data-nitrile**13**

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_chemical_formula_weight           253.68

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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'
 'Cl'  'Cl'   0.1484   0.1585
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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 '-x+1/2, -y, z+1/2'
 '-x, y+1/2, -z+1/2'
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'x+1/2, -y+1/2, -z'

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_cell_length_b 10.4147(6)
_cell_length_c 15.7193(8)
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
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_cell_volume 1113.49(11)
_cell_formula_units_Z 4
_cell_measurement_temperature 213(2)
_cell_measurement_reflns_used ?
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_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     ?
_computing_publication_material   ?

_refine_special_details
;
 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.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0454P)^2^+0.0976P] where
P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      none
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 'Flack H D (1983), Acta Cryst. A39, 876-881'
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_refine_ls_goodness_of_fit_ref    1.037
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 _atom_site_adp_type
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.
C7 C -0.7432(2) -0.42062(15) -0.24242(9) 0.0274(3) Uani 1 1 d . . .
H7A H -0.8538 -0.4251 -0.2833 0.033 Uiso 1 1 calc R . .
N2 N -0.22074(19) -0.48035(14) -0.31889(8) 0.0323(3) Uani 1 1 d . .
.
C5 C -0.9497(2) -0.54425(16) -0.13726(9) 0.0329(3) Uani 1 1 d . . .
O1 O -1.05466(18) -0.63839(13) -0.13762(7) 0.0417(3) Uani 1 1 d . .
.
C8 C -0.5570(2) -0.41565(14) -0.29469(8) 0.0258(3) Uani 1 1 d . . .
C10 C -0.3890(2) -0.35257(17) -0.42251(10) 0.0324(3) Uani 1 1 d . .
.
H10A H -0.3844 -0.3092 -0.4749 0.039 Uiso 1 1 calc R . .
C6 C -0.7577(2) -0.54123(15) -0.18616(10) 0.0324(3) Uani 1 1 d . . .
H6A H -0.7481 -0.6180 -0.2220 0.039 Uiso 1 1 calc R . .
H6B H -0.6476 -0.5424 -0.1460 0.039 Uiso 1 1 calc R . .
C11 C -0.2303(2) -0.42216(15) -0.39301(9) 0.0286(3) Uani 1 1 d . . .
C12 C -0.3844(2) -0.47562(16) -0.27089(10) 0.0311(3) Uani 1 1 d . .
.
H12A H -0.3810 -0.5160 -0.2174 0.037 Uiso 1 1 calc R . .
C1 C -0.6081(3) -0.27773(16) -0.13017(10) 0.0352(4) Uani 1 1 d . . .
N1 N -0.4760(3) -0.26310(17) -0.08664(10) 0.0531(4) Uani 1 1 d . . .
C3 C -0.9719(3) -0.30318(16) -0.14106(11) 0.0363(4) Uani 1 1 d . . .
H3A H -1.0794 -0.2989 -0.1825 0.044 Uiso 1 1 calc R . .
H3B H -0.9827 -0.2281 -0.1038 0.044 Uiso 1 1 calc R . .
C9 C -0.5538(2) -0.34932(16) -0.37217(10) 0.0314(3) Uani 1 1 d . . .
H9A H -0.6648 -0.3025 -0.3897 0.038 Uiso 1 1 calc R . .
C4 C -0.9953(3) -0.42497(17) -0.08754(10) 0.0389(4) Uani 1 1 d . . .
H4A H -0.9072 -0.4201 -0.0383 0.047 Uiso 1 1 calc R . .
H4B H -1.1305 -0.4299 -0.0663 0.047 Uiso 1 1 calc R . .
C2 C -0.7756(2) -0.29761(15) -0.18840(10) 0.0290(3) Uani 1 1 d . . .
H2B H -0.7805 -0.2236 -0.2278 0.035 Uiso 1 1 calc R . .

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0.00199(18)
C7 0.0264(7) 0.0277(8) 0.0281(7) -0.0026(6) -0.0021(6) 0.0003(6)
N2 0.0288(6) 0.0338(7) 0.0345(7) 0.0024(6) 0.0004(5) 0.0033(6)
C5 0.0361(8) 0.0341(9) 0.0284(7) 0.0051(6) -0.0015(6) -0.0038(7)
O1 0.0451(7) 0.0405(7) 0.0394(6) 0.0040(5) 0.0019(5) -0.0150(6)
C8 0.0287(7) 0.0246(7) 0.0241(7) -0.0028(6) -0.0020(5) -0.0019(6)
C10 0.0368(8) 0.0343(9) 0.0261(7) 0.0046(7) -0.0035(6) -0.0025(7)
C6 0.0349(8) 0.0250(8) 0.0374(8) -0.0008(6) 0.0040(7) -0.0005(7)
C11 0.0291(7) 0.0278(8) 0.0291(7) -0.0047(6) 0.0031(6) -0.0046(6)
C12 0.0298(7) 0.0347(9) 0.0287(7) 0.0040(7) 0.0006(6) 0.0026(6)
C1 0.0404(9) 0.0308(9) 0.0344(9) -0.0052(7) 0.0024(8) -0.0016(7)
N1 0.0477(10) 0.0599(11) 0.0519(10) -0.0182(8) -0.0085(9) -
0.0032(9)
C3 0.0335(8) 0.0332(8) 0.0423(9) -0.0046(7) 0.0054(7) 0.0040(7)
C9 0.0303(7) 0.0337(8) 0.0301(8) 0.0044(7) -0.0044(6) 0.0033(7)
C4 0.0404(9) 0.0407(9) 0.0357(8) -0.0018(7) 0.0099(7) -0.0037(8)
C2 0.0312(8) 0.0241(8) 0.0317(8) -0.0001(6) 0.0003(7) 0.0008(6)

_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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 _geom_bond_atom_site_label_2
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C7 C8 1.5107(19) . ?
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N2 C11 1.315(2) . ?
N2 C12 1.346(2) . ?
C5 O1 1.213(2) . ?
C5 C4 1.500(2) . ?
C5 C6 1.515(2) . ?
C8 C12 1.382(2) . ?
C8 C9 1.400(2) . ?
C10 C9 1.373(2) . ?
C10 C11 1.381(2) . ?
C1 N1 1.139(2) . ?
C1 C2 1.476(2) . ?
C3 C2 1.530(2) . ?
C3 C4 1.530(2) . ?

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C8 C7 C6 113.21(12) . . ?
C8 C7 C2 112.84(13) . . ?
C6 C7 C2 110.49(12) . . ?
C11 N2 C12 116.06(13) . . ?
O1 C5 C4 123.38(15) . . ?
O1 C5 C6 121.45(15) . . ?
C4 C5 C6 115.16(14) . . ?
C12 C8 C9 116.45(14) . . ?
C12 C8 C7 123.35(13) . . ?
C9 C8 C7 120.20(13) . . ?
C9 C10 C11 117.26(13) . . ?
C5 C6 C7 111.31(13) . . ?
N2 C11 C10 125.31(14) . . ?
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N2 C11 Cl1 115.61(12) . . ?
C10 C11 Cl1 119.06(11) . . ?
N2 C12 C8 124.58(14) . . ?
N1 C1 C2 178.49(17) . . ?
C2 C3 C4 112.92(14) . . ?
C10 C9 C8 120.13(14) . . ?
C5 C4 C3 112.24(13) . . ?
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C3 C2 C7 111.02(13) . . ?

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 _geom_torsion_site_symmetry_1
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 _geom_torsion_site_symmetry_3
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C6 C7 C8 C12 -26.6(2) . . . . ?
C2 C7 C8 C12 99.89(18) . . . . ?
C6 C7 C8 C9 152.56(14) . . . . ?
C2 C7 C8 C9 -81.01(16) . . . . ?
O1 C5 C6 C7 129.45(16) . . . . ?
C4 C5 C6 C7 -52.12(17) . . . . ?
C8 C7 C6 C5 -178.07(12) . . . . ?
C2 C7 C6 C5 54.26(16) . . . . ?
C12 N2 C11 C10 3.5(2) . . . . ?
C12 N2 C11 Cl1 -175.08(12) . . . . ?
C9 C10 C11 N2 -3.5(2) . . . . ?
C9 C10 C11 Cl1 175.04(11) . . . . ?
C11 N2 C12 C8 0.5(2) . . . . ?
C9 C8 C12 N2 -4.0(2) . . . . ?
C7 C8 C12 N2 175.14(14) . . . . ?
C11 C10 C9 C8 -0.5(2) . . . . ?
C12 C8 C9 C10 3.9(2) . . . . ?
C7 C8 C9 C10 -175.31(14) . . . . ?
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O1 C5 C4 C3 -132.31(17) . . . . ?
C6 C5 C4 C3 49.30(19) . . . . ?
C2 C3 C4 C5 -49.83(19) . . . . ?
N1 C1 C2 C3 167(7) . . . . ?
N1 C1 C2 C7 42(7) . . . . ?
C4 C3 C2 C1 -70.01(18) . . . . ?
C4 C3 C2 C7 53.76(17) . . . . ?
C8 C7 C2 C1 -58.75(16) . . . . ?
C6 C7 C2 C1 69.12(16) . . . . ?
C8 C7 C2 C3 176.35(12) . . . . ?
C6 C7 C2 C3 -55.77(16) . . . . ?

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'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'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'
'Si'  'Si'   0.0817   0.0704
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Cl'  'Cl'   0.1484   0.1585
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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loop_
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 'x, y, z'
 '-x, y+1/2, -z'

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_cell_formula_units_Z              2
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_exptl_special_details
;
 ?
;

_diffrn_ambient_temperature      213(2)
_diffrn_radiation_wavelength     0.71073
_diffrn_radiation_type           MoK\a
_diffrn_radiation_source         'fine-focus sealed tube'
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_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     ?
_computing_publication_material   ?

_refine_special_details
;
 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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_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
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P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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 'Flack H D (1983), Acta Cryst. A39, 876-881'
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Si1 Si 0.68667(8) 0.81929(17) 0.41719(8) 0.0385(3) Uani 1 1 d . . .
Cl1 Cl 1.30788(8) 0.6276(2) 0.93433(9) 0.0600(4) Uani 1 1 d . . .
Cl1S Cl 1.04632(16) 0.8863(3) 0.96389(15) 0.1029(8) Uani 1 1 d . . .
C1S C 1.1220(7) 1.0720(13) 0.9515(6) 0.104(3) Uani 1 1 d . . .
H1SA H 1.1353 1.0670 0.8915 0.124 Uiso 1 1 calc R . .
H1SB H 1.0879 1.1842 0.9558 0.124 Uiso 1 1 calc R . .
O2 O 0.76358(18) 0.8005(4) 0.51663(17) 0.0314(5) Uani 1 1 d . . .
N3 N 0.8969(2) 0.6283(4) 0.5112(2) 0.0285(6) Uani 1 1 d . . .
H3A H 0.9018 0.6912 0.4646 0.034 Uiso 1 1 calc R . .
C5 C 0.8168(2) 0.6534(5) 0.5546(2) 0.0265(7) Uani 1 1 d . . .
O1 O 1.0376(2) 0.4826(4) 0.5240(2) 0.0411(7) Uani 1 1 d . . .
O5 O 0.8798(2) 1.1472(4) 0.8353(2) 0.0425(7) Uani 1 1 d . . .
O4 O 0.9550(2) 1.0281(4) 0.7372(2) 0.0389(6) Uani 1 1 d . . .
C2 C 0.9318(3) 0.3999(5) 0.6201(3) 0.0319(8) Uani 1 1 d . . .
H2A H 0.9776 0.3028 0.6434 0.038 Uiso 1 1 calc R . .
```

C28 C 1.1954(3) 0.6109(6) 0.8625(3) 0.0384(9) Uani 1 1 d . . .
O3 O 0.7257(2) 0.6628(5) 0.7138(2) 0.0453(7) Uani 1 1 d . . .
C4 C 0.7619(3) 0.4764(5) 0.5460(3) 0.0327(8) Uani 1 1 d . . .
H4A H 0.7314 0.4540 0.4829 0.039 Uiso 1 1 calc R . .
H4B H 0.7122 0.4829 0.5801 0.039 Uiso 1 1 calc R . .
C1 C 0.9626(2) 0.5040(5) 0.5467(2) 0.0284(7) Uani 1 1 d . . .
N2 N 0.8120(2) 0.9103(5) 0.7597(2) 0.0316(7) Uani 1 1 d . . .
C14 C 0.8896(3) 1.0262(5) 0.7730(3) 0.0331(8) Uani 1 1 d . . .
C24 C 0.9237(3) 0.5339(5) 0.6962(2) 0.0289(7) Uani 1 1 d . . .
H24A H 0.8874 0.4732 0.7353 0.035 Uiso 1 1 calc R . .
C26 C 1.0836(3) 0.6970(6) 0.7312(3) 0.0347(8) Uani 1 1 d . . .
H26A H 1.0658 0.7675 0.6792 0.042 Uiso 1 1 calc R . .
C13 C 0.7961(3) 0.7520(5) 0.7097(2) 0.0297(7) Uani 1 1 d . . .
N1 N 1.1368(3) 0.4951(6) 0.8873(2) 0.0481(10) Uani 1 1 d . . .
C12 C 0.8648(2) 0.6987(5) 0.6540(2) 0.0252(6) Uani 1 1 d . . .
H12A H 0.9092 0.7999 0.6540 0.030 Uiso 1 1 calc R . .
C16 C 0.7434(3) 0.9702(6) 0.8121(3) 0.0351(8) Uani 1 1 d . . .
H16A H 0.7222 0.8675 0.8436 0.042 Uiso 1 1 calc R . .
C25 C 1.0207(3) 0.5765(5) 0.7530(2) 0.0299(7) Uani 1 1 d . . .
C15 C 0.8055(3) 1.0954(7) 0.8786(3) 0.0425(9) Uani 1 1 d . . .
H15A H 0.7693 1.2004 0.8904 0.051 Uiso 1 1 calc R . .
H15B H 0.8316 1.0337 0.9353 0.051 Uiso 1 1 calc R . .
C18 C 0.5881(3) 1.1201(7) 0.8051(3) 0.0409(9) Uani 1 1 d . . .
C3 C 0.8312(3) 0.3229(6) 0.5823(3) 0.0365(8) Uani 1 1 d . . .
H3B H 0.8332 0.2376 0.5340 0.044 Uiso 1 1 calc R . .
H3C H 0.8094 0.2588 0.6298 0.044 Uiso 1 1 calc R . .
C27 C 1.1745(3) 0.7144(6) 0.7870(3) 0.0397(9) Uani 1 1 d . . .
H27A H 1.2194 0.7942 0.7730 0.048 Uiso 1 1 calc R . .
C29 C 1.0511(3) 0.4827(6) 0.8335(3) 0.0406(9) Uani 1 1 d . . .
H29A H 1.0074 0.4047 0.8508 0.049 Uiso 1 1 calc R . .
C17 C 0.6579(3) 1.0632(8) 0.7509(3) 0.0446(10) Uani 1 1 d . . .
H17A H 0.6795 1.1685 0.7227 0.054 Uiso 1 1 calc R . .
H17B H 0.6270 0.9806 0.7033 0.054 Uiso 1 1 calc R . .
C10 C 0.6841(3) 1.0649(7) 0.3988(3) 0.0461(11) Uani 1 1 d . . .
H10A H 0.6714 1.1239 0.4520 0.055 Uiso 1 1 calc R . .
H10B H 0.7473 1.1034 0.3928 0.055 Uiso 1 1 calc R . .
C23 C 0.5318(3) 0.9955(8) 0.8358(3) 0.0506(11) Uani 1 1 d . . .
H23A H 0.5357 0.8737 0.8211 0.061 Uiso 1 1 calc R . .
C19 C 0.5786(4) 1.2964(7) 0.8276(3) 0.0498(11) Uani 1 1 d . . .
H19A H 0.6157 1.3840 0.8075 0.060 Uiso 1 1 calc R . .

C8 C 0.5669(4) 0.7355(7) 0.4243(4) 0.0620(15) Uani 1 1 d . . .
H8A H 0.5201 0.7745 0.3707 0.074 Uiso 1 1 calc R . .
H8B H 0.5677 0.6040 0.4245 0.074 Uiso 1 1 calc R . .
C22 C 0.4694(4) 1.0487(10) 0.8883(4) 0.0608(14) Uani 1 1 d . . .
H22A H 0.4316 0.9625 0.9085 0.073 Uiso 1 1 calc R . .
C20 C 0.5154(4) 1.3491(9) 0.8793(4) 0.0585(14) Uani 1 1 d . . .
H20A H 0.5094 1.4711 0.8926 0.070 Uiso 1 1 calc R . .
C21 C 0.4629(4) 1.2245(10) 0.9106(4) 0.0621(16) Uani 1 1 d . . .
H21A H 0.4221 1.2591 0.9474 0.074 Uiso 1 1 calc R . .
C6 C 0.7152(5) 0.6788(10) 0.3250(4) 0.0707(16) Uani 1 1 d . . .
H6A H 0.6793 0.5760 0.3038 0.085 Uiso 1 1 calc R . .
C7 C 0.7945(6) 0.7340(13) 0.2877(5) 0.092(2) Uani 1 1 d . . .
H7A H 0.8019 0.6502 0.2413 0.138 Uiso 1 1 calc R . .
H7B H 0.8522 0.7358 0.3347 0.138 Uiso 1 1 calc R . .
H7C H 0.7824 0.8532 0.2620 0.138 Uiso 1 1 calc R . .
C11 C 0.6110(4) 1.1292(9) 0.3168(4) 0.0723(19) Uani 1 1 d . . .
H11A H 0.6142 1.2589 0.3126 0.108 Uiso 1 1 calc R . .
H11B H 0.5479 1.0943 0.3224 0.108 Uiso 1 1 calc R . .
H11C H 0.6242 1.0755 0.2632 0.108 Uiso 1 1 calc R . .
C9 C 0.5356(5) 0.8010(9) 0.5071(7) 0.084(2) Uani 1 1 d . . .
H9A H 0.4732 0.7527 0.5072 0.125 Uiso 1 1 calc R . .
H9B H 0.5327 0.9311 0.5066 0.125 Uiso 1 1 calc R . .
H9C H 0.5808 0.7611 0.5606 0.125 Uiso 1 1 calc R . .
Cl3S Cl 1.2244(5) 1.0748(5) 1.0275(5) 0.336(5) Uani 1 1 d . . .

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Cl1 0.0339(5) 0.0830(9) 0.0537(7) -0.0156(6) -0.0096(4) 0.0019(6)
Cl1S 0.0991(14) 0.1193(17) 0.0979(14) 0.0467(13) 0.0382(11)
0.0406(13)
C1S 0.140(8) 0.083(5) 0.080(5) -0.007(4) 0.007(5) 0.019(5)
O2 0.0292(12) 0.0345(13) 0.0284(12) 0.0012(11) 0.0022(9)
0.0070(11)

N3 0.0322(14) 0.0311(14) 0.0239(13) 0.0015(12) 0.0099(11) -0.0015(12)
C5 0.0259(15) 0.0288(16) 0.0238(15) 0.0003(13) 0.0037(12) 0.0015(13)
O1 0.0385(15) 0.0389(15) 0.0498(17) -0.0023(13) 0.0180(13) 0.0069(12)
O5 0.0461(16) 0.0388(15) 0.0435(16) -0.0083(13) 0.0123(12) -0.0039(13)
O4 0.0421(15) 0.0338(14) 0.0438(15) -0.0020(12) 0.0160(12) -0.0076(12)
C2 0.0341(18) 0.0242(16) 0.0341(18) 0.0042(14) 0.0008(14) 0.0016(14)
C28 0.0244(16) 0.045(2) 0.041(2) -0.0128(18) -0.0030(14) 0.0034(16)
O3 0.0421(16) 0.0528(18) 0.0464(17) -0.0150(15) 0.0214(13) -0.0145(14)
C4 0.0307(18) 0.0289(17) 0.0362(19) 0.0004(15) 0.0030(14) -0.0047(14)
C1 0.0293(17) 0.0258(16) 0.0291(17) -0.0075(13) 0.0046(13) 0.0003(13)
N2 0.0309(15) 0.0363(16) 0.0291(15) -0.0028(13) 0.0097(12) 0.0006(13)
C14 0.0368(19) 0.0279(17) 0.0314(18) 0.0029(14) 0.0014(15) -0.0026(15)
C24 0.0335(18) 0.0292(17) 0.0236(15) 0.0026(13) 0.0052(13) 0.0001(14)
C26 0.0315(18) 0.040(2) 0.0312(18) 0.0012(15) 0.0048(14) 0.0042(16)
C13 0.0261(16) 0.0365(18) 0.0267(16) -0.0013(14) 0.0064(12) -0.0010(14)
N1 0.047(2) 0.057(2) 0.0329(18) 0.0033(17) -0.0069(15) 0.0055(18)
C12 0.0241(15) 0.0294(16) 0.0222(15) 0.0002(13) 0.0053(12) -0.0029(13)
C16 0.0346(19) 0.042(2) 0.0292(18) -0.0006(16) 0.0082(14) 0.0046(16)
C25 0.0314(17) 0.0339(18) 0.0235(16) -0.0016(13) 0.0043(13) 0.0018(14)
C15 0.044(2) 0.051(2) 0.033(2) -0.0077(18) 0.0090(16) -0.0005(19)

C18 0.0311(18) 0.059(3) 0.0280(18) -0.0043(18) -0.0029(14)
0.0065(19)
C3 0.0363(19) 0.0273(16) 0.042(2) 0.0019(16) 0.0003(15) -
0.0088(16)
C27 0.0280(18) 0.045(2) 0.045(2) -0.0041(18) 0.0066(16) -
0.0070(17)
C29 0.038(2) 0.044(2) 0.035(2) 0.0090(17) -0.0022(15) -0.0072(17)
C17 0.039(2) 0.062(3) 0.0313(19) -0.0049(19) 0.0054(15) 0.015(2)
C10 0.035(2) 0.051(2) 0.044(2) 0.019(2) -0.0074(17) -0.0065(18)
C23 0.040(2) 0.067(3) 0.041(2) -0.009(2) 0.0019(18) 0.007(2)
C19 0.053(3) 0.052(3) 0.040(2) 0.009(2) 0.0012(18) 0.011(2)
C8 0.044(3) 0.046(3) 0.081(4) 0.002(3) -0.017(3) -0.008(2)
C22 0.039(2) 0.083(4) 0.060(3) 0.004(3) 0.009(2) 0.003(3)
C20 0.049(3) 0.072(4) 0.050(3) -0.013(3) 0.002(2) 0.023(3)
C21 0.039(2) 0.101(5) 0.047(3) -0.006(3) 0.010(2) 0.020(3)
C6 0.078(4) 0.077(4) 0.054(3) -0.012(3) 0.008(3) -0.015(3)
C7 0.110(6) 0.096(5) 0.069(4) 0.001(4) 0.019(4) -0.021(5)
C11 0.067(3) 0.057(3) 0.072(4) 0.027(3) -0.028(3) -0.011(3)
C9 0.061(4) 0.051(3) 0.150(7) -0.013(4) 0.048(4) -0.010(3)
Cl3S 0.346(7) 0.0700(16) 0.428(9) 0.026(3) -0.250(7) -0.022(3)

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;
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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Si1 C10 1.851(5) . ?

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Cl1 C28 1.747(4) . ?
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C1S Cl3S 1.662(10) . ?
O2 C5 1.388(4) . ?
N3 C1 1.349(5) . ?
N3 C5 1.471(4) . ?
C5 C4 1.529(5) . ?
C5 C12 1.559(5) . ?
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O5 C14 1.343(5) . ?
O5 C15 1.437(5) . ?
O4 C14 1.194(5) . ?
C2 C1 1.512(5) . ?
C2 C3 1.547(5) . ?
C2 C24 1.559(5) . ?
C28 N1 1.323(6) . ?
C28 C27 1.364(7) . ?
O3 C13 1.229(5) . ?
C4 C3 1.538(6) . ?
N2 C14 1.392(5) . ?
N2 C13 1.396(5) . ?
N2 C16 1.479(5) . ?
C24 C25 1.505(5) . ?
C24 C12 1.549(5) . ?
C26 C25 1.371(6) . ?
C26 C27 1.400(6) . ?
C13 C12 1.501(5) . ?
N1 C29 1.324(5) . ?
C16 C15 1.514(6) . ?
C16 C17 1.535(6) . ?
C25 C29 1.398(5) . ?
C18 C19 1.373(7) . ?
C18 C23 1.385(8) . ?
C18 C17 1.505(6) . ?
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C23 C22 1.393(7) . ?
C19 C20 1.394(7) . ?
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C20 C21 1.353(9) . ?
C6 C7 1.452(10) . ?

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C10 Si1 C8 110.7(2) . . ?
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C10 Si1 C6 115.9(3) . . ?
C8 Si1 C6 102.8(3) . . ?
Cl3S C1S Cl1S 113.6(6) . . ?
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C14 O5 C15 110.9(3) . . ?
C1 C2 C3 108.8(3) . . ?
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C3 C2 C24 107.0(3) . . ?
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C14 N2 C16 110.5(3) . . ?
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C13 N2 C16 120.3(3) . . ?
O4 C14 O5 122.6(4) . . ?
O4 C14 N2 129.4(4) . . ?
O5 C14 N2 108.0(3) . . ?
C25 C24 C12 115.1(3) . . ?
C25 C24 C2 110.4(3) . . ?
C12 C24 C2 108.9(3) . . ?
C25 C26 C27 119.6(4) . . ?
O3 C13 N2 117.7(3) . . ?
O3 C13 C12 123.2(3) . . ?
N2 C13 C12 119.2(3) . . ?
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C13 C12 C24 110.1(3) . . ?
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C24 C12 C5 108.4(3) . . ?
N2 C16 C15 100.5(3) . . ?
N2 C16 C17 110.5(3) . . ?
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C26 C25 C24 125.4(3) . . ?
C29 C25 C24 118.0(3) . . ?
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C4 C3 C2 109.8(3) . . ?
C28 C27 C26 117.4(4) . . ?
N1 C29 C25 125.1(4) . . ?
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C18 C23 C22 120.8(5) . . ?
C18 C19 C20 121.9(5) . . ?
C9 C8 Si1 113.4(4) . . ?
C21 C22 C23 120.5(6) . . ?
C21 C20 C19 120.0(6) . . ?
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C7 C6 Si1 117.8(5) . . ?

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C5 N3 C1 C2 6.5(4) . . . . ?
C3 C2 C1 O1 -128.1(4) . . . . ?
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C3 C2 C1 N3 53.7(4) . . . . ?
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C13 N2 C14 O5 -171.9(4) . . . . ?
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C14 N2 C13 O3 173.9(4) . . . . ?
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C14 N2 C13 C12 -6.2(6) . . . . ?
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N2 C13 C12 C24 109.0(4) . . . . ?
O3 C13 C12 C5 51.1(5) . . . . ?
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C25 C24 C12 C13 -98.0(4) . . . . ?
C2 C24 C12 C13 137.5(3) . . . . ?
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N3 C5 C12 C13 173.0(3) . . . . ?
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O2 C5 C12 C24 179.7(3) . . . . ?
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C14 N2 C16 C17 102.9(4) . . . . ?
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C27 C26 C25 C24 -175.3(4) . . . . ?
C12 C24 C25 C26 -43.5(5) . . . . ?
C2 C24 C25 C26 80.2(5) . . . . ?
C12 C24 C25 C29 138.4(4) . . . . ?
C2 C24 C25 C29 -97.9(4) . . . . ?
C14 O5 C15 C16 -22.5(4) . . . . ?
N2 C16 C15 O5 23.0(4) . . . . ?
C17 C16 C15 O5 -95.2(4) . . . . ?
C5 C4 C3 C2 3.2(5) . . . . ?
C1 C2 C3 C4 -57.3(4) . . . . ?
C24 C2 C3 C4 59.3(4) . . . . ?
N1 C28 C27 C26 0.1(7) . . . . ?
Cl1 C28 C27 C26 180.0(3) . . . . ?
C25 C26 C27 C28 -1.3(6) . . . . ?
C28 N1 C29 C25 2.3(7) . . . . ?
C26 C25 C29 N1 -3.5(7) . . . . ?
C24 C25 C29 N1 174.7(4) . . . . ?
C19 C18 C17 C16 105.5(5) . . . . ?

C23 C18 C17 C16 -73.3(5) . . . . ?
N2 C16 C17 C18 179.0(4) . . . . ?
C15 C16 C17 C18 -68.8(5) . . . . ?
O2 Si1 C10 C11 -173.5(4) . . . . ?
C8 Si1 C10 C11 -55.9(5) . . . . ?
C6 Si1 C10 C11 60.7(5) . . . . ?
C19 C18 C23 C22 -0.9(6) . . . . ?
C17 C18 C23 C22 178.0(4) . . . . ?
C23 C18 C19 C20 0.2(7) . . . . ?
C17 C18 C19 C20 -178.6(4) . . . . ?
O2 Si1 C8 C9 44.8(5) . . . . ?
C10 Si1 C8 C9 -67.4(5) . . . . ?
C6 Si1 C8 C9 168.1(5) . . . . ?
C18 C23 C22 C21 -0.1(8) . . . . ?
C18 C19 C20 C21 1.4(7) . . . . ?
C19 C20 C21 C22 -2.5(8) . . . . ?
C23 C22 C21 C20 1.9(8) . . . . ?
O2 Si1 C6 C7 -72.9(6) . . . . ?
C10 Si1 C6 C7 45.8(7) . . . . ?
C8 Si1 C6 C7 166.8(6) . . . . ?

_diffrn_measured_fraction_theta_max 0.997
_diffrn_reflns_theta_full 28.35
_diffrn_measured_fraction_theta_full 0.997
_refine_diff_density_max 1.438
_refine_diff_density_min -0.868
_refine_diff_density_rms 0.092