Electronic Supplementary Material (ESI) for Chemical Science


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#  to carry out CIF format checking respectively.
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 Mercury: visualization and analysis of crystal structures, C. F. Macrae,
 P. R. Edgington, P. McCabe, E. Pidcock, G. P. Shields, R. Taylor,
 M. Towler and J. van de Streek, J. Appl. Cryst., 39, 453-457, 2006.
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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C16 C 0.3497(4) 0.2179(2) 0.64159(11) 0.0266(8) Uani 1 1 d . . .
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C18 C 0.3658(4) 0.1141(2) 0.69086(12) 0.0341(9) Uani 1 1 d . . .
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C20 C 0.8002(5) 0.3302(3) 0.66153(12) 0.0371(10) Uani 1 1 d . . .
C21 C 0.9303(4) 0.2721(3) 0.67367(14) 0.0403(10) Uani 1 1 d . . .
H21B H 0.8897 0.2170 0.6832 0.048 Uiso 1 1 calc R . .
H21A H 0.9925 0.2611 0.6488 0.048 Uiso 1 1 calc R . .
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H22A H 1.0760 0.3615 0.6972 0.053 Uiso 1 1 calc R . .
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H23A H 0.8970 0.2742 0.7564 0.044 Uiso 1 1 calc R . .
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C25 C 0.8529(6) 0.4094(4) 0.63835(15) 0.0542(14) Uani 1 1 d . . .
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H25C H 0.9479 0.4288 0.6501 0.081 Uiso 1 1 calc R . .
H25B H 0.7778 0.4543 0.6411 0.081 Uiso 1 1 calc R . .
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H26C H 0.6550 0.2310 0.6475 0.069 Uiso 1 1 calc R . .
H26A H 0.7547 0.2589 0.6086 0.069 Uiso 1 1 calc R . .
C27 C 0.8532(5) 0.4788(3) 0.72822(14) 0.0398(10) Uani 1 1 d . . .
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C18 0.036(2) 0.0241(18) 0.042(2) -0.0014(16) -0.0022(16) 0.0039(15)
C19 0.0217(18) 0.0210(16) 0.0314(17) 0.0001(13) -0.0037(14) 0.0027(15)
C20 0.026(2) 0.052(3) 0.034(2) -0.0081(18) 0.0030(16) 0.0003(19)
C21 0.023(2) 0.049(3) 0.049(2) -0.011(2) 0.0056(18) 0.0013(18)
C22 0.024(2) 0.052(3) 0.055(3) 0.002(2) -0.0026(18) 0.003(2)
C23 0.027(2) 0.046(2) 0.038(2) 0.0016(18) -0.0030(16) 0.0001(18)
C24 0.0221(18) 0.032(2) 0.0325(19) 0.0051(15) -0.0019(14) -0.0019(16)
C25 0.047(3) 0.078(4) 0.038(3) 0.011(2) 0.002(2) -0.006(3)
C26 0.032(2) 0.065(3) 0.042(2) -0.012(2) 0.0079(19) 0.002(2)
C27 0.039(2) 0.037(2) 0.043(2) -0.0056(19) -0.0041(19) -0.0100(19)
C28 0.032(2) 0.045(3) 0.035(2) -0.0062(18) -0.0011(17) -0.0049(19)
C29 0.033(2) 0.0260(19) 0.038(2) -0.0048(16) 0.0024(17) -0.0018(17)
C30 0.033(2) 0.0316(19) 0.0314(18) -0.0020(15) 0.0022(18) -0.0011(19)
C31 0.041(2) 0.039(2) 0.0291(19) -0.0034(16) -0.0005(18) -0.002(2)
C32 0.051(3) 0.049(3) 0.038(2) -0.012(2) 0.010(2) -0.002(2)
C33 0.038(3) 0.051(3) 0.046(2) -0.017(2) 0.0081(19) 0.000(2)
C34 0.031(2) 0.040(2) 0.041(2) -0.0028(19) 0.0019(18) -0.0020(18)
C35 0.033(2) 0.0253(19) 0.0332(19) -0.0007(15) -0.0016(15) -0.0025(16)
C36 0.033(2) 0.034(2) 0.045(2) 0.0011(18) 0.0006(18) 0.0005(18)
C37 0.040(2) 0.031(2) 0.059(3) 0.0004(19) -0.009(2) 0.006(2)
C38 0.054(3) 0.027(2) 0.040(2) 0.0097(17) -0.007(2) 0.000(2)
C39 0.056(3) 0.033(2) 0.039(2) 0.0047(18) 0.005(2) -0.006(2)
C40 0.037(2) 0.030(2) 0.037(2) -0.0041(16) 0.0012(17) 0.0022(18)
C41 0.031(2) 0.0293(19) 0.0274(19) -0.0018(15) 0.0011(15) -0.0012(17)
C42 0.031(2) 0.038(2) 0.032(2) 0.0008(17) 0.0017(16) 0.0005(17)
C43 0.041(2) 0.040(2) 0.032(2) -0.0020(16) -0.0102(18) -0.005(2)
C44 0.052(3) 0.043(2) 0.0272(19) -0.0034(19) -0.0046(17) -0.004(2)
C45 0.049(3) 0.038(2) 0.0315(19) -0.0048(18) 0.0076(17) 0.004(2)
C46 0.035(2) 0.040(2) 0.0323(19) -0.0020(16) 0.0005(18) 0.001(2)

_geom_special_details
;
All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
;

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Ge1 N3 1.941(3) . ?
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F3 C32 1.339(5) . ?
F4 C33 1.331(5) . ?
F5 C34 1.342(5) . ?
F6 C36 1.344(5) . ?
F7 C37 1.350(5) . ?
F8 C38 1.339(5) . ?
F9 C39 1.344(5) . ?
F10 C40 1.340(5) . ?
F11 C42 1.344(4) . ?
F12 C43 1.338(5) . ?
F13 C44 1.336(5) . ?
F14 C45 1.344(5) . ?
F15 C46 1.346(5) . ?
O1 N5 1.477(4) . ?
N1 C1 1.375(5) . ?
N1 C4 1.385(5) . ?
N2 C16 1.365(5) . ?
N2 C19 1.387(4) . ?
N3 C11 1.382(5) . ?
N3 C14 1.407(5) . ?
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N4 C6 1.421(5) . ?
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C3 H3 0.9500 . ?
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C7 H7 0.9500 . ?
C8 C9 1.424(5) . ?
C8 H8 0.9500 . ?
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C12 H12 0.9500 . ?
C13 C14 1.425(5) . ?

C13 H13 0.9500 . ?
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C27 H27C 0.9800 . ?
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C28 H28A 0.9800 . ?
C28 H28C 0.9800 . ?
C28 H28B 0.9800 . ?
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C32 C33 1.384(7) . ?
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C16 N2 C19 109.1(3) . . ?
C16 N2 Ge1 134.3(3) . . ?
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C11 N3 C14 106.9(3) . . ?
C11 N3 Ge1 125.1(3) . . ?
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C9 N4 Ge1 124.8(3) . . ?
C6 N4 Ge1 126.9(3) . . ?
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O1 N5 C20 106.6(3) . . ?
C24 N5 C20 115.9(3) . . ?
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C7 C8 C9 107.0(4) . . ?
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C10 C9 C8 126.5(4) . . ?
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C28 C24 C27 107.9(3) . . ?
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C20 C25 H25B 109.5 . . ?
H25A C25 H25B 109.5 . . ?
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H26C C26 H26A 109.5 . . ?
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H28C C28 H28B 109.5 . . ?
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C2 C3 C4 C5 173.9(4) . . . . ?
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C7 C8 C9 C10 173.8(4) . . . . ?
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C14 N3 C11 C12 -2.0(4) . . . . ?
Ge1 N3 C11 C12 169.6(3) . . . . ?
C9 C10 C11 N3 -5.5(7) . . . . ?
C35 C10 C11 N3 178.5(4) . . . . ?
C9 C10 C11 C12 170.0(4) . . . . ?
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C11 N3 C14 C15 -177.5(4) . . . . ?
Ge1 N3 C14 C15 11.2(5) . . . . ?
C11 N3 C14 C13 2.2(4) . . . . ?
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C12 C13 C14 C15 178.1(4) . . . . ?
C12 C13 C14 N3 -1.6(4) . . . . ?
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C13 C14 C15 C41 -3.4(6) . . . . ?
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Ge1 N2 C16 C17 -178.7(3) . . . . ?
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C41 C15 C16 N2 -179.7(3) . . . . ?
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C16 N2 C19 C18 2.9(4) . . . . ?
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N1 C1 C19 N2 1.2(5) . . . . ?

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C22 C23 C24 N5 54.0(5) . . . . ?
C22 C23 C24 C28 168.7(4) . . . . ?
C22 C23 C24 C27 -73.3(5) . . . . ?
C4 C5 C29 C30 67.9(5) . . . . ?
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C4 C5 C29 C34 -113.0(5) . . . . ?
C6 C5 C29 C34 66.1(6) . . . . ?
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C5 C29 C30 F1 1.7(6) . . . . ?
C34 C29 C30 C31 -1.1(6) . . . . ?
C5 C29 C30 C31 178.1(4) . . . . ?
F1 C30 C31 F2 -2.0(6) . . . . ?
C29 C30 C31 F2 -178.4(4) . . . . ?
F1 C30 C31 C32 177.8(4) . . . . ?
C29 C30 C31 C32 1.4(7) . . . . ?
F2 C31 C32 F3 -1.9(7) . . . . ?
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F2 C31 C32 C33 178.6(4) . . . . ?
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F8 C38 C39 C40 178.6(4) . . . . ?
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F9 C39 C40 F10 -0.7(6) . . . . ?
C38 C39 C40 F10 -178.7(4) . . . . ?
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C10 C35 C40 C39 180.0(4) . . . . ?
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C14 C15 C41 C42 -69.3(5) . . . . ?
C16 C15 C41 C46 -73.1(5) . . . . ?
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C46 C41 C42 F11 179.8(4) . . . . ?
C15 C41 C42 F11 0.1(6) . . . . ?
C46 C41 C42 C43 1.6(6) . . . . ?
C15 C41 C42 C43 -178.2(4) . . . . ?
F11 C42 C43 F12 0.6(6) . . . . ?
C41 C42 C43 F12 178.9(4) . . . . ?
F11 C42 C43 C44 -178.2(4) . . . . ?
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C42 C43 C44 C45 -2.1(7) . . . . ?
F13 C44 C45 F14 -1.0(7) . . . . ?
C43 C44 C45 F14 -178.2(4) . . . . ?
F13 C44 C45 C46 179.5(4) . . . . ?
C43 C44 C45 C46 2.3(7) . . . . ?
F14 C45 C46 F15 -0.2(6) . . . . ?
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F14 C45 C46 C41 180.0(4) . . . . ?
C44 C45 C46 C41 -0.5(7) . . . . ?
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C15 C41 C46 F15 -1.5(6) . . . . ?
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C15 C41 C46 C45 178.4(4) . . . . ?

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SQUEEZE RESULTS (APPEND TO CIF)
Note: Data are Listed for all Voids in the P1 Unit Cell
i.e. Centre of Gravity, Solvent Accessible Volume,
Recovered number of Electrons in the Void and
Details about the Squeezed Material
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loop_
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H H 0.0000 0.0000 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
N N 0.0061 0.0033 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
O O 0.0106 0.0060 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
F F 0.0171 0.0103 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Ge Ge 0.1547 1.8001 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_space_group_name_H-M   P-1

loop_
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'x, y, z'
'-x, -y, -z'

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_cell_length_c                  18.314(6)
_cell_angle_alpha               102.173(4)
_cell_angle_beta                103.316(5)
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_cell_volume                    3503.9(19)
_cell_formula_units_Z           2
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_diffrn_measurement_device_type  'Saturn724+ CCD'
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 Mercury: visualization and analysis of crystal structures, C. F. Macrae,
 P. R. Edgington, P. McCabe, E. Pidcock, G. P. Shields, R. Taylor,
 M. Towler and J. van de Streek, J. Appl. Cryst., 39, 453-457, 2006.
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_computing_publication_material  'SHELX-97 (Sheldrick, 2008)'
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_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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_atom_sites_solution_secondary   difmap
_atom_sites_solution_hydrogens   geom
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_refine_ls_extinction_method     none
_refine_ls_extinction_coef       ?
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loop_
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Ge2 Ge 0.23573(4) 0.66915(3) 0.07962(3) 0.03335(16) Uani 1 1 d . . .
F1 F 0.7116(3) 0.7754(2) -0.07538(18) 0.0493(8) Uani 1 1 d . . .
F2 F 0.6227(3) 0.8429(2) -0.19025(19) 0.0609(10) Uani 1 1 d . . .
F3 F 0.4506(3) 0.9200(2) -0.1829(2) 0.0658(10) Uani 1 1 d . . .
F4 F 0.3738(3) 0.9314(2) -0.0571(2) 0.0547(9) Uani 1 1 d . . .
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F5 F 0.4600(3) 0.8639(2) 0.05838(18) 0.0459(8) Uani 1 1 d . . .
F6 F 0.9473(3) 0.9875(3) 0.4017(2) 0.0690(11) Uani 1 1 d . . .
F7 F 0.9713(4) 1.1413(3) 0.5082(3) 0.0905(14) Uani 1 1 d . . .
F8 F 0.8054(4) 1.1745(2) 0.5686(2) 0.0803(13) Uani 1 1 d . . .
F9 F 0.6152(3) 1.0537(3) 0.5218(2) 0.0731(11) Uani 1 1 d . . .
F10 F 0.5910(3) 0.9011(2) 0.4163(2) 0.0610(10) Uani 1 1 d . . .
F11 F 0.9009(4) 0.4545(4) 0.3503(3) 0.0998(16) Uani 1 1 d . . .
F12 F 0.9249(5) 0.3503(4) 0.4479(4) 0.148(3) Uani 1 1 d . . .
F13 F 0.7775(6) 0.3241(4) 0.5301(3) 0.139(2) Uani 1 1 d . . .
F14 F 0.6076(4) 0.4024(3) 0.5123(3) 0.1012(16) Uani 1 1 d . . .
F15 F 0.5843(3) 0.5083(3) 0.4160(2) 0.0673(10) Uani 1 1 d . . .
F16 F -0.0686(3) 0.8127(3) -0.1022(2) 0.0668(11) Uani 1 1 d . . .
F17 F -0.1419(4) 0.8679(3) -0.2287(3) 0.0950(15) Uani 1 1 d . . .
F18 F -0.0225(4) 0.8762(3) -0.3323(2) 0.1001(16) Uani 1 1 d . . .
F19 F 0.1727(4) 0.8309(3) -0.3052(2) 0.0767(12) Uani 1 1 d . . .
F20 F 0.2472(3) 0.7771(2) -0.1777(2) 0.0553(9) Uani 1 1 d . . .
F21 F 0.1780(3) 0.9617(2) 0.3074(2) 0.0598(9) Uani 1 1 d . . .
F22 F 0.2727(3) 1.1201(2) 0.4059(2) 0.0729(11) Uani 1 1 d . . .
F23 F 0.4861(3) 1.1897(2) 0.4291(2) 0.0741(12) Uani 1 1 d . . .
F24 F 0.6020(3) 1.0981(2) 0.3494(2) 0.0690(11) Uani 1 1 d . . .
F25 F 0.5072(3) 0.9378(2) 0.2510(2) 0.0609(10) Uani 1 1 d . . .
F26 F 0.4275(3) 0.4545(3) 0.2229(2) 0.0642(10) Uani 1 1 d . . .
F27 F 0.4538(4) 0.3376(3) 0.3097(2) 0.0837(13) Uani 1 1 d . . .
F28 F 0.3165(4) 0.3081(3) 0.3987(3) 0.1014(16) Uani 1 1 d . . .
F29 F 0.1534(4) 0.3953(3) 0.3979(2) 0.0860(14) Uani 1 1 d . . .
F30 F 0.1276(3) 0.5118(2) 0.31202(19) 0.0567(9) Uani 1 1 d . . .
O1 O 0.5156(3) 0.6554(2) 0.1954(2) 0.0428(9) Uani 1 1 d . . .
H1 H 0.5137 0.6781 0.2407 0.051 Uiso 1 1 d R . .
O2 O 0.3646(3) 0.6760(2) 0.0646(2) 0.0367(8) Uani 1 1 d . . .
H2A H 0.4087 0.6745 0.1055 0.044 Uiso 1 1 d R . .
N1 N 0.7261(4) 0.6956(3) 0.3123(2) 0.0370(10) Uani 1 1 d . . .
N2 N 0.6848(3) 0.5539(3) 0.1928(2) 0.0360(10) Uani 1 1 d . . .
N3 N 0.6526(4) 0.6395(3) 0.0962(2) 0.0376(10) Uani 1 1 d . . .
N4 N 0.6939(3) 0.7914(3) 0.2016(2) 0.0339(10) Uani 1 1 d . . .
N5 N 0.2607(4) 0.6950(3) 0.1906(2) 0.0360(10) Uani 1 1 d . . .
N6 N 0.2061(3) 0.7831(3) 0.0767(2) 0.0348(10) Uani 1 1 d . . .
N7 N 0.1444(3) 0.6254(3) -0.0248(2) 0.0342(10) Uani 1 1 d . . .
N8 N 0.1846(3) 0.5475(3) 0.0767(2) 0.0368(10) Uani 1 1 d . . .
C1 C 0.6429(4) 0.5510(3) 0.0629(3) 0.0363(12) Uani 1 1 d . . .
C2 C 0.6128(4) 0.5368(4) -0.0189(3) 0.0393(13) Uani 1 1 d . . .
H2 H 0.6030 0.4825 -0.0564 0.047 Uiso 1 1 calc R . .
C3 C 0.6006(4) 0.6166(4) -0.0334(3) 0.0382(12) Uani 1 1 d . . .
H3 H 0.5785 0.6269 -0.0834 0.046 Uiso 1 1 calc R . .
C4 C 0.6265(4) 0.6816(3) 0.0388(3) 0.0354(12) Uani 1 1 d . . .
C5 C 0.6307(4) 0.7729(3) 0.0586(3) 0.0358(12) Uani 1 1 d . . .
C6 C 0.5884(4) 0.8155(3) -0.0041(3) 0.0369(12) Uani 1 1 d . . .
C7 C 0.6274(4) 0.8130(4) -0.0695(3) 0.0392(13) Uani 1 1 d . . .
C8 C 0.5823(5) 0.8477(4) -0.1281(3) 0.0469(15) Uani 1 1 d . . .
C9 C 0.4966(5) 0.8868(4) -0.1253(3) 0.0471(15) Uani 1 1 d . . .
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C11 C 0.5028(5) 0.8571(4) -0.0022(3) 0.0402(13) Uani 1 1 d . . .
C12 C 0.6692(4) 0.8243(3) 0.1356(3) 0.0363(12) Uani 1 1 d . . .
C13 C 0.6893(4) 0.9177(3) 0.1612(3) 0.0355(12) Uani 1 1 d . . .
H13 H 0.6801 0.9570 0.1288 0.043 Uiso 1 1 calc R . .

C14 C 0.7240(4) 0.9417(4) 0.2402(3) 0.0399(13) Uani 1 1 d . . .
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C15 C 0.7259(4) 0.8637(3) 0.2665(3) 0.0389(13) Uani 1 1 d . . .
C16 C 0.7496(4) 0.8568(3) 0.3427(3) 0.0391(13) Uani 1 1 d . . .
C17 C 0.7677(5) 0.9398(4) 0.4053(3) 0.0425(14) Uani 1 1 d . . .
C18 C 0.8631(5) 1.0024(4) 0.4305(4) 0.0530(16) Uani 1 1 d . . .
C19 C 0.8760(6) 1.0815(4) 0.4853(4) 0.0606(18) Uani 1 1 d . . .
C20 C 0.7925(6) 1.0978(4) 0.5164(3) 0.0565(18) Uani 1 1 d . . .
C21 C 0.6978(5) 1.0366(4) 0.4922(3) 0.0509(15) Uani 1 1 d . . .
C22 C 0.6859(5) 0.9593(4) 0.4390(3) 0.0436(14) Uani 1 1 d . . .
C23 C 0.7515(4) 0.7782(4) 0.3651(3) 0.0392(13) Uani 1 1 d . . .
C24 C 0.7830(5) 0.7666(4) 0.4410(3) 0.0454(14) Uani 1 1 d . . .
H24 H 0.8049 0.8124 0.4879 0.055 Uiso 1 1 calc R . .
C25 C 0.7766(5) 0.6792(4) 0.4358(3) 0.0445(14) Uani 1 1 d . . .
H25 H 0.7924 0.6532 0.4782 0.053 Uiso 1 1 calc R . .
C26 C 0.7421(4) 0.6328(4) 0.3552(3) 0.0410(13) Uani 1 1 d . . .
C27 C 0.7267(5) 0.5419(4) 0.3245(3) 0.0428(14) Uani 1 1 d . . .
C28 C 0.7412(5) 0.4842(4) 0.3798(3) 0.0489(15) Uani 1 1 d . . .
C29 C 0.8264(7) 0.4421(5) 0.3896(4) 0.071(2) Uani 1 1 d . . .
C30 C 0.8404(8) 0.3885(6) 0.4402(5) 0.094(3) Uani 1 1 d . . .
C31 C 0.7653(9) 0.3753(5) 0.4806(5) 0.091(3) Uani 1 1 d . . .
C32 C 0.6812(7) 0.4158(5) 0.4720(4) 0.075(2) Uani 1 1 d . . .
C33 C 0.6682(6) 0.4701(4) 0.4229(4) 0.0552(16) Uani 1 1 d . . .
C34 C 0.7001(4) 0.5028(4) 0.2449(3) 0.0403(13) Uani 1 1 d . . .
C35 C 0.6861(5) 0.4146(4) 0.1994(3) 0.0447(14) Uani 1 1 d . . .
H35 H 0.6915 0.3642 0.2192 0.054 Uiso 1 1 calc R . .
C36 C 0.6634(5) 0.4143(4) 0.1225(3) 0.0433(14) Uani 1 1 d . . .
H36 H 0.6507 0.3642 0.0799 0.052 Uiso 1 1 calc R . .
C37 C 0.6624(4) 0.5021(3) 0.1183(3) 0.0358(12) Uani 1 1 d . . .
C38 C 0.1090(4) 0.5346(3) -0.0529(3) 0.0371(12) Uani 1 1 d . . .
C39 C 0.0576(4) 0.5161(4) -0.1331(3) 0.0413(13) Uani 1 1 d . . .
H39 H 0.0266 0.4591 -0.1677 0.050 Uiso 1 1 calc R . .
C40 C 0.0607(5) 0.5964(4) -0.1520(3) 0.0435(14) Uani 1 1 d . . .
H40 H 0.0324 0.6043 -0.2021 0.052 Uiso 1 1 calc R . .
C41 C 0.1139(4) 0.6653(4) -0.0828(3) 0.0391(13) Uani 1 1 d . . .
C42 C 0.1311(4) 0.7572(3) -0.0666(3) 0.0380(12) Uani 1 1 d . . .
C43 C 0.0936(5) 0.7951(3) -0.1339(3) 0.0396(13) Uani 1 1 d . . .
C44 C 0.1507(5) 0.8005(4) -0.1880(3) 0.0447(14) Uani 1 1 d . . .
C45 C 0.1133(6) 0.8275(4) -0.2544(3) 0.0550(17) Uani 1 1 d . . .
C46 C 0.0141(6) 0.8504(5) -0.2678(4) 0.0652(19) Uani 1 1 d . . .
C47 C -0.0458(6) 0.8461(5) -0.2160(4) 0.0653(19) Uani 1 1 d . . .
C48 C -0.0055(5) 0.8188(4) -0.1500(3) 0.0491(15) Uani 1 1 d . . .
C49 C 0.1728(4) 0.8121(3) 0.0084(3) 0.0351(12) Uani 1 1 d . . .
C50 C 0.1883(4) 0.9057(3) 0.0319(3) 0.0402(13) Uani 1 1 d . . .
H50 H 0.1711 0.9426 -0.0017 0.048 Uiso 1 1 calc R . .
C51 C 0.2312(4) 0.9339(3) 0.1096(3) 0.0386(13) Uani 1 1 d . . .
H51 H 0.2491 0.9936 0.1398 0.046 Uiso 1 1 calc R . .
C52 C 0.2451(4) 0.8583(4) 0.1384(3) 0.0393(13) Uani 1 1 d . . .
C53 C 0.2892(4) 0.8571(3) 0.2155(3) 0.0371(12) Uani 1 1 d . . .
C54 C 0.3386(4) 0.9443(3) 0.2742(3) 0.0357(12) Uani 1 1 d . . .
C55 C 0.2831(5) 0.9934(4) 0.3151(3) 0.0427(13) Uani 1 1 d . . .
C56 C 0.3312(5) 1.0761(4) 0.3674(3) 0.0474(15) Uani 1 1 d . . .
C57 C 0.4385(6) 1.1100(4) 0.3782(4) 0.0540(16) Uani 1 1 d . . .
C58 C 0.4962(5) 1.0645(4) 0.3397(4) 0.0477(14) Uani 1 1 d . . .

C59 C 0.4471(5) 0.9822(4) 0.2880(3) 0.0431(13) Uani 1 1 d . . .
C60 C 0.2976(4) 0.7792(3) 0.2401(3) 0.0360(12) Uani 1 1 d . . .
C61 C 0.3407(5) 0.7727(4) 0.3165(3) 0.0427(13) Uani 1 1 d . . .
H61 H 0.3716 0.8207 0.3614 0.051 Uiso 1 1 calc R . .
C62 C 0.3302(5) 0.6859(4) 0.3142(3) 0.0438(14) Uani 1 1 d . . .
H62 H 0.3525 0.6625 0.3575 0.053 Uiso 1 1 calc R . .
C63 C 0.2804(4) 0.6354(3) 0.2367(3) 0.0361(12) Uani 1 1 d . . .
C64 C 0.2553(4) 0.5431(4) 0.2089(3) 0.0374(12) Uani 1 1 d . . .
C65 C 0.2761(4) 0.4867(4) 0.2635(3) 0.0398(13) Uani 1 1 d . . .
C66 C 0.3588(5) 0.4408(4) 0.2660(3) 0.0476(15) Uani 1 1 d . . .
C67 C 0.3726(6) 0.3809(4) 0.3106(4) 0.0607(18) Uani 1 1 d . . .
C68 C 0.3033(6) 0.3662(4) 0.3551(4) 0.0627(19) Uani 1 1 d . . .
C69 C 0.2220(6) 0.4104(5) 0.3551(4) 0.0597(18) Uani 1 1 d . . .
C70 C 0.2095(5) 0.4704(4) 0.3104(3) 0.0452(14) Uani 1 1 d . . .
C71 C 0.2050(4) 0.4998(3) 0.1307(3) 0.0371(12) Uani 1 1 d . . .
C72 C 0.1631(4) 0.4084(4) 0.0907(3) 0.0415(13) Uani 1 1 d . . .
H72 H 0.1661 0.3599 0.1134 0.050 Uiso 1 1 calc R . .
C73 C 0.1180(4) 0.4028(4) 0.0141(3) 0.0391(13) Uani 1 1 d . . .
H73 H 0.0835 0.3501 -0.0257 0.047 Uiso 1 1 calc R . .
C74 C 0.1325(4) 0.4907(3) 0.0054(3) 0.0373(12) Uani 1 1 d . . .
C75 C -0.0025(6) 0.6834(4) 0.3032(4) 0.0611(18) Uani 1 1 d . . .
H75B H -0.0679 0.6377 0.2743 0.092 Uiso 1 1 calc R . .
H75C H 0.0049 0.6935 0.3590 0.092 Uiso 1 1 calc R . .
H75A H 0.0610 0.6638 0.2916 0.092 Uiso 1 1 calc R . .
C76 C -0.0110(5) 0.7691(4) 0.2794(4) 0.0574(17) Uani 1 1 d . . .
H76B H -0.0700 0.7920 0.2972 0.069 Uiso 1 1 calc R . .
H76A H 0.0573 0.8135 0.3065 0.069 Uiso 1 1 calc R . .
C77 C -0.0327(5) 0.7597(4) 0.1934(3) 0.0485(15) Uani 1 1 d . . .
H77B H -0.1014 0.7158 0.1662 0.058 Uiso 1 1 calc R . .
H77A H 0.0260 0.7366 0.1754 0.058 Uiso 1 1 calc R . .
C78 C -0.0402(5) 0.8467(4) 0.1709(4) 0.0526(16) Uani 1 1 d . . .
H78B H -0.0942 0.8722 0.1933 0.063 Uiso 1 1 calc R . .
H78A H 0.0307 0.8888 0.1950 0.063 Uiso 1 1 calc R . .
C79 C -0.0708(5) 0.8397(4) 0.0852(4) 0.0511(15) Uani 1 1 d . . .
H79B H -0.1413 0.7974 0.0604 0.061 Uiso 1 1 calc R . .
H79A H -0.0159 0.8161 0.0624 0.061 Uiso 1 1 calc R . .
C80 C -0.0789(6) 0.9285(4) 0.0674(4) 0.0630(18) Uani 1 1 d . . .
H80A H -0.1000 0.9204 0.0111 0.095 Uiso 1 1 calc R . .
H80B H -0.0086 0.9701 0.0903 0.095 Uiso 1 1 calc R . .
H80C H -0.1335 0.9520 0.0896 0.095 Uiso 1 1 calc R . .

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Ge1 0.0463(4) 0.0332(3) 0.0342(3) 0.0147(2) 0.0116(3) 0.0172(3)
Ge2 0.0424(3) 0.0284(3) 0.0329(3) 0.0118(2) 0.0100(2) 0.0134(2)
F1 0.060(2) 0.052(2) 0.0477(19) 0.0231(16) 0.0223(16) 0.0203(17)
F2 0.086(3) 0.062(2) 0.046(2) 0.0246(18) 0.0257(19) 0.022(2)
F3 0.094(3) 0.066(2) 0.050(2) 0.0356(19) 0.012(2) 0.036(2)

F4 0.063(2) 0.048(2) 0.062(2) 0.0251(17) 0.0128(17) 0.0307(17)
F5 0.058(2) 0.0449(19) 0.0497(19) 0.0219(15) 0.0241(16) 0.0261(16)
F6 0.061(2) 0.069(3) 0.075(3) 0.021(2) 0.019(2) 0.005(2)
F7 0.091(3) 0.062(3) 0.093(3) 0.009(2) 0.006(3) -0.013(2)
F8 0.122(4) 0.044(2) 0.058(2) -0.0051(18) 0.003(2) 0.026(2)
F9 0.095(3) 0.076(3) 0.057(2) 0.005(2) 0.028(2) 0.049(2)
F10 0.058(2) 0.062(2) 0.055(2) -0.0008(18) 0.0155(18) 0.0140(19)
F11 0.102(4) 0.137(4) 0.110(4) 0.073(3) 0.050(3) 0.083(3)
F12 0.190(6) 0.165(6) 0.153(5) 0.105(5) 0.051(5) 0.133(5)
F13 0.244(7) 0.114(4) 0.106(4) 0.091(4) 0.053(4) 0.077(5)
F14 0.147(5) 0.088(3) 0.087(3) 0.049(3) 0.056(3) 0.010(3)
F15 0.075(3) 0.071(3) 0.072(3) 0.031(2) 0.035(2) 0.024(2)
F16 0.061(2) 0.088(3) 0.076(3) 0.045(2) 0.029(2) 0.039(2)
F17 0.082(3) 0.132(4) 0.100(3) 0.069(3) 0.019(3) 0.063(3)
F18 0.128(4) 0.123(4) 0.070(3) 0.069(3) 0.015(3) 0.042(3)
F19 0.113(3) 0.074(3) 0.055(2) 0.031(2) 0.036(2) 0.018(2)
F20 0.061(2) 0.055(2) 0.062(2) 0.0210(18) 0.0272(18) 0.0214(18)
F21 0.057(2) 0.053(2) 0.071(2) 0.0038(18) 0.0286(19) 0.0170(18)
F22 0.098(3) 0.049(2) 0.073(3) -0.0018(19) 0.034(2) 0.028(2)
F23 0.095(3) 0.040(2) 0.066(3) -0.0009(18) 0.000(2) 0.006(2)
F24 0.058(2) 0.061(2) 0.075(3) 0.019(2) 0.0006(19) 0.0011(19)
F25 0.052(2) 0.060(2) 0.074(2) 0.0106(19) 0.0253(19) 0.0185(18)
F26 0.071(2) 0.075(3) 0.065(2) 0.031(2) 0.027(2) 0.041(2)
F27 0.106(3) 0.071(3) 0.084(3) 0.033(2) 0.010(2) 0.054(3)
F28 0.147(4) 0.081(3) 0.096(3) 0.068(3) 0.023(3) 0.039(3)
F29 0.096(3) 0.109(4) 0.077(3) 0.064(3) 0.037(2) 0.018(3)
F30 0.059(2) 0.072(2) 0.055(2) 0.0293(19) 0.0253(17) 0.0267(19)
O1 0.042(2) 0.051(2) 0.044(2) 0.0212(19) 0.0133(18) 0.0176(18)
O2 0.042(2) 0.035(2) 0.036(2) 0.0114(16) 0.0106(16) 0.0149(17)
N1 0.055(3) 0.033(2) 0.029(2) 0.0136(19) 0.010(2) 0.022(2)
N2 0.047(3) 0.034(2) 0.030(2) 0.0114(19) 0.008(2) 0.016(2)
N3 0.049(3) 0.031(2) 0.037(2) 0.015(2) 0.012(2) 0.014(2)
N4 0.047(3) 0.033(2) 0.027(2) 0.0145(19) 0.0109(19) 0.017(2)
N5 0.053(3) 0.027(2) 0.034(2) 0.0116(19) 0.014(2) 0.014(2)
N6 0.045(3) 0.030(2) 0.032(2) 0.0119(19) 0.009(2) 0.012(2)
N7 0.043(3) 0.030(2) 0.029(2) 0.0087(18) 0.0073(19) 0.011(2)
N8 0.045(3) 0.032(2) 0.036(2) 0.014(2) 0.008(2) 0.011(2)
C1 0.039(3) 0.032(3) 0.046(3) 0.015(2) 0.017(2) 0.013(2)
C2 0.055(3) 0.034(3) 0.038(3) 0.013(2) 0.019(3) 0.020(3)
C3 0.048(3) 0.043(3) 0.030(3) 0.015(2) 0.015(2) 0.017(3)
C4 0.040(3) 0.037(3) 0.037(3) 0.019(2) 0.012(2) 0.016(2)
C5 0.039(3) 0.038(3) 0.040(3) 0.018(2) 0.016(2) 0.018(2)
C6 0.044(3) 0.033(3) 0.040(3) 0.016(2) 0.013(2) 0.014(2)
C7 0.044(3) 0.035(3) 0.045(3) 0.012(3) 0.018(3) 0.016(3)
C8 0.070(4) 0.041(3) 0.038(3) 0.020(3) 0.019(3) 0.014(3)
C9 0.064(4) 0.037(3) 0.042(3) 0.022(3) 0.005(3) 0.016(3)
C10 0.053(4) 0.030(3) 0.047(3) 0.014(3) 0.005(3) 0.020(3)
C11 0.049(3) 0.038(3) 0.034(3) 0.014(2) 0.006(3) 0.013(3)
C12 0.045(3) 0.034(3) 0.041(3) 0.018(2) 0.017(3) 0.020(2)
C13 0.046(3) 0.030(3) 0.038(3) 0.017(2) 0.013(2) 0.018(2)
C14 0.046(3) 0.034(3) 0.042(3) 0.012(2) 0.011(3) 0.016(3)
C15 0.048(3) 0.030(3) 0.046(3) 0.015(2) 0.018(3) 0.016(2)
C16 0.054(3) 0.030(3) 0.035(3) 0.010(2) 0.009(3) 0.015(3)
C17 0.060(4) 0.038(3) 0.029(3) 0.014(2) 0.003(3) 0.012(3)

C18 0.062(4) 0.055(4) 0.046(4) 0.016(3) 0.015(3) 0.020(3)
C19 0.067(5) 0.045(4) 0.057(4) 0.016(3) -0.002(3) -0.001(3)
C20 0.089(5) 0.040(4) 0.036(3) 0.004(3) 0.004(3) 0.030(4)
C21 0.068(4) 0.044(4) 0.041(3) 0.012(3) 0.007(3) 0.021(3)
C22 0.063(4) 0.035(3) 0.034(3) 0.006(2) 0.013(3) 0.018(3)
C23 0.048(3) 0.036(3) 0.036(3) 0.010(2) 0.012(3) 0.016(3)
C24 0.063(4) 0.045(3) 0.031(3) 0.011(3) 0.013(3) 0.018(3)
C25 0.062(4) 0.044(3) 0.037(3) 0.023(3) 0.015(3) 0.019(3)
C26 0.049(3) 0.046(3) 0.038(3) 0.024(3) 0.014(3) 0.020(3)
C27 0.057(4) 0.040(3) 0.040(3) 0.022(3) 0.010(3) 0.023(3)
C28 0.076(4) 0.035(3) 0.041(3) 0.018(3) 0.011(3) 0.025(3)
C29 0.092(6) 0.077(5) 0.073(5) 0.047(4) 0.034(4) 0.045(4)
C30 0.140(8) 0.106(7) 0.073(6) 0.052(5) 0.031(5) 0.085(6)
C31 0.158(9) 0.070(5) 0.073(6) 0.052(5) 0.034(6) 0.052(6)
C32 0.122(7) 0.057(5) 0.052(4) 0.025(4) 0.031(4) 0.012(5)
C33 0.081(5) 0.046(4) 0.045(4) 0.020(3) 0.020(3) 0.017(3)
C34 0.048(3) 0.041(3) 0.043(3) 0.021(3) 0.015(3) 0.022(3)
C35 0.057(4) 0.033(3) 0.056(4) 0.021(3) 0.021(3) 0.025(3)
C36 0.055(4) 0.035(3) 0.049(3) 0.015(3) 0.019(3) 0.023(3)
C37 0.042(3) 0.034(3) 0.037(3) 0.012(2) 0.011(2) 0.020(2)
C38 0.041(3) 0.025(3) 0.043(3) 0.008(2) 0.008(2) 0.008(2)
C39 0.048(3) 0.031(3) 0.043(3) 0.006(2) 0.011(3) 0.010(3)
C40 0.050(3) 0.046(3) 0.033(3) 0.009(3) 0.005(3) 0.014(3)
C41 0.043(3) 0.045(3) 0.031(3) 0.014(2) 0.006(2) 0.015(3)
C42 0.046(3) 0.035(3) 0.041(3) 0.019(2) 0.009(3) 0.020(3)
C43 0.049(3) 0.032(3) 0.040(3) 0.015(2) 0.009(3) 0.014(3)
C44 0.055(4) 0.036(3) 0.047(3) 0.016(3) 0.012(3) 0.016(3)
C45 0.083(5) 0.043(4) 0.044(4) 0.019(3) 0.027(3) 0.003(3)
C46 0.081(5) 0.072(5) 0.051(4) 0.040(4) 0.008(4) 0.025(4)
C47 0.065(4) 0.076(5) 0.062(4) 0.037(4) 0.004(4) 0.030(4)
C48 0.059(4) 0.052(4) 0.045(3) 0.023(3) 0.015(3) 0.020(3)
C49 0.044(3) 0.033(3) 0.037(3) 0.016(2) 0.015(2) 0.018(2)
C50 0.052(3) 0.033(3) 0.044(3) 0.016(2) 0.016(3) 0.019(3)
C51 0.048(3) 0.030(3) 0.044(3) 0.013(2) 0.017(3) 0.016(2)
C52 0.046(3) 0.035(3) 0.044(3) 0.015(3) 0.016(3) 0.018(3)
C53 0.048(3) 0.032(3) 0.037(3) 0.008(2) 0.017(3) 0.015(2)
C54 0.047(3) 0.031(3) 0.035(3) 0.018(2) 0.009(2) 0.016(2)
C55 0.045(3) 0.040(3) 0.047(3) 0.015(3) 0.012(3) 0.016(3)
C56 0.072(4) 0.036(3) 0.040(3) 0.005(3) 0.020(3) 0.026(3)
C57 0.066(4) 0.031(3) 0.053(4) 0.012(3) -0.004(3) 0.009(3)
C58 0.048(4) 0.039(3) 0.052(4) 0.015(3) 0.003(3) 0.006(3)
C59 0.053(4) 0.042(3) 0.040(3) 0.015(3) 0.015(3) 0.017(3)
C60 0.043(3) 0.035(3) 0.036(3) 0.010(2) 0.016(2) 0.015(2)
C61 0.054(4) 0.039(3) 0.036(3) 0.009(2) 0.012(3) 0.013(3)
C62 0.060(4) 0.041(3) 0.037(3) 0.018(3) 0.015(3) 0.017(3)
C63 0.042(3) 0.036(3) 0.035(3) 0.017(2) 0.011(2) 0.013(2)
C64 0.044(3) 0.036(3) 0.039(3) 0.020(2) 0.013(2) 0.013(2)
C65 0.045(3) 0.035(3) 0.041(3) 0.013(2) 0.010(3) 0.014(3)
C66 0.059(4) 0.054(4) 0.036(3) 0.016(3) 0.018(3) 0.017(3)
C67 0.076(5) 0.043(4) 0.066(4) 0.024(3) 0.000(4) 0.033(3)
C68 0.086(5) 0.050(4) 0.057(4) 0.035(3) 0.012(4) 0.013(4)
C69 0.069(5) 0.062(4) 0.054(4) 0.035(3) 0.015(3) 0.009(4)
C70 0.055(4) 0.041(3) 0.039(3) 0.019(3) 0.007(3) 0.008(3)
C71 0.045(3) 0.037(3) 0.040(3) 0.019(2) 0.020(3) 0.014(3)

C72 0.053(3) 0.031(3) 0.044(3) 0.015(2) 0.015(3) 0.013(3)
C73 0.042(3) 0.032(3) 0.046(3) 0.012(2) 0.013(3) 0.013(2)
C74 0.045(3) 0.038(3) 0.036(3) 0.013(2) 0.015(2) 0.019(3)
C75 0.071(5) 0.055(4) 0.059(4) 0.018(3) 0.014(3) 0.020(3)
C76 0.062(4) 0.056(4) 0.054(4) 0.017(3) 0.012(3) 0.014(3)
C77 0.048(4) 0.048(4) 0.051(4) 0.012(3) 0.015(3) 0.012(3)
C78 0.048(4) 0.053(4) 0.059(4) 0.019(3) 0.013(3) 0.018(3)
C79 0.052(4) 0.040(3) 0.065(4) 0.019(3) 0.014(3) 0.016(3)
C80 0.081(5) 0.053(4) 0.073(5) 0.027(4) 0.034(4) 0.032(4)

_geom_special_details
;
All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
;

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Ge1 N3 1.903(4) . ?
Ge1 N4 1.905(4) . ?
Ge1 N1 1.918(4) . ?
Ge1 N2 1.920(4) . ?
Ge2 O2 1.751(3) . ?
Ge2 N6 1.915(4) . ?
Ge2 N7 1.918(4) . ?
Ge2 N8 1.921(4) . ?
Ge2 N5 1.925(4) . ?
F1 C7 1.344(6) . ?
F2 C8 1.353(6) . ?
F3 C9 1.338(6) . ?
F4 C10 1.348(6) . ?
F5 C11 1.344(6) . ?
F6 C18 1.353(7) . ?
F7 C19 1.351(7) . ?
F8 C20 1.338(7) . ?
F9 C21 1.350(7) . ?
F10 C22 1.336(7) . ?
F11 C29 1.347(8) . ?
F12 C30 1.332(9) . ?
F13 C31 1.338(8) . ?
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F17 C47 1.333(7) . ?
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F21 C55 1.343(6) . ?
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F24 C58 1.350(7) . ?
F25 C59 1.337(6) . ?
F26 C66 1.343(6) . ?
F27 C67 1.351(7) . ?
F28 C68 1.346(7) . ?
F29 C69 1.343(7) . ?
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O2 H2A 0.8400 . ?
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N7 C41 1.362(6) . ?
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C79 H79B 0.9900 . ?
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H75B C75 H75A 109.5 . . ?
H75C C75 H75A 109.5 . . ?
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H76B C76 H76A 107.6 . . ?
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C78 C77 H77A 108.9 . . ?
H77B C77 H77A 107.7 . . ?
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H79B C79 H79A 107.8 . . ?
C79 C80 H80A 109.5 . . ?
C79 C80 H80B 109.5 . . ?
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H80B C80 H80C 109.5 . . ?

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O1 Ge1 N1 C23 -83.4(5) . . . . ?
N3 Ge1 N1 C23 110.8(5) . . . . ?
N4 Ge1 N1 C23 19.8(5) . . . . ?
N2 Ge1 N1 C23 172.1(5) . . . . ?
O1 Ge1 N1 C26 84.3(4) . . . . ?
N3 Ge1 N1 C26 -81.6(6) . . . . ?
N4 Ge1 N1 C26 -172.6(4) . . . . ?
N2 Ge1 N1 C26 -20.3(4) . . . . ?
O1 Ge1 N2 C37 82.7(4) . . . . ?
N3 Ge1 N2 C37 -15.0(4) . . . . ?
N4 Ge1 N2 C37 -79.1(5) . . . . ?
N1 Ge1 N2 C37 -172.0(4) . . . . ?
O1 Ge1 N2 C34 -80.1(5) . . . . ?
N3 Ge1 N2 C34 -177.8(5) . . . . ?
N4 Ge1 N2 C34 118.2(5) . . . . ?
N1 Ge1 N2 C34 25.2(5) . . . . ?

O1 Ge1 N3 C4 70.7(5) . . . . ?
N4 Ge1 N3 C4 -30.9(5) . . . . ?
N1 Ge1 N3 C4 -123.1(5) . . . . ?
N2 Ge1 N3 C4 173.9(5) . . . . ?
O1 Ge1 N3 C1 -87.6(4) . . . . ?
N4 Ge1 N3 C1 170.8(4) . . . . ?
N1 Ge1 N3 C1 78.6(6) . . . . ?
N2 Ge1 N3 C1 15.6(4) . . . . ?
O1 Ge1 N4 C15 88.6(4) . . . . ?
N3 Ge1 N4 C15 -171.7(4) . . . . ?
N1 Ge1 N4 C15 -17.7(4) . . . . ?
N2 Ge1 N4 C15 -109.4(5) . . . . ?
O1 Ge1 N4 C12 -75.0(4) . . . . ?
N3 Ge1 N4 C12 24.7(4) . . . . ?
N1 Ge1 N4 C12 178.7(4) . . . . ?
N2 Ge1 N4 C12 87.0(5) . . . . ?
O2 Ge2 N5 C60 77.4(4) . . . . ?
N6 Ge2 N5 C60 -27.8(4) . . . . ?
N7 Ge2 N5 C60 -117.2(5) . . . . ?
N8 Ge2 N5 C60 -177.1(4) . . . . ?
O2 Ge2 N5 C63 -79.9(4) . . . . ?
N6 Ge2 N5 C63 174.9(4) . . . . ?
N7 Ge2 N5 C63 85.5(6) . . . . ?
N8 Ge2 N5 C63 25.6(4) . . . . ?
O2 Ge2 N6 C52 -80.7(4) . . . . ?
N7 Ge2 N6 C52 178.1(4) . . . . ?
N8 Ge2 N6 C52 113.9(5) . . . . ?
N5 Ge2 N6 C52 25.4(4) . . . . ?
O2 Ge2 N6 C49 77.9(4) . . . . ?
N7 Ge2 N6 C49 -23.4(4) . . . . ?
N8 Ge2 N6 C49 -87.6(5) . . . . ?
N5 Ge2 N6 C49 -176.0(4) . . . . ?
O2 Ge2 N7 C41 -79.9(5) . . . . ?
N6 Ge2 N7 C41 24.0(5) . . . . ?
N8 Ge2 N7 C41 176.0(5) . . . . ?
N5 Ge2 N7 C41 114.5(5) . . . . ?
O2 Ge2 N7 C38 92.0(4) . . . . ?
N6 Ge2 N7 C38 -164.1(4) . . . . ?
N8 Ge2 N7 C38 -12.0(4) . . . . ?
N5 Ge2 N7 C38 -73.6(5) . . . . ?
O2 Ge2 N8 C74 -86.8(4) . . . . ?
N6 Ge2 N8 C74 78.5(5) . . . . ?
N7 Ge2 N8 C74 12.2(4) . . . . ?
N5 Ge2 N8 C74 168.4(4) . . . . ?
O2 Ge2 N8 C71 79.9(5) . . . . ?
N6 Ge2 N8 C71 -114.8(5) . . . . ?
N7 Ge2 N8 C71 178.9(5) . . . . ?
N5 Ge2 N8 C71 -24.9(5) . . . . ?
C4 N3 C1 C37 -176.6(4) . . . . ?
Ge1 N3 C1 C37 -13.6(6) . . . . ?
C4 N3 C1 C2 2.0(6) . . . . ?
Ge1 N3 C1 C2 164.9(3) . . . . ?
N3 C1 C2 C3 -2.5(6) . . . . ?
C37 C1 C2 C3 175.5(6) . . . . ?

C1 C2 C3 C4 2.0(6) . . . . ?
C1 N3 C4 C5 -179.9(5) . . . . ?
Ge1 N3 C4 C5 20.7(7) . . . . ?
C1 N3 C4 C3 -0.7(6) . . . . ?
Ge1 N3 C4 C3 -160.2(4) . . . . ?
C2 C3 C4 N3 -0.9(6) . . . . ?
C2 C3 C4 C5 178.1(6) . . . . ?
N3 C4 C5 C12 5.1(8) . . . . ?
C3 C4 C5 C12 -173.7(5) . . . . ?
N3 C4 C5 C6 -172.2(5) . . . . ?
C3 C4 C5 C6 8.9(9) . . . . ?
C12 C5 C6 C11 -58.4(7) . . . . ?
C4 C5 C6 C11 119.0(6) . . . . ?
C12 C5 C6 C7 124.7(6) . . . . ?
C4 C5 C6 C7 -57.9(7) . . . . ?
C11 C6 C7 F1 178.8(5) . . . . ?
C5 C6 C7 F1 -4.2(8) . . . . ?
C11 C6 C7 C8 -1.3(8) . . . . ?
C5 C6 C7 C8 175.7(5) . . . . ?
F1 C7 C8 F2 0.4(8) . . . . ?
C6 C7 C8 F2 -179.6(5) . . . . ?
F1 C7 C8 C9 -179.9(5) . . . . ?
C6 C7 C8 C9 0.2(9) . . . . ?
F2 C8 C9 F3 0.6(9) . . . . ?
C7 C8 C9 F3 -179.1(5) . . . . ?
F2 C8 C9 C10 -179.5(5) . . . . ?
C7 C8 C9 C10 0.7(9) . . . . ?
F3 C9 C10 F4 -1.3(8) . . . . ?
C8 C9 C10 F4 178.9(5) . . . . ?
F3 C9 C10 C11 179.4(5) . . . . ?
C8 C9 C10 C11 -0.4(9) . . . . ?
F4 C10 C11 F5 0.9(8) . . . . ?
C9 C10 C11 F5 -179.8(5) . . . . ?
F4 C10 C11 C6 179.9(5) . . . . ?
C9 C10 C11 C6 -0.8(9) . . . . ?
C7 C6 C11 F5 -179.4(5) . . . . ?
C5 C6 C11 F5 3.6(8) . . . . ?
C7 C6 C11 C10 1.7(8) . . . . ?
C5 C6 C11 C10 -175.4(5) . . . . ?
C4 C5 C12 N4 -8.8(8) . . . . ?
C6 C5 C12 N4 168.5(5) . . . . ?
C4 C5 C12 C13 171.7(5) . . . . ?
C6 C5 C12 C13 -10.9(8) . . . . ?
C15 N4 C12 C5 -178.0(5) . . . . ?
Ge1 N4 C12 C5 -12.0(7) . . . . ?
C15 N4 C12 C13 1.5(6) . . . . ?
Ge1 N4 C12 C13 167.6(3) . . . . ?
C5 C12 C13 C14 178.9(5) . . . . ?
N4 C12 C13 C14 -0.7(6) . . . . ?
C12 C13 C14 C15 -0.4(6) . . . . ?
C12 N4 C15 C16 175.4(5) . . . . ?
Ge1 N4 C15 C16 9.3(8) . . . . ?
C12 N4 C15 C14 -1.8(6) . . . . ?
Ge1 N4 C15 C14 -167.9(3) . . . . ?

C13 C14 C15 C16 -175.6(5) . . . . ?
C13 C14 C15 N4 1.4(6) . . . . ?
N4 C15 C16 C23 4.3(9) . . . . ?
C14 C15 C16 C23 -179.1(6) . . . . ?
N4 C15 C16 C17 -171.7(5) . . . . ?
C14 C15 C16 C17 4.8(9) . . . . ?
C15 C16 C17 C18 -78.3(7) . . . . ?
C23 C16 C17 C18 105.3(7) . . . . ?
C15 C16 C17 C22 99.0(6) . . . . ?
C23 C16 C17 C22 -77.4(7) . . . . ?
C22 C17 C18 F6 178.7(5) . . . . ?
C16 C17 C18 F6 -3.9(8) . . . . ?
C22 C17 C18 C19 -1.5(9) . . . . ?
C16 C17 C18 C19 175.9(5) . . . . ?
F6 C18 C19 F7 0.1(9) . . . . ?
C17 C18 C19 F7 -179.7(5) . . . . ?
F6 C18 C19 C20 -179.1(5) . . . . ?
C17 C18 C19 C20 1.1(10) . . . . ?
F7 C19 C20 F8 1.3(9) . . . . ?
C18 C19 C20 F8 -179.5(5) . . . . ?
F7 C19 C20 C21 179.9(6) . . . . ?
C18 C19 C20 C21 -0.9(10) . . . . ?
F8 C20 C21 F9 -0.1(9) . . . . ?
C19 C20 C21 F9 -178.7(5) . . . . ?
F8 C20 C21 C22 179.8(5) . . . . ?
C19 C20 C21 C22 1.2(9) . . . . ?
F9 C21 C22 F10 0.4(8) . . . . ?
C20 C21 C22 F10 -179.4(5) . . . . ?
F9 C21 C22 C17 178.1(5) . . . . ?
C20 C21 C22 C17 -1.7(9) . . . . ?
C18 C17 C22 F10 179.5(5) . . . . ?
C16 C17 C22 F10 2.1(8) . . . . ?
C18 C17 C22 C21 1.8(8) . . . . ?
C16 C17 C22 C21 -175.6(5) . . . . ?
C26 N1 C23 C16 177.0(5) . . . . ?
Ge1 N1 C23 C16 -13.4(8) . . . . ?
C26 N1 C23 C24 -0.2(6) . . . . ?
Ge1 N1 C23 C24 169.3(4) . . . . ?
C15 C16 C23 N1 -2.1(9) . . . . ?
C17 C16 C23 N1 173.9(5) . . . . ?
C15 C16 C23 C24 174.5(6) . . . . ?
C17 C16 C23 C24 -9.5(9) . . . . ?
N1 C23 C24 C25 -0.4(7) . . . . ?
C16 C23 C24 C25 -177.5(6) . . . . ?
C23 C24 C25 C26 0.9(7) . . . . ?
C23 N1 C26 C27 -179.4(5) . . . . ?
Ge1 N1 C26 C27 11.1(8) . . . . ?
C23 N1 C26 C25 0.7(6) . . . . ?
Ge1 N1 C26 C25 -168.7(4) . . . . ?
C24 C25 C26 C27 179.2(6) . . . . ?
C24 C25 C26 N1 -1.0(7) . . . . ?
N1 C26 C27 C34 4.8(9) . . . . ?
C25 C26 C27 C34 -175.3(6) . . . . ?
N1 C26 C27 C28 -176.3(5) . . . . ?

C25 C26 C27 C28 3.5(9) . . . . ?
C26 C27 C28 C29 -111.0(7) . . . . ?
C34 C27 C28 C29 67.9(9) . . . . ?
C26 C27 C28 C33 69.6(8) . . . . ?
C34 C27 C28 C33 -111.5(7) . . . . ?
C33 C28 C29 F11 -178.9(6) . . . . ?
C27 C28 C29 F11 1.8(11) . . . . ?
C33 C28 C29 C30 -0.5(12) . . . . ?
C27 C28 C29 C30 -179.8(7) . . . . ?
F11 C29 C30 F12 -0.9(13) . . . . ?
C28 C29 C30 F12 -179.3(8) . . . . ?
F11 C29 C30 C31 180.0(8) . . . . ?
C28 C29 C30 C31 1.6(14) . . . . ?
F12 C30 C31 F13 1.2(15) . . . . ?
C29 C30 C31 F13 -179.7(8) . . . . ?
F12 C30 C31 C32 179.4(9) . . . . ?
C29 C30 C31 C32 -1.5(15) . . . . ?
F13 C31 C32 F14 -1.7(13) . . . . ?
C30 C31 C32 F14 -179.8(8) . . . . ?
F13 C31 C32 C33 178.6(7) . . . . ?
C30 C31 C32 C33 0.4(14) . . . . ?
C31 C32 C33 F15 179.8(7) . . . . ?
F14 C32 C33 F15 0.1(10) . . . . ?
C31 C32 C33 C28 0.7(12) . . . . ?
F14 C32 C33 C28 -179.0(6) . . . . ?
C29 C28 C33 F15 -179.8(6) . . . . ?
C27 C28 C33 F15 -0.4(9) . . . . ?
C29 C28 C33 C32 -0.7(10) . . . . ?
C27 C28 C33 C32 178.7(6) . . . . ?
C37 N2 C34 C27 178.4(5) . . . . ?
Ge1 N2 C34 C27 -18.0(8) . . . . ?
C37 N2 C34 C35 -0.1(6) . . . . ?
Ge1 N2 C34 C35 163.5(4) . . . . ?
C26 C27 C34 N2 -2.0(9) . . . . ?
C28 C27 C34 N2 179.1(5) . . . . ?
C26 C27 C34 C35 175.9(6) . . . . ?
C28 C27 C34 C35 -2.9(10) . . . . ?
N2 C34 C35 C36 0.2(6) . . . . ?
C27 C34 C35 C36 -178.0(6) . . . . ?
C34 C35 C36 C37 -0.2(6) . . . . ?
C34 N2 C37 C1 178.2(4) . . . . ?
Ge1 N2 C37 C1 11.8(6) . . . . ?
C34 N2 C37 C36 -0.1(6) . . . . ?
Ge1 N2 C37 C36 -166.5(4) . . . . ?
N3 C1 C37 N2 1.1(6) . . . . ?
C2 C1 C37 N2 -176.8(6) . . . . ?
N3 C1 C37 C36 178.5(6) . . . . ?
C2 C1 C37 C36 0.6(12) . . . . ?
C35 C36 C37 N2 0.2(6) . . . . ?
C35 C36 C37 C1 -177.3(7) . . . . ?
C41 N7 C38 C74 -176.4(4) . . . . ?
Ge2 N7 C38 C74 9.9(6) . . . . ?
C41 N7 C38 C39 2.5(6) . . . . ?
Ge2 N7 C38 C39 -171.3(3) . . . . ?

N7 C38 C39 C40 -1.3(6) . . . . ?
C74 C38 C39 C40 177.1(7) . . . . ?
C38 C39 C40 C41 -0.3(6) . . . . ?
C38 N7 C41 C42 173.6(5) . . . . ?
Ge2 N7 C41 C42 -14.0(8) . . . . ?
C38 N7 C41 C40 -2.6(6) . . . . ?
Ge2 N7 C41 C40 169.7(4) . . . . ?
C39 C40 C41 N7 1.8(6) . . . . ?
C39 C40 C41 C42 -173.8(6) . . . . ?
N7 C41 C42 C49 -4.2(8) . . . . ?
C40 C41 C42 C49 170.9(6) . . . . ?
N7 C41 C42 C43 -179.2(5) . . . . ?
C40 C41 C42 C43 -4.1(9) . . . . ?
C41 C42 C43 C44 -76.8(7) . . . . ?
C49 C42 C43 C44 108.0(6) . . . . ?
C41 C42 C43 C48 96.7(7) . . . . ?
C49 C42 C43 C48 -78.4(7) . . . . ?
C48 C43 C44 F20 -178.7(5) . . . . ?
C42 C43 C44 F20 -4.8(8) . . . . ?
C48 C43 C44 C45 -0.1(9) . . . . ?
C42 C43 C44 C45 173.8(5) . . . . ?
F20 C44 C45 F19 -0.9(8) . . . . ?
C43 C44 C45 F19 -179.6(5) . . . . ?
F20 C44 C45 C46 178.8(6) . . . . ?
C43 C44 C45 C46 0.1(10) . . . . ?
F19 C45 C46 F18 -0.1(10) . . . . ?
C44 C45 C46 F18 -179.8(6) . . . . ?
F19 C45 C46 C47 179.6(6) . . . . ?
C44 C45 C46 C47 -0.1(11) . . . . ?
F18 C46 C47 F17 -0.1(12) . . . . ?
C45 C46 C47 F17 -179.8(7) . . . . ?
F18 C46 C47 C48 179.8(7) . . . . ?
C45 C46 C47 C48 0.1(11) . . . . ?
C44 C43 C48 F16 177.7(5) . . . . ?
C42 C43 C48 F16 3.8(9) . . . . ?
C44 C43 C48 C47 0.1(9) . . . . ?
C42 C43 C48 C47 -173.8(6) . . . . ?
F17 C47 C48 F16 2.2(10) . . . . ?
C46 C47 C48 F16 -177.8(6) . . . . ?
F17 C47 C48 C43 179.8(6) . . . . ?
C46 C47 C48 C43 -0.1(11) . . . . ?
C41 C42 C49 C50 -176.4(5) . . . . ?
C43 C42 C49 C50 -1.6(9) . . . . ?
C41 C42 C49 N6 2.2(9) . . . . ?
C43 C42 C49 N6 177.0(5) . . . . ?
C52 N6 C49 C42 178.4(5) . . . . ?
Ge2 N6 C49 C42 16.7(7) . . . . ?
C52 N6 C49 C50 -2.8(6) . . . . ?
Ge2 N6 C49 C50 -164.5(4) . . . . ?
C42 C49 C50 C51 -179.6(5) . . . . ?
N6 C49 C50 C51 1.6(6) . . . . ?
C49 C50 C51 C52 0.2(6) . . . . ?
C49 N6 C52 C53 -177.6(5) . . . . ?
Ge2 N6 C52 C53 -15.8(7) . . . . ?

C49 N6 C52 C51 2.9(6) . . . . ?
Ge2 N6 C52 C51 164.8(3) . . . . ?
C50 C51 C52 N6 -2.0(6) . . . . ?
C50 C51 C52 C53 178.6(5) . . . . ?
N6 C52 C53 C60 -1.2(9) . . . . ?
C51 C52 C53 C60 178.1(5) . . . . ?
N6 C52 C53 C54 173.6(5) . . . . ?
C51 C52 C53 C54 -7.1(8) . . . . ?
C52 C53 C54 C55 88.1(7) . . . . ?
C60 C53 C54 C55 -96.7(6) . . . . ?
C52 C53 C54 C59 -89.5(6) . . . . ?
C60 C53 C54 C59 85.7(6) . . . . ?
C59 C54 C55 F21 -178.3(5) . . . . ?
C53 C54 C55 F21 4.0(8) . . . . ?
C59 C54 C55 C56 0.0(8) . . . . ?
C53 C54 C55 C56 -177.6(5) . . . . ?
F21 C55 C56 F22 -0.9(8) . . . . ?
C54 C55 C56 F22 -179.4(5) . . . . ?
F21 C55 C56 C57 178.7(5) . . . . ?
C54 C55 C56 C57 0.2(9) . . . . ?
F22 C56 C57 C58 179.3(5) . . . . ?
C55 C56 C57 C58 -0.3(9) . . . . ?
F22 C56 C57 F23 0.1(9) . . . . ?
C55 C56 C57 F23 -179.5(5) . . . . ?
F23 C57 C58 F24 -1.6(9) . . . . ?
C56 C57 C58 F24 179.2(5) . . . . ?
F23 C57 C58 C59 179.3(5) . . . . ?
C56 C57 C58 C59 0.1(9) . . . . ?
C55 C54 C59 F25 179.2(5) . . . . ?
C53 C54 C59 F25 -3.1(7) . . . . ?
C55 C54 C59 C58 -0.3(8) . . . . ?
C53 C54 C59 C58 177.5(5) . . . . ?
C57 C58 C59 F25 -179.2(5) . . . . ?
F24 C58 C59 F25 1.6(8) . . . . ?
C57 C58 C59 C54 0.2(9) . . . . ?
F24 C58 C59 C54 -178.9(5) . . . . ?
C63 N5 C60 C53 -178.3(5) . . . . ?
Ge2 N5 C60 C53 20.7(7) . . . . ?
C63 N5 C60 C61 0.4(6) . . . . ?
Ge2 N5 C60 C61 -160.6(4) . . . . ?
C52 C53 C60 N5 -1.4(8) . . . . ?
C54 C53 C60 N5 -176.3(5) . . . . ?
C52 C53 C60 C61 -179.9(5) . . . . ?
C54 C53 C60 C61 5.3(8) . . . . ?
N5 C60 C61 C62 -0.3(6) . . . . ?
C53 C60 C61 C62 178.4(5) . . . . ?
C60 C61 C62 C63 0.1(7) . . . . ?
C60 N5 C63 C64 -179.8(5) . . . . ?
Ge2 N5 C63 C64 -19.2(7) . . . . ?
C60 N5 C63 C62 -0.3(6) . . . . ?
Ge2 N5 C63 C62 160.2(4) . . . . ?
C61 C62 C63 C64 179.6(5) . . . . ?
C61 C62 C63 N5 0.2(6) . . . . ?
N5 C63 C64 C71 -1.2(9) . . . . ?

C62 C63 C64 C71 179.4(5) . . . . ?
N5 C63 C64 C65 -177.7(5) . . . . ?
C62 C63 C64 C65 3.0(9) . . . . ?
C63 C64 C65 C70 77.0(7) . . . . ?
C71 C64 C65 C70 -99.6(7) . . . . ?
C63 C64 C65 C66 -108.5(7) . . . . ?
C71 C64 C65 C66 74.8(7) . . . . ?
C70 C65 C66 F26 -179.0(5) . . . . ?
C64 C65 C66 F26 6.3(9) . . . . ?
C70 C65 C66 C67 1.6(9) . . . . ?
C64 C65 C66 C67 -173.2(6) . . . . ?
F26 C66 C67 F27 -0.2(9) . . . . ?
C65 C66 C67 F27 179.2(6) . . . . ?
F26 C66 C67 C68 179.8(6) . . . . ?
C65 C66 C67 C68 -0.8(10) . . . . ?
F27 C67 C68 F28 0.2(10) . . . . ?
C66 C67 C68 F28 -179.9(6) . . . . ?
F27 C67 C68 C69 -179.9(6) . . . . ?
C66 C67 C68 C69 0.1(11) . . . . ?
F28 C68 C69 F29 -0.9(11) . . . . ?
C67 C68 C69 F29 179.2(6) . . . . ?
F28 C68 C69 C70 179.6(6) . . . . ?
C67 C68 C69 C70 -0.3(11) . . . . ?
F29 C69 C70 F30 0.0(9) . . . . ?
C68 C69 C70 F30 179.6(6) . . . . ?
F29 C69 C70 C65 -178.2(6) . . . . ?
C68 C69 C70 C65 1.3(10) . . . . ?
C66 C65 C70 F30 179.9(5) . . . . ?
C64 C65 C70 F30 -5.4(8) . . . . ?
C66 C65 C70 C69 -1.9(9) . . . . ?
C64 C65 C70 C69 172.8(6) . . . . ?
C74 N8 C71 C64 -178.3(5) . . . . ?
Ge2 N8 C71 C64 14.3(8) . . . . ?
C74 N8 C71 C72 -0.1(6) . . . . ?
Ge2 N8 C71 C72 -167.6(4) . . . . ?
C63 C64 C71 N8 4.3(8) . . . . ?
C65 C64 C71 N8 -179.1(5) . . . . ?
C63 C64 C71 C72 -173.3(6) . . . . ?
C65 C64 C71 C72 3.3(9) . . . . ?
N8 C71 C72 C73 -0.4(6) . . . . ?
C64 C71 C72 C73 177.5(6) . . . . ?
C71 C72 C73 C74 0.7(6) . . . . ?
C71 N8 C74 C38 -179.9(4) . . . . ?
Ge2 N8 C74 C38 -10.3(6) . . . . ?
C71 N8 C74 C73 0.5(6) . . . . ?
Ge2 N8 C74 C73 170.2(3) . . . . ?
N7 C38 C74 N8 0.2(7) . . . . ?
C39 C38 C74 N8 -178.1(6) . . . . ?
N7 C38 C74 C73 179.6(6) . . . . ?
C39 C38 C74 C73 1.3(13) . . . . ?
C72 C73 C74 N8 -0.7(6) . . . . ?
C72 C73 C74 C38 179.8(6) . . . . ?
C75 C76 C77 C78 -179.6(5) . . . . ?
C76 C77 C78 C79 -175.2(5) . . . . ?

C77 C78 C79 C80 178.8(5) . . . . ?

loop_
_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
_geom_hbond_atom_site_label_A
_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_site_symmetry_A
O2 H2A O1 0.84 2.01 2.841(5) 172.4 .

_diffrn_measured_fraction_theta_max 0.999
_diffrn_reflns_theta_full 25.00
_diffrn_measured_fraction_theta_full 0.999
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_refine_diff_density_min -0.611
_refine_diff_density_rms 0.083
_database_code_depnum_ccdc_archive 'CCDC 945439'