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data_dop61
_publ_requested_journal          'test'
_audit_creation_method             SHELXL
_chemical_name_systematic
;
Bis(2,2'-difluoro-propylenedithio)-tetrathiafulvalene
;
_chemical_name_common                 'F4-BPDT-TTF 5'
_chemical_formula_moiety              'C12 H8 F4 S8'
_chemical_formula_sum                 'C12 H8 F4 S8'
_chemical_formula_weight              484.66
_chemical_melting_point               306

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'
 'F'  'F'   0.0171   0.0103
 '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'

_symmetry_cell_setting                monoclinic
_symmetry_space_group_name_H-M        'P21/c'

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

_cell_length_a                        15.460(2)
_cell_length_b                        4.5991(5)
_cell_length_c                        13.0492(13)
_cell_angle_alpha                     90.00
_cell_angle_beta                      109.201(13)
_cell_angle_gamma                     90.00
_cell_volume                          876.2(2)
_cell_formula_units_Z                 2
_cell_measurement_temperature         293(2)
_cell_measurement_reflns_used         3252
_cell_measurement_theta_min           2.8
_cell_measurement_theta_max           27.75

_exptl_crystal_description            'platelet'
_exptl_crystal_colour                 red
_exptl_crystal_size_max               0.17
_exptl_crystal_size_mid               0.15
_exptl_crystal_size_min               0.08
_exptl_crystal_density_meas           'not measured'
_exptl_crystal_density_diffrn         1.837
_exptl_crystal_density_method         ?
_exptl_crystal_F_000                  488
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```
_exptl_absorpt_coefficient_mu     1.051
_exptl_absorpt_correction_type    numerical
_exptl_absorpt_process_details    'FACEIT, STOE-IPDS'
_exptl_absorpt_correction_T_min   0.8940
_exptl_absorpt_correction_T_max   0.9920

_diffrn_ambient_temperature       293(2)
_diffrn_radiation_wavelength      0.71073
_diffrn_radiation_type            MoK\a
_diffrn_radiation_source          'fine-focus sealed tube'
_diffrn_radiation_monochromator   graphite
_diffrn_radiation_detector        'area detector'
_diffrn_detector_area_resol_mean  6.66
_diffrn_measurement_device_type   'STOE-IPDS'
_diffrn_measurement_method        'Oscillation, Phi incr.=1.4'
_diffrn_standards_number          ?
_diffrn_standards_interval_count  ?
_diffrn_standards_interval_time   ?
_diffrn_standards_decay_%         ?
_diffrn_reflns_number             7811
_diffrn_reflns_av_R_equivalents   0.0736
_diffrn_reflns_av_sigmaI/netI     0.0793
_diffrn_reflns_limit_h_min        -20
_diffrn_reflns_limit_h_max        20
_diffrn_reflns_limit_k_min        -6
_diffrn_reflns_limit_k_max        6
_diffrn_reflns_limit_l_min        -16
_diffrn_reflns_limit_l_max        17
_diffrn_reflns_theta_min          2.79
_diffrn_reflns_theta_max          28.02
_reflns_number_total              2091
_reflns_special_details
;
Friedel equivalent reflections have not been averaged in the _refln_ list
;
_reflns_number_gt           1134
_reflns_observed_criterion        >2sigma(I)

_computing_data_collection        'EXPOSE [STOE-IPDS]'
_computing_cell_refinement        'SELECT, CELL [STOE-IPDS]'
_computing_data_reduction         'INTEGRATE [STOE-IPDS]'
_computing_structure_solution     'SHELXS-86 (Sheldrick, 1990)'
_computing_structure_refinement   'SHELXL-93 (Sheldrick, 1993)'
_computing_molecular_graphics     ?
_computing_publication_material   ?

_refine_special_details
;
 Refinement on F^2^ for ALL reflections except for 0 with very negative F^2^
 or flagged by the user for potential systematic errors.  Weighted R-factors
 wR and all goodnesses 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 observed criterion
 of F^2^ > 2sigma(F^2^) is used only for calculating _R_factor_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 w=1/[\s^2^(Fo^2^)+(0.0190P)^2^+0.0000P] 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     constr
 _refine_ls_extinction_method      none
 _refine_ls_extinction_coef        ?
 _refine_ls_number_reflns          2091
 _refine_ls_number_parameters      109
 _refine_ls_number_restraints      0
 _refine_ls_R_factor_all           0.0897
 _refine_ls_R_factor_gt            0.0350
 _refine_ls_wR_factor_all          0.0670
 _refine_ls_wR_factor_ref          0.0564
 _refine_ls_goodness_of_fit_all    0.826
 _refine_ls_goodness_of_fit_ref    0.965
 _refine_ls_restrained_S_all       0.826
 _refine_ls_restrained_S_obs       0.965
 _refine_ls_shift/su_max           0.000
 _refine_ls_shift/esd_mean         0.000

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  _atom_site_type_symbol
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_U_iso_or_equiv
  _atom_site_thermal_displace_type
  _atom_site_occupancy
  _atom_site_calc_flag
  _atom_site_refinement_flags
  _atom_site_disorder_group
S1 S 0.38678(5) 0.8450(3) 0.35958(7) 0.0559(3) Uani 1 d . .
S2 S 0.41902(5) 0.8246(3) 0.59613(7) 0.0566(3) Uani 1 d . .
S3 S 0.21805(5) 0.4765(2) 0.30466(7) 0.0446(2) Uani 1 d . .
S4 S 0.25451(6) 0.4555(2) 0.57287(7) 0.0494(2) Uani 1 d . .
F1 F 0.06742(11) 0.3104(4) 0.40209(15) 0.0484(5) Uani 1 d . .
F2 F 0.00749(11) 0.7406(4) 0.3930(2) 0.0560(5) Uani 1 d . .
C1 C 0.4602(2) 0.9287(8) 0.4909(2) 0.0489(9) Uani 1 d . .
C2 C 0.3242(2) 0.6339(8) 0.5106(2) 0.0424(8) Uani 1 d . .
C3 C 0.3101(2) 0.6426(8) 0.4040(2) 0.0420(8) Uani 1 d . .
C4 C 0.1503(2) 0.6656(8) 0.5244(3) 0.0460(8) Uani 1 d . .
H4A H 0.1150(2) 0.6327(8) 0.5725(3) 0.055 Uiso 1 calc R .
H4B H 0.1664(2) 0.8701(8) 0.5288(3) 0.055 Uiso 1 calc R .
C5 C 0.0901(2) 0.5992(7) 0.4094(3) 0.0403(8) Uani 1 d . .
C6 C 0.1227(2) 0.6833(8) 0.3166(3) 0.0420(8) Uani 1 d . .
H6A H 0.1400(2) 0.8870(8) 0.3245(3) 0.050 Uiso 1 calc R .
H6B H 0.0719(2) 0.6635(8) 0.2495(3) 0.050 Uiso 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
S1 0.0352(4) 0.1013(8) 0.0318(4) 0.0014(5) 0.0117(3) -0.0160(5)
S2 0.0358(4) 0.1013(8) 0.0316(4) 0.0010(5) 0.0096(3) -0.0199(5)
S3 0.0414(4) 0.0529(6) 0.0386(4) -0.0083(4) 0.0119(3) -0.0050(4)
```

```
S4 0.0433(5) 0.0638(6) 0.0398(5) 0.0102(5) 0.0121(3) -0.0109(4)
F1 0.0469(10) 0.0375(10) 0.0575(12) -0.0024(10) 0.0126(8) -0.0135(8)
F2 0.0396(10) 0.0515(13) 0.0791(14) 0.0043(10) 0.0226(9) 0.0016(9)
C1 0.0312(15) 0.079(3) 0.037(2) 0.003(2) 0.0116(13) -0.004(2)
C2 0.0326(15) 0.057(2) 0.038(2) 0.005(2) 0.0120(13) -0.0033(14)
C3 0.0328(15) 0.056(2) 0.037(2) 0.002(2) 0.0108(12) 0.0014(15)
C4 0.042(2) 0.055(2) 0.046(2) -0.008(2) 0.0215(14) -0.015(2)
C5 0.035(2) 0.032(2) 0.053(2) -0.001(2) 0.0127(14) -0.0036(13)
C6 0.037(2) 0.040(2) 0.045(2) 0.001(2) 0.0094(14) -0.0083(14)

_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
S1 C3 1.750(3) . ?
S1 C1 1.759(3) . ?
S2 C2 1.757(3) . ?
S2 C1 1.760(3) . ?
S3 C3 1.754(3) . ?
S3 C6 1.803(3) . ?
S4 C2 1.752(3) . ?
S4 C4 1.805(3) . ?
F1 C5 1.369(3) . ?
F2 C5 1.386(3) . ?
C1 C1 1.344(6) 3_676 ?
C2 C3 1.335(4) . ?
C4 C5 1.514(4) . ?
C5 C6 1.508(4) . ?

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
C3 S1 C1 94.83(14) . . ?
C2 S2 C1 94.62(14) . . ?
C3 S3 C6 101.2(2) . . ?
C2 S4 C4 101.57(15) . . ?
C1 C1 S1 122.6(3) 3_676 . ?
C1 C1 S2 122.6(3) 3_676 . ?
S1 C1 S2 114.7(2) . . ?
C3 C2 S4 125.6(2) . . ?
C3 C2 S2 117.6(2) . . ?
S4 C2 S2 116.8(2) . . ?
C2 C3 S1 117.7(2) . . ?
C2 C3 S3 124.9(2) . . ?
```

```
S1 C3 S3 117.4(2) . . ?
C5 C4 S4 115.3(2) . . ?
F1 C5 F2 104.0(2) . . ?
F1 C5 C6 109.8(3) . . ?
F2 C5 C6 106.8(2) . . ?
F1 C5 C4 109.0(3) . . ?
F2 C5 C4 107.1(2) . . ?
C6 C5 C4 119.0(2) . . ?
C5 C6 S3 115.7(2) . . ?

_refine_diff_density_max    0.222
_refine_diff_density_min   -0.277
_refine_diff_density_rms    0.059
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data_dop102c
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_audit_creation_method               SHELXL-97
_chemical_name_systematic
;
 ?
;
_chemical_name_common                'F2PDT-TTF 8'
_chemical_melting_point              ?
_chemical_formula_moiety             'C9H6F2S6'
_chemical_formula_sum
 'C9 H6 F2 S6'
_chemical_formula_weight             344.50

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 _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'
 'F'  'F'   0.0171   0.0103
 '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'

_symmetry_cell_setting               monoclinic
_symmetry_space_group_name_H-M       'P 21/c'

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

_cell_length_a                       13.649(3)
_cell_length_b                       10.996(2)
_cell_length_c                       9.1740(18)
_cell_angle_alpha                    90.00
_cell_angle_beta                     108.44(3)
_cell_angle_gamma                    90.00
_cell_volume                         1306.2(4)
_cell_formula_units_Z                4
_cell_measurement_temperature        293(2)
_cell_measurement_reflns_used        25
_cell_measurement_theta_min          6.1
_cell_measurement_theta_max          11.5

_exptl_crystal_description           plate
_exptl_crystal_colour                red
_exptl_crystal_size_max              0.26
_exptl_crystal_size_mid              0.24
_exptl_crystal_size_min              0.04
_exptl_crystal_density_meas          'not measured'
_exptl_crystal_density_diffrn        1.752
_exptl_crystal_density_method        'not measured'
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_exptl_crystal_F_000                696
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_exptl_absorpt_correction_type      none
_exptl_absorpt_correction_T_min     ?
_exptl_absorpt_correction_T_max     ?
_exptl_absorpt_process_details      'SHELXTL [Sheldrick, 1995]'

_exptl_special_details
;
 ?
;

_diffrn_ambient_temperature         293(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     'Enraf Nonius CAD4'
_diffrn_measurement_method          w--2q
_diffrn_refln_scan_width            1.00
_diffrn_standards_number            3
_diffrn_standards_interval_time     60
_diffrn_standards_decay_%           0
_diffrn_reflns_number               3664
_diffrn_reflns_av_R_equivalents     0.0318
_diffrn_reflns_av_sigmaI/netI       0.0629
_diffrn_reflns_limit_h_min          -17
_diffrn_reflns_limit_h_max          16
_diffrn_reflns_limit_k_min          -14
_diffrn_reflns_limit_k_max          1
_diffrn_reflns_limit_l_min          -1
_diffrn_reflns_limit_l_max          11
_diffrn_reflns_theta_min            1.57
_diffrn_reflns_theta_max            26.96
_reflns_number_total                2810
_reflns_number_gt                   1717
_reflns_threshold_expression        >2sigma(I)

_computing_data_collection          'CAD4 Express'
_computing_cell_refinement          'CAD4 Express'
_computing_data_reduction           'XCAD4 [Harms, 1993]'
_computing_structure_solution       'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement     'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics       'Diamonds...'
_computing_publication_material     'SHELXL-97 (Sheldrick, 1997)'


_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^)+(0.0487P)^2^+0.0840P] 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          2810
_refine_ls_number_parameters      154
_refine_ls_number_restraints      0
_refine_ls_R_factor_all           0.1009
_refine_ls_R_factor_gt            0.0345
_refine_ls_wR_factor_ref          0.0932
_refine_ls_wR_factor_gt           0.0794
_refine_ls_goodness_of_fit_ref    0.987
_refine_ls_restrained_S_all       0.987
_refine_ls_shift/su_max           0.001
_refine_ls_shift/su_mean          0.000

loop_
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 _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
S1 S 0.64986(7) 0.01138(9) 0.39668(11) 0.0560(3) Uani 1 1 d . . .
S2 S 0.68361(6) 0.21015(8) 0.20310(12) 0.0547(2) Uani 1 1 d . . .
S3 S 0.41021(6) -0.00478(7) 0.18714(10) 0.0458(2) Uani 1 1 d . . .
S4 S 0.43896(6) 0.20018(8) -0.00141(10) 0.0470(2) Uani 1 1 d . . .
S5 S 0.18143(6) 0.02735(8) 0.09980(9) 0.0405(2) Uani 1 1 d . . .
S6 S 0.21535(6) 0.26542(8) -0.11114(10) 0.0476(2) Uani 1 1 d . . .
F1 F 0.00166(13) 0.1474(2) -0.1564(2) 0.0633(6) Uani 1 1 d . . .
F2 F 0.00675(16) 0.0227(2) -0.3382(2) 0.0796(7) Uani 1 1 d . . .
C1 C 0.7654(3) 0.0909(4) 0.4601(4) 0.0598(10) Uani 1 1 d . . .
H1 H 0.8153 0.0711 0.5526 0.072 Uiso 1 1 calc R . .
C2 C 0.7806(3) 0.1795(3) 0.3743(5) 0.0595(10) Uani 1 1 d . . .
H2 H 0.8414 0.2245 0.4040 0.071 Uiso 1 1 calc R . .
C3 C 0.5954(2) 0.1079(3) 0.2393(4) 0.0402(7) Uani 1 1 d . . .
C4 C 0.4962(2) 0.1031(3) 0.1546(3) 0.0386(7) Uani 1 1 d . . .
C5 C 0.2999(2) 0.0770(3) 0.0849(3) 0.0371(7) Uani 1 1 d . . .
C6 C 0.3127(2) 0.1709(3) 0.0000(3) 0.0382(7) Uani 1 1 d . . .
C7 C 0.1406(2) 0.1618(3) -0.2560(4) 0.0516(9) Uani 1 1 d . . .
H7A H 0.1000 0.2090 -0.3437 0.062 Uiso 1 1 calc R . .
H7B H 0.1879 0.1120 -0.2900 0.062 Uiso 1 1 calc R . .
C8 C 0.0688(2) 0.0790(4) -0.2072(4) 0.0489(8) Uani 1 1 d . . .
C9 C 0.1134(2) -0.0206(3) -0.0938(4) 0.0453(8) Uani 1 1 d . . .
H9A H 0.1605 -0.0677 -0.1314 0.054 Uiso 1 1 calc R . .
H9B H 0.0577 -0.0742 -0.0908 0.054 Uiso 1 1 calc R . .

loop_
 _atom_site_aniso_label
 _atom_site_aniso_U_11
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 _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
S1 0.0424(5) 0.0604(6) 0.0568(5) 0.0126(5) 0.0039(4) 0.0016(4)
S2 0.0389(4) 0.0474(5) 0.0818(7) 0.0048(5) 0.0249(4) -0.0029(4)
S3 0.0338(4) 0.0454(5) 0.0545(5) 0.0180(4) 0.0087(4) -0.0010(3)
S4 0.0359(4) 0.0523(5) 0.0550(5) 0.0186(4) 0.0175(4) 0.0023(4)
S5 0.0336(4) 0.0508(5) 0.0388(4) 0.0000(4) 0.0140(3) -0.0057(3)
S6 0.0404(4) 0.0483(5) 0.0503(5) 0.0128(4) 0.0091(4) 0.0076(4)
F1 0.0382(10) 0.0806(14) 0.0754(14) 0.0101(12) 0.0242(10) 0.0175(10)
F2 0.0591(13) 0.118(2) 0.0471(12) -0.0136(13) -0.0041(10) -0.0158(13)
C1 0.0404(19) 0.070(3) 0.058(2) -0.017(2) 0.0008(18) 0.0027(18)
C2 0.0362(17) 0.058(2) 0.079(3) -0.026(2) 0.0109(18) -0.0062(16)
C3 0.0345(15) 0.0386(17) 0.0479(19) 0.0044(15) 0.0135(14) 0.0023(13)
C4 0.0331(15) 0.0409(17) 0.0423(17) 0.0079(14) 0.0124(14) 0.0006(12)
C5 0.0318(15) 0.0432(17) 0.0355(16) 0.0026(14) 0.0092(13) 0.0008(13)
C6 0.0303(14) 0.0453(18) 0.0383(17) 0.0063(14) 0.0097(13) 0.0012(13)
C7 0.0409(17) 0.076(3) 0.0352(18) 0.0104(17) 0.0076(15) 0.0094(17)
C8 0.0307(15) 0.075(2) 0.0361(18) -0.0076(17) 0.0039(14) -0.0003(16)
C9 0.0380(16) 0.0503(19) 0.0479(19) -0.0120(16) 0.0140(15) -0.0045(14)

_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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S3 C4 1.759(3) . ?
S4 C6 1.758(3) . ?
S4 C4 1.758(3) . ?
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S5 C9 1.803(3) . ?
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S6 C7 1.802(3) . ?
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F2 C8 1.379(4) . ?
C1 C2 1.309(5) . ?
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 C5 S5 C9 102.36(14) . . ?
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 C1 C2 S2 117.9(3) . . ?
 C4 C3 S2 123.1(2) . . ?
 C4 C3 S1 122.9(2) . . ?
 S2 C3 S1 113.92(17) . . ?
 C3 C4 S4 124.0(2) . . ?
 C3 C4 S3 122.5(2) . . ?
 S4 C4 S3 113.52(16) . . ?
 C6 C5 S3 117.4(2) . . ?
 C6 C5 S5 125.4(2) . . ?
 S3 C5 S5 117.17(17) . . ?
 C5 C6 S6 125.9(2) . . ?
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 S6 C6 S4 117.06(17) . . ?
 C8 C7 S6 115.6(2) . . ?
 F1 C8 F2 104.4(2) . . ?
 F1 C8 C9 109.4(3) . . ?
 F2 C8 C9 106.2(3) . . ?
 F1 C8 C7 109.6(3) . . ?
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 'H'  'H'   0.0000   0.0000
 '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'
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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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

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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
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S3 S 0.85269(8) 0.16094(14) 1.06552(8) 0.0594(3) Uani 1 1 d . . .
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S7 S 0.16884(8) 0.30893(14) 0.65688(8) 0.0597(3) Uani 1 1 d . . .
S8 S 0.29957(9) 0.06331(16) 0.54645(7) 0.0655(4) Uani 1 1 d . . .
F1 F 0.95251(18) 0.3163(3) 1.2671(2) 0.0776(8) Uani 1 1 d . . .
F2 F 0.9384(2) 0.1261(3) 1.35596(18) 0.0843(9) Uani 1 1 d . . .
C1 C 0.4457(3) 0.1327(4) 0.8493(2) 0.0413(9) Uani 1 1 d . . .
C2 C 0.5293(3) 0.1455(4) 0.9283(2) 0.0416(9) Uani 1 1 d . . .
C3 C 0.7184(3) 0.1667(4) 1.0364(3) 0.0423(9) Uani 1 1 d . . .
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H4B H 0.9628 0.0522 1.2032 0.067 Uiso 1 1 calc R . .
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C7 C 0.6660(3) 0.2537(4) 1.0801(3) 0.0417(9) Uani 1 1 d . . .
C8 C 0.2818(3) 0.2084(4) 0.7113(2) 0.0401(9) Uani 1 1 d . . .
C9 C 0.1324(5) 0.2386(8) 0.5354(4) 0.146(4) Uani 1 1 d . . .
H9A H 0.0582 0.2232 0.5170 0.175 Uiso 1 1 calc R . .
H9B H 0.1430 0.3211 0.4951 0.175 Uiso 1 1 calc R . .
C10 C 0.1699(4) 0.1170(10) 0.5043(4) 0.117(3) Uani 1 1 d . . .
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S4 0.0566(6) 0.0462(6) 0.0522(6) -0.0093(5) 0.0034(5) 0.0041(5)
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F2 0.0669(16) 0.101(2) 0.0605(16) 0.0144(16) -0.0165(13) 0.0065(16)
C1 0.041(2) 0.047(2) 0.0327(18) 0.0014(17) 0.0070(16) 0.0030(18)
C2 0.044(2) 0.042(2) 0.0360(19) 0.0020(16) 0.0084(16) 0.0041(17)
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C5 0.039(2) 0.057(3) 0.053(2) 0.005(2) -0.0035(18) -0.009(2)
C6 0.050(2) 0.069(3) 0.040(2) -0.001(2) 0.0038(18) -0.009(2)
C7 0.0405(19) 0.041(2) 0.0383(19) 0.0026(16) 0.0041(16) 0.0018(18)
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C9 0.138(6) 0.128(6) 0.096(4) -0.068(4) -0.077(4) 0.074(5)
C10 0.052(3) 0.214(8) 0.067(3) -0.050(4) -0.009(2) 0.023(4)
C11 0.040(2) 0.047(2) 0.0344(18) 0.0014(17) 0.0059(15) -0.0060(18)

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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)
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S2 C2 1.753(4) . ?
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S3 C4 1.793(4) . ?
S4 C7 1.743(4) . ?
S4 C6 1.796(4) . ?
S5 C7 1.752(4) . ?
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S6 C1 1.749(4) . ?
S6 C8 1.760(3) . ?
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F2 C5 1.380(4) . ?
C1 C2 1.339(5) . ?
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C7 S5 C2 94.23(17) . . ?
C1 S6 C8 94.16(17) . . ?
C8 S7 C9 101.6(2) . . ?
C11 S8 C10 101.5(2) . . ?
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S6 C1 S1 113.59(19) . . ?
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F1 C5 F2 104.0(3) . . ?
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F2 C5 C4 106.6(3) . . ?
F1 C5 C6 109.5(4) . . ?
F2 C5 C6 106.8(3) . . ?
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S7 C8 S6 114.7(2) . . ?
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