Structural and photophysical characterisation of coordination and optical isomers of mononuclear ruthenium(II) polypyridyl 1,2,4-triazole complexes

Browne, Wesley R.; Hesek, Dusan; Gallagher, John F.; O'Connor, Christine M.; Killeen, J. Scott; Aoki, Fumiko; Ishida, Hitoshi; Inoue, Yoshihisa; Villani, Claudio; Vos, Johannes G.

Published in:
Dalton Transactions

DOI:
10.1039/ b301961f

Supplementary Material (ESI) for Dalton Transactions


```
data_global
_journal_name_full               'Dalton Trans.'
_journal_coden_Cambridge         0222

_publ_contact_author_name        'Dr. John F. Gallagher'
_publ_contact_author_address
;
School of Chemical Sciences,
Dublin City University, Dublin 9, Ireland
;
_publ_contact_author_phone       '353 1 7005114'
_publ_contact_author_fax         '353 1 7005503'
_publ_contact_author_email       john.gallagher@dcu.ie
_publ_requested_category         FM
_publ_requested_coeditor_name    'CSD internal review/RSC review'
_publ_contact_letter
;
February 24th, 2003

Please consider this CIF file for deposition in the Cambridge Structural
Database for submitted crystal structures.  Two CIF files form this
submission.  We request a CSD code and number for the compound
for future reference in future publications and theses.

The authors are Browne, Hesek, Gallagher,
O'Connor, Killeen, Villani and Vos.

The crystals diffracted reasonably well and absorption effects were
corrected for using psi-scan reflections at 5 degree intervals.

Note:
There is considerable disorder in the hexafluorophosphate anions
in both structures and there are partial occupancy solvent molecules
as well.

I was collected on an Enraf Nonius CAD4 diffractometer in Guelph, Canada.
II was collected on a Siemens P4 diffractometer in DCU, Dublin, Ireland.

Yours sincerely,

John Gallagher

;

_publ_section_title
;
Structural and photophysical characterisation of coordination and optical
isomers of mononuclear ruthenium(II) polypyridyl 1,2,4-triazole complexes
;

loop_
_publ_author_name
'Johannes G. Vos'
'Wesley R Browne'
'D Hesek'
'J. F. Gallagher'
'Christine M O-Connor'
'J. Scott Killeen'
```

```
'Fumiko Aoki'
'Hitoshi Ishida'
'Yoshihisa Inoue'
'Claudio Villani'

data_I
_database_code_CSD               204725

_audit_creation_method           SHELXL-97
_chemical_name_systematic
;
?
;
_chemical_name_common            ?
_chemical_formula_moiety         ?
_chemical_formula_sum            'C33.40 H29.20 F6 N9 O1.20 P Ru'
_chemical_formula_weight         821.90

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'
O O 0.0106 0.0060 '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'
P P 0.1023 0.0942 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Ru Ru -1.2594 0.8363 '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
_symmetry_space_group_name_Hall  -p-1

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

_cell_length_a                   12.2324(17)
_cell_length_b                   12.301(2)
_cell_length_c                   13.296(2)
_cell_angle_alpha                78.996(12)
_cell_angle_beta                 64.996(10)
_cell_angle_gamma                77.151(10)
_cell_volume                     1757.0(5)
_cell_formula_units_Z            2
_cell_measurement_temperature    293(2)

_exptl_crystal_density_diffrn    1.554
_exptl_crystal_density_method    'not measured'
_exptl_crystal_F_000             830
_exptl_absorpt_coefficient_mu    0.566

_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  'Bruker P4 diffractometer'
_diffrn_measurement_method       ?
_diffrn_detector_area_resol_mean ?
_diffrn_standards_number         4
_diffrn_standards_interval_count ?
_diffrn_standards_interval_time  296
_diffrn_standards_decay_%        none
_diffrn_reflns_number            7145
_diffrn_reflns_av_R_equivalents  0.0433
_diffrn_reflns_av_sigmaI/netI    0.0837
_diffrn_reflns_limit_h_min       -14
_diffrn_reflns_limit_h_max       1
_diffrn_reflns_limit_k_min       -14
_diffrn_reflns_limit_k_max       14
_diffrn_reflns_limit_l_min       -15
_diffrn_reflns_limit_l_max       14
_diffrn_reflns_theta_min         1.9
_diffrn_reflns_theta_max         25.3
_reflns_number_total             6202
_reflns_number_gt                4344
_reflns_threshold_expression     >2\s(I)

_computing_data_collection       'Bruker Nonius (1996)'
_computing_cell_refinement       'XSCANS (1996)'
_computing_data_reduction        'XSCANS (1996)'
_computing_structure_solution    'SHELXS97 (Sheldrick, 1990)'
_computing_structure_refinement  'SHELXL97 (Sheldrick, 1997)'
_computing_molecular_graphics    'PLATON (Spek, 2002)'
_computing_publication_material  'PLATON (Spek, 2002)'

_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^)+(0.0948P)^2^+2.1459P] 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         6202
_refine_ls_number_parameters     596
_refine_ls_number_restraints     162
_refine_ls_R_factor_all          0.1059
```

```
_refine_ls_R_factor_gt           0.0653
_refine_ls_wR_factor_ref         0.1794
_refine_ls_wR_factor_gt          0.1540
_refine_ls_goodness_of_fit_ref   1.023
_refine_ls_restrained_S_all      1.623

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_calc_flag
_atom_site_refinement_flags
_atom_site_disorder_assembly
_atom_site_disorder_group
Ru1 Ru 0.11468(9) 0.15168(8) 0.14601(9) 0.0356(3) Uani 1 d . . .
N11A N 0.2914(9) 0.1112(8) 0.1305(8) 0.039(2) Uani 1 d . . .
C2A C 0.3660(12) 0.1859(11) 0.1171(12) 0.053(3) Uani 1 d . . .
H2A H 0.3377 0.2623 0.1077 0.064 Uiso 1 calc R . .
C3A C 0.4802(13) 0.1522(13) 0.1170(13) 0.059(4) Uani 1 d . . .
H3A H 0.5285 0.2052 0.1070 0.071 Uiso 1 calc R . .
C4A C 0.5238(13) 0.0399(13) 0.1315(13) 0.063(4) Uani 1 d . . .
H4A H 0.6012 0.0161 0.1321 0.075 Uiso 1 calc R . .
C5A C 0.4498(12) -0.0374(12) 0.1455(13) 0.056(4) Uani 1 d . . .
H5A H 0.4776 -0.1138 0.1552 0.067 Uiso 1 calc R . .
C6A C 0.3358(11) -0.0005(10) 0.1447(10) 0.042(3) Uani 1 d . . .
C7A C 0.2511(11) -0.0735(10) 0.1544(10) 0.041(3) Uani 1 d . . .
C8A C 0.2796(12) -0.1893(10) 0.1596(11) 0.048(3) Uani 1 d . . .
H8A H 0.3571 -0.2247 0.1545 0.057 Uiso 1 calc R . .
C9A C 0.1936(13) -0.2521(11) 0.1724(13) 0.056(4) Uani 1 d . . .
H9A H 0.2120 -0.3300 0.1778 0.067 Uiso 1 calc R . .
C10A C 0.0814(13) -0.1993(11) 0.1773(12) 0.054(3) Uani 1 d . . .
H10A H 0.0224 -0.2402 0.1850 0.065 Uiso 1 calc R . .
C11A C 0.0569(12) -0.0826(10) 0.1704(10) 0.043(3) Uani 1 d . . .
H11A H -0.0198 -0.0467 0.1739 0.052 Uiso 1 calc R . .
N12A N 0.1395(8) -0.0193(7) 0.1588(8) 0.034(2) Uani 1 d . . .
N11B N 0.0392(9) 0.1505(8) 0.3174(9) 0.042(2) Uani 1 d . . .
C2B C 0.1006(13) 0.1276(11) 0.3843(11) 0.051(3) Uani 1 d . . .
H2B H 0.1848 0.1054 0.3529 0.061 Uiso 1 calc R . .
C3B C 0.0445(16) 0.1356(14) 0.4957(13) 0.067(4) Uani 1 d . . .
H3B H 0.0902 0.1220 0.5389 0.080 Uiso 1 calc R . .
C4B C -0.0800(16) 0.1640(15) 0.5437(12) 0.071(5) Uani 1 d . . .
H4B H -0.1197 0.1686 0.6202 0.085 Uiso 1 calc R . .
C5B C -0.1462(14) 0.1855(14) 0.4781(12) 0.064(4) Uani 1 d . . .
H5B H -0.2308 0.2046 0.5093 0.077 Uiso 1 calc R . .
C6B C -0.0834(12) 0.1780(10) 0.3646(11) 0.045(3) Uani 1 d . . .
C7B C -0.1431(11) 0.2012(10) 0.2842(11) 0.043(3) Uani 1 d . . .
C8B C -0.2671(13) 0.2394(13) 0.3137(13) 0.060(4) Uani 1 d . . .
H8B H -0.3175 0.2523 0.3871 0.072 Uiso 1 calc R . .
C9B C -0.3156(13) 0.2584(14) 0.2339(15) 0.068(4) Uani 1 d . . .
H9B H -0.3982 0.2857 0.2526 0.082 Uiso 1 calc R . .
C10B C -0.2401(14) 0.2365(13) 0.1269(14) 0.062(4) Uani 1 d . . .
H10B H -0.2712 0.2461 0.0724 0.074 Uiso 1 calc R . .
C11B C -0.1163(11) 0.1996(11) 0.1009(11) 0.048(3) Uani 1 d . . .
H11B H -0.0648 0.1859 0.0279 0.057 Uiso 1 calc R . .
N12B N -0.0682(9) 0.1828(7) 0.1800(8) 0.037(2) Uani 1 d . . .
N1 N 0.1086(9) 0.3238(8) 0.1180(9) 0.039(2) Uani 1 d . . .
```

```
C2 C 0.0696(12) 0.3974(10) 0.1945(12) 0.048(3) Uani 1 d . . .
H2 H 0.0442 0.3706 0.2698 0.057 Uiso 1 calc R . .
C3 C 0.0666(14) 0.5105(11) 0.1634(13) 0.058(4) Uani 1 d . . .
H3 H 0.0361 0.5578 0.2194 0.070 Uiso 1 calc R . .
N4 N 0.1042(12) 0.5556(9) 0.0598(12) 0.061(3) Uani 1 d . . .
C5 C 0.1453(13) 0.4845(11) -0.0186(13) 0.055(3) Uani 1 d . . .
H5 H 0.1738 0.5132 -0.0935 0.067 Uiso 1 calc R . .
C6 C 0.1466(11) 0.3683(10) 0.0094(11) 0.044(3) Uani 1 d . . .
C7 C 0.1801(11) 0.2865(10) -0.0684(10) 0.042(3) Uani 1 d . . .
C8 C 0.2279(11) 0.1955(11) -0.2008(11) 0.045(3) Uani 1 d . . .
N2 N 0.1715(9) 0.1799(8) -0.0243(8) 0.039(2) Uani 1 d . . .
N3 N 0.2148(10) 0.3026(9) -0.1791(9) 0.050(3) Uani 1 d . . .
N5 N 0.2021(9) 0.1193(8) -0.1103(8) 0.042(2) Uani 1 d . . .
C31 C 0.2685(12) 0.1658(12) -0.3157(11) 0.051(3) Uani 1 d . . .
C32 C 0.2797(18) 0.2485(16) -0.4038(14) 0.080(5) Uani 1 d . . .
H32 H 0.2575 0.3235 -0.3907 0.096 Uiso 1 calc R . .
C33 C 0.3244(19) 0.2205(18) -0.5130(15) 0.087(6) Uani 1 d . . .
H33 H 0.3336 0.2768 -0.5723 0.104 Uiso 1 calc R . .
C34 C 0.3541(16) 0.1119(19) -0.5321(14) 0.081(5) Uani 1 d . . .
H34 H 0.3825 0.0930 -0.6044 0.097 Uiso 1 calc R . .
C35 C 0.3424(15) 0.0304(15) -0.4459(14) 0.073(5) Uani 1 d . . .
H35 H 0.3649 -0.0443 -0.4598 0.087 Uiso 1 calc R . .
C36 C 0.2983(13) 0.0557(13) -0.3389(12) 0.060(4) Uani 1 d . . .
H36 H 0.2882 -0.0019 -0.2807 0.072 Uiso 1 calc R . .
P1 P 0.5000 0.5000 -1.0000 0.077(2) Uani 1 d SD . .
F11A F 0.3754(18) 0.4780(19) -0.905(2) 0.147(11) Uani 0.81(5) d PDU A -1
F12A F 0.505(3) 0.5997(17) -0.9438(19) 0.140(11) Uani 0.81(5) d PDU A -1
F13A F 0.570(2) 0.4132(16) -0.938(2) 0.143(12) Uani 0.81(5) d PDU A -1
F11B F 0.404(10) 0.604(8) -0.951(13) 0.29(9) Uani 0.19(5) d PDU A -2
F12B F 0.592(8) 0.543(7) -0.969(10) 0.16(5) Uani 0.19(5) d PDU A -2
F13B F 0.455(13) 0.430(6) -0.884(6) 0.15(5) Uani 0.19(5) d PDU A -2
P2 P 0.001(5) 0.502(4) 0.500(4) 0.093(3) Uani 1 d SD B -2
F21A F 0.122(7) 0.458(10) 0.413(5) 0.16(3) Uani 0.42(13) d PDU C -1
F22A F 0.066(9) 0.554(8) 0.549(6) 0.12(2) Uani 0.42(13) d PDU C -1
F23A F 0.010(9) 0.398(6) 0.579(6) 0.14(3) Uani 0.42(13) d PDU C -1
F21B F 0.099(5) 0.411(4) 0.422(4) 0.129(17) Uani 0.58(13) d PDU B -2
F22B F 0.100(6) 0.514(7) 0.545(6) 0.16(2) Uani 0.58(13) d PDU B -2
F23B F -0.047(9) 0.405(4) 0.600(4) 0.14(2) Uani 0.58(13) d PDU B -2
C1S C 0.635(10) 0.418(7) 0.571(10) 0.22(5) Uani 0.35 d PDU D -1
H1S1 H 0.6908 0.4379 0.4959 0.323 Uiso 0.35 calc PR D -1
H1S2 H 0.6799 0.3732 0.6126 0.323 Uiso 0.35 calc PR D -1
H1S3 H 0.5914 0.4855 0.6056 0.323 Uiso 0.35 calc PR D -1
C2S C 0.553(11) 0.358(8) 0.568(11) 0.26(5) Uani 0.35 d PDU D -1
H2S1 H 0.5699 0.3534 0.4909 0.307 Uiso 0.35 calc PR D -1
H2S2 H 0.4711 0.4002 0.6008 0.307 Uiso 0.35 calc PR D -1
O3S O 0.553(4) 0.247(6) 0.625(5) 0.15(2) Uani 0.35 d PDU D -1
H3S H 0.5227 0.2104 0.6010 0.218 Uiso 0.35 calc PR D -1
O4S O 0.514(11) 0.323(10) 0.705(10) 0.25(5) Uani 0.35 d PDU E -2
H4S1 H 0.5424 0.3060 0.7532 0.375 Uiso 0.35 calc PR E -2
C5S C 0.511(11) 0.438(9) 0.670(14) 0.23(6) Uani 0.35 d PDU E -2
H5S1 H 0.4928 0.4550 0.6032 0.279 Uiso 0.35 calc PR E -2
H5S2 H 0.4458 0.4800 0.7274 0.279 Uiso 0.35 calc PR E -2
C6S C 0.620(11) 0.471(9) 0.646(10) 0.22(5) Uani 0.35 d PDU E -2
H6S1 H 0.6691 0.4113 0.6737 0.330 Uiso 0.35 calc PR E -2
H6S2 H 0.6047 0.5365 0.6818 0.330 Uiso 0.35 calc PR E -2
H6S3 H 0.6613 0.4868 0.5670 0.330 Uiso 0.35 calc PR E -2
O1W O 0.366(9) 0.469(7) 0.673(7) 0.15(3) Uani 0.25 d PDU F -1
H1W H 0.46(9) 0.51(8) 0.64(7) 0.218 Uiso 0.25 d PD G -1
H2W H 0.55(11) 0.45(6) 0.48(7) 0.218 Uiso 0.25 d PD H -1
O2W O 0.253(8) 0.513(4) 0.682(5) 0.11(2) Uani 0.25 d PDU I -2
H3W H 0.15(3) 0.53(7) 0.71(7) 0.162 Uiso 0.25 d PD J -2
```

```
H4W H 0.29(4) 0.42(4) 0.73(10) 0.162 Uiso 0.25 d PD K -2

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
Ru1 0.0364(5) 0.0329(5) 0.0389(6) -0.0019(4) -0.0167(4) -0.0064(4)
N11A 0.045(6) 0.037(5) 0.036(6) -0.005(4) -0.012(5) -0.013(4)
C2A 0.043(7) 0.048(7) 0.071(10) -0.006(7) -0.025(7) -0.011(6)
C3A 0.050(8) 0.064(9) 0.067(10) 0.001(8) -0.025(8) -0.023(7)
C4A 0.041(7) 0.072(10) 0.076(11) -0.008(8) -0.026(8) -0.003(7)
C5A 0.047(7) 0.052(8) 0.066(10) -0.008(7) -0.025(7) 0.002(6)
C6A 0.040(7) 0.047(7) 0.037(7) -0.009(6) -0.013(6) -0.006(5)
C7A 0.052(7) 0.035(6) 0.036(7) -0.001(5) -0.019(6) -0.007(5)
C8A 0.048(7) 0.044(7) 0.046(8) -0.002(6) -0.016(6) -0.005(6)
C9A 0.070(9) 0.031(6) 0.069(10) -0.008(6) -0.031(8) -0.005(6)
C10A 0.067(9) 0.047(8) 0.060(9) -0.008(7) -0.033(8) -0.016(7)
C11A 0.048(7) 0.040(7) 0.045(8) -0.007(6) -0.019(6) -0.010(5)
N12A 0.037(5) 0.029(5) 0.035(6) -0.002(4) -0.016(4) -0.004(4)
N11B 0.050(6) 0.032(5) 0.049(7) -0.006(5) -0.021(5) -0.008(4)
C2B 0.060(8) 0.056(8) 0.045(8) 0.003(6) -0.031(7) -0.012(7)
C3B 0.079(11) 0.082(11) 0.055(10) -0.007(8) -0.040(9) -0.017(9)
C4B 0.080(11) 0.100(13) 0.030(8) -0.012(8) -0.013(8) -0.025(10)
C5B 0.051(8) 0.090(12) 0.042(9) -0.014(8) -0.007(7) -0.013(8)
C6B 0.053(8) 0.039(7) 0.049(8) -0.011(6) -0.021(7) -0.007(6)
C7B 0.034(6) 0.046(7) 0.048(8) -0.007(6) -0.014(6) -0.004(5)
C8B 0.045(8) 0.073(10) 0.056(9) -0.013(8) -0.013(7) -0.003(7)
C9B 0.039(8) 0.075(10) 0.089(13) -0.008(9) -0.030(9) 0.002(7)
C10B 0.056(9) 0.075(10) 0.065(11) 0.001(8) -0.036(8) -0.013(8)
C11B 0.042(7) 0.061(8) 0.042(8) 0.006(6) -0.020(6) -0.018(6)
N12B 0.046(6) 0.030(5) 0.034(6) -0.005(4) -0.016(5) -0.005(4)
N1 0.040(5) 0.032(5) 0.042(6) -0.003(5) -0.017(5) -0.001(4)
C2 0.061(8) 0.035(6) 0.048(8) -0.006(6) -0.023(7) -0.007(6)
C3 0.079(10) 0.039(7) 0.060(10) -0.010(7) -0.027(8) -0.014(7)
N4 0.071(8) 0.039(6) 0.073(9) -0.004(6) -0.032(7) -0.003(6)
C5 0.063(9) 0.046(8) 0.057(9) -0.002(7) -0.023(8) -0.013(7)
C6 0.047(7) 0.037(6) 0.049(8) -0.003(6) -0.021(6) -0.004(5)
C7 0.042(7) 0.041(7) 0.034(7) -0.002(5) -0.008(6) -0.005(5)
C8 0.043(7) 0.049(7) 0.041(8) -0.003(6) -0.018(6) -0.002(6)
N2 0.038(5) 0.038(5) 0.037(6) -0.004(4) -0.012(5) -0.007(4)
N3 0.058(7) 0.045(6) 0.045(7) 0.000(5) -0.019(6) -0.008(5)
N5 0.039(5) 0.046(6) 0.037(6) -0.004(5) -0.014(5) -0.004(5)
C31 0.048(8) 0.063(9) 0.039(8) 0.004(7) -0.017(6) -0.010(6)
C32 0.104(14) 0.081(12) 0.054(11) -0.004(9) -0.036(10) -0.004(10)
C33 0.112(16) 0.097(15) 0.048(11) 0.004(10) -0.033(11) -0.018(12)
C34 0.070(11) 0.131(18) 0.039(10) -0.018(11) -0.016(8) -0.017(11)
C35 0.069(10) 0.081(12) 0.065(12) -0.030(10) -0.016(9) -0.010(9)
C36 0.064(9) 0.070(10) 0.041(8) -0.012(7) -0.018(7) -0.005(8)
P1 0.056(3) 0.045(3) 0.118(6) -0.008(4) -0.031(4) 0.006(3)
F11A 0.088(13) 0.104(18) 0.17(2) -0.024(15) 0.022(13) -0.009(11)
F12A 0.17(3) 0.088(14) 0.164(19) -0.038(12) -0.059(18) -0.020(16)
F13A 0.13(2) 0.101(14) 0.20(3) 0.015(14) -0.10(2) 0.019(12)
F11B 0.27(14) 0.13(8) 0.41(17) -0.17(10) -0.07(12) 0.07(9)
F12B 0.08(6) 0.10(6) 0.30(13) -0.09(7) -0.05(7) -0.01(4)
F13B 0.22(12) 0.05(4) 0.11(6) -0.02(4) 0.00(6) -0.01(5)
P2 0.152(8) 0.071(5) 0.066(5) -0.013(4) -0.052(5) -0.014(5)
F21A 0.16(4) 0.14(6) 0.12(3) -0.05(3) 0.01(3) 0.01(4)
```

```
F22A 0.14(4) 0.15(5) 0.10(3) -0.04(3) -0.06(3) -0.03(4)
F23A 0.17(5) 0.11(4) 0.11(4) 0.02(3) -0.06(4) 0.01(3)
F21B 0.20(4) 0.09(2) 0.11(2) -0.049(18) -0.09(3) 0.03(2)
F22B 0.21(5) 0.14(4) 0.17(4) -0.05(3) -0.12(4) 0.01(3)
F23B 0.27(6) 0.10(3) 0.07(2) 0.008(16) -0.05(3) -0.08(3)
C1S 0.28(11) 0.15(7) 0.28(12) -0.07(7) -0.17(9) 0.00(6)
C2S 0.23(8) 0.26(8) 0.28(9) -0.04(7) -0.11(7) -0.04(6)
O3S 0.04(2) 0.23(6) 0.13(4) 0.02(4) -0.02(3) -0.03(3)
O4S 0.23(8) 0.30(9) 0.23(9) 0.08(8) -0.14(8) -0.07(8)
C5S 0.24(9) 0.27(9) 0.21(9) -0.08(7) -0.09(7) -0.01(7)
C6S 0.21(9) 0.20(9) 0.18(9) -0.04(8) -0.01(8) -0.01(7)
O1W 0.18(6) 0.11(5) 0.12(5) 0.00(4) -0.01(5) -0.07(5)
O2W 0.18(6) 0.05(3) 0.07(3) 0.01(2) -0.02(4) -0.05(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
Ru1 N11A 2.036(10) . ?
Ru1 N12A 2.042(9) . ?
Ru1 N12B 2.046(10) . ?
Ru1 N2 2.051(10) . ?
Ru1 N11B 2.064(11) . ?
Ru1 N1 2.069(9) . ?
N11A C6A 1.369(15) . ?
N11A C2A 1.372(15) . ?
C2A C3A 1.366(18) . ?
C2A H2A 0.9300 . ?
C3A C4A 1.37(2) . ?
C3A H3A 0.9300 . ?
C4A C5A 1.389(19) . ?
C4A H4A 0.9300 . ?
C5A C6A 1.371(17) . ?
C5A H5A 0.9300 . ?
C6A C7A 1.468(16) . ?
C7A N12A 1.361(15) . ?
C7A C8A 1.385(16) . ?
C8A C9A 1.375(18) . ?
C8A H8A 0.9300 . ?
C9A C10A 1.362(19) . ?
C9A H9A 0.9300 . ?
C10A C11A 1.392(17) . ?
C10A H10A 0.9300 . ?
C11A N12A 1.350(14) . ?
C11A H11A 0.9300 . ?
N11B C2B 1.344(15) . ?
N11B C6B 1.348(16) . ?
C2B C3B 1.36(2) . ?
C2B H2B 0.9300 . ?
```

```
C3B C4B 1.37(2) . ?
C3B H3B 0.9300 . ?
C4B C5B 1.38(2) . ?
C4B H4B 0.9300 . ?
C5B C6B 1.385(19) . ?
C5B H5B 0.9300 . ?
C6B C7B 1.487(17) . ?
C7B N12B 1.328(16) . ?
C7B C8B 1.388(17) . ?
C8B C9B 1.38(2) . ?
C8B H8B 0.9300 . ?
C9B C10B 1.37(2) . ?
C9B H9B 0.9300 . ?
C10B C11B 1.389(19) . ?
C10B H10B 0.9300 . ?
C11B N12B 1.372(15) . ?
C11B H11B 0.9300 . ?
N1 C2 1.353(16) . ?
N1 C6 1.358(16) . ?
C2 C3 1.371(17) . ?
C2 H2 0.9300 . ?
C3 N4 1.305(18) . ?
C3 H3 0.9300 . ?
N4 C5 1.347(18) . ?
C5 C6 1.406(17) . ?
C5 H5 0.9300 . ?
C6 C7 1.451(17) . ?
C7 N3 1.336(16) . ?
C7 N2 1.338(15) . ?
C8 N5 1.344(15) . ?
C8 N3 1.362(16) . ?
C8 C31 1.485(18) . ?
N2 N5 1.358(14) . ?
C31 C32 1.38(2) . ?
C31 C36 1.38(2) . ?
C32 C33 1.40(2) . ?
C32 H32 0.9300 . ?
C33 C34 1.35(3) . ?
C33 H33 0.9300 . ?
C34 C35 1.35(2) . ?
C34 H34 0.9300 . ?
C35 C36 1.36(2) . ?
C35 H35 0.9300 . ?
C36 H36 0.9300 . ?

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
N11A Ru1 N12A 78.6(4) . . ?
N11A Ru1 N12B 173.3(4) . . ?
N12A Ru1 N12B 98.4(4) . . ?
N11A Ru1 N2 90.5(4) . . ?
N12A Ru1 N2 97.2(4) . . ?
N12B Ru1 N2 95.8(4) . . ?
N11A Ru1 N11B 95.7(4) . . ?
N12A Ru1 N11B 91.6(4) . . ?
```

```
N12B Ru1 N11B 78.4(4) . . ?
N2 Ru1 N11B 170.1(4) . . ?
N11A Ru1 N1 96.8(4) . . ?
N12A Ru1 N1 173.5(4) . . ?
N12B Ru1 N1 86.7(4) . . ?
N2 Ru1 N1 78.2(4) . . ?
N11B Ru1 N1 93.4(4) . . ?
C6A N11A C2A 117.1(10) . . ?
C6A N11A Ru1 116.9(7) . . ?
C2A N11A Ru1 125.7(8) . . ?
C3A C2A N11A 122.4(13) . . ?
C3A C2A H2A 118.8 . . ?
N11A C2A H2A 118.8 . . ?
C2A C3A C4A 120.0(12) . . ?
C2A C3A H3A 120.0 . . ?
C4A C3A H3A 120.0 . . ?
C3A C4A C5A 118.7(12) . . ?
C3A C4A H4A 120.6 . . ?
C5A C4A H4A 120.6 . . ?
C6A C5A C4A 119.7(13) . . ?
C6A C5A H5A 120.2 . . ?
C4A C5A H5A 120.1 . . ?
N11A C6A C5A 122.1(11) . . ?
N11A C6A C7A 112.9(10) . . ?
C5A C6A C7A 125.0(12) . . ?
N12A C7A C8A 121.2(11) . . ?
N12A C7A C6A 115.2(10) . . ?
C8A C7A C6A 123.6(11) . . ?
C9A C8A C7A 120.1(12) . . ?
C9A C8A H8A 119.9 . . ?
C7A C8A H8A 119.9 . . ?
C10A C9A C8A 119.4(12) . . ?
C10A C9A H9A 120.3 . . ?
C8A C9A H9A 120.3 . . ?
C9A C10A C11A 118.6(12) . . ?
C9A C10A H10A 120.7 . . ?
C11A C10A H10A 120.7 . . ?
N12A C11A C10A 123.0(12) . . ?
N12A C11A H11A 118.5 . . ?
C10A C11A H11A 118.5 . . ?
C11A N12A C7A 117.6(10) . . ?
C11A N12A Ru1 126.4(8) . . ?
C7A N12A Ru1 115.9(7) . . ?
C2B N11B C6B 118.1(11) . . ?
C2B N11B Ru1 126.3(9) . . ?
C6B N11B Ru1 115.5(8) . . ?
N11B C2B C3B 122.6(14) . . ?
N11B C2B H2B 118.7 . . ?
C3B C2B H2B 118.7 . . ?
C2B C3B C4B 119.3(13) . . ?
C2B C3B H3B 120.3 . . ?
C4B C3B H3B 120.3 . . ?
C3B C4B C5B 119.6(14) . . ?
C3B C4B H4B 120.2 . . ?
C5B C4B H4B 120.2 . . ?
C4B C5B C6B 118.3(14) . . ?
C4B C5B H5B 120.9 . . ?
C6B C5B H5B 120.8 . . ?
N11B C6B C5B 122.0(12) . . ?
N11B C6B C7B 114.2(11) . . ?
C5B C6B C7B 123.8(12) . . ?
```

```
N12B C7B C8B 121.7(12) . . ?
N12B C7B C6B 114.7(10) . . ?
C8B C7B C6B 123.5(12) . . ?
C9B C8B C7B 119.9(14) . . ?
C9B C8B H8B 120.0 . . ?
C7B C8B H8B 120.0 . . ?
C10B C9B C8B 119.0(13) . . ?
C10B C9B H9B 120.5 . . ?
C8B C9B H9B 120.5 . . ?
C9B C10B C11B 119.0(13) . . ?
C9B C10B H10B 120.5 . . ?
C11B C10B H10B 120.5 . . ?
N12B C11B C10B 121.8(13) . . ?
N12B C11B H11B 119.1 . . ?
C10B C11B H11B 119.1 . . ?
C7B N12B C11B 118.5(10) . . ?
C7B N12B Ru1 116.4(7) . . ?
C11B N12B Ru1 124.5(9) . . ?
C2 N1 C6 116.2(10) . . ?
C2 N1 Ru1 128.0(9) . . ?
C6 N1 Ru1 115.8(8) . . ?
N1 C2 C3 121.5(13) . . ?
N1 C2 H2 119.3 . . ?
C3 C2 H2 119.3 . . ?
N4 C3 C2 123.7(13) . . ?
N4 C3 H3 118.1 . . ?
C2 C3 H3 118.1 . . ?
C3 N4 C5 116.3(12) . . ?
N4 C5 C6 122.0(13) . . ?
N4 C5 H5 119.0 . . ?
C6 C5 H5 119.0 . . ?
N1 C6 C5 120.3(12) . . ?
N1 C6 C7 113.8(10) . . ?
C5 C6 C7 125.9(12) . . ?
N3 C7 N2 114.3(11) . . ?
N3 C7 C6 129.1(11) . . ?
N2 C7 C6 116.5(11) . . ?
N5 C8 N3 114.8(12) . . ?
N5 C8 C31 122.9(12) . . ?
N3 C8 C31 122.3(12) . . ?
C7 N2 N5 106.7(10) . . ?
C7 N2 Ru1 115.7(8) . . ?
N5 N2 Ru1 137.6(8) . . ?
C7 N3 C8 100.2(10) . . ?
C8 N5 N2 104.1(10) . . ?
C32 C31 C36 117.6(14) . . ?
C32 C31 C8 120.5(14) . . ?
C36 C31 C8 121.9(12) . . ?
C31 C32 C33 120.5(18) . . ?
C31 C32 H32 119.8 . . ?
C33 C32 H32 119.8 . . ?
C34 C33 C32 119.9(17) . . ?
C34 C33 H33 120.1 . . ?
C32 C33 H33 120.0 . . ?
C33 C34 C35 119.8(17) . . ?
C33 C34 H34 120.1 . . ?
C35 C34 H34 120.1 . . ?
C34 C35 C36 121.2(17) . . ?
C34 C35 H35 119.4 . . ?
C36 C35 H35 119.4 . . ?
C35 C36 C31 120.9(15) . . ?
```

```
C35 C36 H36 119.6 . . ?
C31 C36 H36 119.6 . . ?

loop_
_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
N12A Ru1 N11A C6A -5.3(8) . . . . ?
N12B Ru1 N11A C6A 58(4) . . . . ?
N2 Ru1 N11A C6A -102.6(9) . . . . ?
N11B Ru1 N11A C6A 85.2(9) . . . . ?
N1 Ru1 N11A C6A 179.3(8) . . . . ?
N12A Ru1 N11A C2A -179.0(11) . . . . ?
N12B Ru1 N11A C2A -116(3) . . . . ?
N2 Ru1 N11A C2A 83.7(11) . . . . ?
N11B Ru1 N11A C2A -88.5(11) . . . . ?
N1 Ru1 N11A C2A 5.5(11) . . . . ?
C6A N11A C2A C3A 0(2) . . . . ?
Ru1 N11A C2A C3A 174.1(11) . . . . ?
N11A C2A C3A C4A -1(2) . . . . ?
C2A C3A C4A C5A 0(2) . . . . ?
C3A C4A C5A C6A 0(2) . . . . ?
C2A N11A C6A C5A -0.2(19) . . . . ?
Ru1 N11A C6A C5A -174.5(10) . . . . ?
C2A N11A C6A C7A -178.0(11) . . . . ?
Ru1 N11A C6A C7A 7.7(13) . . . . ?
C4A C5A C6A N11A 0(2) . . . . ?
C4A C5A C6A C7A 177.6(13) . . . . ?
N11A C6A C7A N12A -6.2(16) . . . . ?
C5A C6A C7A N12A 176.0(12) . . . . ?
N11A C6A C7A C8A 174.2(11) . . . . ?
C5A C6A C7A C8A -3(2) . . . . ?
N12A C7A C8A C9A -1.7(19) . . . . ?
C6A C7A C8A C9A 177.8(13) . . . . ?
C7A C8A C9A C10A 2(2) . . . . ?
C8A C9A C10A C11A -1(2) . . . . ?
C9A C10A C11A N12A 0(2) . . . . ?
C10A C11A N12A C7A -0.3(18) . . . . ?
C10A C11A N12A Ru1 179.2(10) . . . . ?
C8A C7A N12A C11A 1.1(17) . . . . ?
C6A C7A N12A C11A -178.5(10) . . . . ?
C8A C7A N12A Ru1 -178.5(9) . . . . ?
C6A C7A N12A Ru1 1.9(13) . . . . ?
N11A Ru1 N12A C11A -177.9(10) . . . . ?
N12B Ru1 N12A C11A 8.1(10) . . . . ?
N2 Ru1 N12A C11A -88.8(10) . . . . ?
N11B Ru1 N12A C11A 86.6(10) . . . . ?
N1 Ru1 N12A C11A -133(3) . . . . ?
N11A Ru1 N12A C7A 1.6(8) . . . . ?
N12B Ru1 N12A C7A -172.3(8) . . . . ?
N2 Ru1 N12A C7A 90.7(9) . . . . ?
N11B Ru1 N12A C7A -93.8(9) . . . . ?
N1 Ru1 N12A C7A 46(4) . . . . ?
N11A Ru1 N11B C2B -0.4(10) . . . . ?
```

```
N12A Ru1 N11B C2B 78.3(10) . . . . ?
N12B Ru1 N11B C2B 176.5(10) . . . . ?
N2 Ru1 N11B C2B -129(2) . . . . ?
N1 Ru1 N11B C2B -97.6(10) . . . . ?
N11A Ru1 N11B C6B 178.0(8) . . . . ?
N12A Ru1 N11B C6B -103.3(8) . . . . ?
N12B Ru1 N11B C6B -5.1(8) . . . . ?
N2 Ru1 N11B C6B 49(2) . . . . ?
N1 Ru1 N11B C6B 80.8(8) . . . . ?
C6B N11B C2B C3B -2.7(19) . . . . ?
Ru1 N11B C2B C3B 175.7(11) . . . . ?
N11B C2B C3B C4B 3(2) . . . . ?
C2B C3B C4B C5B -1(3) . . . . ?
C3B C4B C5B C6B 0(2) . . . . ?
C2B N11B C6B C5B 1.4(18) . . . . ?
Ru1 N11B C6B C5B -177.1(11) . . . . ?
C2B N11B C6B C7B -179.6(10) . . . . ?
Ru1 N11B C6B C7B 1.8(13) . . . . ?
C4B C5B C6B N11B 0(2) . . . . ?
C4B C5B C6B C7B -178.8(13) . . . . ?
N11B C6B C7B N12B 5.0(15) . . . . ?
C5B C6B C7B N12B -176.1(12) . . . . ?
N11B C6B C7B C8B -174.7(12) . . . . ?
C5B C6B C7B C8B 4(2) . . . . ?
N12B C7B C8B C9B 1(2) . . . . ?
C6B C7B C8B C9B -179.7(13) . . . . ?
C7B C8B C9B C10B 1(2) . . . . ?
C8B C9B C10B C11B -2(2) . . . . ?
C9B C10B C11B N12B 1(2) . . . . ?
C8B C7B N12B C11B -1.7(18) . . . . ?
C6B C7B N12B C11B 178.5(10) . . . . ?
C8B C7B N12B Ru1 170.2(10) . . . . ?
C6B C7B N12B Ru1 -9.5(13) . . . . ?
C10B C11B N12B C7B 0.9(18) . . . . ?
C10B C11B N12B Ru1 -170.4(10) . . . . ?
N11A Ru1 N12B C7B 36(4) . . . . ?
N12A Ru1 N12B C7B 98.0(9) . . . . ?
N2 Ru1 N12B C7B -163.8(8) . . . . ?
N11B Ru1 N12B C7B 8.1(8) . . . . ?
N1 Ru1 N12B C7B -86.0(9) . . . . ?
N11A Ru1 N12B C11B -153(3) . . . . ?
N12A Ru1 N12B C11B -90.5(10) . . . . ?
N2 Ru1 N12B C11B 7.7(10) . . . . ?
N11B Ru1 N12B C11B 179.5(10) . . . . ?
N1 Ru1 N12B C11B 85.4(10) . . . . ?
N11A Ru1 N1 C2 -94.5(10) . . . . ?
N12A Ru1 N1 C2 -138(3) . . . . ?
N12B Ru1 N1 C2 79.8(10) . . . . ?
N2 Ru1 N1 C2 176.4(11) . . . . ?
N11B Ru1 N1 C2 1.7(10) . . . . ?
N11A Ru1 N1 C6 86.8(8) . . . . ?
N12A Ru1 N1 C6 43(4) . . . . ?
N12B Ru1 N1 C6 -99.0(8) . . . . ?
N2 Ru1 N1 C6 -2.4(8) . . . . ?
N11B Ru1 N1 C6 -177.1(8) . . . . ?
C6 N1 C2 C3 1.2(18) . . . . ?
Ru1 N1 C2 C3 -177.5(10) . . . . ?
N1 C2 C3 N4 -2(2) . . . . ?
C2 C3 N4 C5 1(2) . . . . ?
C3 N4 C5 C6 1(2) . . . . ?
C2 N1 C6 C5 0.7(17) . . . . ?
```

```
Ru1 N1 C6 C5 179.6(9) . . . . ?
C2 N1 C6 C7 -176.4(10) . . . . ?
Ru1 N1 C6 C7 2.6(13) . . . . ?
N4 C5 C6 N1 -2(2) . . . . ?
N4 C5 C6 C7 174.9(12) . . . . ?
N1 C6 C7 N3 176.2(12) . . . . ?
C5 C6 C7 N3 -1(2) . . . . ?
N1 C6 C7 N2 -1.1(16) . . . . ?
C5 C6 C7 N2 -177.9(12) . . . . ?
N3 C7 N2 N5 -0.1(14) . . . . ?
C6 C7 N2 N5 177.6(10) . . . . ?
N3 C7 N2 Ru1 -178.6(8) . . . . ?
C6 C7 N2 Ru1 -0.9(14) . . . . ?
N11A Ru1 N2 C7 -95.1(8) . . . . ?
N12A Ru1 N2 C7 -173.6(8) . . . . ?
N12B Ru1 N2 C7 87.2(8) . . . . ?
N11B Ru1 N2 C7 34(3) . . . . ?
N1 Ru1 N2 C7 1.7(8) . . . . ?
N11A Ru1 N2 N5 87.1(11) . . . . ?
N12A Ru1 N2 N5 8.5(11) . . . . ?
N12B Ru1 N2 N5 -90.7(11) . . . . ?
N11B Ru1 N2 N5 -144.1(19) . . . . ?
N1 Ru1 N2 N5 -176.1(11) . . . . ?
N2 C7 N3 C8 -0.3(14) . . . . ?
C6 C7 N3 C8 -177.7(12) . . . . ?
N5 C8 N3 C7 0.6(14) . . . . ?
C31 C8 N3 C7 -179.0(11) . . . . ?
N3 C8 N5 N2 -0.7(13) . . . . ?
C31 C8 N5 N2 178.9(11) . . . . ?
C7 N2 N5 C8 0.5(12) . . . . ?
Ru1 N2 N5 C8 178.5(9) . . . . ?
N5 C8 C31 C32 172.2(13) . . . . ?
N3 C8 C31 C32 -8(2) . . . . ?
N5 C8 C31 C36 -9.1(19) . . . . ?
N3 C8 C31 C36 170.5(13) . . . . ?
C36 C31 C32 C33 -2(2) . . . . ?
C8 C31 C32 C33 176.5(15) . . . . ?
C31 C32 C33 C34 1(3) . . . . ?
C32 C33 C34 C35 -1(3) . . . . ?
C33 C34 C35 C36 2(3) . . . . ?
C34 C35 C36 C31 -2(2) . . . . ?
C32 C31 C36 C35 3(2) . . . . ?
C8 C31 C36 C35 -176.0(13) . . . . ?

_diffrn_measured_fraction_theta_max 1.00
_diffrn_reflns_theta_full        25.2
_diffrn_measured_fraction_theta_full 1.00
_refine_diff_density_max         1.31
_refine_diff_density_min         -0.76
_refine_diff_density_rms         0.11

#=============================================================

data_II
_database_code_CSD               204726

_audit_creation_method           SHELXL-97
_chemical_name_systematic
;
?
;
```

```
_chemical_name_common            ?
_chemical_formula_moiety         ?
_chemical_formula_sum            'C26 H21.24 F9 N9 O0.37 P1.50 Ru'
_chemical_formula_weight         784.25

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'
Ru Ru -1.2594 0.8363 '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'
P P 0.1023 0.0942 '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'

_symmetry_cell_setting           Orthorhombic
_symmetry_space_group_name_H-M   'B2cb '
# Alternative setting of Aba2 (No. 41)

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

_cell_length_a                   17.4944(15)
_cell_length_b                   17.5143(16)
_cell_length_c                   19.5605(19)
_cell_angle_alpha                90
_cell_angle_beta                 90
_cell_angle_gamma                90
_cell_volume                     5993.4(10)
_cell_formula_units_Z            8
_cell_measurement_temperature    293(2)
_cell_measurement_reflns_used    25
_cell_measurement_theta_min      10
_cell_measurement_theta_max      15

_exptl_crystal_description       block
_exptl_crystal_colour            red
_exptl_crystal_size_max          0.25
_exptl_crystal_size_mid          0.15
_exptl_crystal_size_min          0.10
_exptl_crystal_density_meas      ?
_exptl_crystal_density_diffrn    1.738
_exptl_crystal_density_method    'not measured'
_exptl_crystal_F_000             3126
_exptl_absorpt_coefficient_mu    0.697
_exptl_absorpt_correction_type   psi-scans
_exptl_absorpt_correction_T_min  0.845
_exptl_absorpt_correction_T_max  0.933
```

```
_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       ?
_diffrn_detector_area_resol_mean ?
_diffrn_standards_number         3
_diffrn_standards_interval_count 120
_diffrn_standards_interval_time  ?
_diffrn_standards_decay_%        1
_diffrn_reflns_number            3430
_diffrn_reflns_av_R_equivalents  0.0000
_diffrn_reflns_av_sigmaI/netI    0.0522
_diffrn_reflns_limit_h_min       0
_diffrn_reflns_limit_h_max       22
_diffrn_reflns_limit_k_min       0
_diffrn_reflns_limit_k_max       22
_diffrn_reflns_limit_l_min       0
_diffrn_reflns_limit_l_max       25
_diffrn_reflns_theta_min         2.08
_diffrn_reflns_theta_max         27.14
_reflns_number_total             3430
_reflns_number_gt                2184
_reflns_threshold_expression     >2\s(I)

_computing_data_collection       'DATCOL (Nonius)'
_computing_cell_refinement       'SET4 (nonius)'
_computing_data_reduction        'NRCVAX (Gabe et al., 1989)'
_computing_structure_solution    'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement  'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics    'PLATON, (Spek 2002)'
_computing_publication_material  'PLATON, (Spek 2002)'

_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^)+(0.0281P)^2^] 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_abs_structure_details Flack
_refine_ls_abs_structure_Flack   0.00(4)
_refine_ls_number_reflns         3430
_refine_ls_number_parameters     533
_refine_ls_number_restraints     88
_refine_ls_R_factor_all          0.0732
_refine_ls_R_factor_gt           0.0351
_refine_ls_wR_factor_ref         0.0635
_refine_ls_wR_factor_gt          0.0568
_refine_ls_goodness_of_fit_ref   0.977
_refine_ls_restrained_S_all      0.969
_refine_ls_shift/su_max          <0.02
_refine_ls_shift/su_mean         0.004

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_calc_flag
_atom_site_refinement_flags
_atom_site_disorder_assembly
_atom_site_disorder_group
Ru1 Ru 0.46800(15) 0.798320(19) 0.801924(18) 0.04564(10) Uani 1 d . . .
N1 N 0.4318(3) 0.8389(3) 0.8932(2) 0.0497(11) Uani 1 d . . .
N2 N 0.3923(3) 0.8106(3) 0.9479(2) 0.0607(13) Uani 1 d . . .
N3 N 0.4173(3) 0.9334(3) 0.9667(2) 0.0607(13) Uani 1 d . . .
H3 H 0.4190 0.9776 0.9858 0.073 Uiso 0.50 calc PR . .
N4 N 0.4999(3) 0.9120(2) 0.7961(2) 0.0477(10) Uani 1 d . . .
N11 N 0.4991(3) 0.7727(2) 0.7028(2) 0.0546(12) Uani 1 d . . .
N21 N 0.3694(3) 0.8255(2) 0.7503(3) 0.0544(12) Uani 1 d . . .
N31 N 0.5652(3) 0.7630(2) 0.8509(2) 0.0507(11) Uani 1 d . . .
N41 N 0.4390(3) 0.6873(2) 0.8268(2) 0.0543(13) Uani 1 d . . .
C1 C 0.3859(4) 0.8694(4) 0.9907(3) 0.0669(17) Uani 1 d . . .
H1 H 0.3620 0.8661 1.0331 0.080 Uiso 1 calc R . .
C2 C 0.4458(3) 0.9126(3) 0.9055(3) 0.0509(15) Uani 1 d . . .
C3 C 0.4835(4) 0.9552(3) 0.8523(3) 0.0532(18) Uani 1 d . . .
C4 C 0.5047(4) 1.0316(3) 0.8528(4) 0.0736(19) Uani 1 d . . .
H4 H 0.4933 1.0602 0.8915 0.088 Uiso 1 calc R . .
N5 N 0.5394(4) 1.0656(3) 0.8026(4) 0.0811(16) Uani 1 d . . .
C6 C 0.5546(4) 1.0219(4) 0.7492(4) 0.0713(18) Uani 1 d . . .
H6 H 0.5803 1.0439 0.7126 0.086 Uiso 1 calc R . .
C7 C 0.5351(4) 0.9464(3) 0.7443(3) 0.0608(15) Uani 1 d . . .
H7 H 0.5464 0.9192 0.7047 0.073 Uiso 1 calc R . .
C12 C 0.5649(4) 0.7453(3) 0.6815(3) 0.0651(18) Uani 1 d . . .
H12 H 0.6026 0.7351 0.7138 0.078 Uiso 1 calc R . .
C13 C 0.5807(5) 0.7310(4) 0.6133(4) 0.083(2) Uani 1 d . . .
H13 H 0.6281 0.7119 0.6001 0.100 Uiso 1 calc R . .
C14 C 0.5268(6) 0.7451(5) 0.5667(3) 0.093(2) Uani 1 d . . .
H14 H 0.5362 0.7349 0.5209 0.111 Uiso 1 calc R . .
C15 C 0.4560(7) 0.7753(4) 0.5865(3) 0.091(3) Uani 1 d . . .
H15 H 0.4183 0.7856 0.5543 0.109 Uiso 1 calc R . .
C16 C 0.4433(4) 0.7895(3) 0.6552(3) 0.064(2) Uani 1 d . . .
C22 C 0.3067(4) 0.8532(4) 0.7796(4) 0.078(2) Uani 1 d . . .
H22 H 0.3048 0.8564 0.8270 0.093 Uiso 1 calc R . .
C23 C 0.2443(5) 0.8773(5) 0.7420(5) 0.099(3) Uani 1 d . . .
H23 H 0.2001 0.8949 0.7632 0.119 Uiso 1 calc R . .
```

```
C24 C 0.2502(7) 0.8743(5) 0.6714(6) 0.099(3) Uani 1 d . . .
H24 H 0.2105 0.8928 0.6445 0.119 Uiso 1 calc R . .
C25 C 0.3128(5) 0.8448(5) 0.6413(4) 0.085(2) Uani 1 d . . .
H25 H 0.3158 0.8408 0.5939 0.102 Uiso 1 calc R . .
C26 C 0.3720(5) 0.8209(3) 0.6817(3) 0.0647(18) Uani 1 d . . .
C32 C 0.6296(4) 0.8025(4) 0.8609(3) 0.0664(16) Uani 1 d . . .
H32 H 0.6337 0.8501 0.8401 0.080 Uiso 1 calc R . .
C33 C 0.6900(4) 0.7776(4) 0.8995(4) 0.082(2) Uani 1 d . . .
H33 H 0.7338 0.8074 0.9040 0.098 Uiso 1 calc R . .
C34 C 0.6849(5) 0.7097(5) 0.9308(4) 0.090(2) Uani 1 d . . .
H34 H 0.7249 0.6922 0.9580 0.108 Uiso 1 calc R . .
C35 C 0.6201(5) 0.6658(4) 0.9223(4) 0.083(2) Uani 1 d . . .
H35 H 0.6163 0.6181 0.9430 0.100 Uiso 1 calc R . .
C36 C 0.5607(4) 0.6934(3) 0.8828(3) 0.0562(14) Uani 1 d . . .
C42 C 0.3742(4) 0.6523(3) 0.8092(3) 0.0726(18) Uani 1 d . . .
H42 H 0.3423 0.6748 0.7770 0.087 Uiso 1 calc R . .
C43 C 0.3535(5) 0.5824(4) 0.8382(5) 0.099(3) Uani 1 d . . .
H43 H 0.3079 0.5588 0.8259 0.118 Uiso 1 calc R . .
C44 C 0.4006(6) 0.5496(5) 0.8845(5) 0.106(3) Uani 1 d . . .
H44 H 0.3871 0.5035 0.9046 0.128 Uiso 1 calc R . .
C45 C 0.4694(7) 0.5846(3) 0.9022(3) 0.0889(19) Uani 1 d . . .
H45 H 0.5021 0.5625 0.9341 0.107 Uiso 1 calc R . .
C46 C 0.4879(4) 0.6536(3) 0.8707(3) 0.0577(19) Uani 1 d . . .
O1W O 0.6122(7) 1.0000 0.5000 0.145(7) Uani 0.748(18) d SPD . .
H1W1 H 0.6219 0.9698 0.5327 0.174 Uiso 0.374(9) d PD . .
H1W2 H 0.6572 1.0093 0.4845 0.174 Uiso 0.374(9) d PD . .
P1A P 0.6782(15) 0.9942(17) 0.9988(16) 0.098(15) Uani 0.17 d PD A -1
F11A F 0.6878(18) 0.9785(18) 0.9243(15) 0.145(18) Uani 0.34 d PDU A -1
F12A F 0.5981(13) 0.9651(11) 0.9970(13) 0.120(7) Uani 0.34 d PDU A -1
F13A F 0.7063(16) 0.9156(9) 1.0134(10) 0.102(6) Uani 0.34 d PDU A -1
P1B P 0.6767(7) 1.0027(15) 0.9985(12) 0.080(5) Uani 0.33 d PD B -2
F11B F 0.6754(9) 0.9805(9) 0.9206(5) 0.127(6) Uani 0.66 d PD B -2
F12B F 0.6283(10) 0.9296(7) 1.0168(7) 0.165(7) Uani 0.66 d PD B -2
F13B F 0.7522(6) 0.9546(7) 1.0099(5) 0.148(4) Uani 0.66 d PD B -2
P2A P 0.7313(8) 0.9207(7) 0.6361(6) 0.101(4) Uani 0.522(16) d PD C -3
F21A F 0.6473(8) 0.9001(10) 0.6179(9) 0.141(7) Uani 0.522(16) d PD C -3
F22A F 0.7537(13) 0.8363(8) 0.6258(13) 0.222(14) Uani 0.522(16) d PD C -3
F23A F 0.7136(8) 0.9077(14) 0.7127(6) 0.159(9) Uani 0.522(16) d PD C -3
F24A F 0.7072(9) 1.0050(6) 0.6438(9) 0.158(7) Uani 0.522(16) d PD C -3
F25A F 0.7469(10) 0.9368(11) 0.5581(6) 0.146(7) Uani 0.522(16) d PD C -3
F26A F 0.8145(7) 0.9416(14) 0.6519(10) 0.195(9) Uani 0.522(16) d PD C -3
P2B P 0.7438(9) 0.9055(8) 0.6486(8) 0.110(5) Uani 0.478(16) d PD C -4
F21B F 0.6600(10) 0.9334(14) 0.6392(11) 0.210(14) Uani 0.478(16) d PDU C -4
F22B F 0.7328(11) 0.8507(12) 0.5874(7) 0.158(10) Uani 0.478(16) d PDU C -4
F23B F 0.7172(10) 0.8430(9) 0.6993(8) 0.147(7) Uani 0.478(16) d PDU C -4
F24B F 0.7534(14) 0.9609(10) 0.7079(10) 0.216(15) Uani 0.478(16) d PD C -4
F25B F 0.7707(12) 0.9672(10) 0.5960(11) 0.162(9) Uani 0.478(16) d PD C -4
F26B F 0.8273(7) 0.8785(10) 0.6553(7) 0.123(6) Uani 0.478(16) d PD C -4

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
Ru1 0.04604(19) 0.04527(16) 0.04560(17) -0.0057(2) 0.0003(4) -0.0012(4)
N1 0.046(3) 0.053(3) 0.049(3) -0.004(2) -0.001(2) 0.002(2)
N2 0.060(3) 0.069(3) 0.053(3) -0.007(3) 0.008(3) -0.007(3)
N3 0.064(3) 0.066(3) 0.052(3) -0.020(2) -0.002(3) -0.004(3)
```

```
N4 0.043(2) 0.054(2) 0.046(2) -0.001(2) -0.005(2) -0.0032(19)
N11 0.066(3) 0.046(2) 0.051(3) -0.009(2) 0.008(3) -0.002(2)
N21 0.050(3) 0.047(2) 0.066(3) 0.000(2) -0.007(3) -0.004(2)
N31 0.046(3) 0.056(3) 0.050(3) -0.002(2) 0.001(2) 0.005(2)
N41 0.057(3) 0.049(3) 0.057(3) -0.010(2) 0.006(2) -0.004(2)
C1 0.064(4) 0.085(5) 0.052(4) -0.012(3) 0.009(3) -0.002(4)
C2 0.048(4) 0.057(3) 0.047(3) -0.010(2) -0.009(2) 0.008(3)
C3 0.053(5) 0.051(3) 0.056(3) -0.009(2) -0.007(3) 0.002(3)
C4 0.083(5) 0.053(3) 0.086(5) -0.015(3) 0.001(4) -0.008(3)
N5 0.097(4) 0.051(3) 0.095(4) 0.006(3) -0.004(4) -0.018(3)
C6 0.070(5) 0.068(4) 0.075(4) 0.010(4) 0.006(4) -0.013(4)
C7 0.066(4) 0.054(3) 0.063(4) 0.001(3) 0.004(4) -0.007(3)
C12 0.075(5) 0.058(3) 0.062(4) -0.008(3) 0.014(3) -0.003(4)
C13 0.091(6) 0.082(5) 0.076(5) -0.007(4) 0.026(5) -0.009(4)
C14 0.105(7) 0.123(6) 0.049(4) -0.011(5) 0.020(4) -0.019(6)
C15 0.104(8) 0.117(6) 0.052(4) -0.005(3) -0.016(5) -0.022(6)
C16 0.084(6) 0.056(3) 0.053(3) -0.006(3) -0.010(3) -0.017(3)
C22 0.055(5) 0.069(4) 0.109(6) -0.014(4) -0.014(4) 0.008(4)
C23 0.063(5) 0.090(6) 0.145(9) -0.007(6) -0.027(6) 0.020(5)
C24 0.082(7) 0.086(6) 0.130(8) 0.030(6) -0.058(7) 0.000(6)
C25 0.073(6) 0.092(6) 0.091(5) 0.010(5) -0.025(5) -0.008(5)
C26 0.073(5) 0.056(4) 0.065(4) -0.003(3) -0.016(4) -0.007(3)
C32 0.051(4) 0.076(4) 0.072(4) -0.007(4) -0.005(3) -0.010(4)
C33 0.046(4) 0.105(6) 0.095(5) 0.002(4) -0.012(4) 0.002(4)
C34 0.062(5) 0.122(6) 0.086(5) 0.021(5) -0.017(4) 0.018(5)
C35 0.081(6) 0.085(5) 0.084(5) 0.021(4) -0.005(4) 0.021(5)
C36 0.061(4) 0.055(3) 0.052(3) 0.001(3) 0.011(3) 0.003(3)
C42 0.064(4) 0.061(4) 0.092(5) -0.010(4) -0.010(4) -0.017(3)
C43 0.087(6) 0.075(5) 0.134(7) -0.003(5) 0.000(6) -0.023(5)
C44 0.118(8) 0.071(5) 0.130(8) 0.021(5) 0.008(6) -0.025(5)
C45 0.098(5) 0.077(4) 0.092(4) 0.019(3) 0.003(8) -0.016(7)
C46 0.066(6) 0.051(3) 0.055(3) -0.001(3) 0.008(3) 0.005(3)
O1W 0.164(13) 0.108(9) 0.163(12) -0.066(8) 0.000 0.000
P1A 0.06(3) 0.055(19) 0.18(3) 0.019(16) 0.07(3) -0.01(2)
F11A 0.17(3) 0.10(2) 0.17(3) -0.03(2) 0.04(2) 0.05(2)
F12A 0.096(12) 0.116(18) 0.148(15) 0.029(17) -0.014(12) -0.046(11)
F13A 0.15(2) 0.070(9) 0.087(11) 0.003(7) -0.041(15) 0.009(11)
P1B 0.096(12) 0.098(10) 0.045(4) 0.011(4) -0.015(17) -0.03(2)
F11B 0.188(13) 0.142(12) 0.052(6) 0.009(6) -0.020(7) -0.050(9)
F12B 0.240(19) 0.115(10) 0.142(11) 0.018(7) 0.066(12) -0.058(12)
F13B 0.118(9) 0.196(13) 0.131(8) -0.001(10) -0.009(8) 0.055(7)
P2A 0.090(7) 0.106(6) 0.108(7) -0.022(5) 0.036(5) -0.005(5)
F21A 0.110(11) 0.187(13) 0.127(11) -0.023(10) 0.008(9) -0.059(10)
F22A 0.26(3) 0.095(11) 0.31(3) 0.039(17) 0.09(3) 0.040(15)
F23A 0.117(12) 0.27(3) 0.091(10) 0.022(14) 0.031(8) 0.021(17)
F24A 0.169(15) 0.125(10) 0.180(15) -0.039(10) 0.026(12) 0.024(10)
F25A 0.132(12) 0.195(18) 0.111(10) 0.010(10) 0.049(9) 0.029(11)
F26A 0.072(10) 0.27(3) 0.24(2) -0.01(2) 0.012(10) -0.033(14)
P2B 0.089(8) 0.136(10) 0.104(7) 0.006(6) 0.031(5) 0.002(6)
F21B 0.109(18) 0.36(4) 0.16(2) 0.00(2) 0.048(14) 0.07(2)
F22B 0.158(16) 0.21(2) 0.103(10) -0.060(13) 0.027(9) -0.063(16)
F23B 0.168(16) 0.151(13) 0.123(12) 0.014(10) 0.044(10) -0.063(12)
F24B 0.34(4) 0.122(13) 0.19(2) -0.085(14) 0.03(2) 0.006(17)
F25B 0.20(2) 0.139(14) 0.151(18) 0.038(14) 0.054(19) -0.001(14)
F26B 0.108(11) 0.158(13) 0.105(9) -0.011(9) 0.014(7) 0.001(11)

_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
Ru1 N1 2.023(4) . ?
Ru1 N31 2.048(5) . ?
Ru1 N21 2.055(5) . ?
Ru1 N11 2.063(5) . ?
Ru1 N41 2.067(4) . ?
Ru1 N4 2.071(4) . ?
N1 C2 1.335(7) . ?
N1 N2 1.367(6) . ?
N2 C1 1.331(7) . ?
N3 C1 1.335(7) . ?
N3 C2 1.346(6) . ?
N3 H3 0.8600 . ?
N4 C7 1.330(7) . ?
N4 C3 1.365(6) . ?
N11 C12 1.315(7) . ?
N11 C16 1.380(7) . ?
N21 C22 1.329(8) . ?
N21 C26 1.344(8) . ?
N31 C32 1.336(7) . ?
N31 C36 1.371(7) . ?
N41 C42 1.334(7) . ?
N41 C46 1.348(7) . ?
C1 H1 0.9300 . ?
C2 C3 1.441(7) . ?
C3 C4 1.388(7) . ?
C4 N5 1.299(8) . ?
C4 H4 0.9300 . ?
N5 C6 1.322(8) . ?
C6 C7 1.368(8) . ?
C6 H6 0.9300 . ?
C7 H7 0.9300 . ?
C12 C13 1.386(8) . ?
C12 H12 0.9300 . ?
C13 C14 1.334(10) . ?
C13 H13 0.9300 . ?
C14 C15 1.401(12) . ?
C14 H14 0.9300 . ?
C15 C16 1.384(8) . ?
C15 H15 0.9300 . ?
C16 C26 1.458(9) . ?
C22 C23 1.383(10) . ?
C22 H22 0.9300 . ?
C23 C24 1.386(15) . ?
C23 H23 0.9300 . ?
C24 C25 1.346(13) . ?
C24 H24 0.9300 . ?
C25 C26 1.370(10) . ?
C25 H25 0.9300 . ?
C32 C33 1.370(9) . ?
C32 H32 0.9300 . ?

```
C33 C34 1.341(9) . ?
C33 H33 0.9300 . ?
C34 C35 1.381(10) . ?
C34 H34 0.9300 . ?
C35 C36 1.382(9) . ?
C35 H35 0.9300 . ?
C36 C46 1.472(8) . ?
C42 C43 1.397(9) . ?
C42 H42 0.9300 . ?
C43 C44 1.353(11) . ?
C43 H43 0.9300 . ?
C44 C45 1.394(14) . ?
C44 H44 0.9300 . ?
C45 C46 1.395(8) . ?
C45 H45 0.9300 . ?
O1W H1W1 0.846(3) . ?
O1W H1W2 0.859(12) . ?
P1A F13A 1.49(3) . ?
P1A F12A 1.49(3) . ?
P1A F11A 1.49(3) . ?
P1B F11B 1.57(2) . ?
P1B F12B 1.58(2) . ?
P1B F13B 1.584(18) . ?
P2A F26A 1.534(14) . ?
P2A F22A 1.541(14) . ?
P2A F24A 1.543(14) . ?
P2A F23A 1.548(13) . ?
P2A F21A 1.554(14) . ?
P2A F25A 1.575(14) . ?
P2B F24B 1.521(15) . ?
P2B F26B 1.541(15) . ?
P2B F22B 1.546(15) . ?
P2B F23B 1.549(15) . ?
P2B F21B 1.555(15) . ?
P2B F25B 1.566(15) . ?

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
N1 Ru1 N31 87.33(17) . . ?
N1 Ru1 N21 95.15(19) . . ?
N31 Ru1 N21 175.70(18) . . ?
N1 Ru1 N11 171.18(18) . . ?
N31 Ru1 N11 98.92(19) . . ?
N21 Ru1 N11 79.0(2) . . ?
N1 Ru1 N41 92.65(18) . . ?
N31 Ru1 N41 79.01(19) . . ?
N21 Ru1 N41 97.33(19) . . ?
N11 Ru1 N41 94.65(16) . . ?
N1 Ru1 N4 78.18(18) . . ?
N31 Ru1 N4 95.31(17) . . ?
N21 Ru1 N4 88.64(16) . . ?
N11 Ru1 N4 94.95(17) . . ?
N41 Ru1 N4 169.51(18) . . ?
C2 N1 N2 107.5(4) . . ?
C2 N1 Ru1 116.2(4) . . ?
```

```
N2 N1 Ru1 136.2(4) . . ?
C1 N2 N1 104.8(5) . . ?
C1 N3 C2 103.7(5) . . ?
C1 N3 H3 128.1 . . ?
C2 N3 H3 128.1 . . ?
C7 N4 C3 117.3(5) . . ?
C7 N4 Ru1 127.1(4) . . ?
C3 N4 Ru1 115.6(4) . . ?
C12 N11 C16 118.9(5) . . ?
C12 N11 Ru1 127.4(5) . . ?
C16 N11 Ru1 113.6(4) . . ?
C22 N21 C26 118.7(6) . . ?
C22 N21 Ru1 124.4(5) . . ?
C26 N21 Ru1 116.6(5) . . ?
C32 N31 C36 116.2(5) . . ?
C32 N31 Ru1 127.8(4) . . ?
C36 N31 Ru1 115.7(4) . . ?
C42 N41 C46 120.2(5) . . ?
C42 N41 Ru1 125.5(4) . . ?
C46 N41 Ru1 114.0(4) . . ?
N2 C1 N3 113.1(5) . . ?
N2 C1 H1 123.4 . . ?
N3 C1 H1 123.4 . . ?
N1 C2 N3 110.8(5) . . ?
N1 C2 C3 117.0(5) . . ?
N3 C2 C3 132.1(5) . . ?
N4 C3 C4 118.9(5) . . ?
N4 C3 C2 113.0(5) . . ?
C4 C3 C2 128.1(5) . . ?
N5 C4 C3 124.2(6) . . ?
N5 C4 H4 117.9 . . ?
C3 C4 H4 117.9 . . ?
C4 N5 C6 115.2(5) . . ?
N5 C6 C7 124.4(6) . . ?
N5 C6 H6 117.8 . . ?
C7 C6 H6 117.8 . . ?
N4 C7 C6 119.9(6) . . ?
N4 C7 H7 120.0 . . ?
C6 C7 H7 120.0 . . ?
N11 C12 C13 123.0(7) . . ?
N11 C12 H12 118.5 . . ?
C13 C12 H12 118.5 . . ?
C14 C13 C12 118.9(8) . . ?
C14 C13 H13 120.6 . . ?
C12 C13 H13 120.6 . . ?
C13 C14 C15 120.4(7) . . ?
C13 C14 H14 119.8 . . ?
C15 C14 H14 119.8 . . ?
C16 C15 C14 118.5(8) . . ?
C16 C15 H15 120.7 . . ?
C14 C15 H15 120.7 . . ?
N11 C16 C15 120.2(7) . . ?
N11 C16 C26 116.4(5) . . ?
C15 C16 C26 123.4(7) . . ?
N21 C22 C23 122.3(8) . . ?
N21 C22 H22 118.9 . . ?
C23 C22 H22 118.9 . . ?
C22 C23 C24 117.3(10) . . ?
C22 C23 H23 121.3 . . ?
C24 C23 H23 121.3 . . ?
C25 C24 C23 120.8(9) . . ?
```

```
C25 C24 H24 119.6 . . ?
C23 C24 H24 119.6 . . ?
C24 C25 C26 118.7(8) . . ?
C24 C25 H25 120.7 . . ?
C26 C25 H25 120.7 . . ?
N21 C26 C25 122.2(7) . . ?
N21 C26 C16 114.0(6) . . ?
C25 C26 C16 123.8(7) . . ?
N31 C32 C33 124.5(7) . . ?
N31 C32 H32 117.7 . . ?
C33 C32 H32 117.7 . . ?
C34 C33 C32 118.8(8) . . ?
C34 C33 H33 120.6 . . ?
C32 C33 H33 120.6 . . ?
C33 C34 C35 119.6(7) . . ?
C33 C34 H34 120.2 . . ?
C35 C34 H34 120.2 . . ?
C34 C35 C36 119.3(7) . . ?
C34 C35 H35 120.4 . . ?
C36 C35 H35 120.4 . . ?
N31 C36 C35 121.5(6) . . ?
N31 C36 C46 113.4(5) . . ?
C35 C36 C46 125.0(6) . . ?
N41 C42 C43 121.3(7) . . ?
N41 C42 H42 119.4 . . ?
C43 C42 H42 119.4 . . ?
C44 C43 C42 119.0(8) . . ?
C44 C43 H43 120.5 . . ?
C42 C43 H43 120.5 . . ?
C43 C44 C45 120.4(8) . . ?
C43 C44 H44 119.8 . . ?
C45 C44 H44 119.8 . . ?
C44 C45 C46 118.2(9) . . ?
C44 C45 H45 120.9 . . ?
C46 C45 H45 120.9 . . ?
N41 C46 C45 120.9(7) . . ?
N41 C46 C36 116.4(5) . . ?
C45 C46 C36 122.7(7) . . ?
H1W1 O1W H1W2 101.7(12) . . ?
F13A P1A F12A 89.8(15) . . ?
F13A P1A F11A 88.8(15) . . ?
F12A P1A F11A 91.0(16) . . ?
F11B P1B F12B 90.6(13) . . ?
F11B P1B F13B 91.0(12) . . ?
F12B P1B F13B 89.0(13) . . ?
F26A P2A F22A 90.8(10) . . ?
F26A P2A F24A 90.6(9) . . ?
F22A P2A F24A 177.9(13) . . ?
F26A P2A F23A 91.7(10) . . ?
F22A P2A F23A 92.1(11) . . ?
F24A P2A F23A 89.5(9) . . ?
F26A P2A F21A 178.4(12) . . ?
F22A P2A F21A 89.4(9) . . ?
F24A P2A F21A 89.2(9) . . ?
F23A P2A F21A 89.9(9) . . ?
F26A P2A F25A 89.3(8) . . ?
F22A P2A F25A 90.1(11) . . ?
F24A P2A F25A 88.3(9) . . ?
F23A P2A F25A 177.6(12) . . ?
F21A P2A F25A 89.1(9) . . ?
F24B P2B F26B 91.5(10) . . ?
```

```
F24B P2B F22B 178.6(14) . . ?
F26B P2B F22B 89.6(10) . . ?
F24B P2B F23B 89.8(10) . . ?
F26B P2B F23B 90.8(10) . . ?
F22B P2B F23B 91.1(10) . . ?
F24B P2B F21B 89.7(11) . . ?
F26B P2B F21B 178.0(12) . . ?
F22B P2B F21B 89.2(11) . . ?
F23B P2B F21B 90.9(10) . . ?
F24B P2B F25B 91.6(11) . . ?
F26B P2B F25B 89.0(9) . . ?
F22B P2B F25B 87.5(13) . . ?
F23B P2B F25B 178.6(14) . . ?
F21B P2B F25B 89.3(11) . . ?

loop_
_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
N31 Ru1 N1 C2 94.9(4) . . . . ?
N21 Ru1 N1 C2 -88.6(4) . . . . ?
N11 Ru1 N1 C2 -40.4(14) . . . . ?
N41 Ru1 N1 C2 173.7(4) . . . . ?
N4 Ru1 N1 C2 -1.1(4) . . . . ?
N31 Ru1 N1 N2 -88.2(5) . . . . ?
N21 Ru1 N1 N2 88.3(5) . . . . ?
N11 Ru1 N1 N2 136.5(11) . . . . ?
N41 Ru1 N1 N2 -9.3(5) . . . . ?
N4 Ru1 N1 N2 175.9(5) . . . . ?
C2 N1 N2 C1 -1.0(6) . . . . ?
Ru1 N1 N2 C1 -178.1(4) . . . . ?
N1 Ru1 N4 C7 180.0(5) . . . . ?
N31 Ru1 N4 C7 93.8(5) . . . . ?
N21 Ru1 N4 C7 -84.5(5) . . . . ?
N11 Ru1 N4 C7 -5.6(5) . . . . ?
N41 Ru1 N4 C7 150.5(9) . . . . ?
N1 Ru1 N4 C3 1.0(4) . . . . ?
N31 Ru1 N4 C3 -85.2(4) . . . . ?
N21 Ru1 N4 C3 96.5(4) . . . . ?
N11 Ru1 N4 C3 175.4(4) . . . . ?
N41 Ru1 N4 C3 -28.5(12) . . . . ?
N1 Ru1 N11 C12 131.7(12) . . . . ?
N31 Ru1 N11 C12 -3.0(5) . . . . ?
N21 Ru1 N11 C12 -179.1(5) . . . . ?
N41 Ru1 N11 C12 -82.5(5) . . . . ?
N4 Ru1 N11 C12 93.2(5) . . . . ?
N1 Ru1 N11 C16 -46.0(14) . . . . ?
N31 Ru1 N11 C16 179.3(4) . . . . ?
N21 Ru1 N11 C16 3.1(4) . . . . ?
N41 Ru1 N11 C16 99.7(4) . . . . ?
N4 Ru1 N11 C16 -84.6(4) . . . . ?
N1 Ru1 N21 C22 -5.6(5) . . . . ?
N31 Ru1 N21 C22 119(3) . . . . ?
N11 Ru1 N21 C22 -179.0(5) . . . . ?
```

```
N41 Ru1 N21 C22 87.7(5) . . . . ?
N4 Ru1 N21 C22 -83.6(5) . . . . ?
N1 Ru1 N21 C26 168.2(4) . . . . ?
N31 Ru1 N21 C26 -67(3) . . . . ?
N11 Ru1 N21 C26 -5.1(4) . . . . ?
N41 Ru1 N21 C26 -98.4(4) . . . . ?
N4 Ru1 N21 C26 90.2(4) . . . . ?
N1 Ru1 N31 C32 -88.7(5) . . . . ?
N21 Ru1 N31 C32 146(3) . . . . ?
N11 Ru1 N31 C32 85.0(5) . . . . ?
N41 Ru1 N31 C32 178.1(5) . . . . ?
N4 Ru1 N31 C32 -10.8(5) . . . . ?
N1 Ru1 N31 C36 84.5(4) . . . . ?
N21 Ru1 N31 C36 -41(3) . . . . ?
N11 Ru1 N31 C36 -101.8(4) . . . . ?
N41 Ru1 N31 C36 -8.7(4) . . . . ?
N4 Ru1 N31 C36 162.4(4) . . . . ?
N1 Ru1 N41 C42 96.8(5) . . . . ?
N31 Ru1 N41 C42 -176.4(5) . . . . ?
N21 Ru1 N41 C42 1.3(5) . . . . ?
N11 Ru1 N41 C42 -78.2(5) . . . . ?
N4 Ru1 N41 C42 125.6(10) . . . . ?
N1 Ru1 N41 C46 -75.5(4) . . . . ?
N31 Ru1 N41 C46 11.3(4) . . . . ?
N21 Ru1 N41 C46 -171.0(4) . . . . ?
N11 Ru1 N41 C46 109.5(4) . . . . ?
N4 Ru1 N41 C46 -46.7(12) . . . . ?
N1 N2 C1 N3 1.1(7) . . . . ?
C2 N3 C1 N2 -0.8(7) . . . . ?
N2 N1 C2 N3 0.5(6) . . . . ?
Ru1 N1 C2 N3 178.3(3) . . . . ?
N2 N1 C2 C3 -176.7(5) . . . . ?
Ru1 N1 C2 C3 1.1(6) . . . . ?
C1 N3 C2 N1 0.1(6) . . . . ?
C1 N3 C2 C3 176.8(6) . . . . ?
C7 N4 C3 C4 -0.5(8) . . . . ?
Ru1 N4 C3 C4 178.6(5) . . . . ?
C7 N4 C3 C2 -179.8(5) . . . . ?
Ru1 N4 C3 C2 -0.7(6) . . . . ?
N1 C2 C3 N4 -0.3(7) . . . . ?
N3 C2 C3 N4 -176.8(6) . . . . ?
N1 C2 C3 C4 -179.5(6) . . . . ?
N3 C2 C3 C4 4.1(10) . . . . ?
N4 C3 C4 N5 0.2(10) . . . . ?
C2 C3 C4 N5 179.4(7) . . . . ?
C3 C4 N5 C6 -0.6(11) . . . . ?
C4 N5 C6 C7 1.3(11) . . . . ?
C3 N4 C7 C6 1.2(9) . . . . ?
Ru1 N4 C7 C6 -177.8(5) . . . . ?
N5 C6 C7 N4 -1.6(11) . . . . ?
C16 N11 C12 C13 -1.3(9) . . . . ?
Ru1 N11 C12 C13 -179.0(5) . . . . ?
N11 C12 C13 C14 -0.4(10) . . . . ?
C12 C13 C14 C15 1.3(12) . . . . ?
C13 C14 C15 C16 -0.5(12) . . . . ?
C12 N11 C16 C15 2.1(8) . . . . ?
Ru1 N11 C16 C15 -179.9(5) . . . . ?
C12 N11 C16 C26 -179.0(5) . . . . ?
Ru1 N11 C16 C26 -1.0(6) . . . . ?
C14 C15 C16 N11 -1.2(10) . . . . ?
C14 C15 C16 C26 179.9(7) . . . . ?
```

```
C26 N21 C22 C23 0.0(10) . . . . ?
Ru1 N21 C22 C23 173.8(5) . . . . ?
N21 C22 C23 C24 -2.3(12) . . . . ?
C22 C23 C24 C25 3.7(14) . . . . ?
C23 C24 C25 C26 -2.8(14) . . . . ?
C22 N21 C26 C25 1.0(9) . . . . ?
Ru1 N21 C26 C25 -173.3(5) . . . . ?
C22 N21 C26 C16 -179.8(6) . . . . ?
Ru1 N21 C26 C16 6.0(7) . . . . ?
C24 C25 C26 N21 0.4(12) . . . . ?
C24 C25 C26 C16 -178.7(7) . . . . ?
N11 C16 C26 N21 -3.2(8) . . . . ?
C15 C16 C26 N21 175.7(6) . . . . ?
N11 C16 C26 C25 176.0(6) . . . . ?
C15 C16 C26 C25 -5.1(11) . . . . ?
C36 N31 C32 C33 0.6(9) . . . . ?
Ru1 N31 C32 C33 173.8(5) . . . . ?
N31 C32 C33 C34 -1.0(11) . . . . ?
C32 C33 C34 C35 1.3(11) . . . . ?
C33 C34 C35 C36 -1.3(11) . . . . ?
C32 N31 C36 C35 -0.6(8) . . . . ?
Ru1 N31 C36 C35 -174.6(5) . . . . ?
C32 N31 C36 C46 179.0(5) . . . . ?
Ru1 N31 C36 C46 5.0(6) . . . . ?
C34 C35 C36 N31 1.0(10) . . . . ?
C34 C35 C36 C46 -178.6(6) . . . . ?
C46 N41 C42 C43 3.5(9) . . . . ?
Ru1 N41 C42 C43 -168.4(5) . . . . ?
N41 C42 C43 C44 -0.7(12) . . . . ?
C42 C43 C44 C45 -0.9(14) . . . . ?
C43 C44 C45 C46 -0.2(13) . . . . ?
C42 N41 C46 C45 -4.6(9) . . . . ?
Ru1 N41 C46 C45 168.2(5) . . . . ?
C42 N41 C46 C36 175.1(5) . . . . ?
Ru1 N41 C46 C36 -12.1(6) . . . . ?
C44 C45 C46 N41 3.0(10) . . . . ?
C44 C45 C46 C36 -176.7(7) . . . . ?
N31 C36 C46 N41 4.9(7) . . . . ?
C35 C36 C46 N41 -175.6(6) . . . . ?
N31 C36 C46 C45 -175.4(6) . . . . ?
C35 C36 C46 C45 4.1(10) . . . . ?

_diffrn_measured_fraction_theta_max 1.00
_diffrn_reflns_theta_full        27.14
_diffrn_measured_fraction_theta_full 1.00
_refine_diff_density_max         0.30
_refine_diff_density_min         -0.37
_refine_diff_density_rms         0.06
```