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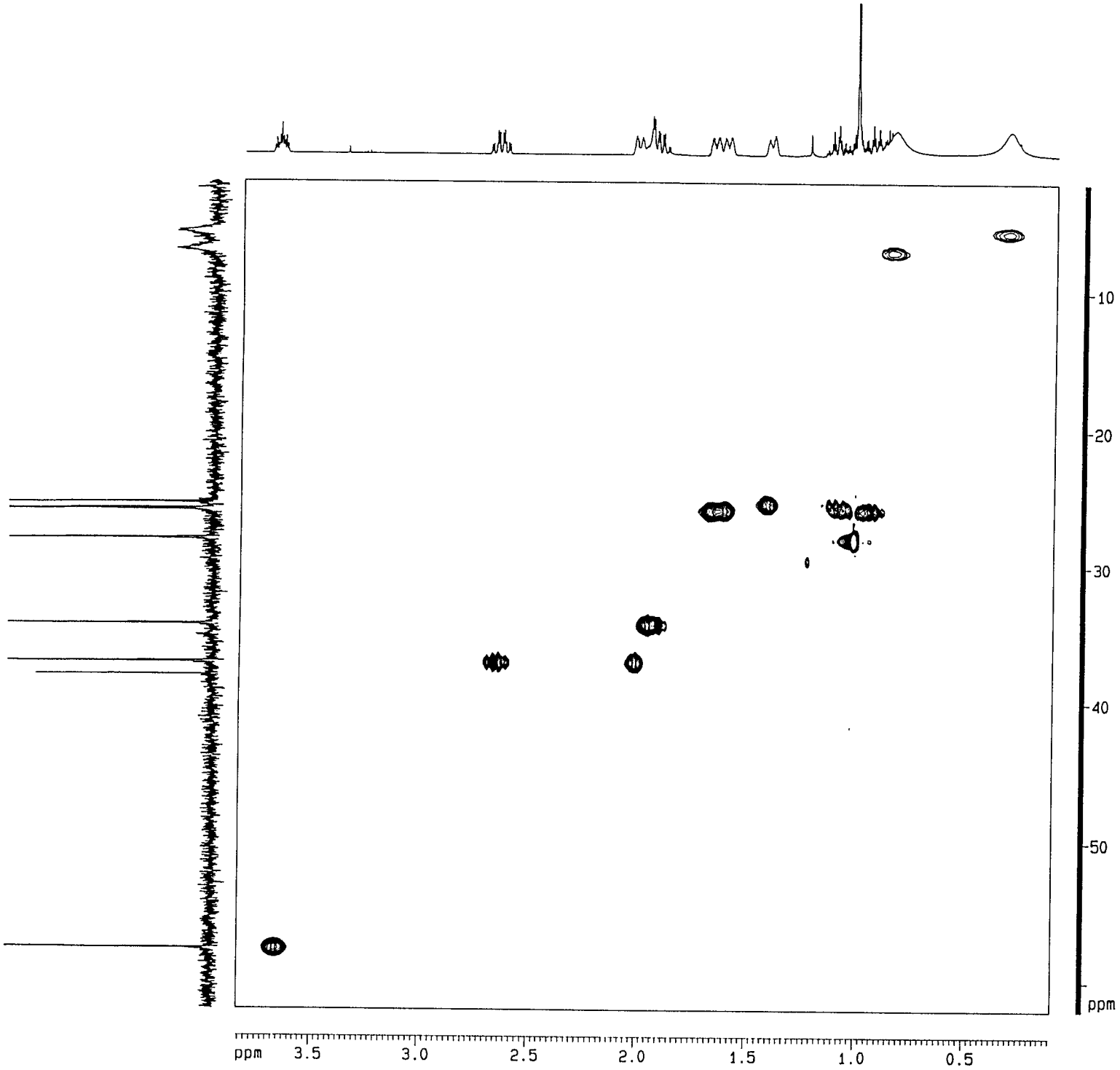
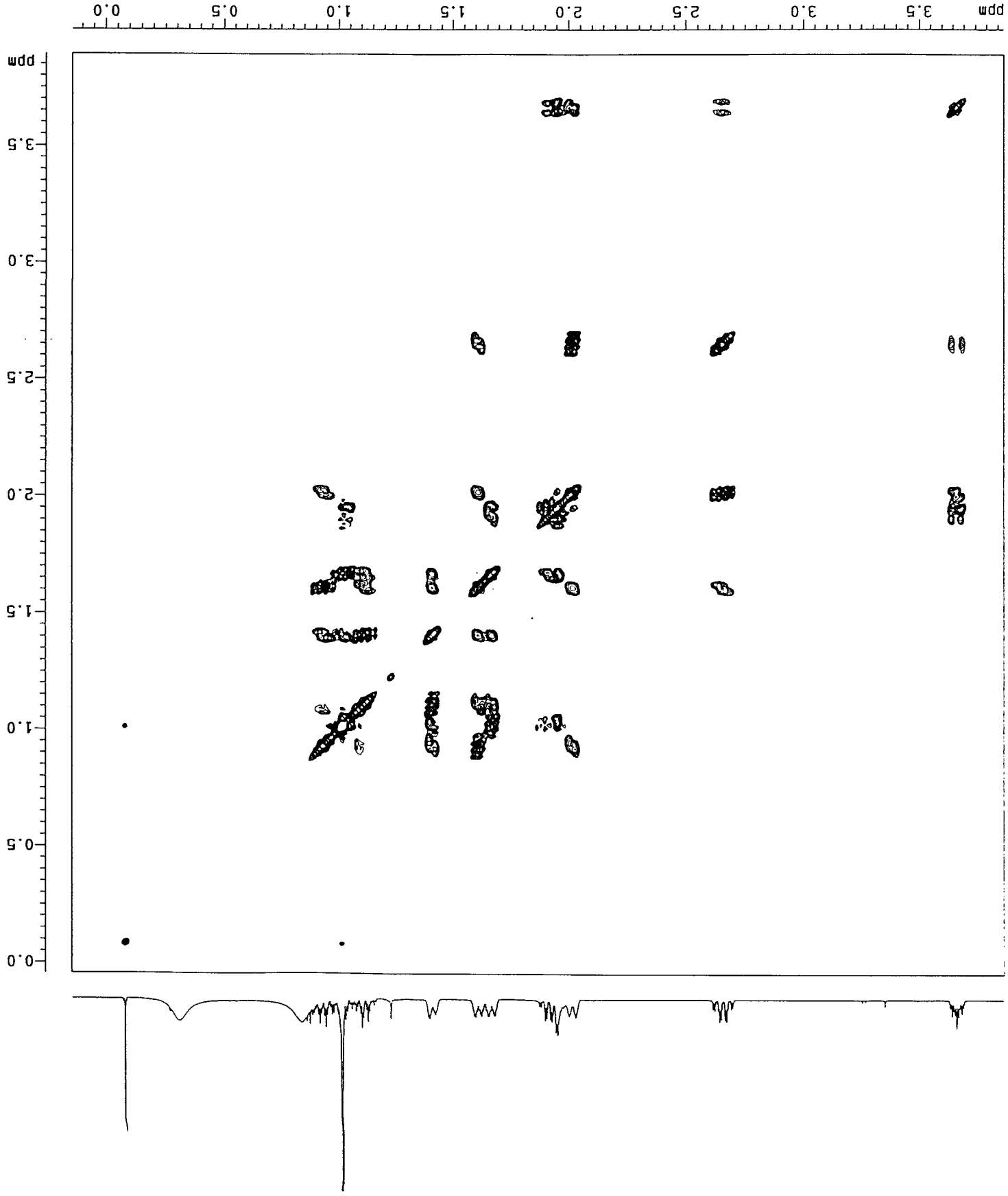
J. Am. Chem. Soc., 1997, 119(43), 10359-10363, DOI:10.1021/ja9719891

$[C_6H_{11}NC(CMe_3)NC_6H_{11}]Ge[N(SiMe_3)_2]Se$

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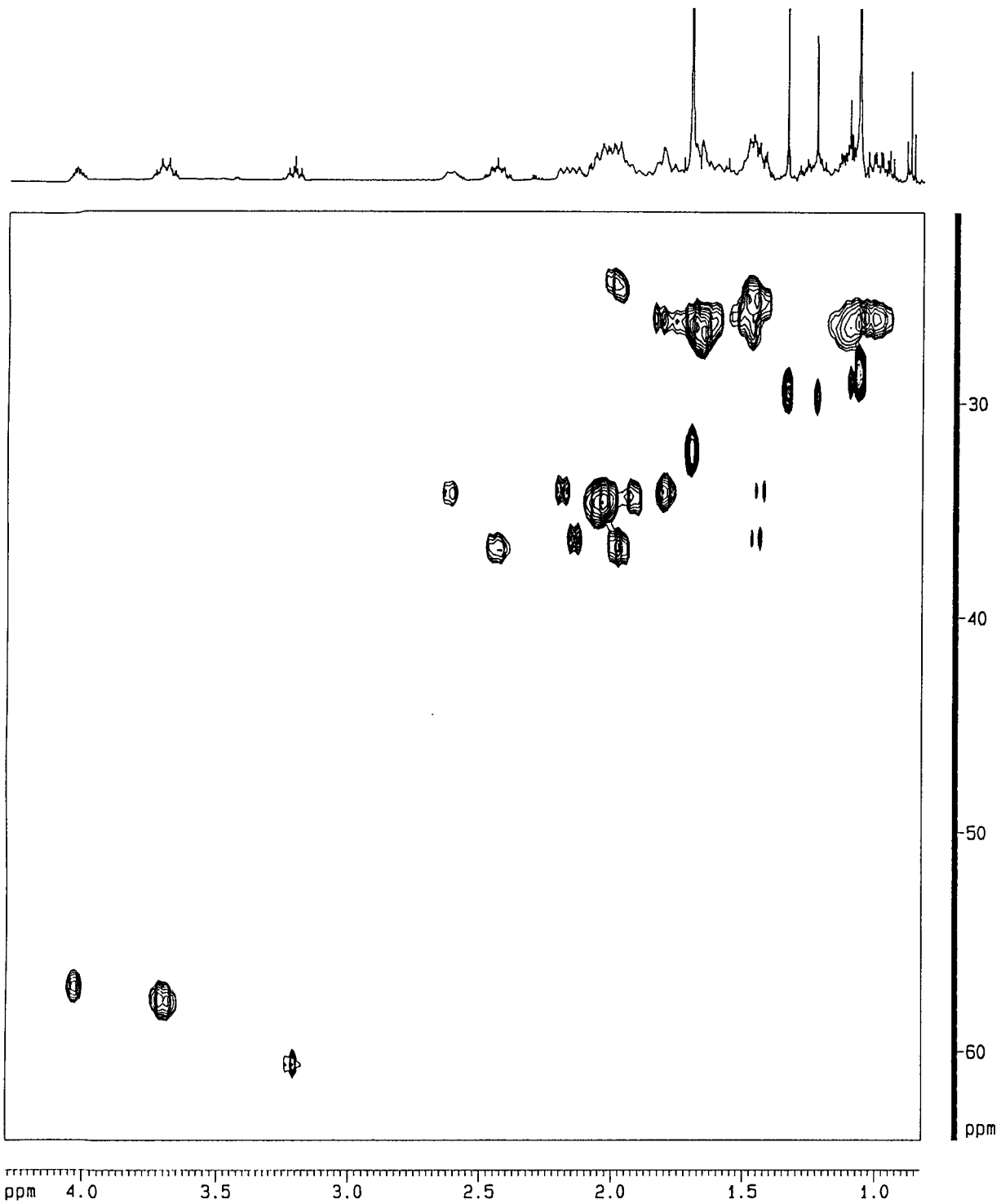
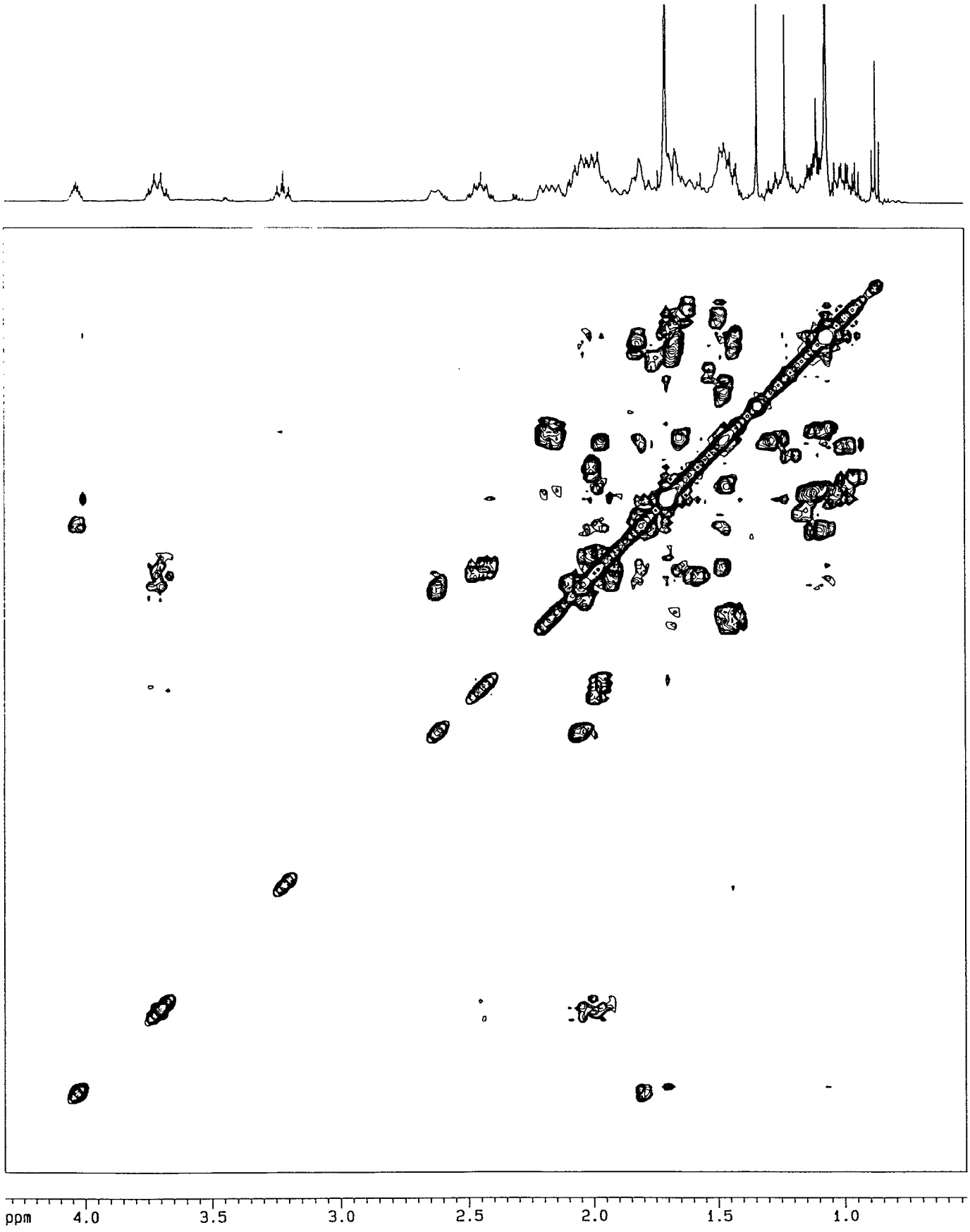
$[C_6H_{11}NC(CMe_3)NC_6H_{11}]_2GeS$

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1

Space Group and Cell Dimensions Monoclinic, P 21/c
a 15.1666(6) b 11.5652(4) c 16.0374(6)
beta 99.856(3)
Volume 2771.51(2)A**3

Empirical formula : Ge N4 C28 H50

Cell dimensions were obtained from 24 reflections with 2Theta angle
in the range 80.00 - 100.00 degrees.

Crystal dimensions : 0.20 X 0.20 X 0.20 mm

FW = 515.31 Z = 4 F(000) = 1109.77

Dcalc 1.235Mg.m-3, mu 1.62mm-1, lambda 1.54056A, 2Theta(max) 99.9

The intensity data were collected on a Rigaku diffractometer,
using the theta/2theta scan mode.
The h,k,l ranges used during structure solution and refinement are :--
Hmin,max -12 12; Kmin,max 0 11; Lmin,max 0 15
No. of reflections measured 2509
No. of unique reflections 2373
No. of reflections with Inet > 2.5sigma(Inet) 1129
Merging R-value on intensities 0.029
No correction was made for absorption

The last least squares cycle was calculated with
83 atoms, 298 parameters and 1128 out of 2373 reflections.
Weights based on counting-statistics were used.

The residuals are as follows :--
For significant reflections, RF 0.074, Rw 0.052 GoF 2.84
For all reflections, RF 0.088, Rw 0.057.
where RF = Sum(Fo-Fc)/Sum(Fo),
Rw = Sqrt[Sum(w(Fo-Fc)**2)/Sum(wFo**2)] and
GoF = Sqrt[Sum(w(Fo-Fc)**2)/(No. of reflns - No. of params.)]
The maximum shift/sigma ratio was 0.232.

In the last D-map, the deepest hole was -0.780e/A**3,
and the highest peak 0.560e/A**3.

The following references are relevant to the NRCVAX System.

1. Full System Reference :
Gabe, E.J., Le Page, Y., Charland,.J.-P., Lee, F.L. and White, P.S.
(1989) J. Appl. Cryst., 22, 384-387.

2. Scattering Factors from Int. Tab. Vol. 4 :
International Tables for X-ray Crystallography, Vol. IV, (1974)
Kynoch Press, Birmingham, England.

The following references may also be relevant.

3. ORTEP Plotting :
Johnson, C.K., (1976) ORTEP - A Fortran Thermal Ellipsoid Plot Program, Technical Report ORNL-5138, Oak Ridge

4. Pluto Plotting :
S. Motherwell, University Chemical Laboratory, Cambridge, 1978

5. Missing Symmetry Treatment by MISSYM :
Le Page, Y., (1988) J. Appl. Cryst., 21, 983-984.

6. Grouping of Equivalent Reflections in DATRD2 :
Le Page, Y. and Gabe, E.J., (1979) J. Appl. Cryst., 12, 464-466.

Table of Atomic Parameters x,y,z and Biso.
E.S.Ds. refer to the last digit printed.

	x	y	z	Biso
GE1	0.66588(16)	0.16161(17)	0.16565(13)	3.99(11)
N1	0.6712 (9)	0.0044 (10)	0.1094 (7)	2.8 (7)
N2	0.5553 (9)	0.0447 (9)	0.1674 (7)	2.8 (7)
N3	0.7258 (8)	0.1286 (9)	0.2797 (7)	2.1 (7)
N4	0.8281 (8)	0.1976 (10)	0.2088 (7)	2.7 (7)
C1	0.7354 (10)	-0.0610 (12)	0.0688 (9)	2.0 (9)
C2	0.7848 (11)	0.0246 (13)	0.0176 (9)	2.9 (9)
C3	0.8568 (11)	-0.0360 (13)	-0.0209 (9)	3.4 (10)
C4	0.9211 (11)	-0.1022 (14)	0.0448 (10)	3.4 (10)
C5	0.8694 (10)	-0.1886 (13)	0.0908 (10)	3.0 (10)
C6	0.7997 (11)	-0.1259 (13)	0.1306 (9)	3.3 (9)
C7	0.5910 (10)	-0.0276 (13)	0.1181 (9)	2.3 (9)
C8	0.5394 (11)	-0.1276 (12)	0.0698 (9)	3.3 (10)
C9	0.4603 (11)	0.0493 (12)	0.1740 (8)	2.5 (9)
C10	0.4366 (11)	0.1700 (14)	0.1986 (8)	3.0 (9)
C11	0.3406 (12)	0.1871 (13)	0.2055 (9)	4.5 (11)
C12	0.3084 (11)	0.0969 (13)	0.2632 (9)	3.2 (10)
C13	0.3318 (11)	-0.0249 (13)	0.2391 (9)	3.6 (10)
C14	0.4298 (12)	-0.0390 (12)	0.2338 (9)	3.2 (10)
C15	0.6863 (13)	0.0806 (14)	0.3516 (10)	4.7 (11)
C16	0.6501 (12)	0.1689 (16)	0.4048 (9)	4.9 (11)
C17	0.5959 (12)	0.1135 (15)	0.4655 (10)	4.5 (11)
C18	0.6351 (13)	0.0126 (19)	0.5085 (11)	7.1 (13)
C19	0.6698 (15)	-0.0745 (14)	0.4519 (10)	6.6 (14)
C20	0.7258 (12)	-0.0244 (14)	0.3906 (11)	4.7 (11)
C21	0.8077 (11)	0.1794 (13)	0.2849 (9)	3.4 (10)
C22	0.8666 (11)	0.2083 (14)	0.3665 (8)	3.3 (10)
C23	0.9021 (10)	0.2746 (13)	0.1990 (8)	2.8 (9)
C24	0.8657 (12)	0.3653 (13)	0.1331 (10)	4.3 (11)
C25	0.9419 (13)	0.4471 (14)	0.1195 (11)	5.2 (12)
C26	1.0167 (12)	0.3826 (13)	0.0920 (9)	3.5 (10)
C27	1.0528 (12)	0.2885 (14)	0.1557 (9)	4.2 (10)
C28	0.9786 (11)	0.2076 (12)	0.1717 (9)	3.1 (10)
H1	0.698	-0.120	0.023	4.3
H2a	0.736	0.070	-0.030	4.8
H2b	0.816	0.093	0.062	4.8
H3a	0.892	0.025	-0.055	5.1
H3b	0.823	-0.098	-0.070	5.1
H4a	0.970	-0.143	0.016	5.3
H4b	0.952	-0.037	0.090	5.3
H5a	0.915	-0.235	0.140	4.9
H5b	0.835	-0.254	0.047	4.9
H6a	0.832	-0.066	0.177	4.2
H6b	0.762	-0.188	0.163	4.2
H8a	0.476	-0.137	0.091	4.3
H8b	0.529	-0.113	0.003	4.3
H8c	0.578	-0.208	0.084	4.3
H9	0.424	0.032	0.111	4.1
H10a	0.456	0.233	0.155	4.8
H10b	0.478	0.191	0.262	4.8

H11a	0.331	0.271	0.230	5.9
H11b	0.303	0.177	0.143	5.9
H12a	0.336	0.115	0.329	4.5
H12b	0.234	0.106	0.258	4.5
H13a	0.292	-0.050	0.179	4.6
H13b	0.314	-0.088	0.287	4.6
H14a	0.467	-0.023	0.297	5.3
H14b	0.442	-0.125	0.215	5.3
H15	0.624	0.047	0.317	6.0
H16a	0.609	0.234	0.368	5.9
H16b	0.707	0.217	0.445	5.9
H17a	0.533	0.088	0.430	5.0
H17b	0.583	0.179	0.513	5.0
H18a	0.693	0.046	0.558	7.9
H18b	0.587	-0.022	0.546	7.9
H19a	0.704	-0.142	0.491	7.1
H19b	0.608	-0.116	0.415	7.1
H20a	0.734	-0.086	0.341	6.3
H20b	0.793	-0.003	0.425	6.3
H22a	0.929	0.246	0.354	5.2
H22b	0.836	0.264	0.405	5.2
H22c	0.885	0.127	0.402	5.2
H23	0.926	0.320	0.259	3.8
H24a	0.838	0.318	0.073	6.3
H24b	0.808	0.410	0.151	6.3
H25a	0.961	0.495	0.177	7.1
H25b	0.912	0.511	0.070	7.1
H26a	0.996	0.347	0.030	5.5
H26b	1.071	0.447	0.087	5.5
H27a	1.104	0.240	0.132	5.8
H27b	1.083	0.329	0.215	5.8
H28a	1.002	0.144	0.219	4.9
H28b	0.950	0.161	0.113	4.9

Biso is the Mean of the Principal Axes of the Thermal Ellipsoid

Table of u(i,j) or U values *100.
E.S.Ds. refer to the last digit printed

	u11(U)	u22	u33	u12	u13	u23
GE1	8.59(17)	3.00(10)	4.03(11)	-0.57(19)	2.39(11)	0.25(15)
N1	6.8 (12)	0.7 (8)	4.1 (9)	-0.8 (8)	3.9 (9)	-0.1 (7)
N2	6.7 (12)	2.3 (8)	2.3 (8)	2.3 (9)	2.5 (8)	0.7 (7)
N3	1.5 (10)	1.9 (9)	4.9 (9)	-0.2 (7)	1.0 (8)	0.1 (7)
N4	4.4 (11)	4.3 (10)	2.3 (8)	-1.4 (8)	2.9 (8)	-1.4 (7)
C1	2.0 (13)	1.6 (10)	4.6 (12)	1.0 (10)	1.9 (10)	0.1 (9)
C2	5.2 (15)	2.3 (11)	4.1 (12)	0.4 (11)	2.4 (11)	0.3 (9)
C3	6.0 (16)	4.0 (13)	4.3 (12)	0.1 (12)	4.6 (11)	0.5 (10)
C4	4.9 (15)	3.8 (11)	4.5 (12)	0.1 (11)	2.2 (11)	-0.5 (10)
C5	2.8 (13)	2.4 (12)	6.5 (13)	1.0 (10)	1.7 (10)	-0.2 (10)
C6	4.7 (14)	3.2 (13)	5.2 (12)	3.7 (10)	2.8 (11)	2.4 (9)
C7	2.7 (13)	2.9 (11)	3.4 (11)	-1.7 (10)	1.3 (10)	1.2 (9)
C8	7.8 (16)	2.9 (12)	2.9 (11)	-2.0 (11)	3.9 (11)	-0.7 (9)
C9	5.0 (15)	3.2 (11)	1.7 (10)	1.9 (11)	2.2 (10)	-0.2 (9)
C10	7.1 (15)	2.0 (10)	3.1 (10)	1.5 (12)	3.3 (10)	0.1 (10)
C11	11.7 (18)	2.7 (12)	4.3 (12)	2.0 (13)	6.0 (12)	-0.4 (10)
C12	6.8 (16)	2.9 (11)	3.0 (11)	2.2 (11)	2.4 (11)	1.0 (9)
C13	7.0 (17)	4.4 (12)	3.3 (12)	0.1 (12)	3.9 (11)	0.9 (10)
C14	9.1 (17)	1.9 (11)	2.1 (10)	-1.2 (12)	3.4 (11)	0.4 (9)
C15	11.4 (19)	2.1 (11)	5.7 (14)	1.1 (13)	5.8 (14)	0.4 (10)
C16	10.7 (18)	6.3 (13)	2.6 (10)	2.6 (16)	4.0 (11)	1.3 (12)
C17	7.5 (16)	6.8 (15)	3.2 (11)	-0.7 (13)	2.0 (11)	-1.3 (11)
C18	9.0 (19)	12.6 (19)	6.3 (14)	4.3 (17)	4.3 (14)	7.8 (14)
C19	19. (3)	2.6 (12)	3.2 (12)	-1.6 (16)	1.8 (15)	2.1 (10)
C20	5.8 (17)	4.5 (13)	8.1 (15)	3.3 (12)	3.3 (13)	2.9 (12)
C21	7.8 (15)	2.1 (11)	2.6 (10)	0.4 (12)	0.2 (10)	-0.9 (9)
C22	4.8 (15)	6.4 (14)	1.3 (10)	-1.6 (11)	0.4 (9)	0.1 (9)
C23	3.8 (14)	5.7 (12)	1.2 (10)	-3.0 (11)	0.8 (9)	-0.2 (9)
C24	6.3 (16)	2.5 (13)	7.9 (14)	-0.5 (11)	2.2 (12)	0.9 (10)
C25	9.4 (19)	2.7 (13)	8.7 (16)	0.8 (13)	4.9 (14)	-0.4 (11)
C26	7.2 (16)	3.4 (12)	2.9 (11)	-3.0 (11)	1.4 (11)	-0.7 (9)
C27	6.9 (16)	5.3 (13)	4.6 (12)	-1.7 (12)	3.3 (12)	-1.3 (10)
C28	6.2 (16)	3.6 (12)	2.8 (11)	0.6 (11)	2.6 (10)	0.6 (9)

Anisotropic Temperature Factors are of the form
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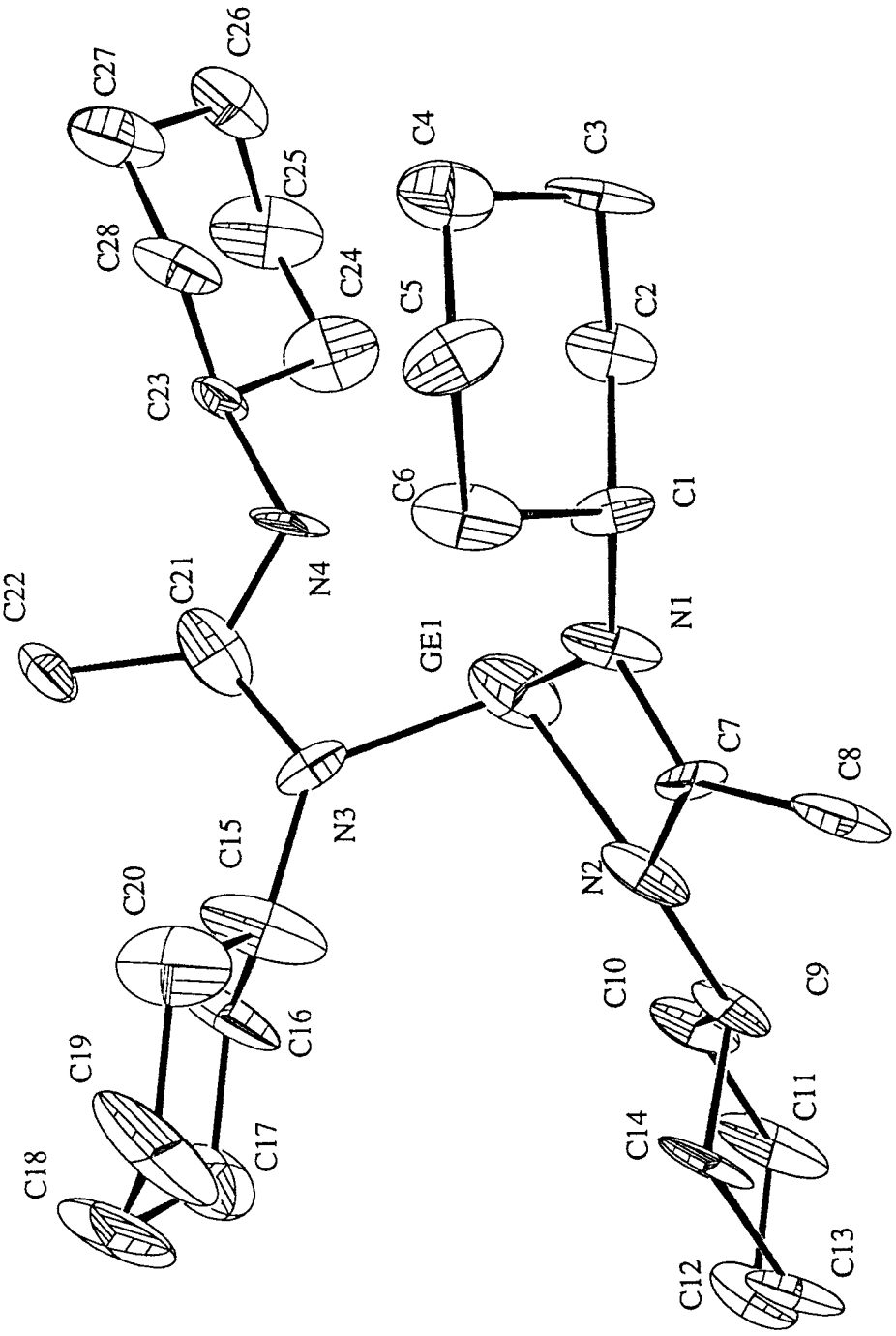
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C25
C28
C24
C4
C3
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C5
C2
C22
C21
N4
C6
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N1
C7
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C11
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C18
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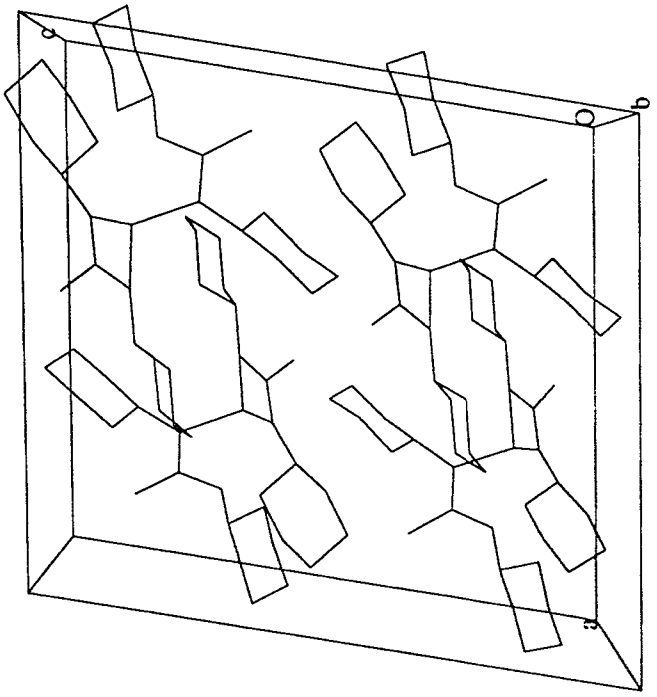
C12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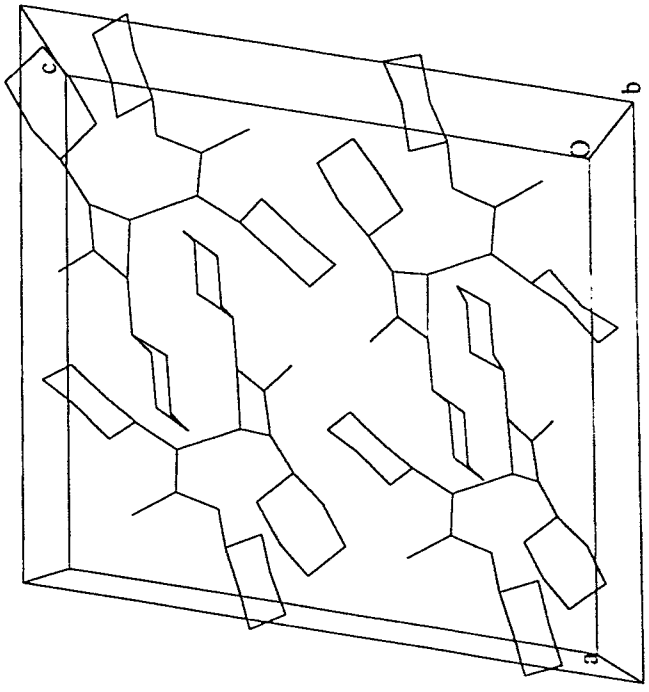
c
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a

Table of Atomic Bond Distances in Angstroms

GE1-N1	2.037(11)	C13-C14	1.512(24)
GE1-N2	2.158(13)	C13-H13a	1.092(16)
GE1-N3	1.935(12)	C13-H13b	1.119(14)
N1-C1	1.470(18)	C14-H14a	1.095(15)
N1-C7	1.302(19)	C14-H14b	1.065(14)
N2-C7	1.329(18)	C15-C16	1.495(22)
N2-C9	1.464(20)	C15-C20	1.448(23)
N3-C15	1.493(18)	C15-H15	1.085(19)
N3-C21	1.364(20)	C16-C17	1.520(22)
N4-C21	1.327(18)	C16-H16a	1.086(17)
N4-C23	1.462(19)	C16-H16b	1.126(19)
C1-C2	1.558(20)	C17-C18	1.43(3)
C1-C6	1.472(21)	C17-H17a	1.069(18)
C1-H1	1.091(15)	C17-H17b	1.114(16)
C2-C3	1.515(21)	C18-C19	1.51(3)
C2-H2a	1.100(16)	C18-H18a	1.138(21)
C2-H2b	1.113(15)	C18-H18b	1.098(18)
C3-C4	1.516(23)	C19-C20	1.519(24)
C3-H3a	1.097(15)	C19-H19a	1.083(17)
C3-H3b	1.119(16)	C19-H19b	1.129(21)
C4-C5	1.535(21)	C20-H20a	1.091(17)
C4-H4a	1.054(15)	C20-H20b	1.100(18)
C4-H4b	1.096(16)	C21-C22	1.489(20)
C5-C6	1.511(20)	C22-H22a	1.091(16)
C5-H5a	1.094(15)	C22-H22b	1.058(15)
C5-H5b	1.098(15)	C22-H22c	1.116(16)
C6-H6a	1.079(16)	C23-C24	1.524(22)
C6-H6b	1.106(15)	C23-C28	1.520(22)
C7-C8	1.530(21)	C23-H23	1.096(14)
C8-H8a	1.075(15)	C24-C25	1.538(24)
C8-H8b	1.071(14)	C24-H24a	1.127(17)
C8-H8c	1.100(15)	C24-H24b	1.094(17)
C9-C10	1.511(21)	C25-C26	1.487(24)
C9-C14	1.526(19)	C25-H25a	1.069(17)
C9-H9	1.081(14)	C25-H25b	1.126(17)
C10-C11	1.491(23)	C26-C27	1.529(23)
C10-H10a	1.093(14)	C26-H26a	1.072(14)
C10-H10b	1.126(15)	C26-H26b	1.122(15)
C11-C12	1.530(21)	C27-C28	1.519(22)
C11-H11a	1.070(14)	C27-H27a	1.081(16)
C11-H11b	1.069(17)	C27-H27b	1.093(15)
C12-C13	1.518(21)	C28-H28a	1.078(14)
C12-H12a	1.086(15)	C28-H28b	1.110(15)
C12-H12b	1.122(17)		

Table of Atomic Bond Angles in Degrees

N1-GE1-N2	62.4(4)	C9-C14-C13	111.7(13)
N1-GE1-N3	101.2(5)	C9-C14-H14a	107.8(12)
N2-GE1-N3	96.0(4)	C9-C14-H14b	111.1(11)
GE1-N1-C1	137.3(10)	C13-C14-H14a	106.6(12)
GE1-N1-C7	95.6(9)	C13-C14-H14b	110.0(13)
C1-N1-C7	127.0(12)	H14a-C14-H14b	109.5(14)
GE1-N2-C7	89.4(9)	N3-C15-C16	115.0(13)
GE1-N2-C9	139.0(9)	N3-C15-C20	117.0(13)
C7-N2-C9	124.9(12)	N3-C15-H15	99.7(12)
GE1-N3-C15	128.1(10)	C16-C15-C20	119.4(14)
GE1-N3-C21	104.4(9)	C16-C15-H15	99.5(14)
C15-N3-C21	126.4(12)	C20-C15-H15	100.3(14)
C21-N4-C23	120.0(12)	C15-C16-C17	111.7(15)
N1-C1-C2	108.7(11)	C15-C16-H16a	113.1(12)
N1-C1-C6	112.1(11)	C15-C16-H16b	110.1(15)
N1-C1-H1	108.4(12)	C17-C16-H16a	109.0(14)
C2-C1-C6	110.8(13)	C17-C16-H16b	106.9(12)
C2-C1-H1	106.6(11)	H16a-C16-H16b	105.7(16)
C6-C1-H1	110.1(12)	C16-C17-C18	115.3(15)
C1-C2-C3	111.5(12)	C16-C17-H17a	107.9(13)
C1-C2-H2a	109.7(13)	C16-C17-H17b	109.2(14)
C1-C2-H2b	107.5(12)	C18-C17-H17a	107.0(16)
C3-C2-H2a	112.8(12)	C18-C17-H17b	109.5(14)
C3-C2-H2b	109.4(13)	H17a-C17-H17b	107.8(15)
H2a-C2-H2b	105.7(12)	C17-C18-C19	114.4(14)
C2-C3-C4	112.0(12)	C17-C18-H18a	105.5(17)
C2-C3-H3a	111.0(13)	C17-C18-H18b	107.6(16)
C2-C3-H3b	108.1(14)	C19-C18-H18a	109.7(16)
C4-C3-H3a	111.4(14)	C19-C18-H18b	114.8(18)
C4-C3-H3b	108.8(13)	H18a-C18-H18b	104.1(14)
H3a-C3-H3b	105.4(12)	C18-C19-C20	115.2(14)
C3-C4-C5	110.0(13)	C18-C19-H19a	108.6(14)
C3-C4-H4a	109.6(13)	C18-C19-H19b	104.9(18)
C3-C4-H4b	105.3(13)	C20-C19-H19a	112.5(18)
C5-C4-H4a	112.2(13)	C20-C19-H19b	109.2(14)
C5-C4-H4b	109.3(12)	H19a-C19-H19b	105.7(14)
H4a-C4-H4b	110.3(14)	C15-C20-C19	111.4(14)
C4-C5-C6	110.0(12)	C15-C20-H20a	109.3(14)
C4-C5-H5a	110.9(13)	C15-C20-H20b	108.0(15)
C4-C5-H5b	111.1(13)	C19-C20-H20a	111.6(14)
C6-C5-H5a	109.2(12)	C19-C20-H20b	109.2(14)
C6-C5-H5b	108.4(13)	H20a-C20-H20b	107.2(14)
H5a-C5-H5b	107.1(12)	N3-C21-N4	111.4(12)
C1-C6-C5	113.1(12)	N3-C21-C22	123.6(13)
C1-C6-H6a	108.3(12)	N4-C21-C22	125.0(14)
C1-C6-H6b	108.0(13)	C21-C22-H22a	109.9(12)
C5-C6-H6a	109.4(13)	C21-C22-H22b	113.1(14)
C5-C6-H6b	110.4(12)	C21-C22-H22c	108.7(13)
H6a-C6-H6b	107.6(12)	H22a-C22-H22b	110.3(14)
N1-C7-N2	111.6(13)	H22a-C22-H22c	106.1(14)
N1-C7-C8	124.6(13)	H22b-C22-H22c	108.4(11)

N2-C7-C8	123.5(13)	N4-C23-C24	107.4(12)
C7-C8-H8a	108.9(11)	N4-C23-C28	111.0(12)
C7-C8-H8b	110.9(11)	N4-C23-H23	110.0(11)
C7-C8-H8c	109.5(14)	C24-C23-C28	110.8(12)
H8a-C8-H8b	110.6(15)	C24-C23-H23	107.6(13)
H8a-C8-H8c	108.4(12)	C28-C23-H23	109.9(13)
H8b-C8-H8c	108.6(12)	C23-C24-C25	109.3(14)
N2-C9-C10	109.5(12)	C23-C24-H24a	107.4(12)
N2-C9-C14	115.3(12)	C23-C24-H24b	110.4(13)
N2-C9-H9	106.2(11)	C25-C24-H24a	110.7(13)
C10-C9-C14	110.1(11)	C25-C24-H24b	113.8(13)
C10-C9-H9	108.2(12)	H24a-C24-H24b	105.1(14)
C14-C9-H9	107.2(13)	C24-C25-C26	111.3(13)
C9-C10-C11	114.9(14)	C24-C25-H25a	107.5(13)
C9-C10-H10a	110.3(11)	C24-C25-H25b	106.3(15)
C9-C10-H10b	108.0(12)	C26-C25-H25a	113.7(16)
C11-C10-H10a	109.7(13)	C26-C25-H25b	110.7(13)
C11-C10-H10b	108.2(11)	H25a-C25-H25b	106.9(13)
H10a-C10-H10b	105.2(14)	C25-C26-C27	111.3(12)
C10-C11-C12	111.8(13)	C25-C26-H26a	110.4(15)
C10-C11-H11a	109.8(15)	C25-C26-H26b	106.9(13)
C10-C11-H11b	107.1(12)	C27-C26-H26a	111.3(13)
C12-C11-H11a	108.9(12)	C27-C26-H26b	109.8(14)
C12-C11-H11b	108.2(14)	H26a-C26-H26b	107.0(12)
H11a-C11-H11b	111.1(14)	C26-C27-C28	111.1(14)
C11-C12-C13	111.4(11)	C26-C27-H27a	109.0(12)
C11-C12-H12a	110.3(14)	C26-C27-H27b	109.1(13)
C11-C12-H12b	108.0(13)	C28-C27-H27a	110.2(13)
C13-C12-H12a	110.8(13)	C28-C27-H27b	108.9(12)
C13-C12-H12b	110.1(14)	H27a-C27-H27b	108.4(15)
H12a-C12-H12b	106.0(12)	C23-C28-C27	111.0(12)
C12-C13-C14	113.0(13)	C23-C28-H28a	108.7(12)
C12-C13-H13a	110.5(14)	C23-C28-H28b	106.7(13)
C12-C13-H13b	109.7(12)	C27-C28-H28a	112.3(14)
C14-C13-H13a	108.9(12)	C27-C28-H28b	110.6(12)
C14-C13-H13b	108.7(13)	H28a-C28-H28b	107.4(12)
H13a-C13-H13b	105.8(13)		

2

Space Group and Cell Dimensions Monoclinic, P c
a 17.2075(21) b 11.055(4) c 18.223(3)
beta 97.029(12)
Volume 3440.6(14)A**3

Empirical formula : Ge2 N8 C68 H124

Cell dimensions were obtained from 24 reflections with 2Theta angle
in the range 40.00 - 50.00 degrees.

Crystal dimensions : 0.20 X 0.20 X 0.20 mm

FW = 1198.95 Z = 2 F(000) = 1302.18

Dcalc 1.157Mg.m-3, mu 1.37mm-1, lambda 1.54056A, 2Theta(max) 100.0

The intensity data were collected on a Rigaku diffractometer,
using the theta/2theta scan mode.
The h,k,l ranges used during structure solution and refinement are :--
Hmin,max -17 16; Kmin,max -10 10; Lmin,max -17 18
No. of reflections measured 3690
No. of unique reflections 3690
No. of reflections with Inet > 2.5sigma(Inet) 3416
Merging R-value on intensities 0.000
No correction was made for absorption

The last least squares cycle was calculated with
202 atoms, 702 parameters and 3415 out of 3690 reflections.
Weights based on counting-statistics were used.

The residuals are as follows :--
For significant reflections, RF 0.057, Rw 0.043 GoF 3.65
For all reflections, RF 0.062, Rw 0.043.
where RF = Sum(Fo-Fc)/Sum(Fo),
Rw = Sqrt[Sum(w(Fo-Fc)**2)/Sum(wFo**2)] and
GoF = Sqrt[Sum(w(Fo-Fc)**2)/(No. of reflns - No. of params.)]
The maximum shift/sigma ratio was 0.466.

In the last D-map, the deepest hole was -0.590e/A**3,
and the highest peak 0.900e/A**3.

Secondary ext. coeff. 0.5313microns sigma 0.0215

The following references are relevant to the NRCVAX System.

1. Full System Reference :
Gabe, E.J., Le Page, Y., Charland,.J.-P., Lee, F.L. and White, P.S.
(1989) J. Appl. Cryst., 22, 384-387.

2. Scattering Factors from Int. Tab. Vol. 4 :
International Tables for X-ray Crystallography, Vol. IV, (1974)

Kynoch Press, Birmingham, England.

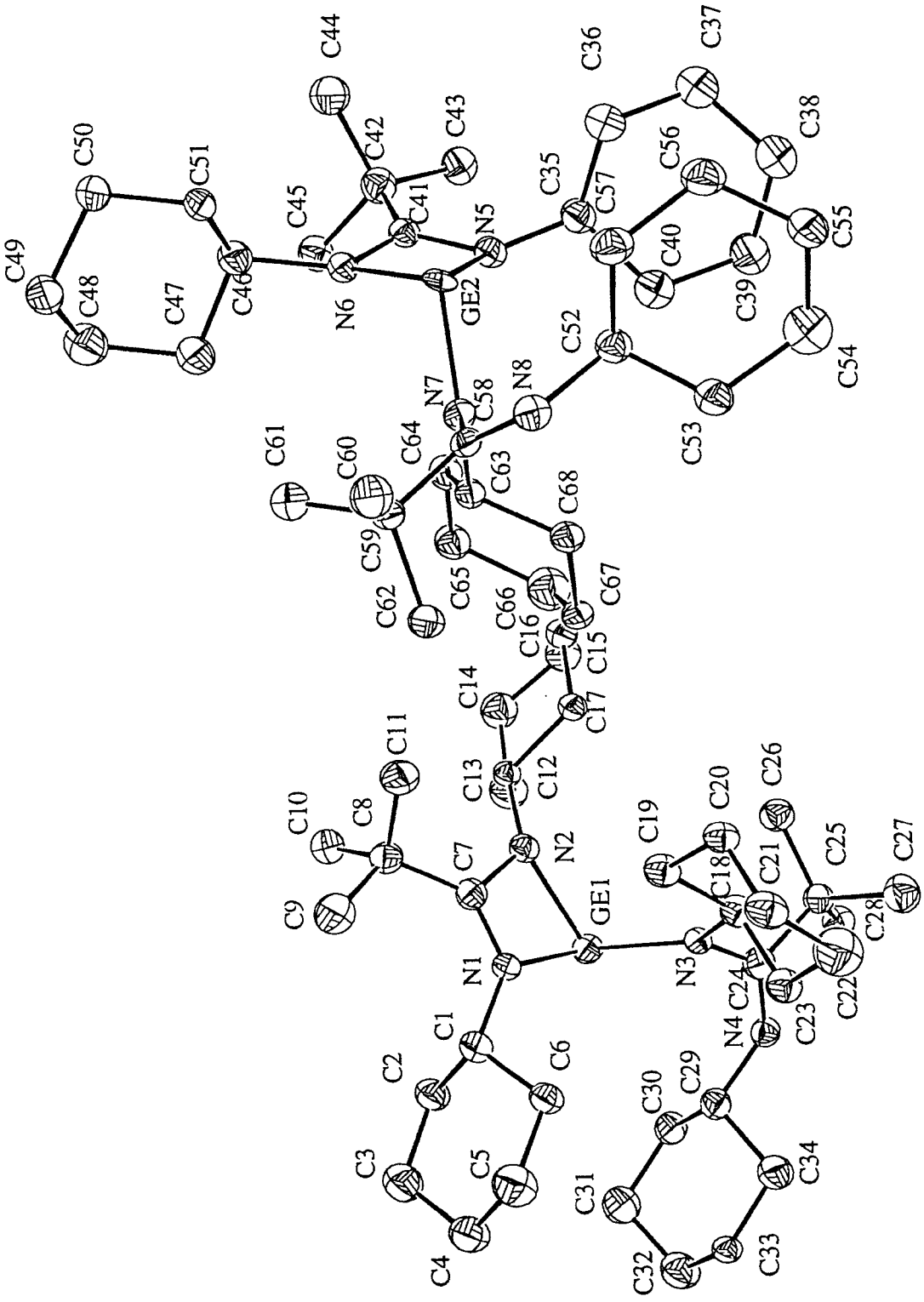
The following references may also be relevant.

3. ORTEP Plotting :
Johnson, C.K., (1976) ORTEP - A Fortran Thermal Ellipsoid Plot Program, Technical Report ORNL-5138, Oak Ridge

4. Pluto Plotting :
S. Motherwell, University Chemical Laboratory, Cambridge, 1978

5. Missing Symmetry Treatment by MISSYM :
Le Page, Y., (1988) J. Appl. Cryst., 21, 983-984.

7. Extinction Treatment :
Larson, A.C., (1970) p.293, Crystallographic Computing, Munksgaard, Copenhagen.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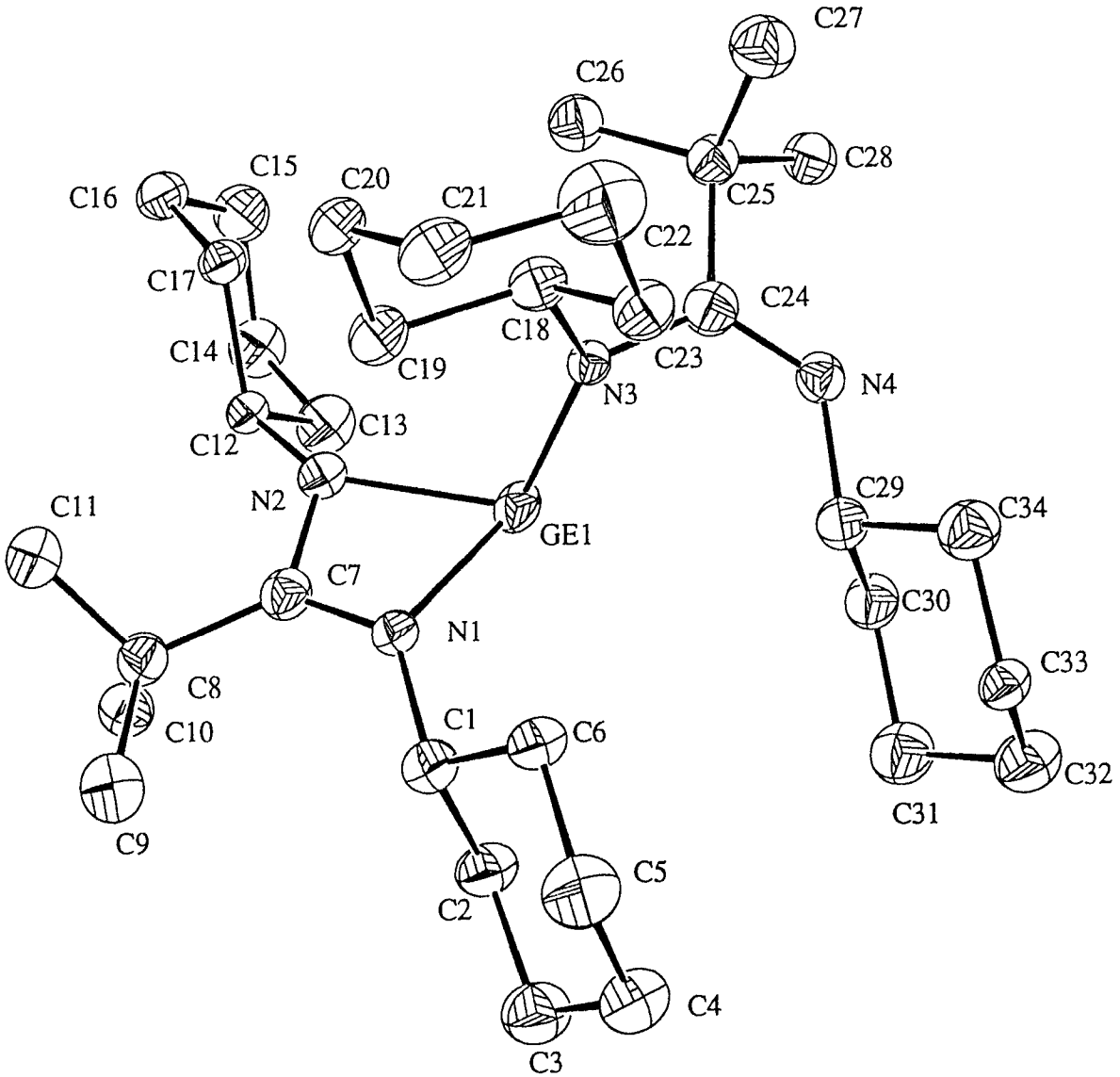
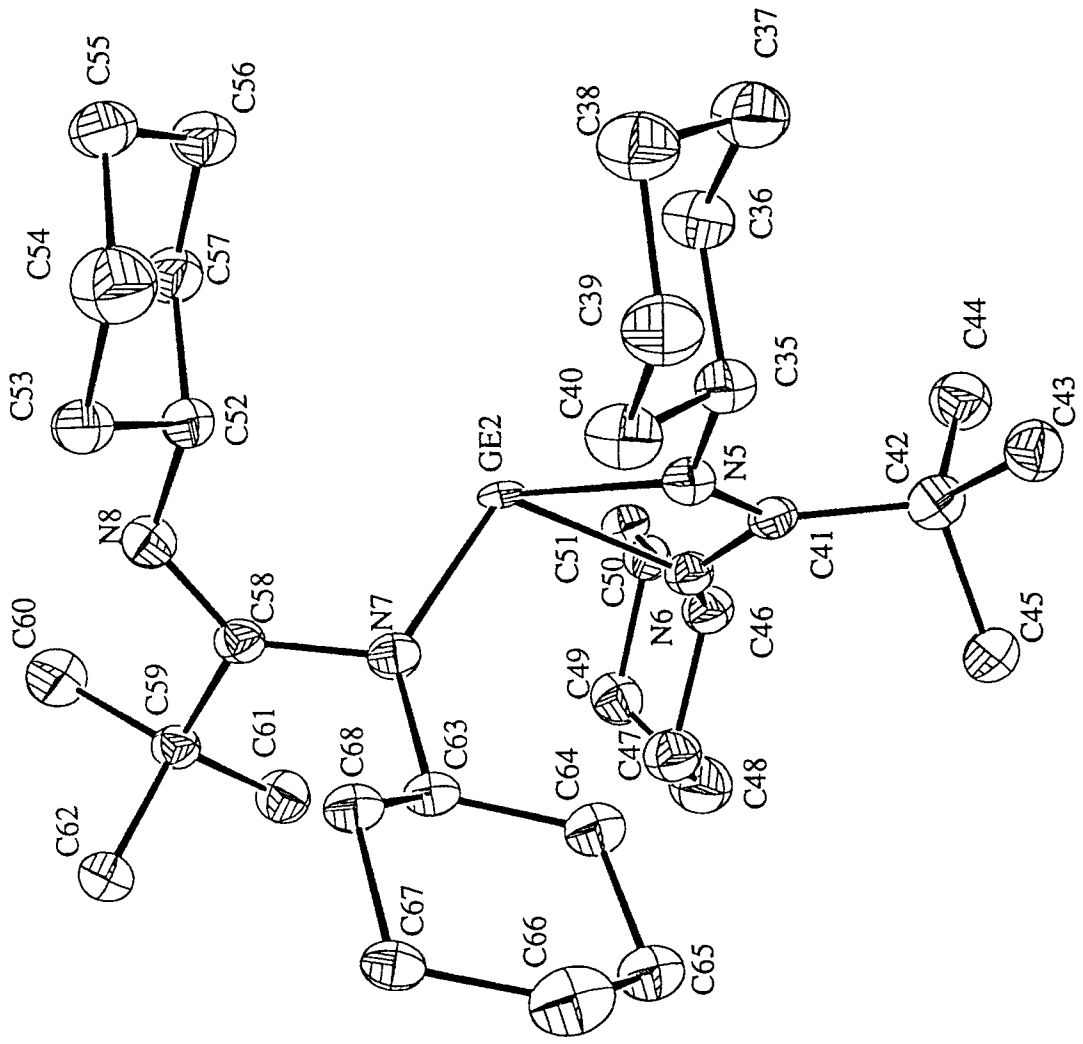
C43
C42
C50
C51
C45
C41
C36
C37
C35
N5
C57
C56
C38
C49
C48
C47
C46
N6
GE2
C40
C39
C55
C52
C54
N7
C58
N8
C53
C61
C60
C64
C63
C68
C59
C65
C67
C62
C66
C16
C15
C14
C17
C13
C12
C11
C10
C8
C7
N2
C19
C20
C26
C18
C21
C25
C27
C9
GE1
C28
N1
N3
C24
C22
C1
N4
C23
C2
C6
C29
C30
C3
C5
C34
C31
C33
C4
C32




C55
C56
C54
C57
C53
C52
N8
C58
C60
C59
C61
C62
C68
C63
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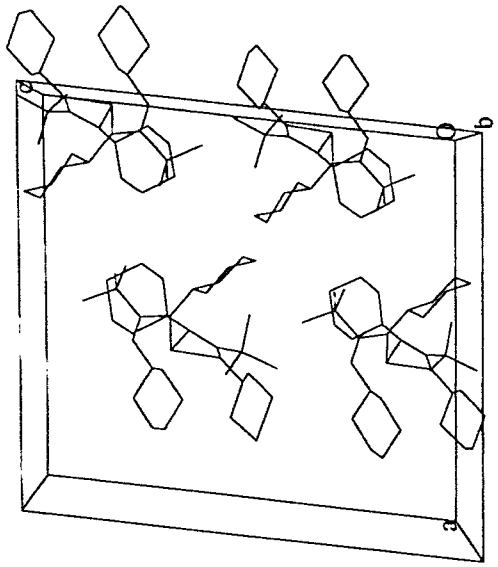
C67
C66
C65
N7
GE2
C38
C37
C36
C39
C35
C40
N5
C42
C44
C43
C41
C51
C50
N6
C46
C45
C49
C47
C48


b
a

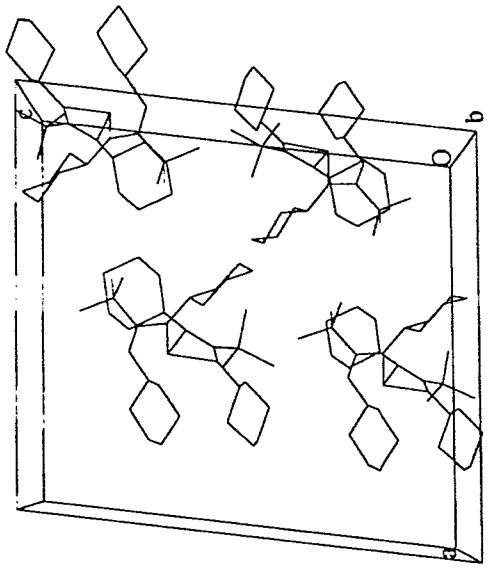

c
b

Table of Atomic Parameters x,y,z and Biso.
E.S.Ds. refer to the last digit printed.

	x	y	z	Biso
GE1	0.02260	0.31720(13)	0.30530	2.05(6)
GE2	0.59694(8)	0.81334(12)	0.67819(8)	1.42(5)
N1	0.0174 (5)	0.3545 (8)	0.4142 (5)	1.7 (4)
N2	0.0805 (5)	0.4656 (9)	0.3420 (5)	1.9 (4)
N3	0.0967 (5)	0.1901 (8)	0.3017 (5)	1.5 (4)
N4	0.0216 (6)	0.0595 (9)	0.2155 (5)	2.0 (4)
N5	0.6007 (5)	0.8484 (9)	0.5686 (5)	1.8 (4)
N6	0.5386 (5)	0.9682 (8)	0.6348 (5)	1.7 (4)
N7	0.5190 (5)	0.6925 (9)	0.6806 (5)	1.7 (4)
N8	0.5937 (6)	0.5562 (9)	0.7696 (5)	2.1 (4)
C1	-0.0341 (7)	0.3019 (11)	0.4660 (7)	2.3 (6)
C2	-0.1199 (8)	0.3313 (12)	0.4340 (7)	2.6 (6)
C3	-0.1775 (8)	0.2727 (13)	0.4820 (8)	3.3 (7)
C4	-0.1608 (8)	0.1408 (13)	0.5014 (8)	3.3 (6)
C5	-0.0772 (9)	0.1168 (14)	0.5275 (8)	3.8 (7)
C6	-0.0223 (7)	0.1706 (11)	0.4764 (7)	2.2 (5)
C7	0.0483 (7)	0.4611 (11)	0.4101 (7)	2.1 (6)
C8	0.0524 (7)	0.5688 (11)	0.4646 (7)	2.2 (5)
C9	0.0188 (8)	0.5488 (13)	0.5361 (8)	3.4 (7)
C10	0.0016 (8)	0.6740 (12)	0.4260 (7)	2.6 (6)
C11	0.1350 (8)	0.6047 (12)	0.4885 (7)	2.8 (6)
C12	0.1115 (7)	0.5672 (10)	0.3094 (6)	1.6 (5)
C13	0.0598 (8)	0.5897 (13)	0.2330 (8)	3.2 (6)
C14	0.0970 (9)	0.6965 (12)	0.1887 (8)	3.2 (6)
C15	0.1787 (8)	0.6673 (13)	0.1765 (7)	3.1 (6)
C16	0.2287 (7)	0.6482 (12)	0.2507 (7)	2.3 (6)
C17	0.1979 (7)	0.5476 (11)	0.2950 (6)	1.8 (5)
C18	0.1692 (7)	0.1499 (11)	0.3535 (7)	2.2 (5)
C19	0.1880 (7)	0.2448 (12)	0.4187 (7)	2.4 (5)
C20	0.2676 (7)	0.1864 (11)	0.4616 (6)	2.0 (5)
C21	0.2550 (8)	0.0674 (12)	0.4905 (7)	2.9 (6)
C22	0.2339 (9)	-0.0236 (15)	0.4261 (9)	4.4 (7)
C23	0.1560 (7)	0.0231 (12)	0.3831 (7)	2.4 (5)
C24	0.0833 (7)	0.1220 (11)	0.2356 (7)	2.3 (6)
C25	0.1444 (7)	0.1250 (11)	0.1807 (7)	2.1 (5)
C26	0.1858 (8)	0.2489 (12)	0.1833 (7)	2.6 (6)
C27	0.2058 (8)	0.0236 (13)	0.1932 (7)	3.2 (6)
C28	0.1016 (7)	0.1059 (12)	0.1033 (7)	2.4 (6)
C29	-0.0426 (7)	0.0415 (11)	0.2609 (7)	2.2 (6)
C30	-0.1178 (7)	0.0898 (12)	0.2142 (7)	2.4 (6)
C31	-0.1881 (8)	0.0672 (13)	0.2585 (7)	3.2 (7)
C32	-0.1945 (8)	-0.0668 (13)	0.2705 (8)	3.3 (7)
C33	-0.1187 (7)	-0.1167 (11)	0.3167 (6)	1.8 (5)
C34	-0.0500 (8)	-0.0939 (12)	0.2761 (7)	2.7 (6)
C35	0.6536 (7)	0.8033 (11)	0.5200 (7)	2.2 (6)
C36	0.7393 (8)	0.8222 (12)	0.5475 (7)	2.8 (6)
C37	0.7906 (8)	0.7783 (13)	0.4906 (8)	3.2 (7)
C38	0.7800 (8)	0.6404 (13)	0.4837 (8)	3.3 (6)
C39	0.6920 (8)	0.6140 (13)	0.4547 (7)	3.1 (6)
C40	0.6376 (8)	0.6662 (12)	0.5085 (7)	3.0 (6)

C41	0.5708 (7)	0.9638 (10)	0.5747 (6)	1.6 (5)
C42	0.5703 (7)	1.0701 (12)	0.5213 (7)	2.3 (5)
C43	0.6002 (8)	1.0386 (12)	0.4456 (7)	2.5 (6)
C44	0.6199 (8)	1.1720 (12)	0.5551 (7)	2.7 (6)
C45	0.4806 (7)	1.1106 (11)	0.5039 (7)	2.3 (5)
C46	0.5068 (7)	1.0714 (11)	0.6783 (7)	2.0 (5)
C47	0.4229 (8)	1.0411 (12)	0.6881 (7)	2.6 (6)
C48	0.3897 (8)	1.1510 (13)	0.7280 (8)	3.3 (7)
C49	0.4383 (7)	1.1697 (12)	0.8039 (7)	2.5 (6)
C50	0.5261 (7)	1.1919 (11)	0.7918 (6)	2.0 (5)
C51	0.5558 (7)	1.0915 (11)	0.7513 (6)	1.7 (5)
C52	0.6586 (7)	0.5409 (11)	0.7264 (6)	1.8 (5)
C53	0.6664 (7)	0.4095 (11)	0.7077 (7)	2.2 (6)
C54	0.7373 (9)	0.3829 (14)	0.6619 (8)	3.8 (7)
C55	0.8139 (7)	0.4321 (12)	0.7030 (7)	2.5 (6)
C56	0.8054 (7)	0.5629 (12)	0.7256 (7)	2.6 (6)
C57	0.7354 (7)	0.5860 (12)	0.7675 (7)	2.4 (6)
C58	0.5329 (7)	0.6217 (10)	0.7486 (6)	1.6 (5)
C59	0.4712 (7)	0.6239 (10)	0.8029 (6)	1.6 (5)
C60	0.5106 (8)	0.6017 (12)	0.8827 (7)	2.6 (6)
C61	0.4282 (7)	0.7428 (11)	0.8018 (7)	2.3 (5)
C62	0.4121 (7)	0.5196 (11)	0.7845 (6)	2.0 (5)
C63	0.4500 (7)	0.6546 (11)	0.6310 (6)	1.7 (5)
C64	0.4242 (7)	0.7376 (11)	0.5704 (7)	2.1 (5)
C65	0.3549 (7)	0.7091 (12)	0.5173 (7)	2.4 (6)
C66	0.3634 (8)	0.5719 (14)	0.4892 (8)	3.5 (7)
C67	0.3885 (7)	0.4845 (11)	0.5502 (6)	1.9 (5)
C68	0.4601 (7)	0.5265 (11)	0.6029 (6)	1.9 (5)
H1	-0.022	0.348	0.519	3.3
H2A	-0.129	0.429	0.431	3.8
H2B	-0.131	0.295	0.378	3.8
H3A	-0.237	0.283	0.456	5.2
H3B	-0.173	0.324	0.535	5.2
H4A	-0.177	0.089	0.451	4.4
H4B	-0.197	0.112	0.542	4.4
H5A	-0.063	0.157	0.583	4.6
H5B	-0.068	0.020	0.533	4.6
H6A	-0.034	0.126	0.423	3.5
H6B	0.038	0.153	0.499	3.5
H9C	0.052	0.479	0.569	4.3
H9A	0.023	0.632	0.570	4.3
H9B	-0.042	0.523	0.526	4.3
H10C	0.020	0.694	0.373	3.7
H10A	-0.060	0.643	0.417	3.7
H10B	0.005	0.753	0.460	3.7
H11C	0.165	0.622	0.439	4.1
H11A	0.139	0.687	0.521	4.1
H11B	0.166	0.533	0.519	4.1
H12	0.109	0.648	0.344	2.6
H13A	0.056	0.507	0.200	4.0
H13B	0.000	0.614	0.242	4.0
H14A	0.098	0.779	0.221	4.2
H14B	0.062	0.711	0.136	4.2
H15A	0.179	0.584	0.145	4.0

H15B	0.203	0.739	0.146	4.0
H16A	0.228	0.732	0.284	3.1
H16B	0.289	0.630	0.243	3.1
H17A	0.202	0.464	0.264	3.2
H17B	0.235	0.538	0.348	3.2
H18	0.219	0.147	0.322	3.0
H19A	0.197	0.334	0.396	3.3
H19B	0.141	0.247	0.452	3.3
H20A	0.288	0.249	0.508	3.3
H20B	0.313	0.184	0.426	3.3
H21A	0.306	0.040	0.526	3.5
H21B	0.205	0.073	0.523	3.5
H22A	0.281	-0.021	0.390	5.6
H22B	0.230	-0.113	0.447	5.6
H23A	0.111	0.026	0.420	3.4
H23B	0.136	-0.038	0.338	3.4
H26C	0.144	0.321	0.174	3.6
H26A	0.222	0.263	0.236	3.6
H26B	0.225	0.254	0.139	3.6
H27C	0.239	0.031	0.247	4.4
H27A	0.178	-0.065	0.189	4.4
H27B	0.246	0.029	0.151	4.4
H28C	0.071	0.020	0.100	3.4
H28A	0.058	0.177	0.091	3.4
H28B	0.141	0.108	0.062	3.4
H29	-0.033	0.091	0.312	2.9
H30A	-0.112	0.186	0.203	3.4
H30B	-0.127	0.043	0.161	3.4
H31A	-0.242	0.102	0.227	4.5
H31B	-0.179	0.115	0.311	4.5
H32A	-0.246	-0.086	0.301	4.9
H32B	-0.204	-0.114	0.218	4.9
H33A	-0.125	-0.213	0.328	2.9
H33B	-0.110	-0.070	0.370	2.9
H34A	0.003	-0.125	0.309	3.8
H34B	-0.057	-0.144	0.225	3.8
H35	0.642	0.847	0.467	3.0
H36A	0.750	0.918	0.559	4.0
H36B	0.753	0.773	0.600	4.0
H37A	0.776	0.821	0.439	4.5
H37B	0.853	0.798	0.511	4.5
H38A	0.818	0.604	0.445	4.3
H38B	0.796	0.596	0.537	4.3
H39A	0.681	0.515	0.450	4.2
H39B	0.677	0.653	0.400	4.2
H40A	0.648	0.621	0.561	3.9
H40B	0.576	0.654	0.486	3.9
H43C	0.567	0.964	0.419	3.4
H43A	0.594	1.117	0.409	3.4
H43B	0.662	1.013	0.454	3.4
H44C	0.680	1.144	0.567	3.5
H44A	0.617	1.247	0.516	3.5
H44B	0.598	1.203	0.605	3.5
H45C	0.456	1.132	0.553	3.3

H45A	0.476	1.188	0.467	3.3
H45B	0.447	1.036	0.475	3.3
H46	0.506	1.154	0.645	3.0
H47A	0.388	1.025	0.635	3.5
H47B	0.421	0.960	0.722	3.5
H48A	0.329	1.136	0.735	4.2
H48B	0.394	1.232	0.695	4.2
H49A	0.416	1.247	0.832	3.7
H49B	0.435	1.090	0.838	3.7
H50A	0.562	1.202	0.845	3.2
H50B	0.530	1.275	0.760	3.2
H51A	0.615	1.110	0.742	2.7
H51B	0.554	1.010	0.784	2.7
H52	0.647	0.592	0.675	2.8
H53A	0.675	0.359	0.759	3.5
H53B	0.613	0.379	0.676	3.5
H54A	0.726	0.429	0.609	5.0
H54B	0.742	0.287	0.653	5.0
H55A	0.861	0.424	0.670	3.7
H55B	0.829	0.378	0.754	3.7
H56A	0.796	0.617	0.675	3.6
H56B	0.857	0.594	0.759	3.6
H57A	0.746	0.539	0.820	3.4
H57B	0.731	0.682	0.778	3.4
H60C	0.543	0.517	0.886	3.6
H60A	0.553	0.675	0.899	3.6
H60B	0.468	0.601	0.922	3.6
H61C	0.471	0.816	0.815	3.4
H61A	0.397	0.760	0.748	3.4
H61B	0.388	0.743	0.843	3.4
H62C	0.383	0.530	0.728	3.1
H62A	0.443	0.433	0.787	3.1
H62B	0.369	0.518	0.823	3.1
H63	0.403	0.651	0.665	2.6
H64A	0.473	0.748	0.537	3.1
H64B	0.414	0.827	0.593	3.1
H65A	0.303	0.714	0.547	4.1
H65B	0.348	0.770	0.472	4.1
H66A	0.406	0.569	0.450	4.7
H66B	0.307	0.540	0.460	4.7
H67A	0.340	0.472	0.584	2.8
H67B	0.401	0.396	0.528	2.8
H68A	0.470	0.464	0.648	3.1
H68B	0.510	0.525	0.572	3.1

Biso is the Mean of the Principal Axes of the Thermal Ellipsoid

Table of u(i,j) or U values *100.
E.S.Ds. refer to the last digit printed

	u11(U)	u22	u33	u12	u13	u23
GE1	1.69(7)	2.59(8)	3.33(8)	0.02(7)	-0.40(6)	-0.16(7)
GE2	0.71(6)	2.42(7)	2.15(7)	-0.26(6)	-0.33(5)	0.27(6)
N1	1.9 (5)	2.3 (6)	2.4 (5)	-0.1 (5)	0.3 (4)	0.0 (4)
N2	2.1 (6)	2.5 (6)	2.5 (6)	0.0 (5)	0.2 (5)	0.1 (5)
N3	1.6 (5)	2.0 (5)	1.8 (5)	0.1 (4)	-0.1 (4)	0.1 (4)
N4	2.5 (6)	2.3 (6)	2.7 (6)	0.1 (5)	0.2 (5)	-0.1 (5)
N5	2.0 (6)	2.5 (6)	2.5 (6)	0.0 (5)	0.3 (5)	0.1 (5)
N6	1.8 (5)	2.0 (6)	2.4 (5)	0.1 (5)	0.2 (4)	0.0 (4)
N7	2.0 (5)	2.4 (6)	2.1 (5)	-0.2 (5)	0.0 (4)	-0.3 (4)
N8	2.6 (6)	2.5 (6)	2.7 (6)	-0.1 (5)	0.3 (5)	0.1 (5)
C1	2.4 (7)	3.1 (8)	3.0 (7)	-0.1 (6)	0.4 (6)	0.1 (6)
C2	2.6 (8)	3.3 (8)	4.1 (8)	0.1 (7)	0.7 (6)	0.4 (7)
C3	3.5 (9)	4.3 (9)	4.8 (9)	0.2 (7)	0.9 (7)	0.2 (7)
C4	3.6 (8)	4.5 (9)	4.7 (9)	-0.2 (7)	0.8 (7)	0.4 (7)
C5	4.5 (9)	5.1 (10)	4.9 (9)	0.0 (8)	0.8 (8)	0.5 (8)
C6	2.3 (7)	3.0 (8)	3.2 (7)	0.0 (6)	0.5 (6)	0.4 (6)
C7	2.2 (7)	2.8 (8)	3.0 (7)	0.1 (6)	0.1 (6)	0.0 (6)
C8	2.6 (7)	2.9 (7)	2.9 (7)	-0.1 (6)	0.2 (6)	-0.1 (6)
C9	4.4 (9)	4.3 (9)	4.3 (9)	-0.2 (8)	0.5 (7)	-0.3 (7)
C10	3.2 (8)	3.2 (8)	3.6 (8)	0.1 (7)	0.5 (6)	-0.1 (6)
C11	3.3 (8)	3.7 (8)	3.7 (8)	-0.4 (7)	0.2 (6)	-0.4 (7)
C12	1.7 (6)	2.2 (7)	2.2 (6)	-0.1 (6)	0.1 (5)	0.0 (5)
C13	3.7 (9)	4.2 (9)	4.2 (8)	-0.1 (7)	0.3 (7)	0.2 (7)
C14	4.0 (8)	4.0 (8)	4.1 (8)	0.0 (7)	0.4 (7)	0.1 (7)
C15	4.1 (9)	3.6 (9)	4.2 (8)	-0.3 (7)	0.9 (7)	0.0 (7)
C16	2.5 (7)	2.7 (7)	3.7 (7)	0.0 (6)	0.6 (6)	0.1 (6)
C17	2.0 (7)	2.3 (7)	2.8 (7)	0.0 (6)	0.3 (5)	0.1 (6)
C18	2.4 (7)	3.1 (8)	2.8 (7)	0.2 (6)	0.1 (6)	0.3 (6)
C19	2.5 (7)	3.3 (8)	3.0 (7)	0.0 (6)	0.0 (6)	0.2 (6)
C20	2.1 (7)	2.9 (7)	2.6 (7)	-0.1 (6)	-0.2 (6)	0.2 (6)
C21	2.7 (8)	4.2 (8)	3.8 (8)	0.0 (7)	-0.1 (6)	0.7 (7)
C22	5.2 (10)	5.6 (11)	5.7 (10)	0.6 (9)	0.4 (8)	0.8 (9)
C23	2.7 (7)	3.3 (8)	3.2 (7)	0.2 (6)	0.0 (6)	0.3 (6)
C24	2.7 (7)	2.7 (8)	3.4 (7)	0.2 (6)	0.1 (6)	0.2 (6)
C25	2.4 (7)	2.5 (7)	2.9 (7)	0.1 (6)	0.2 (6)	0.2 (6)
C26	3.4 (8)	3.2 (8)	3.2 (7)	-0.1 (7)	0.5 (6)	0.0 (7)
C27	3.8 (9)	4.0 (9)	4.3 (9)	0.3 (7)	0.6 (7)	0.1 (7)
C28	3.1 (8)	3.0 (8)	3.1 (7)	0.0 (6)	0.5 (6)	0.0 (6)
C29	2.4 (7)	2.7 (7)	3.0 (7)	0.1 (6)	0.2 (6)	-0.2 (6)
C30	2.7 (7)	3.0 (8)	3.5 (7)	0.2 (6)	0.0 (6)	0.0 (6)
C31	3.2 (8)	4.2 (9)	4.6 (9)	0.3 (7)	0.1 (7)	0.1 (7)
C32	3.2 (8)	4.7 (9)	4.8 (9)	-0.1 (7)	0.5 (7)	0.1 (7)
C33	1.9 (7)	2.2 (7)	2.8 (7)	0.0 (6)	0.2 (5)	0.3 (6)
C34	3.0 (8)	3.5 (8)	4.0 (8)	0.1 (7)	0.4 (6)	0.2 (7)
C35	2.4 (7)	3.0 (8)	2.9 (7)	0.0 (6)	0.3 (6)	-0.1 (6)
C36	2.9 (8)	3.5 (8)	4.3 (8)	-0.2 (7)	0.7 (6)	-0.3 (7)
C37	3.4 (9)	4.2 (9)	4.7 (8)	0.0 (7)	0.8 (7)	-0.1 (7)
C38	3.4 (8)	4.3 (9)	4.7 (8)	0.2 (7)	0.9 (7)	-0.3 (7)
C39	3.5 (8)	4.2 (9)	4.2 (8)	0.1 (7)	0.6 (7)	-0.5 (7)

C40	3.3 (8)	3.9 (9)	4.2 (8)	-0.1 (7)	0.6 (7)	-0.4 (7)
C41	1.6 (6)	2.1 (7)	2.3 (7)	0.0 (5)	0.0 (5)	0.1 (5)
C42	2.8 (7)	3.0 (8)	3.0 (7)	0.2 (6)	0.2 (6)	0.0 (6)
C43	3.3 (8)	3.1 (8)	3.2 (8)	0.2 (7)	0.5 (6)	0.3 (6)
C44	3.3 (8)	3.4 (8)	3.7 (8)	-0.1 (7)	0.4 (6)	0.0 (7)
C45	2.7 (7)	2.9 (8)	3.1 (7)	0.4 (6)	0.1 (6)	0.3 (6)
C46	2.3 (7)	2.6 (7)	2.9 (7)	0.2 (6)	0.3 (6)	0.1 (6)
C47	2.8 (8)	3.3 (8)	3.6 (8)	0.2 (6)	0.3 (6)	0.0 (6)
C48	3.7 (9)	4.0 (9)	4.9 (9)	0.0 (7)	0.7 (7)	0.0 (7)
C49	3.2 (8)	2.9 (8)	3.3 (8)	0.1 (6)	0.8 (6)	0.0 (6)
C50	2.5 (7)	2.3 (7)	2.7 (7)	0.1 (6)	0.4 (6)	0.0 (6)
C51	1.7 (7)	2.2 (7)	2.4 (7)	0.2 (6)	0.1 (5)	-0.1 (5)
C52	2.1 (7)	2.3 (7)	2.5 (7)	0.0 (6)	0.2 (6)	0.1 (6)
C53	2.3 (7)	2.9 (7)	3.1 (7)	0.0 (6)	0.3 (6)	0.0 (6)
C54	4.4 (9)	4.8 (10)	5.4 (9)	0.1 (8)	0.6 (8)	-0.3 (8)
C55	2.4 (7)	3.3 (8)	3.6 (8)	0.2 (6)	0.2 (6)	0.0 (6)
C56	2.5 (7)	3.3 (8)	3.8 (8)	-0.3 (6)	0.0 (6)	0.0 (6)
C57	2.7 (7)	2.8 (8)	3.4 (7)	-0.3 (6)	-0.1 (6)	0.0 (6)
C58	1.9 (7)	1.8 (7)	2.4 (6)	-0.2 (6)	0.0 (5)	-0.2 (5)
C59	1.9 (7)	1.9 (7)	2.4 (6)	-0.2 (6)	0.1 (5)	-0.2 (5)
C60	3.4 (8)	3.4 (8)	3.2 (8)	-0.1 (7)	0.5 (6)	-0.1 (6)
C61	2.8 (7)	2.8 (8)	3.0 (7)	0.0 (6)	0.4 (6)	0.0 (6)
C62	2.3 (7)	2.6 (7)	2.7 (7)	-0.3 (6)	0.4 (6)	0.0 (6)
C63	1.6 (7)	2.4 (7)	2.2 (7)	-0.1 (6)	0.0 (5)	-0.4 (5)
C64	2.4 (7)	3.0 (7)	2.7 (7)	0.0 (6)	0.1 (6)	-0.3 (6)
C65	2.5 (7)	3.6 (8)	3.1 (7)	-0.1 (6)	0.0 (6)	-0.3 (6)
C66	3.6 (9)	5.1 (9)	4.4 (9)	0.1 (7)	0.0 (7)	-0.6 (7)
C67	2.0 (7)	2.5 (7)	2.5 (7)	-0.5 (6)	0.2 (5)	-0.6 (6)
C68	1.9 (7)	2.7 (7)	2.4 (7)	-0.2 (6)	0.0 (6)	-0.3 (6)

Anisotropic Temperature Factors are of the form
Temp=-2*Pi*Pi*(h*h*u11*astar*astar+---+2*h*k*u12*astar*bstar+---)

Table of Atomic Bond Distances in Angstroms

GE1-N1	2.040(9)	C31-C32	1.504(20)
GE1-N2	1.993(10)	C31-H31A	1.099(14)
GE1-N3	1.903(9)	C31-H31B	1.086(14)
GE2-N5	2.043(9)	C32-C33	1.564(18)
GE2-N6	2.090(9)	C32-H32A	1.111(14)
GE2-N7	1.898(9)	C32-H32B	1.078(14)
N1-C1	1.490(15)	C33-C34	1.492(17)
N1-C7	1.299(15)	C33-H33A	1.086(12)
N2-C7	1.420(15)	C33-H33B	1.099(12)
N2-C12	1.405(15)	C34-H34A	1.091(13)
N3-C18	1.535(15)	C34-H34B	1.082(13)
N3-C24	1.415(15)	C35-C36	1.514(18)
N4-C24	1.282(16)	C35-C40	1.549(19)
N4-C29	1.472(15)	C35-H35	1.085(12)
N5-C35	1.436(15)	C36-C37	1.520(19)
N5-C41	1.385(15)	C36-H36A	1.090(14)
N6-C41	1.287(14)	C36-H36B	1.106(13)
N6-C46	1.528(15)	C37-C38	1.539(20)
N7-C58	1.460(14)	C37-H37A	1.050(14)
N7-C63	1.463(14)	C37-H37B	1.114(14)
N8-C52	1.454(15)	C38-C39	1.568(19)
N8-C58	1.292(15)	C38-H38A	1.096(14)
C1-C2	1.554(18)	C38-H38B	1.097(14)
C1-C6	1.475(18)	C39-C40	1.548(19)
C1-H1	1.097(12)	C39-H39A	1.107(14)
C2-C3	1.542(19)	C39-H39B	1.086(14)
C2-H2A	1.092(13)	C40-H40A	1.077(14)
C2-H2B	1.086(13)	C40-H40B	1.097(13)
C3-C4	1.520(20)	C41-C42	1.526(17)
C3-H3A	1.077(14)	C42-C43	1.570(18)
C3-H3B	1.117(14)	C42-C44	1.499(18)
C4-C5	1.483(21)	C42-C45	1.601(18)
C4-H4A	1.095(14)	C43-H43C	1.079(13)
C4-H4B	1.077(14)	C43-H43A	1.084(13)
C5-C6	1.526(19)	C43-H43B	1.092(13)
C5-H5A	1.098(15)	C44-H44C	1.079(13)
C5-H5B	1.088(15)	C44-H44A	1.090(13)
C6-H6A	1.086(12)	C44-H44B	1.082(13)
C6-H6B	1.083(12)	C45-H45C	1.064(12)
C7-C8	1.547(17)	C45-H45A	1.085(12)
C8-C9	1.505(19)	C45-H45B	1.105(13)
C8-C10	1.568(18)	C46-C47	1.514(18)
C8-C11	1.489(18)	C46-C51	1.500(16)
C9-H9C	1.090(15)	C46-H46	1.094(12)
C9-H9A	1.102(14)	C47-C48	1.560(19)
C9-H9B	1.076(14)	C47-H47A	1.083(13)
C10-H10C	1.073(13)	C47-H47B	1.089(13)
C10-H10A	1.108(13)	C48-C49	1.541(19)
C10-H10B	1.068(13)	C48-H48A	1.077(14)
C11-H11C	1.113(13)	C48-H48B	1.087(14)
C11-H11A	1.074(13)	C49-C50	1.573(17)
C11-H11B	1.076(13)	C49-H49A	1.091(13)

C12-C13	1.578(18)	C49-H49B	1.085(13)
C12-C17	1.556(16)	C50-C51	1.460(16)
C12-H12	1.095(11)	C50-H50A	1.086(12)
C13-C14	1.606(20)	C50-H50B	1.090(12)
C13-H13A	1.088(14)	C51-H51A	1.076(11)
C13-H13B	1.100(14)	C51-H51B	1.082(12)
C14-C15	1.485(20)	C52-C53	1.501(17)
C14-H14A	1.089(14)	C52-C57	1.521(17)
C14-H14B	1.078(14)	C52-H52	1.096(12)
C15-C16	1.525(18)	C53-C54	1.587(19)
C15-H15A	1.092(14)	C53-H53A	1.081(12)
C15-H15B	1.081(14)	C53-H53B	1.086(12)
C16-C17	1.508(17)	C54-C55	1.534(20)
C16-H16A	1.104(13)	C54-H54A	1.087(15)
C16-H16B	1.085(12)	C54-H54B	1.074(15)
C17-H17A	1.088(12)	C55-C56	1.516(18)
C17-H17B	1.093(12)	C55-H55A	1.074(13)
C18-C19	1.589(18)	C55-H55B	1.105(13)
C18-C23	1.529(18)	C56-C57	1.525(18)
C18-H18	1.093(12)	C56-H56A	1.091(13)
C19-C20	1.625(17)	C56-H56B	1.071(13)
C19-H19A	1.083(13)	C57-H57A	1.091(12)
C19-H19B	1.071(13)	C57-H57B	1.082(13)
C20-C21	1.443(18)	C58-C59	1.537(16)
C20-H20A	1.120(12)	C59-C60	1.547(17)
C20-H20B	1.074(12)	C59-C61	1.507(17)
C21-C22	1.554(21)	C59-C62	1.547(17)
C21-H21A	1.072(13)	C60-H60C	1.085(13)
C21-H21B	1.097(13)	C60-H60A	1.103(13)
C22-C23	1.556(20)	C60-H60B	1.078(13)
C22-H22A	1.110(16)	C61-H61C	1.098(12)
C22-H22B	1.065(16)	C61-H61A	1.076(12)
C23-H23A	1.092(13)	C61-H61B	1.079(12)
C23-H23B	1.093(13)	C62-H62C	1.088(12)
C24-C25	1.538(17)	C62-H62A	1.093(12)
C25-C26	1.542(18)	C62-H62B	1.073(12)
C25-C27	1.538(18)	C63-C64	1.462(17)
C25-C28	1.525(17)	C63-C68	1.524(17)
C26-H26C	1.080(13)	C63-H63	1.085(11)
C26-H26A	1.080(13)	C64-C65	1.475(17)
C26-H26B	1.105(13)	C64-H64A	1.106(12)
C27-H27C	1.080(14)	C64-H64B	1.094(12)
C27-H27A	1.087(14)	C65-C66	1.614(20)
C27-H27B	1.096(14)	C65-H65A	1.103(13)
C28-H28C	1.089(13)	C65-H65B	1.062(13)
C28-H28A	1.099(13)	C66-C67	1.495(19)
C28-H28B	1.076(12)	C66-H66A	1.090(14)
C29-C30	1.554(17)	C66-H66B	1.108(14)
C29-C34	1.530(18)	C67-C68	1.538(16)
C29-H29	1.073(12)	C67-H67A	1.099(12)
C30-C31	1.554(19)	C67-H67B	1.089(12)
C30-H30A	1.092(13)	C68-H68A	1.074(12)
C30-H30B	1.086(13)	C68-H68B	1.090(12)

Table of Atomic Bond Angles in Degrees

N1-GE1-N2	65.6(4)	H32A-C32-H32B	107.3(12)
N1-GE1-N3	107.0(4)	C32-C33-C34	109.4(10)
N2-GE1-N3	108.1(4)	C32-C33-H33A	110.5(10)
N5-GE2-N6	63.0(4)	C32-C33-H33B	109.0(10)
N5-GE2-N7	105.2(4)	C34-C33-H33A	110.7(10)
N6-GE2-N7	106.1(4)	C34-C33-H33B	109.5(10)
GE1-N1-C1	129.7(7)	H33A-C33-H33B	107.6(10)
GE1-N1-C7	93.4(7)	C29-C34-C33	110.1(10)
C1-N1-C7	132.1(10)	C29-C34-H34A	109.0(11)
GE1-N2-C7	91.8(7)	C29-C34-H34B	110.2(11)
GE1-N2-C12	135.7(7)	C33-C34-H34A	109.8(11)
C7-N2-C12	127.3(10)	C33-C34-H34B	109.2(11)
GE1-N3-C18	133.6(7)	H34A-C34-H34B	108.5(11)
GE1-N3-C24	112.5(7)	N5-C35-C36	114.4(10)
C18-N3-C24	113.9(9)	N5-C35-C40	107.9(10)
C24-N4-C29	124.3(10)	N5-C35-H35	109.4(10)
GE2-N5-C35	129.5(8)	C36-C35-C40	109.3(10)
GE2-N5-C41	92.3(7)	C36-C35-H35	107.9(10)
C35-N5-C41	129.7(10)	C40-C35-H35	107.8(10)
GE2-N6-C41	93.1(7)	C35-C36-C37	110.7(11)
GE2-N6-C46	127.0(7)	C35-C36-H36A	109.5(11)
C41-N6-C46	133.5(10)	C35-C36-H36B	108.6(11)
GE2-N7-C58	110.7(7)	C37-C36-H36A	110.5(11)
GE2-N7-C63	135.2(7)	C37-C36-H36B	110.6(11)
C58-N7-C63	114.0(9)	H36A-C36-H36B	106.9(11)
C52-N8-C58	123.6(10)	C36-C37-C38	107.4(11)
N1-C1-C2	107.0(9)	C36-C37-H37A	111.4(12)
N1-C1-C6	112.4(10)	C36-C37-H37B	109.1(11)
N1-C1-H1	108.5(10)	C38-C37-H37A	111.1(12)
C2-C1-C6	111.3(10)	C38-C37-H37B	108.6(11)
C2-C1-H1	107.5(10)	H37A-C37-H37B	109.1(12)
C6-C1-H1	109.9(10)	C37-C38-C39	108.2(11)
C1-C2-C3	110.3(10)	C37-C38-H38A	110.2(12)
C1-C2-H2A	110.3(11)	C37-C38-H38B	111.0(12)
C1-C2-H2B	109.1(11)	C39-C38-H38A	110.4(11)
C3-C2-H2A	110.5(11)	C39-C38-H38B	110.0(11)
C3-C2-H2B	108.6(11)	H38A-C38-H38B	107.1(12)
H2A-C2-H2B	108.1(11)	C38-C39-C40	110.5(11)
C2-C3-C4	114.7(11)	C38-C39-H39A	110.7(11)
C2-C3-H3A	110.1(12)	C38-C39-H39B	110.7(11)
C2-C3-H3B	107.4(11)	C40-C39-H39A	108.2(11)
C4-C3-H3A	110.3(12)	C40-C39-H39B	109.7(12)
C4-C3-H3B	106.9(11)	H39A-C39-H39B	107.0(11)
H3A-C3-H3B	107.0(12)	C35-C40-C39	109.8(11)
C3-C4-C5	113.2(12)	C35-C40-H40A	109.0(11)
C3-C4-H4A	106.5(11)	C35-C40-H40B	108.4(11)
C3-C4-H4B	109.7(12)	C39-C40-H40A	110.5(11)
C5-C4-H4A	108.1(12)	C39-C40-H40B	110.5(11)
C5-C4-H4B	110.5(12)	H40A-C40-H40B	108.4(12)
H4A-C4-H4B	108.5(12)	N5-C41-N6	107.8(10)
C4-C5-C6	112.6(12)	N5-C41-C42	129.2(10)

C4-C5-H5A	108.2(12)	N6-C41-C42	122.9(10)
C4-C5-H5B	109.4(13)	C41-C42-C43	114.4(10)
C6-C5-H5A	108.8(12)	C41-C42-C44	111.0(10)
C6-C5-H5B	110.2(12)	C41-C42-C45	105.8(10)
H5A-C5-H5B	107.5(12)	C43-C42-C44	107.3(10)
C1-C6-C5	112.0(11)	C43-C42-C45	107.4(10)
C1-C6-H6A	109.1(10)	C44-C42-C45	111.0(10)
C1-C6-H6B	109.9(11)	C42-C43-H43C	110.6(11)
C5-C6-H6A	107.8(11)	C42-C43-H43A	109.7(10)
C5-C6-H6B	109.1(11)	C42-C43-H43B	110.3(10)
H6A-C6-H6B	108.8(11)	H43C-C43-H43A	109.3(11)
N1-C7-N2	106.8(10)	H43C-C43-H43B	108.6(11)
N1-C7-C8	130.4(11)	H43A-C43-H43B	108.3(11)
N2-C7-C8	122.8(10)	C42-C44-H44C	110.8(11)
C7-C8-C9	116.8(11)	C42-C44-H44A	109.0(11)
C7-C8-C10	107.7(10)	C42-C44-H44B	110.3(11)
C7-C8-C11	111.1(10)	H44C-C44-H44A	108.8(11)
C9-C8-C10	104.2(10)	H44C-C44-H44B	109.4(11)
C9-C8-C11	103.9(10)	H44A-C44-H44B	108.6(11)
C10-C8-C11	113.1(11)	C42-C45-H45C	111.6(10)
C8-C9-H9C	110.4(12)	C42-C45-H45A	109.7(10)
C8-C9-H9A	110.6(12)	C42-C45-H45B	109.0(10)
C8-C9-H9B	111.4(12)	H45C-C45-H45A	110.3(11)
H9C-C9-H9A	107.2(12)	H45C-C45-H45B	108.8(11)
H9C-C9-H9B	109.0(13)	H45A-C45-H45B	107.3(10)
H9A-C9-H9B	108.1(12)	N6-C46-C47	107.6(10)
C8-C10-H10C	110.3(11)	N6-C46-C51	111.9(9)
C8-C10-H10A	108.2(10)	N6-C46-H46	108.1(9)
C8-C10-H10B	111.2(11)	C47-C46-C51	111.7(10)
H10C-C10-H10A	107.9(11)	C47-C46-H46	107.7(10)
H10C-C10-H10B	110.9(12)	C51-C46-H46	109.7(10)
H10A-C10-H10B	108.2(11)	C46-C47-C48	106.9(10)
C8-C11-H11C	108.9(11)	C46-C47-H47A	111.4(11)
C8-C11-H11A	111.9(11)	C46-C47-H47B	109.7(11)
C8-C11-H11B	110.8(11)	C48-C47-H47A	110.4(11)
H11C-C11-H11A	107.5(11)	C48-C47-H47B	109.8(11)
H11C-C11-H11B	107.4(11)	H47A-C47-H47B	108.6(11)
H11A-C11-H11B	110.2(11)	C47-C48-C49	109.5(11)
N2-C12-C13	107.3(9)	C47-C48-H48A	110.2(12)
N2-C12-C17	112.3(9)	C47-C48-H48B	109.0(11)
N2-C12-H12	111.1(9)	C49-C48-H48A	109.8(11)
C13-C12-C17	108.6(9)	C49-C48-H48B	109.0(11)
C13-C12-H12	108.6(10)	H48A-C48-H48B	109.2(12)
C17-C12-H12	108.8(9)	C48-C49-C50	108.6(10)
C12-C13-C14	110.1(11)	C48-C49-H49A	110.4(11)
C12-C13-H13A	109.8(11)	C48-C49-H49B	110.4(11)
C12-C13-H13B	109.9(11)	C50-C49-H49A	109.8(10)
C14-C13-H13A	109.9(11)	C50-C49-H49B	109.5(10)
C14-C13-H13B	109.7(11)	H49A-C49-H49B	108.3(10)
H13A-C13-H13B	107.4(12)	C49-C50-C51	110.8(10)
C13-C14-C15	111.0(11)	C49-C50-H50A	110.2(10)
C13-C14-H14A	108.7(11)	C49-C50-H50B	109.2(10)
C13-C14-H14B	110.1(12)	C51-C50-H50A	109.3(10)
C15-C14-H14A	108.5(12)	C51-C50-H50B	109.1(10)

C15-C14-H14B	109.6(12)	H50A-C50-H50B	108.3(10)
H14A-C14-H14B	108.9(12)	C46-C51-C50	111.6(10)
C14-C15-C16	109.8(11)	C46-C51-H51A	108.9(10)
C14-C15-H15A	109.5(12)	C46-C51-H51B	108.4(10)
C14-C15-H15B	110.6(12)	C50-C51-H51A	109.7(10)
C16-C15-H15A	108.4(11)	C50-C51-H51B	108.6(10)
C16-C15-H15B	110.0(11)	H51A-C51-H51B	109.6(10)
H15A-C15-H15B	108.5(11)	N8-C52-C53	109.3(10)
C15-C16-C17	112.3(10)	N8-C52-C57	111.9(10)
C15-C16-H16A	109.1(11)	N8-C52-H52	109.7(10)
C15-C16-H16B	111.1(11)	C53-C52-C57	109.5(10)
C17-C16-H16A	107.4(10)	C53-C52-H52	108.4(10)
C17-C16-H16B	109.4(10)	C57-C52-H52	108.0(10)
H16A-C16-H16B	107.3(11)	C52-C53-C54	113.2(10)
C12-C17-C16	113.1(10)	C52-C53-H53A	108.3(10)
C12-C17-H17A	108.9(10)	C52-C53-H53B	109.0(10)
C12-C17-H17B	109.4(9)	C54-C53-H53A	108.6(10)
C16-C17-H17A	107.8(10)	C54-C53-H53B	108.7(10)
C16-C17-H17B	109.6(10)	H53A-C53-H53B	109.0(11)
H17A-C17-H17B	107.9(10)	C53-C54-C55	110.3(11)
N3-C18-C19	110.2(9)	C53-C54-H54A	108.8(12)
N3-C18-C23	109.7(9)	C53-C54-H54B	109.7(12)
N3-C18-H18	108.4(9)	C55-C54-H54A	108.4(12)
C19-C18-C23	111.5(10)	C55-C54-H54B	110.3(12)
C19-C18-H18	108.3(10)	H54A-C54-H54B	109.3(13)
C23-C18-H18	108.6(10)	C54-C55-C56	111.4(11)
C18-C19-C20	100.4(9)	C54-C55-H55A	111.0(11)
C18-C19-H19A	109.7(10)	C54-C55-H55B	108.9(11)
C18-C19-H19B	109.6(10)	C56-C55-H55A	109.6(11)
C20-C19-H19A	113.5(10)	C56-C55-H55B	107.8(10)
C20-C19-H19B	113.3(10)	H55A-C55-H55B	108.0(11)
H19A-C19-H19B	109.9(11)	C55-C56-C57	113.8(11)
C19-C20-C21	112.4(10)	C55-C56-H56A	107.9(10)
C19-C20-H20A	106.6(10)	C55-C56-H56B	110.8(11)
C19-C20-H20B	110.5(10)	C57-C56-H56A	106.5(10)
C21-C20-H20A	109.5(10)	C57-C56-H56B	108.4(10)
C21-C20-H20B	110.7(11)	H56A-C56-H56B	109.3(11)
H20A-C20-H20B	107.0(10)	C52-C57-C56	112.9(10)
C20-C21-C22	110.3(11)	C52-C57-H57A	108.4(10)
C20-C21-H21A	109.5(11)	C52-C57-H57B	109.7(10)
C20-C21-H21B	107.8(11)	C56-C57-H57A	107.9(10)
C22-C21-H21A	111.9(12)	C56-C57-H57B	109.4(11)
C22-C21-H21B	108.5(11)	H57A-C57-H57B	108.5(11)
H21A-C21-H21B	108.8(11)	N7-C58-N8	126.5(10)
C21-C22-C23	105.8(12)	N7-C58-C59	118.9(9)
C21-C22-H22A	108.1(13)	N8-C58-C59	114.6(10)
C21-C22-H22B	110.7(13)	C58-C59-C60	110.1(9)
C23-C22-H22A	110.1(12)	C58-C59-C61	112.4(10)
C23-C22-H22B	113.7(13)	C58-C59-C62	109.6(9)
H22A-C22-H22B	108.3(14)	C60-C59-C61	108.0(10)
C18-C23-C22	109.0(11)	C60-C59-C62	106.7(9)
C18-C23-H23A	109.9(11)	C61-C59-C62	109.9(10)
C18-C23-H23B	110.3(10)	C59-C60-H60C	111.0(10)
C22-C23-H23A	109.7(11)	C59-C60-H60A	109.6(10)

C22-C23-H23B	110.4(11)	C59-C60-H60B	111.5(11)
H23A-C23-H23B	107.6(11)	H60C-C60-H60A	107.4(11)
N3-C24-N4	125.0(11)	H60C-C60-H60B	109.3(11)
N3-C24-C25	119.3(10)	H60A-C60-H60B	107.9(11)
N4-C24-C25	115.7(11)	C59-C61-H61C	109.0(10)
C24-C25-C26	110.5(10)	C59-C61-H61A	110.8(10)
C24-C25-C27	113.6(10)	C59-C61-H61B	110.5(10)
C24-C25-C28	108.0(10)	H61C-C61-H61A	108.4(11)
C26-C25-C27	109.7(10)	H61C-C61-H61B	108.2(10)
C26-C25-C28	108.7(10)	H61A-C61-H61B	109.9(11)
C27-C25-C28	106.3(10)	C59-C62-H62C	110.0(10)
C25-C26-H26C	110.8(11)	C59-C62-H62A	109.5(10)
C25-C26-H26A	111.2(11)	C59-C62-H62B	110.8(10)
C25-C26-H26B	109.9(10)	H62C-C62-H62A	107.9(10)
H26C-C26-H26A	109.5(11)	H62C-C62-H62B	109.5(10)
H26C-C26-H26B	107.6(11)	H62A-C62-H62B	109.0(10)
H26A-C26-H26B	107.6(11)	N7-C63-C64	115.8(10)
C25-C27-H27C	110.9(11)	N7-C63-C68	110.9(9)
C25-C27-H27A	110.8(11)	N7-C63-H63	105.4(9)
C25-C27-H27B	110.1(11)	C64-C63-C68	111.4(9)
H27C-C27-H27A	109.0(12)	C64-C63-H63	106.1(10)
H27C-C27-H27B	108.2(12)	C68-C63-H63	106.5(10)
H27A-C27-H27B	107.8(12)	C63-C64-C65	120.5(11)
C25-C28-H28C	110.7(10)	C63-C64-H64A	107.7(10)
C25-C28-H28A	109.5(10)	C63-C64-H64B	109.3(10)
C25-C28-H28B	111.5(11)	C65-C64-H64A	105.2(10)
H28C-C28-H28A	107.4(11)	C65-C64-H64B	106.7(10)
H28C-C28-H28B	109.1(11)	H64A-C64-H64B	106.5(10)
H28A-C28-H28B	108.4(11)	C64-C65-C66	108.1(10)
N4-C29-C30	106.1(9)	C64-C65-H65A	107.9(10)
N4-C29-C34	108.6(10)	C64-C65-H65B	112.7(11)
N4-C29-H29	111.4(10)	C66-C65-H65A	108.1(10)
C30-C29-C34	110.7(10)	C66-C65-H65B	110.8(11)
C30-C29-H29	109.3(10)	H65A-C65-H65B	109.1(11)
C34-C29-H29	110.7(10)	C65-C66-C67	113.6(11)
C29-C30-C31	108.0(10)	C65-C66-H66A	109.6(12)
C29-C30-H30A	109.9(10)	C65-C66-H66B	109.9(11)
C29-C30-H30B	110.3(10)	C67-C66-H66A	108.4(12)
C31-C30-H30A	110.4(11)	C67-C66-H66B	108.3(12)
C31-C30-H30B	110.0(11)	H66A-C66-H66B	106.7(12)
H30A-C30-H30B	108.2(11)	C66-C67-C68	113.9(10)
C30-C31-C32	108.0(11)	C66-C67-H67A	108.8(10)
C30-C31-H31A	109.8(11)	C66-C67-H67B	110.8(10)
C30-C31-H31B	110.1(11)	C68-C67-H67A	107.1(9)
C32-C31-H31A	110.4(12)	C68-C67-H67B	108.6(10)
C32-C31-H31B	110.9(12)	H67A-C67-H67B	107.4(10)
H31A-C31-H31B	107.7(12)	C63-C68-C67	112.0(9)
C31-C32-C33	110.8(11)	C63-C68-H68A	110.4(10)
C31-C32-H32A	109.4(12)	C63-C68-H68B	108.9(10)
C31-C32-H32B	110.7(12)	C67-C68-H68A	109.3(10)
C33-C32-H32A	109.0(11)	C67-C68-H68B	106.9(9)
C33-C32-H32B	109.5(11)	H68A-C68-H68B	109.2(10)

Torsion angles

N2	GE1	N1	C1	167.4(14)	N2	GE1	N1	C7	10.3(10)
N3	GE1	N1	C1	-90.0(12)	N3	GE1	N1	C7	112.8(14)
N1	GE1	N2	C7	-9.4(9)	N1	GE1	N2	C12	-163.6(14)
N3	GE1	N2	C7	-110.3(13)	N3	GE1	N2	C12	95.5(12)
N1	GE1	N3	C18	-28.0(9)	N1	GE1	N3	C24	155.2(14)
N2	GE1	N3	C18	41.2(10)	N2	GE1	N3	C24	-135.6(14)
N6	GE2	N5	C35	161.2(14)	N6	GE2	N5	C41	11.7(9)
N7	GE2	N5	C35	-98.2(13)	N7	GE2	N5	C41	112.3(13)
N5	GE2	N6	C41	-12.6(10)	N5	GE2	N6	C46	-167.2(13)
N7	GE2	N6	C41	-111.8(14)	N7	GE2	N6	C46	93.6(12)
N5	GE2	N7	C58	154.8(13)	N5	GE2	N7	C63	-25.0(9)
N6	GE2	N7	C58	-139.4(13)	N6	GE2	N7	C63	40.8(9)
GE1	N1	C1	C2	-61.0(12)	GE1	N1	C1	C6	61.5(12)
C7	N1	C1	C2	87.5(19)	C7	N1	C1	C6	-150.0(24)
GE1	N1	C7	N2	-13.8(7)	GE1	N1	C7	C8	166.1(18)
C1	N1	C7	N2	-170.0(22)	C1	N1	C7	C8	9.8(11)
GE1	N2	C7	N1	14.1(8)	GE1	N2	C7	C8	-165.8(18)
C12	N2	C7	N1	171.7(24)	C12	N2	C7	C8	-8.2(11)
GE1	N2	C12	C13	28.8(10)	GE1	N2	C12	C17	-90.5(14)
C7	N2	C12	C13	-118.1(20)	C7	N2	C12	C17	122.6(20)
GE1	N3	C18	C19	-6.7(8)	GE1	N3	C18	C23	116.4(17)
C24	N3	C18	C19	170.1(22)	C24	N3	C18	C23	-66.7(16)
GE1	N3	C24	N4	-62.9(13)	GE1	N3	C24	C25	114.4(16)
C18	N3	C24	N4	119.6(21)	C18	N3	C24	C25	-63.1(15)
C29	N4	C24	N3	-4.8(10)	C29	N4	C24	C25	177.8(23)
C24	N4	C29	C30	121.9(22)	C24	N4	C29	C34	-119.0(22)
GE2	N5	C35	C36	-53.8(12)	GE2	N5	C35	C40	68.0(13)
C41	N5	C35	C36	84.9(18)	C41	N5	C35	C40	-153.3(23)
GE2	N5	C41	N6	-18.0(8)	GE2	N5	C41	C42	164.5(18)
C35	N5	C41	N6	-167.3(23)	C35	N5	C41	C42	15.1(12)
GE2	N6	C41	N5	17.6(8)	GE2	N6	C41	C42	-164.7(17)
C46	N6	C41	N5	169.3(21)	C46	N6	C41	C42	-13.0(11)
GE2	N6	C46	C47	-91.0(14)	GE2	N6	C46	C51	32.0(9)
C41	N6	C46	C47	125.2(22)	C41	N6	C46	C51	-111.7(21)
GE2	N7	C58	N8	-61.5(12)	GE2	N7	C58	C59	117.5(16)
C63	N7	C58	N8	118.3(20)	C63	N7	C58	C59	-62.7(14)
GE2	N7	C63	C64	-12.7(8)	GE2	N7	C63	C68	115.5(16)
C58	N7	C63	C64	167.5(22)	C58	N7	C63	C68	-64.2(14)
C58	N8	C52	C53	-119.2(21)	C58	N8	C52	C57	119.4(21)
C52	N8	C58	N7	-1.4(10)	C52	N8	C58	C59	179.5(22)
N1	C1	C2	C3	176.4(25)	C6	C1	C2	C3	53.2(16)
N1	C1	C6	C5	-178.1(25)	C2	C1	C6	C5	-58.1(16)
C1	C2	C3	C4	-47.4(15)	C2	C3	C4	C5	46.5(16)
C3	C4	C5	C6	-49.3(16)	C4	C5	C6	C1	56.3(17)
N1	C7	C8	C9	2.9(12)	N1	C7	C8	C10	-113.8(22)
N1	C7	C8	C11	121.8(23)	N2	C7	C8	C9	-177. (3)
N2	C7	C8	C10	66.0(16)	N2	C7	C8	C11	-58.4(15)
N2	C12	C13	C14	-174. (3)	C17	C12	C13	C14	-52.7(15)
N2	C12	C17	C16	172.1(24)	C13	C12	C17	C16	53.6(15)

C12	C13	C14	C15	57.9(16)	C13	C14	C15	C16	-59.0(16)
C14	C15	C16	C17	58.9(17)	C15	C16	C17	C12	-56.8(15)
N3	C18	C19	C20	-177.2(23)	C23	C18	C19	C20	60.7(15)
N3	C18	C23	C22	171.9(24)	C19	C18	C23	C22	-65.7(17)
C18	C19	C20	C21	-62.2(16)	C19	C20	C21	C22	66.7(17)
C20	C21	C22	C23	-62.2(18)	C21	C22	C23	C18	60.6(17)
N3	C24	C25	C26	-31.6(12)	N3	C24	C25	C27	92.1(19)
N3	C24	C25	C28	-150.3(24)	N4	C24	C25	C26	145.9(25)
N4	C24	C25	C27	-90.4(20)	N4	C24	C25	C28	27.2(12)
N4	C29	C30	C31	177.4(25)	C34	C29	C30	C31	59.8(16)
N4	C29	C34	C33	-175. (3)	C30	C29	C34	C33	-59.3(15)
C29	C30	C31	C32	-60.7(17)	C30	C31	C32	C33	61.6(16)
C31	C32	C33	C34	-60.7(17)	C32	C33	C34	C29	57.6(16)
N5	C35	C36	C37	-177. (3)	C40	C35	C36	C37	62.1(17)
N5	C35	C40	C39	179. (3)	C36	C35	C40	C39	-56.4(16)
C35	C36	C37	C38	-65.4(17)	C36	C37	C38	C39	62.4(17)
C37	C38	C39	C40	-59.2(17)	C38	C39	C40	C35	55.9(16)
N5	C41	C42	C43	6.9(10)	N5	C41	C42	C44	-114.6(22)
N5	C41	C42	C45	125.0(22)	N6	C41	C42	C43	-170.2(25)
N6	C41	C42	C44	68.3(17)	N6	C41	C42	C45	-52.2(14)
N6	C46	C47	C48	-176.4(24)	C51	C46	C47	C48	60.5(16)
N6	C46	C51	C50	178.8(23)	C47	C46	C51	C50	-60.5(16)
C46	C47	C48	C49	-60.7(16)	C47	C48	C49	C50	58.8(16)
C48	C49	C50	C51	-56.8(16)	C49	C50	C51	C46	57.0(15)
N8	C52	C53	C54	-178.7(24)	C57	C52	C53	C54	-55.8(15)
N8	C52	C57	C56	176.0(24)	C53	C52	C57	C56	54.6(15)
C52	C53	C54	C55	55.0(16)	C53	C54	C55	C56	-50.8(15)
C54	C55	C56	C57	51.8(16)	C55	C56	C57	C52	-53.8(15)
N7	C58	C59	C60	-151.7(22)	N7	C58	C59	C61	-31.2(11)
N7	C58	C59	C62	91.3(17)	N8	C58	C59	C60	27.5(12)
N8	C58	C59	C61	147.9(24)	N8	C58	C59	C62	-89.6(18)
N7	C63	C64	C65	-179.6(24)	C68	C63	C64	C65	52.4(14)
N7	C63	C68	C67	-179.7(23)	C64	C63	C68	C67	-49.1(14)
C63	C64	C65	C66	-48.7(14)	C64	C65	C66	C67	45.4(14)
C65	C66	C67	C68	-49.2(14)	C66	C67	C68	C63	50.7(15)

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6

Space Group and Cell Dimensions Monoclinic, P 21/c
a 17.806(3) b 9.9000(23) c 20.425(5)
beta 94.920(16)
Volume 3587.3(14)A**3

Empirical formula : Se Ge N4 C34 H62

Cell dimensions were obtained from 24 reflections with 2Theta angle in the range 80.00 - 100.00 degrees.

Crystal dimensions : 0.20 X 0.20 X 0.20 mm

FW = 678.43 Z = 4 F(000) = 1434.74

Dcalc 1.256Mg.m-3, mu 2.52mm-1, lambda 1.54056A, 2Theta(max) 100.0

The intensity data were collected on a Rigaku diffractometer, using the theta/2theta scan mode.
The h,k,l ranges used during structure solution and refinement are :--
Hmin,max -15 15; Kmin,max 0 9; Lmin,max 0 20
No. of reflections measured 3740
No. of unique reflections 3588
No. of reflections with Inet > 2.5sigma(Inet) 1998
Merging R-value on intensities 0.126
Absorption corrections were made.
The minimum and maximum transmission factors are 0.566009 and 0.583563.

The last least squares cycle was calculated with
102 atoms, 361 parameters and 1998 out of 3588 reflections.
Weights based on counting-statistics were used.

The residuals are as follows :--
For significant reflections, RF 0.111, Rw 0.087 GoF 6.36
For all reflections, RF 0.209, Rw 0.089.
where RF = Sum(Fo-Fc)/Sum(Fo),
Rw = Sqrt[Sum(w(Fo-Fc)**2)/Sum(wFo**2)] and
GoF = Sqrt[Sum(w(Fo-Fc)**2)/(No. of reflns - No. of params.)]
The maximum shift/sigma ratio was 0.724.

In the last D-map, the deepest hole was -0.770e/A**3,
and the highest peak 1.180e/A**3.

The following references are relevant to the NRCVAX System.

1. Full System Reference :
Gabe, E.J., Le Page, Y., Charland,.J.-P., Lee, F.L. and White, P.S. (1989) J. Appl. Cryst., 22, 384-387.

2. Scattering Factors from Int. Tab. Vol. 4 :
International Tables for X-ray Crystallography, Vol. IV, (1974)

Kynoch Press, Birmingham, England.

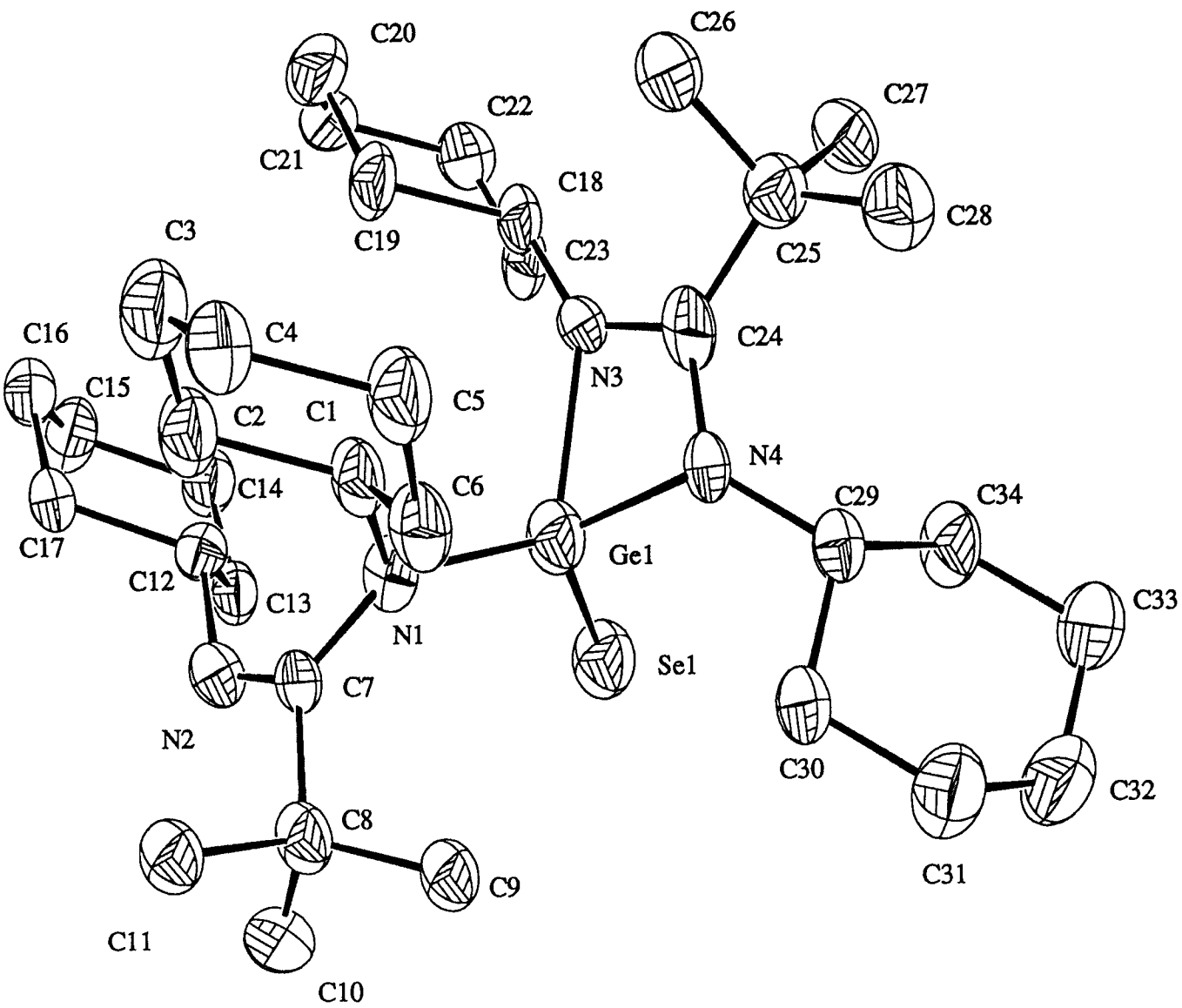
The following references may also be relevant.

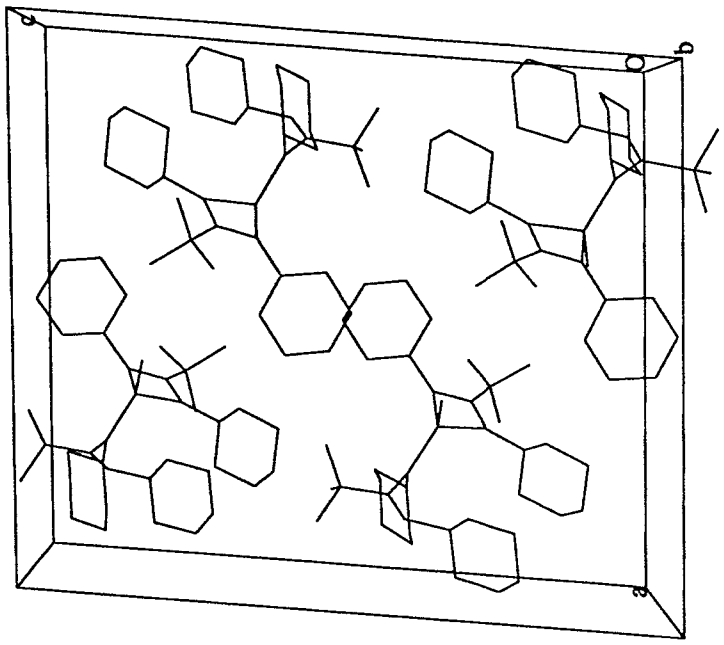
3. ORTEP Plotting :
Johnson, C.K., (1976) ORTEP - A Fortran Thermal Ellipsoid Plot Program, Technical Report ORNL-5138, Oak Ridge

4. Pluto Plotting :
S. Motherwell, University Chemical Laboratory, Cambridge, 1978

5. Missing Symmetry Treatment by MISSYM :
Le Page, Y., (1988) J. Appl. Cryst., 21, 983-984.

6. Grouping of Equivalent Reflections in DATRD2 :
Le Page, Y. and Gabe, E.J., (1979) J. Appl. Cryst., 12, 464-466.




c
b
a

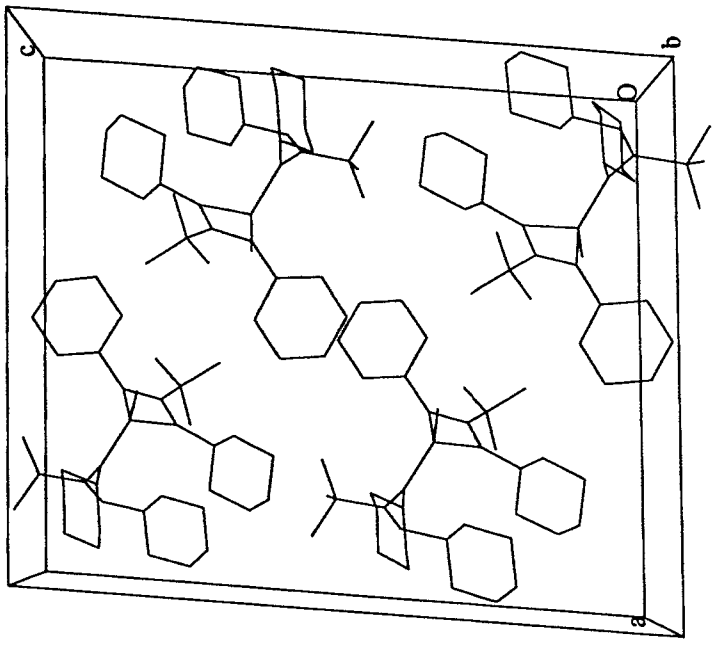

c
b
a

Table of Atomic Parameters x,y,z and Biso.
E.S.Ds. refer to the last digit printed.

	x	y	z	Biso
Se1	0.36437(13)	1.1292(3)	0.14654(11)	4.52(12)
Ge1	0.30628(13)	0.9334(3)	0.14300(11)	3.71(12)
N1	0.2133 (8)	0.9148(16)	0.0948 (6)	2.9 (8)
N2	0.1429 (8)	1.1246(16)	0.0864 (7)	3.3 (8)
N3	0.3027 (8)	0.8153(15)	0.2229 (7)	2.8 (8)
N4	0.3629 (8)	0.7608(15)	0.1389 (7)	3.0 (8)
C1	0.1788 (10)	0.7778(20)	0.0941 (9)	3.2 (10)
C2	0.0918 (11)	0.7833(22)	0.0984 (9)	4.1 (12)
C3	0.0605 (11)	0.6392(24)	0.1037 (9)	4.8 (13)
C4	0.0858 (10)	0.5400(21)	0.0546 (9)	3.6 (11)
C5	0.1716 (10)	0.5411(22)	0.0531 (9)	4.1 (12)
C6	0.2009 (10)	0.6843(20)	0.0430 (9)	3.5 (11)
C7	0.1788 (9)	1.0286(19)	0.0624 (8)	2.7 (10)
C8	0.1882 (10)	1.0461(21)	-0.0135 (8)	3.3 (11)
C9	0.2581 (10)	0.9776(21)	-0.0358 (8)	3.4 (11)
C10	0.1928 (11)	1.1961(22)	-0.0277 (9)	4.3 (13)
C11	0.1160 (10)	0.9920(20)	-0.0523 (8)	3.5 (11)
C12	0.1294 (10)	1.1337(20)	0.1570 (8)	2.8 (10)
C13	0.1610 (10)	1.2674(20)	0.1818 (9)	3.1 (11)
C14	0.1426 (10)	1.2908(21)	0.2535 (9)	3.7 (12)
C15	0.0578 (10)	1.2830(22)	0.2600 (9)	4.1 (12)
C16	0.0259 (10)	1.1538(22)	0.2335 (9)	3.8 (12)
C17	0.0434 (10)	1.1266(20)	0.1645 (8)	3.0 (10)
C18	0.2691 (10)	0.8350(20)	0.2847 (9)	3.3 (11)
C19	0.1831 (10)	0.8148(21)	0.2762 (9)	3.7 (12)
C20	0.1506 (11)	0.8317(22)	0.3434 (10)	4.2 (13)
C21	0.1716 (10)	0.9660(22)	0.3723 (9)	3.7 (11)
C22	0.2570 (10)	0.9873(21)	0.3816 (9)	3.9 (11)
C23	0.2911 (10)	0.9691(21)	0.3155 (9)	3.4 (11)
C24	0.3484 (10)	0.7280(21)	0.2010 (9)	3.4 (11)
C25	0.3734 (10)	0.5971(21)	0.2369 (9)	3.7 (12)
C26	0.3029 (10)	0.5197(21)	0.2542 (9)	4.0 (11)
C27	0.4228 (10)	0.6401(23)	0.3002 (9)	4.0 (11)
C28	0.4187 (11)	0.4969(23)	0.2009 (9)	4.6 (12)
C29	0.4273 (10)	0.7289(20)	0.1011 (8)	2.9 (11)
C30	0.4167 (10)	0.7871(21)	0.0321 (9)	3.8 (12)
C31	0.4852 (12)	0.7495(23)	-0.0069 (11)	5.0 (14)
C32	0.5581 (12)	0.8012(24)	0.0286 (10)	5.8 (15)
C33	0.5698 (11)	0.7475(23)	0.0968 (10)	4.9 (13)
C34	0.5020 (10)	0.7813(22)	0.1364 (9)	4.2 (12)
H1	0.201	0.731	0.141	4.1
H2a	0.065	0.835	0.056	4.8
H2b	0.079	0.846	0.142	4.8
H3a	-0.001	0.645	0.101	5.7
H3b	0.078	0.603	0.154	5.7
H4a	0.068	0.437	0.067	4.8
H4b	0.059	0.564	0.007	4.8
H5a	0.189	0.476	0.014	4.7
H5b	0.199	0.505	0.100	4.7
H6a	0.177	0.722	-0.005	4.4

H6b	0.263	0.683	0.042	4.4
H9a	0.258	0.870	-0.026	4.2
H9b	0.262	0.994	-0.088	4.2
H9c	0.309	1.021	-0.010	4.2
H10a	0.242	1.239	-0.001	5.1
H10b	0.195	1.213	-0.080	5.1
H10c	0.143	1.247	-0.012	5.1
H11a	0.066	1.040	-0.035	4.7
H11b	0.117	1.012	-0.104	4.7
H11c	0.110	0.883	-0.046	4.7
H12	0.158	1.048	0.185	3.5
H13a	0.222	1.267	0.180	3.9
H13b	0.137	1.347	0.152	3.9
H14a	0.172	1.215	0.285	4.4
H14b	0.164	1.390	0.270	4.4
H15a	0.030	1.367	0.234	4.8
H15b	0.047	1.292	0.312	4.8
H16a	-0.036	1.155	0.234	5.1
H16b	0.048	1.071	0.265	5.1
H17a	0.023	1.024	0.150	3.2
H17b	0.016	1.198	0.131	3.2
H18	0.292	0.756	0.319	3.7
H19a	0.169	0.716	0.256	4.5
H19b	0.159	0.891	0.242	4.5
H20a	0.172	0.752	0.376	4.6
H20b	0.089	0.820	0.336	4.6
H21a	0.147	1.046	0.339	5.0
H21b	0.147	0.977	0.419	5.0
H22a	0.283	0.911	0.417	4.9
H22b	0.272	1.086	0.403	4.9
H23a	0.352	0.980	0.320	4.0
H23b	0.268	1.049	0.282	4.0
H26a	0.268	0.491	0.211	4.6
H26b	0.318	0.431	0.283	4.6
H26c	0.268	0.585	0.284	4.6
H27a	0.392	0.714	0.328	4.8
H27b	0.436	0.554	0.332	4.8
H27c	0.475	0.688	0.289	4.8
H28a	0.470	0.544	0.186	5.9
H28b	0.433	0.412	0.232	5.9
H28c	0.385	0.463	0.157	5.9
H29	0.433	0.620	0.097	3.5
H30a	0.364	0.752	0.007	4.1
H30b	0.413	0.899	0.036	4.1
H31a	0.478	0.794	-0.057	6.1
H31b	0.488	0.641	-0.012	6.1
H32a	0.554	0.913	0.033	6.2
H32b	0.605	0.778	0.002	6.2
H33a	0.573	0.637	0.094	5.2
H33b	0.621	0.785	0.121	5.2
H34a	0.498	0.893	0.141	4.8
H34b	0.510	0.742	0.186	4.8

Biso is the Mean of the Principal Axes of the Thermal Ellipsoid