Supporting Information

N-doped Nonalternant Aromatic Belt via a Six-fold Double N-Arylation

Hiroki Sato,¹ Rie Suizu,²,³ Tomoki Kato,² Akiko Yagi,¹ Yasutomo Segawa,²,⁴,⁵,⁶,,* Kunio Awaga,²,⁷ and Kenichiro Itami¹,²,⁶,⁷,*

¹ Institute of Transformative Bio-Molecules (WPI-ITbM), Nagoya University, Chikusa, Nagoya 464-8602, Japan
² Graduate School of Science, Nagoya University, Chikusa, Nagoya 464-8602, Japan
³ Japan Science and Technology Agency (JST), PRESTO, 4-1-8 Honcho, Kawaguchi, Saitama, 332-0012, Japan
⁴ Institute for Molecular Science, Myodaiji, Okazaki, 444-8787, Japan.
⁵ Department of Structural Molecular Science, SOKENDAI (The Graduate University for Advanced Studies), Myodaiji, Okazaki, 444-8787, Japan.
⁶ JST-ERATO, Itami Molecular Nanocarbon Project, Nagoya University, Chikusa, Nagoya 464-8602, Japan
⁷ Integrated Research Consortium on Chemical Sciences (IRCCS), Nagoya University, Chikusa, Nagoya 464-8602, Japan

*E-mail: segawa@ims.ac.jp (Y.S.), itami@chem.nagoya-u.ac.jp (K.I.)

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1. Instrumentation and chemicals

**Materials.** Unless otherwise noted, all reactions were performed with dry solvents under an atmosphere of nitrogen in dried glassware with standard vacuum-line techniques. Materials were obtained from commercial suppliers and used without further purification. Silver salt Ag[B(C₆F₅)₄] was prepared following the known procedure.¹ Macrocycle precursor 1 was prepared following our previous paper.² Dichloromethane (DCM) for reactions was purified by passing through a solvent purification system (Glass Contour). All work-up and purification procedures were carried out with reagent-grade solvents in air. Analytical thin-layer chromatography (TLC) was performed using E. Merck silica gel 60 F₂₅₄ coated plates (0.25 mm). The developed chromatogram was analyzed by UV lamp (254 nm and 365 nm). Flash column chromatography was performed with E. Merck silica gel 60 (230–400 mesh). Membrane filtration was performed with Merck Milipore Ltd. Millex® LH 0.45 µm. Preparative HPLC was performed using YMC Multiple preparative HPLC LC-Forte/R instrument equipped with YMC-Actus SIL 250 × 30.0 mm S-5 µm 12 nm column.

**Measurements.** Melting points were measured on a MPA100 Optimelt automated melting point system. High-resolution mass spectra (HRMS) were determined on a JEOL JMS-S3000 SpiralTOF (MALDI-TOF MS) using polyethylene glycol mixture (PEG) as internal standards and trans-2-[3-(4-tert-butylphenyl)-2-methyl-2-propenylidene] malononitrile (DCTB) as matrix with NaI as cationizing agent. Nuclear magnetic resonance (NMR) spectra were recorded on JEOL spectrometers (JNM-ECA-600: ¹H 600 MHz, ¹³C 150 MHz; JEOL ECA 500II: ¹H 500 MHz, ¹³C 125 MHz). Chemical shifts for ¹H NMR are expressed in parts per million (ppm) relative to CHDCl₂ (δ 5.32 ppm). ¹³C NMR spectra were run using a proton-decoupled pulse sequence. Chemical shifts for ¹³C NMR are expressed in ppm relative to CD₂Cl₂ (δ 54.0 ppm). The following abbreviations were used to explain the multiplicities: s (singlet), d (doublet), t (triplet), sept (septuplet), m (multiplet). Coupling constants, J, are reported in Hz and with an accuracy of one unit of the last digit.

For photophysical measurements, dilute solutions in degassed spectral grade dichloromethane in a 1 cm square quartz cell were used. UV–vis absorption spectra were recorded on a Shimadzu UV-3510 spectrometer with a resolution of 0.2. UV-Vis-NIR absorption spectra were recorded on a JASCO UV V-570 spectrometer with a resolution of 2 nm between 250 nm to 2500 nm. Fluorescence spectra were recorded with a Shimadzu RF6000 spectrofluorometer using a 0.1
nm bandwidth in both excitation and emission. Absolute FL quantum yields were determined with the same instrument equipped with a calibrated integrating sphere. Electron paramagnetic resonance (EPR) spectra were recorded on JEOL ESR JES TE-200 instruments using quartz Schlenk tube filled with Ar.
2. Synthesis of N-belt (2) and dications salt 2^{2+} \cdot 2[B(C_6F_5)_4]^-

Synthesis of N-belt 2 via a palladium catalyzed 6-fold double N-arylation

To a dry Schlenk tube equipped with argon containing a magnetic stirring bar were added 1 (122.0 mg, 78.1 µmol), p-anisidine (56.7 mg, 460 µmol), Pd(dbaf)_2 (26.4 mg, 45.9 µmol), PMe('Bu)_2\cdot HBF_4 (23.0 mg, 92.7 µmol), and NaO'Bu (211 mg, 2.19 mmol). Then, the flask was replaced by argon gas with a balloon. To this flask was added m-xylene (4.8 mL), and Schlenk tube was capped. After stirring at 140 °C for 8 h, 3.0 g silica gel was added and the solvent was removed by rotary evaporation. After removal of the solvent, the product on silica was put on silica pad and eluted with toluene/EtOAc = 90:10. Then, the filtrate was concentrated and further purified by preparative HPLC (42 mL/min, toluene/EtOAc = 95:5) to afford N-belt 2 (2.4 mg, 1.8 µmol, 2.3%) as a yellow powder. $^1$H NMR (600 MHz, CD$_2$Cl$_2$) δ 7.36 (s, 12H), 6.77 (s, 12H), 6.69 (d, $J = 8.9$ Hz, 12 H), 6.44 (d, $J = 8.9$ Hz, 12H), 3.71 (s, 18H). $^{13}$C NMR (150 MHz, CD$_2$Cl$_2$) δ 153.3, 143.02, 142.97, 138.8, 132.2, 130.7, 114.6, 113.6, 56.1. HRMS (MALDI-TOF, DCTB matrix): Exact mass calculated for C$_{90}$H$_{66}$N$_6$O$_6$ ([M$^+$]): $m/z = 1326.5038$, mass found: 1326.5020; melting point: decomposed ~210 °C. $R_t = 0.2–0.4$ (dichloromethane).
$^1$H NMR spectrum of 2

$^{13}$C NMR spectrum of 2
HRMS (MALDI-TOF) of 2
N-Belt dication $2^{2+}\cdot2[B(C_6F_5)_4]^-$

To a dry Schlenk tube equipped with argon containing a magnetic stirring bar was added N-belt $2$ (2.0 mg, 1.5 μmol). Then, dichloromethane (DCM, 1.5 mL) was added, and the mixture was cooled down to $-30\,^\circ\text{C}$. To the reaction mixture was slowly added 1.0 mM Ag[$B(C_6F_5)_4]$ (3.0 mL, 3.0 μmol) at $-30\,^\circ\text{C}$. Then, the mixture was gradually warmed up to ambient temperature and stirred for 30 min. After stirring, the mixture was concentrated under vacuum until 0.5 mL solvent remained and transferred to a glass tube through membrane filter via syringe. Then, the mixture was slowly diffused in hexane under argon atmosphere at $-30\,^\circ\text{C}$ in dark. After 1 week, purple crystal appeared in the solution, which was filtered and washed by hexane under N$_2$ atmosphere. After dried under vacuum, N-belt dication $2^{2+}\cdot2[B(C_6F_5)_4]^-$ was obtained as a purple crystal.
3. X-ray crystallography

Details of the crystal data and a summary of the intensity data collection parameters are listed in Table S1. A suitable crystal was mounted with mineral oil on a MiTeGen MicroMounts and transferred to the goniometer of the kappa goniometer of a RIGAKU XtaLAB Synergy-S system with 1.2 kW MicroMax-007HF microfocus rotating anode (Graphite-monochromated Mo Kα radiation (λ = 0.71073 Å)) and PILATUS200K hybrid photon-counting detector. Cell parameters were determined and refined, and raw frame data were integrated using CrysAlisPro (Agilent Technologies, 2010). The structures were solved by direct methods with SHELXT³ and refined by full-matrix least-squares techniques against $F^2$ (SHELXL-2018/3)⁴ by using Olex2 software package.⁵ The intensities were corrected for Lorentz and polarization effects. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed using AFIX instructions.

The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed using AFIX instructions. CCDC 2133103 (2) and 2133104 (2²⁺·2[B(C₆F₅)₄]⁻) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystallographic data for 2 and dication salt 2²⁺·2[B(C₆F₅)₄]⁻.

|                     | 2             | 2²⁺·2[B(C₆F₅)₄]⁻ |
|---------------------|---------------|------------------|
| formula             | C95H78N6O6    | C79H55.5BCl2F20N3O3 |
| fw                  | 1399.63       | 1556.47          |
| T (K)               | 123(2)        | 123(2)           |
| λ (Å)               | 0.71073       | 0.71073          |
| cryst syst          | Trigonal      | Monoclinic       |
| space group         | R-3           | i2/a             |
| a (Å)               | 22.2142 (14)  | 32.5289(11)      |
| b (Å)               | 22.2142 (14)  | 13.8777(4)       |
| c (Å)               | 12.977 (2)    | 32.5269(15)      |
| α (deg)             | 90            | 90               |
| β (deg)             | 90            | 96.618(4)        |
| γ (deg)             | 120           | 90               |
| V (Å³)              | 5545.8 (12)   | 14585.7(9)       |
| Z                   | 3             | 8                |
| Dcalc (g / cm³)     | 1.257         | 1.418            |
| μ (mm⁻¹)            | 0.079         | 0.1192           |
| F(000)              | 2214          | 6348.0           |
| cryst size (mm)     | 0.010 × 0.010 × 0.010 | 0.15 × 0.10 × 0.05 |
| θ range (deg)       | 1.833–24.992  | 2.384–31.26      |
| reflns collected    | 6084          | 68811            |
| indep reflns/Rint  | 2175 / 0.0965 | 21919 / 0.0908   |
| params              | 200           | 1017             |
| GOF on $F^2$        | 0.988         | 1.021            |
| R₁, wR₂ [$I>2σ(I)$] | 0.0815, 0.1882 | 0.1162, 0.2728   |
| R₁, wR₂ (all data)  | 0.1804, 0.2443 | 0.3059, 0.3935   |
4. Photophysical properties of N-belt 2

Absorption spectrum of 2

Fig S1. Absorption spectrum of 2. Measurement was carried out under following conditions; solvent: DCM, concentration of 2: \(5.0 \times 10^{-6}\) M, room temperature.
**Titration of the N-belt (2) with oxidant**

Dichloromethane solutions of cationic species of N-belt 2 prepared by chemical oxidation with AgSbF$_6$ were used for measurement. The samples were prepared as following the procedure: To the 0.2 mM solution of 2 in DCM was added 2.0 mM AgSbF$_6$ solution in DCM at –30 °C under argon atmosphere. Then, the reaction mixture was warmed gradually to the ambient temperature and stirred for 30 minutes at the same temperature. After stirring, the reaction mixture was diluted to 5.0 × 10$^{-5}$ M in DCM and transferred to quartz cell through membrane filter by syringe.

**Fig S2.** The UV-Vis-NIR measurement was carried out under following conditions; solvent: DCM, concentration of 2: 5.0 × 10$^{-5}$ M, oxidant: AgSbF$_6$, room temperature.
5. Electrochemical measurements of N-belt 2

Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) of N-belt 2 were measured under the following conditions: 0.1 M TBAPF₆ and 1.0 mM 2 in DCM, Pt reference electrode, Pt working electrode, titanium counter electrode and scan rate of 100 mV·s⁻¹ for CV and 20 mV·s⁻¹ for DPV. The measurements were carried out under a nitrogen atmosphere.

![Cyclic Voltammogram and Differential Pulse Voltammogram](image)

**Fig S3.** Cyclic voltammogram and differential pulse voltammogram of 2. $E^{Ox1} = 0.43$ V (vs Fe/Fc⁺), $E^{Ox2}$ (V) = 0.54 V (vs Fe/Fc⁺), where $E^{Ox}$ were determined as the peak values in DPV.
6. Computational study

For DFT calculation, the Gaussian 16 suite of programs running on a NEC LX system was used. All molecules were fully optimized using (U)B3LYP level of theory with 6-31G(d) basis set. For singlet biradical states, symmetry-broken UB3LYP/6–31G(d) method was employed with a keyword “guess=mix”. Harmonic vibration frequency calculation at the same level was performed to verify all stationary points as local minima (with no imaginary frequency) or transition states (with one imaginary frequency). Time-dependent DFT (TD-DFT) calculations were performed at (U)B3LYP level of theory with 6-31G(d) basis set. Visualization of the results was performed by the use of GaussView 6.0.16 software.

Fig S4. (a) Hypothetical homodesmotic reactions for the calculation of the strain energies of \([n]N\)-belt. (b)

\[
\begin{align*}
\text{[\(n\)]N-belt} & \quad + n \\
\text{PhN} \quad \text{PhN} & \quad \rightarrow \\
\text{PhN} & \quad \text{PhN}
\end{align*}
\]

\[
\begin{array}{c|c}
 n & \text{strain energy (kcal·mol}^{-1}) \\
\hline
4 & 26.0 \\
6 & 1.3 \\
8 & 0.4 \\
10 & 9.1 \\
12 & 22.7 \\
14 & 39.2 \\
16 & 57.8 \\
\end{array}
\]

Fig S5. Optimized structure of 2. (a) Top view; (b) side view.
Fig S6. Frontier molecular orbitals (isovalue = 0.02) and energy diagram of 2.
Fig S7. Optimized structure of N-belt 2 cations (a) 2$^+$ UB3LYP (b) 2$^{2+}$ UB3LYP_T (c) 2$^{3+}$ UB3LYP_Q. (T, triplet; Q, quartet).

Fig S8. Spin density maps (isovalue = 0.0004) calculated for N-belt 2 cations (a) 2$^+$ UB3LYP (b) 2$^{2+}$ UB3LYP_T (c) 2$^{3+}$ UB3LYP_Q. (T, triplet; Q, quartet).
Fig S9. Time dependent-DFT (TD-DFT) calculations. Calculated stick spectra at B3LYP/6-31G(d) of (a) neutral $2^-$, (b) radical cation $2^+$ with triplet state, and (d) trication $2^{3+}$ with quartet state.

Table S2. The TD-DFT calculation results. (a) $2^-$ (B3LYP/6-31G(d)) (b) $2^+$ (UB3LYP/6-31G(d)) (c) $2^{2+}$ (UB3LYP/6-31G(d)$_T$) (d) $2^{3+}$ (UB3LYP/6-31G(d)$_Q$)

(a) $2^-$ (B3LYP/6-31G(d))

| Excited State | Singlet-AG | 2.2523 eV | 550.47 nm | f=0.0000 | $<S^2>=0.000$ |
|---------------|------------|------------|------------|----------|----------------|
| 346 $\rightarrow$ 351 | -0.16653 | |
| 347 $\rightarrow$ 350 | 0.16653 |
| 348 $\rightarrow$ 349 | 0.65796 |

This state for optimization and/or second-order correction.

Total Energy, $E$(TD-HF/TD-DFT) = -4248.95256587

Copying the excited state density for this state as the 1-particle RhoCl density.

(b) $2^+$ (UB3LYP/6-31G(d))

| Excited State | Singlet-EU | 3.4383 eV | 360.59 nm | f=0.9802 | $<S^2>=0.000$ |
|---------------|------------|------------|------------|----------|----------------|
| 340 $\rightarrow$ 349 | 0.18851 | |
| 341 $\rightarrow$ 349 | -0.35697 | |
| 342 $\rightarrow$ 350 | 0.45244 | |
| 342 $\rightarrow$ 351 | -0.21802 | |
| 343 $\rightarrow$ 355 | -0.10423 | |
| 344 $\rightarrow$ 352 | 0.21848 | |
Excited State 28:  Singlet-EU  3.4383 eV  360.59 nm  f=0.9803  <S**2>=0.000
340 -> 349  -0.35698
341 -> 349  -0.18851
342 -> 350  0.21802
342 -> 351  0.45244
343 -> 356  0.10423
345 -> 352  -0.21847

2*(UB3LYP/6-31G(d))  E = -4248.83612625 Hartree
Excited State  1:  2.003-EU  0.2119 eV 5850.74 nm  f=0.0775  <S**2>=0.753
346B -> 348B  1.19210
346B <-> 348B  -0.65006
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -4248.82833863
Copying the excited state density for this state as the 1-particle RhoCl density.

Excited State  23:  2.007-EU  2.1514 eV  576.29 nm  f=0.0962  <S**2>=0.757
328B -> 348B  0.20034
329B -> 348B  0.97110

Excited State  24:  2.007-EU  2.1514 eV  576.29 nm  f=0.0962  <S**2>=0.757
328B -> 348B  0.97110
329B -> 348B  -0.20034

Excited State  97:  2.101-EU  3.4640 eV  357.92 nm  f=0.7351  <S**2>=0.854
341A -> 349A  0.14285
342A -> 350A  0.66516
343A -> 355A  -0.10238
344A -> 352A  -0.10233
341B -> 349B  0.22718
342B -> 350B  0.58138

Excited State  98:  2.101-EU  3.4640 eV  357.92 nm  f=0.7351  <S**2>=0.854
$2^2$ (UB3LYP/6-31G(d) T) $E = -4248.57604166$ Hartree

Excited State 1: 3.006-AG  0.0719 eV  17233.21 nm  f=0.0000  $<S^{*2}> = 2.010$

345B -> 348B  -0.28510
346B -> 347B  -1.00106
346B <- 347B  0.28289

This state for optimization and/or second-order correction.

Total Energy, $E(TD-HF/TD-DFT) = -4248.57339774$

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 30: 3.014-AU  2.1740 eV  570.31 nm  f=0.2159  $<S^{*2}> = 2.021$

326B -> 347B  -0.13981
327B -> 347B  -0.20382
328B -> 348B  0.30062
329B -> 347B  0.39020
330B -> 348B  0.18853
331B -> 348B  0.36492
333B -> 347B  0.59224
334B -> 347B  0.18647
335B -> 347B  -0.17587
336B -> 348B  -0.17326
338B -> 347B  0.21487

Excited State 127: 3.260-AU  3.4726 eV  357.03 nm  f=0.6545  $<S^{*2}> = 2.406$

340A -> 349A  0.47986
342A -> 350A  0.26839
342A -> 351A  0.18806
344A -> 357A  -0.11914
340B --> 349B 0.45980
342B --> 350B 0.32007
342B --> 351B 0.17824
343B --> 354B -0.25344
343B --> 359B -0.15090
344B --> 357B 0.15959
345B --> 358B 0.16565
346B --> 355B -0.12020

Excited State 129: 3.297-AU 3.4872 eV 355.54 nm f=0.5965 <S**2>=2.468
342A --> 351A 0.57676
343A --> 355A -0.24949
344A --> 352A -0.34824
347A --> 354A 0.12599
347A --> 356A 0.10108
341B --> 349B 0.12748
342B --> 351B 0.43682
343B --> 356B 0.12317
344B --> 352B -0.12182

$^2+$ (UB3LYP/6-31G(d) Q) E = -4248.25556306 Hartree

Excited State 1: 4.009-AU 0.0993 eV 12490.76 nm f=0.0000 <S**2>=3.767
344B --> 346B -0.73678
344B --> 347B -0.11675
345B --> 346B -0.11663
345B --> 347B 0.73733
344B < 346B -0.23636
345B < 347B 0.23584

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -4248.25191530

Copying the excited state density for this state as the 1-particle RhoCI density

Excited State 138: 4.051-AU 3.4635 eV 357.97 nm f=0.8372 <S**2>=3.854
341A --> 349A 0.25796

S18
342A -> 350A  0.64187
341B -> 349B  0.34661
342B -> 350B  0.55996

Excited State 139:  4.051-AU  3.4637 eV  357.95 nm  f=0.8356  <S**2>=3.854
340A -> 349A  -0.25770
342A -> 351A  0.64207
340B -> 349B  -0.34691
342B -> 351B  0.55980
Table S3. Cartesian coordinates of optimized structures with uncorrected and thermal-corrected (298 K) energies of stationary points (Hartree).

| Structure | E [kcal/mol] | C | H | N |
|-----------|-------------|-----------------|-----------------|---------|
| [4]C-belt | -2374.56844998 | C 2.80585 1.49189 1.06131 | 2.80585 1.49189 1.06131 | 2.80585 1.49189 1.06131 |
| C         | -2373.764196  | C 1.173221 0.28794 | 1.173221 0.28794 | 1.173221 0.28794 |
| N         | -2373.764196  | C 1.49189 2.80858 1.06131 | 1.49189 2.80858 1.06131 | 1.49189 2.80858 1.06131 |
| [5]C-belt | -2373.764196  | C 1.873597 1.318569 | 1.873597 1.318569 | 1.873597 1.318569 |
| C         | -2373.764196  | C 3.57512 3.452184 1.06131 | 3.57512 3.452184 1.06131 | 3.57512 3.452184 1.06131 |
| N         | -2373.764196  | C 3.330152 0.674356 2.173844 | 3.330152 0.674356 2.173844 | 3.330152 0.674356 2.173844 |
| [6]C-belt | -3560.706386  | C 0.00000 0.971967 1.255899 | 0.00000 0.971967 1.255899 | 0.00000 0.971967 1.255899 |
| C         | -3560.706386  | C 9.014140 1.143438 | 9.014140 1.143438 | 9.014140 1.143438 |
| N         | -3560.706386  | C 0.00000 0.971967 1.255899 | 0.00000 0.971967 1.255899 | 0.00000 0.971967 1.255899 |
| [7]C-belt | -3560.706386  | C 2.14887 2.795383 3.28794 | 2.14887 2.795383 3.28794 | 2.14887 2.795383 3.28794 |
| C         | -3560.706386  | C 2.14887 2.795383 3.28794 | 2.14887 2.795383 3.28794 | 2.14887 2.795383 3.28794 |
| N         | -3560.706386  | C 2.14887 2.795383 3.28794 | 2.14887 2.795383 3.28794 | 2.14887 2.795383 3.28794 |
| [8]C-belt | -3560.706386  | C 2.14887 2.795383 3.28794 | 2.14887 2.795383 3.28794 | 2.14887 2.795383 3.28794 |
| C         | -3560.706386  | C 2.14887 2.795383 3.28794 | 2.14887 2.795383 3.28794 | 2.14887 2.795383 3.28794 |
| N         | -3560.706386  | C 2.14887 2.795383 3.28794 | 2.14887 2.795383 3.28794 | 2.14887 2.795383 3.28794 |

S20
| C  | 8.132772 | 9.267128 | -1.304479 |
| C  | 7.656686 | 10.538524 | -1.439512 |
| C  | 6.275381 | 10.675418 | -1.304479 |
| C  | 5.463472 | 9.572992 | -1.040477 |
| C  | 6.020375 | 8.286336 | -0.912790 |
| N  | 5.197204 | 7.153338 | -0.680835 |
| C  | 5.406935 | 6.289530 | 2.157403 |
| C  | 5.310864 | 7.085873 | 2.157403 |
| C  | -4.310864 | 7.085873 | 2.157403 |
| C  | -4.506935 | -6.289530 | 2.157403 |
| C  | -4.310864 | -7.085873 | -2.157403 |
| C  | -9.916198 | -6.77646 | 2.551711 |
| C  | -9.916198 | 0.677646 | 2.551711 |
| C  | -6.677646 | 9.916198 | -2.551711 |
| C  | -1.580321 | 9.696793 | -1.043363 |

N-belt E = -712.80345370, H = -711.380942

| C  | 1.228173 | 9.688754 | 0.314942 |
| C  | 1.590231 | 9.696793 | 0.143363 |
| C  | 2.138076 | 9.549020 | 1.318081 |
| C  | 3.472062 | 9.192284 | 1.043363 |
| C  | 3.870748 | 9.160678 | -0.314942 |
| C  | 2.933233 | 9.393511 | -1.318081 |
| C  | -8.248856 | 5.449585 | -2.155711 |
| C  | -8.265052 | 4.372140 | -2.155711 |
| C  | -9.192284 | 3.472082 | -1.043363 |
| C  | -9.160678 | 3.870748 | 0.314942 |
| N  | -9.096444 | 5.251835 | 0.678073 |
| C  | -7.932505 | 9.909006 | 0.314942 |
| C  | -7.603054 | 6.224711 | 0.314942 |
| C  | -7.204136 | 6.626588 | 0.314942 |
| C  | -6.626588 | 7.201436 | -1.318081 |
| C  | -9.549920 | 2.138076 | -2.155711 |
| C  | -9.868754 | 3.742082 | -0.314942 |
| C  | -10.096444 | 5.251835 | 0.678073 |
| C  | -7.932505 | 8.909006 | -0.314942 |
| C  | -7.603054 | 5.224711 | -0.314942 |
| C  | -7.204136 | 5.626588 | -0.314942 |
| C  | -6.626588 | 5.201436 | 1.318081 |

12N-belt E = -712.80345370, H = -711.380942
| N-C | 3.51279 | 3.05301 | 0.16440 |
|-----|---------|---------|---------|
| C-C | 2.68237 | 2.15342 | 0.908263 |
| C-H | 0.54306 | 4.937833 | 0.309773 |
| C-H | 0.908263 | 4.548909 | 1.321959 |
| C-H | 1.714476 | 2.352283 | 1.978162 |
| C-H | 4.826367 | 1.158361 | 0.307021 |
| C-H | 4.786150 | 0.754669 | 1.047411 |
| H-C | 10.52536 | 0.754669 | 1.047411 |
| H-N | 4.750662 | -0.622266 | 1.399225 |
| N-C | 3.12352 | 3.312819 | 0.141464 |
| C-C | 2.14708 | 3.349469 | 0.055610 |
| C-H | 0.54306 | 4.937833 | 1.321959 |
| C-H | 0.908263 | 4.548909 | 1.321959 |
| H-N | 4.750662 | -0.622266 | 1.399225 |
| C-H | 10.52536 | 0.754669 | 1.047411 |
| H-N | 4.750662 | -0.622266 | 1.399225 |
| N-C | 3.12352 | 3.312819 | 0.141464 |
| C-C | 2.14708 | 3.349469 | 0.055610 |
| C-H | 0.54306 | 4.937833 | 1.321959 |
| C-H | 0.908263 | 4.548909 | 1.321959 |
| H-N | 4.750662 | -0.622266 | 1.399225 |
| C-H | 10.52536 | 0.754669 | 1.047411 |
| H-N | 4.750662 | -0.622266 | 1.399225 |
|   | X       | Y       | Z       |   | X       | Y       | Z       |
|---|---------|---------|---------|---|---------|---------|---------|
| N | 4.368613| -3.382968| -0.607939| C | 6.272520| 2.564070| 1.241316|
| C | 4.340142| -2.506039| 2.173711 | H | -10.098967| 5.754820| 2.493391|
| H | 3.356789| -4.089579| 3.119281 | C | 4.005975| 2.941069| 0.298146|
| C | -6.272520| -2.564070| -1.241316| H | -9.492685| 5.256231| 4.110012|
| C | -6.272520| -2.564070| -1.241316| C | -10.035157| -5.241431| -3.394603|
| H | -10.058570| 6.929274| 3.839156 |
| C | -6.272520| -2.564070| -1.241316| C | -2.682378| 4.027331| -1.059642|
| H | 10.032337| 5.872178| 2.499029 |
| C | -4.916461| -0.709955| -0.299419| H | -3.356789| 4.089579| -3.119281|
| C | 9.292217| 5.602126| 4.114260 |
| C | -4.832123| -0.309773| 1.054516 |
| H | 11.024648| 5.253622| 3.849848 |
| H | -5.225875| -0.862300| 3.113820 | C | -6.624266| 3.605433| 1.537616 |
| H | 2.377903| 8.432101| -2.149476|
| H | 0.089720| -11.624753| 2.491952 | C | -2.197060| 4.261781| 1.318430 |
| H | 3.088637| 6.615769| -1.304753|
| H | 0.204591| -10.851498| 4.108604 | C | 5.533239| -6.076860| -3.386914 |
| H | -0.026214| 8.778079| -2.140179|
| H | -0.962744| -12.177580| 3.841179 | C | 3.664326| 3.163774| -1.056152 |
| H | -1.193386| 7.217750| -1.308957|
| C | 5.355262| -4.150881| -1.235291| H | 4.332932| 3.043590| -3.115065 |
| C | 1.263621| 9.241641| -2.464031|
| C | 4.548909| -1.997917| -0.294679| C | 7.342519| 1.685852| 1.552283 |
| C | 3.643143| 3.937218| 1.539065 |
| H | -0.900503| 9.384022| -2.346106|
| H | 4.799794| -2.226044| 3.118940 | C | 3.259174| 3.522987| 1.321441 |
| O | 1.542355| 10.415505| -3.046527|
| H | -7.342519| -1.685852| -1.552283 | H | -10.032337| -5.872178| -2.499029 |
| C | 0.478618| 11.315584| -3.387722|
| C | -6.434143| -3.937218| -1.539065 | H | -9.292217| -5.602126| -4.114260 |
| H | -0.067920| 11.624753| -2.491952|
| C | -4.789425| 0.227163| -1.323602 | H | -11.024648| -5.253622| -3.849848 |
| H | -0.204591| 10.851498| -4.108604|
| C | -4.680233| 1.061341| 1.318892 | C | -1.419210| 4.581712| -1.324170 |
| O | 0.962744| 12.177580| -3.841179|
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