Bulk spontaneous magnetization in the new radical cation salt TM-TTF[$Cr(NCS)_4$(isoquinoline)$_2$], TM-TTF = tetramethyltetrathiafulvalene

M. Mas-Torrent, S. S. Turner, K. Wurst, J. Vidal-Gancedo, X. Ribas, J. Veciana, P.Day, and

C. Rovira

Crystallographic data as CIF files for [TM-TTF][Cr(NCS)4(isoquinoline)2] at 213 and 123K

```
data_213

_audit_creation_method            SHELXL
_chemical_name_systematic
;
 ?
;
_chemical_name_common             ?
_chemical_formula_moiety          ?
_chemical_formula_structural      ?
_chemical_formula_analytical      ?
_chemical_formula_sum             'C32 H26 Cr N6 S8'
_chemical_formula_weight          803.07
_chemical_melting_point           ?
_chemical_compound_source         ?

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'
'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'
'Cr'  'Cr'   0.3209   0.6236
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting            triclinic
_symmetry_space_group_name_H-M    P-1

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

_cell_length_a                    8.269(1)
_cell_length_b                    10.211(2)
_cell_length_c                    11.176(2)
_cell_angle_alpha                 89.244(9)
```

```
_cell_angle_beta                  88.114(9)
_cell_angle_gamma                 74.227(7)
_cell_volume                      907.6(3)
_cell_formula_units_Z             1
_cell_measurement_temperature     213(2)
_cell_measurement_reflns_used     3440
_cell_measurement_theta_min       1.0
_cell_measurement_theta_max       20.0

_exptl_crystal_description        prism
_exptl_crystal_colour             'dark brown'
_exptl_crystal_size_max           0.2
_exptl_crystal_size_mid           0.1
_exptl_crystal_size_min           0.05
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.469
_exptl_crystal_density_method     ?
_exptl_crystal_F_000              412
_exptl_absorpt_coefficient_mu     0.808
_exptl_absorpt_correction_type    none
_exptl_absorpt_correction_T_min   ?
_exptl_absorpt_correction_T_max   ?

_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'
_diffrn_radiation_monochromator   graphite
_diffrn_measurement_device        'Kappa CCD'
_diffrn_measurement_method        phi-scans
_diffrn_standards_number          ?
_diffrn_standards_interval_count  ?
_diffrn_standards_interval_time   ?
_diffrn_standards_decay_%         0
_diffrn_reflns_number             2849
_diffrn_reflns_av_R_equivalents   0.0310
_diffrn_reflns_av_sigmaI/netI     0.0515
_diffrn_reflns_limit_h_min        0
_diffrn_reflns_limit_h_max        7
_diffrn_reflns_limit_k_min        -9
_diffrn_reflns_limit_k_max        9
_diffrn_reflns_limit_l_min        -10
_diffrn_reflns_limit_l_max        10
_diffrn_reflns_theta_min          1.82
_diffrn_reflns_theta_max          19.99
_reflns_number_total              1629
_reflns_number_observed           1340
_reflns_observed_criterion        >2sigma(I)

_computing_data_collection        'Kappa CCD'
_computing_cell_refinement        ?
_computing_data_reduction         'DENZO and SKALEPACK'
_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 80 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_obs 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^)+(0.0188P)^2^+0.6043P] 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     riding
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          1549
_refine_ls_number_parameters      216
_refine_ls_number_restraints      0
_refine_ls_R_factor_all           0.0465
_refine_ls_R_factor_obs           0.0331
_refine_ls_wR_factor_all          0.0791
_refine_ls_wR_factor_obs          0.0725
_refine_ls_goodness_of_fit_all    1.065
_refine_ls_goodness_of_fit_obs    1.109
_refine_ls_restrained_S_all       1.080
_refine_ls_restrained_S_obs       1.109
_refine_ls_shift/esd_max          0.003
_refine_ls_shift/esd_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_thermal_displace_type
 _atom_site_occupancy
 _atom_site_calc_flag
 _atom_site_refinement_flags
 _atom_site_disorder_group
Cr1 Cr 0.0000 0.5000 0.0000 0.0324(3) Uani 1 d S .
S1 S 0.2319(2) 0.04317(11) 0.53634(10) 0.0442(4) Uani 1 d . .
S2 S 0.4561(2) 0.21496(11) 0.53731(11) 0.0466(4) Uani 1 d . .
S3 S 0.4308(2) 0.45388(15) 0.27507(13) 0.0720(5) Uani 1 d . .
S4 S 0.1259(2) 0.79785(11) -0.29222(10) 0.0452(4) Uani 1 d . .
N1 N 0.1626(5) 0.3190(3) -0.0646(3) 0.0320(9) Uani 1 d . .
N2 N 0.1701(5) 0.5140(3) 0.1172(3) 0.0400(10) Uani 1 d . .
N3 N 0.0917(4) 0.6093(4) -0.1185(3) 0.0388(10) Uani 1 d . .
C1 C 0.4337(5) 0.0553(4) 0.5155(3) 0.0358(11) Uani 1 d . .
C2 C 0.1421(6) 0.2110(4) 0.5770(4) 0.0369(12) Uani 1 d . .
```

C3 C 0.2469(6) 0.2909(4) 0.5764(4) 0.0401(12) Uani 1 d . .
C4 C 0.1027(5) 0.2079(5) -0.0813(4) 0.0360(11) Uani 1 d . .
H4 H -0.0124 0.2166 -0.0670 0.043 Uiso 1 calc . .
C5 C 0.2039(6) 0.0859(4) -0.1178(4) 0.0369(11) Uani 1 d . .
H5 H 0.1576 0.0125 -0.1281 0.044 Uiso 1 calc . .
C6 C 0.3768(6) 0.0676(4) -0.1403(3) 0.0328(11) Uani 1 d . .
C7 C 0.4898(6) -0.0570(4) -0.1776(4) 0.0401(12) Uani 1 d . .
H7 H 0.4501 -0.1337 -0.1896 0.048 Uiso 1 calc . .
C8 C 0.6543(6) -0.0654(5) -0.1960(4) 0.0466(13) Uani 1 d . .
H8 H 0.7283 -0.1485 -0.2207 0.056 Uiso 1 calc . .
C9 C 0.7176(6) 0.0476(5) -0.1790(4) 0.0498(13) Uani 1 d . .
H9 H 0.8328 0.0395 -0.1923 0.060 Uiso 1 calc . .
C10 C 0.6107(6) 0.1700(5) -0.1429(4) 0.0455(13) Uani 1 d . .
H10 H 0.6527 0.2455 -0.1314 0.055 Uiso 1 calc . .
C11 C 0.4396(6) 0.1816(4) -0.1232(4) 0.0333(11) Uani 1 d . .
C12 C 0.3241(6) 0.3042(4) -0.0859(4) 0.0348(11) Uani 1 d . .
H12 H 0.3652 0.3804 -0.0755 0.042 Uiso 1 calc . .
C13 C 0.2786(6) 0.4881(4) 0.1832(4) 0.0363(12) Uani 1 d . .
C14 C 0.1058(5) 0.6886(4) -0.1906(4) 0.0324(11) Uani 1 d . .
C21 C -0.0414(6) 0.2503(5) 0.6093(4) 0.0505(13) Uani 1 d . .
H21A H -0.0697(9) 0.1758(11) 0.6520(21) 0.076 Uiso 1 calc R .
H21B H -0.1055(6) 0.2704(26) 0.5370(4) 0.076 Uiso 1 calc R .
H21C H -0.0682(8) 0.3302(16) 0.6600(19) 0.076 Uiso 1 calc R .
C31 C 0.2028(6) 0.4388(4) 0.6057(4) 0.0594(15) Uani 1 d . .
H31A H 0.2660(28) 0.4525(6) 0.6739(17) 0.089 Uiso 1 calc R .
H31B H 0.0834(9) 0.4711(8) 0.6251(26) 0.089 Uiso 1 calc R .
H31C H 0.2303(35) 0.4891(6) 0.5374(10) 0.089 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
Cr1 0.0321(7) 0.0284(6) 0.0339(6) 0.0013(5) 0.0010(5) -0.0037(5)
S1 0.0487(9) 0.0336(7) 0.0500(8) -0.0008(6) 0.0042(6) -0.0110(6)
S2 0.0483(9) 0.0281(7) 0.0619(8) -0.0043(6) 0.0003(7) -0.0079(6)
S3 0.0513(10) 0.0780(11) 0.0823(11) 0.0155(8) -0.0303(8) -0.0077(8)
S4 0.0545(9) 0.0332(7) 0.0462(8) 0.0066(6) 0.0048(6) -0.0102(6)
N1 0.033(3) 0.031(2) 0.029(2) 0.003(2) 0.000(2) -0.005(2)
N2 0.035(3) 0.038(2) 0.043(2) -0.003(2) -0.006(2) -0.002(2)
N3 0.043(3) 0.030(2) 0.039(2) 0.001(2) 0.008(2) -0.004(2)
C1 0.048(3) 0.029(3) 0.031(3) 0.001(2) 0.001(2) -0.011(2)
C2 0.047(3) 0.031(3) 0.029(3) -0.003(2) -0.002(2) -0.003(3)
C3 0.050(3) 0.029(3) 0.035(3) -0.005(2) -0.003(2) 0.001(3)
C4 0.031(3) 0.040(3) 0.038(3) -0.003(2) -0.004(2) -0.010(3)
C5 0.037(3) 0.028(3) 0.045(3) -0.008(2) -0.004(2) -0.007(2)
C6 0.030(3) 0.036(3) 0.027(2) 0.002(2) -0.003(2) 0.000(3)
C7 0.038(3) 0.034(3) 0.042(3) -0.001(2) -0.004(2) 0.001(3)
C8 0.038(4) 0.044(3) 0.044(3) 0.001(2) 0.006(2) 0.011(3)
C9 0.035(3) 0.054(4) 0.053(3) 0.007(3) 0.007(3) -0.001(3)
C10 0.037(4) 0.041(3) 0.055(3) 0.003(3) 0.005(3) -0.006(3)
C11 0.030(3) 0.034(3) 0.032(3) 0.005(2) 0.000(2) -0.003(3)
C12 0.039(3) 0.031(3) 0.035(3) 0.005(2) -0.002(2) -0.010(3)
C13 0.031(3) 0.030(3) 0.045(3) -0.005(2) 0.002(3) -0.003(2)
C14 0.030(3) 0.030(3) 0.035(3) -0.008(2) 0.002(2) -0.003(2)
C21 0.051(4) 0.050(3) 0.044(3) -0.001(2) 0.003(3) -0.003(3)
C31 0.067(4) 0.042(3) 0.062(3) -0.015(3) -0.007(3) -0.002(3)

```
_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
Cr1 N3 1.982(4) 2_565 ?
Cr1 N3 1.982(4) . ?
Cr1 N2 1.988(4) . ?
Cr1 N2 1.988(4) 2_565 ?
Cr1 N1 2.089(3) 2_565 ?
Cr1 N1 2.089(3) . ?
S1 C1 1.715(4) . ?
S1 C2 1.733(4) . ?
S2 C1 1.712(4) . ?
S2 C3 1.737(5) . ?
S3 C13 1.612(5) . ?
S4 C14 1.617(5) . ?
N1 C12 1.316(5) . ?
N1 C4 1.373(5) . ?
N2 C13 1.152(5) . ?
N3 C14 1.161(5) . ?
C1 C1 1.382(8) 2_656 ?
C2 C3 1.341(6) . ?
C2 C21 1.494(6) . ?
C3 C31 1.493(6) . ?
C4 C5 1.357(6) . ?
C5 C6 1.405(6) . ?
C6 C11 1.415(6) . ?
C6 C7 1.417(6) . ?
C7 C8 1.348(6) . ?
C8 C9 1.408(6) . ?
C9 C10 1.377(6) . ?
C10 C11 1.397(6) . ?
C11 C12 1.411(6) . ?

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
N3 Cr1 N3 180.0 2_565 . ?
N3 Cr1 N2 89.06(14) 2_565 . ?
N3 Cr1 N2 90.94(14) . . ?
N3 Cr1 N2 90.94(14) 2_565 2_565 ?
N3 Cr1 N2 89.06(14) . 2_565 ?
```

N2 Cr1 N2 180.0 . 2_565 ?
N3 Cr1 N1 91.56(13) 2_565 2_565 ?
N3 Cr1 N1 88.44(13) . 2_565 ?
N2 Cr1 N1 90.23(14) . 2_565 ?
N2 Cr1 N1 89.77(14) 2_565 2_565 ?
N3 Cr1 N1 88.44(13) 2_565 . ?
N3 Cr1 N1 91.56(13) . . ?
N2 Cr1 N1 89.77(14) . . ?
N2 Cr1 N1 90.23(14) 2_565 . ?
N1 Cr1 N1 180.0 2_565 . ?
C1 S1 C2 96.8(2) . . ?
C1 S2 C3 96.2(2) . . ?
C12 N1 C4 117.6(4) . . ?
C12 N1 Cr1 122.7(3) . . ?
C4 N1 Cr1 119.6(3) . . ?
C13 N2 Cr1 163.2(4) . . ?
C14 N3 Cr1 163.9(3) . . ?
C1 C1 S2 123.3(4) 2_656 . ?
C1 C1 S1 122.4(4) 2_656 . ?
S2 C1 S1 114.3(2) . . ?
C3 C2 C21 127.4(4) . . ?
C3 C2 S1 115.7(3) . . ?
C21 C2 S1 116.8(3) . . ?
C2 C3 C31 126.9(4) . . ?
C2 C3 S2 116.9(3) . . ?
C31 C3 S2 116.2(4) . . ?
C5 C4 N1 122.3(4) . . ?
C4 C5 C6 121.1(4) . . ?
C5 C6 C11 117.0(4) . . ?
C5 C6 C7 124.0(4) . . ?
C11 C6 C7 118.9(4) . . ?
C8 C7 C6 119.9(4) . . ?
C7 C8 C9 121.5(4) . . ?
C10 C9 C8 119.9(4) . . ?
C9 C10 C11 119.9(4) . . ?
C10 C11 C12 122.5(4) . . ?
C10 C11 C6 119.9(4) . . ?
C12 C11 C6 117.6(4) . . ?
N1 C12 C11 124.4(4) . . ?
N2 C13 S3 179.2(4) . . ?
N3 C14 S4 179.4(4) . . ?

_refine_diff_density_max 0.190
_refine_diff_density_min -0.221
_refine_diff_density_rms 0.045

#===END

data_ee

_audit_creation_method SHELXL
_chemical_name_systematic
;
?
;
_chemical_name_common ?
_chemical_formula_moiety ?
_chemical_formula_structural ?
_chemical_formula_analytical ?

```
_chemical_formula_sum            'C32 H26 Cr N6 S8'
_chemical_formula_weight         803.07
_chemical_melting_point          ?
_chemical_compound_source        ?

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'
 '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'
 'Cr'  'Cr'   0.3209   0.6236
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting           triclinic
_symmetry_space_group_name_H-M    P-1

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

_cell_length_a                   8.112(6)
_cell_length_b                   9.886(6)
_cell_length_c                   11.507(9)
_cell_angle_alpha                 83.89(5)
_cell_angle_beta                 82.37(3)
_cell_angle_gamma                 76.34(6)
_cell_volume                     886.1(11)
_cell_formula_units_Z            1
_cell_measurement_temperature    123(2)
_cell_measurement_reflns_used    10511
_cell_measurement_theta_min      1.0
_cell_measurement_theta_max      20.0

_exptl_crystal_description       prism
_exptl_crystal_colour            'dark brown'
_exptl_crystal_size_max          0.2
_exptl_crystal_size_mid          0.1
_exptl_crystal_size_min          0.05
_exptl_crystal_density_meas      ?
_exptl_crystal_density_diffrn    1.505
_exptl_crystal_density_method    ?
_exptl_crystal_F_000             412
_exptl_absorpt_coefficient_mu    0.828
_exptl_absorpt_correction_type   none
_exptl_absorpt_correction_T_min  ?
_exptl_absorpt_correction_T_max  ?

_exptl_special_details
;
 ?
```

;

_diffrn_ambient_temperature 123(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 'Kappa CCD'
_diffrn_measurement_method phi-scans
_diffrn_standards_number ?
_diffrn_standards_interval_count ?
_diffrn_standards_interval_time ?
_diffrn_standards_decay_% 0
_diffrn_reflns_number 2493
_diffrn_reflns_av_R_equivalents 0.0702
_diffrn_reflns_av_sigmaI/netI 0.1160
_diffrn_reflns_limit_h_min 0
_diffrn_reflns_limit_h_max 7
_diffrn_reflns_limit_k_min -8
_diffrn_reflns_limit_k_max 9
_diffrn_reflns_limit_l_min -10
_diffrn_reflns_limit_l_max 11
_diffrn_reflns_theta_min 1.79
_diffrn_reflns_theta_max 20.00
_reflns_number_total 1562
_reflns_number_observed 1007
_reflns_observed_criterion >2sigma(I)

_computing_data_collection 'Kappa CCD'
_computing_cell_refinement ?
_computing_data_reduction 'DENZO and SCALEPACK'
_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 157 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_obs 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^)+(0.0706P)^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 riding
_refine_ls_extinction_method none
_refine_ls_extinction_coef ?
_refine_ls_number_reflns 1405
_refine_ls_number_parameters 216

```
_refine_ls_number_restraints      0
_refine_ls_R_factor_all           0.1144
_refine_ls_R_factor_obs           0.0636
_refine_ls_wR_factor_all          0.1671
_refine_ls_wR_factor_obs          0.1379
_refine_ls_goodness_of_fit_all    1.069
_refine_ls_goodness_of_fit_obs    1.189
_refine_ls_restrained_S_all       1.113
_refine_ls_restrained_S_obs       1.189
_refine_ls_shift/esd_max          0.000
_refine_ls_shift/esd_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_thermal_displace_type
 _atom_site_occupancy
 _atom_site_calc_flag
 _atom_site_refinement_flags
 _atom_site_disorder_group
Cr1 Cr 0.0000 0.5000 0.0000 0.0439(8) Uani 1 d S .
S1 S 0.2268(4) 0.0797(3) 0.5067(2) 0.0508(9) Uani 1 d . .
S2 S 0.4935(4) 0.2022(3) 0.5615(2) 0.0506(9) Uani 1 d . .
S3 S 0.3888(4) 0.4172(3) 0.2798(3) 0.0613(10) Uani 1 d . .
S4 S 0.1531(4) 0.8183(3) -0.3024(2) 0.0515(9) Uani 1 d . .
N1 N 0.1687(11) 0.3221(7) -0.0600(6) 0.037(2) Uani 1 d . .
N2 N 0.1532(11) 0.5077(8) 0.1193(8) 0.043(2) Uani 1 d . .
N3 N 0.1161(11) 0.6210(8) -0.1128(8) 0.048(3) Uani 1 d . .
C1 C 0.4411(14) 0.0591(10) 0.5146(8) 0.049(3) Uani 1 d . .
C2 C 0.1625(16) 0.2422(10) 0.5653(8) 0.049(3) Uani 1 d . .
C3 C 0.2860(14) 0.2996(10) 0.5887(8) 0.045(3) Uani 1 d . .
C4 C 0.1100(13) 0.2095(11) -0.0812(8) 0.045(3) Uani 1 d . .
H4 H -0.0099 0.2168 -0.0705 0.054 Uiso 1 calc . .
C5 C 0.2123(15) 0.0871(11) -0.1168(9) 0.047(3) Uani 1 d . .
H5 H 0.1640 0.0118 -0.1292 0.056 Uiso 1 calc . .
C6 C 0.3905(15) 0.0736(10) -0.1350(8) 0.043(3) Uani 1 d . .
C7 C 0.5060(15) -0.0480(9) -0.1746(8) 0.041(3) Uani 1 d . .
H7 H 0.4654 -0.1265 -0.1892 0.049 Uiso 1 calc . .
C8 C 0.6756(15) -0.0511(10) -0.1915(9) 0.047(3) Uani 1 d . .
H8 H 0.7535 -0.1330 -0.2173 0.056 Uiso 1 calc . .
C9 C 0.7389(13) 0.0653(11) -0.1714(9) 0.050(3) Uani 1 d . .
H9 H 0.8582 0.0607 -0.1838 0.060 Uiso 1 calc . .
C10 C 0.6298(15) 0.1834(10) -0.1344(9) 0.046(3) Uani 1 d . .
H10 H 0.6726 0.2612 -0.1210 0.055 Uiso 1 calc . .
C11 C 0.4524(14) 0.1900(11) -0.1161(8) 0.044(3) Uani 1 d . .
C12 C 0.3332(15) 0.3123(9) -0.0781(8) 0.037(3) Uani 1 d . .
H12 H 0.3757 0.3906 -0.0653 0.045 Uiso 1 calc . .
C13 C 0.2502(15) 0.4689(9) 0.1871(9) 0.043(3) Uani 1 d . .
C14 C 0.1325(12) 0.7062(11) -0.1933(10) 0.040(3) Uani 1 d . .
C21 C -0.0263(13) 0.3011(10) 0.5818(9) 0.054(3) Uani 1 d . .
H21A H -0.0773(17) 0.2524(43) 0.6509(31) 0.081 Uiso 1 calc R .
H21B H -0.0766(17) 0.2886(55) 0.5119(23) 0.081 Uiso 1 calc R .
H21C H -0.0483(13) 0.4009(17) 0.5934(52) 0.081 Uiso 1 calc R .
C31 C 0.2679(13) 0.4404(10) 0.6310(9) 0.055(3) Uani 1 d . .
H31A H 0.2970(78) 0.5048(19) 0.5649(14) 0.083 Uiso 1 calc R .
H31B H 0.3450(59) 0.4337(16) 0.6912(40) 0.083 Uiso 1 calc R .
```

H31C H 0.1498(23) 0.4751(29) 0.6648(50) 0.083 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
Cr1 0.040(2) 0.037(2) 0.051(2) -0.0087(12) -0.0016(13) -0.0005(12)
S1 0.047(2) 0.043(2) 0.058(2) -0.0074(14) 0.001(2) -0.0036(14)
S2 0.051(2) 0.044(2) 0.054(2) -0.0087(14) -0.003(2) -0.0054(15)
S3 0.060(2) 0.060(2) 0.062(2) -0.010(2) -0.016(2) -0.001(2)
S4 0.052(2) 0.044(2) 0.055(2) -0.0051(14) 0.000(2) -0.0057(15)
N1 0.026(6) 0.034(6) 0.047(6) -0.008(4) -0.002(5) -0.002(5)
N2 0.039(6) 0.031(5) 0.053(7) -0.005(4) 0.002(5) 0.002(4)
N3 0.046(6) 0.039(6) 0.050(6) -0.010(5) -0.002(5) 0.007(5)
C1 0.055(9) 0.054(7) 0.036(7) -0.006(5) -0.001(6) -0.006(6)
C2 0.064(9) 0.040(7) 0.038(7) 0.002(5) -0.004(6) -0.006(7)
C3 0.048(8) 0.040(7) 0.037(7) 0.000(5) -0.004(6) 0.005(6)
C4 0.043(8) 0.051(8) 0.043(7) -0.006(6) -0.005(6) -0.010(7)
C5 0.036(9) 0.046(7) 0.058(8) -0.013(6) -0.009(6) -0.001(6)
C6 0.046(9) 0.040(7) 0.043(7) -0.019(5) -0.009(6) 0.003(6)
C7 0.037(8) 0.035(7) 0.049(7) 0.003(5) -0.005(6) -0.009(6)
C8 0.056(10) 0.034(7) 0.052(7) -0.007(5) 0.000(6) -0.012(6)
C9 0.034(7) 0.053(8) 0.057(8) 0.003(6) -0.005(6) -0.004(7)
C10 0.047(9) 0.043(7) 0.044(7) -0.009(5) -0.012(6) 0.005(6)
C11 0.034(8) 0.057(8) 0.041(7) -0.006(6) -0.010(6) -0.009(7)
C12 0.039(8) 0.027(7) 0.044(7) -0.002(5) -0.008(6) -0.004(6)
C13 0.053(9) 0.026(6) 0.039(8) 0.003(5) 0.005(7) 0.004(6)
C14 0.024(7) 0.045(8) 0.050(8) -0.022(6) -0.013(6) 0.009(5)
C21 0.039(8) 0.063(7) 0.054(8) -0.012(6) -0.001(6) 0.003(6)
C31 0.054(8) 0.054(8) 0.058(8) -0.012(6) -0.012(6) -0.008(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.
;

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
Cr1 N3 1.970(9) 2_565 ?
Cr1 N3 1.970(9) . ?
Cr1 N2 1.989(10) . ?
Cr1 N2 1.989(10) 2_565 ?
Cr1 N1 2.077(7) . ?
Cr1 N1 2.077(7) 2_565 ?
S1 C1 1.715(11) . ?
S1 C2 1.746(10) . ?
S2 C1 1.726(10) . ?

S2 C3 1.737(10) . ?
S3 C13 1.610(13) . ?
S4 C14 1.602(12) . ?
N1 C12 1.305(12) . ?
N1 C4 1.366(12) . ?
N2 C13 1.153(12) . ?
N3 C14 1.200(11) . ?
C1 C1 1.37(2) 2_656 ?
C2 C3 1.331(14) . ?
C2 C21 1.499(14) . ?
C3 C31 1.491(13) . ?
C4 C5 1.365(13) . ?
C5 C6 1.409(14) . ?
C6 C11 1.407(13) . ?
C6 C7 1.415(13) . ?
C7 C8 1.357(13) . ?
C8 C9 1.417(13) . ?
C9 C10 1.358(13) . ?
C10 C11 1.414(14) . ?
C11 C12 1.427(13) . ?

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
N3 Cr1 N3 180.0 2_565 . ?
N3 Cr1 N2 89.5(3) 2_565 . ?
N3 Cr1 N2 90.5(3) . . ?
N3 Cr1 N2 90.5(3) 2_565 2_565 ?
N3 Cr1 N2 89.5(3) . 2_565 ?
N2 Cr1 N2 180.0 . 2_565 ?
N3 Cr1 N1 88.7(3) 2_565 . ?
N3 Cr1 N1 91.3(3) . . ?
N2 Cr1 N1 90.0(3) . . ?
N2 Cr1 N1 90.0(3) 2_565 . ?
N3 Cr1 N1 91.3(3) 2_565 2_565 ?
N3 Cr1 N1 88.7(3) . 2_565 ?
N2 Cr1 N1 90.0(3) . 2_565 ?
N2 Cr1 N1 90.0(3) 2_565 2_565 ?
N1 Cr1 N1 180.0 . 2_565 ?
C1 S1 C2 96.5(5) . . ?
C1 S2 C3 96.7(5) . . ?
C12 N1 C4 117.4(8) . . ?
C12 N1 Cr1 122.1(6) . . ?
C4 N1 Cr1 120.5(7) . . ?
C13 N2 Cr1 159.1(8) . . ?
C14 N3 Cr1 157.7(8) . . ?
C1 C1 S1 123.0(11) 2_656 . ?
C1 C1 S2 123.3(12) 2_656 . ?
S1 C1 S2 113.7(5) . . ?
C3 C2 C21 127.7(9) . . ?
C3 C2 S1 116.6(9) . . ?
C21 C2 S1 115.7(9) . . ?
C2 C3 C31 127.6(10) . . ?
C2 C3 S2 116.3(8) . . ?
C31 C3 S2 116.0(9) . . ?

C5 C4 N1 124.2(10) . . ?
C4 C5 C6 119.2(9) . . ?
C11 C6 C5 117.1(9) . . ?
C11 C6 C7 119.7(10) . . ?
C5 C6 C7 123.2(10) . . ?
C8 C7 C6 119.2(9) . . ?
C7 C8 C9 121.3(9) . . ?
C10 C9 C8 120.3(10) . . ?
C9 C10 C11 119.7(9) . . ?
C6 C11 C10 119.7(10) . . ?
C6 C11 C12 118.7(10) . . ?
C10 C11 C12 121.6(10) . . ?
N1 C12 C11 123.3(9) . . ?
N2 C13 S3 178.5(10) . . ?
N3 C14 S4 178.9(9) . . ?

_refine_diff_density_max 0.488
_refine_diff_density_min -0.293
_refine_diff_density_rms 0.084