```
data_k05kcm23

_audit_creation_method            SHELXL-97
_chemical_name_systematic
;
 ?
;
_chemical_name_common             ?
_chemical_melting_point           ?
_chemical_formula_moiety          ?
_chemical_formula_sum
 'C16 H20 Cl6 N2 O2 Sn'
_chemical_formula_weight          603.73

loop_
 _atom_type_symbol
 _atom_type_description
 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
'C'  'C'   0.0033   0.0016
 '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'
'Cl'  'Cl'   0.1484   0.1585
 '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'
'Sn'  'Sn'  -0.6537   1.4246
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting            ?
_symmetry_space_group_name_H-M    ?

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

_cell_length_a                    7.37800(10)
_cell_length_b                    7.44800(10)
_cell_length_c                    11.5170(2)
_cell_angle_alpha                   97.6240(10)
_cell_angle_beta                  91.4810(10)
_cell_angle_gamma                     117.3890(10)
_cell_volume                      554.243(14)
_cell_formula_units_Z             1
```

```
_cell_measurement_temperature     150(2)
_cell_measurement_reflns_used     ?
_cell_measurement_theta_min       ?
_cell_measurement_theta_max       ?

_exptl_crystal_description        ?
_exptl_crystal_colour             ?
_exptl_crystal_size_max           ?
_exptl_crystal_size_mid           ?
_exptl_crystal_size_min           ?
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.809
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              298
_exptl_absorpt_coefficient_mu     1.891
_exptl_absorpt_correction_type    ?
_exptl_absorpt_correction_T_min   ?
_exptl_absorpt_correction_T_max   ?
_exptl_absorpt_process_details    ?

_exptl_special_details
;
 ?
;

_diffrn_ambient_temperature       150(2)
_diffrn_radiation_wavelength      0.71073
_diffrn_radiation_type            MoK\a
_diffrn_radiation_source          'fine-focus sealed tube'
_diffrn_radiation_monochromator   graphite
_diffrn_measurement_device_type   ?
_diffrn_measurement_method        ?
_diffrn_detector_area_resol_mean  ?
_diffrn_standards_number          ?
_diffrn_standards_interval_count  ?
_diffrn_standards_interval_time   ?
_diffrn_standards_decay_%         ?
_diffrn_reflns_number             8539
_diffrn_reflns_av_R_equivalents   0.0270
_diffrn_reflns_av_sigmaI/netI     0.0261
_diffrn_reflns_limit_h_min        -8
_diffrn_reflns_limit_h_max        8
_diffrn_reflns_limit_k_min        -8
_diffrn_reflns_limit_k_max        8
_diffrn_reflns_limit_l_min        -13
_diffrn_reflns_limit_l_max        13
_diffrn_reflns_theta_min          3.85
_diffrn_reflns_theta_max          24.97
_reflns_number_total              1909
_reflns_number_gt                 1890
```

```
_reflns_threshold_expression      >2sigma(I)

_computing_data_collection        ?
_computing_cell_refinement        ?
_computing_data_reduction         ?
_computing_structure_solution     ?
_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^)+(0.0120P)^2^+0.2090P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          1909
_refine_ls_number_parameters      136
_refine_ls_number_restraints      0
_refine_ls_R_factor_all           0.0156
_refine_ls_R_factor_gt            0.0154
_refine_ls_wR_factor_ref          0.0390
_refine_ls_wR_factor_gt           0.0388
_refine_ls_goodness_of_fit_ref    1.104
_refine_ls_restrained_S_all       1.104
_refine_ls_shift/su_max           0.001
_refine_ls_shift/su_mean          0.000

loop_
 _atom_site_label
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
```

```
 _atom_site_U_iso_or_equiv
 _atom_site_adp_type
 _atom_site_occupancy
 _atom_site_symmetry_multiplicity
 _atom_site_calc_flag
 _atom_site_refinement_flags
 _atom_site_disorder_assembly
 _atom_site_disorder_group
Sn Sn 0.5000 0.0000 0.0000 0.01455(7) Uani 1 2 d S . .
Cl1 Cl 0.16150(6) -0.22514(6) 0.05433(3) 0.02076(10) Uani 1 1 d . . .
Cl2 Cl 0.64998(6) -0.18451(6) 0.09292(3) 0.02024(10) Uani 1 1 d . . .
Cl3 Cl 0.56731(6) 0.22768(6) 0.18357(3) 0.02169(10) Uani 1 1 d . . .
O1 O 1.36508(17) 0.52884(18) 0.36931(10) 0.0281(3) Uani 1 1 d . . .
N1 N 1.2489(2) 0.4143(3) 0.14543(14) 0.0232(3) Uani 1 1 d . . .
H10A H 1.216(4) 0.497(4) 0.120(2) 0.050(7) Uiso 1 1 d . . .
H10B H 1.262(4) 0.338(4) 0.087(2) 0.055(7) Uiso 1 1 d . . .
H10C H 1.366(4) 0.494(4) 0.186(2) 0.052(7) Uiso 1 1 d . . .
C1 C 1.1055(2) 0.2873(3) 0.22441(14) 0.0224(3) Uani 1 1 d . . .
H1A H 1.0878 0.1459 0.2086 0.027 Uiso 1 1 calc R . .
H1B H 0.9697 0.2812 0.2104 0.027 Uiso 1 1 calc R . .
C2 C 1.1941(2) 0.3834(2) 0.35142(14) 0.0199(3) Uani 1 1 d . . .
C3 C 1.0664(2) 0.2936(2) 0.44582(14) 0.0189(3) Uani 1 1 d . . .
C4 C 1.1441(3) 0.3808(2) 0.56302(14) 0.0220(3) Uani 1 1 d . . .
H4 H 1.2768 0.4952 0.5808 0.026 Uiso 1 1 calc R . .
C5 C 1.0272(3) 0.2998(3) 0.65272(14) 0.0255(4) Uani 1 1 d . . .
H5 H 1.0795 0.3592 0.7323 0.031 Uiso 1 1 calc R . .
C6 C 0.8340(3) 0.1323(3) 0.62699(15) 0.0257(4) Uani 1 1 d . . .
H6 H 0.7537 0.0786 0.6891 0.031 Uiso 1 1 calc R . .
C7 C 0.7570(3) 0.0425(3) 0.51110(15) 0.0240(4) Uani 1 1 d . . .
H7 H 0.6257 -0.0741 0.4939 0.029 Uiso 1 1 calc R . .
C8 C 0.8728(2) 0.1238(2) 0.42053(14) 0.0216(3) Uani 1 1 d . . .
H8 H 0.8200 0.0636 0.3410 0.026 Uiso 1 1 calc R . .

loop_
 _atom_site_aniso_label
 _atom_site_aniso_U_11
 _atom_site_aniso_U_22
 _atom_site_aniso_U_33
 _atom_site_aniso_U_23
 _atom_site_aniso_U_13
 _atom_site_aniso_U_12
Sn 0.01356(10) 0.01427(10) 0.01314(10) -0.00040(6) -0.00002(6) 0.00500(7)
Cl1 0.0150(2) 0.0224(2) 0.0208(2) 0.00499(16) 0.00225(15) 0.00495(17)
Cl2 0.0202(2) 0.0200(2) 0.0205(2) 0.00314(15) -0.00052(15) 0.00952(17)
Cl3 0.0228(2) 0.0233(2) 0.01627(19) -0.00566(15) -0.00246(15) 0.01108(17)
O1 0.0199(6) 0.0277(6) 0.0269(6) -0.0001(5) -0.0011(5) 0.0043(5)
N1 0.0233(8) 0.0247(8) 0.0223(8) 0.0046(7) 0.0031(6) 0.0116(7)
C1 0.0190(8) 0.0241(8) 0.0211(8) 0.0038(7) 0.0021(6) 0.0075(7)
C2 0.0193(8) 0.0202(8) 0.0227(8) 0.0005(6) -0.0015(6) 0.0123(7)
C3 0.0203(8) 0.0198(8) 0.0211(8) 0.0015(6) 0.0009(6) 0.0136(7)
```

C4 0.0228(9) 0.0189(8) 0.0233(8) -0.0017(6) -0.0024(7) 0.0105(7)
C5 0.0346(10) 0.0264(9) 0.0182(8) -0.0015(7) 0.0002(7) 0.0180(8)
C6 0.0305(9) 0.0266(9) 0.0247(9) 0.0058(7) 0.0077(7) 0.0167(8)
C7 0.0218(9) 0.0213(8) 0.0301(9) 0.0038(7) 0.0026(7) 0.0111(7)
C8 0.0220(8) 0.0232(8) 0.0209(8) -0.0007(7) -0.0023(7) 0.0129(7)

_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.
;

loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
Sn Cl3 2.4107(4) 2_655 ?
Sn Cl3 2.4107(4) . ?
Sn Cl1 2.4386(4) 2_655 ?
Sn Cl1 2.4386(4) . ?
Sn Cl2 2.4467(4) . ?
Sn Cl2 2.4467(4) 2_655 ?
O1 C2 1.215(2) . ?
N1 C1 1.483(2) . ?
N1 H10A 0.83(3) . ?
N1 H10B 0.86(3) . ?
N1 H10C 0.87(3) . ?
C1 C2 1.524(2) . ?
C1 H1A 0.9900 . ?
C1 H1B 0.9900 . ?
C2 C3 1.478(2) . ?
C3 C8 1.394(2) . ?
C3 C4 1.399(2) . ?
C4 C5 1.381(2) . ?
C4 H4 0.9500 . ?
C5 C6 1.386(2) . ?
C5 H5 0.9500 . ?
C6 C7 1.388(2) . ?
C6 H6 0.9500 . ?
C7 C8 1.386(2) . ?
C7 H7 0.9500 . ?
C8 H8 0.9500 . ?

loop_

```
 _geom_angle_atom_site_label_1
 _geom_angle_atom_site_label_2
 _geom_angle_atom_site_label_3
 _geom_angle
 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_3
 _geom_angle_publ_flag
Cl3 Sn Cl3 180.000(11) 2_655 . ?
Cl3 Sn Cl1 89.722(13) 2_655 2_655 ?
Cl3 Sn Cl1 90.278(13) . 2_655 ?
Cl3 Sn Cl1 90.278(13) 2_655 . ?
Cl3 Sn Cl1 89.722(13) . . ?
Cl1 Sn Cl1 180.00(3) 2_655 . ?
Cl3 Sn Cl2 90.030(13) 2_655 . ?
Cl3 Sn Cl2 89.970(13) . . ?
Cl1 Sn Cl2 88.929(13) 2_655 . ?
Cl1 Sn Cl2 91.071(12) . . ?
Cl3 Sn Cl2 89.970(13) 2_655 2_655 ?
Cl3 Sn Cl2 90.030(13) . 2_655 ?
Cl1 Sn Cl2 91.071(13) 2_655 2_655 ?
Cl1 Sn Cl2 88.929(13) . 2_655 ?
Cl2 Sn Cl2 180.000(19) . 2_655 ?
C1 N1 H10A 114.2(17) . . ?
C1 N1 H10B 110.8(17) . . ?
H10A N1 H10B 109(2) . . ?
C1 N1 H10C 108.3(16) . . ?
H10A N1 H10C 103(2) . . ?
H10B N1 H10C 111(2) . . ?
N1 C1 C2 108.49(13) . . ?
N1 C1 H1A 110.0 . . ?
C2 C1 H1A 110.0 . . ?
N1 C1 H1B 110.0 . . ?
C2 C1 H1B 110.0 . . ?
H1A C1 H1B 108.4 . . ?
O1 C2 C3 123.83(15) . . ?
O1 C2 C1 118.35(14) . . ?
C3 C2 C1 117.82(14) . . ?
C8 C3 C4 119.73(15) . . ?
C8 C3 C2 121.53(15) . . ?
C4 C3 C2 118.73(15) . . ?
C5 C4 C3 119.75(15) . . ?
C5 C4 H4 120.1 . . ?
C3 C4 H4 120.1 . . ?
C4 C5 C6 120.25(16) . . ?
C4 C5 H5 119.9 . . ?
C6 C5 H5 119.9 . . ?
C5 C6 C7 120.43(16) . . ?
C5 C6 H6 119.8 . . ?
C7 C6 H6 119.8 . . ?
C8 C7 C6 119.66(16) . . ?
```

C8 C7 H7 120.2 . . ?
C6 C7 H7 120.2 . . ?
C7 C8 C3 120.15(15) . . ?
C7 C8 H8 119.9 . . ?
C3 C8 H8 119.9 . . ?

_diffrn_measured_fraction_theta_max 0.983
_diffrn_reflns_theta_full 24.97
_diffrn_measured_fraction_theta_full 0.983
_refine_diff_density_max 0.285
_refine_diff_density_min -0.702
_refine_diff_density_rms 0.071