7-Pyridylindoles: Synthesis, Structure and Properties

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Supporting Information

Contents

CIF File for 7-(Pyrid-2'-yl)indole (5)

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 All measurements were made with a Siemens SMART platform
 diffractometer equipped with a 1K CCD area detector.  A
 hemisphere of data (1271 frames at 5 cm detector distance)
 was collected using a narrow-frame method with scan widths of
 0.30\% in omega and an exposure time of 30 s/frame.  The first
 50 frames were re-measured at the end of data collection to
 monitor instrument and crystal stability, and the maximum
 correction on I was <1%.  The data were integrated using the
 Siemens SAINT program, with the intensities corrected for
 Lorentz factor, polarization, air absorption, and absorption
 due to variation in the path length through the detector
 faceplate.  A psi scan absorption correction was applied based
 on the entire data set.  Redundant reflections were averaged.
 Final cell constants were refined using 3739 reflections
 having I>10\s(I), and these, along with other information
 pertinent to data collection and refinement, are listed in
 Table 1.  The Laue symmetry was determined to be mmm, and
 from the systematic absences noted the space group was shown
 to be either Pca2(1) or Pbcm.  The asymmetric unit consists of
 two independent molecules.  The hydogens attached to N were
 allowed to refine freely.

 Acknowledgment for use of MRSEC/TCSUH Facilities:

    This work made use of MRSEC/TCSUH Shared Experimental Facilities
 supported by the National Science Foundation under Award Number
 DMR-9632667 and the Texas Center for Superconductivity at the
 University of Houston.
;

_publ_section_figure_captions
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 Fig. 1 -- View of one molecule showing the atom numbering
   scheme.  Thermal ellipsoids are 40% equiprobability envelopes,
   with hydrogens as spheres of arbitrary diameter.  To obtain
   numbers for the other molecule, add 15 to the values shown.

 Fig. 2 -- Packing of the molecules in the unit cell.
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 F^2^ > 4sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
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C7 C8 C10 N11 175.8(3) . . . . ?
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C8 C10 C15 C14 178.9(3) . . . . ?
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C20 C21 C22 C23 0.8(4) . . . . ?
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C17 N16 C24 C23 178.8(3) . . . . ?
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C18 C19 C24 N16 2.0(3) . . . . ?
C20 C19 C24 C23 1.2(4) . . . . ?
C18 C19 C24 C23 -178.6(2) . . . . ?
C22 C23 C24 N16 179.8(3) . . . . ?
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C22 C23 C24 C19 0.6(3) . . . . ?
C25 C23 C24 C19 -178.2(2) . . . . ?
C22 C23 C25 N26 -175.9(2) . . . . ?
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C22 C23 C25 C30 3.0(4) . . . . ?
C24 C23 C25 C30 -178.3(2) . . . . ?
C30 C25 N26 C27 -0.5(4) . . . . ?
C23 C25 N26 C27 178.4(2) . . . . ?
C25 N26 C27 C28 -0.1(4) . . . . ?
N26 C27 C28 C29 1.0(5) . . . . ?
C27 C28 C29 C30 -1.3(4) . . . . ?
C28 C29 C30 C25 0.7(4) . . . . ?
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N16 H16 N26  0.83(3) 2.28(3) 2.769(3) 119(3) .

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CIF File for 7-(Pyrid-3'-yl)indole (6)

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 '-x, -y, -z'

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 All measurements were made with a Siemens SMART platform
 diffractometer equipped with a 1K CCD area detector.  A
 hemisphere of data (1271 frames at 5 cm detector distance)
 was collected using a narrow-frame method with scan widths of
 0.30\% in omega and an exposure time of 30 s/frame.  The first
 50 frames were re-measured at the end of data collection to
 monitor instrument and crystal stability, and the maximum
 correction on I was <1%.  The data were integrated using the
 Siemens SAINT program, with the intensities corrected for
 Lorentz factor, polarization, air absorption, and absorption
 due to variation in the path length through the detector
 faceplate.  A psi scan absorption correction was applied based
 on the entire data set.  Redundant reflections were averaged.
 Final cell constants were refined using 2195 reflections
 having I>10\s(I), and these, along with other information
 pertinent to data collection and refinement, are listed in
 Table 1.  The Laue symmetry was determined to be -1, and
 the space group was shown to be either P1 or P-1.  The asymmetric
 unit consists of two independent molecules having small but
 significant differences in geometry.  Hydrogens attached to
 nitrogen were refined independently.

 Acknowledgment for use of MRSEC/TCSUH Facilities:

    This work made use of MRSEC/TCSUH Shared Experimental Facilities
 supported by the National Science Foundation under Award Number
 DMR-9632667 and the Texas Center for Superconductivity at the
 University of Houston.
;

_publ_section_figure_captions
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 Fig. 1 -- View of molecule 1 showing the atom numbering
   scheme.  Thermal ellipsoids are 40% equiprobability envelopes,
   with hydrogens as spheres of arbitrary diameter.  To get atom
   labels for molecule 2, add 15 to the numbers shown.

 Fig. 2 -- View of the intermolecular hydrogen bonding arrangement,
   which forms polymeric chains along the a direction.  Only the
   hydrogens attached to N are shown, with hydrogen bonds as thin
   dashed lines.

 Fig. 3 -- Packing of the molecules in the unit cell.
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1999)'
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR
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based
 on F, with F set to zero for negative F^2^. The threshold expression
of
 F^2^ > 4sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
 not relevant to the choice of reflections for refinement.  R-factors
based
 on F^2^ are statistically about twice as large as those based on F,
and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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C2 C 0.7125(4) 0.8744(3) 0.4527(2) 0.0503(8) Uani 1 1 d . . .
H2 H 0.8141 0.8785 0.4881 0.060 Uiso 1 1 calc R . .
C3 C 0.6738(4) 0.9341(3) 0.3555(2) 0.0496(8) Uani 1 1 d . . .
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C4 C 0.5081(4) 0.9038(3) 0.33143(19) 0.0393(7) Uani 1 1 d . . .
C5 C 0.4009(4) 0.9345(3) 0.24395(19) 0.0452(8) Uani 1 1 d . . .
H5 H 0.4323 0.9881 0.1848 0.054 Uiso 1 1 calc R . .
C6 C 0.2492(4) 0.8844(3) 0.2468(2) 0.0479(8) Uani 1 1 d . . .
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C7 C 0.2026(4) 0.8035(3) 0.33351(19) 0.0444(7) Uani 1 1 d . . .
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C8 C 0.3028(4) 0.7714(3) 0.42256(18) 0.0364(7) Uani 1 1 d . . .
C9 C 0.4552(4) 0.8247(3) 0.41829(17) 0.0340(6) Uani 1 1 d . . .
C10 C 0.2489(4) 0.6854(3) 0.51403(18) 0.0354(6) Uani 1 1 d . . .
C11 C 0.2061(4) 0.7319(3) 0.59535(18) 0.0379(7) Uani 1 1 d . . .
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N12 N 0.1509(3) 0.6623(3) 0.67871(15) 0.0433(6) Uani 1 1 d . . .
C13 C 0.1401(4) 0.5374(3) 0.6846(2) 0.0469(8) Uani 1 1 d . . .
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C14 C 0.1813(4) 0.4807(3) 0.6090(2) 0.0487(8) Uani 1 1 d . . .
H14 H 0.1738 0.3921 0.6161 0.058 Uiso 1 1 calc R . .
C15 C 0.2336(4) 0.5563(3) 0.5229(2) 0.0453(7) Uani 1 1 d . . .
H15 H 0.2591 0.5202 0.4701 0.054 Uiso 1 1 calc R . .
N16 N -0.0733(3) 0.2476(2) 0.14566(16) 0.0362(6) Uani 1 1 d . . .
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H16 H -0.090(4) 0.275(3) 0.198(2) 0.043 Uiso 1 1 d . . .
C17 C -0.1989(4) 0.1888(3) 0.1210(2) 0.0423(7) Uani 1 1 d . . .
H17 H -0.3060 0.1757 0.1560 0.051 Uiso 1 1 calc R . .
C18 C -0.1451(4) 0.1528(3) 0.0391(2) 0.0435(7) Uani 1 1 d . . .
H18 H -0.2070 0.1107 0.0079 0.052 Uiso 1 1 calc R . .
C19 C 0.0234(4) 0.1907(3) 0.00897(18) 0.0362(6) Uani 1 1 d . . .
C20 C 0.1367(4) 0.1880(3) -0.07109(19) 0.0440(7) Uani 1 1 d . . .
H20 H 0.1123 0.1487 -0.1174 0.053 Uiso 1 1 calc R . .
C21 C 0.2838(4) 0.2434(3) -0.0817(2) 0.0475(8) Uani 1 1 d . . .
H21 H 0.3600 0.2423 -0.1357 0.057 Uiso 1 1 calc R . .
C22 C 0.3217(4) 0.3014(3) -0.01291(19) 0.0412(7) Uani 1 1 d . . .
H22 H 0.4233 0.3388 -0.0222 0.049 Uiso 1 1 calc R . .
C23 C 0.2151(4) 0.3058(3) 0.06833(17) 0.0330(6) Uani 1 1 d . . .
C24 C 0.0641(4) 0.2496(3) 0.07854(17) 0.0328(6) Uani 1 1 d . . .
C25 C 0.2630(3) 0.3691(3) 0.13892(17) 0.0309(6) Uani 1 1 d . . .
C26 C 0.2945(4) 0.2980(3) 0.23868(17) 0.0348(6) Uani 1 1 d . . .
H26 H 0.2763 0.2108 0.2614 0.042 Uiso 1 1 calc R . .
N27 N 0.3494(3) 0.3483(2) 0.30370(15) 0.0392(6) Uani 1 1 d . . .
C28 C 0.3690(4) 0.4737(3) 0.27051(19) 0.0385(7) Uani 1 1 d . . .
H28 H 0.4058 0.5104 0.3154 0.046 Uiso 1 1 calc R . .
C29 C 0.3381(4) 0.5519(3) 0.17439(19) 0.0407(7) Uani 1 1 d . . .
H29 H 0.3525 0.6403 0.1542 0.049 Uiso 1 1 calc R . .
C30 C 0.2850(4) 0.4982(3) 0.10746(18) 0.0387(7) Uani 1 1 d . . .
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C3 0.0513(18) 0.0539(19) 0.0412(17) -0.0044(14) 0.0025(14) -0.0232(15)
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C7 0.0431(16) 0.0547(18) 0.0410(17) -0.0219(14) -0.0081(13) -0.0154(14)
C8 0.0368(15) 0.0424(16) 0.0317(14) -0.0168(12) -0.0008(11) -0.0098(12)
C9 0.0343(14) 0.0380(15) 0.0277(14) -0.0115(11) -0.0049(11) -0.0071(12)
C10 0.0296(14) 0.0466(16) 0.0328(14) -0.0170(12) -0.0037(11) -
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N12 0.0395(14) 0.0615(17) 0.0342(13) -0.0180(12) 0.0025(10) -0.0203(12)
C13 0.0384(16) 0.058(2) 0.0428(17) -0.0107(15) 0.0036(13) -0.0187(15)
C14 0.0493(18) 0.0498(18) 0.0562(19) -0.0230(15) 0.0083(14) -0.0227(15)
C15 0.0446(17) 0.0570(19) 0.0443(17) -0.0260(14) 0.0051(13) -0.0203(14)
N16 0.0376(13) 0.0478(14) 0.0300(12) -0.0169(10) -0.0007(10) -
0.0182(11)
C17 0.0400(16) 0.0480(17) 0.0404(16) -0.0071(13) -0.0047(12) -
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C18 0.0473(17) 0.0434(17) 0.0440(17) -0.0130(13) -0.0104(13) -
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C25 0.0261(13) 0.0396(15) 0.0287(14) -0.0129(11) -0.0037(10) -
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C28 0.0380(15) 0.0514(18) 0.0349(15) -0.0216(13) -0.0015(12) -
0.0182(13)
C29 0.0473(16) 0.0431(16) 0.0397(16) -0.0162(13) -0.0011(12) -
0.0217(13)
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0.0140(13)

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taken
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angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
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C3 C4 1.434(4) . ?
C4 C9 1.403(4) . ?
C4 C5 1.409(4) . ?
C5 C6 1.375(4) . ?
C6 C7 1.390(4) . ?
C7 C8 1.399(4) . ?
C8 C9 1.401(4) . ?
C8 C10 1.484(4) . ?
C10 C15 1.387(4) . ?
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C21 C22 1.398(4) . ?
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C25 C30 1.376(4) . ?
C25 C26 1.399(3) . ?
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C3 C2 N1 111.0(3) . . ?
C2 C3 C4 106.4(2) . . ?
C9 C4 C5 118.9(3) . . ?
C9 C4 C3 107.1(2) . . ?
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CIF File for 7-(Pyrid-4'-yl)indole (7)

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 All measurements were made with a Siemens SMART platform
 diffractometer equipped with a 1K CCD area detector.  A
 hemisphere of data (1271 frames at 5 cm detector distance)
 was collected using a narrow-frame method with scan widths of
 0.30\% in omega and an exposure time of 35 s/frame.  The first
 50 frames were re-measured at the end of data collection to
 monitor instrument and crystal stability, and the maximum
 correction on I was <1%.  The data were integrated using the
 Siemens SAINT program, with the intensities corrected for
 Lorentz factor, polarization, air absorption, and absorption
 due to variation in the path length through the detector
 faceplate.  A psi scan absorption correction was applied based
 on the entire data set.  Redundant reflections were averaged.
 Final cell constants were refined using 2831 reflections
 having I>10\s(I), and these, along with other information
 pertinent to data collection and refinement, are listed in
 Table 1.  The Laue symmetry was determined to be 2/m, and
 from the systematic absences noted the space group was shown
 unambiguously to be P2(1)/c.  There are two independent molecules
 per asymmetric unit, both forming hydrogen bonded pairs with
 their symmetry relative across an inversion center.  One of the
 molecules was found to be disordered approximately 5:1 with its
 mirror image (ignoring the torsional twist of the pyridyl ring),
 and this was treated by refinement of two ideal rigid bodies for
 the minor component.   Due to the close proximity of many of the
 atoms in the two orientations, all atoms were refined isotropically.

 Acknowledgment for use of MRSEC/TCSUH Facilities:

    This work made use of MRSEC/TCSUH Shared Experimental Facilities
 supported by the National Science Foundation under Award Number
 DMR-9632667 and the Texas Center for Superconductivity at the
 University of Houston.
;

_publ_section_figure_captions
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 Fig. 1 -- View of molecule 1 showing the atom numbering scheme,
   with hydrogens as spheres of arbitrary diameter.  To get atom
   labels for molecule 2, add 15 to the numbers shown.

 Fig. 2 -- View of a mutually hydrogen bonded pair of molecules
   across an inversion center.

 Fig. 3 -- View of the two orientations of molecule 1, and their
   inversion relatives.  The major orientation is depicted with
   solid bonds, and the minor orientation with dashed bonds.
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 Fig. 4 -- Packing of the molecules in the unit cell.  Only the major
   orientation of the disordered molecules are shown at each site.
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of
 F^2^ > 4sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
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and R-
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H17 H 0.2203 0.0276 0.6911 0.053 Uiso 1 1 calc R . .
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C17 0.039(2) 0.052(3) 0.039(2) 0.0039(19) 0.0112(18) 0.0139(19)
C18 0.054(2) 0.041(2) 0.038(2) 0.0101(18) 0.0160(19) 0.0170(19)
C19 0.051(2) 0.031(2) 0.0308(19) 0.0006(16) 0.0188(17) 0.0046(17)
C20 0.071(3) 0.035(2) 0.045(2) 0.0068(19) 0.028(2) 0.000(2)
C21 0.051(2) 0.045(2) 0.055(2) 0.003(2) 0.022(2) -0.009(2)
C22 0.041(2) 0.042(2) 0.040(2) -0.0004(19) 0.0157(17) 0.0007(18)
C23 0.041(2) 0.030(2) 0.0280(18) -0.0015(15) 0.0135(16) 0.0020(16)
C24 0.042(2) 0.0310(19) 0.0261(18) -0.0024(16) 0.0138(16) 0.0020(16)
C25 0.0302(18) 0.038(2) 0.033(2) 0.0028(17) 0.0097(16) 0.0017(16)
C26 0.047(2) 0.038(2) 0.034(2) -0.0002(18) 0.0124(17) 0.0027(18)
C27 0.047(2) 0.044(2) 0.034(2) 0.0016(19) 0.0121(18) 0.0008(19)
N28 0.0442(18) 0.044(2) 0.047(2) 0.0110(16) 0.0151(16) 0.0056(15)
C29 0.056(2) 0.043(3) 0.061(3) 0.014(2) 0.032(2) 0.020(2)
C30 0.055(2) 0.046(3) 0.051(2) 0.009(2) 0.029(2) 0.016(2)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
;

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N1 C2 1.383(5) . ?
C2 C3 1.356(5) . ?
C3 C4 1.4292 . ?
C4 C5 1.3900 . ?
C4 C9 1.420(5) . ?
C5 C6 1.405(5) . ?
C6 C7 1.419(6) . ?
C7 C8 1.402(6) . ?
C8 C9 1.395(6) . ?
C8 C10 1.465(6) . ?
C10 C11 1.388(6) . ?
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C10 C15 1.391(6) . ?
C11 C12 1.378(6) . ?
C12 N13 1.325(6) . ?
N13 C14 1.342(5) . ?
C14 C15 1.372(6) . ?
N1' C9' 1.3700 . ?
N1' C2' 1.3828 . ?
C2' C3' 1.3525 . ?
C3' C4' 1.4100 . ?
C4' C5' 1.4004 . ?
C4' C9' 1.4229 . ?
C5' C6' 1.3747 . ?
C6' C7' 1.3916 . ?
C7' C8' 1.3847 . ?
C8' C9' 1.4111 . ?
C8' C10' 1.418(13) . ?
C10' C11' 1.3859 . ?
C10' C15' 1.3937 . ?
C11' C12' 1.3752 . ?
C12' N13' 1.3438 . ?
N13' C14' 1.3326 . ?
C14' C15' 1.3761 . ?
N16 C17 1.375(4) . ?
N16 C24 1.376(4) . ?
C17 C18 1.356(5) . ?
C18 C19 1.425(5) . ?
C19 C20 1.395(5) . ?
C19 C24 1.425(5) . ?
C20 C21 1.372(5) . ?
C21 C22 1.393(5) . ?
C22 C23 1.387(5) . ?
C23 C24 1.409(5) . ?
C23 C25 1.485(5) . ?
C25 C26 1.387(5) . ?
C25 C30 1.394(5) . ?
C26 C27 1.378(5) . ?
C27 N28 1.341(5) . ?
N28 C29 1.335(5) . ?
C29 C30 1.379(5) . ?

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 _geom_angle_site_symmetry_3
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C3 C2 N1 111.5(4) . . ?
C2 C3 C4 105.4(2) . . ?
C5 C4 C9 119.3(2) . . ?
C5 C4 C3 132.6 . . ?
C9 C4 C3 108.0(2) . . ?
C4 C5 C6 118.8(2) . . ?
C5 C6 C7 120.9(4) . . ?
C8 C7 C6 120.9(4) . . ?
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C9 C8 C7 116.9(4) . . ?
C9 C8 C10 123.6(4) . . ?
C7 C8 C10 119.4(4) . . ?
N1 C9 C8 129.7(4) . . ?
N1 C9 C4 107.1(3) . . ?
C8 C9 C4 123.0(4) . . ?
C11 C10 C15 116.6(4) . . ?
C11 C10 C8 122.1(4) . . ?
C15 C10 C8 121.2(4) . . ?
C12 C11 C10 119.1(4) . . ?
N13 C12 C11 124.6(4) . . ?
C12 N13 C14 116.1(4) . . ?
N13 C14 C15 123.5(4) . . ?
C14 C15 C10 120.0(4) . . ?
C9' N1' C2' 107.9 . . ?
C3' C2' N1' 111.7 . . ?
C2' C3' C4' 105.1 . . ?
C5' C4' C3' 132.0 . . ?
C5' C4' C9' 119.0 . . ?
C3' C4' C9' 108.8 . . ?
C6' C5' C4' 118.6 . . ?
C5' C6' C7' 121.7 . . ?
C8' C7' C6' 122.3 . . ?
C7' C8' C9' 116.0 . . ?
C7' C8' C10' 116.2(9) . . ?
C9' C8' C10' 127.6(9) . . ?
N1' C9' C8' 131.5 . . ?
N1' C9' C4' 106.3 . . ?
C8' C9' C4' 122.2 . . ?
C11' C10' C15' 116.8 . . ?
C11' C10' C8' 123.9(12) . . ?
C15' C10' C8' 119.3(12) . . ?
C12' C11' C10' 120.1 . . ?
N13' C12' C11' 123.3 . . ?
C14' N13' C12' 116.5 . . ?
N13' C14' C15' 124.0 . . ?
C14' C15' C10' 119.4 . . ?
C17 N16 C24 108.3(3) . . ?
C18 C17 N16 110.4(3) . . ?
C17 C18 C19 107.3(3) . . ?
C20 C19 C18 134.4(3) . . ?
C20 C19 C24 119.1(3) . . ?
C18 C19 C24 106.3(3) . . ?
C21 C20 C19 118.9(4) . . ?
C20 C21 C22 121.8(4) . . ?
C23 C22 C21 121.9(3) . . ?
C22 C23 C24 116.4(3) . . ?
C22 C23 C25 122.5(3) . . ?
C24 C23 C25 121.1(3) . . ?
N16 C24 C23 130.2(3) . . ?
N16 C24 C19 107.6(3) . . ?
C23 C24 C19 121.9(3) . . ?
C26 C25 C30 117.1(3) . . ?
C26 C25 C23 122.1(3) . . ?
C30 C25 C23 120.8(3) . . ?
C27 C26 C25 119.9(4) . . ?
N28 C27 C26 123.4(4) . . ?
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C29 N28 C27 116.5(3) . . ?
N28 C29 C30 124.1(4) . . ?
C29 C30 C25 119.1(3) . . ?

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N1 C2 C3 C4 1.1(4) . . . . ?
C2 C3 C4 C5 175.0(3) . . . . ?
C2 C3 C4 C9 -0.5(3) . . . . ?
C9 C4 C5 C6 0.7(3) . . . . ?
C3 C4 C5 C6 -174.3(2) . . . . ?
C4 C5 C6 C7 1.1(5) . . . . ?
C5 C6 C7 C8 -2.9(6) . . . . ?
C6 C7 C8 C9 2.7(6) . . . . ?
C6 C7 C8 C10 -179.8(5) . . . . ?
C2 N1 C9 C8 -174.3(4) . . . . ?
C2 N1 C9 C4 0.9(4) . . . . ?
C7 C8 C9 N1 173.6(4) . . . . ?
C10 C8 C9 N1 -3.7(8) . . . . ?
C7 C8 C9 C4 -0.9(6) . . . . ?
C10 C8 C9 C4 -178.2(5) . . . . ?
C5 C4 C9 N1 -176.4(2) . . . . ?
C3 C4 C9 N1 -0.2(3) . . . . ?
C5 C4 C9 C8 -0.8(5) . . . . ?
C3 C4 C9 C8 175.3(3) . . . . ?
C9 C8 C10 C11 -65.4(7) . . . . ?
C7 C8 C10 C11 117.3(5) . . . . ?
C9 C8 C10 C15 111.9(5) . . . . ?
C7 C8 C10 C15 -65.3(6) . . . . ?
C15 C10 C11 C12 1.8(6) . . . . ?
C8 C10 C11 C12 179.2(4) . . . . ?
C10 C11 C12 N13 -2.1(7) . . . . ?
C11 C12 N13 C14 0.7(7) . . . . ?
C12 N13 C14 C15 0.8(6) . . . . ?
N13 C14 C15 C10 -1.0(7) . . . . ?
C11 C10 C15 C14 -0.4(6) . . . . ?
C8 C10 C15 C14 -177.9(4) . . . . ?
C9' N1' C2' C3' 2.1 . . . . ?
N1' C2' C3' C4' -4.3 . . . . ?
C2' C3' C4' C5' 179.5 . . . . ?
C2' C3' C4' C9' 4.9 . . . . ?
C3' C4' C5' C6' -176.5 . . . . ?
C9' C4' C5' C6' -2.4 . . . . ?
C4' C5' C6' C7' 0.5 . . . . ?
C5' C6' C7' C8' 1.3 . . . . ?
C6' C7' C8' C9' -1.1 . . . . ?
C6' C7' C8' C10' 175.2(18) . . . . ?
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C2' N1' C9' C8' 179.2 . . . . ?
C2' N1' C9' C4' 1.1 . . . . ?
C7' C8' C9' N1' -178.7 . . . . ?
C10' C8' C9' N1' 6(2) . . . . ?
C7' C8' C9' C4' -0.9 . . . . ?
C10' C8' C9' C4' -177(2) . . . . ?
C5' C4' C9' N1' -179.1 . . . . ?
C3' C4' C9' N1' -3.7 . . . . ?
C5' C4' C9' C8' 2.6 . . . . ?
C3' C4' C9' C8' 178.0 . . . . ?
C7' C8' C10' C11' -116.8(11) . . . . ?
C9' C8' C10' C11' 59(2) . . . . ?
C7' C8' C10' C15' 64.8(14) . . . . ?
C9' C8' C10' C15' -119.4(13) . . . . ?
C15' C10' C11' C12' -0.5 . . . . ?
C8' C10' C11' C12' -178.9(14) . . . . ?
C10' C11' C12' N13' 1.5 . . . . ?
C11' C12' N13' C14' -1.2 . . . . ?
C12' N13' C14' C15' 0.0 . . . . ?
N13' C14' C15' C10' 0.9 . . . . ?
C11' C10' C15' C14' -0.6 . . . . ?
C8' C10' C15' C14' 177.9(13) . . . . ?
C24 N16 C17 C18 1.1(4) . . . . ?
N16 C17 C18 C19 -0.6(4) . . . . ?
C17 C18 C19 C20 -176.0(4) . . . . ?
C17 C18 C19 C24 -0.1(4) . . . . ?
C18 C19 C20 C21 173.5(4) . . . . ?
C24 C19 C20 C21 -2.0(5) . . . . ?
C19 C20 C21 C22 0.2(6) . . . . ?
C20 C21 C22 C23 1.5(6) . . . . ?
C21 C22 C23 C24 -1.3(5) . . . . ?
C21 C22 C23 C25 -179.3(3) . . . . ?
C17 N16 C24 C23 173.5(3) . . . . ?
C17 N16 C24 C19 -1.1(4) . . . . ?
C22 C23 C24 N16 -174.5(3) . . . . ?
C25 C23 C24 N16 3.6(5) . . . . ?
C22 C23 C24 C19 -0.6(5) . . . . ?
C25 C23 C24 C19 177.5(3) . . . . ?
C20 C19 C24 N16 177.4(3) . . . . ?
C18 C19 C24 N16 0.7(4) . . . . ?
C20 C19 C24 C23 2.2(5) . . . . ?
C18 C19 C24 C23 -174.4(3) . . . . ?
C22 C23 C25 C26 -121.5(4) . . . . ?
C24 C23 C25 C26 60.5(5) . . . . ?
C22 C23 C25 C30 59.6(5) . . . . ?
C24 C23 C25 C30 -118.4(4) . . . . ?
C30 C25 C26 C27 -0.5(5) . . . . ?
C23 C25 C26 C27 -179.5(3) . . . . ?
C25 C26 C27 N28 1.4(6) . . . . ?
C26 C27 N28 C29 -1.2(5) . . . . ?
C27 N28 C29 C30 0.1(6) . . . . ?
N28 C29 C30 C25 0.7(6) . . . . ?
C26 C25 C30 C29 -0.5(5) . . . . ?
C23 C25 C30 C29 178.5(3) . . . . ?

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N1' H1' N13'  0.90 2.15 3.04(3) 173.3 3_666
N16 H16 N28  0.87 2.06 2.917(4) 167.6 3_566

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_diffrn_reflns_theta_full              23.49
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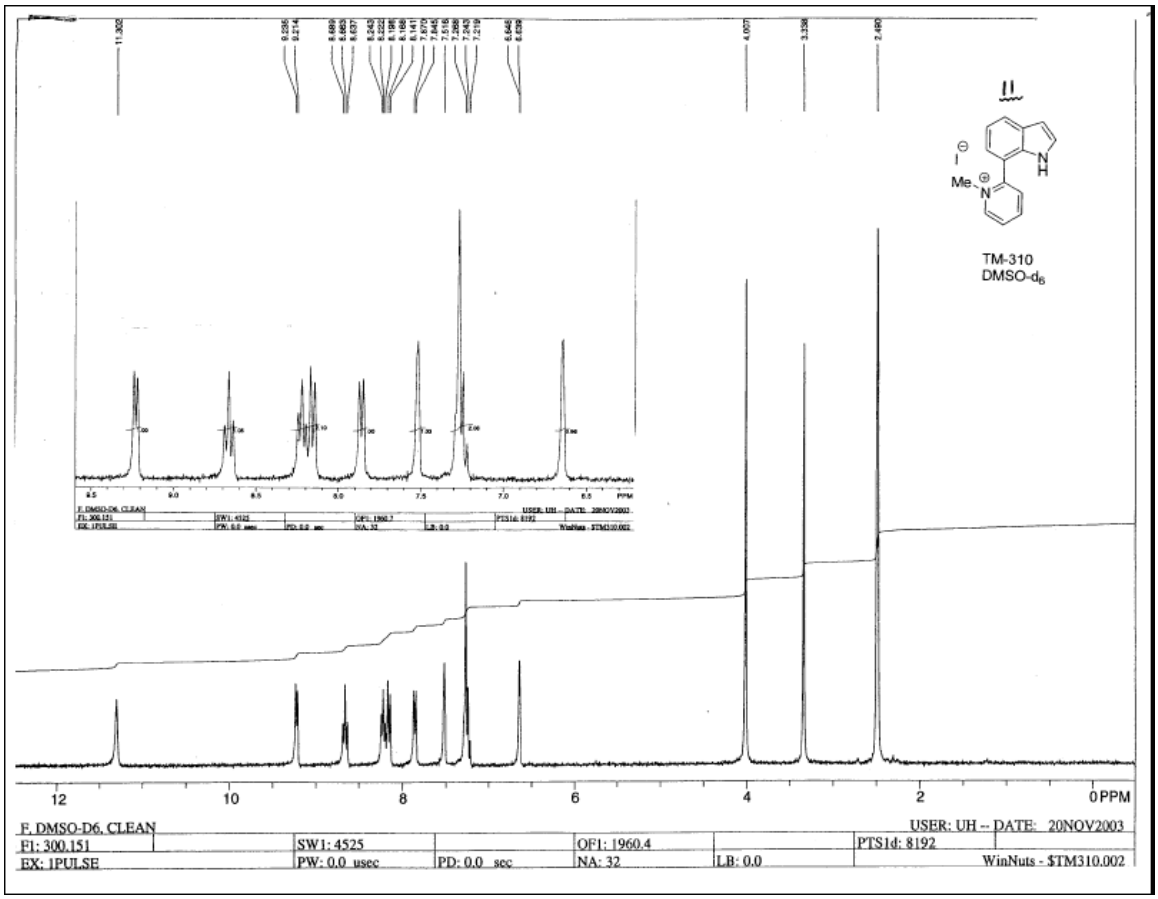
General Experimental Methods

Nuclear magnetic resonance spectra were recorded at 300 MHz for ^{1}H and 75 MHz for ^{13}C, referenced to DMSO-d_6, CD_3CN, CD_3OD and TMS in $CDCl_3$. Melting points are uncorrected. The starting materials vinylmagnesium bromide and 2-nitro-bromobenzene are commercially available. The 2-, 3-, and 4-bromopyridine were purified according to literature procedures,[14] however, the 4-bromopyridine was not distilled and used immediately after purification to avoid decomposition. The bromopyridines were converted to the corresponding tri-*n*-butylstannanes as previously described.[15]

References

14. (a) Ziessel, R.; Suffert, J.; Youinou, M.-T. *J. Org. Chem.* **1996**, 61, 6535-6546. (b) Parks, J. E.; Wagner, B. E.; Holm, R. H. *J. Organomet. Chem*. **1973**, *56*, 53-66.

15. (a) Peters, D.; Hornfeldt, A. –B.; Cronowitz, S. *J. Heterocycl. Chem.* **1990**, *27*, 2165. (b) Guiller, F.; Nivoliers, F.; Godard, A.; Marsais, F.; Quéguiner, G.; Siddiqui, M. A.; Snieckus, V. *J. Org. Chem.* **1995**, *60,* 292-296.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DMSO-d6
12
10
8
6
4
2
0 PPM
F, DMSO-D6, CLEAN
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F1: 300.151
SW1: 4525
OF1: 1960.4
PTS1d: 8192
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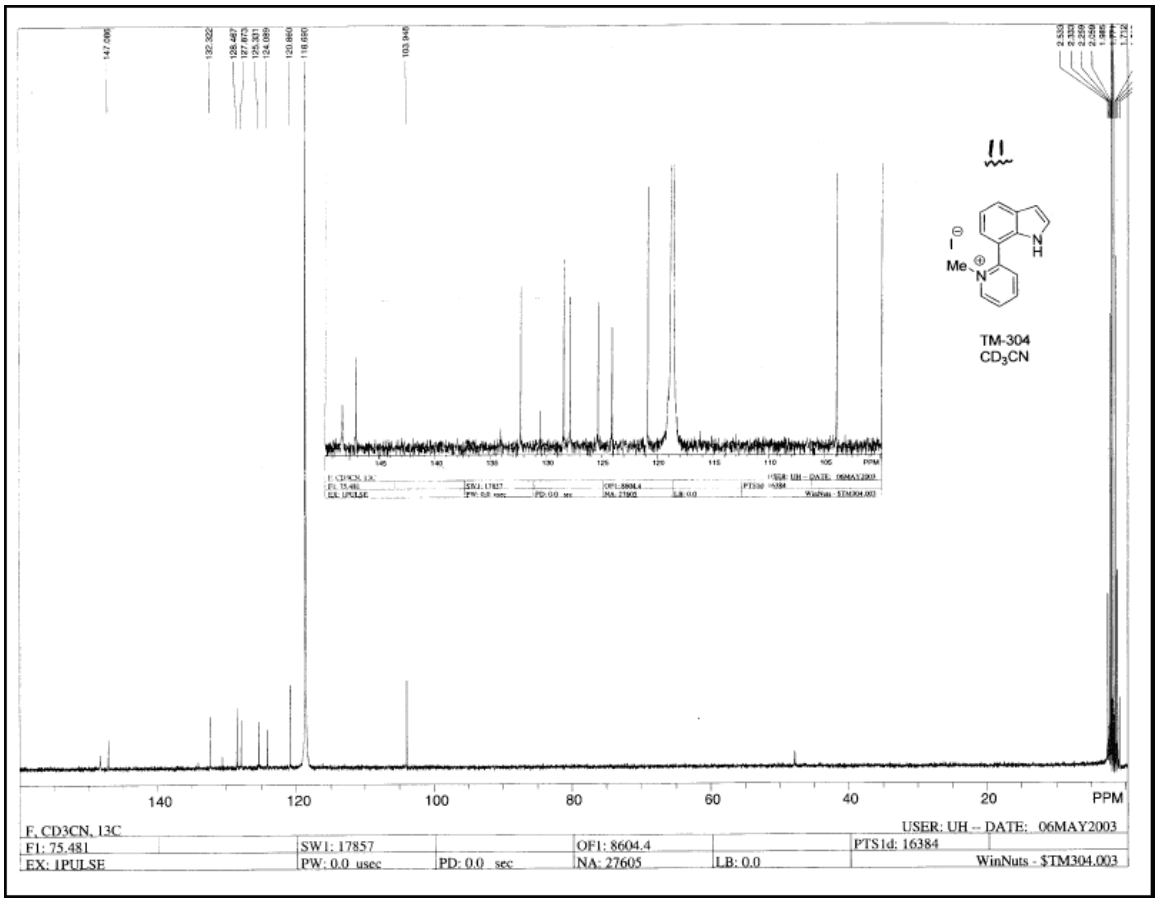
PD: 0.0 sec
NA: 32
LB: 0.0
WinNuts - $TM310.002


TM-304
CD3CN
140
120
100
80
60
40
20
PPM
F, CD3CN, 13C
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SW1: 17857
OF1: 8604.4
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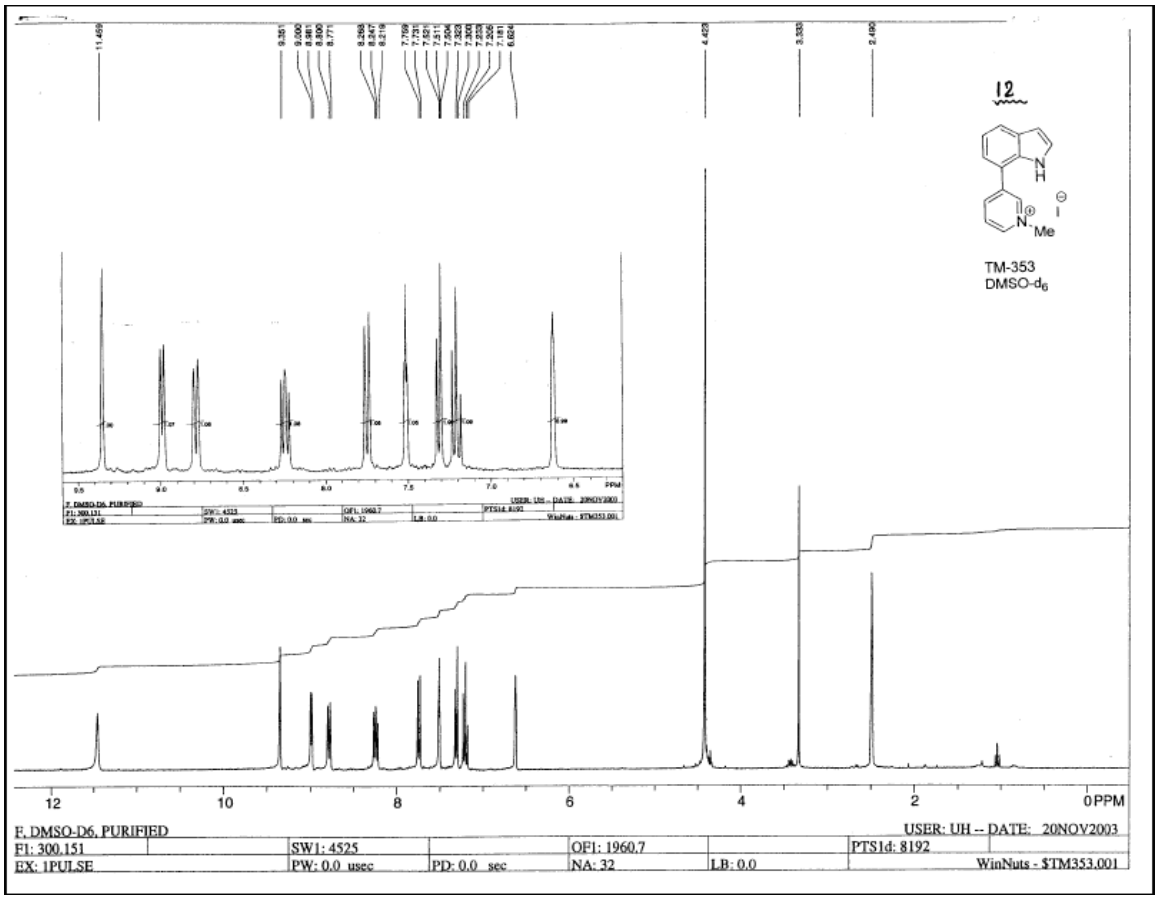
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12
10
8
6
4
2
0PPM
F, DMSO-D6, PURIFIED
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OF1: 1960.7
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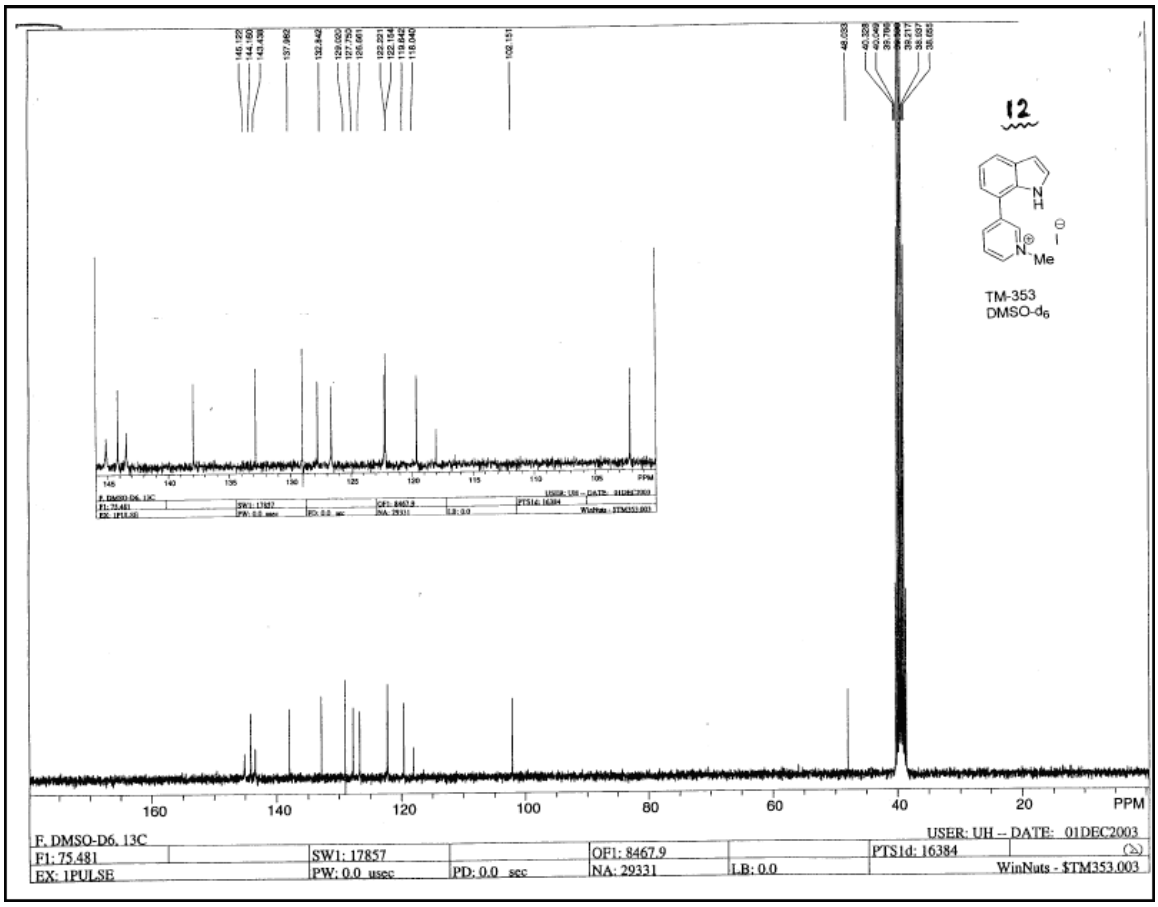
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TM-353
DMSO-d6
Me
160
140
120
100
80
60
40
20
PPM
F, DMSO-D6, 13C
F1: 75.481
EX: 1PULSE
SW1: 17857
PW: 0.0 usec
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NA: 29331
LB: 0.0
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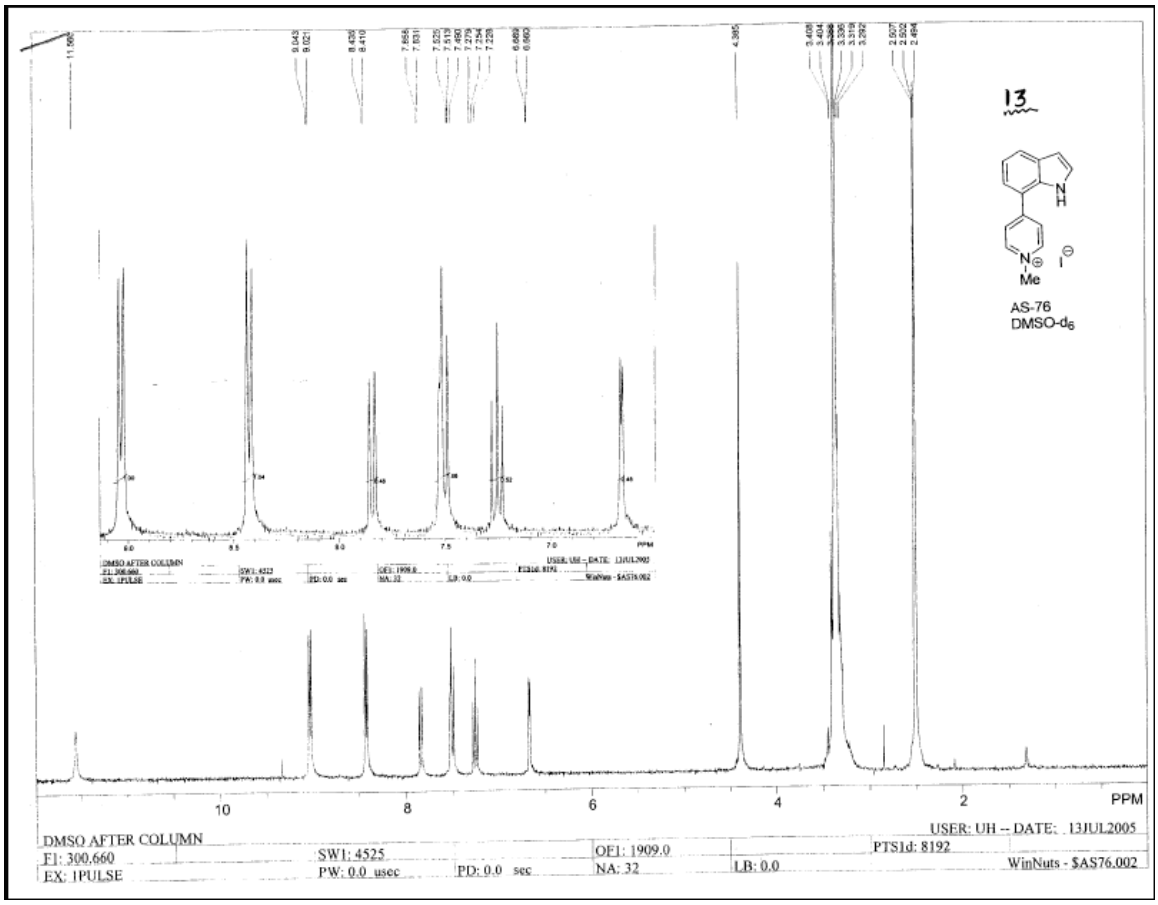
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AS-76
DMSO-d6
PPM
DMSO AFTER COLUMN
F1: 300.660
EX: 1PULSE
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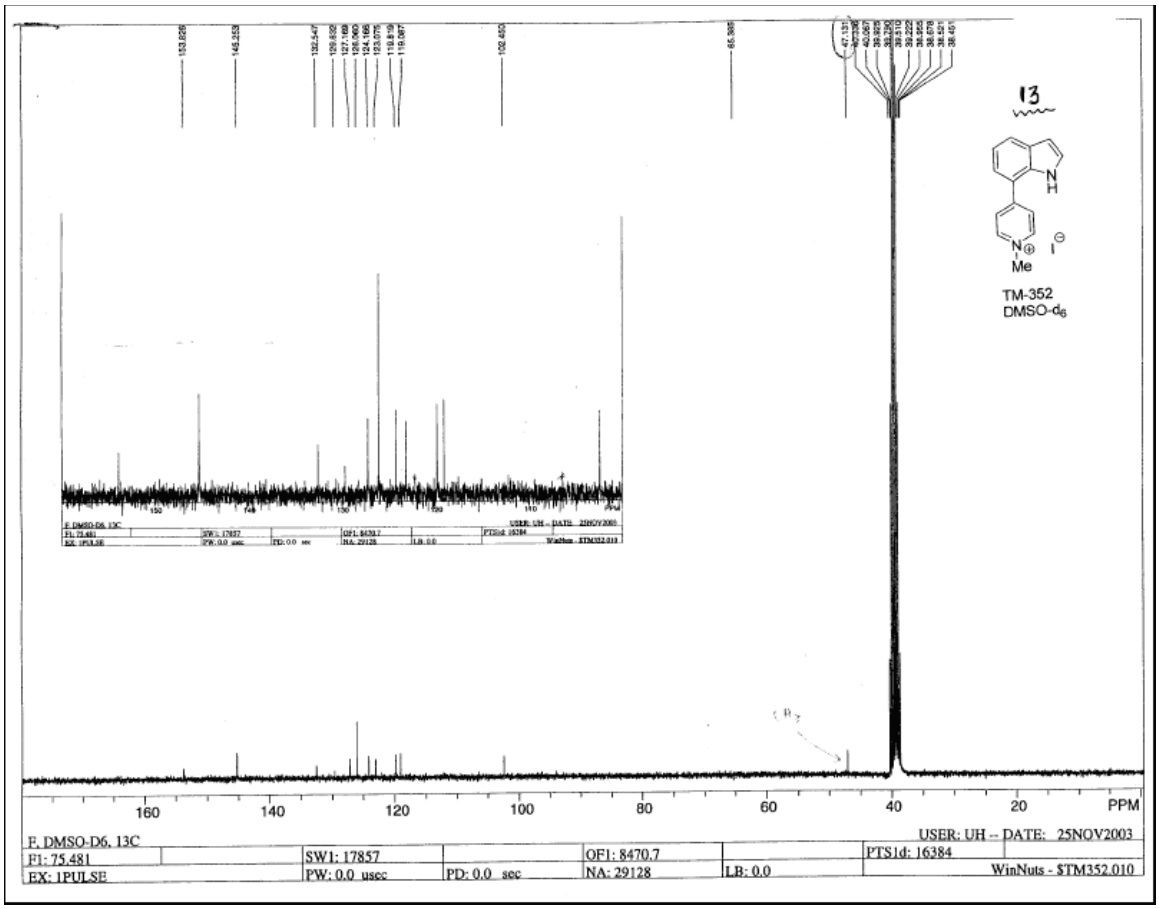
USER: UH -- DATE: 13JUL2005
WinNuts - $AS76.002


13
TM-352
DMSO-d6
Me
160
140
120
100
80
60
40
20
PPM
F, DMSO-D6, 13C
F1: 75.481
EX: 1PULSE
SW1: 17857
PW: 0.0 usec
PD: 0.0 sec
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NA: 29128
LB: 0.0
USER: UH -- DATE: 25NOV2003
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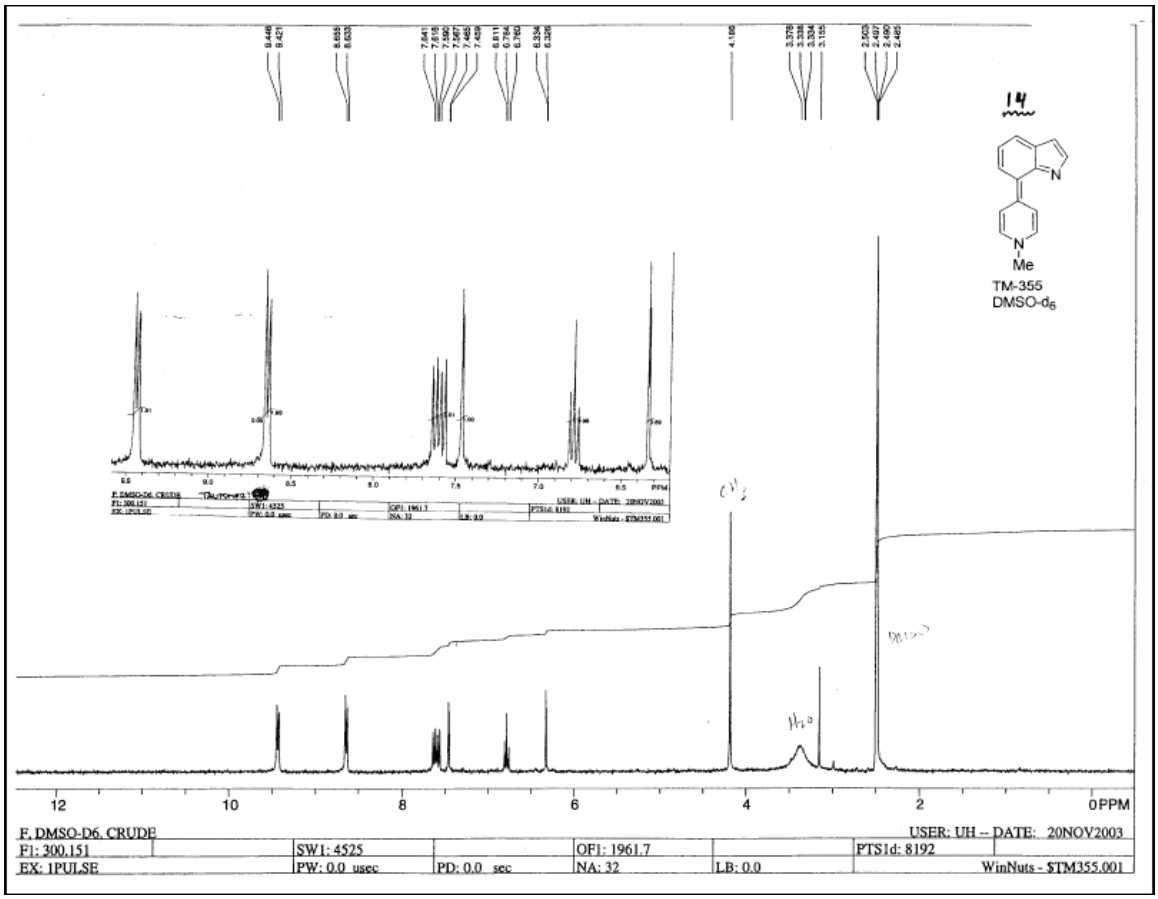
WinNuts - $TM352.010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N
N
Me
TM-355
DMSO-d6
12
10
8
6
4
2
0PPM
F, DMSO-D6, CRUDE
USER: UH -- DATE: 20NOV2003
F1: 300.151
SW1: 4525
OF1: 1961.7
PTS1d: 8192
EX: 1PULSE
PW: 0.0 usec
PD: 0.0 sec
NA: 32
LB: 0.0
WinNuts - $TM355.001