Electronic Supplementary Material (ESI) for ChemComm.
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The Cis/Trans Conformation Approach for Tuning the Magnetic Coupling in a Diradical: Isolation of Pure Pyridine-Based Diradical Dianions

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Electronic Supplementary Information

Content

Experimental details:

General consideration: All oxygen- and moisture-sensitive experiments and manipulations were carried out under N_2 atmosphere using standard Schlenk techniques or in a N_2-filled glovebox. Solvents were dried by the proper drying agents; THF was dried over NaK/benzophenone, and CH_3CN was treated with CaH_2 under refluxing and degassed before use. EPR spectra were obtained using a Bruker EMX plus-6/1 variable-temperature apparatus. UV/Vis spectra were recorded on the Lambda 750 spectrometer at room temperature. All NMR spectra were recorded on Bruker AVQ-400 spectrometers referenced to residual solvent signals as internal standards for ^1H and $^{13}C\{^1H\}$ NMR. Element analyses were performed on an Elementar Vario EL III instrument at Shanghai Institute of Organic Chemistry, the Chinese Academy of Science. For the single crystal X-ray structure analyses, the crystals were each mounted on a glass capillary in perfluorinated oil and measured in a cold N_2 flow. The data were collected on Bruker D8 CMOS detectors. The structures were solved by direct methods and all refined on F^2 with the SHELX-2014/7 software package. SQUEEZE was used to treat the highly disorder solvent molecules in the crystal structures.

Synthesis of 2,6-dimesitylpyridin-4-amine: To a Schlenk pressure tube K_2CO_3 (16.56 g, 120.00 mmol, 4 eq), 2,6-dichloropyridin-4-amine (4.89 g, 30.00 mmol, 1 eq), mesitylboronic acid (11.81 g, 72.00 mmol, 2.4 eq) and $Pt(PPh_3)_2Cl_2$ (0.42 g, 0.60 mmol, 0.02 eq) were added and a degassed solvent mixture [60 mL, toluene, water and ethanol (14:3:3)] was transferred via cannula to the Schlenk pressure tube under an inert atmosphere. The pressure tube was sealed and heated at 115 ℃ for 36 h. The resultant reaction mixture was allowed to cool to room temperature and a saturated solution of NH_4Cl (120 mL) was added to it. The mixture was filtered through a pad of celite and 120 mL of CH_2Cl_2 was used to wash the pad. The solution was then extracted with CH_2Cl_2 (100 mL × 3) and the combined organic layer was washed

successively with water, brine and dried over anhydrous $MgSO_4$. Removal of solvents resulted in an off white solid. After washing with MeOH (50 mL × 3), the product was isolated as a white solid. Yield: 8.91 g, 90 %. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.86 (s, 2H), 6.43 (s, 2H), 4.16 (s, 2H), 2.27 (s, 6H) and 2.07 (s, 12H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 159.9, 149.7, 139.9, 136.9, 135.5, 127.9, 107.6, 21.1, 20.0 ppm.

Synthesis of 4-bromo-2,6-dimesitylpyridine: To a solution of $CuBr_2$ (8.03 g, 36.00 mmol) in dry CH_3CN (100 mL), *t*BuONO (5.1 mL, 45 mmol) was added dropwise under nitrogen. The mixture was allowed to attain at 0 ^{o}C and carefully transferred to a mixture of 2,6-dimesitylpyridin-4-amine (9.90 g, 30.00 mmol) in dry CH_3CN (100 mL) at same temperature under nitrogen. The temperature was kept at 0 ^{o}C for 1 h and allowed to stir overnight at room temperature. The reaction mixture was quenched by an aqueous ammonia solution (15 %, 100 mL) and the resultant mixture was extracted with CH_2Cl_2 (100 mL × 3). The combined organic layer was washed successively with water, brine and dried over anhydrous $MgSO_4$. Removal of solvents resulted in a pale yellow solid and the product was purified by column chromatography with an eluent of toluene to afford a white solid. Yield: 6.62 g, 56 %. ^{1}H NMR ($CDCl_3$, 400MHz): δ 7.39 (s, 2H), 6.90 (s, 4H), 2.30 (s, 6H) and 2.06 (s, 12H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 161.5, 137.9, 136.8, 135.6, 128.4, 125.9, 21.02 and 20.3 ppm.

Synthesis of (2,6-dimesitylpyridin-4-yl)boronic acid: To a solution of 4-bromo-2,6-dimesitylpyridine (1.58 g, 4.00 mmol, 1 eq) in dry THF (60 mL), *n*BuLi (2.6 mL, 1.6 M in hexane, 4.2 mmol, 1.05 eq) was added dropwise at –78 ^{o}C under nitrogen. The temperature was kept –78 ^{o}C for 2 h. $(n\text{BuO})_3\text{B}$ (1.6 mL, 6.0 mmol, 1.5 eq) was added to the mixture and allowed to stir overnight at room temperature. The pale yellow solid was obtained by evaporation of all the volatiles and treated with HCl solution (1 M, 100 mL). The crude product was obtained by adjusting pH to 7 with NaOH solution (2 M). The product was obtained as a white solid by filtering and washed with hexane. Yield: 1.2 g, 84 %. ^{1}H NMR (CD_3OD, 400 MHz): δ 7.85 (s, 2H), 7.06 (s, 4H), 2.35 (s, 6H) and 2.09 (s, 12H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 150.3, 139.9, 135.7, 130.7, 128.2, 123.0, 120.9, 19.7 and 18.6 ppm.

Synthesis of 1: To a Schlenk pressure tube Na_2CO_3 (3.15 g, 29.80 mmol, 8.5 eq), 3,3'-dibromobiphenyl (1.09 g, 3.50 mmol, 1 eq), (2,6-dimesitylpyridin-4-yl)boronic acid (3.77 g, 10.50 mmol, 3 eq) and $Pt(PPh_3)_4$ (0.28 g, 0.24 mmol, 0.07 eq) were added. A degassed solvent mixture (90 mL, toluene, water and ethanol in a volume ratio of 52:24:14) was transferred *via* cannula to the Schlenk pressure tube under an inert atmosphere. The pressure tube was sealed and heated at 105 °C for 48 h. The resultant reaction mixture was cooled to room temperature and filtered through a pad of celite. The solution was then extracted with CH_2Cl_2 (100 mL × 3) and the combined organic layer was washed successively with water, brine and dried over anhydrous $MgSO_4$. Removal of the solvents resulted in a pale yellow solid, which was purified by column chromatography with an eluent of petroleum ether/ ethyl acetate (10:1) to afford the product as a white solid. Yield: 1.83 g, 67%. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.94 (m, 2H), 7.72 (m, 4H), 7.58 (m, 2H), 7.52 (s, 4H), 6.93 (s, 8H)，2.32 (s, 12H), 2.11 (s, 24H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.9, 148.5, 141.7, 138.8, 138.0, 137.4, 135.7, 129.8, 128.2, 128.0, 126.3, 125.9, 120.3, 21.2, 20.4 ppm. Elemental analysis for $C_{58}H_{56}N_2$ (%): cacld: C 89.19; H 7.23; N 3.59; found: C 88.69; H 7.22; N 3.76.

Synthesis of K^+_2•[*trans*-1]$^{\bullet\bullet 2-}$: Under anaerobic and anhydrous conditions, **1** (0.156 g, 0.200 mmol), and potassium (0.017 g, 0.44 mmol) were added into a 100 mL Schlenk flask. Then THF (50 mL) was added and the mixture was stirred at room temperature for 12 h. The resultant mixture was filtered and the filtrate was then concentrated and left at –10 °C for 24 h to form deep blue crystals of K^+_2•[*trans*-**1**]$^{\bullet\bullet 2-}$. Yield: 0.052 g, 23 %. No satisfactory elemental analysis result was obtained.

Synthesis of [K(18-c-6)]$^+_2$•[*cis*-1]$^{\bullet\bullet 2-}$: Under anaerobic and anhydrous conditions, **1** (0.156 g, 0.200 mmol), potassium (0.017 g, 0.44 mmol), and 18-c-6 (0.116 g, 0.440 mmol) were added into a 100 mL Schlenk flask. Then THF (50 mL) was added and the mixture was stirred at room temperature for 24 h. The resultant mixture was filtered and the filtrate was then concentrated and left at –40 °C for 24 h to afford deep blue crystals of [K(18-c-6)]$^+_2$•[*cis*-**1**]$^{\bullet\bullet 2-}$. Yield: 0.120 g, 43 %. Elemental

analysis for $C_{82}H_{104}K_2N_2O_{12}$ (%): Calcld: C 70.96, H 7.55, 2.02; C 70.41; H 8.09; N 1.84.

Detail information of Bleaney-Bowers equation：

$$\chi_M = \frac{2Ng^2\beta^2}{3\kappa T}\left[1+\frac{1}{3}\exp\left(\frac{-2J}{\kappa T}\right)\right]^{-1}$$

χ_M：Magnetic susceptibility

N= Avogadro's number *g*: g-factor β：Bohr magneton k: boltzmann constant

T:absolute temperature *J* :exchange constant

Fig.S1

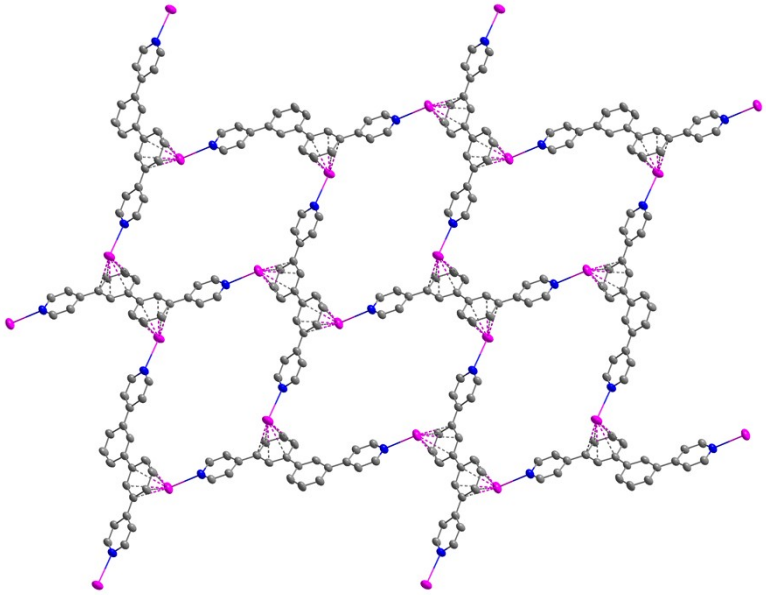


Fig.S1 Depiction of the two-dimensional honeycomb structure of K^{+}_{2}•[trans-1]$^{\bullet\bullet 2-}$. The Mes groups, hydrogen atoms and THF molecules are omitted for clarity.

Fig.S2

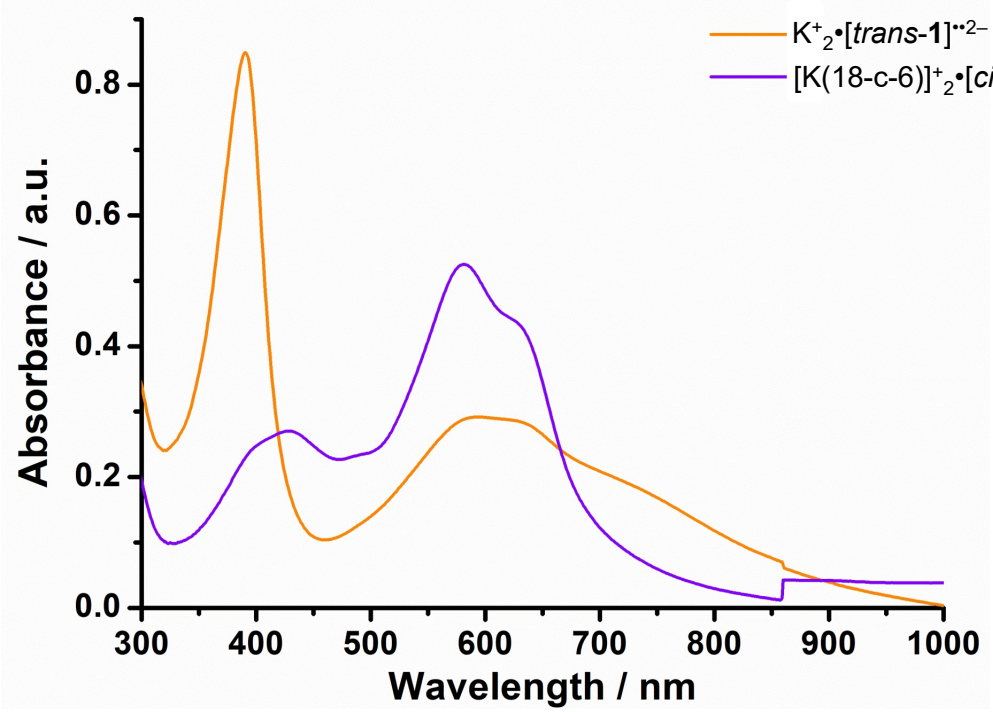
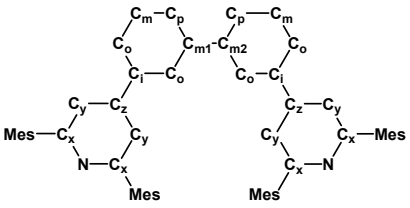


Fig.S2 UV/Vis absorption spectra of K^{+}_{2}•[trans-1]$^{\bullet\bullet 2-}$ (a) and $[K(18\text{-c-}6)]^{+}_{2}$•[cis-1]$^{\bullet\bullet 2-}$ (b) in THF solutions (10–4 M) at room temperature

Table S1. Crystal Data and Structure Refinement for 1, K^+_2•[*trans*-1**]$^{\bullet\bullet 2-}$ and [K(18-c-6)]$^+_2$•[*cis*-**1**]$^{\bullet\bullet 2-}$**

	1	K^+_2•[*trans*-**1**]$^{\bullet\bullet 2-}$	[K(18-c-6)]$^+_2$•[*cis*-**1**]$^{\bullet\bullet 2-}$
formula	$C_{58}H_{56}N_2$	$C_{37}H_{44}KNO_2$	$C_{41}H_{52}KNO_6$
*M*r [g mol^{-1}]	781.04	573.83	693.93
crystal system	monoclinic	monoclinic	monoclinic
space group	*P*2(1)/*n*	*P*2(1)/*n*	*C*2/*c*
Z	4	4	8
Temp. (K)	193	193	193
μ (mm^{-1})	0.054	1.077	0.868
a (Å)	16.6713(8)	11.5553(9)	19.7899(16)
b (Å)	16.2931(6)	17.2021(14)	20.4638(19)
c (Å)	20.9884(8)	17.3420(13)	22.710(2)
α			
β	105.296(1)	107.153(5)	98.184(6)
γ			
V	5499.1(4)	3293.8(5)	9103.3(14)
*R*1 (I > 2σ(I))	0.0573	0.0680	0.1166
*wR*2 (I > 2σ(I))	0.1458	0.1803	0.2827

Table S2. Selected experimental and calculated bond lengths (Å)[a], and relative energy (kcal mol^{-1}) for 1, [*trans*-1]$^{\bullet\bullet 2-}$ and [*cis*-1]$^{\bullet\bullet 2-}$



		ΔEX-OS	N-Cx	Cx-Cy	Cy-Cz	Cz-Ci	Ci-Co	Co-Cm	Cm-Cp	Cm1-Cm2
1	X-ray	—	1.356(2)	1.386(2)	1.392(2)	1.482(2)	1.394(2)	1.385(2)	1.387(2)	1.480(2)
[*trans*-**1**]$^{\bullet\bullet 2-}$	X-ray	—	1.368(4)	1.360(4)	1.433(4)	1.419(4)	1.436(4)	1.369(4)	1.409(4)	1.493(4)
	CS	23.89	1.378	1.366	1.469	1.382	1.473	1.392	1.381	1.485
	OS	0	1.362	1.375	1.437	1.432	1.429	1.381	1.399	1.491
	T	0.30	1.363	1.375	1.436	1.432	1.429	1.390	1.399	1.492
[*cis*-**1**]$^{\bullet\bullet 2-}$	X-ray	—	1.354(7)	1.378(7)	1.426(7)	1.435(8)	1.430(8)	1.382(8)	1.397(8)	1.452(8)
	CS	21.47	1.378	1.367	1.465	1.382	1.461	1.372	1.417	1.487
	OS	0	1.362	1.376	1.436	1.432	1.427	1.389	1.400	1.490
	T	0.55	1.362	1.376	1.437	1.432	1.427	1.389	1.400	1.491

[a] Average values.

Selected NMR spectra

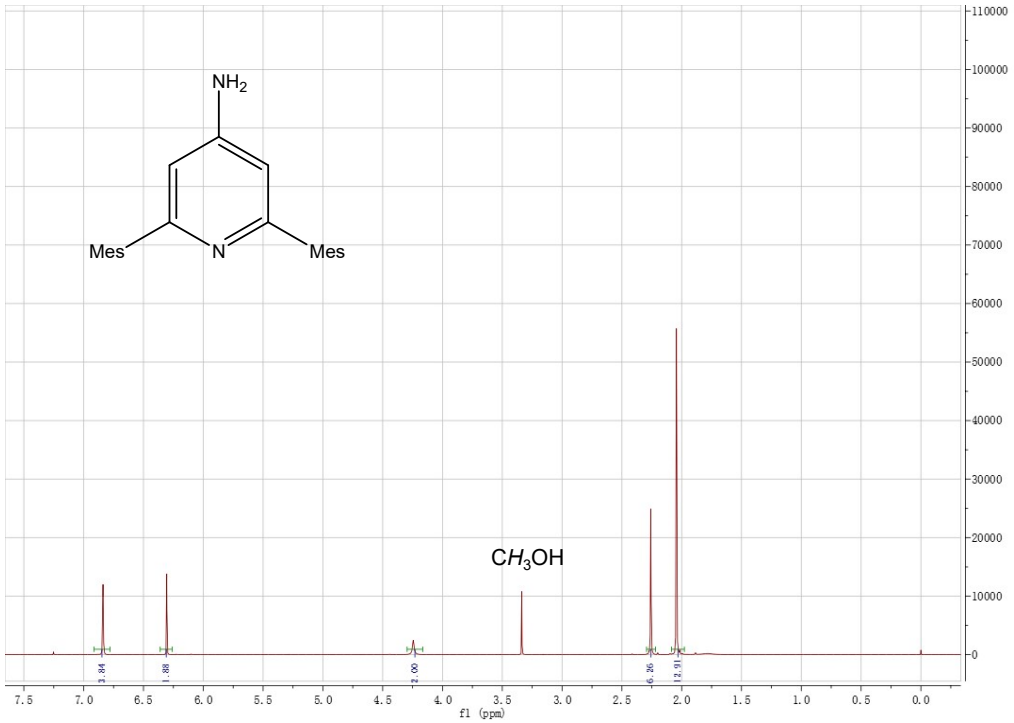


Figure S1. ^{1}H NMR spectrum of 2,6-dimesitylpyridin-4-amine in $CDCl_3$.

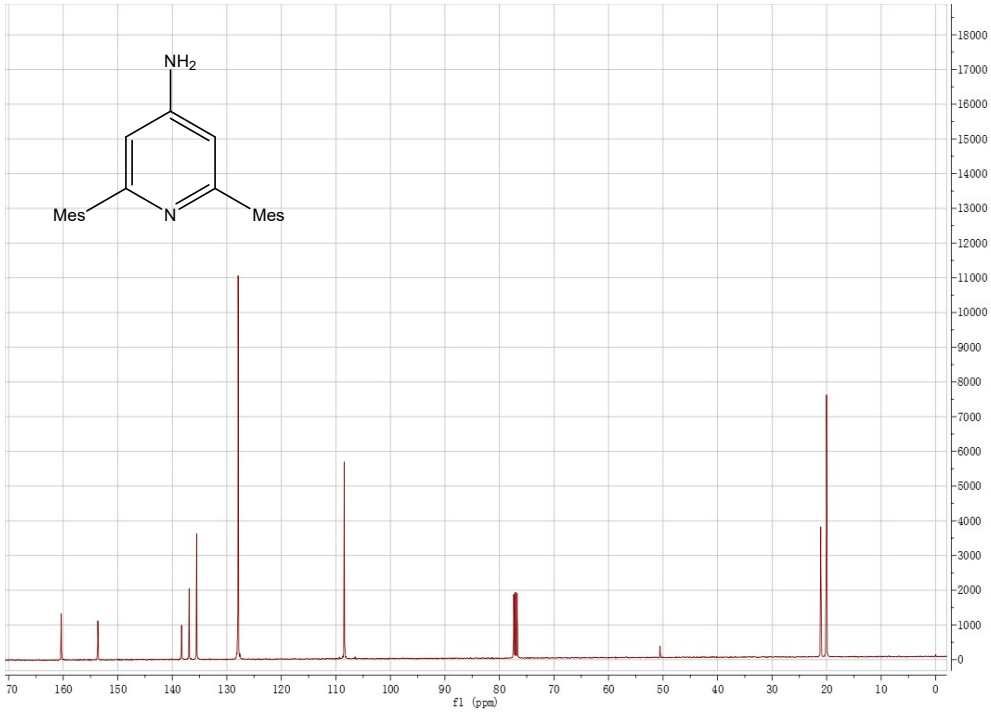


Figure S2. ^{13}C NMR spectrum of 2,6-dimesitylpyridin-4-amine in $CDCl_3$.

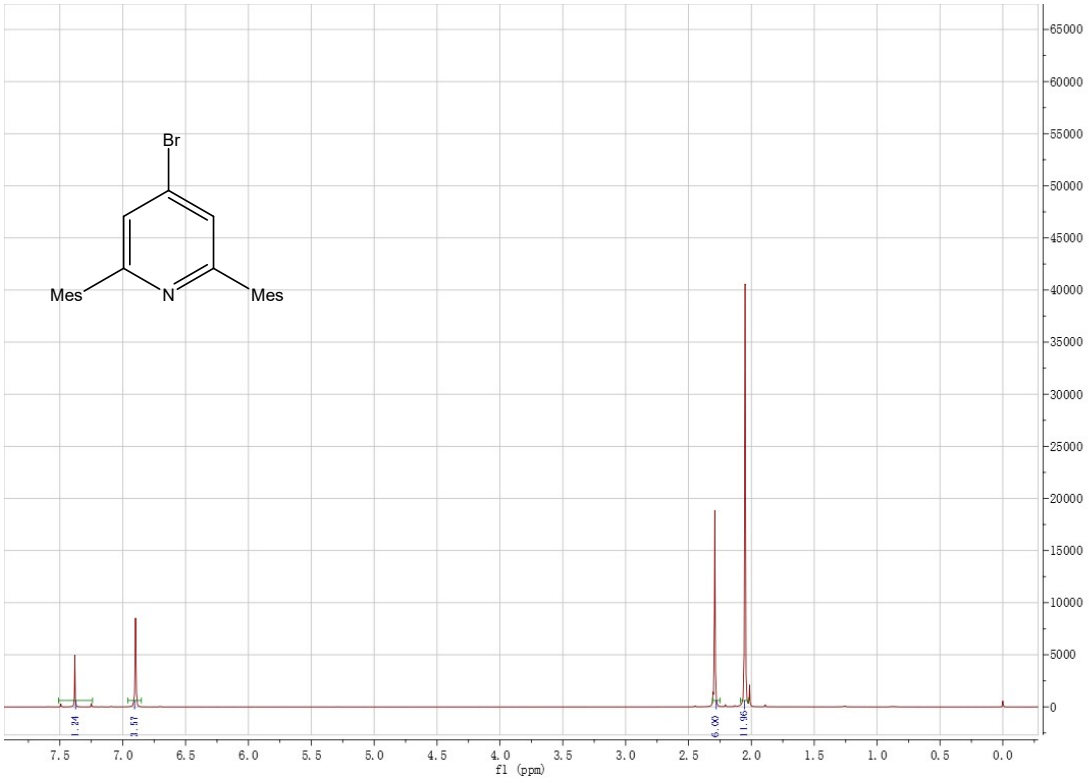


Figure S3. ^{1}H NMR spectrum of 4-bromo-2,6-dimesitylpyridine in $CDCl_3$.

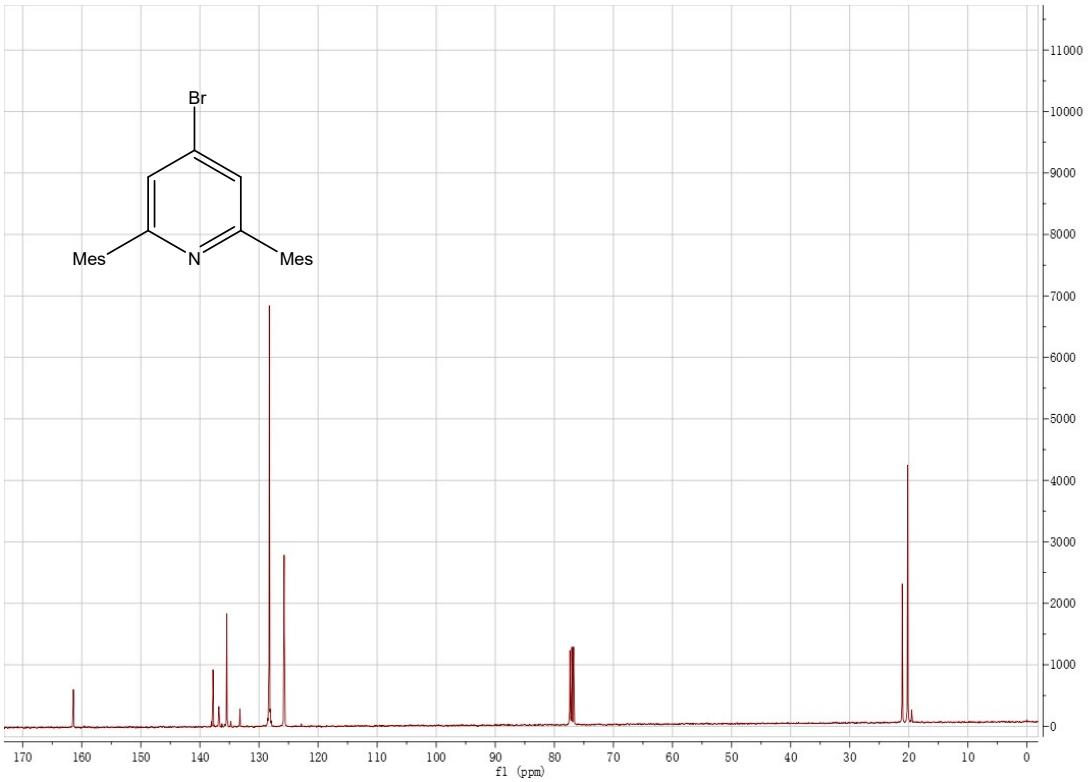


Figure S4. ^{13}C NMR spectrum of 4-bromo-2,6-dimesitylpyridine in $CDCl_3$.

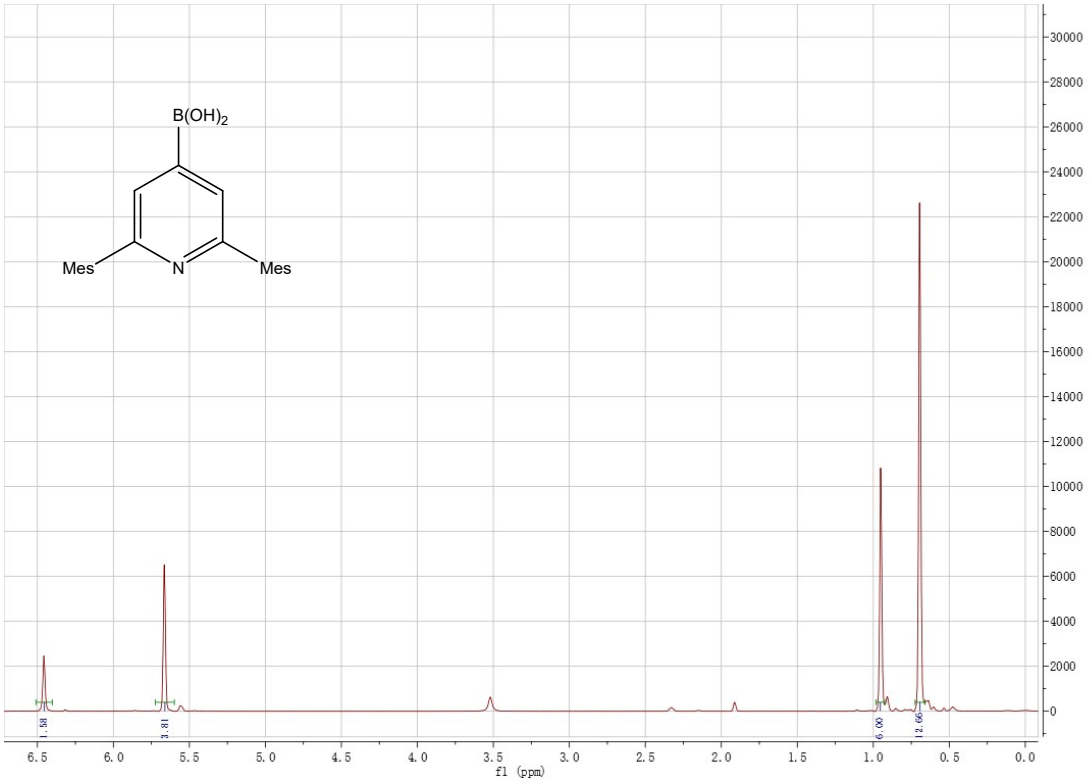


Figure S5. ^{1}H NMR spectrum of (2,6-dimesitylpyridin-4-yl)boronic acid in CD_3OD.

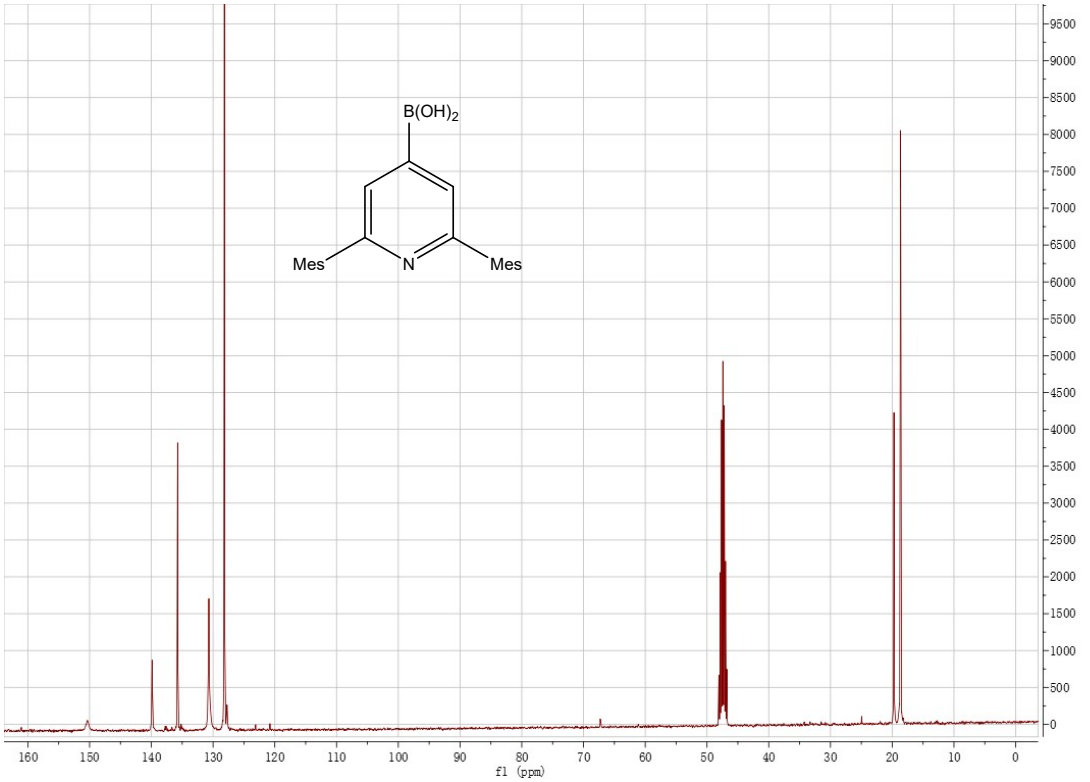


Figure S6. ^{13}C NMR spectrum of (2,6-dimesitylpyridin-4-yl)boronic acid in CD_3OD.

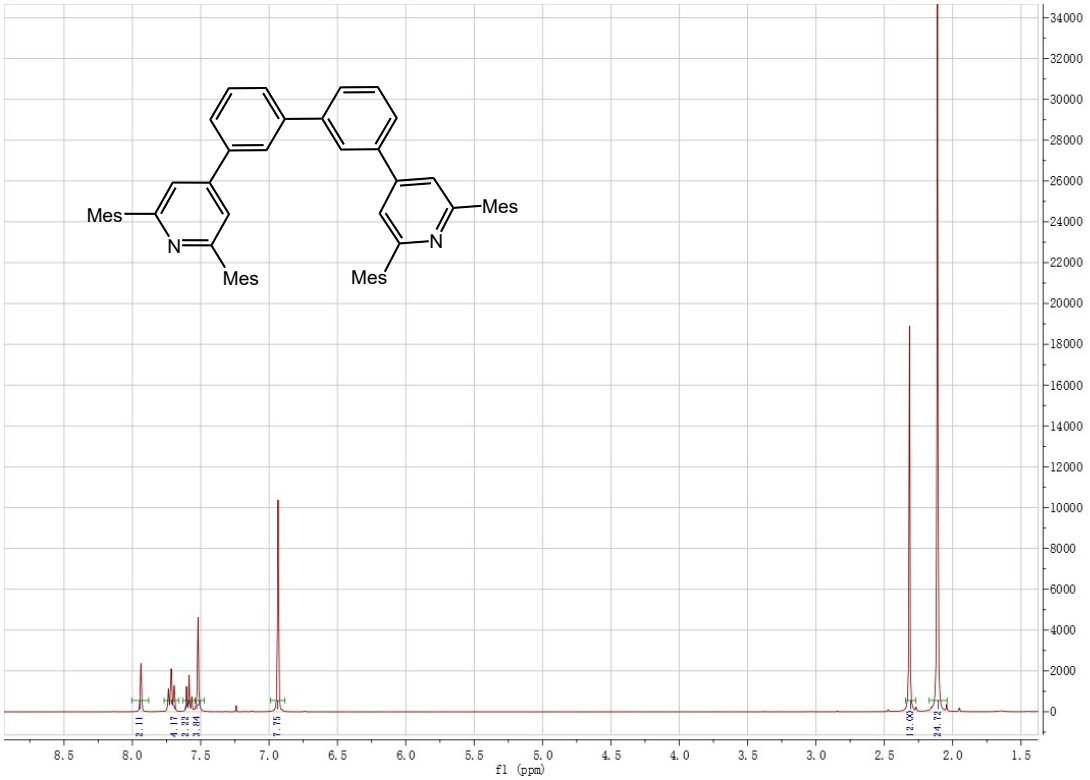


Figure S7. ^{1}H NMR spectrum of **1** in $CDCl_3$.

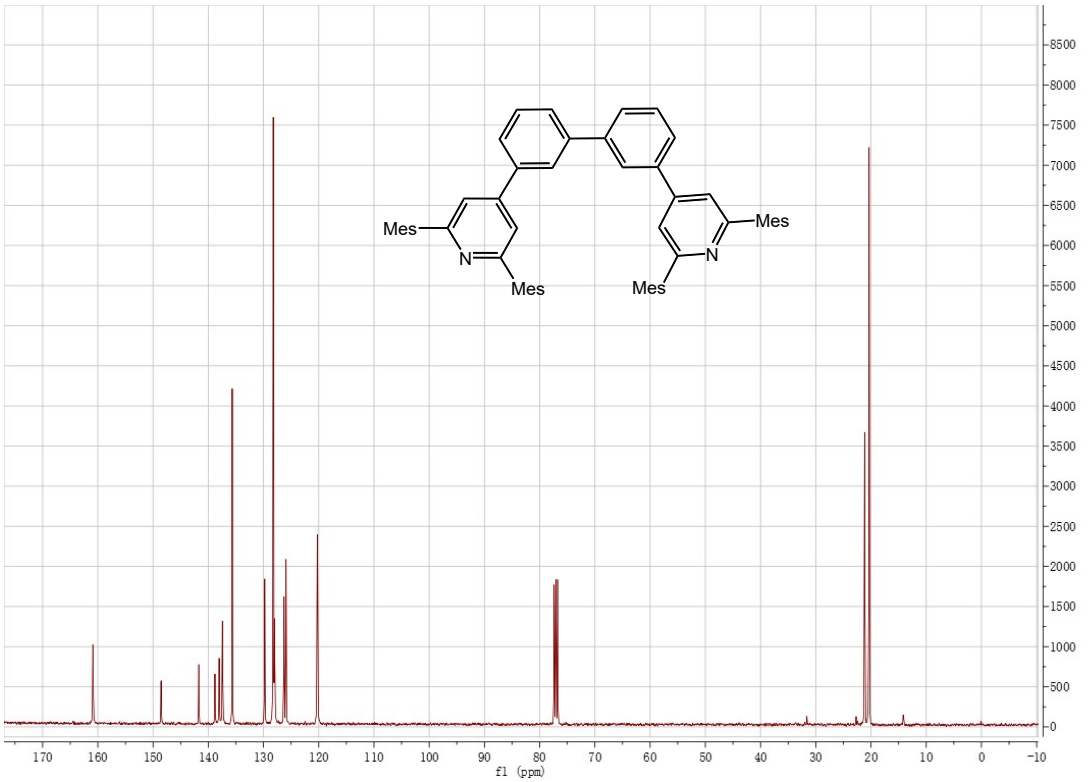


Figure S8. ^{13}C NMR spectrum of **1** in $CDCl_3$.

Theoretical calculations

All the calculations were carried out with Gaussian 09 program suite.[S1] The optimized structures were obtained at the (U)WB97XD/6-31G(d) level of theory,[S2] the Polarizable Continuum Model (PCM) model was used and no imaginary frequency was found. The calculated results show that [*trans*-**1**]$^{\bullet\bullet 2-}$ and [*cis*-**1**]$^{\bullet\bullet 2-}$ possess an open-shell singlet ground state (Table S2). In addition, to further figure out the structure-property relationship of the studied compounds, we also performed the calculations on the UV-vis absorption spectra by using the time-dependent DFT (TD-DFT) method at the UWB97XD/6-31(d) level.[S3] Moreover, in view of the solvent effects (THF in this work), the Polarizable Continuum Model (PCM) model was used in the TD-DFT calculations.[S4]

Table S3. Calculated excited wavelengths (λ) and oscillator strengths (*f*) of selected transitions of [*trans*-1]$^{\bullet\bullet 2-}$ and [*cis*-1]$^{\bullet\bullet 2-}$.

Compound	Excited state	Wavelength/nm	*f*	Transition nature	
[*trans*-**1**]$^{\bullet\bullet 2-}$	S_3	610	0.6634	HOMO(α)->L+3(α)	24%
				HOMO(β)->L+3(β)	28%
	S_5	570	0.3577	HOMO(α)->L+4(α)	20%
				HOMO(α)->L+10(α)	11%
				HOMO(β)->L+4(β)	30%
				HOMO(β)->L+10(β)	12%
	S_4	433.1	0.082	HOMO→LUMO+3	92%
[*cis*-**1**]$^{\bullet\bullet 2-}$	S_5	612	0.3377	HOMO(α)->L+3(α)	15%
				HOMO(α)->L+4(α)	18%
				HOMO(α)->L+3(β)	15%
				HOMO(β)->L+4(β)	18%
	S_6	583	0.3136	HOMO(α)->L+3(α)	25%
				HOMO(α)->L+4(α)	11%
				HOMO(β)->L+3(β)	25%

Coordinates of [*trans*-1]$^{\bullet\bullet 2-}$ and [*cis*-1]$^{\bullet\bullet 2-}$

[*trans*-**1**]$^{\bullet\bullet 2-}$ in closed-shell singlet state

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
N	-6.91419900	0.40283800	0.32260500
C	-6.15503500	2.62577600	-0.26962700
C	-6.61564400	-0.94074000	0.33444100
C	-1.81157300	-0.37403400	-0.86067700
H	-1.92996100	0.70647900	-0.81173400
C	-4.23411200	-0.70449100	-0.32233400
C	-7.75856700	-1.82854000	0.72859100
C	-4.60005300	0.71452400	-0.41905200
H	-3.87205900	1.44383000	-0.77082500
C	-5.41037900	-1.50951500	0.03551600
H	-5.34056800	-2.59528500	0.06780900
C	-0.54991600	-0.87322500	-1.11659100
C	-5.84989400	1.16724800	-0.10321100
C	-5.64215800	3.58106700	0.62203300
C	-7.27476800	4.40581500	-1.47632300
H	-7.91670500	4.72232000	-2.29821100
C	-6.99020400	3.05037400	-1.32127000
C	-2.96801800	-1.21297500	-0.53987900
C	-8.48772700	-2.52985800	-0.24316200
C	-0.27723000	-2.26930400	-1.05993000
H	0.68149300	-2.67357900	-1.37243500
C	-8.12838200	-1.94418900	2.08041300
C	-9.20000600	-2.76161500	2.43722000
H	-9.47728100	-2.84474800	3.48776800
C	-6.75803100	5.36828200	-0.60642500

C	-5.94836500	4.93367700	0.43942400
H	-5.54856200	5.66561100	1.14060100
C	-2.62630700	-2.64329500	-0.45504700
H	-3.39314300	-3.35437000	-0.15318000
C	-7.55975400	2.03725500	-2.28180100
H	-8.17097500	2.51338600	-3.05548400
H	-8.15703000	1.30229200	-1.73368300
H	-6.75173400	1.47503000	-2.76438800
C	-4.77428100	3.16440300	1.78645600
H	-5.18760200	2.28019900	2.28123400
H	-4.68943700	3.97307100	2.52082600
H	-3.76442400	2.89475400	1.46027300
C	-1.36324600	-3.11028600	-0.71901400
H	-1.18673500	-4.18694400	-0.65029500
C	-9.55663200	-3.34324100	0.14646400
H	-10.11893100	-3.88063500	-0.61655600
C	-9.92695200	-3.47541000	1.48227900
C	-7.35142000	-1.19713600	3.13579700
H	-7.83196500	-1.27032900	4.11702200
H	-7.25396300	-0.14494300	2.85154700
H	-6.33295100	-1.59428900	3.21800500
C	-7.05595500	6.83416500	-0.81042400
H	-6.43434100	7.25934900	-1.60851700
H	-6.86150200	7.41154000	0.09931500
H	-8.10149200	6.99413900	-1.09609000
C	-8.12880700	-2.40602900	-1.70477000
H	-7.93773500	-1.36067500	-1.96645600
H	-8.93253100	-2.79052000	-2.34230000
H	-7.21233600	-2.95820200	-1.93900400
C	-11.06855400	-4.37386300	1.89382100

H	-10.70037700	-5.30877000	2.33458100
H	-11.69624800	-4.63913600	1.03693000
H	-11.70597600	-3.89296300	2.64418300
N	6.87550900	-0.23142900	0.20854700
C	6.59000600	-2.59071800	-0.21885100
C	6.41487600	1.02684300	0.20593800
C	1.85978200	-0.18918200	-0.96406100
H	2.02980000	-1.09306200	-0.38569100
C	4.28243900	0.37127900	-0.71674500
C	7.33996600	2.08336000	0.71818700
C	4.77052900	-0.93755000	-0.70657100
H	4.16201700	-1.75849600	-1.07306700
C	5.14127100	1.36601900	-0.24342100
H	4.81894000	2.40176500	-0.19928600
C	0.55393100	0.07988600	-1.39694700
C	6.05807900	-1.19398400	-0.24116000
C	7.02330100	-3.19581200	-1.40722700
C	7.15859600	-4.58584700	1.00619300
H	7.21159900	-5.12589500	1.94967600
C	6.66095800	-3.28339600	0.99927300
C	2.91887600	0.69035300	-1.20464700
C	7.18078700	2.58042700	2.01939600
C	0.34448900	1.27341100	-2.10571500
H	-0.65160800	1.49235400	-2.47929500
C	8.36963500	2.56191600	-0.10573800
C	9.22500900	3.54672800	0.38635700
H	10.02452200	3.91934100	-0.25139400
C	7.58884900	-5.21242100	-0.16327100
C	7.51945100	-4.49901100	-1.35896000
H	7.86315700	-4.96775300	-2.27919600

C	2.67531100	1.87795300	-1.90364700
H	3.49131800	2.56064000	-2.12448100
C	6.21046700	-2.63078700	2.28346200
H	6.24656300	-3.33744300	3.11722900
H	6.84652000	-1.77367400	2.53004300
H	5.18505900	-2.25358700	2.19962600
C	6.97196600	-2.44969400	-2.71920300
H	7.44670600	-1.46588700	-2.63538000
H	7.48254000	-3.00970100	-3.50768600
H	5.93941600	-2.27850200	-3.04346700
C	1.38719300	2.16029600	-2.34895400
H	1.19873400	3.07314800	-2.90778500
C	8.05897300	3.56345900	2.47766200
H	7.94175200	3.94571700	3.48991400
C	9.08308900	4.06293500	1.67467100
C	8.55155300	2.01577700	-1.50090000
H	9.36017900	2.53344800	-2.02441700
H	8.78701100	0.94645000	-1.47402300
H	7.63570800	2.12511200	-2.09294500
C	8.09267200	-6.63411400	-0.13781900
H	7.26792200	-7.34318700	-0.27831000
H	8.81926400	-6.81436800	-0.93619300
H	8.56881600	-6.87146400	0.81866800
C	6.08895400	2.05446400	2.92010700
H	6.11604600	0.96100800	2.98014100
H	6.19008600	2.45502000	3.93264000
H	5.09516400	2.32716200	2.54788600
C	10.00129300	5.15011100	2.17559600
H	9.62939600	6.14045700	1.88609000
H	10.07923000	5.13499600	3.26701800

H	11.00806100	5.04469000	1.75911900

[*trans*-**1**]$^{\bullet 2-}$ in triplet state

N	-6.90373200	0.43211300	0.24547200
C	-6.15635700	2.73237000	0.26784700
C	-6.61066200	-0.87939000	0.02326400
C	-1.83368900	-0.05703300	-1.00712200
H	-1.94251900	0.96540100	-0.65790600
C	-4.26363000	-0.47839500	-0.57107300
C	-7.73623700	-1.84051000	0.25582000
C	-4.58977100	0.89890400	-0.32635600
H	-3.84602200	1.67897500	-0.46206500
C	-5.38113500	-1.35722300	-0.36672300
H	-5.27381100	-2.43099700	-0.49200500
C	-0.56774500	-0.46687000	-1.40844600
C	-5.85471900	1.28064900	0.05538500
C	-5.68793800	3.39931400	1.40983400
C	-7.21100800	4.77938400	-0.47030200
H	-7.80840400	5.31457100	-1.20723800
C	-6.93165300	3.42911500	-0.67565700
C	-2.96668600	-0.92688200	-0.98078800
C	-8.38574900	-2.45384400	-0.82503800
C	-0.36850500	-1.80263100	-1.81031200
H	0.60676500	-2.13067500	-2.15768100
C	-8.15331200	-2.12463500	1.56923100
C	-9.19819400	-3.02258700	1.77719100
H	-9.51153300	-3.24371500	2.79679500
C	-6.74462500	5.46197300	0.65421100
C	-5.98970500	4.75259900	1.58508400
H	-5.62819400	5.26340700	2.47631400

C	-2.71396700	-2.27367900	-1.38759500
H	-3.52633600	-2.99429700	-1.41083400
C	-7.45421900	2.72297500	-1.90269500
H	-7.98060300	3.41667100	-2.56562800
H	-8.13595100	1.91467900	-1.61961100
H	-6.63514500	2.25909600	-2.46421600
C	-4.87504700	2.67129600	2.45463400
H	-5.33395400	1.71126300	2.71247200
H	-4.78474000	3.26989900	3.36667600
H	-3.86489900	2.44937400	2.09408900
C	-1.45483600	-2.68350100	-1.78728000
H	-1.31158400	-3.71538600	-2.10427000
C	-9.43274800	-3.34760800	-0.57949700
H	-9.93469600	-3.81752200	-1.42392700
C	-9.85212800	-3.64757600	0.71333900
C	-7.47053500	-1.46847700	2.74386000
H	-7.85563500	-1.85414800	3.69287300
H	-7.61593200	-0.38406900	2.71600500
H	-6.38868900	-1.64000500	2.71185200
C	-7.03430500	6.93140200	0.84088100
H	-6.34562500	7.54772700	0.24984200
H	-6.92538600	7.22980700	1.88835100
H	-8.05089800	7.18218600	0.51971000
C	-7.97617900	-2.15275700	-2.24764200
H	-7.89284600	-1.07353000	-2.41178100
H	-8.70399800	-2.55725800	-2.95823400
H	-6.99622100	-2.58145600	-2.48317100
C	-10.98286900	-4.61429400	0.96846300
H	-10.65874700	-5.44561800	1.60519100
H	-11.36507300	-5.03665100	0.03403700

H	-11.81825000	-4.12264100	1.48066800
N	6.89689300	-0.43364700	0.25792300
C	6.10841100	-2.71710900	0.37626200
C	6.62288100	0.87499300	-0.00190000
C	1.83381900	0.08436700	-1.00487100
H	1.93841500	-0.94009000	-0.66101300
C	4.26550100	0.49412400	-0.56956300
C	7.77676500	1.81756300	0.15957100
C	4.57373600	-0.88119100	-0.29062100
H	3.81833500	-1.65410200	-0.39927900
C	5.39883200	1.36072200	-0.40011500
H	5.30975600	2.43134200	-0.56217700
C	0.56927100	0.49843100	-1.40577200
C	5.83498700	-1.27121800	0.09377800
C	6.27159200	-3.63023800	-0.67696600
C	6.48916600	-4.50535500	1.95820100
H	6.57638100	-4.84213100	2.99023000
C	6.22537400	-3.15931200	1.70423200
C	2.97045300	0.94966400	-0.97746200
C	7.85067600	2.67042000	1.27185800
C	0.37334600	1.83564400	-1.80412100
H	-0.60107900	2.16737700	-2.15045000
C	8.80480900	1.83562500	-0.79849000
C	9.87653300	2.71369300	-0.63867000
H	10.66790900	2.72467200	-1.38694800
C	6.64330000	-5.42917000	0.92468200
C	6.53607300	-4.97038300	-0.38691200
H	6.66709000	-5.67386100	-1.20795800
C	2.72113600	2.29819800	-1.38145000
H	3.53398100	3.01830000	-1.39921900

C	6.06376400	-2.18575000	2.84524100
H	6.14524900	-2.68938200	3.81332800
H	6.82292800	-1.39926900	2.78819800
H	5.09022300	-1.68537100	2.79423700
C	6.17870100	-3.17444800	-2.11378800
H	6.79774700	-2.28741300	-2.28347900
H	6.50751300	-3.96347500	-2.79758700
H	5.15323900	-2.89786600	-2.38074800
C	1.46286200	2.71276500	-1.77925900
H	1.32258800	3.74627500	-2.09232400
C	8.94000100	3.53534200	1.40167600
H	8.99463600	4.19018000	2.27014500
C	9.96083300	3.57641500	0.45442800
C	8.75127600	0.91292800	-1.99094700
H	9.56192600	1.12563200	-2.69470000
H	8.82529800	-0.13170800	-1.67235000
H	7.79589600	1.01107800	-2.51847700
C	6.89464700	-6.88817200	1.21798600
H	5.95164400	-7.44411800	1.29059700
H	7.48941400	-7.35742600	0.42750700
H	7.42482400	-7.01953700	2.16679100
C	6.77652900	2.65167100	2.33364100
H	6.56485000	1.62805200	2.65969700
H	7.07868100	3.23849600	3.20687000
H	5.83366000	3.06228300	1.95762000
C	11.11324500	4.54119200	0.59262600
H	10.91897100	5.47000100	0.04195900
H	11.28413400	4.81134300	1.63962300
H	12.04040700	4.11535700	0.19507200

[*trans*-1]$^{\bullet\bullet 2-}$ in open-shell singlet state

N	-6.90781700	0.43159500	0.24336300
C	-6.16117300	2.73195300	0.26718300
C	-6.61388300	-0.87990400	0.02171500
C	-1.83475200	-0.05611300	-0.99890900
H	-1.94453000	0.96626700	-0.64992500
C	-4.26586900	-0.47832400	-0.56865100
C	-7.73948300	-1.84138800	0.25260600
C	-4.59297700	0.89901000	-0.32449400
H	-3.84920400	1.67929100	-0.45889800
C	-5.38362800	-1.35739200	-0.36614100
H	-5.27586600	-2.43118000	-0.49104600
C	-0.56757200	-0.46613400	-1.39771400
C	-5.85872500	1.28031100	0.05505300
C	-5.69549600	3.39867000	1.41041200
C	-7.21469700	4.77893200	-0.47267800
H	-7.81060800	5.31417900	-1.21077300
C	-6.93461800	3.42877900	-0.67777700
C	-2.96795100	-0.92611800	-0.97516500
C	-8.38726000	-2.45494800	-0.82916200
C	-0.36773500	-1.80220800	-1.79836900
H	0.60807500	-2.13043000	-2.14399300
C	-8.15828000	-2.12574000	1.56542700
C	-9.20320000	-3.02398600	1.77190100
H	-9.51785700	-3.24527600	2.79106700
C	-6.75092600	5.46132500	0.65303700
C	-5.99793100	4.75184900	1.58538300
H	-5.63851400	5.26247000	2.47756700
C	-2.71408700	-2.27297200	-1.38130600

H	-3.52651500	-2.99348300	-1.40659400
C	-7.45455600	2.72282300	-1.90603600
H	-7.97941000	3.41664100	-2.57005400
H	-8.13700600	1.91457500	-1.62451600
H	-6.63428400	2.25893600	-2.46578100
C	-4.88495800	2.67041600	2.45686400
H	-5.34509900	1.71081400	2.71415300
H	-4.79584600	3.26921400	3.36889300
H	-3.87437300	2.44759900	2.09812700
C	-1.45426200	-2.68320600	-1.77791000
H	-1.31037800	-3.71506700	-2.09459400
C	-9.43435300	-3.34902100	-0.58511800
H	-9.93495400	-3.81909200	-1.43026300
C	-9.85549500	-3.64910800	0.70711700
C	-7.47716100	-1.46961800	2.74104000
H	-7.86332900	-1.85557800	3.68950300
H	-7.62279400	-0.38524300	2.71322200
H	-6.39523200	-1.64085100	2.71029900
C	-7.04143200	6.93062800	0.83944000
H	-6.35323900	7.54723400	0.24813100
H	-6.93253200	7.22932000	1.88682600
H	-8.05823300	7.18074400	0.51838400
C	-7.97561600	-2.15391100	-2.25118300
H	-7.89115600	-1.07473700	-2.41503300
H	-8.70282800	-2.55772000	-2.96279200
H	-6.99571200	-2.58339600	-2.48553900
C	-10.98644600	-4.61601000	0.96061900
H	-10.66362500	-5.44628800	1.59936100
H	-11.36601900	-5.03982400	0.02577900
H	-11.82341000	-4.12403100	1.46993300

N	6.90098400	-0.43316700	0.25615900
C	6.11300800	-2.71665400	0.37572600
C	6.62631300	0.87550200	-0.00340400
C	1.83513400	0.08397200	-0.99667300
H	1.94055200	-0.94027800	-0.65255900
C	4.26804500	0.49430500	-0.56753500
C	7.78020000	1.81832100	0.15661700
C	4.57710700	-0.88109800	-0.28913600
H	3.82172000	-1.65416800	-0.39678300
C	5.40166900	1.36098700	-0.39988600
H	5.31223400	2.43162700	-0.56173300
C	0.56938500	0.49818800	-1.39519600
C	5.83901100	-1.27080700	0.09341500
C	6.27636300	-3.62969200	-0.67753700
C	6.49459900	-4.50479100	1.95758500
H	6.58206900	-4.84155400	2.98959800
C	6.23027700	-3.15883900	1.70366200
C	2.97208900	0.94926800	-0.97231900
C	7.85473600	2.67203800	1.26821600
C	0.37299800	1.83559500	-1.79278000
H	-0.60194100	2.16750800	-2.13743500
C	8.80769300	1.83580300	-0.80206500
C	9.87944300	2.71406900	-0.64354300
H	10.67035300	2.72457200	-1.39232300
C	6.64895800	-5.42852000	0.92402400
C	6.54138500	-4.96974500	-0.38755200
H	6.67252700	-5.67316400	-1.20863100
C	2.72177800	2.29775000	-1.37607200
H	3.53481300	3.01761100	-1.39625000
C	6.06841900	-2.18529900	2.84465400

H	6.15059400	-2.68877600	3.81276400
H	6.82702100	-1.39829700	2.78725700
H	5.09452100	-1.68559200	2.79391500
C	6.18297200	-3.17385700	-2.11430300
H	6.80238000	-2.28712700	-2.28428300
H	6.51104700	-3.96302200	-2.79829400
H	5.15750900	-2.89672900	-2.38068300
C	1.46282200	2.71273400	-1.77083700
H	1.32201200	3.74613100	-2.08393400
C	8.94410200	3.53711100	1.39676800
H	8.99922200	4.19255800	2.26474900
C	9.96436900	3.57756900	0.44889500
C	8.75356200	0.91223900	-1.99380600
H	9.56310500	1.12525200	-2.69874200
H	8.82902100	-0.13209100	-1.67456300
H	7.79739000	1.00904200	-2.52014300
C	6.90086300	-6.88744000	1.21727100
H	5.95806800	-7.44372400	1.29000500
H	7.49569100	-7.35647400	0.42670700
H	7.43121500	-7.01862900	2.16600300
C	6.78122500	2.65415100	2.33065900
H	6.56860900	1.63068700	2.65655500
H	7.08456600	3.24044400	3.20383600
H	5.83856600	3.06593700	1.95537300
C	11.11684300	4.54246800	0.58573300
H	10.92234100	5.47079800	0.03433900
H	11.28820100	4.81353200	1.63241800
H	12.04382800	4.11627800	0.18814200

[*cis*-1]$^{\bullet\bullet 2-}$ in closed-shell singlet state

N	4.86817400	-0.62956400	-0.33507200
C	0.63636800	4.26703700	-0.87676100
C	3.16202500	-1.80280800	-1.58594000
C	2.80423800	3.12168200	-0.74379700
C	5.35969800	0.49325500	0.20597800
C	3.54653400	1.84266200	-0.64641500
C	1.41324700	3.10093900	-0.85619000
C	3.73089100	-0.53495400	-1.03940600
C	6.62637300	0.36389600	0.98937000
C	4.72750900	1.72942400	0.09209400
H	5.14582100	2.58823000	0.60769100
C	3.84727900	-2.50876900	-2.58960500
C	3.07063100	0.67283200	-1.24354100
H	2.17596500	0.68603200	-1.85703600
C	6.60591000	-0.26239400	2.24489900
C	2.09166600	-4.19656400	-2.58959000
C	1.94500000	-2.28754800	-1.08135700
C	3.46257400	4.35861900	-0.69062800
H	4.54710700	4.40445800	-0.64060200
C	1.43370500	-3.48236700	-1.59245600
H	0.49396200	-3.85639100	-1.19341300
C	7.82922500	0.85944500	0.46299600
C	2.71590900	5.52999500	-0.73281400
H	3.22257700	6.49102900	-0.69394300
C	3.29931200	-3.69337400	-3.07713700
H	3.82794100	-4.23851100	-3.85747500
C	1.32565200	5.48885700	-0.81612900
C	8.99968500	0.72634500	1.20972000
H	9.93429600	1.10326100	0.79816500
C	7.79682800	-0.37189600	2.96350700

H	7.78153700	-0.85499200	3.93859800
C	5.31974200	-0.81056500	2.81376500
H	5.47255100	-1.20364800	3.82279500
H	4.92648300	-1.61479300	2.18386900
H	4.54478500	-0.03722900	2.86138300
C	9.00265500	0.11882700	2.46503700
C	1.18107200	-1.56368000	0.00385800
H	0.65277200	-0.68893800	-0.39348100
H	1.84641400	-1.20342200	0.79520500
H	0.43052200	-2.21923500	0.45290000
C	5.15168400	-1.99033900	-3.14590400
H	5.92602700	-1.96546600	-2.37322400
H	5.04194500	-0.96560600	-3.51956900
H	5.50189200	-2.61746300	-3.97080300
C	1.50590300	-5.47212600	-3.14260200
H	1.02571000	-5.29631600	-4.11266000
H	0.74806600	-5.88401600	-2.46886400
H	2.27817500	-6.23367200	-3.29472700
C	7.87156900	1.51184800	-0.89884400
H	7.37530200	0.89128800	-1.65270000
H	8.90404600	1.67873000	-1.21859100
H	7.35979700	2.48078000	-0.89764500
C	10.27562600	0.01838800	3.26845100
H	11.13440000	-0.20579000	2.62733200
H	10.20591100	-0.76292400	4.03123300
H	10.48944800	0.96358300	3.78178800
H	0.90207700	2.14622600	-0.91433300
H	0.75784800	6.41402700	-0.80558200
N	-4.80944100	-0.82511300	0.72170000
C	-0.84639200	4.20509800	-0.96265900

C	-2.65850000	-1.92076800	0.78307700
C	-2.94124600	2.89014000	-0.53601600
C	-5.51603100	0.29895500	0.35368500
C	-3.54219400	1.68813500	-0.21340300
C	-1.49134400	3.06966200	-0.51223500
C	-3.45864300	-0.68111300	0.51160100
C	-7.00684200	0.17102100	0.45892300
C	-4.98751600	1.47366900	-0.10494300
H	-5.67915500	2.27041500	-0.37434000
C	-2.10269700	-2.14511800	2.05239500
C	-2.81648500	0.44439600	0.08109200
H	-1.74053000	0.38588300	-0.07770900
C	-7.71083800	-0.65333600	-0.43689800
C	-1.18472300	-4.27437500	1.30062300
C	-2.48671100	-2.88636800	-0.22202500
C	-3.66155500	4.11879400	-0.90993500
H	-4.74646400	4.15169100	-0.82119100
C	-1.76840800	-4.05053900	0.05358100
H	-1.65334300	-4.80032500	-0.72953000
C	-7.71848800	0.85299700	1.46178300
C	-2.99864300	5.23316400	-1.35863800
H	-3.59228700	6.10317800	-1.65247300
C	-1.36904000	-3.31081800	2.29082000
H	-0.92883100	-3.46881500	3.27455800
C	-1.58693600	5.32478300	-1.43767300
C	-9.10632900	0.71424300	1.54152800
H	-9.64626800	1.24162500	2.32758400
C	-9.09800200	-0.76655500	-0.33250900
H	-9.63254000	-1.40287700	-1.03727600
C	-6.96952200	-1.41023100	-1.50959800

H	-7.65878700	-1.89821600	-2.20658700
H	-6.31798900	-2.16285600	-1.05568200
H	-6.31296100	-0.73679900	-2.07234700
C	-9.81738300	-0.08629300	0.64951600
C	-3.04435800	-2.65618000	-1.60449600
H	-2.40685600	-1.96471500	-2.16758400
H	-4.03815100	-2.20477500	-1.55069600
H	-3.10453700	-3.59356600	-2.16772800
C	-2.29138300	-1.12789700	3.15225700
H	-3.35117200	-0.87437600	3.26027100
H	-1.76831200	-0.19488800	2.91786100
H	-1.91715500	-1.50470800	4.11001200
C	-0.34264100	-5.50255900	1.54400100
H	0.64668000	-5.39298200	1.08076500
H	-0.80404700	-6.39794000	1.11306500
H	-0.18884900	-5.67970500	2.61308600
C	-7.00088900	1.72448000	2.46607800
H	-6.11449700	1.21831700	2.86017000
H	-7.66070400	1.98132100	3.30209700
H	-6.64879800	2.65574200	2.01111200
C	-11.32110100	-0.19297100	0.73176600
H	-11.66622200	-0.18774700	1.77143400
H	-11.68376500	-1.11154200	0.25912100
H	-11.80766600	0.65015800	0.22511500
H	-0.90048600	2.29810400	-0.02500800
H	-1.10284500	6.17743800	-1.90436700

[*cis*-1]$^{\bullet\bullet 2-}$ in triplet state

N	5.02872700	-0.73914100	-0.58208400

C	0.73327400	4.21802900	0.13375200
C	3.02723400	-1.78575200	-1.45174500
C	2.87217000	2.96030700	0.13794600
C	5.61994300	0.37050500	-0.05789300
C	3.58837400	1.74452300	-0.10496000
C	1.47420700	3.07228900	-0.12517000
C	3.70213900	-0.58851000	-0.85699600
C	7.06669000	0.21650500	0.29765800
C	4.98433000	1.56718700	0.18103500
H	5.57213100	2.37562200	0.60707500
C	3.28970400	-2.13759900	-2.78773600
C	2.97928800	0.56071700	-0.64504400
H	1.92477400	0.54204600	-0.90266000
C	7.42553000	-0.54496200	1.42482800
C	1.79051000	-4.04665700	-2.59312500
C	2.15116400	-2.56976500	-0.68614100
C	3.48925400	4.13992400	0.65955700
H	4.55473500	4.14799700	0.87151900
C	1.55520300	-3.69201500	-1.26782100
H	0.89214700	-4.30843200	-0.66392500
C	8.06635300	0.80522600	-0.48938600
C	2.75830200	5.29035000	0.89995800
H	3.26823100	6.16357600	1.30425800
C	2.66600400	-3.25590900	-3.33845100
H	2.86702400	-3.51738800	-4.37644500
C	1.38207500	5.35669200	0.65102100
C	9.40815100	0.63221900	-0.13608600
H	10.18039300	1.08571200	-0.75565700
C	8.77219200	-0.69527300	1.74846500
H	9.04439500	-1.28341700	2.62405000

C	6.35966400	-1.18669600	2.27819900
H	6.79516100	-1.69286000	3.14517700
H	5.78360300	-1.90992200	1.69282600
H	5.64344300	-0.43763100	2.63494800
C	9.78150700	-0.11168300	0.97987600
C	1.84269300	-2.22205500	0.75089400
H	1.12125900	-1.39906100	0.81332300
H	2.74261400	-1.89946700	1.28360000
H	1.40601400	-3.07752500	1.27552700
C	4.22807500	-1.30296900	-3.62380100
H	5.22123600	-1.26751400	-3.16571400
H	3.87520100	-0.26705500	-3.68732900
H	4.31686700	-1.70176000	-4.63905100
C	1.09905200	-5.23506800	-3.21486200
H	0.19440900	-4.92619200	-3.75318000
H	0.79484800	-5.96204100	-2.45501600
H	1.74813300	-5.74536600	-3.93418600
C	7.71052000	1.60853700	-1.71825100
H	6.98979800	1.07085600	-2.34269600
H	8.60104100	1.82113400	-2.31836100
H	7.24395900	2.56339100	-1.45346300
C	11.23193800	-0.28406000	1.36033500
H	11.89862300	0.09254400	0.57845900
H	11.47405300	-1.33878800	1.53234200
H	11.46581100	0.25559100	2.28599500
H	0.94963000	2.22887600	-0.56037300
H	0.81742800	6.25576400	0.88109200
N	-5.02872500	-0.73914400	0.58207600
C	-0.73328000	4.21803400	-0.13371900
C	-3.02725700	-1.78572600	1.45182400

C	-2.87218300	2.96032400	-0.13789300
C	-5.61994100	0.37050100	0.05787800
C	-3.58839100	1.74454600	0.10502600
C	-1.47421100	3.07229000	0.12518200
C	-3.70215500	-0.58848700	0.85706200
C	-7.06667300	0.21648400	-0.29772800
C	-4.98433500	1.56719300	-0.18101600
H	-5.57212900	2.37562300	-0.60707500
C	-3.28973300	-2.13757200	2.78781100
C	-2.97931400	0.56075300	0.64515100
H	-1.92481900	0.54210800	0.90284800
C	-7.42545500	-0.54498600	-1.42491200
C	-1.79053000	-4.04662400	2.59321200
C	-2.15117700	-2.56973600	0.68622400
C	-3.48926900	4.13995300	-0.65947700
H	-4.55475500	4.14803600	-0.87141600
C	-1.55521200	-3.69198000	1.26790700
H	-0.89214400	-4.30839300	0.66402000
C	-8.06637700	0.80520800	0.48926600
C	-2.75831600	5.29037900	-0.89987000
H	-3.26824800	6.16361300	-1.30414800
C	-2.66603200	-3.25588100	3.33853100
H	-2.86705500	-3.51735800	4.37652500
C	-1.38208500	5.35671300	-0.65095000
C	-9.40815700	0.63219600	0.13589700
H	-10.18043200	1.08569100	0.75542500
C	-8.77210000	-0.69530500	-1.74861400
H	-9.04425700	-1.28345400	-2.62420900
C	-6.35954400	-1.18670300	-2.27823900
H	-6.79499800	-1.69289400	-3.14522200

H	-5.78347500	-1.90989700	-1.69283600
H	-5.64333500	-0.43762000	-2.63497900
C	-9.78145500	-0.11171500	-0.98007700
C	-1.84270000	-2.22201300	-0.75080600
H	-1.12129900	-1.39899000	-0.81322400
H	-2.74262900	-1.89945600	-1.28351900
H	-1.40598500	-3.07746500	-1.27543700
C	-4.22811500	-1.30294400	3.62386500
H	-5.22126800	-1.26749400	3.16576000
H	-3.87524700	-0.26702900	3.68740000
H	-4.31692400	-1.70173600	4.63911300
C	-1.09906600	-5.23503000	3.21495100
H	-0.19439000	-4.92615800	3.75321600
H	-0.79491500	-5.96203200	2.45511200
H	-1.74812300	-5.74529100	3.93432300
C	-7.71062000	1.60855000	1.71813300
H	-6.98984100	1.07094800	2.34257900
H	-8.60116100	1.82106100	2.31824300
H	-7.24415700	2.56345300	1.45334500
C	-11.23186700	-0.28409800	-1.36060700
H	-11.89859200	0.09247500	-0.57874900
H	-11.47396200	-1.33882400	-1.53265700
H	-11.46570400	0.25557900	-2.28626000
H	-0.94962400	2.22885300	0.56032800
H	-0.81744100	6.25579000	-0.88100600

[*cis*-1]$^{\bullet\bullet 2-}$ in open-shell singlet state

N	5.02889900	-0.73994400	-0.57905200
C	0.73368100	4.21942400	0.13014100

C	3.02764400	-1.78742500	-1.44784400
C	2.87300900	2.96125700	0.13343700
C	5.62048400	0.37088500	-0.05765200
C	3.58899200	1.74510900	-0.10671800
C	1.47374600	3.07167500	-0.12453200
C	3.70247300	-0.58945200	-0.85439100
C	7.06723800	0.21733100	0.29807500
C	4.98522200	1.56818600	0.17870600
H	5.57324500	2.37729900	0.60318100
C	3.29033100	-2.14073600	-2.78341500
C	2.97969600	0.56020100	-0.64446000
H	1.92536200	0.54148500	-0.90282700
C	7.42584200	-0.54084500	1.42751600
C	1.79184200	-4.05010900	-2.58670900
C	2.15160200	-2.57070500	-0.68148100
C	3.49190100	4.14356000	0.64693500
H	4.55830700	4.15288300	0.85422300
C	1.55623600	-3.69393300	-1.26187000
H	0.89332700	-4.30987500	-0.65737200
C	8.06707700	0.80294000	-0.49103800
C	2.76227100	5.29540100	0.88351100
H	3.27372000	6.17081700	1.28103200
C	2.66705400	-3.25988000	-3.33290400
H	2.86823400	-3.52246700	-4.37058800
C	1.38514100	5.36079200	0.63821600
C	9.40884200	0.63035700	-0.13736800
H	10.18122800	1.08143200	-0.75852100
C	8.77245500	-0.69082500	1.75148800
H	9.04446200	-1.27637300	2.62886900
C	6.35961500	-1.17956200	2.28267000

H	6.79491400	-1.68543300	3.14991900
H	5.78192200	-1.90241500	1.69844500
H	5.64490500	-0.42887800	2.63907200
C	9.78195500	-0.11019100	0.98089300
C	1.84233100	-2.22106900	0.75490600
H	1.12098300	-1.39789100	0.81571600
H	2.74192300	-1.89780700	1.28775000
H	1.40522300	-3.07580000	1.28039900
C	4.22836300	-1.30671600	-3.62047100
H	5.22141100	-1.26995500	-3.16226400
H	3.87480700	-0.27113400	-3.68560700
H	4.31759000	-1.70692600	-4.63512800
C	1.10099800	-5.23959600	-3.20706200
H	0.19746000	-4.93155300	-3.74771400
H	0.79515100	-5.96477400	-2.44616000
H	1.75114300	-5.75178200	-3.92409000
C	7.71148300	1.60231300	-1.72252900
H	6.99263200	1.06144700	-2.34642000
H	8.60242600	1.81472200	-2.32207900
H	7.24285900	2.55705400	-1.46108700
C	11.23235700	-0.28247700	1.36154500
H	11.89910500	0.09564900	0.58046000
H	11.47492000	-1.33738500	1.53191000
H	11.46564100	0.25573800	2.28817000
H	0.94795200	2.22560300	-0.55290500
H	0.82225400	6.26176500	0.86500700
N	-5.02885700	-0.73990600	0.57903500
C	-0.73359100	4.21941100	-0.13036500
C	-3.02760300	-1.78746900	1.44769500
C	-2.87290100	2.96121100	-0.13366600

C	-5.62043900	0.37092700	0.05764700
C	-3.58888300	1.74506400	0.10650400
C	-1.47363900	3.07164800	0.12430200
C	-3.70239000	-0.58949000	0.85420500
C	-7.06723000	0.21742300	-0.29794000
C	-4.98514000	1.56818700	-0.17882100
H	-5.57316700	2.37732000	-0.60325400
C	-3.29018900	-2.14058700	2.78334000
C	-2.97958400	0.56013600	0.64420300
H	-1.92523200	0.54138600	0.90249100
C	-7.42596800	-0.54101000	-1.42716200
C	-1.79202100	-4.05021400	2.58669600
C	-2.15177000	-2.57098400	0.68132200
C	-3.49181400	4.14351200	-0.64714000
H	-4.55822300	4.15282400	-0.85441200
C	-1.55652400	-3.69423900	1.26178800
H	-0.89381000	-4.31037500	0.65727900
C	-8.06697200	0.80327100	0.49111700
C	-2.76220100	5.29536700	-0.88371000
H	-3.27366800	6.17078100	-1.28121200
C	-2.66701700	-3.25975200	3.33289900
H	-2.86811500	-3.52217600	4.37064000
C	-1.38507100	5.36077400	-0.63842500
C	-9.40877600	0.63070100	0.13758100
H	-10.18108500	1.08197600	0.75868300
C	-8.77261500	-0.69099100	-1.75099200
H	-9.04472400	-1.27675700	-2.62819500
C	-6.35984300	-1.18005300	-2.28219800
H	-6.79523400	-1.68614500	-3.14927100
H	-5.78215600	-1.90277700	-1.69780600

H	-5.64511100	-0.42951700	-2.63886800
C	-9.78202200	-0.11009400	-0.98047200
C	-1.84262400	-2.22168000	-0.75517800
H	-1.12112700	-1.39865100	-0.81624600
H	-2.74221600	-1.89837300	-1.28799600
H	-1.40572600	-3.07659900	-1.28054300
C	-4.22796100	-1.30630100	3.62041900
H	-5.22106200	-1.26938500	3.16234300
H	-3.87419100	-0.27078200	3.68540200
H	-4.31713300	-1.70638500	4.63513100
C	-1.10130400	-5.23974200	3.20711000
H	-0.19774300	-4.93176800	3.74776400
H	-0.79552500	-5.96498600	2.44624500
H	-1.75150800	-5.75183600	3.92415200
C	-7.71124100	1.60292000	1.72239000
H	-6.99226400	1.06223400	2.34628900
H	-8.60210900	1.81540800	2.32202400
H	-7.24271200	2.55763600	1.46067700
C	-11.23246200	-0.28238300	-1.36097100
H	-11.89912800	0.09592200	-0.57990200
H	-11.47509000	-1.33731000	-1.53111900
H	-11.46579700	0.25567100	-2.28767800
H	-0.94783300	2.22559000	0.55268800
H	-0.82219900	6.26175900	-0.86520800

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