Supporting Information

First Synthesis of Tetrapyrrolylporphyrin

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Synthetic Procedures of Tetrapyrrolylporphyrins (TPyrPs).

A) 2,4-diformylpyrrole derived TPyrPs (**2-H**, **3-H** + **4-H**, **5-H**)
A mixture of pyrrole (134 mg, 2 mmol) and 2,4-diformylpyrrole[#1] (246 mg, 2 mmol) was dissolved in acetic acid (100 ml) and stirred for 40 min at 110 °C. After removing the solvent, the resulting residue was subjected to silica gel (Wakogel C-300) column chromatography with 3% MeOH-CH_2Cl_2. The four red color bands eluted were separated sequentially. R_f-values were recorded on Merck-Type 60 TLC plate with 10% MeOH-$CHCl_3$.

Formyl-TPyrP (2-H: αβββ**)**: R_f = 0.62; ^{1}HNMR (DMSO-*d*$_6$, 500 MHz, 50 °C): δ (ppm) 13.02 (s, 1H, pyrrole-NH), 12.85 (s, 3H, pyrrole-NH), 10.11 (s, 1H, β-CHO), 9.89 (s, 3H, α-CHO), 9.15 (s, 6H, βH), 9.02 (s, 2H, βH), 8.21 (s, 1H, pyrrole-αH), 8.08 (d, *J* = 7.0 Hz, 3H, pyrrole-αH), 7.91 (d, *J* = 6.0 Hz, 3H, pyrrole-βH), 7.39 (s, 1H, pyrrole-βH), -2.68 (s, 2H, inner-NH); UV/vis (DMF): λ_{max}[nm] 421, 520, 559, 654; MALDI-TOF-MS: m/z = 683.4 (M^++1).

Formyl-TPyrPs (3-H: αβαβ and **4-H:** ααββ**)**: Two isomers are hardly separated: R_f = 0.58; ^{1}HNMR (DMF-*d*$_7$, 500 MHz, 20 °C): δ (ppm) 12.83 (br, 2H, pyrrole-NH), 12.81 (s, 2H, pyrrole-NH), 9.99 (s, 2H, β-CHO), 9.76 (s, 2H, α-CHO), 9.04 (br, 4H, βH), 8.91 (br, 4H, βH), 8.15 (s, 2H, pyrrole-αH), 8.04 (s, 2H, pyrrole-αH), 7.81 (s, 2H, pyrrole-βH), 7.30 (s, 2H, pyrrole-βH), -2.83 or -2.85 (s, 2H, inner-NH).

Formyl-TPyrP (5-H: αααβ): R_f = 0.55; ^{1}HNMR (DMSO-*d*$_6$, 500 MHz, 27 °C): δ (ppm) 13.14 (s, 3H, pyrrole-NH), 13.00 (s, 1H, pyrrole-NH), 10.10 (s, 3H, β-CHO), 9.89 (s, 1H, α-CHO), 9.20 (br, 2H, βH), 9.07 (m, 6H, βH), 8.34 (s, 3H, pyrrole-αH), 8.27 (s, 1H, pyrrole-αH), 8.11 (s, 1H, pyrrole-βH), 7.94 (s, 3H, pyrrole-βH), -2.79 (br, 2H, inner-NH).

B) N-methyl-2,4-diformylpyrrole derived TPyrPs (**2-Me**, **3-Me** + **4-Me**).
Procedures are similar as described above in A). For silica gel column chromatography, 1% MeOH-CH_2Cl_2 was used.

N-Methyl-Formyl-TPyrP (2-Me: αβββ**)**: R_f = 0.78; ^{1}HNMR ($CDCl_3$, 500 MHz, 27 °C): δ (ppm) 10.13 (s, 1H, β-CHO), 9.93 (d, *J* = 3.5 Hz, α-CHO), 9.13 (m, 6H, βH), 8.84 (s, 2H, βH),7.80 (m, pyrrole-αH), 7.69 (d, *J* = 5.5 Hz, 3H, pyrrole-βH), 7.50 (s, 1H, pyrrole-βH), 4.37 (s, 9H, CH_3), 3.42 (s, 3H, CH_3), -2.67 (s, 2H, inner-NH); UV/vis (DMF): λ_{max}[nm] 421, 520, 559, 654; FABMS: m/z (% intensity) = 783.4 (100, M^+).

N-Methyl-Formyl-TPyrPs (3-Me: αβαβ and **4-Me:** ααββ**)**: Two isomers were hardly separated: R_f = 0.71; ^{1}HNMR ($CDCl_3$, 500 MHz, 27 °C): δ (ppm) 10.15 (m, 2H, β-CHO), 9.96 (s, 2H, α-CHO), 9.17 (m, 4H, βH), 8.89 (s, 4H, βH), 7.83 (s, 4H, pyrrole-αH), 7.71 (s, 2H, pyrrole-βH), 7.50 (m, 2H, pyrrole-bH), 4.39 (s, 6H, CH_3), 3.43 (m, 6H, CH_3), -2.66 or -2.71 (br, 2H, inner-NH).

C) N-isopropyl-2,4-diformylpyrrole derived TPyrPs (**1-*i*Pr**, **2-*i*Pr**, **3- *i*Pr** + **4- *i*Pr**).

[Method-1]: Preparation of **1-*i*Pr**

To a solution of 2,4-diformyl-1-isopropylpyrrole[#2] (165 mg, 1.0 mmol) and an equivalent pyrrole in $CHCl_3$ (100 ml) and BF_3OEt_2 (12.6 μl, 0.10 mmol) was added and stirred for 1 h at room temperature. DDQ (170 mg, 0.75 mmol) was then added and stirred for 1 h at room temperature. The violet colored product was separated by silica gel column chromatography (Wakogel C-200, 1% MeOH/CH_2Cl_2), followed by recrystallization from MeOH/CH_2Cl_2 to give **1-*i*Pr** as a violet solid in 20% yield.

N-Isopropyl-Formyl-TPyrP (1- *i*Pr: ββββ**)**: m.p. > 300 °C; ^{1}HNMR ($CDCl_3$, 500 MHz, 27 °C): δ (ppm) 9.94 (d, *J* = 2.0 Hz, 4H, CHO), 9.13 (s, 8H, β-H), 8.00 (s, 4H, pyrrolyl-αH), 7.86 (d, *J* = 2.0 Hz, 4H, pyrrolyl-βH), 5.84 (sept, *J* = 6.5 Hz, 4H, CH), 1.80 (d, *J* = 6.5 Hz, 24H, CH_3), -2.60 (s, 2H, inner NH); ^{13}CNMR ($CDCl_3$, 125.65 MHz, -50 °C): δ (ppm) 180.50 (CHO), 155.07, 138.13, 133.89 (βC), 131.41 (pyrrole-αC), 131.24 (pyrrole-βC), 130.48, 127.66 (βC), 125.82, 112.76, 49.68 (CH), 23.87 (CH_3); IR (KBr): 1662.82 cm^{-1} (ν(C=O)); UV/vis ($CHCl_3$): λ_{max}[nm] (ε x 10^{-4}) 428.5 (57), 526.0 (1.4), 568.5 (2.0), 662.0 (0.87); FABMS: m/z (% intensity) = 850.6 (86, M^+), 851.7 (100, M^++1); HRMS(FAB): calcd for $C_{52}H_{51}N_8O_4$ [M^++H]: 851.4033; found 851.4139; Elemental Analysis: Calcd. for $C_{52}H_{50}N_8O_4H_2O$: C, 71.87; H, 6.03; N, 12.89. Found: C, 72.26; H, 6.00; N, 12.50. **Protonated 1-*i*Pr**: UV/vis (1% TFA-CH_2Cl_2): λ_{max}[nm] 454.0, 709.0.

[Method-2]: Preparation of **2-^{i}Pr**, **3-^{i}Pr** + **4-^{i}Pr**.

To a solution of 2,4-diformyl-1-isopropylpyrrole (165 mg, 1.0 mmol) and $SnCl_2$ (379 mg, 1.0 mmol) in acetic acid (10 ml), pyrrole (67 mg, 1 mmol) was added and stirred for 1 h at room temperature. DDQ (340.5 mg, 1.5 mmol) was then added to the solution and stirred for 30 min. After the solvent was removed, the three products were separated by flash silica gel column chromatography (Merck Type 60; 1% MeOH-CH_2Cl_2). Recrystallization of the second fraction from MeOH/CH_2Cl_2 gave **2**-^{i}Pr as a violet solid. A mixture of **3**-^{i}Pr and **4**-^{i}Pr (1:1) was obtained from the third fraction.

N-Isopropyl-Formyl-TPyrP (**2-^{i}Pr:** αβββ): ^{1}HNMR ($CDCl_3$, 500 MHz, 27 °C): δ (ppm) 10.17 (s, 1H, β-CHO), 9.94 (d, *J* = 1.0 Hz, 1H, α-CHO), 9.93 (d, *J* = 1.0 Hz, 2H, α-CHO), 9.13 (m, 6H, β-H), 8.88 (d, *J* = 4.5 Hz, 2H, β-H), 8.00 (s, 1H, pyrrolyl-αH), 7.98 (s, 2H, pyrrolyl-αH), 7.97 (d, *J* = 2.0 Hz, 1H, pyrrolyl-αH), 7.86 (d, *J* = 2.0 Hz, 1H, pyrrolyl-βH), 7.84 (d, *J* = 2.0 Hz, 2H, pyrrolyl-βH), 7.49 (d, *J* = 2.0 Hz, 1H, pyrrolyl-βH), 5.82 (sept, *J* = 6.5 Hz, 3H, CH), 3.99 (sept, *J* = 6.5 Hz, 1H, CH), 1.80 (d, *J* = 6.5 Hz, 6H, CH_3), 1.79 (d, *J* = 6.5 Hz, 12H, CH_3), 1.27 (d, *J* = 6.5 Hz, 6H, CH_3), -2.59 (s, 2H, inner-NH); UV/vis ($CHCl_3$): λ_{max}[nm] 428.5, 525.0, 565.5, 658.0.

N-Isopropyl-Formyl-TPyrP (**3-^{i}Pr**: αβαβ and **4-^{i}Pr**: ααββ): Two isomers were hardly separated: ^{1}HNMR ($CDCl_3$, 500 MHz, 27 °C): δ (ppm) 10.17 or 10.16 (s, 2H, β-CHO), 9.93 or 9.92 (d, *J* = 2.0 Hz, 2H, α-CHO), 9.14 (m, 4H, βH), 8.89 (m, 4H, βH), 7.97 (m, 4H, pyrrole-αH), 7.84 or 7.82 (d, *J* = 2.0 Hz, 2H, pyrrole-βH), 7.50 or 7.47 (d, *J* = 2.0 Hz, 2H, pyrrole-βH), 5.81 (m, 2H, CH), 3.95 (m, 2H, CH), 1.77 (m, 12H, CH_3), 1.25 (m, 12H, CH_3), -2.62 or -2.68 (br, 2H, inner-NH).

D) Derivatives from formyl-TPyrP.

N-Isopropyl-TPyrP Dipyrromethane Derivative (8): To the solution of **1-^{i}Pr** (17 mg, 0.02 mmol) in pyrrole (2 ml), TFA (6.2 μl, 0.08 mmol) was added and stirred for 30 min at room temperature. After trace amount of Et_3N was added, pyrrole was removed by distillation. The blue-green colored product was separated by silica gel column chromatography (Wakogel C-200); ^{1}HNMR (2% Et_3N/$CDCl_3$, 500 MHz, 27 _): δ (ppm) 9.14 (br, 8H, dipyrromethane-pyrrole-

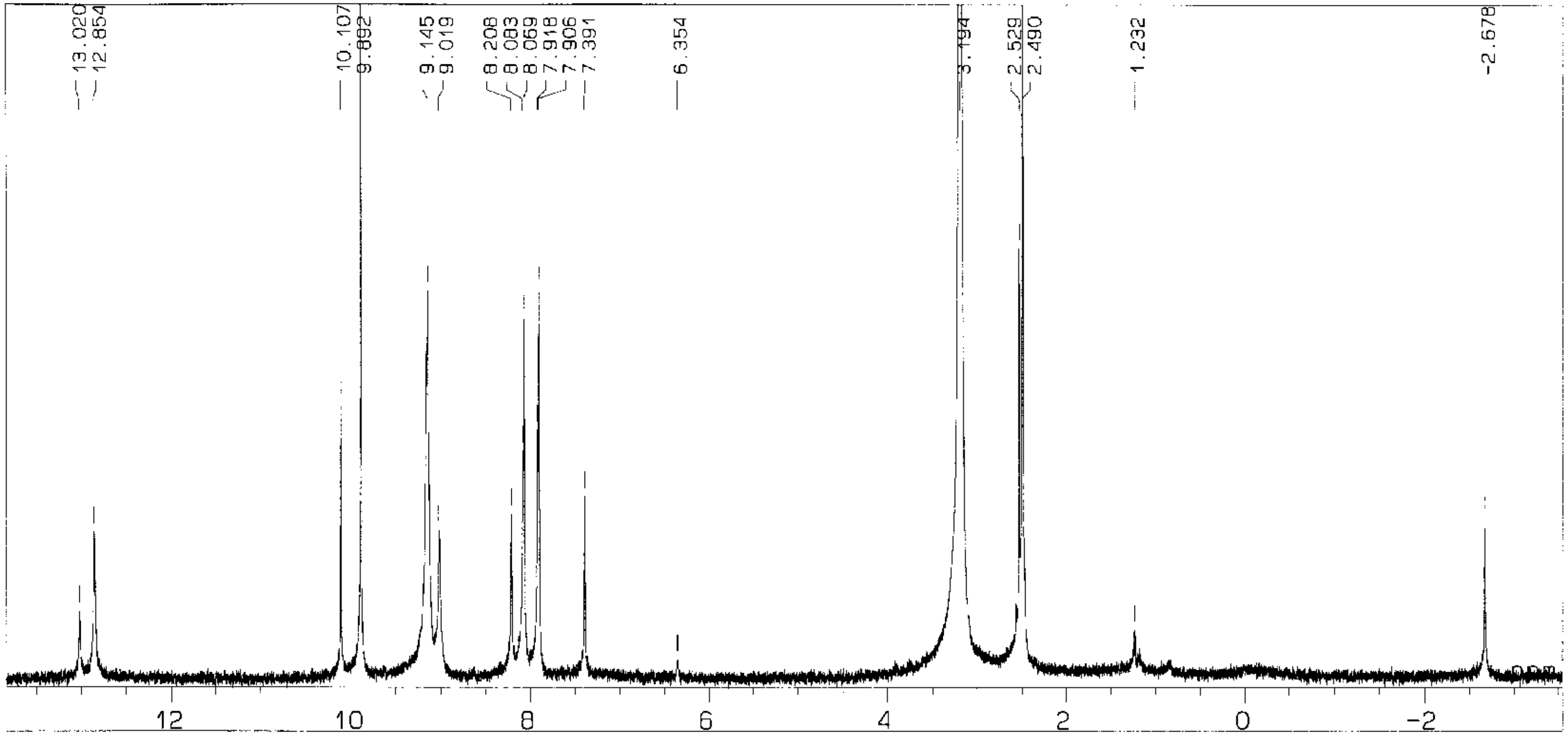
NH), 8.53 (s, 8H, βH), 7.54 (s, 4H, meso-pyrrole-αH), 6.90 (s, 4H, meso-pyrrole-βH), 6.78 (d, *J* = 2.0 Hz, 8H, dipyrromethane-pyrrole-αH), 6.24 (s, 8H, dipyrromethane-pyrrole-βH), 6.24 (d, *J* = 2.0 Hz, dipyrromethane-pyrrole-βH), 5.89 (s, 4H, dipyrromethane-meso-H), 4.64 (sept, *J* = 6.5 Hz, 4H, isopropyl-CH), 1.53 (d, *J* = 6.5 Hz, 24H, isopropyl-CH_3), -2.42 (br, 2H, inner-NH); UV/vis (CH_2Cl_2): λ_{max}[nm] 438.5, 539.5, 588.0, 680.0); MALDI-TOF-MS: m/z = 1315.8 (M^++1). **Protonated type of 8**: UV/vis (CH_2Cl_2): λ_{max}[nm] 454.5, 767.5.

Ni Complex of N-Isopropyl-Formyl-TPyrP (7): To a solution of **1**-^{i}Pr (315 mg, 0.37 mmol) in toluene, nickel acetylacetonate (190 mg, 0.74 mmol) was added and stirred for 0.75 h at a reflux temperature. The solvent was filtrated with basic alumina column to remove excess nickel salt and evaporated. Recrystallization from MeOH/CH_2Cl_2 gave **7** as a red solid in 94% yield: ^{1}HNMR ($CDCl_3$, 500 MHz, 27 _): δ (ppm) 9.86 (d, *J* = 1.0 Hz, 4H, CHO), 8.99 (s, 8H, β-H), 7.73 (s, 4H, pyrrolyl-αH), 7.69 (d, *J* = 2.0 Hz, 4H, pyrrolyl-βH), 6.96 (dd, 4H, pyrrolyl-H), 4.53 (sept, *J* = 6.5 Hz, 4H, CH), 1.69 (d, *J* = 6.5 Hz, 24H, CH_3); UV/vis (CH_2Cl_2): λ_{max}[nm] 429.0, 538.0; FABMS: m/z (% intensity) = 906.4 (93, M^+), 907.4 (100, M^++1).

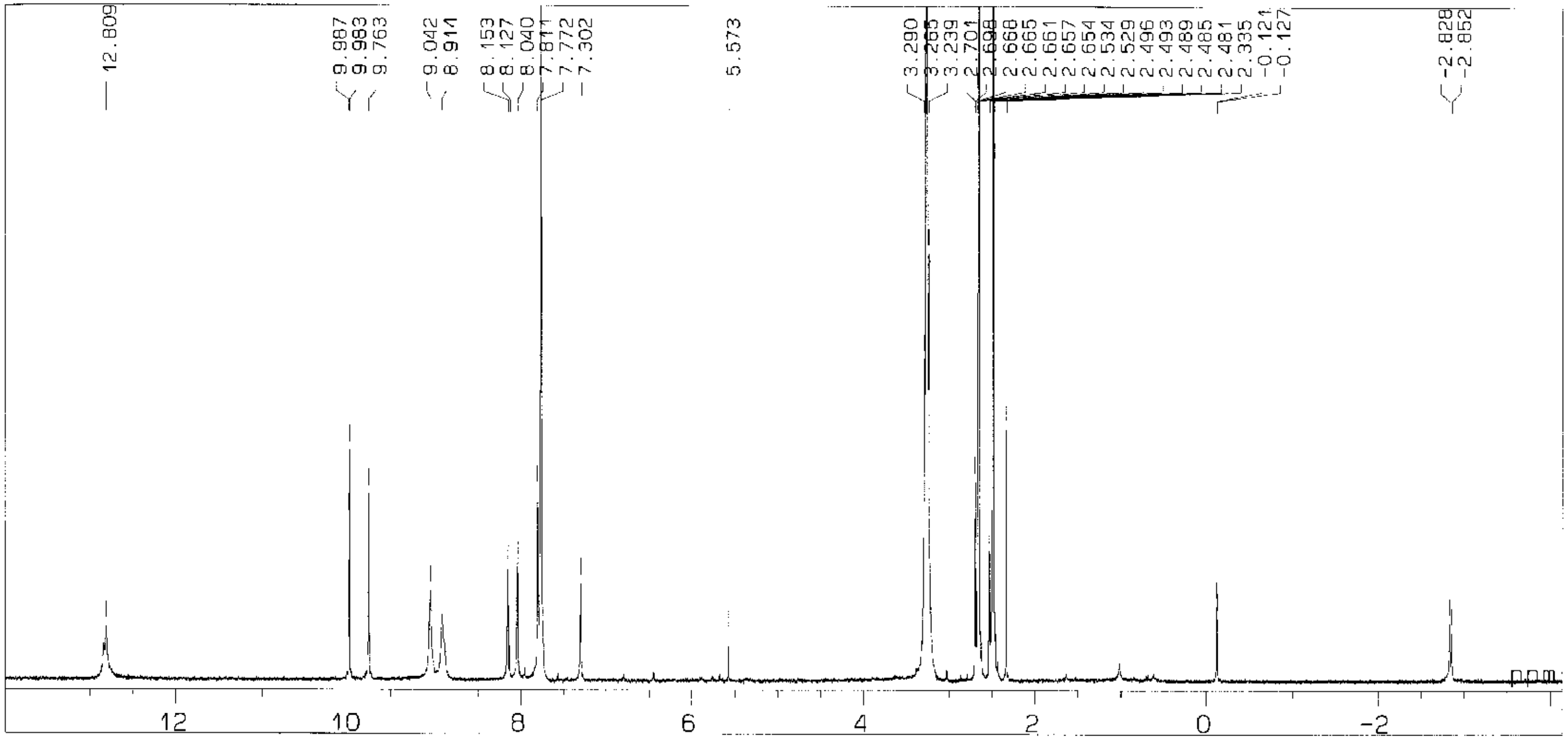
Ni Complex of N-Isopropyl-TPyrP (9): To a solution of **7** (235 mg, 0.26 mmol) in pyrrole (2 ml), TFA (19.9 μl, 0.26 mmol) was added and stirred for 3 h at room temperature. After trace of Et_3N was added, pyrrole was removed by distillation. The purple colored product was separated by flash silica gel column chromatography (Merck Type 60) and evaporated. Recrystallization from MeOH/CH_2Cl_2 gave **9** as a purple solid in 46% yield: ^{1}HNMR ($CDCl_3$, 500 MHz, 27 _): δ (ppm) 9.08 (d, *J* = 3.0 Hz, 8H, β-H), 7.31 (dd, 4H, pyrrolyl-αH), 7.12 (dd, 4H, pyrrolyl-αH), 6.96 (dd, 4H, pyrrolyl-βH), 4.53 (sept, *J* = 6.5 Hz, 4H, CH), 1.69 (d, *J* = 6.5 Hz, 24H, CH_3); UV/vis (CH_2Cl_2): λ_{max}[nm] 433.5, 544.0, 588.5; FABMS: m/z (% intensity) = 794.4 (100,M^+).

#1 Anderson, H. J.; Loader, C. E.: Foster, A. *Can. J. Chem.*, 1980, **58**, 2527.
#2 Elming, N.; Clauson-Kaas, N. *Acta. Chem. Scand.*, 1952, **6**, 867.

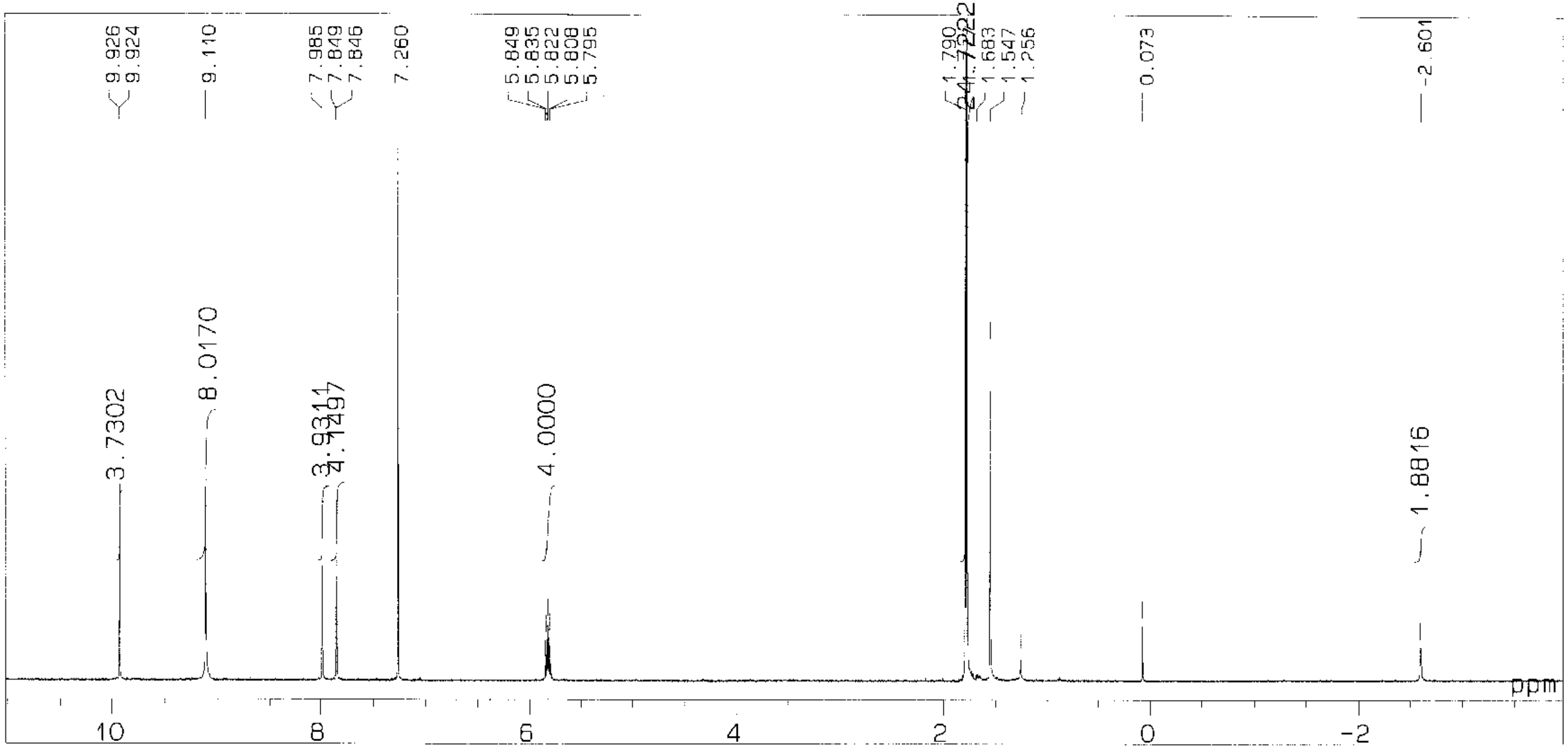
Supporting Figure 1: ^{1}HNMR spectrum of 2-H (500 MHz, DMSO-d_6, 50 ^{o}C)



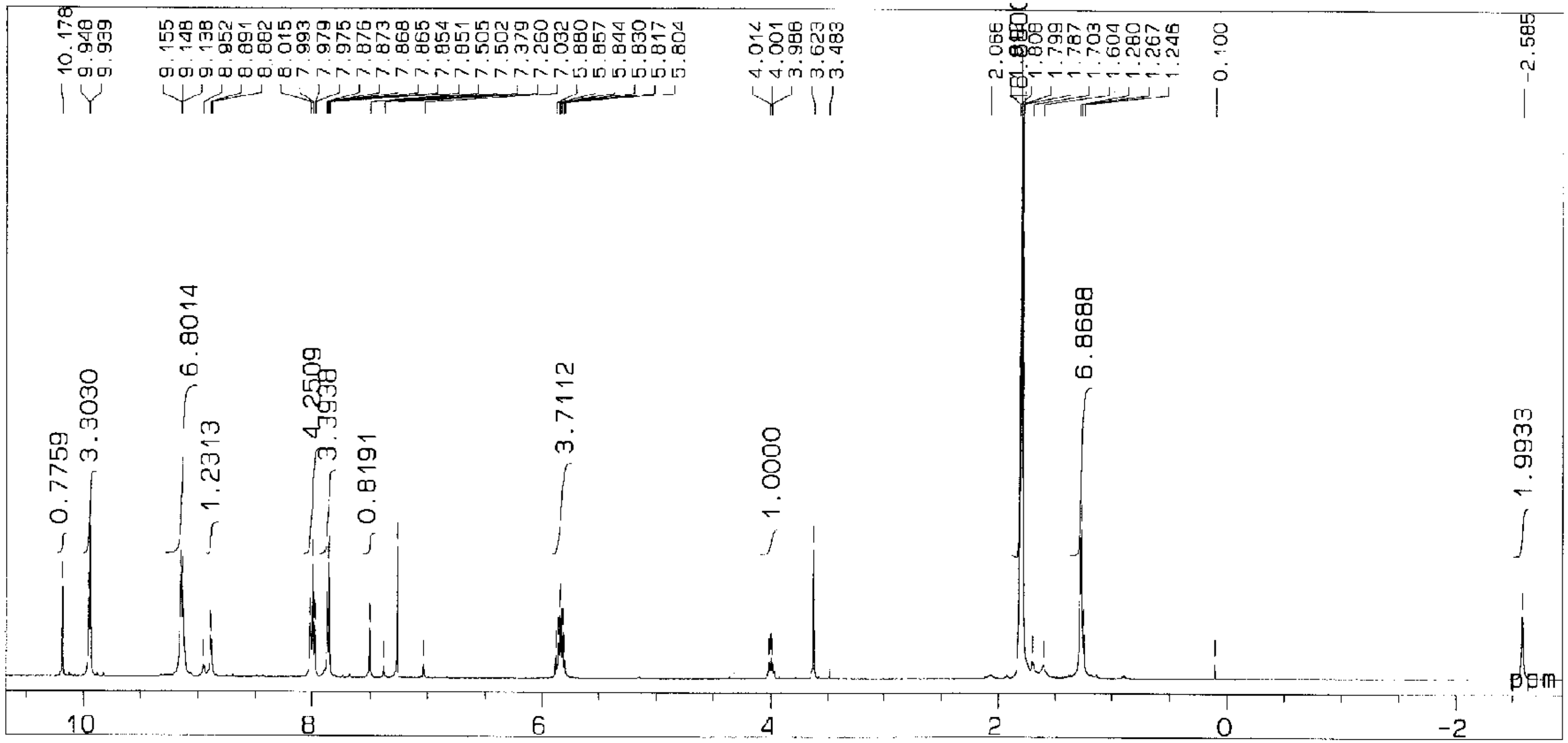
Supporting Figure 2: ^{1}HNMR spectrum of 3-H and 4-H (500 MHz, DMF-d_7, 20 °C)



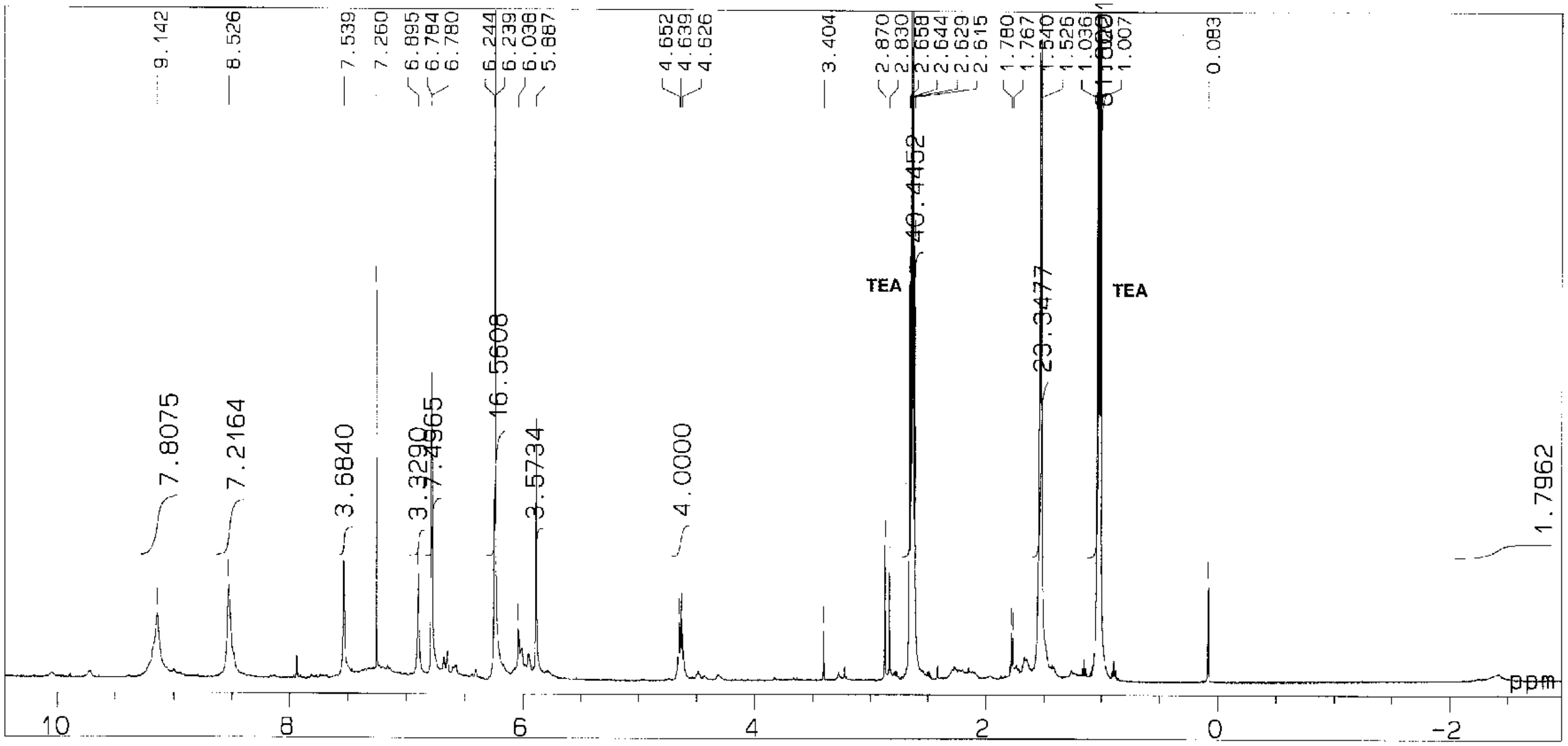
Supporting Figure 3: ^{1}HNMR spectrum of 1-^{i}Pr (500 MHz, $CDCl_3$, 27 °C)



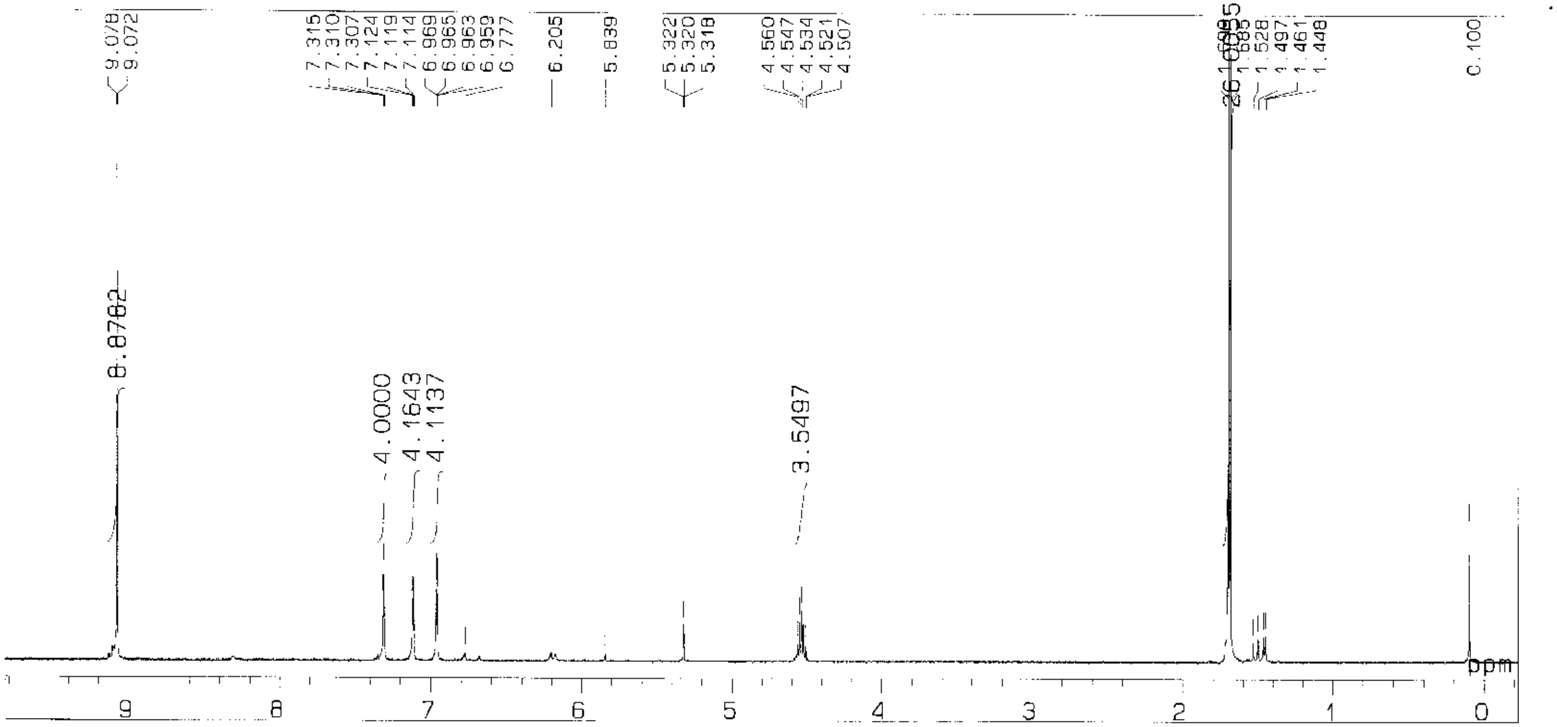
Supporting Figure 4: ^{1}HNMR spectrum of 2-^{i}Pr (500 MHz, $CDCl_3$, 27 °C)



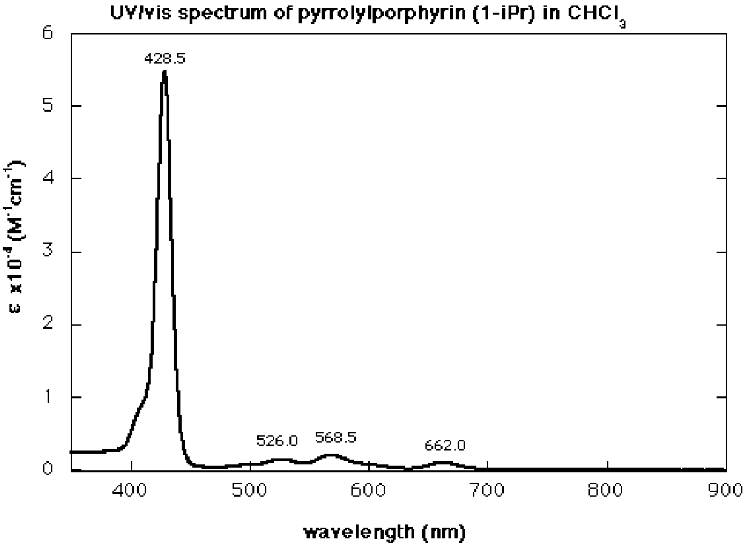
Supporting Figure 5: ^{1}HNMR spectrum of dipyrromethane derivative (8) (500 MHz, $CDCl_3$, r.t.)



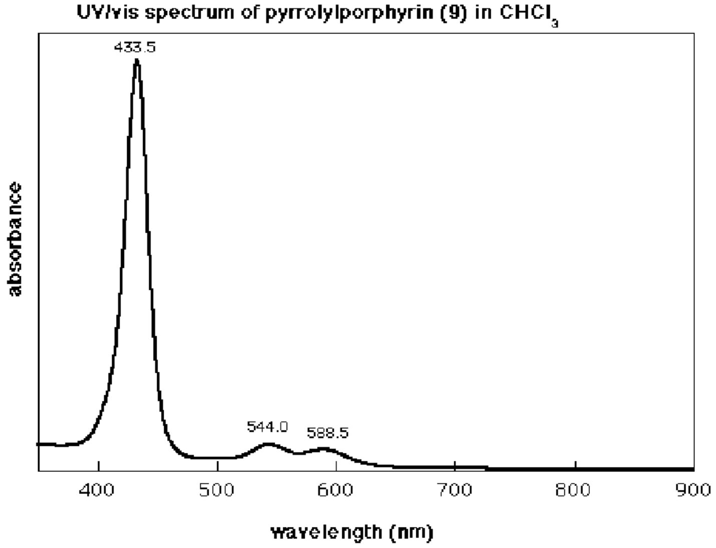
Supporting Figure 6: ^{1}HNMR spectrum of Ni-1-*i*Pr (9) (500 MHz, CD_2Cl_2, r.t.)



Supporting Figure 7



Supporting Figure 8



Supporting X-ray Information for pyrrolylporphyrin (1-*i*Pr)

X-ray Experimental.

Crystallographic Data for pyrrolylporphyrin (**1-*i*Pr**).

Table 1. Atomic Coordinates and Biso/Beq for pyrrolylporphyrin (**1-*i*Pr**).

Table 2. Anisotropic displacement parameters for pyrrolylporphyrin (**1-*i*Pr**).

Table 3. Bond lengths (Å) for pyrrolylporphyrin (**1-*i*Pr**).

Table 4. Bond Angles (°) for pyrrolylporphyrin (**1-*i*Pr**).

Table 5. Tortion Angles (°) for pyrrolylporphyrin (**1-*i*Pr**).

Table 6. Non-bonded Contacts out to 3.60 Å for pyrrolylporphyrin (**1-*i*Pr**).

Table 7. Least Squares Planes.

Supporting Figure 9. View of $C_{52}H_{50}N_8O_4$, pyrrolylporphyrin (**1-*i*Pr**), showing the atom labeling scheme. Thermal ellipsoids are scaled to the 50% probability level. Hydrogen atoms shown are drawn to an arbitrary scale.

Supporting Figure 10. Side view of pyrrolylporphyrin (**1-*i*Pr**).

Supporting Figure 11. Unit cell packing diagram for pyrrolylporphyrin (**1-*i*Pr**).

Experimental

Data Collection

A colorless prismatic crystal of $C_{52}H_{50}N_8O_4$ having approximate dimensions of 0.80 x 0.30 x 0.10 mm was mounted on a glass fiber. All measurements were made on a Rigaku AFC7S diffractometer with graphite monochromated Mo-Kα radiation.

Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the setting angles of 20 carefully centered reflections in the range $6.91 < 2\theta < 12.25^o$ corresponded to a primitive monoclinic cell with dimensions:

a = 7.308(6) Å
b = 23.279(5) Å β = 98.12(5)^o
c = 14.447(6) Å
V = 2433(2) Å^3

For Z = 2 and F.W. = 851.02, the calculated density is 1.16 g/cm^3. The systematic absences of:

h0l: l ± 2n
0k0: k ± 2n

uniquely determine the space group to be:

$P2_1/c$ (#14)

The data were collected at a temperature of 23 $\underline{+}$ 1^{o}C using the ω-2θ scan technique to a maximum 2θ value of 55.0^o. Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.39^o with a take-off angle of 6.0^o. Scans of $(1.42 + 0.30 \tan\theta)^o$ were made at a speed of 8.0^o/min (in ω). The weak reflections ($I < 10.0\sigma(I)$) were rescanned (maximum of 5 scans) and the counts were accumulated to ensure good counting statistics. Stationary background counts were recorded on each side of the reflection. The ratio of peak counting time to background counting time was 2:1. The diameter of the incident beam collimator was 1.0 mm and the crystal to detector distance was 235 mm. The computer-controlled slits were set to 9.0 mm (horizontal) and 13.0 mm (vertical).

Data Reduction

Of the 5065 reflections which were collected, 4631 were unique ($R_{int} = 0.097$); equivalent reflections were merged. The intensities of three representative reflections were measured after every 150 reflections. No decay correction was applied.

The linear absorption coefficient, μ, for Mo-Kα radiation is 0.8 cm^{-1}. Azimuthal scans of several reflections indicated no need for an absorption correction. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement[3] on F was based on 1148 observed reflections ($I > 2.00\sigma(I)$) and 289 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma \,||Fo| - |Fc|| \,/\, \Sigma\, |Fo| = 0.076$$

$$R_W = [\, \Sigma\, w\, (|Fo| - |Fc|)^2 \,/\, \Sigma\, w\, Fo^2]^{1/2} = 0.063$$

The standard deviation of an observation of unit weight[4] was 2.03. The weighting scheme was based on counting statistics and included a factor ($p = 0.004$) to downweight the intense reflections. Plots of $\Sigma\, w\, (|Fo| - |Fc|)^2$ versus $|Fo|$, reflection order in data collection, $\sin \theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.34 and -0.31 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and

Hubbell[8]. All calculations were performed using the teXsan[9] crystallographic software package of Molecular Structure Corporation.

References

(1) SIR92: Altomare, A., Cascarano, M., Giacovazzo, C., Guagliardi, A. (1993). J. Appl. Cryst., 26, 343.

(2) DIRDIF94: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1994). The DIRDIF-94 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least Squares function minimized:

$\Sigma w(|F_o|-|F_c|)^2$ where

$w = 1/[\sigma^2(Fo)] = [\sigma^2{}_c(Fo) + p^2Fo^2/4]^{-1}$

$\sigma_c(Fo)$ = e.s.d. based on counting statistics

p = p-factor

(4) Standard deviation of an observation of unit weight:

$[\Sigma w(|F_o|-|F_c|)^2/(N_o-N_v)]^{1/2}$

where: N_o = number of observations

N_v = number of variables

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) teXsan for Windows: Crystal Structure Analysis Package, Molecular Structure Corporation (1997).

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{52}H_{50}N_8O_4$
Formula Weight	851.02
Crystal Color, Habit	violet, prismatic
Crystal Dimensions	0.80 X 0.30 X 0.10 mm
Crystal System	monoclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	20 (6.9 - 12.3^{o})
Omega Scan Peak Width at Half-height	0.39^{o}
Lattice Parameters	a = 7.308(6) Å b = 23.279(5) Å c = 14.447(6) Å β = 98.12(5) ^{o} V = 2433(2) Å^3
Space Group	$P2_1/c$ (#14)
Z value	2
D_{calc}	1.161 g/cm^3
F_{000}	900.00
μ(MoKα)	0.75 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC7S
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Attenuator	Zr foil (factor = 8.63)

Take-off Angle	6.0^{o}
Detector Aperture	9.0 mm horizontal 13.0 mm vertical
Crystal to Detector Distance	235 mm
Voltage, Current	50 kV, 30 mA
Temperature	23.0^{o}C
Scan Type	ω-2θ
Scan Rate	8.0^{o}/min (in ω) (up to 5 scans)
Scan Width	$(1.42 + 0.30 \tan \theta)^{o}$
$2\theta_{max}$	55.0^{o}
No. of Reflections Measured	Total: 5065 Unique: 4631 (R_{int} = 0.097)
Corrections	Lorentz-polarization

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares on F
Function Minimized	Σ w $(\lvert Fo\rvert - \lvert Fc\rvert)^2$
Least Squares Weights	$w = 1/[\sigma^2(Fo)] = [\sigma^2_c(Fo) + p^2Fo^2/4]^{-1}$
p-factor	0.0041
Anomalous Dispersion	All non-hydrogen atoms
No. Observations ($I>2.00\sigma(I)$)	1148
No. Variables	289
Reflection/Parameter Ratio	3.97
Residuals: R; Rw	0.076 ; 0.063
Goodness of Fit Indicator	2.03
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.34 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.31 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
O(1)	2.1592(7)	-0.0746(3)	1.3754(4)	7.2(2)
O(2)	0.708(1)	0.2191(3)	1.5070(5)	9.7(3)
N(1)	1.2304(8)	-0.0551(3)	0.9943(4)	3.2(2)
N(2)	1.1298(8)	0.0348(3)	1.1182(4)	2.9(2)
N(3)	1.7451(9)	-0.0635(3)	1.3452(4)	4.3(2)
N(4)	0.754(1)	0.2215(3)	1.3000(5)	6.4(3)
C(1)	1.245(1)	-0.0934(3)	0.9236(5)	3.8(2)
C(2)	1.423(1)	-0.1196(4)	0.9461(6)	4.4(3)
C(3)	1.504(1)	-0.0984(4)	1.0312(5)	3.9(2)
C(4)	1.3854(9)	-0.0570(3)	1.0595(5)	3.0(2)
C(5)	1.422(1)	-0.0223(3)	1.1414(5)	3.0(2)
C(6)	1.305(1)	0.0228(4)	1.1620(5)	3.3(2)
C(7)	1.356(1)	0.0616(4)	1.2383(5)	4.2(2)
C(8)	1.211(1)	0.0967(4)	1.2421(5)	4.1(2)
C(9)	1.068(1)	0.0789(4)	1.1673(5)	3.3(2)
C(10)	0.895(1)	0.1044(3)	1.1529(5)	3.5(2)
C(11)	1.873(1)	-0.0554(4)	1.2862(6)	4.1(2)
C(12)	1.769(1)	-0.0398(3)	1.1991(5)	3.9(2)
C(13)	1.585(1)	-0.0366(3)	1.2088(5)	3.2(2)
C(14)	1.574(1)	-0.0514(4)	1.3013(5)	4.0(2)
C(15)	0.774(1)	0.1770(4)	1.3640(6)	5.0(3)
C(16)	0.832(1)	0.1295(4)	1.3177(6)	4.2(2)
C(17)	0.841(1)	0.1432(4)	1.2252(5)	3.9(2)
C(18)	0.795(1)	0.2006(4)	1.2177(6)	6.3(3)
C(19)	1.789(1)	-0.0846(5)	1.4431(6)	6.5(3)
C(20)	1.751(3)	-0.1443(7)	1.446(1)	20.6(8)
C(21)	1.681(3)	-0.0541(8)	1.5042(7)	20.9(8)
C(22)	0.695(3)	0.2830(6)	1.315(1)	12.9(6)
C(23)	0.881(4)	0.3130(7)	1.344(2)	30(1)
C(24)	0.535(4)	0.297(1)	1.268(1)	39(2)
C(25)	2.064(1)	-0.0623(4)	1.3020(6)	5.5(3)
C(26)	0.752(2)	0.1786(5)	1.4624(6)	7.1(3)

H(1)	1.4763	-0.1471	0.9089	5.300
H(2)	1.6193	-0.1100	1.0647	4.699
H(3)	1.4709	0.0622	1.2786	5.015
H(4)	1.2038	0.1272	1.2852	4.802
H(5)	1.1271	-0.0308	0.9974	3.887
H(6)	1.8192	-0.0329	1.1428	4.647
H(7)	1.4639	-0.0529	1.3290	4.824
H(8)	0.8611	0.0928	1.3456	5.011

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(9)	0.7926	0.2226	1.1621	7.597
H(10)	1.9171	-0.0778	1.4639	7.737
H(11)	1.7445	-0.1572	1.5070	24.955
H(12)	1.6408	-0.1538	1.4057	24.955
H(13)	1.8518	-0.1657	1.4227	24.955
H(14)	1.7268	-0.0615	1.5675	25.416
H(15)	1.6918	-0.0129	1.4937	25.416
H(16)	1.5555	-0.0641	1.4908	25.416
H(17)	0.6585	0.2781	1.3749	15.593
H(18)	0.9086	0.3132	1.4132	37.786
H(19)	0.9810	0.2893	1.3249	37.786
H(20)	0.8872	0.3492	1.3219	37.786
H(21)	0.4230	0.3139	1.2855	48.056
H(22)	0.5900	0.3319	1.2254	40.609
H(23)	0.5019	0.2711	1.2207	40.609
H(24)	2.1269	-0.0569	1.2494	6.641
H(25)	0.7755	0.1437	1.4961	8.359

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta$
$+ 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	0.046(4)	0.135(7)	0.086(5)	0.009(4)	-0.008(4)	0.048(5)
O(2)	0.199(8)	0.112(7)	0.066(5)	0.036(6)	0.053(5)	-0.022(5)
N(1)	0.049(4)	0.037(5)	0.035(4)	0.023(4)	0.001(3)	0.003(3)
N(2)	0.032(4)	0.044(5)	0.033(4)	0.005(3)	0.005(3)	-0.003(3)
N(3)	0.044(5)	0.072(6)	0.044(4)	-0.004(4)	-0.002(4)	0.016(4)
N(4)	0.147(8)	0.063(7)	0.036(5)	0.021(6)	0.020(5)	0.007(5)
C(1)	0.071(7)	0.048(7)	0.028(5)	-0.001(5)	0.017(5)	-0.007(4)
C(2)	0.047(6)	0.058(7)	0.060(6)	0.029(5)	-0.003(5)	0.000(5)
C(3)	0.043(5)	0.050(6)	0.050(6)	0.008(5)	-0.016(4)	0.002(5)
C(4)	0.030(5)	0.047(6)	0.038(5)	0.026(4)	0.004(4)	0.012(4)
C(5)	0.041(5)	0.044(6)	0.029(4)	-0.006(5)	0.006(4)	0.005(4)
C(6)	0.042(5)	0.049(6)	0.036(5)	0.001(5)	0.006(4)	0.001(5)
C(7)	0.045(6)	0.062(7)	0.048(6)	0.001(5)	-0.006(4)	-0.007(5)
C(8)	0.065(6)	0.053(7)	0.033(5)	-0.003(5)	-0.006(4)	-0.004(4)
C(9)	0.041(5)	0.057(6)	0.026(5)	0.015(5)	-0.001(4)	-0.007(4)
C(10)	0.077(6)	0.026(5)	0.029(5)	-0.004(5)	0.008(5)	-0.007(4)
C(11)	0.027(5)	0.060(7)	0.070(7)	-0.011(5)	0.009(5)	0.013(5)
C(12)	0.056(6)	0.060(7)	0.030(5)	0.012(5)	0.001(4)	0.009(4)
C(13)	0.026(5)	0.055(6)	0.039(5)	0.004(4)	-0.004(4)	0.004(4)
C(14)	0.028(5)	0.083(7)	0.040(5)	0.002(5)	0.002(4)	-0.001(5)
C(15)	0.086(7)	0.068(8)	0.035(5)	0.018(6)	0.004(5)	-0.015(6)
C(16)	0.067(6)	0.048(6)	0.043(5)	0.003(5)	-0.000(5)	0.009(5)
C(17)	0.074(6)	0.035(6)	0.034(5)	0.003(5)	-0.005(4)	0.008(5)
C(18)	0.134(9)	0.066(9)	0.046(6)	0.003(7)	0.033(6)	0.009(6)
C(19)	0.072(7)	0.13(1)	0.040(6)	-0.002(7)	-0.011(5)	0.041(7)
C(20)	0.40(3)	0.20(2)	0.14(1)	-0.12(2)	-0.11(2)	0.14(1)
C(21)	0.39(2)	0.38(3)	0.024(7)	0.25(2)	0.03(1)	0.06(1)
C(22)	0.26(2)	0.06(1)	0.19(2)	0.06(1)	0.08(2)	-0.06(1)
C(23)	0.59(5)	0.08(1)	0.55(4)	-0.14(2)	0.38(4)	-0.14(2)
C(24)	0.76(6)	0.33(3)	0.29(3)	0.47(4)	-0.31(3)	-0.17(2)
C(25)	0.038(6)	0.107(9)	0.064(6)	0.004(6)	0.003(5)	0.040(6)

C(26)	0.16(1)	0.076(9)	0.037(6)	0.021(8)	0.013(6)	0.016(6)

The general temperature factor expression:
$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 3. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
O(1)	C(25)	1.22(1)	O(2)	C(26)	1.21(1)
N(1)	C(1)	1.37(1)	N(1)	C(4)	1.37(1)
N(1)	H(5)	0.95	N(2)	C(6)	1.37(1)
N(2)	C(9)	1.36(1)	N(3)	C(11)	1.37(1)
N(3)	C(14)	1.35(1)	N(3)	C(19)	1.49(1)
N(4)	C(15)	1.38(1)	N(4)	C(18)	1.36(1)
N(4)	C(22)	1.52(2)	C(1)	C(2)	1.43(1)
C(1)	C(10)	1.42(1)	C(2)	C(3)	1.38(1)
C(2)	H(1)	0.95	C(3)	C(4)	1.40(1)
C(3)	H(2)	0.95	C(4)	C(5)	1.43(1)
C(5)	C(6)	1.41(1)	C(5)	C(13)	1.46(1)
C(6)	C(7)	1.43(1)	C(7)	C(8)	1.35(1)
C(7)	H(3)	0.95	C(8)	C(9)	1.45(1)
C(8)	H(4)	0.95	C(9)	C(10)	1.39(1)
C(10)	C(17)	1.47(1)	C(11)	C(12)	1.42(1)
C(11)	C(25)	1.39(1)	C(12)	C(13)	1.38(1)
C(12)	H(6)	0.95	C(13)	C(14)	1.39(1)
C(14)	H(7)	0.95	C(15)	C(16)	1.39(1)
C(15)	C(26)	1.45(2)	C(16)	C(17)	1.38(1)
C(16)	H(8)	0.95	C(17)	C(18)	1.38(1)

Table 3. Bond Lengths(Å) (continued)

atom	atom	distance	atom	atom	distance
C(18)	H(9)	0.95	C(19)	C(20)	1.42(2)
C(19)	C(21)	1.45(2)	C(19)	H(10)	0.95
C(20)	H(11)	0.93	C(20)	H(12)	0.95
C(20)	H(13)	0.99	C(21)	H(14)	0.94
C(21)	H(15)	0.98	C(21)	H(16)	0.94
C(22)	C(23)	1.54(4)	C(22)	C(24)	1.31(3)
C(22)	H(17)	0.95	C(23)	H(18)	0.99
C(23)	H(19)	0.98	C(23)	H(20)	0.91
C(24)	H(21)	0.97	C(24)	H(22)	1.12
C(24)	H(23)	0.92	C(25)	H(24)	0.95
C(26)	H(25)	0.95			

Table 4. Bond Angles(^{o})

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	N(1)	C(4)	110.3(9)	C(1)	N(1)	H(5)	124.8
C(4)	N(1)	H(5)	124.9	C(6)	N(2)	C(9)	105.6(8)
C(11)	N(3)	C(14)	110.4(9)	C(11)	N(3)	C(19)	124(1)
C(14)	N(3)	C(19)	125(1)	C(15)	N(4)	C(18)	108(1)
C(15)	N(4)	C(22)	128(1)	C(18)	N(4)	C(22)	124(1)
N(1)	C(1)	C(2)	105.8(9)	N(1)	C(1)	C(10)	125(1)
C(2)	C(1)	C(10)	129(1)	C(1)	C(2)	C(3)	108(1)
C(1)	C(2)	H(1)	126.0	C(3)	C(2)	H(1)	125.9
C(2)	C(3)	C(4)	107.7(9)	C(2)	C(3)	H(2)	126.1
C(4)	C(3)	H(2)	126.2	N(1)	C(4)	C(3)	108(1)
N(1)	C(4)	C(5)	126(1)	C(3)	C(4)	C(5)	125.6(9)
C(4)	C(5)	C(6)	123(1)	C(4)	C(5)	C(13)	118(1)
C(6)	C(5)	C(13)	119(1)	N(2)	C(6)	C(5)	127(1)
N(2)	C(6)	C(7)	111(1)	C(5)	C(6)	C(7)	122(1)
C(6)	C(7)	C(8)	107(1)	C(6)	C(7)	H(3)	126.4
C(8)	C(7)	H(3)	126.6	C(7)	C(8)	C(9)	106(1)
C(7)	C(8)	H(4)	126.7	C(9)	C(8)	H(4)	126.9
N(2)	C(9)	C(8)	110.4(9)	N(2)	C(9)	C(10)	127.3(9)
C(8)	C(9)	C(10)	122(1)	C(1)	C(10)	C(9)	126(1)
C(1)	C(10)	C(17)	115(1)	C(9)	C(10)	C(17)	119(1)

Table 4. Bond Angles(^{o}) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
N(3)	C(11)	C(12)	105.0(9)	N(3)	C(11)	C(25)	130(1)
C(12)	C(11)	C(25)	125(1)	C(11)	C(12)	C(13)	109.5(9)
C(11)	C(12)	H(6)	125.3	C(13)	C(12)	H(6)	125.2
C(5)	C(13)	C(12)	131(1)	C(5)	C(13)	C(14)	123.0(9)
C(12)	C(13)	C(14)	105.7(8)	N(3)	C(14)	C(13)	109.3(9)
N(3)	C(14)	H(7)	125.4	C(13)	C(14)	H(7)	125.3
N(4)	C(15)	C(16)	107(1)	N(4)	C(15)	C(26)	128(1)
C(16)	C(15)	C(26)	125(1)	C(15)	C(16)	C(17)	110(1)
C(15)	C(16)	H(8)	124.9	C(17)	C(16)	H(8)	125.1
C(10)	C(17)	C(16)	127(1)	C(10)	C(17)	C(18)	129(1)
C(16)	C(17)	C(18)	105(1)	N(4)	C(18)	C(17)	111(1)
N(4)	C(18)	H(9)	124.6	C(17)	C(18)	H(9)	124.2
N(3)	C(19)	C(20)	110(1)	N(3)	C(19)	C(21)	111(1)
N(3)	C(19)	H(10)	108.4	C(20)	C(19)	C(21)	109(2)
C(20)	C(19)	H(10)	109.9	C(21)	C(19)	H(10)	108.8
C(19)	C(20)	H(11)	112.5	C(19)	C(20)	H(12)	111.0
C(19)	C(20)	H(13)	108.7	H(11)	C(20)	H(12)	110.8
H(11)	C(20)	H(13)	107.6	H(12)	C(20)	H(13)	105.9
C(19)	C(21)	H(14)	110.4	C(19)	C(21)	H(15)	108.9
C(19)	C(21)	H(16)	110.6	H(14)	C(21)	H(15)	107.8

Table 4. Bond Angles(^{o}) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
H(14)	C(21)	H(16)	110.9	H(15)	C(21)	H(16)	108.2
N(4)	C(22)	C(23)	102(2)	N(4)	C(22)	C(24)	115(2)
N(4)	C(22)	H(17)	97.9	C(23)	C(22)	C(24)	136(3)
C(23)	C(22)	H(17)	99.0	C(24)	C(22)	H(17)	99.2
C(22)	C(23)	H(18)	108.9	C(22)	C(23)	H(19)	109.4
C(22)	C(23)	H(20)	114.1	H(18)	C(23)	H(19)	103.8
H(18)	C(23)	H(20)	109.8	H(19)	C(23)	H(20)	110.4
C(22)	C(24)	H(21)	133.4	C(22)	C(24)	H(22)	95.8
C(22)	C(24)	H(23)	109.4	H(21)	C(24)	H(22)	104.2
H(21)	C(24)	H(23)	108.6	H(22)	C(24)	H(23)	98.6
O(1)	C(25)	C(11)	127(1)	O(1)	C(25)	H(24)	116.6
C(11)	C(25)	H(24)	116.1	O(2)	C(26)	C(15)	128(1)
O(2)	C(26)	H(25)	115.8	C(15)	C(26)	H(25)	116.2

Table 5. Torsion Angles(^{o})

atom	atom	atom	atom	angle
O(1)	C(25)	C(11)	N(3)	-4(3)
O(2)	C(26)	C(15)	N(4)	2(3)
N(1)	C(1)	C(2)	C(3)	3(1)
N(1)	C(1)	C(10)	C(17)	174(1)
N(1)	C(4)	C(5)	C(6)	-5(2)
N(2)	C(6)	C(5)	C(4)	11(2)
N(2)	C(6)	C(7)	C(8)	1(1)
N(2)	C(9)	C(10)	C(1)	-8(2)
N(3)	C(11)	C(12)	C(13)	3(1)
N(3)	C(14)	C(13)	C(12)	-0(1)
N(4)	C(18)	C(17)	C(10)	-180(1)
C(1)	N(1)	C(4)	C(3)	-1(1)
C(1)	C(2)	C(3)	C(4)	-4(1)
C(2)	C(1)	N(1)	C(4)	-1(1)
C(2)	C(1)	C(10)	C(17)	-8(2)
C(3)	C(2)	C(1)	C(10)	-175(1)
C(3)	C(4)	C(5)	C(13)	-9(2)
C(4)	C(5)	C(6)	C(7)	-172(1)
C(4)	C(5)	C(13)	C(14)	-120(1)
C(5)	C(6)	C(7)	C(8)	-176(1)
O(1)	C(25)	C(11)	C(12)	179(1)
O(2)	C(26)	C(15)	C(16)	177(2)
N(1)	C(1)	C(10)	C(9)	-1(2)
N(1)	C(4)	C(3)	C(2)	3(1)
N(1)	C(4)	C(5)	C(13)	172(1)
N(2)	C(6)	C(5)	C(13)	-166(1)
N(2)	C(9)	C(8)	C(7)	-2(1)
N(2)	C(9)	C(10)	C(17)	167(1)
N(3)	C(14)	C(13)	C(5)	179(1)
N(4)	C(15)	C(16)	C(17)	-3(2)
N(4)	C(18)	C(17)	C(16)	-1(2)
C(1)	N(1)	C(4)	C(5)	178(1)
C(1)	C(10)	C(9)	C(8)	-173(1)
C(2)	C(1)	C(10)	C(9)	177(1)
C(2)	C(3)	C(4)	C(5)	-176(1)
C(3)	C(4)	C(5)	C(6)	174(1)
C(4)	N(1)	C(1)	C(10)	177(1)
C(4)	C(5)	C(13)	C(12)	58(2)
C(5)	C(6)	N(2)	C(9)	175(1)
C(5)	C(13)	C(12)	C(11)	180(1)

Table 6. Non-bonded Contacts out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
O(1)	H(25)	2.4518	85803	O(1)	H(7)	2.4669	65501
O(1)	H(15)	2.8862	95803	O(1)	H(16)	3.1404	65501
O(1)	H(22)	3.3121	84702	O(1)	H(20)	3.3335	84702
O(1)	H(14)	3.3503	95803	O(1)	C(26)	3.37(2)	85803
O(1)	C(14)	3.40(1)	65501	O(1)	C(21)	3.58(3)	95803
O(2)	H(9)	2.6187	4	O(2)	H(12)	3.3643	75803
O(2)	H(13)	3.4624	85803	O(2)	C(18)	3.55(2)	4
O(2)	H(22)	3.5883	4	O(2)	H(11)	3.5888	75803
N(1)	H(6)	2.8364	85703	N(1)	H(18)	3.5486	74702
N(1)	C(12)	3.56(1)	85703	N(2)	H(6)	2.8270	45501
N(2)	H(24)	2.8568	45501	N(2)	C(12)	3.49(1)	45501
N(2)	C(25)	3.57(1)	45501	N(3)	H(22)	3.5020	74702
N(3)	H(21)	3.5452	74702	C(1)	H(6)	3.1072	85703
C(1)	H(18)	3.5066	74702	C(1)	C(12)	3.57(2)	85703
C(2)	C(6)	3.51(2)	85703	C(2)	C(7)	3.57(2)	85703
C(3)	H(21)	3.3256	74702	C(3)	H(17)	3.4581	74702
C(4)	H(24)	3.5440	45501	C(4)	H(20)	3.5551	74702
C(5)	H(24)	2.9460	45501	C(6)	H(24)	2.6813	45501
C(6)	C(25)	3.48(2)	45501	C(6)	H(1)	3.5269	85703
C(7)	H(14)	2.9542	85803	C(7)	H(24)	3.2425	45501

Table 6. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
C(7)	H(1)	3.2731	85703	C(8)	H(14)	2.8446	85803
C(8)	H(1)	3.5721	85703	C(9)	H(6)	3.1667	45501
C(9)	H(24)	3.3813	45501	C(9)	C(12)	3.59(2)	45501
C(10)	H(6)	3.2416	45501	C(10)	C(12)	3.57(2)	45501
C(11)	H(20)	3.3481	84702	C(11)	H(8)	3.5600	65501
C(12)	H(5)	3.4550	85703	C(13)	H(21)	3.4824	74702
C(13)	H(22)	3.5004	74702	C(13)	H(24)	3.5086	45501
C(14)	H(22)	2.9733	74702	C(14)	H(24)	3.2519	45501
C(14)	H(21)	3.3784	74702	C(15)	H(3)	3.5783	45501
C(16)	H(3)	3.0550	45501	C(17)	H(3)	3.4732	45501
C(19)	H(25)	3.4628	85803	C(20)	H(22)	3.3061	74702
C(20)	H(23)	3.4431	74702	C(20)	H(25)	3.4430	85803
C(20)	H(21)	3.5483	74702	C(21)	H(15)	3.1424	85803
C(21)	H(16)	3.2557	85803	C(21)	H(3)	3.4782	85803
C(21)	H(4)	3.4844	85803	C(23)	H(24)	3.3147	85702
C(24)	H(12)	2.8812	75702	C(24)	H(2)	3.5409	75702
C(25)	H(20)	2.7838	84702	C(25)	H(7)	2.9005	65501
C(25)	H(25)	3.5369	85803	C(25)	H(22)	3.5904	84702
C(26)	H(13)	3.1420	85803	C(26)	H(10)	3.4288	85803
H(1)	H(3)	3.4182	85703	H(2)	H(21)	2.8470	74702

Table 6. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
H(2)	H(17)	3.4882	74702	H(3)	H(14)	2.8179	85803
H(3)	H(8)	2.9660	65501	H(3)	H(16)	3.3643	85803
H(4)	H(14)	2.6112	85803	H(4)	H(11)	3.0544	85803
H(5)	H(6)	2.5832	85703	H(5)	H(6)	3.2895	45501
H(6)	H(20)	3.4773	84702	H(7)	H(24)	2.5684	45501
H(7)	H(22)	2.8080	74702	H(7)	H(15)	3.3201	85803
H(7)	H(14)	3.4435	85803	H(8)	H(10)	3.0112	85803
H(8)	H(14)	3.1795	85803	H(8)	H(15)	3.5938	45501
H(10)	H(25)	2.7142	85803	H(10)	H(15)	3.5368	95803
H(11)	H(25)	3.5285	85803	H(12)	H(22)	2.3748	74702
H(12)	H(23)	2.6335	74702	H(12)	H(21)	2.8376	74702
H(12)	H(25)	3.5418	75803	H(13)	H(25)	2.8562	85803
H(13)	H(21)	3.4054	74702	H(13)	H(23)	3.4080	74702
H(14)	H(15)	3.5182	85803	H(15)	H(16)	2.5784	85803
H(15)	H(15)	2.8982	85803	H(16)	H(25)	3.0741	75803
H(16)	H(16)	3.1160	85803	H(19)	H(21)	3.4068	65501
H(20)	H(24)	2.4124	85702	H(22)	H(24)	3.3023	85702

The ADC (atom designator code) specifies the position of an atom in a crystal. The 5-digit number shown in the table is a composite of three one-digit numbers and one two-digit number: TA (first digit) + TB (second digit) + TC (third digit) + SN (last two digits). TA, TB and TC are the crystal lattice translation digits along cell edges a, b and c. A translation digit of 5 indicates the origin unit cell. If TA = 4, this indicates a translation of one unit cell length along the a-axis in the negative direction. Each translation digit can range in value from 1 to 9 and thus ±4 lattice translations from the origin (TA=5, TB=5, TC=5) can be represented.

The SN, or symmetry operator number, refers to the number of the symmetry operator used to generate the coordinates of the target atom. A list of symmetry operators relevant to this structure is given below.

For a given intermolecular contact, the first atom (origin atom) is located in the origin unit cell and its position can be generated using the identity operator (SN=1). Thus, the ADC for an origin atom is always 55501. The position of the second atom (target atom) can be generated using the ADC and the coordinates of the atom in the parameter table. For example, an ADC of 47502 refers to the target atom moved through symmetry operator two, then translated -1 cell translations along the a axis, +2 cell translations along the b axis, and 0 cell translations along the c axis.

An ADC of 1 indicates an intermolecular contact between two fragments (eg. cation and anion) that reside in the same asymmetric unit.

Symmetry Operators:

(1) +X, +Y, +Z   (2) -X, 1/2+Y, 1/2-Z
(3) -X, -Y, -Z   (4) +X, 1/2-Y, 1/2+Z

Table 7. Least Squares Planes

Plane number 1

Atoms defining plane	Distance
N(1)	0.004(8)
N(2)	-0.034(8)
C(1)	0.08(1)
C(2)	0.09(1)
C(3)	-0.05(1)
C(4)	-0.06(1)
C(5)	-0.12(1)
C(6)	-0.00(1)
C(7)	0.11(1)
C(8)	0.12(1)
C(9)	0.01(1)
C(10)	-0.07(1)

Plane number 2

Atoms defining plane	Distance
N(3)	-0.011(9)
C(11)	0.02(1)
C(12)	-0.01(1)
C(13)	0.00(1)
C(14)	0.01(1)

Plane number 3

Atoms defining plane	Distance
N(4)	0.01(1)
C(15)	-0.01(1)
C(16)	0.01(1)

C(17)	-0.01(1)
C(18)	0.01(1)

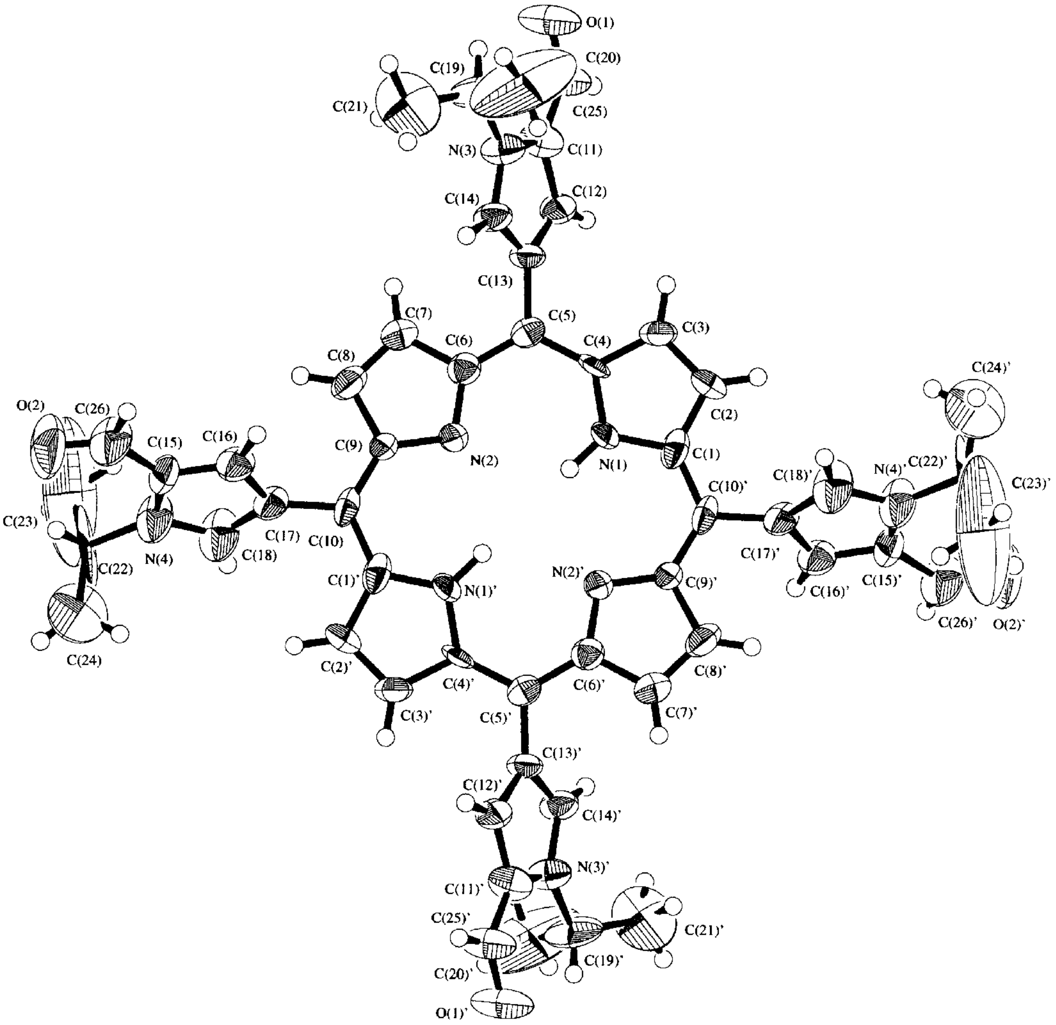
Summary

plane	mean deviation	χ^2
1	0.0635	679.2
2	0.0100	4.6
3	0.0099	3.4

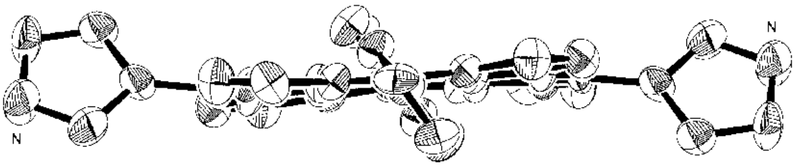
Dihedral angles between planes (°)

plane	1	2
2	57.59	
3	61.41	67.40

Supporting Figure 9: Top view of 1-^{i}Pr



Supporting Figure 10: Side view of 1-^{i}Pr



Supporting Figure 11: Unit cell packing diagram of 1-^{i}Pr