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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 |
|---|---|---|---|---|---|---|
| Se1 | 3.86(15) | 7.08(18) | 6.06(16) | -0.33(16) | -0.61(12) | -0.19(16) |
| Ge1 | 3.13(14) | 6.20(18) | 4.60(15) | -0.08(16) | -0.74(11) | -0.03(15) |
| N1 | 2.6 (10) | 6.3 (13) | 1.9 (10) | -0.2 (10) | -0.9 ( 8) | -2.1 ( 9) |
| N2 | 3.1 (10) | 5.7 (12) | 3.7 (11) | -0.1 (10) | -0.8 ( 8) | 0.3 (10) |
| N3 | 2.2 (10) | 5.4 (13) | 2.9 (10) | 0.1 (10) | -0.7 ( 8) | 1.1 ( 9) |
| N4 | 1.3 (10) | 5.7 (12) | 4.3 (11) | -0.3 (10) | -1.1 ( 8) | 0.7 (10) |
| C1 | 2.5 (13) | 6.0 (17) | 3.3 (13) | 0.3 (12) | -1.0 (10) | -0.5 (12) |
| C2 | 2.8 (14) | 7.9 (18) | 4.6 (14) | 0.3 (14) | -0.6 (11) | -0.4 (13) |
| C3 | 3.4 (15) | 7.9 (19) | 6.9 (16) | -0.1 (15) | -0.2 (12) | -0.2 (15) |
| C4 | 3.1 (13) | 5.3 (17) | 5.2 (14) | 0.1 (13) | -0.5 (11) | -0.5 (13) |
| C5 | 2.9 (14) | 7.2 (18) | 5.2 (14) | 0.1 (14) | -1.0 (11) | -0.3 (14) |
| C6 | 3.2 (14) | 5.7 (17) | 4.1 (14) | 0.2 (13) | -1.1 (11) | -1.4 (12) |
| C7 | 1.7 (11) | 4.9 (16) | 3.4 (13) | -0.8 (11) | -1.0 (10) | 0.4 (12) |
| C8 | 2.8 (13) | 6.3 (17) | 3.1 (13) | 0.1 (13) | -0.9 (10) | -0.5 (12) |
| C9 | 2.9 (13) | 6.4 (17) | 3.2 (13) | 0.0 (12) | -0.8 (11) | -0.2 (12) |
| C10 | 4.7 (16) | 7.5 (18) | 4.0 (16) | 0.1 (14) | -0.1 (12) | 0.8 (14) |
| C11 | 3.3 (14) | 6.4 (16) | 3.4 (13) | -0.4 (13) | -0.7 (11) | -0.5 (12) |
| C12 | 2.8 (12) | 4.4 (14) | 3.3 (12) | 0.2 (12) | 0.4 (10) | 0.2 (12) |
| C13 | 2.4 (13) | 5.1 (16) | 4.1 (14) | 0.3 (12) | -0.2 (10) | -0.1 (12) |
| C14 | 3.1 (14) | 6.5 (17) | 4.5 (15) | -0.1 (13) | 0.0 (11) | -0.2 (13) |
| C15 | 3.0 (15) | 7.6 (18) | 5.0 (15) | 0.0 (14) | 0.6 (12) | -0.6 (14) |
| C16 | 2.9 (14) | 7.2 (18) | 4.3 (15) | 0.5 (14) | 0.1 (11) | 0.8 (14) |
| C17 | 2.3 (12) | 4.8 (15) | 4.0 (13) | 0.2 (12) | -0.5 (10) | 0.5 (12) |
| C18 | 1.9 (13) | 6.2 (18) | 4.2 (14) | 0.3 (13) | -0.6 (10) | 0.6 (12) |
| C19 | 1.8 (13) | 7.4 (18) | 4.7 (15) | -0.2 (13) | -0.5 (11) | 0.0 (13) |
| C20 | 3.1 (15) | 7.4 (19) | 5.6 (16) | -1.1 (14) | 0.1 (12) | 0.7 (14) |
| C21 | 3.6 (14) | 6.4 (18) | 4.3 (14) | 0.0 (13) | 0.4 (11) | 1.3 (13) |
| C22 | 3.7 (14) | 5.9 (17) | 4.9 (14) | -0.1 (13) | -0.5 (12) | 0.7 (13) |
| C23 | 1.9 (13) | 6.0 (17) | 4.9 (14) | -0.1 (12) | -0.8 (11) | -0.5 (13) |
| C24 | 2.2 (13) | 6.0 (17) | 4.4 (14) | -0.1 (13) | -1.8 (11) | -0.9 (13) |
| C25 | 3.4 (13) | 6.5 (19) | 4.0 (14) | 0.2 (13) | -0.3 (11) | 0.4 (13) |
| C26 | 3.4 (14) | 7.0 (18) | 4.5 (14) | -0.2 (13) | -1.2 (12) | 0.8 (13) |
| C27 | 4.1 (14) | 7.3 (17) | 3.7 (14) | 0.6 (14) | -1.1 (11) | 0.9 (14) |
| C28 | 4.3 (15) | 6.3 (19) | 6.6 (16) | 0.3 (14) | -0.3 (13) | 0.6 (14) |
| C29 | 2.3 (13) | 4.3 (16) | 4.5 (13) | 0.2 (12) | -0.4 (10) | -0.1 (12) |
| C30 | 2.3 (14) | 6.9 (17) | 5.3 (15) | 0.4 (13) | -0.4 (11) | 1.0 (13) |
| C31 | 4.4 (16) | 9.1 (20) | 5.7 (16) | 0.5 (15) | 0.4 (13) | -0.9 (16) |
| C32 | 4.1 (17) | 10.7 (22) | 7.2 (18) | 0.1 (17) | 1.4 (14) | 0.7 (16) |
| C33 | 2.7 (15) | 8.2 (19) | 7.5 (17) | -0.5 (15) | 0.0 (13) | 0.6 (15) |
| C34 | 2.4 (14) | 7.6 (18) | 5.5 (15) | -0.5 (14) | -1.1 (12) | -0.4 (14) |

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

| | | | |
|---|---|---|---|
| Se1-Ge1 | 2.196(4) | C15-H15b | 1.098(19) |
| Ge1-N1 | 1.862(13) | C16-C17 | 1.493(25) |
| Ge1-N3 | 2.013(14) | C16-H16a | 1.095(18) |
| Ge1-N4 | 1.989(15) | C16-H16b | 1.087(20) |
| N1-C1 | 1.488(25) | C17-H17a | 1.112(20) |
| N1-C7 | 1.420(24) | C17-H17b | 1.070(18) |
| N2-C7 | 1.268(24) | C18-C19 | 1.540(25) |
| N2-C12 | 1.484(21) | C18-C23 | 1.51(3) |
| N3-C18 | 1.455(22) | C18-H18 | 1.105(19) |
| N3-C24 | 1.294(24) | C19-C20 | 1.54(3) |
| N4-C24 | 1.354(23) | C19-H19a | 1.083(20) |
| N4-C29 | 1.471(22) | C19-H19b | 1.090(19) |
| C1-C2 | 1.56(3) | C20-C21 | 1.49(3) |
| C1-C6 | 1.47(3) | C20-H20a | 1.082(21) |
| C1-H1 | 1.107(18) | C20-H20b | 1.100(19) |
| C2-C3 | 1.54(3) | C21-C22 | 1.53(3) |
| C2-H2a | 1.087(19) | C21-H21a | 1.102(19) |
| C2-H2b | 1.132(19) | C21-H21b | 1.093(18) |
| C3-C4 | 1.50(3) | C22-C23 | 1.54(3) |
| C3-H3a | 1.095(19) | C22-H22a | 1.112(19) |
| C3-H3b | 1.114(20) | C22-H22b | 1.094(20) |
| C4-C5 | 1.53(3) | C23-H23a | 1.081(18) |
| C4-H4a | 1.105(20) | C23-H23b | 1.108(19) |
| C4-H4b | 1.081(18) | C24-C25 | 1.54(3) |
| C5-C6 | 1.53(3) | C25-C26 | 1.54(3) |
| C5-H5a | 1.083(20) | C25-C27 | 1.56(3) |
| C5-H5b | 1.093(19) | C25-C28 | 1.51(3) |
| C6-H6a | 1.098(18) | C26-H26a | 1.076(18) |
| C6-H6b | 1.099(18) | C26-H26b | 1.079(20) |
| C7-C8 | 1.583(24) | C26-H26c | 1.108(20) |
| C8-C9 | 1.52(3) | C27-H27a | 1.109(20) |
| C8-C10 | 1.52(3) | C27-H27b | 1.082(21) |
| C8-C11 | 1.55(3) | C27-H27c | 1.080(20) |
| C9-H9a | 1.079(20) | C28-H28a | 1.086(20) |
| C9-H9b | 1.089(17) | C28-H28b | 1.071(21) |
| C9-H9c | 1.099(18) | C28-H28c | 1.088(19) |
| C10-H10a | 1.083(20) | C29-C30 | 1.52(3) |
| C10-H10b | 1.077(19) | C29-C34 | 1.55(3) |
| C10-H10c | 1.089(20) | C29-H29 | 1.085(19) |
| C11-H11a | 1.092(19) | C30-C31 | 1.56(3) |
| C11-H11b | 1.083(17) | C30-H30a | 1.077(19) |
| C11-H11c | 1.097(20) | C30-H30b | 1.112(21) |
| C12-C13 | 1.51(3) | C31-C32 | 1.52(3) |
| C12-C17 | 1.555(24) | C31-H31a | 1.107(23) |
| C12-H12 | 1.116(18) | C31-H31b | 1.081(23) |
| C13-C14 | 1.54(3) | C32-C33 | 1.49(3) |
| C13-H13a | 1.093(17) | C32-H32a | 1.113(24) |
| C13-H13b | 1.061(19) | C32-H32b | 1.065(21) |
| C14-C15 | 1.53(3) | C33-C34 | 1.55(3) |
| C14-H14a | 1.093(20) | C33-H33a | 1.096(23) |
| C14-H14b | 1.094(20) | C33-H33b | 1.073(20) |
| C15-C16 | 1.48(3) | C34-H34a | 1.117(21) |

C15-H15a 1.089(21) C34-H34b 1.086(19)

Table of Atomic Bond Anglesin Degrees

| | | | |
|---|---|---|---|
| Se1-Ge1-N1 | 120.0(5) | C17-C16-H16b | 108.7(17) |
| Se1-Ge1-N3 | 122.3(4) | H16a-C16-H16b | 107.9(16) |
| Se1-Ge1-N4 | 121.4(4) | C12-C17-C16 | 111.9(14) |
| N1-Ge1-N3 | 106.4(6) | C12-C17-H17a | 108.3(15) |
| N1-Ge1-N4 | 108.9(6) | C12-C17-H17b | 108.2(15) |
| N3-Ge1-N4 | 65.6(6) | C16-C17-H17a | 109.5(16) |
| Ge1-N1-C1 | 116.3(11) | C16-C17-H17b | 111.0(16) |
| Ge1-N1-C7 | 119.8(11) | H17a-C17-H17b | 107.9(14) |
| C1-N1-C7 | 123.9(13) | N3-C18-C19 | 111.3(14) |
| C7-N2-C12 | 123.4(15) | N3-C18-C23 | 111.6(15) |
| Ge1-N3-C18 | 132.0(12) | N3-C18-H18 | 107.4(15) |
| Ge1-N3-C24 | 92.4(11) | C19-C18-C23 | 112.4(16) |
| C18-N3-C24 | 135.0(16) | C19-C18-H18 | 106.7(15) |
| Ge1-N4-C24 | 91.7(11) | C23-C18-H18 | 107.0(14) |
| Ge1-N4-C29 | 128.8(12) | C18-C19-C20 | 109.3(15) |
| C24-N4-C29 | 131.3(15) | C18-C19-H19a | 110.8(16) |
| N1-C1-C2 | 112.2(15) | C18-C19-H19b | 108.7(16) |
| N1-C1-C6 | 116.3(15) | C20-C19-H19a | 110.5(16) |
| N1-C1-H1 | 104.8(14) | C20-C19-H19b | 109.1(16) |
| C2-C1-C6 | 112.9(15) | H19a-C19-H19b | 108.5(15) |
| C2-C1-H1 | 104.8(15) | C19-C20-C21 | 110.4(16) |
| C6-C1-H1 | 104.4(16) | C19-C20-H20a | 108.7(17) |
| C1-C2-C3 | 109.9(16) | C19-C20-H20b | 108.4(16) |
| C1-C2-H2a | 110.5(16) | C21-C20-H20a | 110.4(16) |
| C1-C2-H2b | 109.5(15) | C21-C20-H20b | 111.0(17) |
| C3-C2-H2a | 110.8(16) | H20a-C20-H20b | 107.9(17) |
| C3-C2-H2b | 110.9(16) | C20-C21-C22 | 112.6(16) |
| H2a-C2-H2b | 105.3(17) | C20-C21-H21a | 108.9(15) |
| C2-C3-C4 | 115.3(16) | C20-C21-H21b | 109.3(16) |
| C2-C3-H3a | 108.6(18) | C22-C21-H21a | 108.3(16) |
| C2-C3-H3b | 106.9(16) | C22-C21-H21b | 110.6(15) |
| C4-C3-H3a | 110.6(17) | H21a-C21-H21b | 106.9(17) |
| C4-C3-H3b | 109.0(18) | C21-C22-C23 | 109.8(15) |
| H3a-C3-H3b | 106.0(16) | C21-C22-H22a | 109.7(16) |
| C3-C4-C5 | 111.5(16) | C21-C22-H22b | 112.2(17) |
| C3-C4-H4a | 109.4(16) | C23-C22-H22a | 108.2(16) |
| C3-C4-H4b | 109.1(17) | C23-C22-H22b | 110.7(16) |
| C5-C4-H4a | 109.0(16) | H22a-C22-H22b | 106.1(15) |
| C5-C4-H4b | 110.2(15) | C18-C23-C22 | 111.2(16) |
| H4a-C4-H4b | 107.6(16) | C18-C23-H23a | 110.3(16) |
| C4-C5-C6 | 111.2(16) | C18-C23-H23b | 107.5(14) |
| C4-C5-H5a | 111.0(16) | C22-C23-H23a | 112.2(15) |
| C4-C5-H5b | 110.1(15) | C22-C23-H23b | 108.2(16) |
| C6-C5-H5a | 109.1(16) | H23a-C23-H23b | 107.3(16) |
| C6-C5-H5b | 107.1(16) | N3-C24-N4 | 109.9(16) |
| H5a-C5-H5b | 108.3(18) | N3-C24-C25 | 124.3(16) |
| C1-C6-C5 | 111.7(15) | N4-C24-C25 | 125.4(16) |
| C1-C6-H6a | 108.4(16) | C24-C25-C26 | 108.7(15) |
| C1-C6-H6b | 110.4(15) | C24-C25-C27 | 106.6(16) |
| C5-C6-H6a | 109.0(15) | C24-C25-C28 | 117.8(15) |
| C5-C6-H6b | 110.4(16) | C26-C25-C27 | 111.1(15) |

| | | | |
|---|---|---|---|
| H6a-C6-H6b | 106.8(15) | C26-C25-C28 | 105.4(17) |
| N1-C7-N2 | 128.8(15) | C27-C25-C28 | 107.3(15) |
| N1-C7-C8 | 117.7(15) | C25-C26-H26a | 111.1(15) |
| N2-C7-C8 | 113.4(16) | C25-C26-H26b | 111.0(15) |
| C7-C8-C9 | 113.7(14) | C25-C26-H26c | 109.8(17) |
| C7-C8-C10 | 107.7(15) | H26a-C26-H26b | 109.8(18) |
| C7-C8-C11 | 108.1(14) | H26a-C26-H26c | 107.6(16) |
| C9-C8-C10 | 108.7(15) | H26b-C26-H26c | 107.4(15) |
| C9-C8-C11 | 111.0(15) | C25-C27-H27a | 109.9(15) |
| C10-C8-C11 | 107.3(15) | C25-C27-H27b | 111.0(18) |
| C8-C9-H9a | 111.8(16) | C25-C27-H27c | 111.9(15) |
| C8-C9-H9b | 110.3(15) | H27a-C27-H27b | 107.2(15) |
| C8-C9-H9c | 110.2(15) | H27a-C27-H27c | 107.4(19) |
| H9a-C9-H9b | 108.9(16) | H27b-C27-H27c | 109.3(16) |
| H9a-C9-H9c | 108.2(16) | C25-C28-H28a | 110.0(18) |
| H9b-C9-H9c | 107.5(16) | C25-C28-H28b | 110.1(16) |
| C8-C10-H10a | 110.2(16) | C25-C28-H28c | 109.1(16) |
| C8-C10-H10b | 110.0(17) | H28a-C28-H28b | 109.7(17) |
| C8-C10-H10c | 109.5(16) | H28a-C28-H28c | 108.4(16) |
| H10a-C10-H10b | 109.5(17) | H28b-C28-H28c | 109.6(19) |
| H10a-C10-H10c | 108.6(17) | N4-C29-C30 | 111.4(14) |
| H10b-C10-H10c | 109.0(17) | N4-C29-C34 | 111.2(14) |
| C8-C11-H11a | 110.8(15) | N4-C29-H29 | 109.7(15) |
| C8-C11-H11b | 111.1(15) | C30-C29-C34 | 109.8(15) |
| C8-C11-H11c | 111.1(15) | C30-C29-H29 | 107.8(15) |
| H11a-C11-H11b | 108.3(16) | C34-C29-H29 | 106.7(15) |
| H11a-C11-H11c | 107.3(16) | C29-C30-C31 | 110.0(16) |
| H11b-C11-H11c | 108.0(16) | C29-C30-H30a | 110.3(16) |
| N2-C12-C13 | 107.0(14) | C29-C30-H30b | 108.3(16) |
| N2-C12-C17 | 109.6(13) | C31-C30-H30a | 111.6(16) |
| N2-C12-H12 | 109.9(15) | C31-C30-H30b | 109.1(16) |
| C13-C12-C17 | 110.4(15) | H30a-C30-H30b | 107.3(16) |
| C13-C12-H12 | 111.1(14) | C30-C31-C32 | 110.5(17) |
| C17-C12-H12 | 108.8(15) | C30-C31-H31a | 110.0(17) |
| C12-C13-C14 | 110.3(15) | C30-C31-H31b | 109.8(18) |
| C12-C13-H13a | 109.2(16) | C32-C31-H31a | 109.5(18) |
| C12-C13-H13b | 109.5(15) | C32-C31-H31b | 109.5(18) |
| C14-C13-H13a | 108.6(15) | H31a-C31-H31b | 107.5(19) |
| C14-C13-H13b | 109.3(16) | C31-C32-C33 | 111.7(18) |
| H13a-C13-H13b | 109.9(16) | C31-C32-H32a | 108.1(18) |
| C13-C14-C15 | 111.5(15) | C31-C32-H32b | 111.6(19) |
| C13-C14-H14a | 109.4(16) | C33-C32-H32a | 106.9(18) |
| C13-C14-H14b | 108.7(16) | C33-C32-H32b | 110.2(18) |
| C15-C14-H14a | 109.5(16) | H32a-C32-H32b | 108.2(19) |
| C15-C14-H14b | 110.2(16) | C32-C33-C34 | 111.1(17) |
| H14a-C14-H14b | 107.6(16) | C32-C33-H33a | 107.9(18) |
| C14-C15-C16 | 111.2(16) | C32-C33-H33b | 111.1(18) |
| C14-C15-H15a | 109.5(17) | C34-C33-H33a | 107.1(17) |
| C14-C15-H15b | 109.7(16) | C34-C33-H33b | 110.7(17) |
| C16-C15-H15a | 109.6(16) | H33a-C33-H33b | 108.8(18) |
| C16-C15-H15b | 109.3(17) | C29-C34-C33 | 111.2(15) |
| H15a-C15-H15b | 107.5(17) | C29-C34-H34a | 108.5(16) |
| C15-C16-C17 | 113.3(16) | C29-C34-H34b | 110.7(16) |
| C15-C16-H16a | 109.7(17) | C33-C34-H34a | 108.5(16) |

| | | | |
|---|---|---|---|
| C15-C16-H16b | 109.4(16) | C33-C34-H34b | 111.4(16) |
| C17-C16-H16a | 107.7(15) | H34a-C34-H34b | 106.3(16) |

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Space Group and Cell Dimensions Monoclinic, P 21/a
a 8.8803(1) b 16.5932(2) c 18.2614(3)
beta 97.186(1)
Volume 2669.73(6)A**3

Empirical formula : Ge Se Si2 N3 C20 H43

Cell dimensions were obtained from 8192 reflections with 2Theta angle in the range 3.00 - 57.00 degrees.

Crystal dimensions : 0.20 X 0.20 X 0.20 mm

FW = 533.29 Z = 4 F(000) = 1113.73

Dcalc 1.327Mg.m-3, mu 2.61mm-1, lambda 0.70930A, 2Theta(max) 57.0

The intensity data were collected on a Siemens SMART diffractometer, using the omega scan mode (0.3 deg scans).
The h,k,l ranges used during structure solution and refinement are :--
Hmin,max -11 11; Kmin,max 0 22; Lmin,max 0 24
No. of reflections measured 18456
No. of unique reflections 6781
No. of reflections with Inet > 2.5sigma(Inet) 5253
Merging R-value on intensities 0.021
An empirical absorption correction was applied

The last least squares cycle was calculated with 70 atoms, 417 parameters and 5253 out of 6781 reflections.
Weights based on statistics were used.

The residuals are as follows :--
For significant reflections, RF 0.027, Rw 0.024 GoF 1.53
For all reflections, RF 0.041, Rw 0.025.
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 0.432.

In the last D-map, the deepest hole was -0.340e/A**3, and the highest peak 0.580e/A**3.

Secondary ext. coeff. 13.5176microns sigma 2.8916

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.

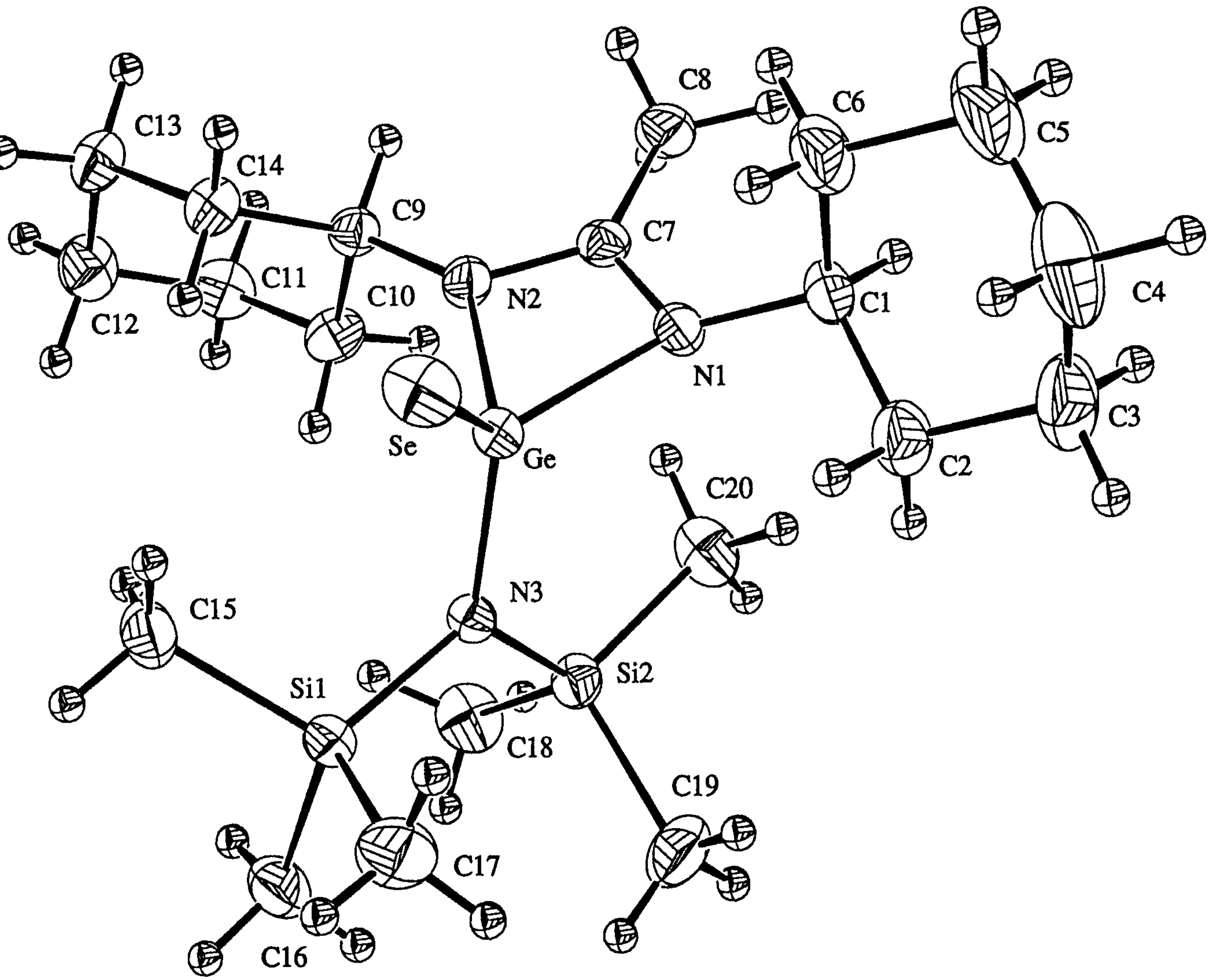
3. ORTEP Plotting :
Johnson, C.K., (1976) ORTEP - A Fortran Thermal Ellipsoid Plot Program, Technical Report ORNL-5138, Oak Ridge

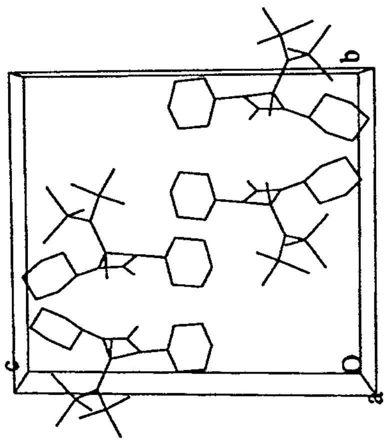
4. Pluto Plotting :
S. Motherwell, University Chemical Laboratory, Cambridge, 1978

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.

7. Extinction Treatment :
Larson, A.C., (1970) p.293, Crystallographic Computing, Munksgaard, Copenhagen.


C13
C14
C9
C12
C11
C10
N2
C8
C7
C6
C5
C4
C1
N1
Se
Ge
C3
C2
C20
N3
C15
Si1
Si2
C18
C19
C17
C16


b
c
a

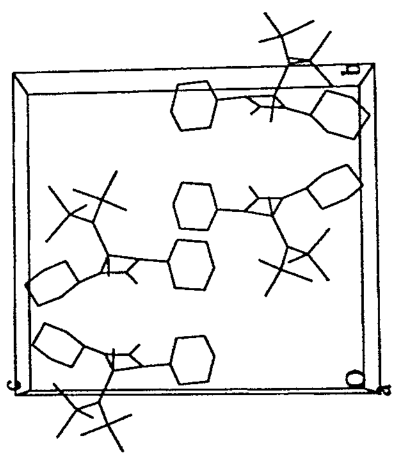

b
c
a

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

| | x | y | z | Biso |
|---|---|---|---|---|
| Ge | 0.159687(21) | 0.567642(12) | 0.262774(11) | 1.564( 7) |
| Se | -0.050239(23) | 0.637548(13) | 0.269207(12) | 2.617( 8) |
| Si1 | -0.01570 ( 6) | 0.44566 ( 3) | 0.15997 ( 3) | 1.930(21) |
| Si2 | 0.28388 ( 6) | 0.38939 ( 3) | 0.24366 ( 3) | 1.988(22) |
| N1 | 0.31524 (17) | 0.57940 ( 9) | 0.34702 ( 8) | 1.82 ( 6) |
| N2 | 0.34384 (17) | 0.61984 ( 9) | 0.23733 ( 8) | 1.82 ( 6) |
| N3 | 0.15085 (16) | 0.46643 ( 9) | 0.22116 ( 8) | 1.57 ( 6) |
| C1 | 0.31599 (23) | 0.58740 (12) | 0.42699 (11) | 2.25 ( 8) |
| C2 | 0.21923 (23) | 0.52173 (14) | 0.45524 (12) | 2.87 (10) |
| C3 | 0.2153 ( 3) | 0.53007 (17) | 0.53833 (13) | 3.94 (12) |
| C4 | 0.1591 ( 3) | 0.61197 (20) | 0.55798 (14) | 5.42 (15) |
| C5 | 0.2553 ( 3) | 0.67855 (17) | 0.53030 (14) | 5.12 (14) |
| C6 | 0.2614 ( 3) | 0.67091 (15) | 0.44724 (12) | 3.54 (11) |
| C7 | 0.40811 (21) | 0.61791 (11) | 0.30656 (11) | 1.81 ( 8) |
| C8 | 0.56122 (22) | 0.65030 (12) | 0.33463 (12) | 2.54 ( 8) |
| C9 | 0.41031 (20) | 0.64791 (11) | 0.17242 (10) | 1.79 ( 7) |
| C10 | 0.47174 (22) | 0.57780 (12) | 0.13117 (12) | 2.43 ( 9) |
| C11 | 0.53379 (23) | 0.60611 (13) | 0.06129 (12) | 2.73 ( 9) |
| C12 | 0.41461 (25) | 0.65298 (14) | 0.01149 (12) | 2.91 (10) |
| C13 | 0.35295 (24) | 0.72309 (12) | 0.05231 (11) | 2.53 ( 8) |
| C14 | 0.29142 (21) | 0.69511 (12) | 0.12232 (11) | 2.11 ( 8) |
| C15 | -0.06111 (24) | 0.52944 (13) | 0.09313 (12) | 2.74 ( 9) |
| C16 | 0.0104 ( 3) | 0.35602 (13) | 0.10061 (12) | 3.06 ( 9) |
| C17 | -0.17735 (24) | 0.42311 (15) | 0.21143 (13) | 3.39 (10) |
| C18 | 0.3672 ( 3) | 0.35202 (14) | 0.16046 (13) | 3.17 (10) |
| C19 | 0.1906 ( 3) | 0.30508 (14) | 0.28819 (13) | 3.45 (11) |
| C20 | 0.45339 (24) | 0.41876 (13) | 0.30893 (13) | 3.05 ( 9) |
| H1 | 0.4274 (19) | 0.5811 (11) | 0.4519 (10) | 2.1 ( 4) |
| H2a | 0.1201 (22) | 0.5274 (13) | 0.4283 (11) | 3.6 ( 5) |
| H2b | 0.2581 (21) | 0.4671 (12) | 0.4438 (10) | 2.9 ( 5) |
| H3a | 0.1552 (24) | 0.4902 (13) | 0.5527 (12) | 4.5 ( 5) |
| H3b | 0.3251 (23) | 0.5219 (13) | 0.5651 (12) | 4.4 ( 5) |
| H4a | 0.170 ( 3) | 0.6159 (14) | 0.6115 (13) | 5.4 ( 6) |
| H4b | 0.052 ( 3) | 0.6218 (15) | 0.5320 (14) | 6.6 ( 7) |
| H5a | 0.218 ( 3) | 0.7279 (14) | 0.5399 (13) | 5.4 ( 6) |
| H5b | 0.3642 (24) | 0.6735 (14) | 0.5557 (12) | 4.6 ( 6) |
| H6a | 0.3260 (22) | 0.7112 (12) | 0.4286 (11) | 3.5 ( 5) |
| H6b | 0.1607 (23) | 0.6777 (13) | 0.4232 (11) | 4.0 ( 5) |
| H8a | 0.5639 (22) | 0.7040 (12) | 0.3238 (11) | 3.5 ( 5) |
| H8b | 0.6338 (22) | 0.6257 (12) | 0.3134 (11) | 3.7 ( 5) |
| H8c | 0.586 ( 3) | 0.6497 (14) | 0.3916 (13) | 5.6 ( 6) |
| H9 | 0.4953 (18) | 0.6841 (11) | 0.1895 ( 9) | 1.7 ( 4) |
| H10a | 0.3926 (21) | 0.5397 (11) | 0.1194 (10) | 2.5 ( 4) |
| H10b | 0.5506 (22) | 0.5511 (12) | 0.1658 (11) | 3.4 ( 5) |
| H11a | 0.6215 (22) | 0.6400 (12) | 0.0765 (11) | 3.3 ( 5) |
| H11b | 0.5703 (22) | 0.5602 (12) | 0.0352 (11) | 3.3 ( 5) |
| H12a | 0.4561 (22) | 0.6709 (13) | -0.0309 (11) | 3.9 ( 5) |
| H12b | 0.3301 (22) | 0.6142 (13) | -0.0059 (11) | 3.7 ( 5) |
| H13a | 0.4362 (20) | 0.7612 (11) | 0.0675 (10) | 2.6 ( 4) |
| H13b | 0.2706 (20) | 0.7505 (11) | 0.0188 (10) | 2.5 ( 4) |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| H14a | 0.2027 | (19) | 0.6604 | (11) | 0.1103 | (10) | 1.9 | ( 4) |
| H14b | 0.2535 | (21) | 0.7408 | (12) | 0.1479 | (11) | 2.9 | ( 5) |
| H15a | -0.0925 | (23) | 0.5757 | (12) | 0.1143 | (12) | 3.9 | ( 5) |
| H15b | -0.1408 | (22) | 0.5143 | (12) | 0.0570 | (11) | 3.5 | ( 5) |
| H15c | 0.0229 | (23) | 0.5401 | (13) | 0.0695 | (12) | 4.2 | ( 5) |
| H16a | 0.0395 | (21) | 0.3077 | (12) | 0.1267 | (11) | 3.1 | ( 5) |
| H16b | 0.0814 | (24) | 0.3661 | (13) | 0.0653 | (12) | 4.4 | ( 6) |
| H16c | -0.0881 | (24) | 0.3450 | (13) | 0.0706 | (12) | 4.7 | ( 6) |
| H17a | -0.2579 | (23) | 0.4150 | (13) | 0.1814 | (12) | 4.0 | ( 5) |
| H17b | -0.1600 | (25) | 0.3764 | (14) | 0.2428 | (12) | 4.9 | ( 6) |
| H17c | -0.1909 | (22) | 0.4669 | (13) | 0.2436 | (11) | 3.6 | ( 5) |
| H18a | 0.3221 | (24) | 0.3085 | (13) | 0.1395 | (12) | 4.5 | ( 5) |
| H18b | 0.350 | ( 3) | 0.3897 | (16) | 0.1161 | (15) | 7.8 | ( 8) |
| H18c | 0.472 | ( 3) | 0.3357 | (15) | 0.1758 | (13) | 5.6 | ( 6) |
| H19a | 0.1566 | (21) | 0.3228 | (12) | 0.3283 | (11) | 3.4 | ( 5) |
| H19b | 0.096 | ( 3) | 0.2843 | (15) | 0.2605 | (14) | 6.5 | ( 7) |
| H19c | 0.261 | ( 3) | 0.2619 | (14) | 0.3016 | (13) | 5.5 | ( 6) |
| H20a | 0.5138 | (24) | 0.3730 | (13) | 0.3149 | (12) | 4.3 | ( 5) |
| H20b | 0.4254 | (23) | 0.4337 | (12) | 0.3568 | (12) | 3.7 | ( 5) |
| H20c | 0.5172 | (22) | 0.4640 | (12) | 0.2912 | (11) | 3.5 | ( 5) |

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 |
|---|---|---|---|---|---|---|
| Ge | 1.885( 9) | 2.039(10) | 2.026(10) | 0.025( 8) | 0.272( 7) | -0.139( 8) |
| Se | 2.473(10) | 3.236(12) | 4.243(13) | 0.759( 9) | 0.448( 9) | -0.796(10) |
| Si1 | 2.29 ( 3) | 2.42 ( 3) | 2.50 ( 3) | -0.289(23) | -0.181(22) | 0.010(22) |
| Si2 | 2.75 ( 3) | 2.24 ( 3) | 2.53 ( 3) | 0.495(23) | 0.176(23) | 0.002(22) |
| N1 | 2.32 ( 8) | 2.52 ( 9) | 2.03 ( 9) | -0.21 ( 7) | 0.13 ( 7) | -0.14 ( 7) |
| N2 | 2.05 ( 8) | 2.58 ( 9) | 2.29 ( 9) | -0.35 ( 7) | 0.23 ( 7) | 0.33 ( 7) |
| N3 | 1.87 ( 8) | 1.98 ( 8) | 2.11 ( 9) | 0.04 ( 6) | 0.18 ( 6) | -0.12 ( 6) |
| C1 | 3.20 (11) | 3.35 (12) | 1.91 (11) | 0.13 ( 9) | -0.11 ( 9) | -0.14 ( 8) |
| C2 | 3.45 (12) | 4.68 (14) | 2.79 (12) | -0.35 (10) | 0.50 (10) | 0.18 (10) |
| C3 | 4.85 (15) | 7.43 (19) | 2.79 (14) | -0.64 (14) | 0.87 (11) | 0.76 (12) |
| C4 | 7.74 (21) | 10.4 ( 3) | 2.58 (15) | 1.67 (18) | 1.25 (14) | -1.14 (14) |
| C5 | 9.91 (23) | 6.49 (19) | 2.88 (15) | 2.07 (17) | 0.16 (14) | -1.91 (12) |
| C6 | 6.44 (16) | 4.25 (14) | 2.63 (13) | 0.90 (12) | 0.07 (11) | -0.84 (10) |
| C7 | 2.30 (10) | 1.73 (10) | 2.78 (11) | 0.21 ( 8) | 0.03 ( 8) | -0.13 ( 8) |
| C8 | 2.59 (11) | 3.10 (12) | 3.76 (13) | -0.62 ( 9) | -0.38 ( 9) | 0.21 ( 9) |
| C9 | 2.03 (10) | 2.34 (10) | 2.45 (11) | -0.31 ( 8) | 0.40 ( 8) | 0.18 ( 8) |
| C10 | 2.93 (11) | 2.63 (11) | 3.75 (13) | 0.44 ( 9) | 0.73 ( 9) | 0.16 ( 9) |
| C11 | 3.15 (12) | 3.74 (13) | 3.66 (13) | 0.29 (10) | 1.16 (10) | -0.64 (10) |
| C12 | 4.09 (13) | 4.40 (14) | 2.73 (12) | -0.01 (11) | 1.10 (10) | -0.09 (10) |
| C13 | 3.75 (12) | 3.11 (12) | 2.82 (12) | 0.22 (10) | 0.69 ( 9) | 0.71 ( 9) |
| C14 | 2.63 (10) | 2.63 (11) | 2.84 (12) | 0.36 ( 9) | 0.69 ( 9) | 0.26 ( 8) |
| C15 | 3.70 (12) | 3.54 (13) | 2.92 (12) | 0.36 (10) | -0.55 (10) | -0.10 ( 9) |
| C16 | 4.44 (13) | 3.11 (12) | 3.74 (14) | -0.03 (10) | -0.81 (11) | -0.64 (10) |
| C17 | 2.84 (12) | 4.79 (15) | 5.21 (16) | -0.99 (11) | 0.31 (11) | 0.35 (11) |
| C18 | 4.06 (13) | 3.90 (14) | 4.20 (14) | 1.18 (11) | 0.90 (11) | -0.98 (10) |
| C19 | 5.89 (16) | 3.14 (13) | 4.14 (15) | 0.40 (11) | 0.84 (12) | 1.17 (10) |
| C20 | 3.32 (12) | 3.83 (14) | 4.16 (14) | 1.42 (10) | -0.54 (10) | -0.68 (10) |

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

| | | | |
|---|---|---|---|
| Ge-Se | 2.2112(3) | C8-H8c | 1.036(24) |
| Ge-N1 | 1.9446(15) | C9-C10 | 1.524(3) |
| Ge-N2 | 1.9572(15) | C9-C14 | 1.524(3) |
| Ge-N3 | 1.8410(15) | C9-H9 | 0.984(17) |
| Si1-N3 | 1.7723(15) | C10-C11 | 1.526(3) |
| Si1-C15 | 1.8606(22) | C10-H10a | 0.949(19) |
| Si1-C16 | 1.8720(22) | C10-H10b | 0.988(20) |
| Si1-C17 | 1.8497(23) | C11-C12 | 1.520(3) |
| Si2-N3 | 1.7542(15) | C11-H11a | 0.972(20) |
| Si2-C18 | 1.8764(22) | C11-H11b | 0.975(20) |
| Si2-C19 | 1.8636(23) | C12-C13 | 1.520(3) |
| Si2-C20 | 1.8642(22) | C12-H12a | 0.946(21) |
| N1-C1 | 1.4656(25) | C12-H12b | 1.010(21) |
| N1-C7 | 1.3367(24) | C13-C14 | 1.524(3) |
| N2-C7 | 1.3209(24) | C13-H13a | 0.987(18) |
| N2-C9 | 1.4648(24) | C13-H13b | 1.002(18) |
| C1-C2 | 1.517(3) | C14-H14a | 0.979(17) |
| C1-C6 | 1.529(3) | C14-H14b | 0.972(19) |
| C1-H1 | 1.041(17) | C15-H15a | 0.918(21) |
| C2-C3 | 1.528(3) | C15-H15b | 0.939(19) |
| C2-H2a | 0.958(20) | C15-H15c | 0.924(22) |
| C2-H2b | 1.001(20) | C16-H16a | 0.951(20) |
| C3-C4 | 1.507(4) | C16-H16b | 0.971(22) |
| C3-H3a | 0.910(22) | C16-H16c | 0.990(21) |
| C3-H3b | 1.043(21) | C17-H17a | 0.856(21) |
| C4-C5 | 1.521(5) | C17-H17b | 0.964(23) |
| C4-H4a | 0.973(24) | C17-H17c | 0.952(21) |
| C4-H4b | 1.022(24) | C18-H18a | 0.889(22) |
| C5-C6 | 1.530(3) | C18-H18b | 1.02(3) |
| C5-H5a | 0.908(24) | C18-H18c | 0.973(23) |
| C5-H5b | 1.022(21) | C19-H19a | 0.877(20) |
| C6-H6a | 0.970(20) | C19-H19b | 0.987(24) |
| C6-H6b | 0.952(20) | C19-H19c | 0.963(23) |
| C7-C8 | 1.492(3) | C20-H20a | 0.929(21) |
| C8-H8a | 0.914(21) | C20-H20b | 0.970(21) |
| C8-H8b | 0.892(20) | C20-H20c | 1.018(20) |

Table of Atomic Bond Angles in Degrees

| | | | |
|---|---|---|---|
| Se-Ge-N1 | 115.18(5) | N2-C9-C10 | 111.26(15) |
| Se-Ge-N2 | 121.03(5) | N2-C9-C14 | 109.28(15) |
| Se-Ge-N3 | 120.52(5) | N2-C9-H9 | 108.0(10) |
| N1-Ge-N2 | 67.14(6) | C10-C9-C14 | 111.07(16) |
| N1-Ge-N3 | 114.05(6) | C10-C9-H9 | 108.3(10) |
| N2-Ge-N3 | 107.42(6) | C14-C9-H9 | 108.8(10) |
| N3-Si1-C15 | 111.32(9) | C9-C10-C11 | 111.55(16) |
| N3-Si1-C16 | 111.43(9) | C9-C10-H10a | 108.6(11) |
| N3-Si1-C17 | 111.01(9) | C9-C10-H10b | 107.2(12) |
| C15-Si1-C16 | 104.25(10) | C11-C10-H10a | 110.5(11) |
| C15-Si1-C17 | 111.48(10) | C11-C10-H10b | 111.9(12) |
| C16-Si1-C17 | 107.08(11) | H10a-C10-H10b | 107.0(16) |
| N3-Si2-C18 | 111.92(9) | C10-C11-C12 | 111.13(17) |
| N3-Si2-C19 | 109.04(9) | C10-C11-H11a | 107.4(12) |
| N3-Si2-C20 | 115.18(9) | C10-C11-H11b | 110.1(12) |
| C18-Si2-C19 | 110.31(11) | C12-C11-H11a | 110.3(12) |
| C18-Si2-C20 | 103.62(10) | C12-C11-H11b | 110.9(12) |
| C19-Si2-C20 | 106.54(11) | H11a-C11-H11b | 106.7(16) |
| Ge-N1-C1 | 135.37(12) | C11-C12-C13 | 111.39(17) |
| Ge-N1-C7 | 92.12(11) | C11-C12-H12a | 109.7(12) |
| C1-N1-C7 | 125.54(15) | C11-C12-H12b | 107.3(12) |
| Ge-N2-C7 | 92.06(11) | C13-C12-H12a | 111.3(13) |
| Ge-N2-C9 | 140.01(12) | C13-C12-H12b | 110.1(12) |
| C7-N2-C9 | 127.78(15) | H12a-C12-H12b | 107.0(17) |
| Ge-N3-Si1 | 115.26(8) | C12-C13-C14 | 111.54(17) |
| Ge-N3-Si2 | 125.13(8) | C12-C13-H13a | 109.0(11) |
| Si1-N3-Si2 | 119.37(9) | C12-C13-H13b | 109.1(11) |
| N1-C1-C2 | 109.97(16) | C14-C13-H13a | 107.1(11) |
| N1-C1-C6 | 111.16(16) | C14-C13-H13b | 109.8(11) |
| N1-C1-H1 | 108.1(10) | H13a-C13-H13b | 110.2(15) |
| C2-C1-C6 | 111.02(18) | C9-C14-C13 | 111.46(16) |
| C2-C1-H1 | 109.1(10) | C9-C14-H14a | 108.1(10) |
| C6-C1-H1 | 107.3(10) | C9-C14-H14b | 111.6(11) |
| C1-C2-C3 | 110.89(18) | C13-C14-H14a | 110.7(10) |
| C1-C2-H2a | 106.2(13) | C13-C14-H14b | 110.3(11) |
| C1-C2-H2b | 110.8(11) | H14a-C14-H14b | 104.4(15) |
| C3-C2-H2a | 111.5(12) | Si1-C15-H15a | 113.6(13) |
| C3-C2-H2b | 109.9(11) | Si1-C15-H15b | 110.1(13) |
| H2a-C2-H2b | 107.5(17) | Si1-C15-H15c | 109.2(13) |
| C2-C3-C4 | 111.57(21) | H15a-C15-H15b | 106.1(18) |
| C2-C3-H3a | 108.0(14) | H15a-C15-H15c | 109.9(19) |
| C2-C3-H3b | 108.5(12) | H15b-C15-H15c | 107.8(18) |
| C4-C3-H3a | 111.3(14) | Si1-C16-H16a | 115.2(12) |
| C4-C3-H3b | 108.9(12) | Si1-C16-H16b | 112.7(13) |
| H3a-C3-H3b | 108.6(18) | Si1-C16-H16c | 107.6(13) |
| C3-C4-C5 | 111.05(22) | H16a-C16-H16b | 108.6(17) |
| C3-C4-H4a | 107.8(14) | H16a-C16-H16c | 106.7(17) |
| C3-C4-H4b | 110.6(14) | H16b-C16-H16c | 105.4(18) |
| C5-C4-H4a | 107.1(14) | Si1-C17-H17a | 110.2(14) |
| C5-C4-H4b | 105.0(14) | Si1-C17-H17b | 112.8(13) |
| H4a-C4-H4b | 115.3(19) | Si1-C17-H17c | 109.0(12) |

| | | | |
|---|---|---|---|
| C4-C5-C6 | 111.13(21) | H17a-C17-H17b | 108.3(20) |
| C4-C5-H5a | 111.1(15) | H17a-C17-H17c | 110.9(19) |
| C4-C5-H5b | 109.2(13) | H17b-C17-H17c | 105.7(18) |
| C6-C5-H5a | 108.9(15) | Si2-C18-H18a | 114.6(14) |
| C6-C5-H5b | 107.1(13) | Si2-C18-H18b | 114.0(15) |
| H5a-C5-H5b | 109.3(19) | Si2-C18-H18c | 108.5(14) |
| C1-C6-C5 | 111.51(20) | H18a-C18-H18b | 98.3(21) |
| C1-C6-H6a | 108.7(12) | H18a-C18-H18c | 105.0(20) |
| C1-C6-H6b | 107.6(13) | H18b-C18-H18c | 116.0(21) |
| C5-C6-H6a | 112.8(12) | Si2-C19-H19a | 109.4(13) |
| C5-C6-H6b | 107.4(13) | Si2-C19-H19b | 115.8(15) |
| H6a-C6-H6b | 108.6(17) | Si2-C19-H19c | 111.2(14) |
| N1-C7-N2 | 108.54(16) | H19a-C19-H19b | 100.6(19) |
| N1-C7-C8 | 125.52(17) | H19a-C19-H19c | 108.5(19) |
| N2-C7-C8 | 125.89(17) | H19b-C19-H19c | 110.7(20) |
| C7-C8-H8a | 108.9(12) | Si2-C20-H20a | 105.7(13) |
| C7-C8-H8b | 111.3(13) | Si2-C20-H20b | 111.4(12) |
| C7-C8-H8c | 114.2(13) | Si2-C20-H20c | 115.2(11) |
| H8a-C8-H8b | 108.2(18) | H20a-C20-H20b | 108.2(18) |
| H8a-C8-H8c | 102.6(18) | H20a-C20-H20c | 107.7(18) |
| H8b-C8-H8c | 111.0(18) | H20b-C20-H20c | 108.3(17) |

Torsion angles

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Se | Ge | N1 | C1 | 37.48(14) | Se | Ge | N1 | C7 | -112.45(20) |
| N2 | Ge | N1 | C1 | 152.31(22) | N2 | Ge | N1 | C7 | 2.38(15) |
| N3 | Ge | N1 | C1 | -108.03(21) | N3 | Ge | N1 | C7 | 102.04(21) |
| Se | Ge | N2 | C7 | 104.16(19) | Se | Ge | N2 | C9 | -80.48(16) |
| N1 | Ge | N2 | C7 | -2.41(16) | N1 | Ge | N2 | C9 | 172.94(22) |
| N3 | Ge | N2 | C7 | -111.75(22) | N3 | Ge | N2 | C9 | 63.60(17) |
| Se | Ge | N3 | Si1 | 21.72( 4) | Se | Ge | N3 | Si2 | -152.54(14) |
| N1 | Ge | N3 | Si1 | 165.22(17) | N1 | Ge | N3 | Si2 | -9.04( 8) |
| N2 | Ge | N3 | Si1 | -122.59(15) | N2 | Ge | N3 | Si2 | 63.15(11) |
| C15 | Si1 | N3 | Ge | 47.30(13) | C15 | Si1 | N3 | Si2 | -138.09(19) |
| C16 | Si1 | N3 | Ge | 163.22(19) | C16 | Si1 | N3 | Si2 | -22.17(12) |
| C17 | Si1 | N3 | Ge | -77.52(16) | C17 | Si1 | N3 | Si2 | 97.09(18) |
| N3 | Si1 | C15 | H15a | -69.4(22) | N3 | Si1 | C15 | H15b | 171.8(20) |
| N3 | Si1 | C15 | H15c | 53.7(22) | C16 | Si1 | C15 | H15a | 170.4(22) |
| C16 | Si1 | C15 | H15b | 51.5(20) | C16 | Si1 | C15 | H15c | -66.5(22) |
| C17 | Si1 | C15 | H15a | 55.2(22) | C17 | Si1 | C15 | H15b | -63.7(20) |
| C17 | Si1 | C15 | H15c | 178.3(22) | N3 | Si1 | C16 | H16a | 56.9(19) |
| N3 | Si1 | C16 | H16b | -68.4(21) | N3 | Si1 | C16 | H16c | 175.8(21) |
| C15 | Si1 | C16 | H16a | 177.1(20) | C15 | Si1 | C16 | H16b | 51.7(21) |
| C15 | Si1 | C16 | H16c | -64.1(21) | C17 | Si1 | C16 | H16a | -64.7(19) |
| C17 | Si1 | C16 | H16b | 170.0(22) | C17 | Si1 | C16 | H16c | 54.2(21) |
| N3 | Si1 | C17 | H17a | 177.8(24) | N3 | Si1 | C17 | H17b | -61.1(22) |
| N3 | Si1 | C17 | H17c | 55.9(21) | C15 | Si1 | C17 | H17a | 53.1(24) |
| C15 | Si1 | C17 | H17b | 174.2(22) | C15 | Si1 | C17 | H17c | -68.8(21) |
| C16 | Si1 | C17 | H17a | -60.4(24) | C16 | Si1 | C17 | H17b | 60.7(22) |
| C16 | Si1 | C17 | H17c | 177.8(21) | C18 | Si2 | N3 | Ge | -123.62(18) |
| C18 | Si2 | N3 | Si1 | 62.34(15) | C19 | Si2 | N3 | Ge | 114.06(18) |
| C19 | Si2 | N3 | Si1 | -59.98(15) | C20 | Si2 | N3 | Ge | -5.60(11) |
| C20 | Si2 | N3 | Si1 | -179.65(20) | N3 | Si2 | C18 | H18a | -95.6(23) |
| N3 | Si2 | C18 | H18b | 17. ( 3) | N3 | Si2 | C18 | H18c | 147.5(23) |
| C19 | Si2 | C18 | H18a | 26.0(23) | C19 | Si2 | C18 | H18b | 138. ( 3) |
| C19 | Si2 | C18 | H18c | -91.0(23) | C20 | Si2 | C18 | H18a | 139.7(23) |
| C20 | Si2 | C18 | H18b | -108. ( 3) | C20 | Si2 | C18 | H18c | 22.7(23) |
| N3 | Si2 | C19 | H19a | -59.8(21) | N3 | Si2 | C19 | H19b | 53.0(24) |
| N3 | Si2 | C19 | H19c | -179.5(23) | C18 | Si2 | C19 | H19a | 176.9(22) |
| C18 | Si2 | C19 | H19b | -70.3(24) | C18 | Si2 | C19 | H19c | 57.2(23) |
| C20 | Si2 | C19 | H19a | 65.1(21) | C20 | Si2 | C19 | H19b | 177.9(24) |
| C20 | Si2 | C19 | H19c | -54.6(23) | N3 | Si2 | C20 | H20a | -178.9(22) |
| N3 | Si2 | C20 | H20b | 63.8(20) | N3 | Si2 | C20 | H20c | -60.1(19) |
| C18 | Si2 | C20 | H20a | -56.3(22) | C18 | Si2 | C20 | H20b | -173.6(21) |
| C18 | Si2 | C20 | H20c | 62.5(19) | C19 | Si2 | C20 | H20a | 60.1(22) |
| C19 | Si2 | C20 | H20b | -57.2(20) | C19 | Si2 | C20 | H20c | 178.9(19) |
| Ge | N1 | C1 | C2 | 50.21(18) | Ge | N1 | C1 | C6 | -73.15(22) |
| Ge | N1 | C1 | H1 | 169.3(16) | C7 | N1 | C1 | C2 | -167.8( 4) |
| C7 | N1 | C1 | C6 | 68.9( 3) | C7 | N1 | C1 | H1 | -48.7(16) |
| Ge | N1 | C7 | N2 | -3.43(12) | Ge | N1 | C7 | C8 | 178.8( 3) |
| C1 | N1 | C7 | N2 | -157.8( 4) | C1 | N1 | C7 | C8 | 24.41(20) |
| Ge | N2 | C7 | N1 | 3.41(12) | Ge | N2 | C7 | C8 | -178.8( 3) |
| C9 | N2 | C7 | N1 | -172.8( 4) | C9 | N2 | C7 | C8 | 4.96(18) |

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|---|---|---|---|---|
| Ge | N2 | C9 | C10 | -76.78(21) |
| Ge | N2 | C9 | H9 | 164.4(17) |
| C7 | N2 | C9 | C14 | -139.7( 4) |
| N1 | C1 | C2 | C3 | -178.7( 4) |
| N1 | C1 | C2 | H2b | 59.0(18) |
| C6 | C1 | C2 | H2a | 66.1(21) |
| H1 | C1 | C2 | C3 | 62.9(16) |
| H1 | C1 | C2 | H2b | -59.4(24) |
| N1 | C1 | C6 | H6a | -57.5(20) |
| C2 | C1 | C6 | C5 | 54.8( 3) |
| C2 | C1 | C6 | H6b | -62.8(21) |
| H1 | C1 | C6 | H6a | 61. ( 3) |
| C1 | C2 | C3 | C4 | 56.5( 3) |
| C1 | C2 | C3 | H3b | -63.4(20) |
| H2a | C2 | C3 | H3a | 61. ( 3) |
| H2b | C2 | C3 | C4 | 179.4(19) |
| H2b | C2 | C3 | H3b | 59. ( 3) |
| C2 | C3 | C4 | H4a | -173.5(24) |
| H3a | C3 | C4 | C5 | -177.1(24) |
| H3a | C3 | C4 | H4b | -61. ( 3) |
| H3b | C3 | C4 | H4a | -54. ( 3) |
| C3 | C4 | C5 | C6 | 55.4( 3) |
| C3 | C4 | C5 | H5b | -62.5(21) |
| H4a | C4 | C5 | H5a | -66. ( 3) |
| H4b | C4 | C5 | C6 | -64.1(23) |
| H4b | C4 | C5 | H5b | 178. ( 3) |
| C4 | C5 | C6 | H6a | -177.3(21) |
| H5a | C5 | C6 | C1 | -177. ( 3) |
| H5a | C5 | C6 | H6b | -60. ( 3) |
| H5b | C5 | C6 | H6a | -58. ( 3) |
| N1 | C7 | C8 | H8a | -124.1(21) |
| N1 | C7 | C8 | H8c | -10.0(22) |
| N2 | C7 | C8 | H8b | -60.7(22) |
| C7 | C8 | H8a | H8b | -121. ( 3) |
| H8b | C8 | H8a | H8b | 0. ( 3) |
| H8c | C8 | H8a | H8b | 117. ( 4) |
| C7 | C8 | H8b | H8a | 120. ( 3) |
| H8c | C8 | H8b | H8a | -112. ( 4) |
| H8a | C8 | H8c | H8a | 0. ( 3) |
| N2 | C9 | C10 | C11 | 177.1( 4) |
| N2 | C9 | C10 | H10b | -60.2(19) |
| C14 | C9 | C10 | H10a | -66.9(19) |
| H9 | C9 | C10 | C11 | -64.4(17) |
| H9 | C9 | C10 | H10b | 58. ( 3) |
| N2 | C9 | C14 | H14a | -56.0(17) |
| C10 | C9 | C14 | C13 | -54.71(24) |
| C10 | C9 | C14 | H14b | -178.5(19) |
| H9 | C9 | C14 | H14a | -173.6(24) |
| C9 | C10 | C11 | C12 | -55.38(25) |
| C9 | C10 | C11 | H11b | -178.7(20) |
| H10a | C10 | C11 | H11a | -174. ( 3) |
| H10b | C10 | C11 | C12 | -175.4(20) |
| H10b | C10 | C11 | H11b | 61. ( 3) |
| C11 | C10 | H10a | H10b | 122.0(24) |

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|---|---|---|---|---|
| Ge | N2 | C9 | C14 | 46.23(16) |
| C7 | N2 | C9 | C10 | 97.3( 3) |
| C7 | N2 | C9 | H9 | -21.4(16) |
| N1 | C1 | C2 | H2a | -57.4(21) |
| C6 | C1 | C2 | C3 | -55.2( 3) |
| C6 | C1 | C2 | H2b | -177.5(19) |
| H1 | C1 | C2 | H2a | -176. ( 3) |
| N1 | C1 | C6 | C5 | 177.5( 4) |
| N1 | C1 | C6 | H6b | 60.0(21) |
| C2 | C1 | C6 | H6a | 179.7(20) |
| H1 | C1 | C6 | C5 | -64.4(16) |
| H1 | C1 | C6 | H6b | 178. ( 3) |
| C1 | C2 | C3 | H3a | 179.2(24) |
| H2a | C2 | C3 | C4 | -61.6(21) |
| H2a | C2 | C3 | H3b | 178. ( 3) |
| H2b | C2 | C3 | H3a | -58. ( 3) |
| C2 | C3 | C4 | C5 | -56.5( 3) |
| C2 | C3 | C4 | H4b | 59.6(23) |
| H3a | C3 | C4 | H4a | 66. ( 3) |
| H3b | C3 | C4 | C5 | 63.2(20) |
| H3b | C3 | C4 | H4b | 179. ( 3) |
| C3 | C4 | C5 | H5a | 177. ( 3) |
| H4a | C4 | C5 | C6 | 172.8(24) |
| H4a | C4 | C5 | H5b | 55. ( 3) |
| H4b | C4 | C5 | H5a | 57. ( 3) |
| C4 | C5 | C6 | C1 | -54.7( 3) |
| C4 | C5 | C6 | H6b | 63.1(21) |
| H5a | C5 | C6 | H6a | 60. ( 3) |
| H5b | C5 | C6 | C1 | 64.5(21) |
| H5b | C5 | C6 | H6b | -178. ( 3) |
| N1 | C7 | C8 | H8b | 116.7(22) |
| N2 | C7 | C8 | H8a | 58.5(21) |
| N2 | C7 | C8 | H8c | 172.6(22) |
| C7 | C8 | H8a | H8c | 121. ( 3) |
| H8b | C8 | H8a | H8c | -117. ( 4) |
| H8c | C8 | H8a | H8c | 0. ( 3) |
| H8a | C8 | H8b | H8a | 0. ( 3) |
| C7 | C8 | H8c | H8a | -118. ( 3) |
| H8b | C8 | H8c | H8a | 115. ( 4) |
| N2 | C9 | C10 | H10a | 55.0(19) |
| C14 | C9 | C10 | C11 | 55.08(24) |
| C14 | C9 | C10 | H10b | 177.8(19) |
| H9 | C9 | C10 | H10a | 174. ( 3) |
| N2 | C9 | C14 | C13 | -177.8( 4) |
| N2 | C9 | C14 | H14b | 58.3(19) |
| C10 | C9 | C14 | H14a | 67.2(17) |
| H9 | C9 | C14 | C13 | 64.5(17) |
| H9 | C9 | C14 | H14b | -59.3(25) |
| C9 | C10 | C11 | H11a | 65.4(19) |
| H10a | C10 | C11 | C12 | 65.5(19) |
| H10a | C10 | C11 | H11b | -58. ( 3) |
| H10b | C10 | C11 | H11a | -55. ( 3) |
| C9 | C10 | H10a | H10b | -115.4(23) |
| H10b | C10 | H10a | H10b | 0.0(23) |

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|---|---|---|---|---|
| C9 | C10 | H10b | H10a | 116.3(24) |
| H10a | C10 | H10b | H10a | 0.0(23) |
| C10 | C11 | C12 | H12a | 178.8(22) |
| H11a | C11 | C12 | C13 | -63.9(20) |
| H11a | C11 | C12 | H12b | 176. ( 3) |
| H11b | C11 | C12 | H12a | -58. ( 3) |
| C11 | C12 | C13 | C14 | -55.1( 3) |
| C11 | C12 | C13 | H13b | -176.6(18) |
| H12a | C12 | C13 | H13a | -60. ( 3) |
| H12b | C12 | C13 | C14 | 63.7(20) |
| H12b | C12 | C13 | H13b | -58. ( 3) |
| C12 | C13 | C14 | H14a | -65.5(17) |
| H13a | C13 | C14 | C9 | -64.3(18) |
| H13a | C13 | C14 | H14b | 60. ( 3) |
| H13b | C13 | C14 | H14a | 55.6(24) |
| C9 | C14 | H14a | H14b | 118.9(22) |
| H14b | C14 | H14a | H14b | 0.0(23) |
| C13 | C14 | H14b | H14a | 119.0(23) |
| Si1 | C15 | H15a | H15b | -121.1(25) |
| H15b | C15 | H15a | H15b | 0. ( 3) |
| H15c | C15 | H15a | H15b | 116. ( 4) |
| Si1 | C15 | H15b | H15a | 123.4(24) |
| H15a | C15 | H15b | H15a | 0. ( 3) |
| H15c | C15 | H15b | H15a | -118. ( 4) |
| Si1 | C15 | H15c | H15a | -125. ( 3) |
| H15a | C15 | H15c | H15a | 0. ( 3) |
| H15b | C15 | H15c | H15a | 115. ( 4) |
| Si1 | C16 | H16a | H16c | 119.4(23) |
| H16c | C16 | H16a | H16c | 0. ( 3) |
| H16a | C16 | H16c | H16a | 0.0(24) |
| Si1 | C17 | H17a | H17b | 124. ( 3) |
| H17b | C17 | H17a | H17b | 0. ( 3) |
| H17c | C17 | H17a | H17b | -115. ( 4) |
| Si1 | C17 | H17b | H17a | -122. ( 3) |
| H17a | C17 | H17b | H17a | 0. ( 3) |
| H17c | C17 | H17b | H17a | 119. ( 4) |
| Si1 | C17 | H17c | H17a | 121.5(25) |
| H17a | C17 | H17c | H17a | 0. ( 3) |
| H17b | C17 | H17c | H17a | -117. ( 4) |
| Si2 | C18 | H18a | H18b | 121. ( 3) |
| H18b | C18 | H18a | H18b | 0. ( 3) |
| H18c | C18 | H18a | H18b | -120. ( 4) |
| Si2 | C18 | H18b | H18a | -122. ( 3) |
| H18c | C18 | H18b | H18a | 111. ( 5) |
| H18a | C18 | H18c | H18a | 0. ( 3) |
| Si2 | C19 | H19a | H19b | 122. ( 3) |
| H19b | C19 | H19a | H19b | 0. ( 3) |
| H19c | C19 | H19a | H19b | -116. ( 4) |
| Si2 | C19 | H19b | H19a | -118. ( 3) |
| H19c | C19 | H19b | H19a | 115. ( 4) |
| H19a | C19 | H19c | H19a | 0. ( 3) |
| Si2 | C20 | H20a | H20b | -119.4(25) |
| H20c | C20 | H20a | H20b | 117. ( 4) |
| H20a | C20 | H20b | H20a | 0. ( 3) |

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|---|---|---|---|---|
| C11 | C10 | H10b | H10a | -121.1(24) |
| C10 | C11 | C12 | C13 | 55.2( 3) |
| C10 | C11 | C12 | H12b | -65.3(20) |
| H11a | C11 | C12 | H12a | 60. ( 3) |
| H11b | C11 | C12 | C13 | 178.1(20) |
| H11b | C11 | C12 | H12b | 58. ( 3) |
| C11 | C12 | C13 | H13a | 63.0(18) |
| H12a | C12 | C13 | C14 | -177.8(22) |
| H12a | C12 | C13 | H13b | 61. ( 3) |
| H12b | C12 | C13 | H13a | -178. ( 3) |
| C12 | C13 | C14 | C9 | 54.88(24) |
| C12 | C13 | C14 | H14b | 179.4(19) |
| H13a | C13 | C14 | H14a | 175. ( 3) |
| H13b | C13 | C14 | C9 | 176.0(18) |
| H13b | C13 | C14 | H14b | -59. ( 3) |
| C13 | C14 | H14a | H14b | -118.7(22) |
| C9 | C14 | H14b | H14a | -116.5(23) |
| H14a | C14 | H14b | H14a | 0.0(21) |
| Si1 | C15 | H15a | H15c | 122.7(25) |
| H15b | C15 | H15a | H15c | -116. ( 4) |
| H15c | C15 | H15a | H15c | 0. ( 3) |
| Si1 | C15 | H15b | H15c | -118.9(24) |
| H15a | C15 | H15b | H15c | 118. ( 4) |
| H15c | C15 | H15b | H15c | 0. ( 3) |
| Si1 | C15 | H15c | H15b | 119.5(25) |
| H15a | C15 | H15c | H15b | -115. ( 4) |
| H15b | C15 | H15c | H15b | 0. ( 3) |
| H16b | C16 | H16a | H16c | -113. ( 4) |
| Si1 | C16 | H16c | H16a | -124.2(25) |
| H16b | C16 | H16c | H16a | 115. ( 4) |
| Si1 | C17 | H17a | H17c | -121. ( 3) |
| H17b | C17 | H17a | H17c | 115. ( 4) |
| H17c | C17 | H17a | H17c | 0. ( 3) |
| Si1 | C17 | H17b | H17c | 119. ( 3) |
| H17a | C17 | H17b | H17c | -119. ( 4) |
| H17c | C17 | H17b | H17c | 0. ( 3) |
| Si1 | C17 | H17c | H17b | -121.5(25) |
| H17a | C17 | H17c | H17b | 117. ( 4) |
| H17b | C17 | H17c | H17b | 0. ( 3) |
| Si2 | C18 | H18a | H18c | -119. ( 3) |
| H18b | C18 | H18a | H18c | 120. ( 4) |
| H18c | C18 | H18a | H18c | 0. ( 3) |
| H18a | C18 | H18b | H18a | 0. ( 3) |
| Si2 | C18 | H18c | H18a | 123. ( 3) |
| H18b | C18 | H18c | H18a | -107. ( 4) |
| Si2 | C19 | H19a | H19c | -121.4(25) |
| H19b | C19 | H19a | H19c | 116. ( 4) |
| H19c | C19 | H19a | H19c | 0. ( 3) |
| H19a | C19 | H19b | H19a | 0. ( 3) |
| Si2 | C19 | H19c | H19a | 120. ( 3) |
| H19b | C19 | H19c | H19a | -110. ( 4) |
| H20b | C20 | H20a | H20b | 0. ( 3) |
| Si2 | C20 | H20b | H20a | 115.8(24) |
| H20c | C20 | H20b | H20a | -117. ( 4) |

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|---|---|---|---|---|---|---|---|---|---|
| C8 | H8a | H8b | C8 | 0.0( 3) | H8c | H8a | H8b | C8 | 41. ( 3) |
| C8 | H8a | H8c | C8 | 0.0( 5) | H8b | H8a | H8c | C8 | -34.8(21) |
| C10 | H10a | H10b | C10 | 0.0( 3) | C14 | H14a | H14b | C14 | 0.0( 3) |
| C15 | H15a | H15b | C15 | 0.0( 3) | C15 | H15a | H15b | H15c | -36.5(23) |
| H15c | H15a | H15b | C15 | 36.5(23) | H15c | H15a | H15b | H15c | 0.0(19) |
| C15 | H15a | H15c | C15 | 0.0( 3) | C15 | H15a | H15c | H15b | 38.8(24) |
| H15b | H15a | H15c | C15 | -38.8(24) | H15b | H15a | H15c | H15b | 0.0(18) |
| C15 | H15b | H15c | C15 | 0.0( 3) | C15 | H15b | H15c | H15a | -37.2(23) |
| H15a | H15b | H15c | C15 | 37.2(23) | H15a | H15b | H15c | H15a | 0.0(19) |
| C16 | H16a | H16c | C16 | 0.0( 3) | C17 | H17a | H17b | C17 | 0.0( 5) |
| C17 | H17a | H17b | H17c | 38. ( 3) | H17c | H17a | H17b | C17 | -37.6(23) |
| H17c | H17a | H17b | H17c | 0.0(18) | C17 | H17a | H17c | C17 | 0.0( 5) |
| C17 | H17a | H17c | H17b | -39. ( 3) | H17b | H17a | H17c | C17 | 39.4(24) |
| H17b | H17a | H17c | H17b | 0.0(20) | C17 | H17b | H17c | C17 | 0.0( 3) |
| C17 | H17b | H17c | H17a | 34.1(22) | H17a | H17b | H17c | C17 | -34.1(23) |
| H17a | H17b | H17c | H17a | 0.0(19) | C18 | H18a | H18b | C18 | 0.0( 6) |
| H18c | H18a | H18b | C18 | -35.8(25) | C18 | H18a | H18c | C18 | 0.0( 4) |
| H18b | H18a | H18c | C18 | 40. ( 3) | C19 | H19a | H19b | C19 | 0.0( 5) |
| H19c | H19a | H19b | C19 | -36.8(24) | C19 | H19a | H19c | C19 | 0.0( 5) |
| H19b | H19a | H19c | C19 | 41. ( 3) | C20 | H20a | H20b | C20 | 0.0( 3) |