2)	20(1)
C(7)	2598(8)	1854(6)	7345(2)	26(1)
C(8)	3324(8)	1762(6)	6850(2)	29(1)
C(9)	2569(8)	2597(6)	6458(2)	31(1)
C(10)	1071(8)	3536(7)	6552(2)	30(1)
C(11)	333(7)	3636(6)	7044(2)	26(1)
C(12)	1796(7)	5001(5)	9359(2)	20(1)
C(13)	2010(7)	4241(6)	9830(2)	27(1)
C(14)	3121(9)	4875(6)	10204(2)	30(1)
C(15)	4001(8)	6243(6)	10121(2)	27(1)
C(16)	3790(8)	7004(6)	9657(2)	26(1)
C(17)	2690(7)	6378(5)	9277(2)	22(1)

Table 3. Bond lengths [Å] and angles [°] for 2.

I(1)-Ge(1)	2.7784(6)
Ge(1)-N(2)	1.959(4)
Ge(1)-N(1)	1.971(4)
N(1)-C(1)	1.345(6)
N(1)-C(6)	1.440(7)
N(2)-C(3)	1.351(6)
N(2)-C(12)	1.441(6)
C(1)-C(2)	1.391(7)
C(1)-C(4)	1.513(7)
C(2)-C(3)	1.397(7)
C(3)-C(5)	1.511(7)
C(6)-C(11)	1.390(7)
C(6)-C(7)	1.390(8)
C(7)-C(8)	1.400(7)
C(8)-C(9)	1.374(8)
C(9)-C(10)	1.392(8)
C(10)-C(11)	1.395(7)
C(12)-C(17)	1.393(7)
C(12)-C(13)	1.409(7)
C(13)-C(14)	1.386(7)
C(14)-C(15)	1.382(8)
C(15)-C(16)	1.391(8)
C(16)-C(17)	1.389(7)
N(2)-Ge(1)-N(1)	91.83(17)
N(2)-Ge(1)-I(1)	92.98(12)
N(1)-Ge(1)-I(1)	98.37(12)
C(1)-N(1)-C(6)	123.1(4)
C(1)-N(1)-Ge(1)	125.5(3)
C(6)-N(1)-Ge(1)	111.4(3)
C(3)-N(2)-C(12)	122.7(4)
C(3)-N(2)-Ge(1)	126.8(3)
C(12)-N(2)-Ge(1)	109.8(3)
N(1)-C(1)-C(2)	123.0(5)
N(1)-C(1)-C(4)	119.9(4)
C(2)-C(1)-C(4)	117.1(5)
C(1)-C(2)-C(3)	128.2(5)
N(2)-C(3)-C(2)	121.7(4)
N(2)-C(3)-C(5)	119.5(4)

C(2)-C(3)-C(5)	118.7(5)
C(11)-C(6)-C(7)	120.1(5)
C(11)-C(6)-N(1)	121.2(4)
C(7)-C(6)-N(1)	118.6(5)
C(6)-C(7)-C(8)	119.7(5)
C(9)-C(8)-C(7)	120.4(5)
C(8)-C(9)-C(10)	120.0(5)
C(9)-C(10)-C(11)	120.2(5)
C(6)-C(11)-C(10)	119.7(5)
C(17)-C(12)-C(13)	119.7(5)
C(17)-C(12)-N(2)	120.2(4)
C(13)-C(12)-N(2)	119.8(4)
C(14)-C(13)-C(12)	119.2(5)
C(15)-C(14)-C(13)	120.7(5)
C(14)-C(15)-C(16)	120.4(5)
C(17)-C(16)-C(15)	119.6(5)
C(16)-C(17)-C(12)	120.4(5)

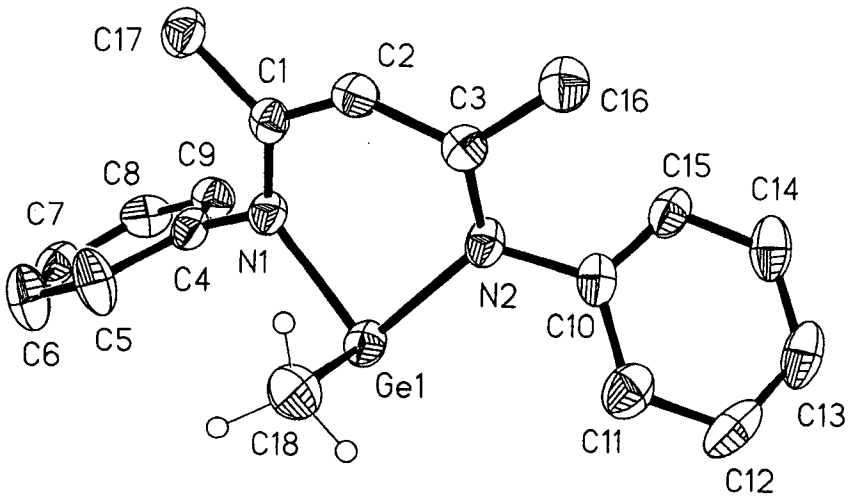
Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 2. 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}
I(1)	25(1)	30(1)	30(1)	7(1)	-4(1)	1(1)
Ge(1)	14(1)	26(1)	17(1)	1(1)	-1(1)	-4(1)
N(1)	18(2)	24(2)	15(2)	-1(2)	-4(2)	-1(2)
N(2)	17(2)	24(2)	16(2)	-4(2)	-1(2)	-3(2)
C(1)	17(2)	22(3)	23(2)	2(2)	0(2)	0(2)
C(2)	14(2)	31(3)	23(2)	3(2)	1(2)	0(2)
C(3)	21(2)	24(3)	22(2)	5(2)	4(2)	3(2)
C(4)	17(2)	39(3)	29(3)	-4(2)	-2(2)	-2(2)
C(5)	24(3)	38(3)	24(3)	-3(2)	4(2)	4(2)
C(6)	16(2)	24(3)	19(2)	-5(2)	-1(2)	-2(2)
C(7)	21(2)	32(3)	27(2)	0(2)	-6(2)	3(2)
C(8)	20(3)	35(3)	30(3)	-9(2)	5(2)	3(3)
C(9)	33(3)	43(3)	17(2)	-9(2)	6(2)	-2(3)
C(10)	31(3)	40(3)	19(2)	0(2)	-1(2)	4(3)
C(11)	25(3)	31(3)	21(2)	-1(2)	2(2)	8(2)
C(12)	18(2)	23(2)	18(2)	-2(2)	1(2)	2(2)
C(13)	31(3)	26(3)	24(2)	4(2)	-1(2)	0(2)
C(14)	39(3)	37(3)	13(2)	2(2)	-4(2)	-2(3)
C(15)	26(3)	34(3)	22(2)	-9(2)	-2(2)	1(2)
C(16)	23(3)	24(3)	30(3)	-6(2)	3(2)	-2(2)
C(17)	22(3)	26(2)	17(2)	-2(2)	4(2)	2(2)

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

	x	y	z	U(eq)
H(2)	-3083	2744	8677	27
H(4A)	-3252	2837	7559	43
H(4B)	-3473	1404	7931	43
H(4C)	-1933	1395	7494	43
H(5A)	-1739	3799	9742	43
H(5B)	-3396	4288	9375	43
H(5C)	-1822	5486	9515	43
H(7)	3117	1269	7615	32
H(8)	4346	1120	6784	34
H(9)	3071	2532	6123	37
H(10)	549	4111	6281	36
H(11)	-698	4270	7108	31
H(13)	1400	3304	9891	32
H(14)	3280	4363	10522	35
H(15)	4754	6666	10381	33
H(16)	4393	7946	9601	31
H(17)	2547	6892	8960	26


C17
C1
C2
C3
C16
C9
C8
C15
C14
C7
C4
N1
N2
C10
C6
C5
Ge1
C13
C18
C11
C12

3

Table 1. Crystal data and structure refinement for 3.

Identification code	3	
Empirical formula	C18 H20 Ge N2	
Formula weight	336.95	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.3713(19) Å	α= 71.289(5)°.
	b = 9.173(3) Å	β= 82.716(6)°.
	c = 13.049(4) Å	γ = 84.495(5)°.
Volume	827.5(4) Å^3	
Z	2	
Density (calculated)	1.352 Mg/m^3	
Absorption coefficient	1.846 mm^{-1}	
F(000)	348	
Crystal size	0.1 x 0.2 x 0.6 mm^3	
Theta range for data collection	1.66 to 24.11°.	
Index ranges	-8<=h<=8, -10<=k<=10, -10<=l<=14	
Reflections collected	3950	
Independent reflections	2593 [R(int) = 0.0455]	
Completeness to theta = 24.11°	98.6 %	
Absorption correction	Semi empirical	
Max. and min. transmission	1.000000 and 0.664309	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2593 / 0 / 193	
Goodness-of-fit on F^2	1.005	
Final R indices [I>2sigma(I)]	R1 = 0.0521, wR2 = 0.1306	
R indices (all data)	R1 = 0.0680, wR2 = 0.1412	
Largest diff. peak and hole	1.227 and -0.872 e.Å^{-3}	

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

	x	y	z	U(eq)
Ge(1)	2378(1)	8545(1)	7771(1)	32(1)
N(1)	3547(5)	8091(4)	9169(3)	28(1)
N(2)	4144(5)	10205(4)	7060(3)	29(1)
C(1)	5289(6)	8312(5)	9218(4)	27(1)
C(10)	3477(6)	11475(5)	6193(4)	28(1)
C(9)	1367(6)	8215(6)	10726(4)	33(1)
C(7)	20(7)	5918(6)	11951(4)	38(1)
C(16)	7302(6)	11156(6)	6565(4)	35(1)
C(11)	2601(7)	11179(7)	5400(4)	40(1)
C(2)	6434(6)	9106(5)	8295(4)	29(1)
C(3)	5875(6)	10115(5)	7321(4)	28(1)
C(18)	3890(7)	6869(6)	7312(4)	40(1)
C(4)	2388(6)	7345(5)	10132(4)	28(1)
C(5)	2206(8)	5773(6)	10435(5)	46(2)
C(12)	1836(8)	12394(8)	4588(4)	50(2)
C(17)	6081(7)	7765(6)	10296(4)	35(1)
C(15)	3550(6)	12997(6)	6162(4)	34(1)
C(8)	198(7)	7493(7)	11638(4)	38(1)
C(13)	1969(7)	13906(7)	4561(4)	47(2)
C(14)	2813(7)	14204(6)	5351(4)	42(1)
C(6)	1022(8)	5065(7)	11347(5)	52(2)

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

Ge(1)-N(2)	2.010(4)
Ge(1)-C(18)	2.014(6)
Ge(1)-N(1)	2.022(4)
N(1)-C(1)	1.332(6)
N(1)-C(4)	1.437(6)
N(2)-C(3)	1.350(6)
N(2)-C(10)	1.438(6)
C(1)-C(2)	1.411(6)
C(1)-C(17)	1.507(7)
C(10)-C(15)	1.389(7)
C(10)-C(11)	1.394(7)
C(9)-C(4)	1.392(7)
C(9)-C(8)	1.393(7)
C(7)-C(8)	1.384(8)
C(7)-C(6)	1.385(8)
C(16)-C(3)	1.522(6)
C(11)-C(12)	1.398(8)
C(2)-C(3)	1.395(7)
C(4)-C(5)	1.383(7)
C(5)-C(6)	1.396(7)
C(12)-C(13)	1.389(9)
C(15)-C(14)	1.386(7)
C(13)-C(14)	1.378(8)
N(2)-Ge(1)-C(18)	96.08(19)
N(2)-Ge(1)-N(1)	88.81(15)
C(18)-Ge(1)-N(1)	94.1(2)
C(1)-N(1)-C(4)	121.2(4)
C(1)-N(1)-Ge(1)	124.3(3)
C(4)-N(1)-Ge(1)	114.2(3)
C(3)-N(2)-C(10)	121.3(4)
C(3)-N(2)-Ge(1)	123.4(3)
C(10)-N(2)-Ge(1)	115.2(3)
N(1)-C(1)-C(2)	122.5(4)
N(1)-C(1)-C(17)	120.0(4)
C(2)-C(1)-C(17)	117.5(4)
C(15)-C(10)-C(11)	118.5(5)
C(15)-C(10)-N(2)	122.0(4)
C(11)-C(10)-N(2)	119.3(5)

C(4)-C(9)-C(8)	119.8(5)
C(8)-C(7)-C(6)	119.1(5)
C(10)-C(11)-C(12)	120.4(6)
C(3)-C(2)-C(1)	126.7(4)
N(2)-C(3)-C(2)	122.3(4)
N(2)-C(3)-C(16)	120.8(4)
C(2)-C(3)-C(16)	116.8(4)
C(5)-C(4)-C(9)	119.8(4)
C(5)-C(4)-N(1)	120.0(5)
C(9)-C(4)-N(1)	120.1(4)
C(4)-C(5)-C(6)	119.7(5)
C(13)-C(12)-C(11)	119.9(6)
C(14)-C(15)-C(10)	121.3(5)
C(7)-C(8)-C(9)	120.6(5)
C(14)-C(13)-C(12)	119.9(5)
C(13)-C(14)-C(15)	120.0(5)
C(7)-C(6)-C(5)	120.8(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 3. 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)	23(1)	36(1)	30(1)	-3(1)	-3(1)	-1(1)
N(1)	26(2)	27(2)	28(2)	-5(2)	-4(2)	2(2)
N(2)	23(2)	30(2)	26(2)	-1(2)	-1(2)	2(2)
C(1)	30(2)	20(2)	30(3)	-9(2)	-3(2)	6(2)
C(10)	21(2)	29(3)	27(3)	-3(2)	6(2)	4(2)
C(9)	32(3)	31(3)	38(3)	-13(2)	-3(2)	0(2)
C(7)	35(3)	46(3)	26(3)	-2(2)	-4(2)	-3(2)
C(16)	28(3)	36(3)	36(3)	-8(2)	-1(2)	2(2)
C(11)	36(3)	52(3)	30(3)	-10(2)	0(2)	-2(3)
C(2)	23(2)	26(2)	41(3)	-13(2)	-7(2)	4(2)
C(3)	23(2)	27(2)	31(3)	-10(2)	-2(2)	2(2)
C(18)	42(3)	35(3)	43(3)	-14(2)	-4(2)	-2(2)
C(4)	27(2)	28(3)	27(2)	-5(2)	-7(2)	3(2)
C(5)	58(3)	23(3)	50(3)	-9(2)	15(3)	3(2)
C(12)	40(3)	80(5)	25(3)	-12(3)	-10(2)	7(3)
C(17)	33(3)	32(3)	36(3)	-5(2)	-7(2)	3(2)
C(15)	30(3)	42(3)	24(2)	-3(2)	-2(2)	1(2)
C(8)	32(3)	51(3)	36(3)	-21(3)	2(2)	-3(2)
C(13)	43(3)	45(4)	34(3)	5(3)	-3(3)	17(3)
C(14)	39(3)	34(3)	39(3)	1(2)	5(2)	10(2)
C(6)	66(4)	33(3)	45(3)	0(3)	10(3)	-7(3)

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

	x	y	z	U(eq)
H(9)	1468	9299	10511	40
H(7)	-778	5429	12573	45
H(16A)	7011	11419	5812	52
H(16B)	8516	10617	6634	52
H(16C)	7297	12101	6762	52
H(11)	2525	10146	5411	48
H(2)	7717	8936	8342	35
H(18A)	3803	7033	6539	60
H(18B)	3431	5864	7744	60
H(18C)	5172	6895	7429	60
H(5)	2884	5178	10025	55
H(12)	1225	12185	4056	60
H(17A)	5705	8504	10694	53
H(17B)	7421	7682	10172	53
H(17C)	5633	6754	10722	53
H(15)	4116	13213	6708	41
H(8)	-483	8087	12048	46
H(13)	1480	14734	3999	56
H(14)	2890	15237	5340	50
H(6)	901	3984	11555	63