Table S(1). Hard copy of Crystallographic Information File (CIF) for $Bi(S_2CN(CH_2)_4)_2Cl.CHCl_3$.

```
data_shelxl

_audit_creation_method            SHELXL-97

_chemical_melting_point           '230-23C'
_chemical_formula_moiety          ?
_chemical_formula_sum
 'C11 H17 Bi C14 N2 S4'
_chemical_formula_weight          656.29

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'
 'Bi'  'Bi'  -4.1077  10.2566
 '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'
 'S'  'S'   0.1246   0.1234
 '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'

_symmetry_cell_setting            monoclinic
_symmetry_space_group_name_H-M    P21/c

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

_cell_length_a                    12.7270(6)
_cell_length_b                    7.7452(4)
_cell_length_c                    21.1854(10)
_cell_angle_alpha                 90
_cell_angle_beta                  100.599(1)
_cell_angle_gamma                 90
_cell_volume                      2052.68(17)
_cell_formula_units_Z             4
_cell_measurement_temperature     183(2)
_cell_measurement_reflns_used     7345
_cell_measurement_theta_min       1.7
_cell_measurement_theta_max       30.0

_exptl_crystal_description        plate
_exptl_crystal_colour             yellow
_exptl_crystal_size_max           0.52
_exptl_crystal_size_mid           0.26
_exptl_crystal_size_min           0.05
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     2.124
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              1248
_exptl_absorpt_coefficient_mu     9.513
```

```
_exptl_absorpt_correction_type    'multi-scan'
_exptl_absorpt_correction_T_min   0.264
_exptl_absorpt_correction_T_max   1
_exptl_absorpt_process_details    '(SADABS; Bruker, 2000)'

_diffrn_ambient_temperature       183(2)
_diffrn_radiation_wavelength      0.71069
_diffrn_radiation_type            MoKalpha
_diffrn_radiation_source          'fine-focus sealed tube'
_diffrn_radiation_monochromator   graphite
_diffrn_measurement_device_type
'Bruker AXS SMART CCD diffractometer'
_diffrn_measurement_method        'omega scans'
_diffrn_detector_area_resol_mean  ?
_diffrn_standards_number          0
_diffrn_standards_interval_count  ?
_diffrn_standards_interval_time   ?
_diffrn_standards_decay_%         0
_diffrn_reflns_number             16366
_diffrn_reflns_av_R_equivalents   0.043
_diffrn_reflns_av_sigmaI/netI     0.069
_diffrn_reflns_limit_h_min        -17
_diffrn_reflns_limit_h_max        17
_diffrn_reflns_limit_k_min        -7
_diffrn_reflns_limit_k_max        10
_diffrn_reflns_limit_l_min        -27
_diffrn_reflns_limit_l_max        29
_diffrn_reflns_theta_min          1.7
_diffrn_reflns_theta_max          30.0
_reflns_number_total              5955
_reflns_number_gt                 5340
_reflns_threshold_expression      >2sigma(I)

_computing_data_collection        'SMART (Bruker, 2000)'
_computing_cell_refinement        'SAINT (Bruker, 2000)'
_computing_data_reduction         'SHELXTL (Bruker, 2000)'
_computing_structure_solution     'PATTY in DIRDIF92 (Beurskens et al., 1992)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     'ORTEPII (Johnson, 1976)'
_computing_publication_material
'SHELXL-97 (Bruker, 2000)'

_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^)+(0.0198P)^2^+2.4228P] 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          5955
_refine_ls_number_parameters      199
_refine_ls_number_restraints      0
_refine_ls_R_factor_all           0.040
_refine_ls_R_factor_gt            0.035
_refine_ls_wR_factor_ref          0.088
_refine_ls_wR_factor_gt           0.084
_refine_ls_goodness_of_fit_ref    1.06
```

```
_refine_ls_restrained_S_all      1.06
_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
Bi Bi 0.184044(10) -0.272051(18) 0.217216(7) 0.01061(6) Uani 1 1 d . . .
Cl1 Cl 0.12076(7) -0.56657(12) 0.28160(5) 0.0187(2) Uani 1 1 d . . .
Cl2 Cl 0.46495(10) 0.03863(18) -0.08820(8) 0.0402(3) Uani 1 1 d . . .
Cl3 Cl 0.58282(13) 0.3258(2) -0.02290(7) 0.0426(3) Uani 1 1 d . . .
Cl4 Cl 0.40540(13) 0.3888(2) -0.12533(9) 0.0589(5) Uani 1 1 d . . .
S1 S -0.02748(8) -0.21005(13) 0.21497(6) 0.0164(2) Uani 1 1 d . . .
S2 S 0.11333(7) 0.03612(12) 0.16211(5) 0.0153(2) Uani 1 1 d . . .
S3 S 0.11282(9) -0.39901(15) 0.10117(6) 0.0235(2) Uani 1 1 d . . .
S4 S 0.32509(7) -0.52819(13) 0.16764(5) 0.01401(19) Uani 1 1 d . . .
N1 N -0.0862(3) 0.1026(4) 0.17279(18) 0.0166(7) Uani 1 1 d . . .
N2 N 0.2125(3) -0.6630(5) 0.06146(17) 0.0156(7) Uani 1 1 d . . .
C1 C -0.0083(3) -0.0121(5) 0.18283(19) 0.0124(7) Uani 1 1 d . . .
C2 C -0.0771(4) 0.2765(5) 0.1459(3) 0.0271(11) Uani 1 1 d . . .
H2A H -0.0826 0.2722 0.0987 0.033 Uiso 1 1 calc R . .
H2B H -0.0089 0.3325 0.1654 0.033 Uiso 1 1 calc R . .
C3 C -0.1719(5) 0.3692(8) 0.1643(5) 0.071(3) Uani 1 1 d . . .
H3A H -0.1513 0.4252 0.2068 0.086 Uiso 1 1 calc R . .
H3B H -0.1993 0.4588 0.1321 0.086 Uiso 1 1 calc R . .
C4 C -0.2532(5) 0.2369(7) 0.1663(5) 0.053(2) Uani 1 1 d . . .
H4A H -0.2973 0.2197 0.1231 0.063 Uiso 1 1 calc R . .
H4B H -0.3006 0.2708 0.1963 0.063 Uiso 1 1 calc R . .
C5 C -0.1929(3) 0.0738(6) 0.1890(2) 0.0222(9) Uani 1 1 d . . .
H5A H -0.1879 0.0579 0.2358 0.027 Uiso 1 1 calc R . .
H5B H -0.2279 -0.0287 0.1664 0.027 Uiso 1 1 calc R . .
C6 C 0.2174(3) -0.5446(5) 0.10625(19) 0.0136(7) Uani 1 1 d . . .
C7 C 0.2949(4) -0.7963(6) 0.0600(2) 0.0211(9) Uani 1 1 d . . .
H7A H 0.3174 -0.8493 0.1029 0.025 Uiso 1 1 calc R . .
H7B H 0.3583 -0.7470 0.0457 0.025 Uiso 1 1 calc R . .
C8 C 0.2397(4) -0.9266(7) 0.0123(3) 0.0368(13) Uani 1 1 d . . .
H8A H 0.2033 -1.0158 0.0339 0.044 Uiso 1 1 calc R . .
H8B H 0.2915 -0.9838 -0.0105 0.044 Uiso 1 1 calc R . .
C9 C 0.1605(6) -0.8229(9) -0.0333(3) 0.0493(17) Uani 1 1 d . . .
H9A H 0.1945 -0.7714 -0.0673 0.059 Uiso 1 1 calc R . .
H9B H 0.0998 -0.8958 -0.0536 0.059 Uiso 1 1 calc R . .
C10 C 0.1233(4) -0.6836(7) 0.0076(2) 0.0279(10) Uani 1 1 d . . .
H10A H 0.1089 -0.5745 -0.0168 0.033 Uiso 1 1 calc R . .
H10B H 0.0576 -0.7197 0.0228 0.033 Uiso 1 1 calc R . .
C11 C 0.5118(4) 0.2479(6) -0.0965(3) 0.0263(11) Uani 1 1 d . . .
H11 H 0.5611 0.2454 -0.1282 0.032 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
Bi 0.01090(8) 0.00649(8) 0.01394(9) -0.00038(4) 0.00096(6) 0.00060(4)
Cl1 0.0157(4) 0.0121(4) 0.0298(6) 0.0044(4) 0.0084(4) 0.0014(3)
Cl2 0.0329(6) 0.0348(7) 0.0539(9) 0.0078(6) 0.0109(6) -0.0060(5)
Cl3 0.0585(9) 0.0330(7) 0.0331(8) -0.0014(6) 0.0001(6) 0.0042(7)
Cl4 0.0435(8) 0.0607(11) 0.0690(12) 0.0232(9) 0.0013(8) 0.0299(8)
S1 0.0126(4) 0.0123(5) 0.0242(6) 0.0032(4) 0.0035(4) 0.0002(3)
```

```
S2 0.0135(4) 0.0102(4) 0.0223(5) 0.0028(4) 0.0040(4) 0.0007(3)
S3 0.0224(5) 0.0224(6) 0.0210(6) -0.0084(4) -0.0081(4) 0.0131(4)
S4 0.0113(4) 0.0144(4) 0.0154(5) 0.0012(3) -0.0001(3) -0.0004(3)
N1 0.0123(15) 0.0092(16) 0.027(2) 0.0012(13) 0.0006(13) 0.0037(12)
N2 0.0163(15) 0.0149(17) 0.0143(17) -0.0036(13) -0.0005(13) 0.0048(13)
C1 0.0129(16) 0.0103(17) 0.0128(19) -0.0030(13) -0.0008(14) -0.0011(13)
C2 0.020(2) 0.009(2) 0.050(4) 0.0058(18) 0.000(2) 0.0022(15)
C3 0.028(3) 0.022(3) 0.169(9) 0.019(4) 0.031(4) 0.013(2)
C4 0.027(3) 0.025(3) 0.111(7) 0.010(3) 0.027(4) 0.012(2)
C5 0.0178(19) 0.019(2) 0.031(3) -0.0014(18) 0.0058(18) 0.0036(16)
C6 0.0188(18) 0.0101(17) 0.0113(19) 0.0005(13) 0.0015(14) 0.0010(14)
C7 0.023(2) 0.016(2) 0.024(2) -0.0005(16) 0.0043(18) 0.0084(16)
C8 0.043(3) 0.028(3) 0.040(3) -0.016(2) 0.008(2) 0.008(2)
C9 0.065(4) 0.041(3) 0.035(3) -0.025(3) -0.009(3) 0.020(3)
C10 0.032(2) 0.029(2) 0.018(2) -0.0104(19) -0.0069(19) 0.011(2)
C11 0.021(2) 0.028(2) 0.030(3) 0.0024(19) 0.008(2) 0.0087(17)

_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
Bi S3 2.6483(11) . ?
Bi S1 2.7263(10) . ?
Bi S2 2.7356(10) . ?
Bi Cl1 2.8490(10) . ?
Bi Cl1 2.9466(9) 2 ?
Bi S4 2.9924(10) . ?
Bi S4 3.1041(10) 2 ?
Cl1 Bi 2.9466(9) 2_545 ?
Cl2 C11 1.747(5) . ?
Cl3 C11 1.760(6) . ?
Cl4 C11 1.758(5) . ?
S1 C1 1.713(4) . ?
S2 C1 1.726(4) . ?
S3 C6 1.733(4) . ?
S4 C6 1.712(4) . ?
S4 Bi 3.1041(10) 2_545 ?
N1 C1 1.319(5) . ?
N1 C5 1.478(5) . ?
N1 C2 1.476(5) . ?
N2 C6 1.313(5) . ?
N2 C10 1.463(6) . ?
N2 C7 1.475(5) . ?
C2 C3 1.516(7) . ?
C3 C4 1.462(8) . ?
C4 C5 1.510(7) . ?
C7 C8 1.507(7) . ?
C8 C9 1.495(8) . ?
C9 C10 1.513(7) . ?

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
S3 Bi S1 83.16(3) . . ?
S3 Bi S2 84.16(3) . . ?
```

```
S1 Bi S2 65.96(3) . . ?
S3 Bi Cl1 93.93(4) . . ?
S1 Bi Cl1 77.54(3) . . ?
S2 Bi Cl1 143.43(3) . . ?
S3 Bi Cl1 110.64(3) . 2 ?
S1 Bi Cl1 137.16(3) . 2 ?
S2 Bi Cl1 75.11(3) . 2 ?
Cl1 Bi Cl1 137.777(17) . 2 ?
S3 Bi S4 63.45(3) . . ?
S1 Bi S4 139.89(3) . . ?
S2 Bi S4 126.88(3) . . ?
Cl1 Bi S4 82.99(3) . . ?
Cl1 Bi S4 78.57(3) 2 . ?
S3 Bi S4 154.10(3) . 2 ?
S1 Bi S4 74.16(3) . 2 ?
S2 Bi S4 75.38(3) . 2 ?
Cl1 Bi S4 93.22(3) . 2 ?
Cl1 Bi S4 79.52(3) 2 2 ?
S4 Bi S4 142.258(11) . 2 ?
Bi Cl1 Bi 97.14(3) . 2_545 ?
C1 S1 Bi 87.25(13) . . ?
C1 S2 Bi 86.71(13) . . ?
C6 S3 Bi 93.21(14) . . ?
C6 S4 Bi 82.41(13) . . ?
C6 S4 Bi 114.30(14) . 2_545 ?
Bi S4 Bi 90.92(3) . 2_545 ?
C1 N1 C5 123.8(3) . . ?
C1 N1 C2 124.5(4) . . ?
C5 N1 C2 111.6(3) . . ?
C6 N2 C10 124.5(3) . . ?
C6 N2 C7 124.3(4) . . ?
C10 N2 C7 111.1(3) . . ?
N1 C1 S1 120.6(3) . . ?
N1 C1 S2 119.7(3) . . ?
S1 C1 S2 119.7(2) . . ?
N1 C2 C3 102.1(4) . . ?
C4 C3 C2 106.0(5) . . ?
C3 C4 C5 105.9(5) . . ?
N1 C5 C4 103.6(4) . . ?
N2 C6 S4 121.7(3) . . ?
N2 C6 S3 118.4(3) . . ?
S4 C6 S3 119.8(2) . . ?
N2 C7 C8 103.7(4) . . ?
C7 C8 C9 104.4(4) . . ?
C10 C9 C8 105.0(5) . . ?
N2 C10 C9 104.1(4) . . ?
Cl3 C11 Cl2 111.0(3) . . ?
Cl3 C11 Cl4 109.4(3) . . ?
Cl2 C11 Cl4 110.8(3) . . ?

_diffrn_measured_fraction_theta_max    0.994
_diffrn_reflns_theta_full              30.0
_diffrn_measured_fraction_theta_full   0.994
_refine_diff_density_max    2.87
_refine_diff_density_min   -3.71
_refine_diff_density_rms    0.276
```