Ruthenium and osmium complexes of hemilabile chiral monophosphinite ligands derived from 1D-pinitol or 1D-*chiro*-inositol as catalysts for asymmetric hydrogenation reactions

Angela T. Slade [a], Cornelis Lensink [b], Andrew Falshaw [b], George R. Clark [a], L. James Wright [a*]

[a] School of Chemical Sciences, University of Auckland, Private Bag 92019, Auckland 1142, New Zealand. E-mail: lj.wright@auckland.ac.nz; Fax: +64 9 373 7422; Tel: +64 9 373 7599
[b] A Industrial Research Limited, PO Box 31-310, Lower Hutt, New Zealand.

SUPPLEMENTARY INFORMATION

Crystallographic data for $RuCl_2$(D-P1)$_2$ (**1**) in CIF format.

```
data_global
_audit_creation_method     shelxl-97
_publ_section_title
;
title
;
_publ_section_abstract        ' abstract  '
_publ_section_comment         ' comment  '
_publ_requested_journal
_publ_contact_author_name        'george r. clark'
_publ_contact_author_address
;
department of chemistry
the university of auckland
private bag 92019
auckland
new zealand
;
_publ_contact_author_email       'g.clark@auckland.ac.nz'
_publ_contact_author_phone       '0064 9 3737599 ext 88294'
_publ_contact_author_fax         '0064 9 3737422'
loop_
_publ_author_name
_publ_author_address

'slade, angela t.'
;
department of chemistry
the university of auckland
private bag 92019
auckland
new zealand
;

'lensink, cornelius.'
;
Industrial Research Limited
PO Box 31-310
Lower hutt
new zealand
;



'falshaw, andrew.'
;
Industrial Research Limited
PO Box 31-310
lower hutt
new zealand
;
```

```
'clark, george r.'
;
department of chemistry
the university of auckland
private bag 92019
auckland
new zealand
;
'wright, l. james.'
;
department of chemistry
the university of auckland
private bag 92019
auckland
new zealand
;
_publ_section_exptl_refinement
;
There were 4943 Friedel pairs. The absolute structure is
established.
;
_publ_section_references
;
burnett, m.n. and johnson, c.k., ortep-iii: oak ridge thermal
ellipsoid
plot program for crystal structure illustrations, oak ridge national
laboratory report ornl-6895, 1996.
sheldrick, g.m. (1997). sadabs. program for semi-empirical
absorption
correction.  univ. of g\"ottingen, germany.
sheldrick, g.m. (1997). shelxs97 and shelxl97. program for solution
and
refinement of crystal structures.  univ. of g\"ottingen, germany.
siemens (1995). shelxtl. siemens analytical instruments inc.,
madison,
wisconsin, usa.
siemens (1995). smart and saint. siemens analytical instruments
inc.,
madison, wisconsin, usa.
;
data_ats157
_audit_creation_method            shelxl-97
_chemical_name_systematic
;
 ?
;
_chemical_name_common             ?
_chemical_melting_point           ?
_chemical_formula_moiety          'C58 H70 Cl2 O12 P2 Ru, C2 H6 O'
_chemical_formula_sum
 'C60 H76 Cl2 O13 P2 Ru'
_chemical_formula_weight          1239.12
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'
 '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'
 'cl'  'cl'   0.1484   0.1585
 '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'
_cell_length_a                    11.5760(2)
_cell_length_b                    11.9927(2)
_cell_length_c                    12.0811(2)
_cell_angle_alpha                 104.793(1)
_cell_angle_beta                  115.370(1)
_cell_angle_gamma                 91.577(1)
_cell_volume                      1447.10(4)
_cell_formula_units_z             1
_cell_measurement_temperature     85(2)
_cell_measurement_reflns_used     6014
_cell_measurement_theta_min       1.78
_cell_measurement_theta_max       26.42
_exptl_crystal_description        prism
_exptl_crystal_colour             orange
_exptl_crystal_size_max           0.28
_exptl_crystal_size_mid           0.18
_exptl_crystal_size_min           0.12
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.422
_exptl_crystal_density_method     'not measured'
_exptl_absorpt_correction_type    empirical
_exptl_absorpt_process_details   'sheldrick, 1997'
_exptl_special_details
;
 ?
;
_exptl_crystal_f_000              648
_exptl_absorpt_coefficient_mu     0.482
_exptl_absorpt_correction_t_min   0.7603
_exptl_absorpt_correction_t_max   0.9377
```

```
_diffrn_ambient_temperature       85(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   'siemens smart ccd'
_diffrn_measurement_method        'area detector \w scans'
_diffrn_detector_area_resol_mean  ?
_diffrn_standards_decay_%         0
_diffrn_standards_number          0
_diffrn_standards_interval_count  0
_diffrn_standards_interval_time   0
_diffrn_reflns_number             14202
_diffrn_reflns_av_r_equivalents   0.0257
_diffrn_reflns_av_sigmai/neti     0.0572
_diffrn_reflns_limit_h_min        -14
_diffrn_reflns_limit_h_max        14
_diffrn_reflns_limit_k_min        -15
_diffrn_reflns_limit_k_max        15
_diffrn_reflns_limit_l_min        -15
_diffrn_reflns_limit_l_max        15
_diffrn_reflns_theta_min          1.78
_diffrn_reflns_theta_max          26.42
_reflns_number_total              10839
_reflns_number_gt                 10282
_reflns_threshold_expression      >2sigma(i)
_computing_data_collection        'siemens smart (siemens, 1995)'
_computing_cell_refinement        'siemens smart (siemens, 1995)'
_computing_data_reduction         'siemens saint (siemens, 1995)'
_computing_structure_solution     'shelxs (sheldrick, 1990)'
_computing_structure_refinement   'shelxl-97 (sheldrick, 1997)'
_computing_molecular_graphics     'ortep-iii (burnett & johnson,
1996)'
_computing_publication_material   'siemens smart (siemens, 1995)'
_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^)+(0.0762p)^2^+1.1352p] 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_abs_structure_details
;
The absolute structure is determined.
flack h d (1983), acta cryst. a39, 876-881
;
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_abs_structure_flack    -0.04(2)
_refine_ls_number_reflns          10839
_refine_ls_number_parameters      703
_refine_ls_number_restraints      3
_refine_ls_r_factor_all           0.0513
_refine_ls_r_factor_gt            0.0475
_refine_ls_wr_factor_ref          0.1226
_refine_ls_wr_factor_gt           0.1189
_refine_ls_goodness_of_fit_ref    1.038
_refine_ls_restrained_s_all       1.038
_refine_ls_shift/su_max           0.001
_refine_ls_shift/su_mean          0.000
loop_
 _atom_site_label
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_u_iso_or_equiv
 _atom_site_adp_type
 _atom_site_occupancy
 _atom_site_symmetry_multiplicity
 _atom_site_calc_flag
 _atom_site_refinement_flags
 _atom_site_disorder_assembly
 _atom_site_disorder_group
ru ru 0.59342(2) 0.61395(2) 0.59859(2) 0.01275(9) uani 1 1 d . . .
cl1 cl 0.51258(10) 0.46974(10) 0.66526(11) 0.0160(2) uani 1 1 d . .
.
cl2 cl 0.67378(10) 0.73798(10) 0.51079(10) 0.0155(2) uani 1 1 d . .
.
p1 p 0.75488(11) 0.69717(10) 0.79273(11) 0.0130(2) uani 1 1 d . . .
p2 p 0.43223(11) 0.71168(10) 0.59350(11) 0.0132(2) uani 1 1 d . . .
o1 o 0.8706(3) 0.6168(3) 0.8100(3) 0.0150(6) uani 1 1 d . . .
o2 o 0.3153(3) 0.6679(3) 0.4452(3) 0.0149(6) uani 1 1 d . . .
o3 o 0.7237(3) 0.4819(3) 0.5591(3) 0.0153(7) uani 1 1 d . . .
o4 o 0.4657(3) 0.5095(3) 0.3909(3) 0.0142(7) uani 1 1 d . . .
o5 o 0.9465(3) 0.2208(3) 0.6657(3) 0.0191(7) uani 1 1 d . . .
o6 o 0.7563(3) 0.2298(3) 0.5015(3) 0.0199(7) uani 1 1 d . . .
o7 o 0.8511(3) 0.3084(3) 0.9176(3) 0.0174(7) uani 1 1 d . . .
o8 o 0.9606(3) 0.4958(3) 1.0068(3) 0.0166(6) uani 1 1 d . . .
```

```
o9 o 0.3165(4) 0.7999(3) 0.1490(3) 0.0203(8) uani 1 1 d . . .
o10 o 0.2100(3) 0.8131(3) 0.2728(3) 0.0174(7) uani 1 1 d . . .
o11 o 0.4634(3) 0.4619(3) 0.1386(3) 0.0176(7) uani 1 1 d . . .
o12 o 0.2587(3) 0.4877(3) 0.0099(3) 0.0160(6) uani 1 1 d . . .
c1 c 0.8359(4) 0.4942(4) 0.7858(4) 0.0128(8) uani 1 1 d . . .
h1a h 0.7583 0.4794 0.7966 0.015 uiso 1 1 calc r . .
c2 c 0.9489(4) 0.4539(4) 0.8799(4) 0.0150(9) uani 1 1 d . . .
h2a h 1.0293 0.4790 0.8783 0.018 uiso 1 1 calc r . .
c3 c 0.9269(4) 0.3207(4) 0.8541(4) 0.0158(9) uani 1 1 d . . .
h3a h 1.0101 0.2947 0.8961 0.019 uiso 1 1 calc r . .
c4 c 0.8565(4) 0.2464(4) 0.7173(4) 0.0162(9) uani 1 1 d . . .
h4a h 0.8125 0.1734 0.7130 0.019 uiso 1 1 calc r . .
c5 c 0.7604(5) 0.3008(4) 0.6192(4) 0.0173(9) uani 1 1 d . . .
h5a h 0.6751 0.2925 0.6173 0.021 uiso 1 1 calc r . .
c6 c 0.8126(4) 0.4296(4) 0.6495(4) 0.0147(9) uani 1 1 d . . .
h6a h 0.8952 0.4346 0.6452 0.018 uiso 1 1 calc r . .
c7 c 0.8684(5) 0.1710(4) 0.5318(4) 0.0194(10) uani 1 1 d . . .
c8 c 0.9454(5) 0.1891(5) 0.4602(5) 0.0274(11) uani 1 1 d . . .
h8a h 1.0249 0.2433 0.5178 0.033 uiso 1 1 calc r . .
h8b h 0.8949 0.2201 0.3904 0.033 uiso 1 1 calc r . .
c9 c 0.9758(6) 0.0668(5) 0.4076(5) 0.0336(13) uani 1 1 d . . .
h9a h 0.9193 0.0334 0.3166 0.040 uiso 1 1 calc r . .
h9b h 1.0651 0.0713 0.4218 0.040 uiso 1 1 calc r . .
c10 c 0.9506(5) -0.0042(5) 0.4846(5) 0.0292(12) uani 1 1 d . . .
h10a h 1.0243 0.0102 0.5681 0.035 uiso 1 1 calc r . .
h10b h 0.9319 -0.0871 0.4398 0.035 uiso 1 1 calc r . .
c11 c 0.8332(5) 0.0392(4) 0.4971(5) 0.0235(10) uani 1 1 d . . .
h11a h 0.8220 0.0172 0.5642 0.028 uiso 1 1 calc r . .
h11b h 0.7549 0.0092 0.4170 0.028 uiso 1 1 calc r . .
c12 c 0.8944(5) 0.4074(4) 1.0301(5) 0.0205(11) uani 1 1 d . . .
c13 c 0.7767(5) 0.4403(5) 1.0496(5) 0.0274(11) uani 1 1 d . . .
h13a h 0.7618 0.5175 1.0408 0.033 uiso 1 1 calc r . .
h13b h 0.6999 0.3846 0.9873 0.033 uiso 1 1 calc r . .
c14 c 0.8086(10) 0.4382(10) 1.1852(9) 0.075(3) uani 1 1 d . . .
h14a h 0.7312 0.4143 1.1912 0.090 uiso 1 1 calc r . .
h14b h 0.8507 0.5141 1.2469 0.090 uiso 1 1 calc r . .
c15 c 0.9015(8) 0.3468(8) 1.2070(7) 0.059(2) uani 1 1 d . . .
h15a h 0.9504 0.3541 1.2975 0.071 uiso 1 1 calc r . .
h15b h 0.8550 0.2679 1.1614 0.071 uiso 1 1 calc r . .
c16 c 0.9880(6) 0.3797(5) 1.1520(5) 0.0292(12) uani 1 1 d . . .
h16a h 1.0316 0.3154 1.1316 0.035 uiso 1 1 calc r . .
h16b h 1.0524 0.4474 1.2116 0.035 uiso 1 1 calc r . .
c17 c 0.7543(5) 0.4789(4) 0.4545(4) 0.0199(10) uani 1 1 d . . .
h17a h 0.8083 0.4205 0.4489 0.030 uiso 1 1 calc r . .
h17b h 0.7991 0.5538 0.4693 0.030 uiso 1 1 calc r . .
h17c h 0.6757 0.4603 0.3757 0.030 uiso 1 1 calc r . .
c18 c 0.3489(4) 0.6711(4) 0.3455(4) 0.0134(8) uani 1 1 d . . .
h18a h 0.4223 0.7330 0.3772 0.016 uiso 1 1 calc r . .
c19 c 0.2297(4) 0.6947(4) 0.2383(4) 0.0141(9) uani 1 1 d . . .
h19a h 0.1528 0.6411 0.2169 0.017 uiso 1 1 calc r . .
c20 c 0.2485(4) 0.6863(4) 0.1178(4) 0.0168(9) uani 1 1 d . . .
h20a h 0.1643 0.6735 0.0425 0.020 uiso 1 1 calc r . .
c21 c 0.3325(4) 0.6009(4) 0.0885(4) 0.0156(9) uani 1 1 d . . .
h21a h 0.3741 0.6307 0.0440 0.019 uiso 1 1 calc r . .
```

```
c22 c 0.4354(4) 0.5687(4) 0.2015(4) 0.0152(9) uani 1 1 d . . .
h22a h 0.5126 0.6288 0.2474 0.018 uiso 1 1 calc r . .
c23 c 0.3805(4) 0.5533(4) 0.2906(4) 0.0150(9) uani 1 1 d . . .
h23a h 0.2997 0.4978 0.2401 0.018 uiso 1 1 calc r . .
c24 c 0.2764(5) 0.8825(4) 0.2304(4) 0.0184(10) uani 1 1 d . . .
c25 c 0.3956(5) 0.9678(4) 0.3360(5) 0.0229(10) uani 1 1 d . . .
h25a h 0.4696 0.9577 0.3184 0.027 uiso 1 1 calc r . .
h25b h 0.4166 0.9556 0.4184 0.027 uiso 1 1 calc r . .
c26 c 0.3598(7) 1.0902(5) 0.3358(6) 0.0443(17) uani 1 1 d . . .
h26a h 0.3170 1.1152 0.3895 0.053 uiso 1 1 calc r . .
h26b h 0.4358 1.1471 0.3651 0.053 uiso 1 1 calc r . .
c27 c 0.2675(7) 1.0725(5) 0.1939(6) 0.0433(16) uani 1 1 d . . .
h27a h 0.2166 1.1354 0.1831 0.052 uiso 1 1 calc r . .
h27b h 0.3143 1.0670 0.1431 0.052 uiso 1 1 calc r . .
c28 c 0.1829(5) 0.9569(4) 0.1585(5) 0.0265(11) uani 1 1 d . . .
h28a h 0.1429 0.9196 0.0667 0.032 uiso 1 1 calc r . .
h28b h 0.1155 0.9689 0.1858 0.032 uiso 1 1 calc r . .
c29 c 0.3556(4) 0.4140(4) 0.0139(4) 0.0160(9) uani 1 1 d . . .
c30 c 0.3016(5) 0.2876(4) -0.0089(4) 0.0174(9) uani 1 1 d . . .
h30a h 0.2266 0.2850 0.0073 0.021 uiso 1 1 calc r . .
h30b h 0.3666 0.2516 0.0470 0.021 uiso 1 1 calc r . .
c31 c 0.2637(5) 0.2240(4) -0.1505(4) 0.0212(10) uani 1 1 d . . .
h31a h 0.3206 0.1676 -0.1573 0.025 uiso 1 1 calc r . .
h31b h 0.1752 0.1838 -0.1942 0.025 uiso 1 1 calc r . .
c32 c 0.2783(5) 0.3207(4) -0.2080(4) 0.0206(10) uani 1 1 d . . .
h32a h 0.2993 0.2908 -0.2785 0.025 uiso 1 1 calc r . .
h32b h 0.1996 0.3546 -0.2383 0.025 uiso 1 1 calc r . .
c33 c 0.3894(5) 0.4098(4) -0.0962(4) 0.0197(9) uani 1 1 d . . .
h33a h 0.3910 0.4854 -0.1114 0.024 uiso 1 1 calc r . .
h33b h 0.4723 0.3839 -0.0799 0.024 uiso 1 1 calc r . .
c34 c 0.4357(5) 0.3827(4) 0.3579(5) 0.0210(10) uani 1 1 d . . .
h34a h 0.3812 0.3511 0.2674 0.031 uiso 1 1 calc r . .
h34b h 0.3916 0.3637 0.4039 0.031 uiso 1 1 calc r . .
h34c h 0.5145 0.3500 0.3809 0.031 uiso 1 1 calc r . .
c41 c 0.7477(4) 0.7159(4) 0.9440(4) 0.0150(9) uani 1 1 d . . .
c42 c 0.8624(5) 0.7455(4) 1.0561(4) 0.0180(9) uani 1 1 d . . .
h42a h 0.9404 0.7520 1.0516 0.022 uiso 1 1 calc r . .
c43 c 0.8642(5) 0.7661(4) 1.1762(4) 0.0210(10) uani 1 1 d . . .
h43a h 0.9421 0.7841 1.2508 0.025 uiso 1 1 calc r . .
c44 c 0.7453(5) 0.7589(5) 1.1811(5) 0.0274(11) uani 1 1 d . . .
h44a h 0.7438 0.7735 1.2598 0.033 uiso 1 1 calc r . .
c45 c 0.6303(5) 0.7301(5) 1.0691(5) 0.0305(12) uani 1 1 d . . .
h45a h 0.5519 0.7259 1.0732 0.037 uiso 1 1 calc r . .
c46 c 0.6308(5) 0.7074(4) 0.9508(5) 0.0221(10) uani 1 1 d . . .
h46a h 0.5530 0.6865 0.8760 0.026 uiso 1 1 calc r . .
c51 c 0.8569(4) 0.8333(4) 0.8298(4) 0.0157(9) uani 1 1 d . . .
c52 c 0.8484(5) 0.9374(4) 0.9089(5) 0.0202(10) uani 1 1 d . . .
h52a h 0.7918 0.9374 0.9450 0.024 uiso 1 1 calc r . .
c53 c 0.9252(5) 1.0417(4) 0.9336(5) 0.0262(11) uani 1 1 d . . .
h53a h 0.9188 1.1110 0.9853 0.031 uiso 1 1 calc r . .
c54 c 1.0091(5) 1.0414(4) 0.8822(5) 0.0269(12) uani 1 1 d . . .
h54a h 1.0612 1.1105 0.9006 0.032 uiso 1 1 calc r . .
c55 c 1.0182(5) 0.9372(4) 0.8009(5) 0.0228(10) uani 1 1 d . . .
h55a h 1.0755 0.9376 0.7657 0.027 uiso 1 1 calc r . .
```

```
c56 c 0.9407(4) 0.8354(4) 0.7749(4) 0.0186(9) uani 1 1 d . . .
h56a h 0.9444 0.7670 0.7198 0.022 uiso 1 1 calc r . .
c61 c 0.3283(4) 0.6813(4) 0.6646(4) 0.0160(9) uani 1 1 d . . .
c62 c 0.3330(5) 0.7605(4) 0.7746(4) 0.0198(9) uani 1 1 d . . .
h62a h 0.3912 0.8300 0.8144 0.024 uiso 1 1 calc r . .
c63 c 0.2503(5) 0.7350(5) 0.8242(5) 0.0267(11) uani 1 1 d . . .
h63a h 0.2547 0.7870 0.8981 0.032 uiso 1 1 calc r . .
c64 c 0.1630(5) 0.6345(5) 0.7656(5) 0.0267(11) uani 1 1 d . . .
h64a h 0.1078 0.6185 0.7991 0.032 uiso 1 1 calc r . .
c65 c 0.1567(5) 0.5553(5) 0.6547(5) 0.0251(10) uani 1 1 d . . .
h65a h 0.0964 0.4872 0.6140 0.030 uiso 1 1 calc r . .
c66 c 0.2398(4) 0.5782(4) 0.6060(4) 0.0192(9) uani 1 1 d . . .
h66a h 0.2367 0.5245 0.5336 0.023 uiso 1 1 calc r . .
c71 c 0.4449(4) 0.8700(4) 0.6269(4) 0.0148(9) uani 1 1 d . . .
c72 c 0.5649(5) 0.9403(4) 0.6835(4) 0.0191(9) uani 1 1 d . . .
h72a h 0.6397 0.9065 0.7020 0.023 uiso 1 1 calc r . .
c73 c 0.5734(5) 1.0617(4) 0.7128(5) 0.0230(10) uani 1 1 d . . .
h73a h 0.6539 1.1086 0.7530 0.028 uiso 1 1 calc r . .
c74 c 0.4627(5) 1.1116(4) 0.6821(5) 0.0232(10) uani 1 1 d . . .
h74a h 0.4685 1.1924 0.7010 0.028 uiso 1 1 calc r . .
c75 c 0.3416(5) 1.0418(4) 0.6228(5) 0.0225(10) uani 1 1 d . . .
h75a h 0.2666 1.0756 0.6006 0.027 uiso 1 1 calc r . .
c76 c 0.3341(5) 0.9211(4) 0.5972(4) 0.0191(9) uani 1 1 d . . .
h76a h 0.2537 0.8744 0.5599 0.023 uiso 1 1 calc r . .
o13 o 0.5904(6) 1.1693(7) 1.2241(5) 0.078(2) uani 1 1 d . . .
h13 h 0.6265 1.1728 1.3003 0.117 uiso 1 1 calc r . .
c80 c 0.6150(8) 1.0774(8) 1.1572(8) 0.063(2) uani 1 1 d . . .
h80a h 0.5857 1.0095 1.1735 0.075 uiso 1 1 calc r . .
h80b h 0.7082 1.0837 1.1905 0.075 uiso 1 1 calc r . .
c81 c 0.5563(11) 1.0531(9) 1.0099(11) 0.122(6) uani 1 1 d . . .
h81a h 0.5864 0.9860 0.9742 0.182 uiso 1 1 calc r . .
h81b h 0.5826 1.1197 0.9910 0.182 uiso 1 1 calc r . .
h81c h 0.4636 1.0385 0.9733 0.182 uiso 1 1 calc r . .
loop_
 _atom_site_aniso_label
 _atom_site_aniso_u_11
 _atom_site_aniso_u_22
 _atom_site_aniso_u_33
 _atom_site_aniso_u_23
 _atom_site_aniso_u_13
 _atom_site_aniso_u_12
ru 0.01420(16) 0.00936(16) 0.01397(16) 0.00310(12) 0.00589(13)
0.00154(12)
cl1 0.0151(5) 0.0137(5) 0.0196(5) 0.0066(4) 0.0071(4) 0.0017(4)
cl2 0.0165(5) 0.0133(5) 0.0165(5) 0.0051(4) 0.0070(4) 0.0007(4)
p1 0.0141(5) 0.0091(5) 0.0141(5) 0.0017(4) 0.0057(4) 0.0015(4)
p2 0.0157(6) 0.0099(5) 0.0139(5) 0.0030(4) 0.0069(5) 0.0026(4)
o1 0.0179(16) 0.0075(15) 0.0191(15) 0.0013(12) 0.0093(13) 0.0037(12)
o2 0.0163(15) 0.0118(15) 0.0148(15) 0.0031(12) 0.0059(13) 0.0006(12)
o3 0.0183(16) 0.0151(16) 0.0163(16) 0.0070(13) 0.0096(13) 0.0095(13)
o4 0.0189(16) 0.0044(14) 0.0146(15) 0.0021(11) 0.0038(13) 0.0007(12)
o5 0.0214(16) 0.0145(16) 0.0198(16) 0.0031(13) 0.0090(14) 0.0056(13)
o6 0.0233(17) 0.0147(16) 0.0173(16) 0.0012(12) 0.0069(14) 0.0046(13)
o7 0.0226(17) 0.0117(16) 0.0195(16) 0.0046(13) 0.0111(14) 0.0010(13)
```

o8 0.0187(16) 0.0121(16) 0.0183(15) 0.0024(12) 0.0089(13) 0.0003(13)
o9 0.0299(19) 0.0123(17) 0.0203(17) 0.0064(14) 0.0120(15) 0.0010(14)
o10 0.0231(16) 0.0085(15) 0.0202(16) 0.0032(12) 0.0099(14)
0.0030(13)
o11 0.0144(15) 0.0171(16) 0.0150(15) -0.0004(12) 0.0038(13)
0.0035(12)
o12 0.0147(15) 0.0117(15) 0.0194(15) 0.0024(12) 0.0070(13)
0.0028(12)
c1 0.018(2) 0.0035(19) 0.018(2) 0.0009(16) 0.0110(18) 0.0022(16)
c2 0.018(2) 0.010(2) 0.016(2) 0.0001(17) 0.0083(18) 0.0027(17)
c3 0.018(2) 0.010(2) 0.018(2) 0.0037(17) 0.0071(18) 0.0053(17)
c4 0.017(2) 0.010(2) 0.020(2) 0.0041(17) 0.0070(18) 0.0015(17)
c5 0.019(2) 0.009(2) 0.018(2) 0.0011(17) 0.0053(19) 0.0028(17)
c6 0.016(2) 0.010(2) 0.018(2) 0.0044(17) 0.0069(18) 0.0025(17)
c7 0.021(2) 0.017(2) 0.016(2) 0.0036(18) 0.0054(19) 0.0032(18)
c8 0.030(3) 0.024(3) 0.026(3) 0.002(2) 0.013(2) 0.003(2)
c9 0.034(3) 0.041(3) 0.020(3) 0.000(2) 0.012(2) 0.012(3)
c10 0.036(3) 0.024(3) 0.023(3) 0.000(2) 0.012(2) 0.014(2)
c11 0.031(3) 0.010(2) 0.024(2) 0.0031(18) 0.009(2) 0.0064(19)
c12 0.025(3) 0.012(2) 0.020(2) 0.0035(19) 0.007(2) -0.0002(19)
c13 0.033(3) 0.021(3) 0.031(3) 0.008(2) 0.018(2) 0.002(2)
c14 0.093(7) 0.105(8) 0.076(6) 0.046(6) 0.069(6) 0.035(6)
c15 0.076(5) 0.070(5) 0.043(4) 0.032(4) 0.030(4) 0.007(4)
c16 0.037(3) 0.022(3) 0.023(3) 0.010(2) 0.007(2) 0.000(2)
c17 0.028(2) 0.021(2) 0.019(2) 0.0067(18) 0.017(2) 0.009(2)
c18 0.018(2) 0.006(2) 0.017(2) 0.0033(16) 0.0082(18) 0.0005(16)
c19 0.017(2) 0.007(2) 0.016(2) 0.0018(16) 0.0072(18) 0.0028(17)
c20 0.022(2) 0.011(2) 0.016(2) 0.0058(17) 0.0066(18) 0.0044(18)
c21 0.020(2) 0.013(2) 0.0111(19) 0.0012(16) 0.0055(18) 0.0003(17)
c22 0.019(2) 0.010(2) 0.013(2) 0.0016(17) 0.0053(18) 0.0012(17)
c23 0.015(2) 0.010(2) 0.018(2) 0.0019(16) 0.0057(18) 0.0029(17)
c24 0.028(3) 0.011(2) 0.014(2) 0.0026(17) 0.008(2) 0.0042(19)
c25 0.025(2) 0.018(2) 0.019(2) 0.0029(19) 0.005(2) -0.002(2)
c26 0.061(4) 0.011(3) 0.031(3) 0.002(2) -0.003(3) -0.003(3)
c27 0.058(4) 0.018(3) 0.039(3) 0.015(2) 0.005(3) 0.000(3)
c28 0.034(3) 0.017(2) 0.025(2) 0.010(2) 0.008(2) 0.007(2)
c29 0.013(2) 0.018(2) 0.016(2) 0.0045(18) 0.0062(18) 0.0066(18)
c30 0.021(2) 0.012(2) 0.018(2) 0.0043(17) 0.0080(19) 0.0006(18)
c31 0.027(2) 0.014(2) 0.019(2) 0.0015(18) 0.009(2) 0.0065(19)
c32 0.021(2) 0.016(2) 0.020(2) 0.0007(18) 0.0071(19) 0.0062(19)
c33 0.019(2) 0.019(2) 0.020(2) 0.0025(18) 0.0108(19) 0.0035(18)
c34 0.028(2) 0.005(2) 0.023(2) 0.0045(17) 0.005(2) 0.0004(18)
c41 0.021(2) 0.010(2) 0.015(2) 0.0016(16) 0.0106(18) 0.0029(17)
c42 0.021(2) 0.012(2) 0.021(2) 0.0030(17) 0.0103(19) 0.0032(18)
c43 0.022(2) 0.020(3) 0.016(2) 0.0023(19) 0.006(2) 0.001(2)
c44 0.031(3) 0.032(3) 0.015(2) 0.001(2) 0.011(2) -0.004(2)
c45 0.025(3) 0.037(3) 0.031(3) 0.006(2) 0.017(2) -0.003(2)
c46 0.018(2) 0.027(3) 0.019(2) 0.0042(19) 0.0077(19) 0.001(2)
c51 0.014(2) 0.012(2) 0.014(2) 0.0052(16) -0.0006(17) 0.0025(17)
c52 0.020(2) 0.014(2) 0.023(2) 0.0062(18) 0.0068(19) 0.0060(18)
c53 0.030(3) 0.008(2) 0.030(3) 0.0050(19) 0.004(2) 0.0037(19)
c54 0.026(3) 0.010(2) 0.031(3) 0.0103(19) -0.001(2) -0.0063(19)
c55 0.019(2) 0.025(3) 0.025(2) 0.015(2) 0.005(2) 0.0010(19)
c56 0.021(2) 0.016(2) 0.019(2) 0.0061(17) 0.0076(19) 0.0045(18)

```
c61 0.016(2) 0.021(2) 0.017(2) 0.0101(18) 0.0103(18) 0.0068(18)
c62 0.023(2) 0.018(2) 0.022(2) 0.0062(18) 0.013(2) 0.0075(19)
c63 0.030(3) 0.036(3) 0.024(2) 0.017(2) 0.016(2) 0.016(2)
c64 0.022(2) 0.039(3) 0.036(3) 0.026(2) 0.019(2) 0.012(2)
c65 0.022(2) 0.025(3) 0.034(3) 0.016(2) 0.015(2) 0.007(2)
c66 0.018(2) 0.017(2) 0.021(2) 0.0075(18) 0.0060(19) 0.0031(18)
c71 0.019(2) 0.011(2) 0.016(2) 0.0024(17) 0.0112(18) -0.0010(17)
c72 0.020(2) 0.014(2) 0.023(2) 0.0045(18) 0.0103(19) 0.0028(18)
c73 0.021(2) 0.016(2) 0.029(3) 0.0045(19) 0.010(2) 0.0007(19)
c74 0.028(3) 0.010(2) 0.029(3) 0.0017(19) 0.014(2) 0.0047(19)
c75 0.024(2) 0.015(2) 0.027(3) 0.0029(19) 0.011(2) 0.0036(19)
c76 0.020(2) 0.014(2) 0.021(2) 0.0016(18) 0.0091(19) 0.0004(18)
o13 0.063(3) 0.115(5) 0.021(2) -0.012(3) 0.006(2) 0.019(4)
c80 0.064(5) 0.072(6) 0.063(5) 0.035(4) 0.028(4) 0.034(4)
c81 0.086(8) 0.061(6) 0.103(9) -0.015(6) -0.040(6) 0.031(5)
_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
ru p2 2.2177(12) . ?
ru p1 2.2217(12) . ?
ru o4 2.273(3) . ?
ru o3 2.318(3) . ?
ru cl2 2.4038(11) . ?
ru cl1 2.4050(12) . ?
p1 o1 1.643(3) . ?
p1 c41 1.821(4) . ?
p1 c51 1.824(5) . ?
p2 o2 1.649(3) . ?
p2 c71 1.825(5) . ?
p2 c61 1.827(5) . ?
o1 c1 1.434(5) . ?
o2 c18 1.425(5) . ?
o3 c6 1.437(5) . ?
o3 c17 1.443(5) . ?
o4 c23 1.429(5) . ?
o4 c34 1.462(5) . ?
```

```
o5 c7 1.419(6) . ?
o5 c4 1.430(6) . ?
o6 c5 1.439(5) . ?
o6 c7 1.446(6) . ?
o7 c3 1.416(6) . ?
o7 c12 1.438(6) . ?
o8 c2 1.431(5) . ?
o8 c12 1.443(6) . ?
o9 c20 1.429(6) . ?
o9 c24 1.443(6) . ?
o10 c19 1.429(5) . ?
o10 c24 1.438(6) . ?
o11 c22 1.435(5) . ?
o11 c29 1.437(5) . ?
o12 c21 1.434(5) . ?
o12 c29 1.439(5) . ?
c1 c2 1.509(6) . ?
c1 c6 1.531(6) . ?
c1 h1a 0.9800 . ?
c2 c3 1.540(6) . ?
c2 h2a 0.9800 . ?
c3 c4 1.498(6) . ?
c3 h3a 0.9800 . ?
c4 c5 1.539(6) . ?
c4 h4a 0.9800 . ?
c5 c6 1.536(6) . ?
c5 h5a 0.9800 . ?
c6 h6a 0.9800 . ?
c7 c11 1.524(6) . ?
c7 c8 1.528(7) . ?
c8 c9 1.558(8) . ?
c8 h8a 0.9700 . ?
c8 h8b 0.9700 . ?
c9 c10 1.516(9) . ?
c9 h9a 0.9700 . ?
c9 h9b 0.9700 . ?
c10 c11 1.521(7) . ?
c10 h10a 0.9700 . ?
c10 h10b 0.9700 . ?
c11 h11a 0.9700 . ?
c11 h11b 0.9700 . ?
c12 c13 1.525(7) . ?
c12 c16 1.535(7) . ?
c13 c14 1.524(9) . ?
c13 h13a 0.9700 . ?
c13 h13b 0.9700 . ?
c14 c15 1.547(12) . ?
c14 h14a 0.9700 . ?
c14 h14b 0.9700 . ?
c15 c16 1.512(9) . ?
c15 h15a 0.9700 . ?
c15 h15b 0.9700 . ?
c16 h16a 0.9700 . ?
c16 h16b 0.9700 . ?
```

```
c17 h17a 0.9600 . ?
c17 h17b 0.9600 . ?
c17 h17c 0.9600 . ?
c18 c23 1.526(6) . ?
c18 c19 1.529(6) . ?
c18 h18a 0.9800 . ?
c19 c20 1.541(6) . ?
c19 h19a 0.9800 . ?
c20 c21 1.511(6) . ?
c20 h20a 0.9800 . ?
c21 c22 1.528(6) . ?
c21 h21a 0.9800 . ?
c22 c23 1.509(6) . ?
c22 h22a 0.9800 . ?
c23 h23a 0.9800 . ?
c24 c25 1.524(7) . ?
c24 c28 1.538(7) . ?
c25 c26 1.537(7) . ?
c25 h25a 0.9700 . ?
c25 h25b 0.9700 . ?
c26 c27 1.535(8) . ?
c26 h26a 0.9700 . ?
c26 h26b 0.9700 . ?
c27 c28 1.526(8) . ?
c27 h27a 0.9700 . ?
c27 h27b 0.9700 . ?
c28 h28a 0.9700 . ?
c28 h28b 0.9700 . ?
c29 c33 1.530(6) . ?
c29 c30 1.533(6) . ?
c30 c31 1.540(6) . ?
c30 h30a 0.9700 . ?
c30 h30b 0.9700 . ?
c31 c32 1.535(7) . ?
c31 h31a 0.9700 . ?
c31 h31b 0.9700 . ?
c32 c33 1.523(6) . ?
c32 h32a 0.9700 . ?
c32 h32b 0.9700 . ?
c33 h33a 0.9700 . ?
c33 h33b 0.9700 . ?
c34 h34a 0.9600 . ?
c34 h34b 0.9600 . ?
c34 h34c 0.9600 . ?
c41 c42 1.382(7) . ?
c41 c46 1.393(7) . ?
c42 c43 1.400(7) . ?
c42 h42a 0.9300 . ?
c43 c44 1.403(8) . ?
c43 h43a 0.9300 . ?
c44 c45 1.384(8) . ?
c44 h44a 0.9300 . ?
c45 c46 1.388(7) . ?
c45 h45a 0.9300 . ?
```

```
c46 h46a 0.9300 . ?
c51 c56 1.394(7) . ?
c51 c52 1.400(6) . ?
c52 c53 1.402(7) . ?
c52 h52a 0.9300 . ?
c53 c54 1.358(8) . ?
c53 h53a 0.9300 . ?
c54 c55 1.416(8) . ?
c54 h54a 0.9300 . ?
c55 c56 1.377(7) . ?
c55 h55a 0.9300 . ?
c56 h56a 0.9300 . ?
c61 c66 1.393(7) . ?
c61 c62 1.401(6) . ?
c62 c63 1.392(7) . ?
c62 h62a 0.9300 . ?
c63 c64 1.363(8) . ?
c63 h63a 0.9300 . ?
c64 c65 1.401(8) . ?
c64 h64a 0.9300 . ?
c65 c66 1.378(7) . ?
c65 h65a 0.9300 . ?
c66 h66a 0.9300 . ?
c71 c76 1.383(7) . ?
c71 c72 1.391(6) . ?
c72 c73 1.398(7) . ?
c72 h72a 0.9300 . ?
c73 c74 1.373(7) . ?
c73 h73a 0.9300 . ?
c74 c75 1.396(7) . ?
c74 h74a 0.9300 . ?
c75 c76 1.393(7) . ?
c75 h75a 0.9300 . ?
c76 h76a 0.9300 . ?
o13 c80 1.307(10) . ?
o13 h13 0.8200 . ?
c80 c81 1.550(14) . ?
c80 h80a 0.9700 . ?
c80 h80b 0.9700 . ?
c81 h81a 0.9600 . ?
c81 h81b 0.9600 . ?
c81 h81c 0.9600 . ?
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
p2 ru p1 104.49(4) . . ?
p2 ru o4 88.70(9) . . ?
p1 ru o4 166.46(8) . . ?
p2 ru o3 166.34(8) . . ?
```

```
p1 ru o3 88.93(9) . . ?
o4 ru o3 78.05(11) . . ?
p2 ru cl2 93.91(4) . . ?
p1 ru cl2 90.78(4) . . ?
o4 ru cl2 85.18(9) . . ?
o3 ru cl2 88.34(9) . . ?
p2 ru cl1 90.41(4) . . ?
p1 ru cl1 93.71(4) . . ?
o4 ru cl1 89.18(9) . . ?
o3 ru cl1 86.13(9) . . ?
cl2 ru cl1 172.81(4) . . ?
o1 p1 c41 100.77(19) . . ?
o1 p1 c51 95.11(18) . . ?
c41 p1 c51 100.6(2) . . ?
o1 p1 ru 106.79(12) . . ?
c41 p1 ru 125.77(16) . . ?
c51 p1 ru 121.77(14) . . ?
o2 p2 c71 101.03(19) . . ?
o2 p2 c61 94.32(19) . . ?
c71 p2 c61 101.8(2) . . ?
o2 p2 ru 107.46(12) . . ?
c71 p2 ru 123.84(15) . . ?
c61 p2 ru 122.49(15) . . ?
c1 o1 p1 117.1(3) . . ?
c18 o2 p2 117.2(3) . . ?
c6 o3 c17 112.3(3) . . ?
c6 o3 ru 126.1(3) . . ?
c17 o3 ru 118.3(3) . . ?
c23 o4 c34 111.8(3) . . ?
c23 o4 ru 126.9(3) . . ?
c34 o4 ru 119.1(3) . . ?
c7 o5 c4 104.8(3) . . ?
c5 o6 c7 108.7(3) . . ?
c3 o7 c12 107.8(4) . . ?
c2 o8 c12 109.1(3) . . ?
c20 o9 c24 108.6(4) . . ?
c19 o10 c24 109.3(3) . . ?
c22 o11 c29 108.0(3) . . ?
c21 o12 c29 103.9(3) . . ?
o1 c1 c2 107.5(3) . . ?
o1 c1 c6 109.0(3) . . ?
c2 c1 c6 109.0(3) . . ?
o1 c1 h1a 110.4 . . ?
c2 c1 h1a 110.4 . . ?
c6 c1 h1a 110.4 . . ?
o8 c2 c1 111.1(4) . . ?
o8 c2 c3 101.9(4) . . ?
c1 c2 c3 111.8(4) . . ?
o8 c2 h2a 110.6 . . ?
c1 c2 h2a 110.6 . . ?
c3 c2 h2a 110.6 . . ?
o7 c3 c4 108.9(4) . . ?
o7 c3 c2 101.9(3) . . ?
c4 c3 c2 117.6(4) . . ?
```

```
o7 c3 h3a 109.3 . . ?
c4 c3 h3a 109.4 . . ?
c2 c3 h3a 109.3 . . ?
o5 c4 c3 109.7(4) . . ?
o5 c4 c5 100.6(4) . . ?
c3 c4 c5 117.8(4) . . ?
o5 c4 h4a 109.4 . . ?
c3 c4 h4a 109.4 . . ?
c5 c4 h4a 109.4 . . ?
o6 c5 c6 112.1(4) . . ?
o6 c5 c4 101.4(3) . . ?
c6 c5 c4 110.4(4) . . ?
o6 c5 h5a 110.9 . . ?
c6 c5 h5a 110.9 . . ?
c4 c5 h5a 110.9 . . ?
o3 c6 c1 110.5(3) . . ?
o3 c6 c5 111.2(4) . . ?
c1 c6 c5 108.5(4) . . ?
o3 c6 h6a 108.9 . . ?
c1 c6 h6a 108.9 . . ?
c5 c6 h6a 108.9 . . ?
o5 c7 o6 105.1(4) . . ?
o5 c7 c11 111.2(4) . . ?
o6 c7 c11 112.8(4) . . ?
o5 c7 c8 109.5(4) . . ?
o6 c7 c8 112.9(4) . . ?
c11 c7 c8 105.4(4) . . ?
c7 c8 c9 106.2(4) . . ?
c7 c8 h8a 110.5 . . ?
c9 c8 h8a 110.5 . . ?
c7 c8 h8b 110.5 . . ?
c9 c8 h8b 110.5 . . ?
h8a c8 h8b 108.7 . . ?
c10 c9 c8 103.2(4) . . ?
c10 c9 h9a 111.1 . . ?
c8 c9 h9a 111.1 . . ?
c10 c9 h9b 111.1 . . ?
c8 c9 h9b 111.1 . . ?
h9a c9 h9b 109.1 . . ?
c9 c10 c11 103.5(4) . . ?
c9 c10 h10a 111.1 . . ?
c11 c10 h10a 111.1 . . ?
c9 c10 h10b 111.1 . . ?
c11 c10 h10b 111.1 . . ?
h10a c10 h10b 109.0 . . ?
c10 c11 c7 102.1(4) . . ?
c10 c11 h11a 111.3 . . ?
c7 c11 h11a 111.3 . . ?
c10 c11 h11b 111.3 . . ?
c7 c11 h11b 111.3 . . ?
h11a c11 h11b 109.2 . . ?
o7 c12 o8 105.5(4) . . ?
o7 c12 c13 108.1(4) . . ?
o8 c12 c13 115.2(4) . . ?
```

```
o7 c12 c16 112.4(4) . . ?
o8 c12 c16 109.4(4) . . ?
c13 c12 c16 106.4(4) . . ?
c14 c13 c12 105.6(5) . . ?
c14 c13 h13a 110.6 . . ?
c12 c13 h13a 110.6 . . ?
c14 c13 h13b 110.6 . . ?
c12 c13 h13b 110.6 . . ?
h13a c13 h13b 108.8 . . ?
c13 c14 c15 103.1(6) . . ?
c13 c14 h14a 111.2 . . ?
c15 c14 h14a 111.2 . . ?
c13 c14 h14b 111.2 . . ?
c15 c14 h14b 111.2 . . ?
h14a c14 h14b 109.1 . . ?
c16 c15 c14 101.6(6) . . ?
c16 c15 h15a 111.5 . . ?
c14 c15 h15a 111.5 . . ?
c16 c15 h15b 111.5 . . ?
c14 c15 h15b 111.5 . . ?
h15a c15 h15b 109.3 . . ?
c15 c16 c12 103.8(5) . . ?
c15 c16 h16a 111.0 . . ?
c12 c16 h16a 111.0 . . ?
c15 c16 h16b 111.0 . . ?
c12 c16 h16b 111.0 . . ?
h16a c16 h16b 109.0 . . ?
o3 c17 h17a 109.5 . . ?
o3 c17 h17b 109.5 . . ?
h17a c17 h17b 109.5 . . ?
o3 c17 h17c 109.5 . . ?
h17a c17 h17c 109.5 . . ?
h17b c17 h17c 109.5 . . ?
o2 c18 c23 110.8(3) . . ?
o2 c18 c19 107.0(4) . . ?
c23 c18 c19 107.7(3) . . ?
o2 c18 h18a 110.4 . . ?
c23 c18 h18a 110.4 . . ?
c19 c18 h18a 110.4 . . ?
o10 c19 c18 111.3(3) . . ?
o10 c19 c20 101.8(3) . . ?
c18 c19 c20 112.0(4) . . ?
o10 c19 h19a 110.5 . . ?
c18 c19 h19a 110.5 . . ?
c20 c19 h19a 110.5 . . ?
o9 c20 c21 105.9(4) . . ?
o9 c20 c19 101.8(3) . . ?
c21 c20 c19 117.8(4) . . ?
o9 c20 h20a 110.2 . . ?
c21 c20 h20a 110.2 . . ?
c19 c20 h20a 110.2 . . ?
o12 c21 c20 111.8(4) . . ?
o12 c21 c22 100.3(3) . . ?
c20 c21 c22 117.0(4) . . ?
```

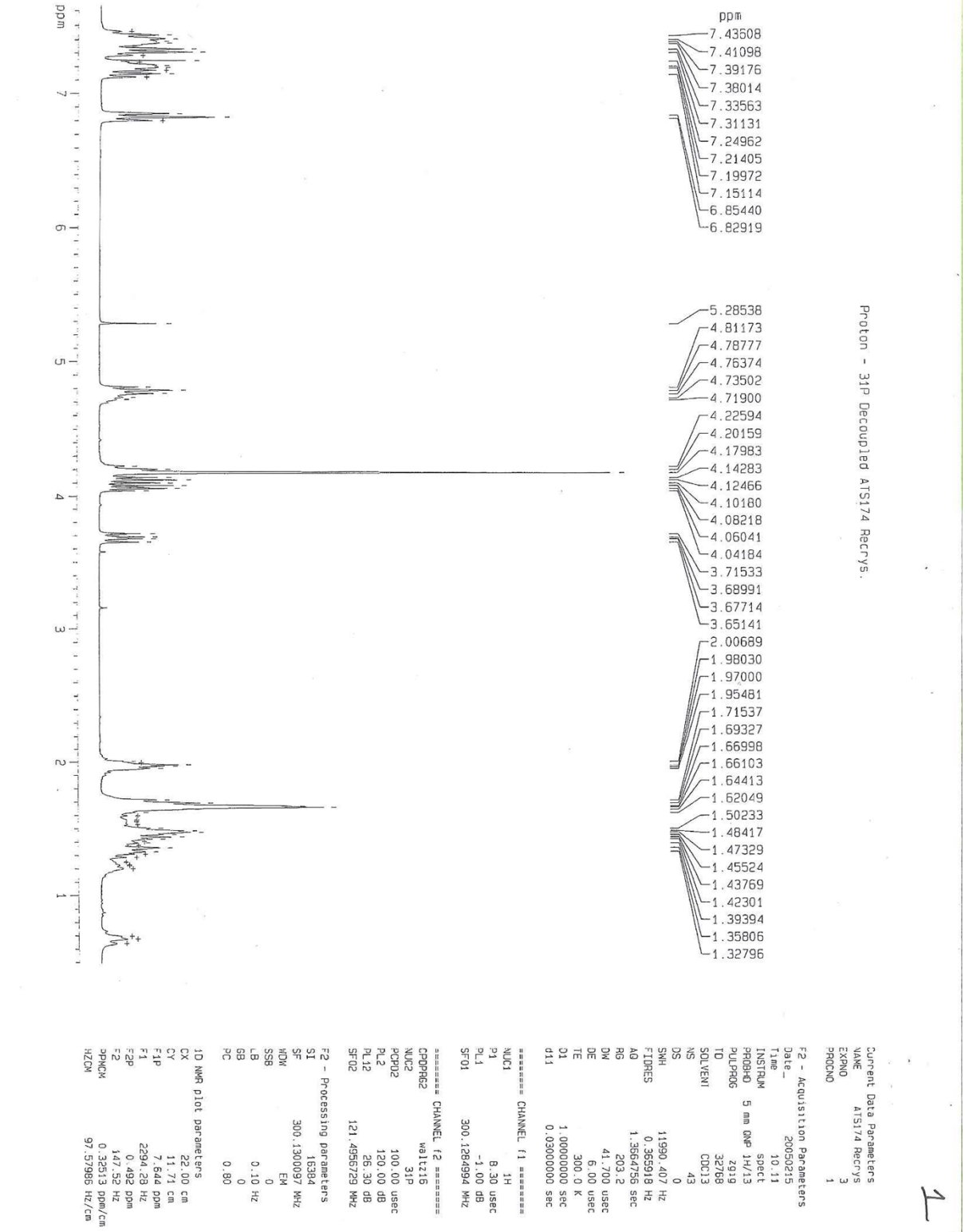
```
o12 c21 h21a 109.1 . . ?
c20 c21 h21a 109.1 . . ?
c22 c21 h21a 109.1 . . ?
o11 c22 c23 113.1(4) . . ?
o11 c22 c21 102.1(3) . . ?
c23 c22 c21 109.7(4) . . ?
o11 c22 h22a 110.6 . . ?
c23 c22 h22a 110.6 . . ?
c21 c22 h22a 110.6 . . ?
o4 c23 c22 113.1(4) . . ?
o4 c23 c18 111.0(3) . . ?
c22 c23 c18 107.7(4) . . ?
o4 c23 h23a 108.3 . . ?
c22 c23 h23a 108.3 . . ?
c18 c23 h23a 108.3 . . ?
o10 c24 o9 105.4(3) . . ?
o10 c24 c25 115.7(4) . . ?
o9 c24 c25 108.4(4) . . ?
o10 c24 c28 108.7(4) . . ?
o9 c24 c28 112.6(4) . . ?
c25 c24 c28 106.1(4) . . ?
c24 c25 c26 105.7(4) . . ?
c24 c25 h25a 110.6 . . ?
c26 c25 h25a 110.6 . . ?
c24 c25 h25b 110.6 . . ?
c26 c25 h25b 110.6 . . ?
h25a c25 h25b 108.7 . . ?
c27 c26 c25 102.6(4) . . ?
c27 c26 h26a 111.2 . . ?
c25 c26 h26a 111.2 . . ?
c27 c26 h26b 111.2 . . ?
c25 c26 h26b 111.2 . . ?
h26a c26 h26b 109.2 . . ?
c28 c27 c26 101.8(5) . . ?
c28 c27 h27a 111.4 . . ?
c26 c27 h27a 111.4 . . ?
c28 c27 h27b 111.4 . . ?
c26 c27 h27b 111.4 . . ?
h27a c27 h27b 109.3 . . ?
c27 c28 c24 104.7(4) . . ?
c27 c28 h28a 110.8 . . ?
c24 c28 h28a 110.8 . . ?
c27 c28 h28b 110.8 . . ?
c24 c28 h28b 110.8 . . ?
h28a c28 h28b 108.9 . . ?
o11 c29 o12 105.7(3) . . ?
o11 c29 c33 113.5(4) . . ?
o12 c29 c33 110.2(4) . . ?
o11 c29 c30 112.2(4) . . ?
o12 c29 c30 110.1(4) . . ?
c33 c29 c30 105.2(4) . . ?
c29 c30 c31 105.9(4) . . ?
c29 c30 h30a 110.6 . . ?
c31 c30 h30a 110.6 . . ?
```

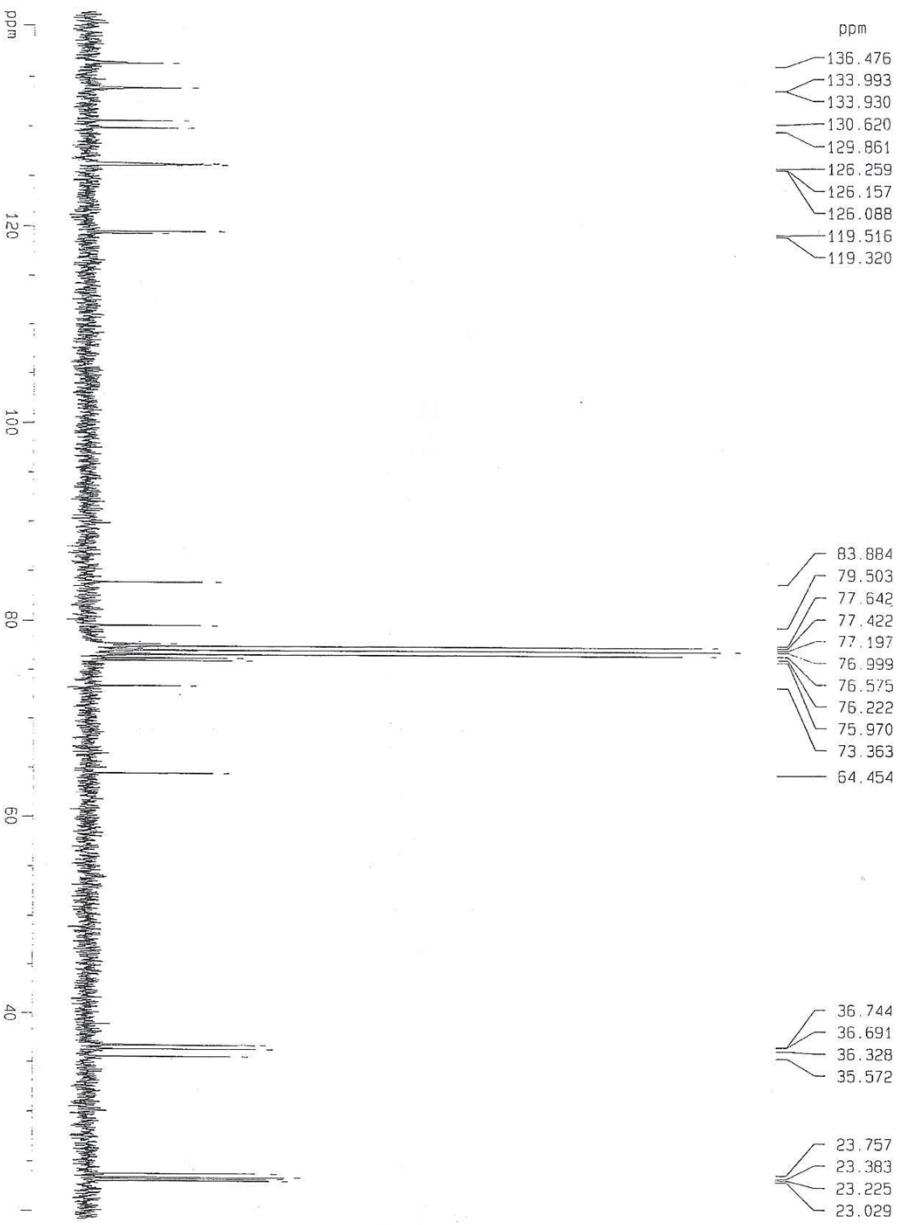
```
c29 c30 h30b 110.6 . . ?
c31 c30 h30b 110.6 . . ?
h30a c30 h30b 108.7 . . ?
c32 c31 c30 105.0(4) . . ?
c32 c31 h31a 110.7 . . ?
c30 c31 h31a 110.7 . . ?
c32 c31 h31b 110.7 . . ?
c30 c31 h31b 110.7 . . ?
h31a c31 h31b 108.8 . . ?
c33 c32 c31 103.6(4) . . ?
c33 c32 h32a 111.0 . . ?
c31 c32 h32a 111.0 . . ?
c33 c32 h32b 111.0 . . ?
c31 c32 h32b 111.0 . . ?
h32a c32 h32b 109.0 . . ?
c32 c33 c29 101.6(4) . . ?
c32 c33 h33a 111.4 . . ?
c29 c33 h33a 111.4 . . ?
c32 c33 h33b 111.4 . . ?
c29 c33 h33b 111.4 . . ?
h33a c33 h33b 109.3 . . ?
o4 c34 h34a 109.5 . . ?
o4 c34 h34b 109.5 . . ?
h34a c34 h34b 109.5 . . ?
o4 c34 h34c 109.5 . . ?
h34a c34 h34c 109.5 . . ?
h34b c34 h34c 109.5 . . ?
c42 c41 c46 119.1(4) . . ?
c42 c41 p1 118.5(4) . . ?
c46 c41 p1 122.2(4) . . ?
c41 c42 c43 121.7(5) . . ?
c41 c42 h42a 119.1 . . ?
c43 c42 h42a 119.1 . . ?
c42 c43 c44 118.2(5) . . ?
c42 c43 h43a 120.9 . . ?
c44 c43 h43a 120.9 . . ?
c45 c44 c43 120.3(5) . . ?
c45 c44 h44a 119.9 . . ?
c43 c44 h44a 119.9 . . ?
c44 c45 c46 120.6(5) . . ?
c44 c45 h45a 119.7 . . ?
c46 c45 h45a 119.7 . . ?
c45 c46 c41 120.1(5) . . ?
c45 c46 h46a 120.0 . . ?
c41 c46 h46a 120.0 . . ?
c56 c51 c52 119.2(4) . . ?
c56 c51 p1 119.9(3) . . ?
c52 c51 p1 120.8(4) . . ?
c51 c52 c53 120.0(5) . . ?
c51 c52 h52a 120.0 . . ?
c53 c52 h52a 120.0 . . ?
c54 c53 c52 120.0(5) . . ?
c54 c53 h53a 120.0 . . ?
c52 c53 h53a 120.0 . . ?
```

```
c53 c54 c55 120.9(5) . . ?
c53 c54 h54a 119.6 . . ?
c55 c54 h54a 119.6 . . ?
c56 c55 c54 119.0(5) . . ?
c56 c55 h55a 120.5 . . ?
c54 c55 h55a 120.5 . . ?
c55 c56 c51 121.0(4) . . ?
c55 c56 h56a 119.5 . . ?
c51 c56 h56a 119.5 . . ?
c66 c61 c62 119.2(4) . . ?
c66 c61 p2 119.2(3) . . ?
c62 c61 p2 121.6(4) . . ?
c63 c62 c61 119.7(5) . . ?
c63 c62 h62a 120.1 . . ?
c61 c62 h62a 120.1 . . ?
c64 c63 c62 120.8(5) . . ?
c64 c63 h63a 119.6 . . ?
c62 c63 h63a 119.6 . . ?
c63 c64 c65 119.9(5) . . ?
c63 c64 h64a 120.1 . . ?
c65 c64 h64a 120.1 . . ?
c66 c65 c64 120.1(5) . . ?
c66 c65 h65a 120.0 . . ?
c64 c65 h65a 120.0 . . ?
c65 c66 c61 120.4(5) . . ?
c65 c66 h66a 119.8 . . ?
c61 c66 h66a 119.8 . . ?
c76 c71 c72 119.4(4) . . ?
c76 c71 p2 119.7(3) . . ?
c72 c71 p2 120.9(4) . . ?
c71 c72 c73 120.2(4) . . ?
c71 c72 h72a 119.9 . . ?
c73 c72 h72a 119.9 . . ?
c74 c73 c72 119.9(5) . . ?
c74 c73 h73a 120.0 . . ?
c72 c73 h73a 120.0 . . ?
c73 c74 c75 120.4(5) . . ?
c73 c74 h74a 119.8 . . ?
c75 c74 h74a 119.8 . . ?
c76 c75 c74 119.4(5) . . ?
c76 c75 h75a 120.3 . . ?
c74 c75 h75a 120.3 . . ?
c71 c76 c75 120.7(4) . . ?
c71 c76 h76a 119.7 . . ?
c75 c76 h76a 119.7 . . ?
c80 o13 h13 109.5 . . ?
o13 c80 c81 118.6(7) . . ?
o13 c80 h80a 107.7 . . ?
c81 c80 h80a 107.7 . . ?
o13 c80 h80b 107.7 . . ?
c81 c80 h80b 107.7 . . ?
h80a c80 h80b 107.1 . . ?
c80 c81 h81a 109.5 . . ?
c80 c81 h81b 109.5 . . ?
```

```
h81a c81 h81b 109.5 . . ?
c80 c81 h81c 109.5 . . ?
h81a c81 h81c 109.5 . . ?
h81b c81 h81c 109.5 . . ?
loop_
 _geom_hbond_atom_site_label_d
 _geom_hbond_atom_site_label_h
 _geom_hbond_atom_site_label_a
 _geom_hbond_distance_dh
 _geom_hbond_distance_ha
 _geom_hbond_distance_da
 _geom_hbond_angle_dha
 _geom_hbond_site_symmetry_a
o13 h13 o6  0.82 2.14 2.934(6) 161.7 1_566
_diffrn_measured_fraction_theta_max    0.992
_diffrn_reflns_theta_full              26.42
_diffrn_measured_fraction_theta_full   0.992
_refine_diff_density_max    1.053
_refine_diff_density_min   -1.096
_refine_diff_density_rms    0.091
```

NMR spectra of $RuCl_2$(D-P1)$_2$ (**1**)

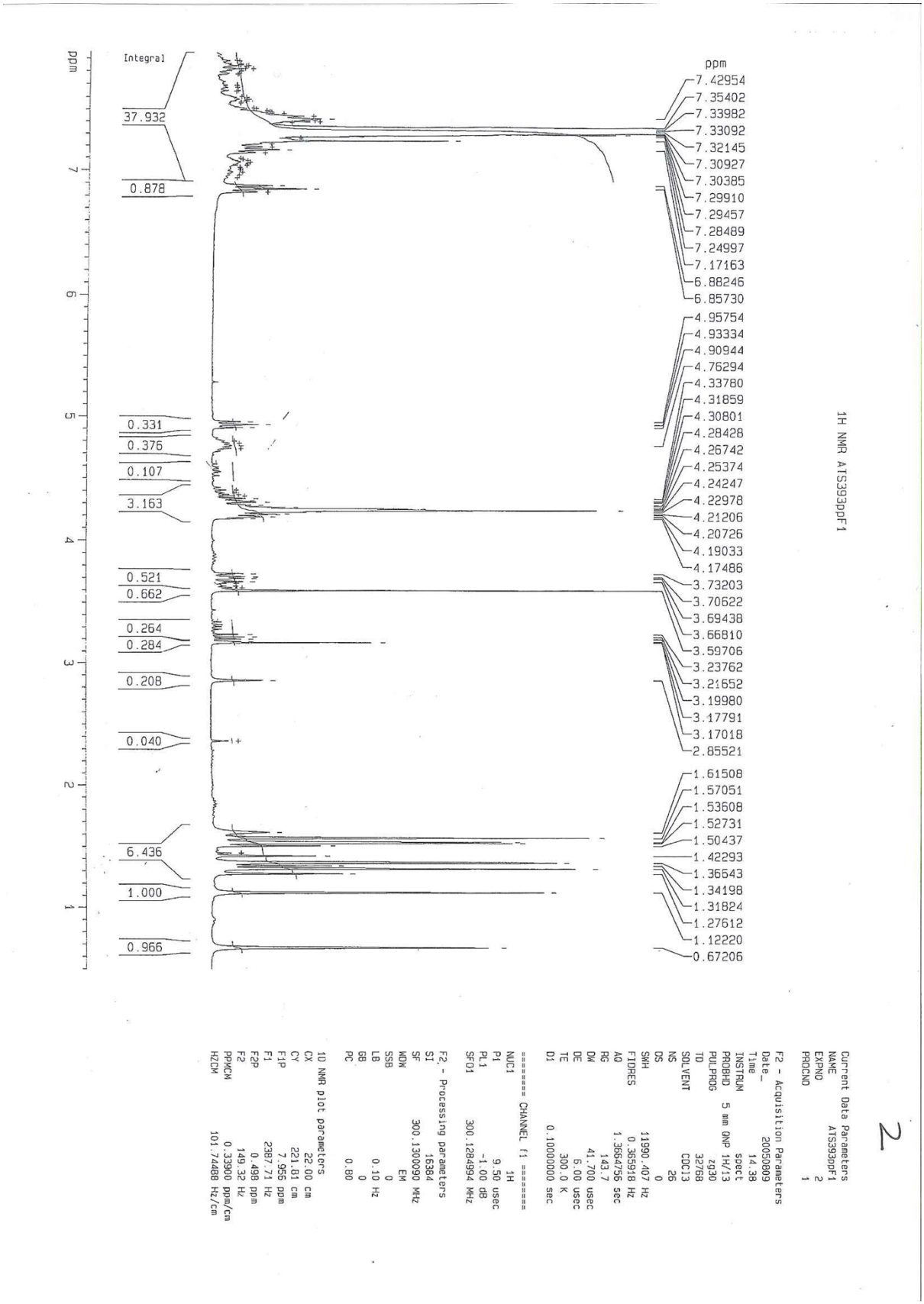




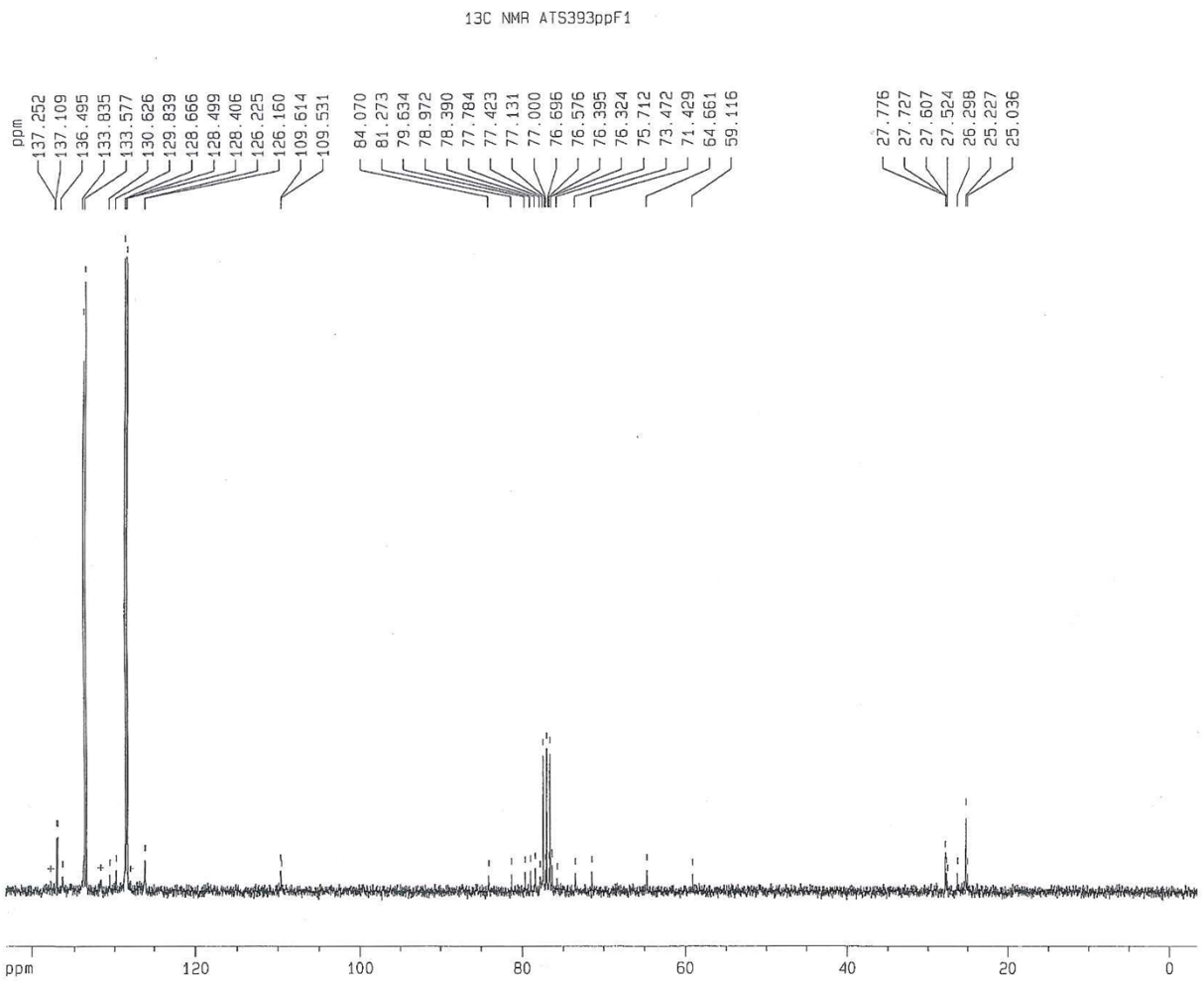

```
Current Data Parameters
NAME          ATS174 Recrys.
EXPNO                      4
PROCNO                     1

F2 - Acquisition Parameters
Date_               20050215
Time                   10.14
INSTRUM                spect
PROBHD     5 mm QNP 1H/13
PULPROG                zgpg
TD                    65536
SOLVENT               CDCl3
NS                      538
DS                        0
SWH               17985.611 Hz
FIDRES                0.274439 Hz
AQ                1.8219508 sec
RG                     16384
DW                   27.800 usec
DE                   20.00 usec
TE                   300.0 K
D1                0.17593171 sec
d11               0.03000000 sec
d12               0.00002000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                       5.44 usec
PL1                      4.00 dB
SF01           75.4760973 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                 102.00 usec
PL2                   120.00 dB
PL12                   20.20 dB
PL13                   25.80 dB
SF02           300.1312005 MHz

F2 - Processing parameters
SI                        32768
SF             75.4677499 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                     22.00 cm
CY                     11.57 cm
F1P                  141.460 ppm
F1                   10675.68 Hz
F2P                   19.186 ppm
F2                   1447.91 Hz
PPMCM                5.55793 ppm/cm
HZCM                 419.44418 Hz/cm
```

1

NMR spectra of $RuCl_2(D\text{-}P2)_2$ (**2**)



2



Current Data Parameters

NAME	ATS393ppF1
EXPNO	4
PROCNO	1

F2 - Acquisition Parameters

Date_	20050809
Time	14.41
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg
TD	65536
SOLVENT	CDCl3
NS	165
DS	0
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	16384
DW	27.800 usec
DE	20.00 usec
TE	300.0 K
D1	0.17593171 sec
d11	0.03000000 sec
d12	0.00002000 sec

======== CHANNEL f1 ========

NUC1	13C
P1	5.44 usec
PL1	4.00 dB
SFO1	75.4760973 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	-1.00 dB
PL12	19.00 dB
PL13	25.20 dB
SFO2	300.1312005 MHz

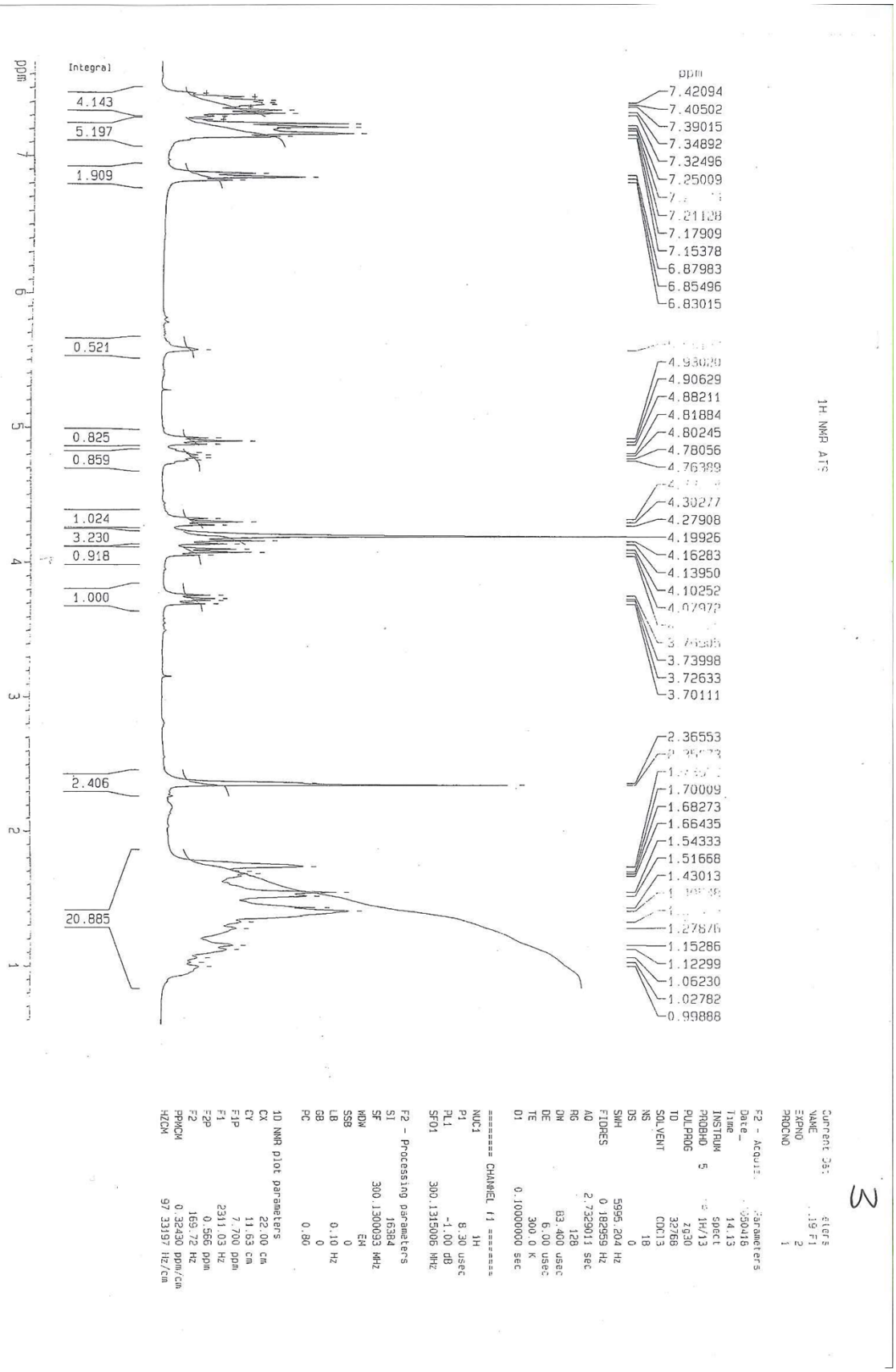
F2 - Processing parameters

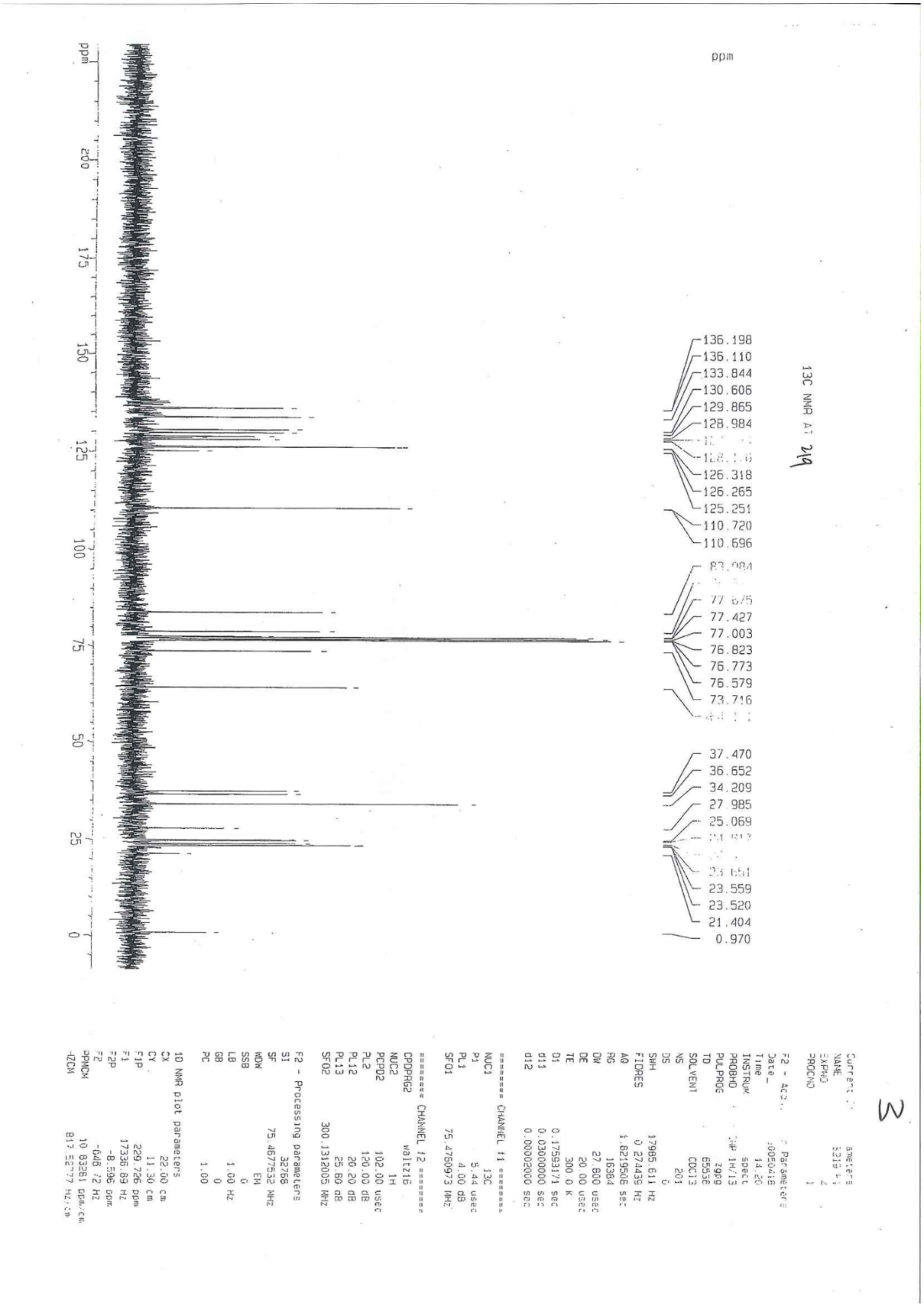
SI	32768
SF	75.4677532 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

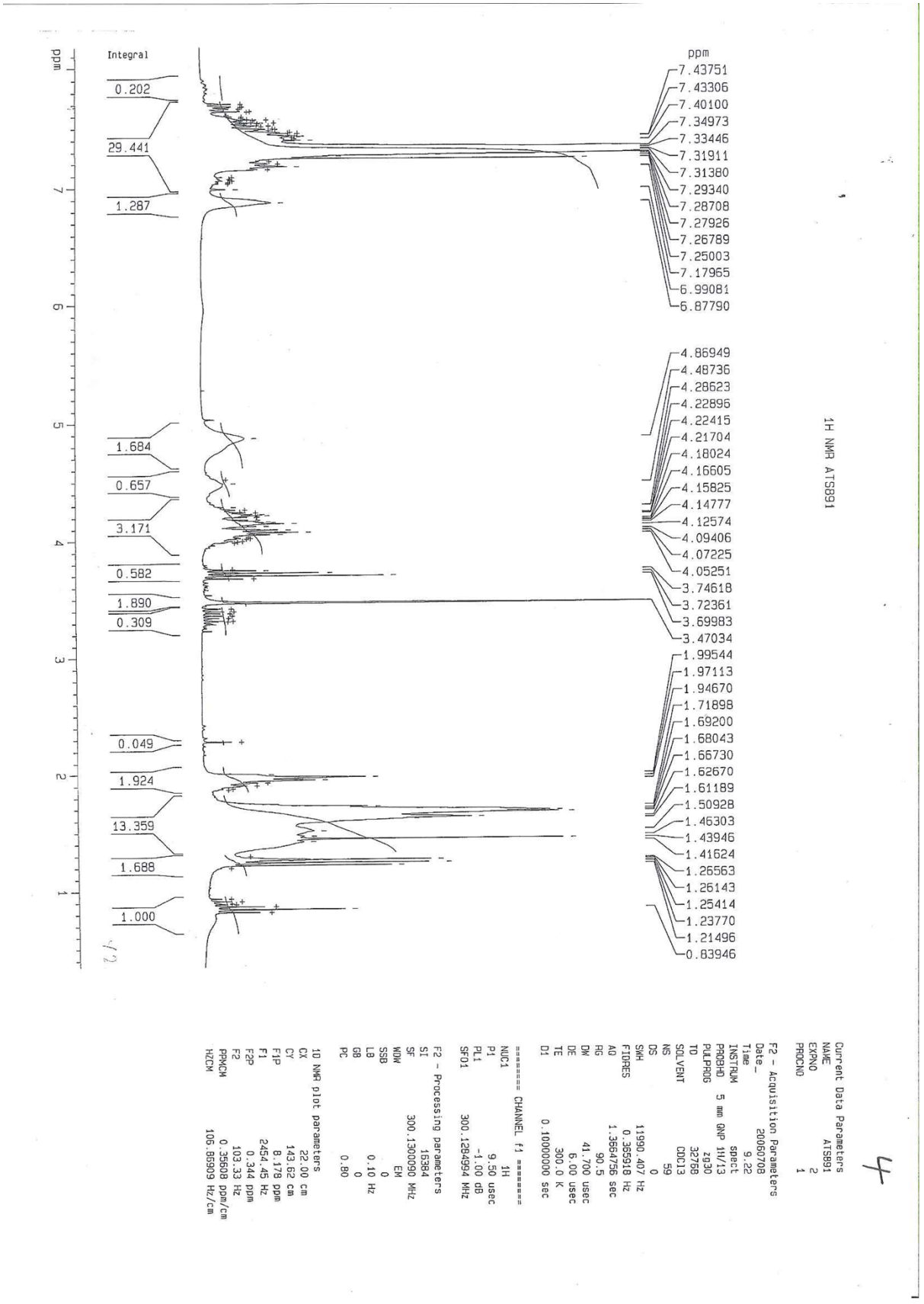
CX	22.00 cm
CY	11.74 cm
F1P	143.242 ppm
F1	10810.15 Hz
F2P	-3.436 ppm
F2	-259.34 Hz
PPMCM	6.66720 ppm/cm
HZCM	503.15884 Hz/cm

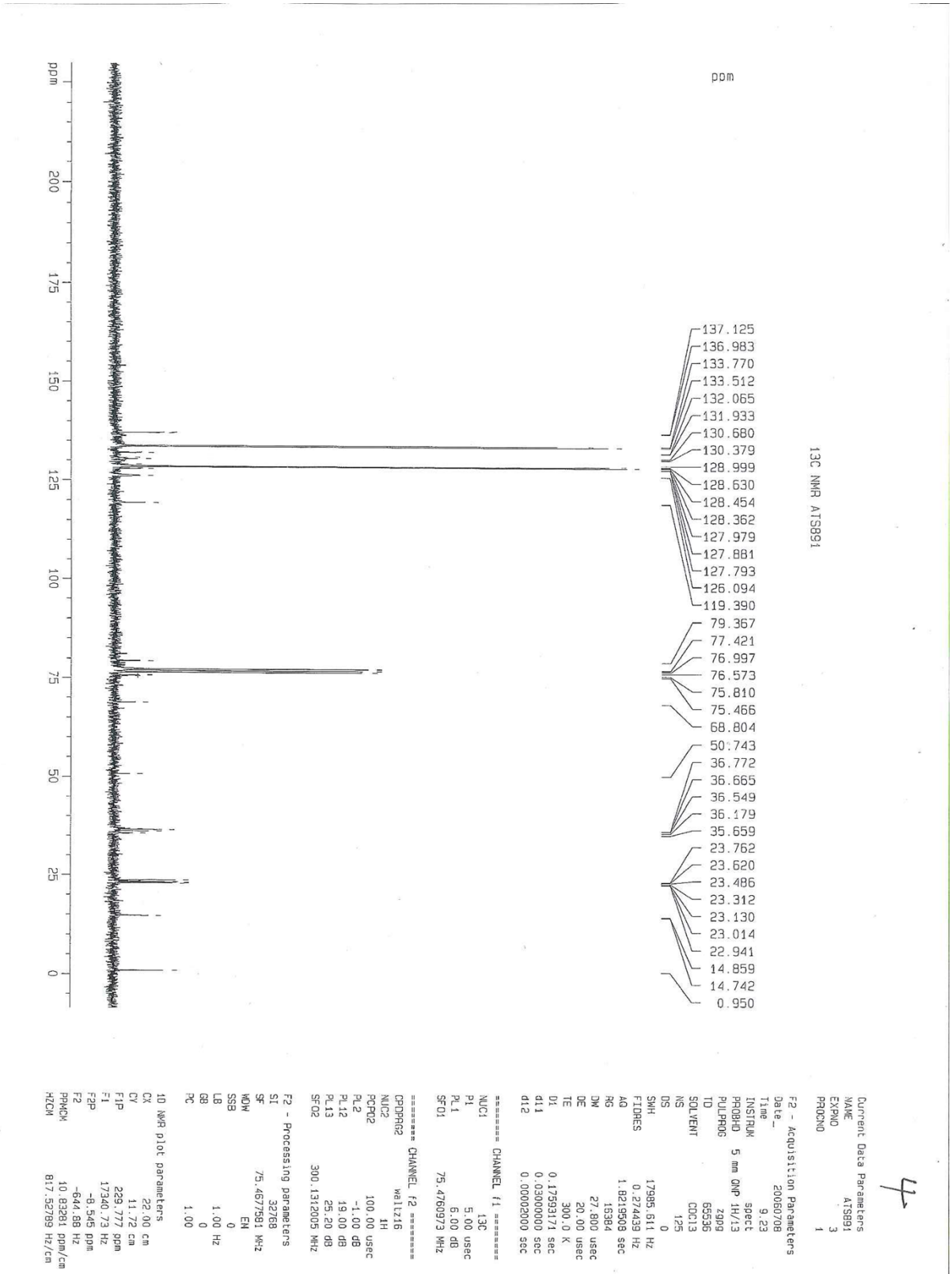
NMR spectra of $RuCl_2(D\text{-}P3)_2$ (**3**)



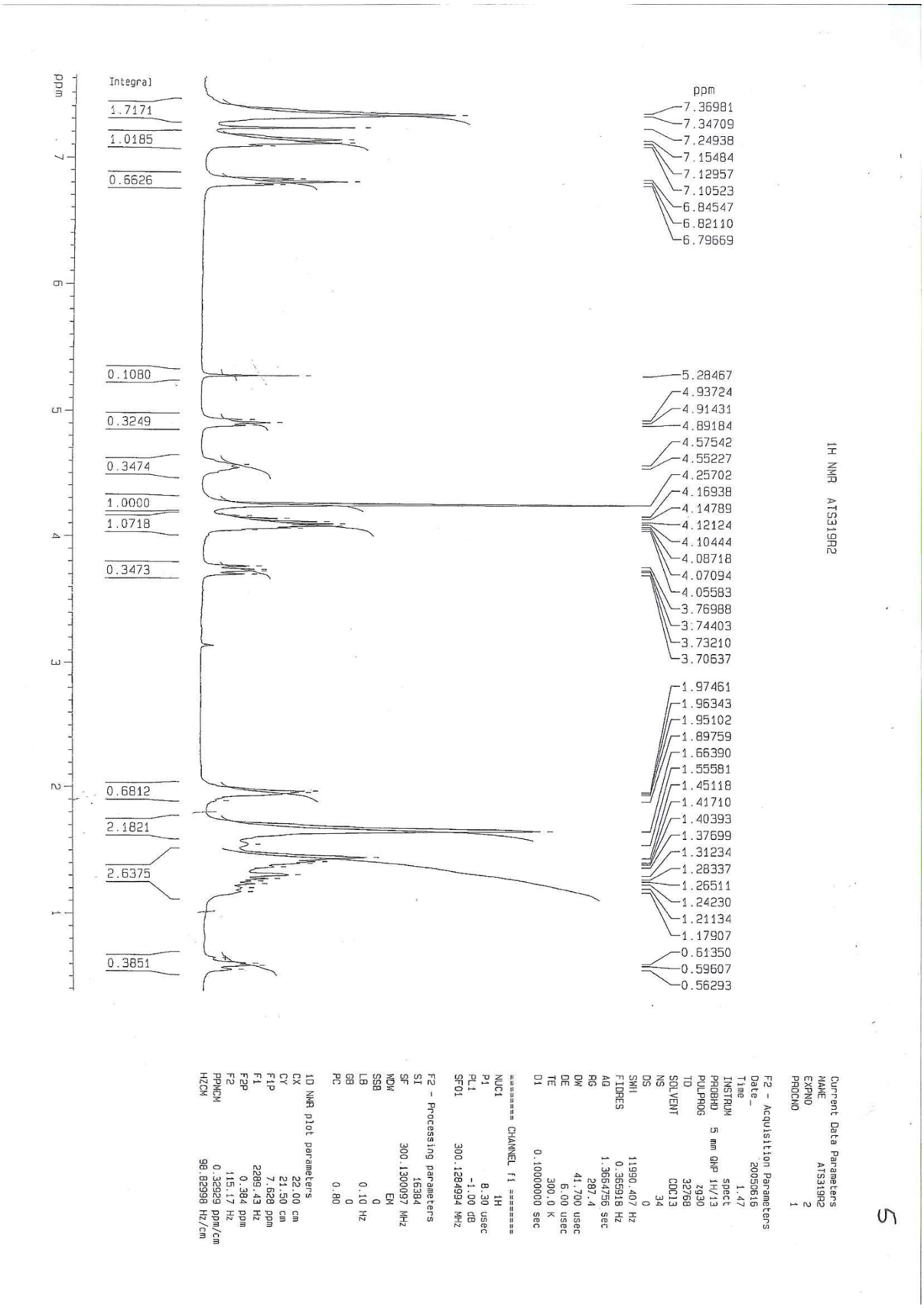

13C NMR at 219
ppm
136.198
136.110
133.844
130.606
129.865
128.984
126.318
126.265
125.251
110.720
110.696
77.427
77.003
76.823
76.773
76.579
37.470
36.652
34.209
27.985
25.069
23.559
23.520
21.404
0.970
ppm
200
175
150
125
100
75
50
25
0

NMR spectra of $RuCl_2(D\text{-}P4)_2$ (**4**)

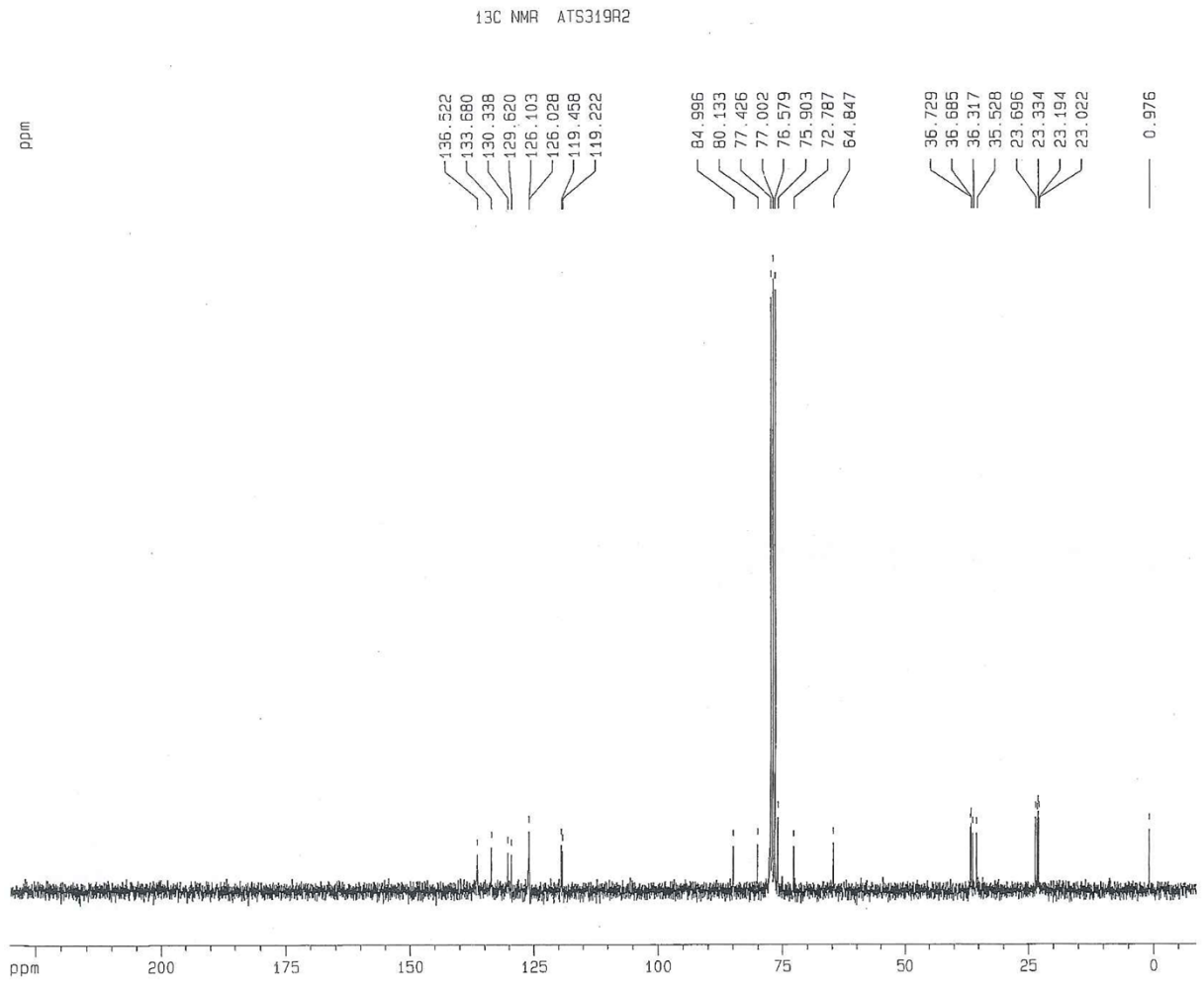



13C NMR ATS891
ppm
137.125
136.983
133.770
133.512
132.065
131.933
130.680
130.379
128.999
128.630
128.454
128.362
127.979
127.881
127.793
126.094
119.390
79.367
77.421
76.997
76.573
75.810
75.466
68.804
50.743
36.772
36.665
36.549
36.179
35.659
23.762
23.620
23.486
23.312
23.130
23.014
22.941
14.859
14.742
0.950
ppm
200
175
150
125
100
75
50
25
0
Current Data Parameters
NAME ATS891
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060708
Time 9.23
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 125
DS 0
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.821908 sec
RG 16384
DW 27.800 usec
DE 20.00 usec
TE 300.0 K
D1 0.17593171 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 5.00 usec
PL1 6.00 dB
SFO1 75.476973 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -1.00 dB
PL12 19.00 dB
PL13 25.20 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677581 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.00 cm
CY 11.72 cm
F1P 229.777 ppm
F1 17340.73 Hz
F2P -8.545 ppm
F2 -644.88 Hz
PPMCM 10.83281 ppm/cm
HZCM 817.52789 Hz/cm

NMR spectra of $OsCl_2(D\text{-}P1)_2$ (**5**)

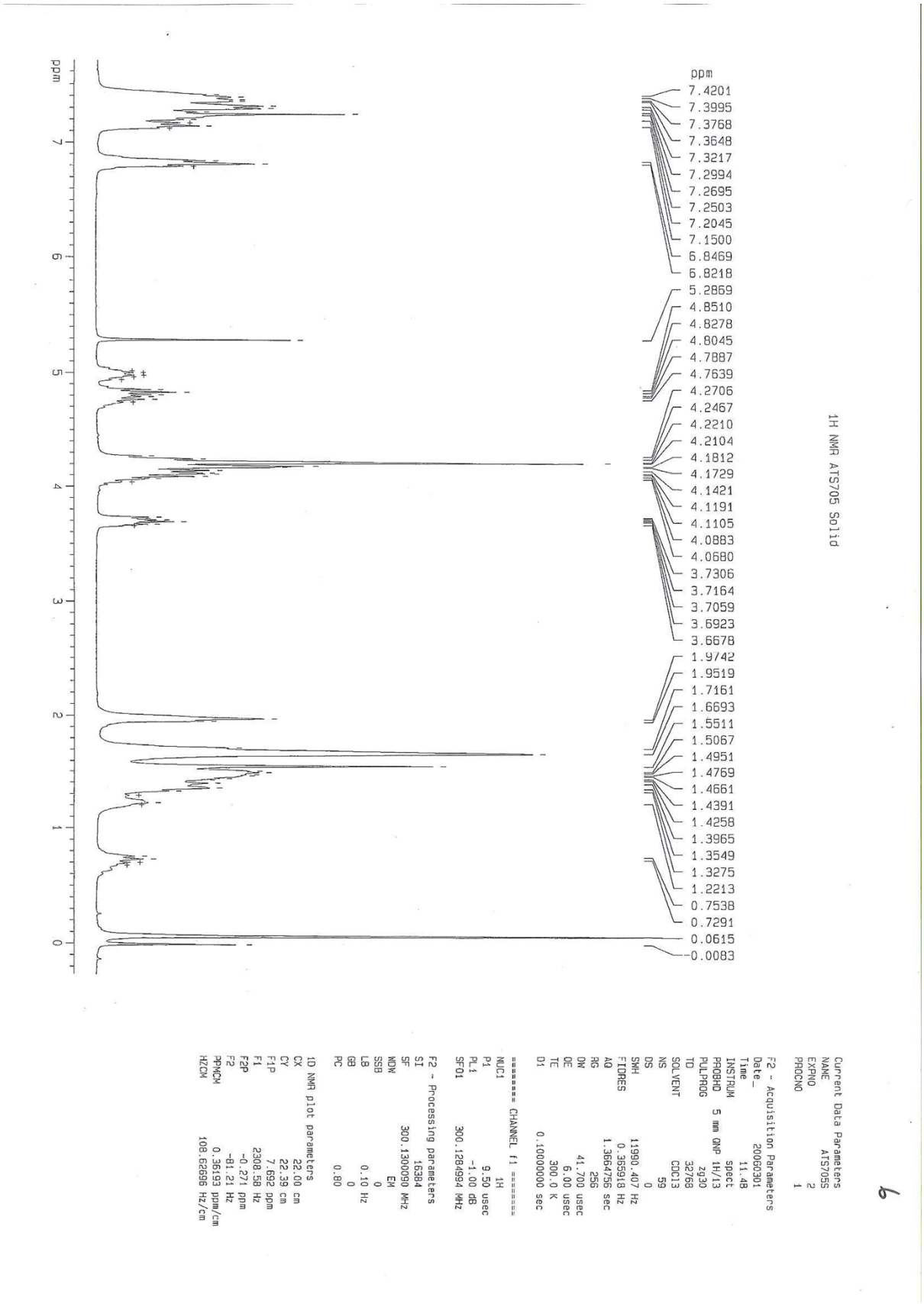


5

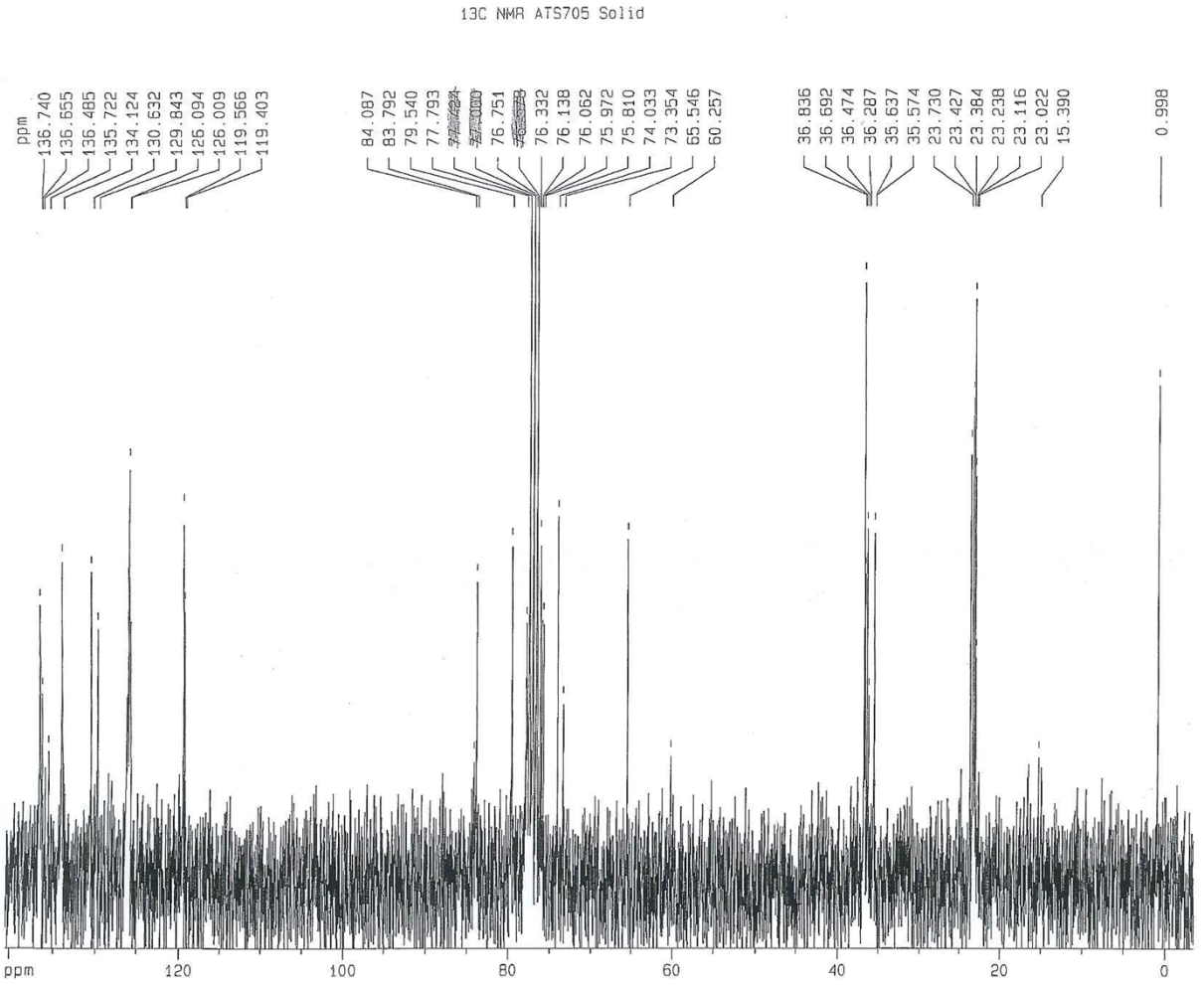



```
Current Data Parameters
NAME                 ATS319R2
EXPNO                       3
PROCNO                      1

F2 - Acquisition Parameters
Date_               20050616
Time                    1.54
INSTRUM                 spect
PROBHD   5 mm QNP 1H/13
PULPROG                 zgpg
TD                      65536
SOLVENT                 CDCl3
NS                        214
DS                          0
SWH                 17985.611 Hz
FIDRES                0.274439 Hz
AQ                    1.8219508 sec
RG                        16384
DW                       27.800 usec
DE                       20.00 usec
TE                       300.0 K
D1                  0.17593171 sec
d11                 0.03000000 sec
d12                 0.00002000 sec

======== CHANNEL f1 ========
NUC1                       13C
P1                        5.44 usec
PL1                       4.00 dB
SFO1                75.4760973 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                    102.00 usec
PL2                      120.00 dB
PL12                      20.20 dB
PL13                      25.80 dB
SFO2               300.1312005 MHz

F2 - Processing parameters
SI                        32768
SF                 75.4677510 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.00

1D NMR plot parameters
CX                       22.00 cm
CY                       11.34 cm
F1P                     229.755 ppm
F1                    17339.09 Hz
F2P                      -8.567 ppm
F2                     -646.52 Hz
PPMCM                  10.83281 ppm/cm
HZCM                  817.52783 Hz/cm
```

NMR spectra of $RuBr_2(D\text{-}P1)_2$ (**6**)



6



Current Data Parameters

NAME	ATS705S
EXPNO	4
PROCNO	1

F2 - Acquisition Parameters

Date_	20060301
Time	11.53
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg
TD	65536
SOLVENT	CDCl3
NS	316
DS	0
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	16384
DW	27.800 usec
DE	20.00 usec
TE	300.0 K
D1	0.17593171 sec
d11	0.03000000 sec
d12	0.00002000 sec

======== CHANNEL f1 ========

NUC1	13C
P1	5.44 usec
PL1	4.00 dB
SFO1	75.4760973 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	-1.00 dB
PL12	19.00 dB
PL13	25.20 dB
SFO2	300.1312005 MHz

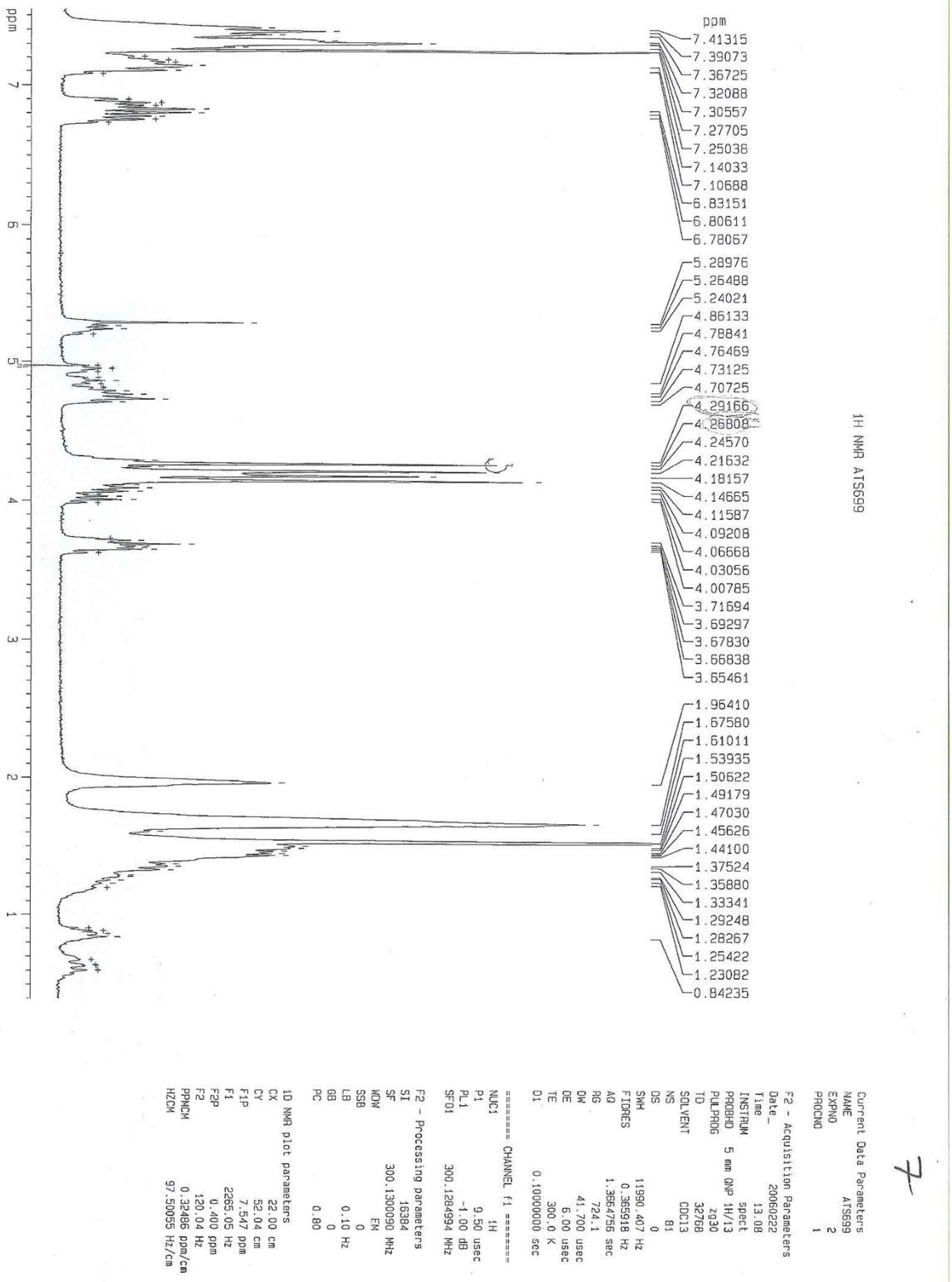
F2 - Processing parameters

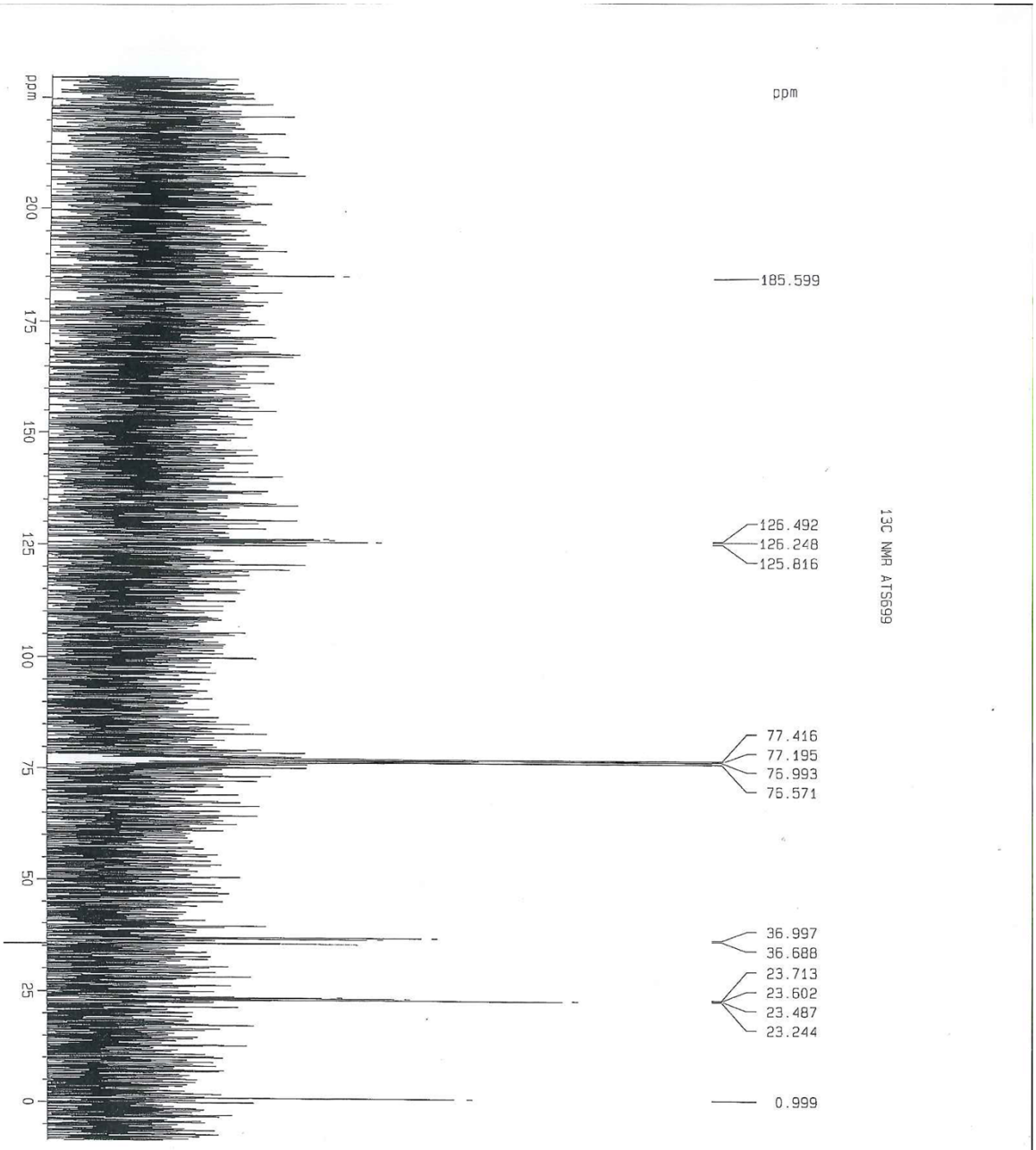
SI	32768
SF	75.4677499 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	22.00 cm
CY	48.29 cm
F1P	140.478 ppm
F1	10601.56 Hz
F2P	-3.476 ppm
F2	-262.31 Hz
PPMCM	6.54335 ppm/cm
HZCM	493.81207 Hz/cm

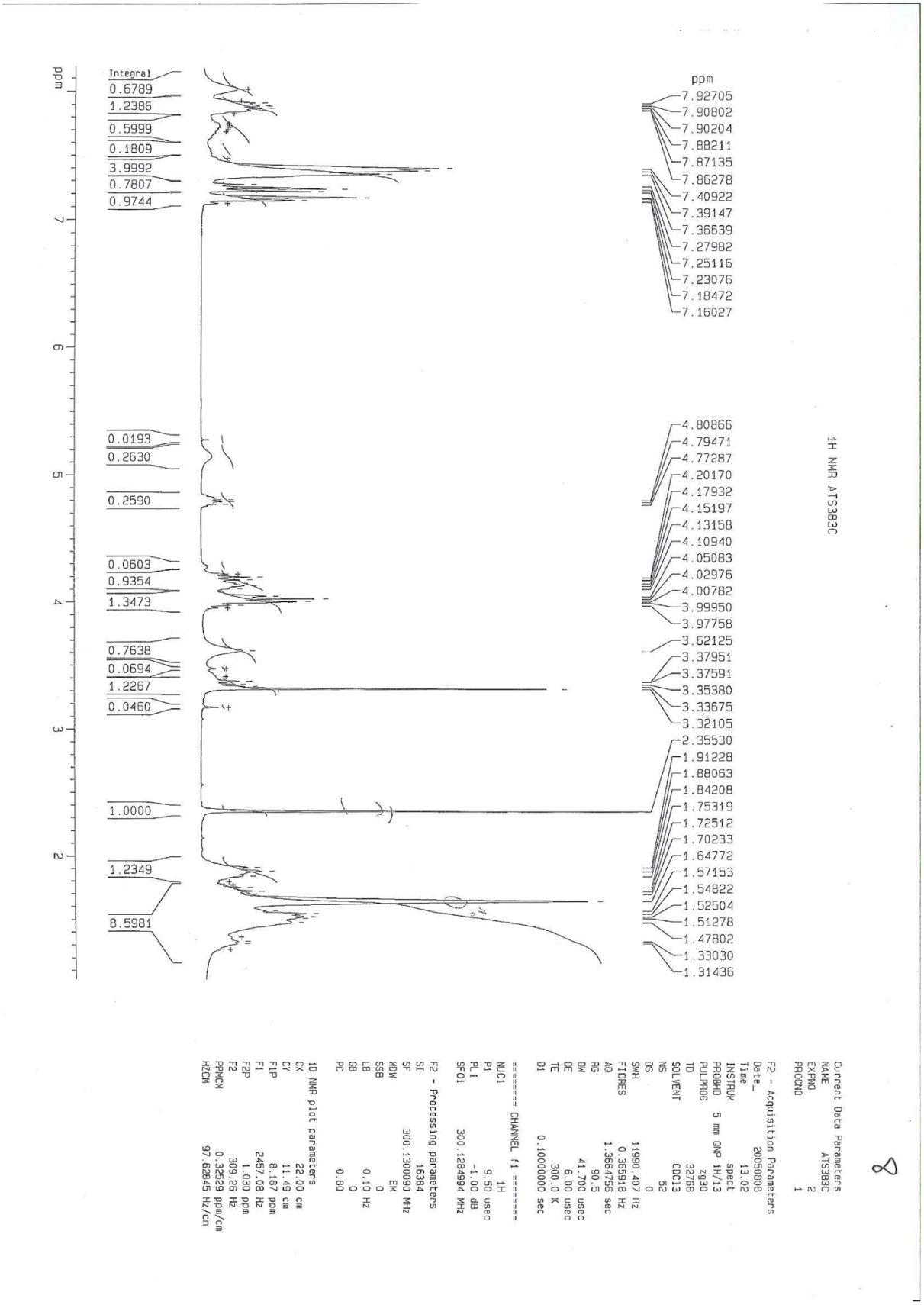
NMR spectra of RuI_2(D-P1)$_2$ (**7**)

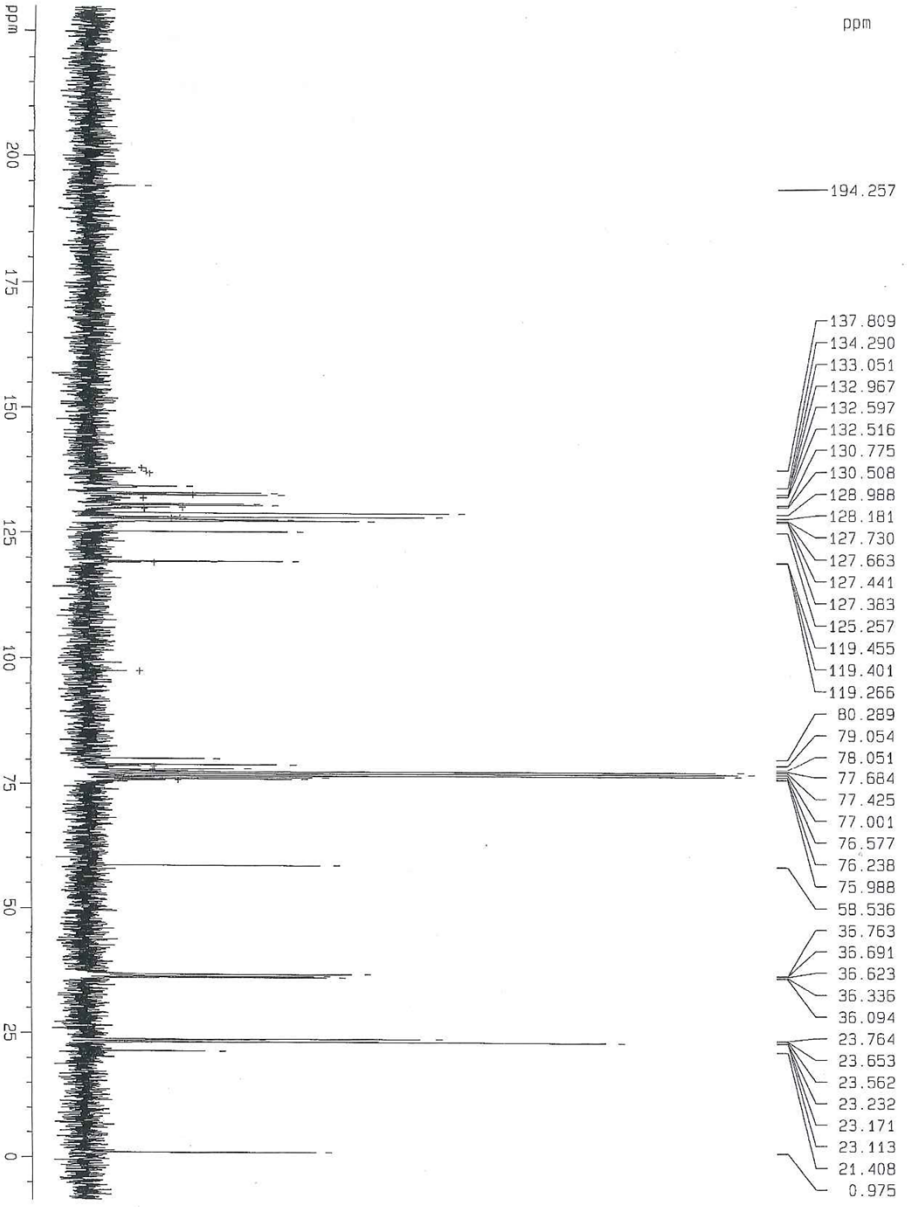





```
Current Data Parameters
NAME                  ATS699
EXPNO                      5
PROCNO                     1

F2 - Acquisition Parameters
Date_              20060222
Time                  13.38
INSTRUM                spect
PROBHD  5 mm QNP 1H/13
PULPROG                zgpg
TD                    65536
SOLVENT                CDCl3
NS                       800
DS                         0
SWH               17985.611 Hz
FIDRES                0.274439 Hz
AQ                1.8219508 sec
RG                       16384
DW                    27.800 usec
DE                    20.00 usec
TE                     300.0 K
D1                0.17593171 sec
d11               0.03000000 sec
d12               0.00002000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                     5.44 usec
PL1                    4.00 dB
SF01           75.4750973 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                100.00 usec
PL2                   -1.00 dB
PL12                  19.00 dB
PL13                  25.20 dB
SFO2           300.1312005 MHz

F2 - Processing parameters
SI                       32768
SF             75.4677499 MHz
WDW                         EM
SSB                          0
LB                    1.00 Hz
GB                           0
PC                        1.00

1D NMR plot parameters
CX                    22.00 cm
CY                    19.15 cm
F1P                  229.769 ppm
F1                 17340.19 Hz
F2P                   -8.552 ppm
F2                  -645.43 Hz
PPMCM                10.83281 ppm/cm
HZCM               817.52783 Hz/cm
```

NMR spectra of $RuCl_2(D\text{-}P1)_2(CO)_2$ (**8**)





Current Data Parameters
NAME ATS383C
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050808
Time 13.05
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 167
DS 0
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219608 sec
RG 16384
DW 27.800 usec
DE 20.00 usec
TE 300.0 K
D1 0.1759171 sec
d11 0.03000000 sec
d12 0.00002000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 5.44 usec
PL1 4.00 dB
SFO1 75.4760973 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -1.00 dB
PL12 19.00 dB
PL13 25.20 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677532 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
CY 11.82 cm
F1P 229.777 ppm
F1 17340.73 Hz
F2P -8.545 ppm
F2 -644.88 Hz
PPMCM 10.83281 ppm/cm
HZCM 817.52783 Hz/cm

8