Organo-Catalytic Asymmetric Conjugate Addition of Nitroalkanes to α,β -Unsaturated Enones Using Novel Imidazoline Catalysts

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Supporting Information

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X-Ray Structure of 4-(4-Chloro-Phenyl)-5-Methyl-5-Nitro-Hexan-2-One, 3j.

```

#      CCDC ELECTRONIC DATA DEPOSITION FORM (CIF, VERSION DEC95)

#      This electronic data deposition form must be associated with CIF
#      output and can be used :
#      (a) WHEN SUBMITTING A PAPER TO A JOURNAL FOR PUBLICATION or
#      (b) WHEN SUBMITTING A PRIVATE COMMUNICATION TO THE CCDC

#      A comprehensive archive of CIF resources is maintained by the IUCr
#      at its Chester office. This can be accessed
#      by anonymous ftp to ftp.iucr.ac.uk
#      or via the WWW at http://www.iucr.ac.uk/cif/home.html

#      If data items in this form are not available or not applicable
#      then ignore these items

#      A few items specific to CCDC input are indicated by _ccdc_

#      Submission and help information is provided at the end of this for
#-----
#1      Data block identification for start of deposition
data_cpd-3j
#-----
#2      Person making the deposition

_publ_contact_author      'Rita Hazell'
_publ_contact_author_email      haz@chem.au.dk
#-----
#3      Publication details

#      Provide these details if the structure has been published,
#      accepted or submitted for publication

#      The CCDC journal deposition number, eg. 182/357,
#      should be included only if it has been assigned by the journal

loop
  _publ_author_name
  'Nis Halland'
  'Rita Hazell'
  'Karl Anker Jorgensen'

  _journal_name_full      'J. Org. Chem.'
  _journal_volume      '?'
  _journal_page_first      '?'
  _journal_page_last      '?'
  _journal_year      '2002'
  _ccdc_journal_depnumber      '?'

#=====
# 4. TEXT

_publ_section_references
;
Altomare,A., Cascarano,G., Giacovazzo,C., Guagliardi,A.,

```

Moliterni, A.G.G., Burla, M.C., Polidori, G., Camalli, M.
& Spagna, R. (1997). SIR97. University of Bari, Italy.

Becker, P.J. & Coppens, P. (1974). Acta Cryst. A30, 129-153.

Burnett, M.N. & Johnson, C.K. (1996). ORTEP-III. Report ORNL-6895.
Oak Ridge National Laboratory, Tennessee, USA.

Busing, W.R., Martin, K.O. & Levy, H.A. (1962). ORFLS. Report
ORNL-TM-305. Oak Ridge National Laboratory, Tennessee, USA.

Hazell, A. (1995). KRYSTAL, An integrated system of
crystallographic programs. Aarhus University, Denmark.

Rogers, D. (1981). Acta Cryst. A37, 734-741.

Siemens (1995) SMART, SAINT and XPREP Area-Detector Control and
Integration Software. Siemens Analytical X-ray Instruments Inc.
Madison, Wisconsin, USA.

#=====

data_cpd-3j

#=====

5. CHEMICAL DATA

_chemical_name_systematic

;

4-(4-Chloro-phenyl)-5-methyl-5-nitro-hexan-2-one

;

_chemical_formula_sum C13H16ClNO3

_chemical_formula_weight 269.74

#=====

6. CRYSTAL DATA

_symmetry_cell_setting

orthorhombic

_symmetry_space_group_name_H-M

'P212121'

loop_

_symmetry_equiv_pos_as_xyz

'+x,+y,+z'

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

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

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

_cell_length_a

5.975(2)

_cell_length_b

10.869(4)

_cell_length_c

20.746(8)

_cell_angle_alpha

90.000

_cell_angle_beta

90.000

_cell_angle_gamma

90.000

_cell_volume

1347(1)

_cell_formula_units_Z

4

_cell_measurement_temperature

120

_cell_measurement_reflns_used

6339

_cell_measurement_theta_min

2.1

_cell_measurement_theta_max

26.3

_exptl_crystal_description

needle

_exptl_crystal_colour

colourless

_exptl_crystal_size_max

0.44

_exptl_crystal_size_mid

0.12

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_exptl_crystal_size_min          0.06
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_exptl_crystal_density_diffn     1.330
_exptl_crystal_density_method    'not measured'
_exptl_crystal_F_000             568
_exptl_absorpt_coefficient_mu     0.283
_exptl_absorpt_correction_type    'none'

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# 7. EXPERIMENTAL DATA

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_diffn_radiation_monochromator    'graphite'
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_diffn_reflns_limit_l_min        -24
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_diffn_reflns_theta_max          27.0
_diffn_reflns_reduction_process   19398
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_computing_data_reduction        'SAINT (Siemens, 1995)'
_computing_structure_solution
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_computing_molecular_graphics
;
      ORTEP-III (Burnett & Johnson, 1996), KRYSTAL
;
_computing_publication_material   KRYSTAL
_atom_type_scatter_source         IntTabIV

#=====

# 8. REFINEMENT DATA

_refine_ls_structure_factor_coef   F
_refine_ls_matrix_type             full
_refine_ls_weighting_scheme        calc
_refine_ls_weighting_details
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w= 1/{[\sigma^2(F^2)+1.03F^2]^1/2+|F|}^2
;
_refine_ls_hydrogen_treatment      refall
_refine_ls_extinction_method
;
      Type 1 Lorentzian isotropic (Becker and Coppens, 1974)
;

```

```

_refine_ls_extinction_coef      103(17)
_refine_ls_abs_structure_details
; Least squares refinement included a factor according to Rogers
(1982). The 2107 significant reflections used included 826
Bijvoet pairs.
;
_refine_ls_abs_structure_Rogers  0.83(15)
_refine_ls_number_reflms        2107
_refine_ls_number_parameters     229
_refine_ls_number_restraints     0
_refine_ls_number_constraints    0
_refine_ls_R_factor_gt          0.039
_refine_ls_wR_factor_ref        0.041
_refine_ls_goodness_of_fit_ref   1.25
_refine_ls_shift/su_max         0.0010
_refine_ls_shift/su_mean        0.0001
_refine_diff_density_max        0.47(8)
_refine_diff_density_min       -0.45(8)

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#=====

9. ATOMIC COORDINATES AND THERMAL PARAMETERS

```

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_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_thermal_displace_type
CL1      0.0406(1)  -0.08628(6)  0.45928(4)  0.0336(4)  Uij
O2       -0.4569(3) -0.4202(2)   0.22104(9)  0.033(1)   Uij
C3       -0.2822(4) -0.5519(2)   0.3301(1)   0.019(1)   Uij
O4       -0.1166(4) -0.3639(2)   0.2078(1)   0.044(1)   Uij
C5       -0.0596(5) -0.2239(2)   0.4260(1)   0.023(1)   Uij
N6       -0.2556(4) -0.4361(2)   0.2275(1)   0.022(1)   Uij
C7       -0.1787(4) -0.5560(2)   0.2607(1)   0.021(1)   Uij
C8       -0.3392(4) -0.3358(2)   0.3689(1)   0.020(1)   Uij
C9       -0.2686(5) -0.2270(2)   0.3981(1)   0.023(1)   Uij
C10      -0.4365(5) -0.7115(2)   0.4085(1)   0.026(1)   Uij
C11      -0.2798(5) -0.6572(3)   0.2193(2)   0.027(2)   Uij
O12      -0.5984(4) -0.6467(2)   0.4160(1)   0.052(1)   Uij
C13      -0.2047(4) -0.4401(2)   0.3678(1)   0.020(1)   Uij
C14       0.0755(5) -0.3274(3)   0.4284(1)   0.026(2)   Uij
C15       0.0027(4) -0.4349(2)   0.3994(1)   0.024(1)   Uij
C16      -0.2463(5) -0.6752(2)   0.3648(2)   0.026(2)   Uij
C17       0.0759(5) -0.5597(3)   0.2590(2)   0.027(2)   Uij
C18      -0.4160(6) -0.8340(3)   0.4416(2)   0.040(2)   Uij
H3       -0.434(4)  -0.546(2)    0.324(1)    0.010(6)   Uiso
H8       -0.487(4)  -0.340(2)    0.348(1)   -0.001(5)   Uiso
H9       -0.357(4)  -0.151(2)    0.397(1)    0.025(7)   Uiso
H11a     -0.244(5)  -0.646(2)    0.171(2)    0.031(8)   Uiso
H11b     -0.208(5)  -0.725(3)    0.230(2)    0.045(10)  Uiso
H11c     -0.439(6)  -0.664(3)    0.226(1)    0.039(8)   Uiso
H14       0.211(4)  -0.322(2)    0.447(1)    0.015(7)   Uiso
H15       0.097(5)  -0.505(2)    0.402(1)    0.014(6)   Uiso
H16a     -0.211(6)  -0.742(3)    0.334(2)    0.052(10)  Uiso
H16b     -0.124(5)  -0.678(2)    0.391(1)    0.027(8)   Uiso
H17a      0.126(4)  -0.559(2)    0.213(1)    0.027(8)   Uiso
H17b      0.140(5)  -0.488(3)    0.282(1)    0.034(8)   Uiso
H17c      0.123(6)  -0.635(3)    0.285(1)    0.053(10)  Uiso
H18a     -0.570(8)  -0.868(4)    0.459(2)    0.084(12)  Uiso
H18b     -0.367(7)  -0.900(4)    0.411(2)    0.081(13)  Uiso

```

H18c -0.339(7) -0.821(4) 0.477(2) 0.077(15) Uiso

```

loop_
  _atom_site_aniso_label
  _atom_site_aniso_U_11
  _atom_site_aniso_U_22
  _atom_site_aniso_U_33
  _atom_site_aniso_U_12
  _atom_site_aniso_U_13
  _atom_site_aniso_U_23
CL1  0.0360(4)  0.0278(3)  0.0371(4) -0.0069(3) -0.0014(3) -0.0080(3)
O2   0.024(1)  0.034(1)   0.042(1)  0.005(1)  -0.001(1)  0.011(1)
C3   0.008(1)  0.020(1)   0.030(2)  0.003(1)  0.000(1)  0.005(1)
O4   0.036(1)  0.035(1)   0.061(2) -0.015(1)  0.001(1)  0.017(1)
C5   0.025(1)  0.021(1)   0.022(1) -0.003(1)  0.000(1) -0.004(1)
N6   0.024(1)  0.018(1)   0.025(1) -0.004(1)  0.002(1) -0.003(1)
C7   0.015(1)  0.016(1)   0.032(2)  0.000(1)  0.001(1) -0.002(1)
C8   0.019(1)  0.020(1)   0.020(2)  0.004(1) -0.002(1)  0.001(1)
C9   0.025(1)  0.018(1)   0.026(2)  0.006(1)  0.003(1)  0.001(1)
C10  0.028(1)  0.020(1)   0.029(2)  0.005(1)  0.002(1)  0.004(1)
C11  0.018(2)  0.025(2)   0.040(2) -0.002(1)  0.000(1) -0.008(1)
O12  0.039(1)  0.046(1)   0.071(2)  0.024(1)  0.032(1)  0.029(1)
C13  0.017(1)  0.021(1)   0.021(1)  0.003(1)  0.004(1)  0.002(1)
C14  0.014(1)  0.037(2)   0.027(2)  0.002(1) -0.002(1) -0.003(1)
C15  0.018(1)  0.025(1)   0.028(2)  0.007(1)  0.002(1)  0.000(1)
C16  0.017(1)  0.021(1)   0.039(2)  0.007(1) -0.001(1)  0.006(1)
C17  0.019(1)  0.029(2)   0.034(2) -0.001(1)  0.005(1) -0.006(1)
C18  0.043(2)  0.029(2)   0.047(2)  0.002(2)  0.001(2)  0.016(2)

```

#=====

10. MOLECULAR GEOMETRY

```

loop_
  _geom_bond_atom_site_label_1
  _geom_bond_atom_site_label_2
  _geom_bond_distance
CL1  C5      1.753(3)
O2   N6      1.222(3)
C3   C13     1.517(4)
C3   C16     1.537(4)
C3   C7      1.567(4)
O4   N6      1.213(3)
C5   C9      1.376(4)
C5   C14     1.385(4)
N6   C7      1.544(4)
C7   C11     1.521(4)
C7   C17     1.522(4)
C8   C13     1.390(4)
C8   C9      1.393(4)
C10  O12     1.207(3)
C10  C18     1.503(4)
C10  C16     1.507(4)
C13  C15     1.403(4)
C14  C15     1.385(4)
C3   H3      0.921(25)
C8   H8      0.984(21)
C9   H9      0.984(26)
C11  H11b    0.886(33)
C11  H11c    0.966(34)
C11  H11a    1.031(31)
C14  H14     0.899(26)
C15  H15     0.947(27)
C16  H16b    0.914(29)

```

C16	H16a	0.984 (34)
C17	H17b	0.991 (30)
C17	H17a	0.994 (28)
C17	H17c	1.023 (35)
C18	H18c	0.873 (42)
C18	H18b	1.000 (44)
C18	H18a	1.058 (49)

```

loop_
  _geom_angle_atom_site_label_1
  _geom_angle_atom_site_label_2
  _geom_angle_atom_site_label_3
  _geom_angle
C13      C3      C16      114.5 (2)
C7       C3      C13      112.0 (2)
C7       C3      C16      110.5 (2)
C9       C5      C14      121.6 (3)
CL1      C5      C9       119.7 (2)
CL1      C5      C14      118.6 (2)
O2       N6      O4       123.1 (2)
O4       N6      C7       119.5 (2)
O2       N6      C7       117.4 (2)
C11      C7      C17      111.3 (2)
N6       C7      C11      103.9 (2)
C3       C7      C11      112.5 (2)
N6       C7      C17      108.0 (2)
C3       C7      C17      114.7 (2)
C3       C7      N6       105.6 (2)
C9       C8      C13      121.6 (2)
C5       C9      C8       118.6 (3)
O12      C10     C18      121.6 (3)
O12      C10     C16      121.9 (2)
C16      C10     C18      116.4 (3)
C8       C13     C15      118.0 (2)
C3       C13     C8       119.1 (2)
C3       C13     C15      122.8 (2)
C5       C14     C15      119.1 (3)
C13      C15     C14      121.0 (2)
C3       C16     C10      113.9 (2)
C13      C3      H3       108.9 (15)
C16      C3      H3       105.1 (15)
C7       C3      H3       105.1 (15)
C13      C8      H8       118.6 (12)
C9       C8      H8       119.8 (12)
C5       C9      H9       118.5 (16)
C8       C9      H9       122.8 (16)
H11b     C11     H11c     112.1 (28)
H11a     C11     H11b     103.9 (26)
C7       C11     H11b     105.8 (22)
H11a     C11     H11c     111.3 (24)
C7       C11     H11c     111.1 (18)
C7       C11     H11a     112.3 (15)
C15      C14     H14      121.5 (16)
C5       C14     H14      119.4 (16)
C14      C15     H15      117.9 (15)
C13      C15     H15      121.1 (15)
H16a     C16     H16b     100.9 (26)
C10      C16     H16b     103.8 (18)
C3       C16     H16b     114.5 (17)
C10      C16     H16a     110.7 (20)
C3       C16     H16a     112.0 (19)
H17a     C17     H17b     110.1 (23)
H17b     C17     H17c     104.9 (24)
C7       C17     H17b     110.8 (17)

```


H17a	C17	H17c	115.6(25)
C7	C17	H17a	108.9(16)
C7	C17	H17c	106.4(20)
H18b	C18	H18c	120(4)
H18a	C18	H18c	102.7(32)
C10	C18	H18c	106.3(30)
H18a	C18	H18b	103.5(30)
C10	C18	H18b	111.3(23)
C10	C18	H18a	113.2(22)

#=====

data_cpd-5b

#=====

5. CHEMICAL DATA

_chemical_name_systematic
;
 cis-5-Methyl-2,3-diphenyl-pyrrolidine
;
 _chemical_formula_sum C17H19N
_chemical_formula_weight 237.35

#=====

6. CRYSTAL DATA

_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P21/n'

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

_cell_length_a	13.7301(8)
_cell_length_b	6.1319(4)
_cell_length_c	16.064(1)
_cell_angle_alpha	90.000
_cell_angle_beta	102.584(1)
_cell_angle_gamma	90.000
_cell_volume	1320.0(1)
_cell_formula_units_Z	4
_cell_measurement_temperature	120
_cell_measurement_reflns_used	4884
_cell_measurement_theta_min	2.6
_cell_measurement_theta_max	29.8
_exptl_crystal_description	'thick plate'
_exptl_crystal_colour	colourless
_exptl_crystal_size_max	0.54
_exptl_crystal_size_mid	0.40
_exptl_crystal_size_min	0.16
_exptl_crystal_density_meas	'not measured'
_exptl_crystal_density_diffn	1.194
_exptl_crystal_density_method	'not measured'
_exptl_crystal_F_000	512
_exptl_absorpt_coefficient_mu	0.069
_exptl_absorpt_correction_type	'none'

#=====

``` # 7. EXPERIMENTAL DATA ```

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_diffn_ambient_temperature      120
_diffn_radiation_wavelength     0.71073
_diffn_radiation_type           'Mo K\alpha'
_diffn_radiation_source         'x-ray tube'
_diffn_radiation_monochromator   'graphite'
_diffn_measurement_device       'Siemens SMART CCD diffractometer'
_diffn_measurement_method       '\omega rotation scans with narrow frames'
_diffn_reflns_number            12427
_diffn_reflns_av_R_equivalents  0.052
_diffn_reflns_limit_h_min       -19
_diffn_reflns_limit_h_max       19
_diffn_reflns_limit_k_min       -8
_diffn_reflns_limit_k_max       8
_diffn_reflns_limit_l_min       -22
_diffn_reflns_limit_l_max       19
_diffn_reflns_theta_min         2.6
_diffn_reflns_theta_max         29.8
_diffn_reflns_reduction_process 12427
_reflns_number_total            4078
_reflns_number_gt               2695
_reflns_threshold_expression     I>3\sigma(I)
_computing_data_collection       'SMART (Siemens, 1995)'
_computing_cell_refinement       'SAINT (Siemens, 1995)'
_computing_data_reduction       'SAINT (Siemens, 1995)'
_computing_structure_solution
;
    SIR97 (Altomare et al., 1997), KRYSTAL
;
_computing_structure_refinement  'modified ORFLS(1962), KRYSTAL'
_computing_molecular_graphics
;
    ORTEP-III (Burnett & Johnson, 1996), KRYSTAL
;
_computing_publication_material  KRYSTAL
_atom_type_scatter_source        IntTabIV
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#=====
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``` # 8. REFINEMENT DATA ```

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_refine_ls_structure_factor_coef F
_refine_ls_matrix_type           full
_refine_ls_weighting_scheme      calc
_refine_ls_weighting_details
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w= 1/{[\sigma^2(F^2)+1.03F^2]}^1/2+ |F|^2
;
_refine_ls_hydrogen_treatment    reffall
_refine_ls_extinction_method
;
    Type 1 Lorentzian isotropic (Becker and Coppens, 1974)
;
_refine_ls_extinction_coef       34(13)
_refine_ls_number_reflns        2695
_refine_ls_number_parameters     240
_refine_ls_number_restraints     0
_refine_ls_number_constraints    0
_refine_ls_R_factor_gt           0.038
_refine_ls_wR_factor_ref         0.047
_refine_ls_goodness_of_fit_ref   1.48
_refine_ls_shift/su_max          0.0003
_refine_ls_shift/su_mean         0.00003
```

```

_refine_diff_density_max          0.34(4)
_refine_diff_density_min          -0.22(4)
#=====

data_cpd-5b

#=====

# 5. CHEMICAL DATA

_chemical_name_systematic
;
cis-5-Methyl-2,3-diphenyl-pyrrolidine
;
_chemical_formula_sum              C17H19N
_chemical_formula_weight           237.35
#=====

# 6. CRYSTAL DATA

_symmetry_cell_setting             monoclinic
_symmetry_space_group_name_H-M    'P21/n'

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

_cell_length_a                     13.7301(8)
_cell_length_b                     6.1319(4)
_cell_length_c                     16.064(1)
_cell_angle_alpha                  90.000
_cell_angle_beta                   102.584(1)
_cell_angle_gamma                  90.000
_cell_volume                       1320.0(1)
_cell_formula_units_Z              4
_cell_measurement_temperature      120
_cell_measurement_reflns_used      4884
_cell_measurement_theta_min        2.6
_cell_measurement_theta_max        29.8
_exptl_crystal_description         'thick plate'
_exptl_crystal_colour              colourless
_exptl_crystal_size_max            0.54
_exptl_crystal_size_mid            0.40
_exptl_crystal_size_min            0.16
_exptl_crystal_density_meas        'not measured'
_exptl_crystal_density_diffn       1.194
_exptl_crystal_density_method      'not measured'
_exptl_crystal_F_000               512
_exptl_absorpt_coefficient_mu       0.069
_exptl_absorpt_correction_type     'none'
#=====

# 7. EXPERIMENTAL DATA

_diffn_ambient_temperature         120
_diffn_radiation_wavelength        0.71073
_diffn_radiation_type              'Mo K\alpha'
_diffn_radiation_source             'x-ray tube'
_diffn_radiation_monochromator      'graphite'
_diffn_measurement_device           'Siemens SMART CCD diffractometer'

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_diffrn_measurement_method      '\w rotation scans with narrow frames'
_diffrn_reflms_number           12427
_diffrn_reflms_av_R_equivalents 0.052
_diffrn_reflms_limit_h_min      -19
_diffrn_reflms_limit_h_max      19
_diffrn_reflms_limit_k_min      -8
_diffrn_reflms_limit_k_max      8
_diffrn_reflms_limit_l_min      -22
_diffrn_reflms_limit_l_max      19
_diffrn_reflms_theta_min        2.6
_diffrn_reflms_theta_max        29.8
_diffrn_reflms_reduction_process 12427
_reflms_number_total            4078
_reflms_number_gt               2695
_reflms_threshold_expression     I>3\s(I)
_computing_data_collection      'SMART (Siemens, 1995)'
_computing_cell_refinement      'SAINT (Siemens, 1995)'
_computing_data_reduction       'SAINT (Siemens, 1995)'
_computing_structure_solution
;
    SIR97 (Altomare et al., 1997 ), KRYSTAL
;
_computing_structure_refinement 'modified ORFLS(1962), KRYSTAL'
_computing_molecular_graphics
;
    ORTEP-III (Burnett & Johnson, 1996), KRYSTAL
;
_computing_publication_material KRYSTAL
_atom_type_scatter_source       IntTabIV

#=====

# 8. REFINEMENT DATA

_refine_ls_structure_factor_coef F
_refine_ls_matrix_type          full
_refine_ls_weighting_scheme     calc
_refine_ls_weighting_details
;
w= 1/{ [\s~cs~(F^2^)+1.03F^2^]^1/2^- |F| }^2^
;
_refine_ls_hydrogen_treatment   reffall
_refine_ls_extinction_method
;
    Type 1 Lorentzian isotropic (Becker and Coppens, 1974)
;
_refine_ls_extinction_coef      34(13)
_refine_ls_number_reflms       2695
_refine_ls_number_parameters    240
_refine_ls_number_restraints    0
_refine_ls_number_constraints    0
_refine_ls_R_factor_gt         0.038
_refine_ls_wR_factor_ref       0.047
_refine_ls_goodness_of_fit_ref  1.48
_refine_ls_shift/su_max         0.0003
_refine_ls_shift/su_mean        0.00003
_refine_diff_density_max        0.34(4)
_refine_diff_density_min        -0.22(4)

#=====

# 9. ATOMIC COORDINATES AND THERMAL PARAMETERS

loop_

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_atom_site_label	_atom_site_fract_x	_atom_site_fract_y	_atom_site_fract_z	_atom_site_U_iso_or_equiv	_atom_site_thermal_displace_type
N1	0.61769(7)	-0.0354(2)	0.41675(6)	0.0212(5)	Uij
C1	0.78113(10)	-0.2081(2)	0.41733(9)	0.0300(7)	Uij
C2	0.72525(8)	0.0019(2)	0.42377(7)	0.0221(6)	Uij
C3	0.72646(8)	0.1663(2)	0.35199(8)	0.0242(6)	Uij
C4	0.62267(8)	0.2758(2)	0.33229(7)	0.0202(6)	Uij
C5	0.57518(8)	0.1845(2)	0.40502(7)	0.0200(6)	Uij
C6	0.46283(8)	0.1957(2)	0.38791(7)	0.0198(6)	Uij
C7	0.40192(9)	0.0193(2)	0.35744(7)	0.0229(6)	Uij
C8	0.29847(9)	0.0402(2)	0.34062(8)	0.0260(6)	Uij
C9	0.25527(9)	0.2379(2)	0.35311(8)	0.0272(6)	Uij
C10	0.31516(9)	0.4151(2)	0.38325(8)	0.0269(7)	Uij
C11	0.41819(9)	0.3938(2)	0.40037(7)	0.0236(6)	Uij
C12	0.56049(7)	0.2271(2)	0.24422(7)	0.0189(5)	Uij
C13	0.55690(9)	0.0200(2)	0.20775(7)	0.0225(6)	Uij
C14	0.49809(9)	-0.0199(2)	0.12720(8)	0.0252(6)	Uij
C15	0.44131(9)	0.1454(2)	0.08197(8)	0.0260(6)	Uij
C16	0.44368(9)	0.3513(2)	0.11757(8)	0.0267(6)	Uij
C17	0.50273(8)	0.3912(2)	0.19810(8)	0.0234(6)	Uij
H1n	0.6062(10)	-0.098(2)	0.4650(9)	0.031(4)	Uiso
H1a	0.8506(11)	-0.176(2)	0.4226(9)	0.040(4)	Uiso
H1b	0.7555(10)	-0.280(2)	0.3606(10)	0.035(4)	Uiso
H1c	0.7740(11)	-0.313(2)	0.4631(10)	0.046(4)	Uiso
H2	0.7538(9)	0.075(2)	0.4797(8)	0.025(3)	Uiso
H3a	0.7407(10)	0.092(2)	0.3016(9)	0.039(4)	Uiso
H3b	0.7811(10)	0.277(2)	0.3688(9)	0.036(4)	Uiso
H4	0.6296(9)	0.436(2)	0.3388(8)	0.025(3)	Uiso
H5	0.6023(8)	0.275(2)	0.4564(8)	0.017(3)	Uiso
H7	0.4327(9)	-0.123(2)	0.3497(8)	0.023(3)	Uiso
H8	0.2562(10)	-0.081(2)	0.3190(8)	0.029(3)	Uiso
H9	0.1841(10)	0.257(2)	0.3398(9)	0.034(4)	Uiso
H10	0.2848(10)	0.556(2)	0.3916(9)	0.037(4)	Uiso
H11	0.4598(9)	0.520(2)	0.4202(8)	0.023(3)	Uiso
H13	0.5963(9)	-0.099(2)	0.2381(8)	0.025(3)	Uiso
H14	0.4970(10)	-0.165(2)	0.1023(9)	0.034(4)	Uiso
H15	0.3998(9)	0.119(2)	0.0255(8)	0.028(3)	Uiso
H16	0.4040(10)	0.468(2)	0.0864(9)	0.032(4)	Uiso
H17	0.5042(10)	0.540(2)	0.2230(8)	0.030(4)	Uiso

loop	_atom_site_aniso_label	_atom_site_aniso_U_11	_atom_site_aniso_U_22	_atom_site_aniso_U_33	_atom_site_aniso_U_12	_atom_site_aniso_U_13	_atom_site_aniso_U_23
N1	0.0203(5)	0.0238(5)	0.0203(5)	0.0024(4)	0.0063(4)	0.0045(4)	
C1	0.0252(6)	0.0340(7)	0.0322(7)	0.0069(5)	0.0089(5)	0.0033(6)	
C2	0.0185(5)	0.0278(6)	0.0191(5)	0.0009(4)	0.0023(4)	0.0000(5)	
C3	0.0186(5)	0.0284(6)	0.0256(6)	-0.0024(5)	0.0044(4)	0.0029(5)	
C4	0.0201(5)	0.0186(5)	0.0211(6)	-0.0028(4)	0.0024(4)	0.0002(4)	
C5	0.0204(5)	0.0215(6)	0.0176(5)	0.0004(4)	0.0032(4)	-0.0022(4)	
C6	0.0213(5)	0.0238(6)	0.0150(5)	0.0010(4)	0.0056(4)	0.0006(4)	
C7	0.0242(6)	0.0227(6)	0.0231(6)	0.0010(5)	0.0076(4)	-0.0017(5)	
C8	0.0241(6)	0.0298(6)	0.0243(6)	-0.0042(5)	0.0057(5)	0.0003(5)	
C9	0.0205(6)	0.0358(7)	0.0258(6)	0.0037(5)	0.0065(5)	0.0057(5)	
C10	0.0283(6)	0.0265(6)	0.0274(6)	0.0081(5)	0.0090(5)	0.0033(5)	
C11	0.0267(6)	0.0224(6)	0.0217(6)	0.0003(5)	0.0054(4)	-0.0007(5)	

C12	0.0168(5)	0.0217(5)	0.0194(5)	-0.0034(4)	0.0064(4)	0.0013(4)
C13	0.0248(6)	0.0209(6)	0.0227(6)	-0.0004(4)	0.0071(4)	0.0019(5)
C14	0.0283(6)	0.0245(6)	0.0245(6)	-0.0058(5)	0.0094(5)	-0.0039(5)
C15	0.0215(5)	0.0352(7)	0.0205(6)	-0.0053(5)	0.0030(4)	-0.0013(5)
C16	0.0219(6)	0.0314(7)	0.0252(6)	0.0028(5)	0.0014(5)	0.0034(5)
C17	0.0229(5)	0.0226(6)	0.0245(6)	0.0014(4)	0.0047(4)	-0.0005(5)

#=====

10. MOLECULAR GEOMETRY

loop_
 _geom_bond_atom_site_label_1
 _geom_bond_atom_site_label_2
 _geom_bond_distance

N1	C5	1.465(2)
N1	C2	1.474(2)
C1	C2	1.514(2)
C2	C3	1.534(2)
C3	C4	1.545(2)
C4	C12	1.514(2)
C4	C5	1.561(2)
C5	C6	1.508(2)
C6	C7	1.390(2)
C6	C11	1.395(2)
C7	C8	1.393(2)
C8	C9	1.383(2)
C9	C10	1.385(2)
C10	C11	1.387(2)
C12	C17	1.391(2)
C12	C13	1.395(2)
C13	C14	1.390(2)
C14	C15	1.385(2)
C15	C16	1.383(2)
C16	C17	1.390(2)
N1	H1n	0.910(15)
C1	H1a	0.959(15)
C1	H1c	0.998(17)
C1	H1b	1.005(15)
C2	H2	1.003(13)
C3	H3a	0.985(16)
C3	H3b	1.003(14)
C4	H4	0.990(14)
C5	H5	0.997(12)
C7	H7	0.990(14)
C8	H8	0.961(14)
C9	H9	0.960(14)
C10	H10	0.983(15)
C11	H11	0.973(13)
C13	H13	0.973(13)
C14	H14	0.972(15)
C15	H15	0.974(13)
C16	H16	0.971(14)
C17	H17	0.997(14)

loop_
 _geom_angle_atom_site_label_1
 _geom_angle_atom_site_label_2
 _geom_angle_atom_site_label_3
 _geom_angle

C2	N1	C5	103.39(9)
N1	C2	C1	112.2(1)
N1	C2	C3	102.65(9)
C1	C2	C3	114.7(1)

C2	C3	C4	106.2(1)
C3	C4	C12	114.4(1)
C5	C4	C12	112.73(9)
C3	C4	C5	102.01(9)
N1	C5	C6	115.4(1)
N1	C5	C4	101.92(9)
C4	C5	C6	115.13(9)
C7	C6	C11	118.6(1)
C5	C6	C7	122.8(1)
C5	C6	C11	118.5(1)
C6	C7	C8	120.4(1)
C7	C8	C9	120.3(1)
C8	C9	C10	119.8(1)
C9	C10	C11	119.9(1)
C6	C11	C10	121.0(1)
C13	C12	C17	118.1(1)
C4	C12	C17	119.7(1)
C4	C12	C13	122.2(1)
C12	C13	C14	120.8(1)
C13	C14	C15	120.4(1)
C14	C15	C16	119.4(1)
C15	C16	C17	120.1(1)
C12	C17	C16	121.2(1)
C5	N1	H1n	111.1(9)
C2	N1	H1n	110.9(8)
H1a	C1	H1c	108.9(12)
H1a	C1	H1b	108.4(12)
C2	C1	H1a	109.0(9)
H1b	C1	H1c	108.1(12)
C2	C1	H1c	111.5(9)
C2	C1	H1b	110.8(8)
N1	C2	H2	109.1(7)
C1	C2	H2	109.6(7)
C3	C2	H2	108.3(8)
H3a	C3	H3b	105.2(12)
C2	C3	H3a	110.6(9)
C4	C3	H3a	111.8(8)
C2	C3	H3b	111.7(8)
C4	C3	H3b	111.3(8)
C12	C4	H4	108.4(7)
C3	C4	H4	110.3(8)
C5	C4	H4	108.9(8)
N1	C5	H5	109.8(7)
C6	C5	H5	107.9(7)
C4	C5	H5	106.2(7)
C6	C7	H7	119.4(7)
C8	C7	H7	120.2(7)
C9	C8	H8	119.2(8)
C7	C8	H8	120.5(8)
C8	C9	H9	121.4(9)
C10	C9	H9	118.8(9)
C9	C10	H10	120.1(8)
C11	C10	H10	120.0(9)
C10	C11	H11	119.4(8)
C6	C11	H11	119.6(7)
C14	C13	H13	118.8(8)
C12	C13	H13	120.4(8)
C15	C14	H14	119.8(8)
C13	C14	H14	119.8(8)
C16	C15	H15	119.6(8)
C14	C15	H15	121.0(8)
C15	C16	H16	120.1(8)
C17	C16	H16	119.8(8)
C16	C17	H17	119.4(8)

C12 C17 H17 119.4 (8)

X-Ray Structure of *cis*-5-Methyl-2,3-Diphenyl-Pyrrolidine, 5b.