Electronic Supplementary Information for

Synthesis and Isolation of a Stable, Axially-Chiral 7-Membered N-Heterocyclic Carbene

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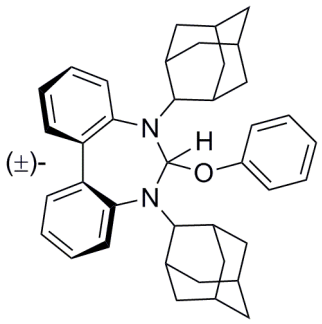
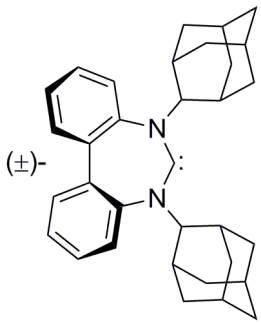
General considerations. Complexes $\mathbf{3}^{\mathbf{OPh}}$, **4**, and **5** were synthesized in a glove box using dry solvents. NMR spectra were recorded on 300 MHz or 500 MHz spectrometers; ^{1}H NMR spectra are referenced to TMS (0.0 ppm), while ^{13}C NMR spectra were referenced to C_6D_6 (128.06 ppm). The FTIR spectrum of **6** (0.025 M in C_6D_6) was recorded on an Hamilton Sundstrand Analect ChemEye FTIR analyzer. Flash chromatography was performed on silica gel 60 (particle size 0.040-0.063mm, 230-400 mesh ASTM, purchased from Sorbent Technology). Complexes $\mathbf{3}^{\mathbf{OMe}}$ and $\mathbf{3}^{\mathbf{O}t\mathbf{Bu}}$ have been reported previously.[1]



$\mathbf{3}^{\mathbf{OPh}}$. Amidinium salt (1.00 g, 1.822 mmol) was combined with 279 mg NaOPh (2.41 mmol) in a glove box. 10 mL dry Et_2O was added, and the suspension stirred until it had clarified (about 20 minutes).

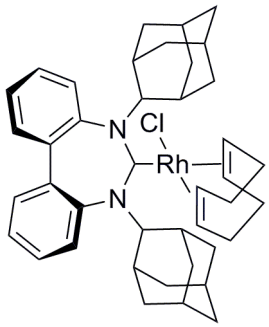
[1] C. C. Scarborough, M. J. W. Grady, I. A. Guzei, B. A. Gandhi, E. E. Bunel and S. S. Stahl, *Angew. Chem. Int. Ed.*, 2005, **44**, 5269-5272.

The solution was dried under vacuum, and the residue was suspended in 10 mL pentane. This suspension was filtered over celite and the filtrate was dried under vacuum to afford 1.00 g **3**$^{\mathbf{OPh}}$ as a white powder, 99% yield. This material used without further purification for the synthesis of free NHC **4**. ^{1}H NMR (C_6D_6, 297K, 300 MHz): δ 1.07 (d, J = 12.6 Hz, 1H), δ 1.16 (d, J = 12.6 Hz, 2H), δ 1.24 - 1.29 (m, 2H), δ 1.25 (s, 4H), δ 1.43 - 1.60 (m, 12H), δ 1.63 (s, 1H), δ 1.73 (s, 1H), δ 1.85 (d, J = 12.6 Hz, 1H), δ 1.97 (s, 2H), δ 2.20 (d, J = 12.6 Hz, 1H), δ 2.28 (s, 1H), δ 3.41 (s, 1H), δ 3.90 (s, 1H), δ 6.47 (s, 1H), δ 6.87 (t, J = 7.0 Hz, 1H), δ 7.11 (t, J = 7.0 Hz, 1H), δ 7.18 - 7.25 (m, 5H), δ 7.34 (d, J = 8.4 Hz, 2H), δ 7.43 (d, J = 7.7 Hz, 2H), δ 7.46 (d, J = 7.7 Hz, 1H). ^{13}C NMR (C_6D_6, 297K, 300 MHz): δ 27.4, δ 27.5, δ 29.0, δ 29.8, δ 30.8, δ 31.4, δ 31.6, δ 31.9, δ 32.1, δ 32.7, δ 36.7, δ 37.1, δ 37.5, δ 37.6, δ 37.9, δ 38.9, δ 59.5, δ 61.1, δ 104.9, δ 117.2, δ 122.0, δ 124.4, δ 126.3, δ 126.4, δ 127.2, δ 127.56, δ 127.63, δ 128.3, δ 129.2, δ 129.9, δ 139.3, δ 143.2, δ 145.8, δ 158.9.

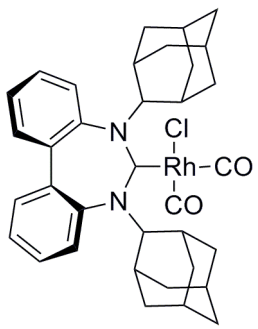


4. Complex **2** (201 mg, 0.365 mmol) was combined with 46 mg NaOPh (1.09 equiv) in 6 mL Et_2O in a glove box. This solution was stirred for 30 minutes, after which the solvent was removed under vacuum. Pentane (~3 mL) was added and removed in vacuo 3x to drive off any remaining Et_2O. The residue was suspended in 6 mL pentane, and the off-white precipitate was removed by filtration through celite. 1.05 equivalents of *n*-BuLi (2.0 M in pentane) was added in one portion via syringe. Immediately, a white solid formed and the solution turned bright yellow. After stirring at room temperature for 20 minutes, the solvent was removed in vacuo and benzene was added to the residue. Filtration over celite afforded free NHC **4** in 87% yield as a yellow solid. Crystals of **4** suitable for X-ray diffraction analysis were obtained by slow evaporation of a benzene solution of **4** under a nitrogen atmosphere. NMR (C_6D_6, 297K,

300 MHz): δ 1.09 (s, 2H), δ 1.44 - 1.73 (m, 16H), δ 1.90 (s, 4H), δ 2.09 (s, 2H), δ 2.35 (d, J = 12.3 H, 2H), δ 3.37 (s, 2H), δ 4.49 (s, 2H), δ 6.95 - 7.02 (m, 4H), δ 7.05 - 7.08 (m, 2H), δ 7.20 - 7.23 (m, 2H). ^{13}C NMR ($CDCl_3$, 297K, 300 MHz): δ 28.0, δ 30.4, δ 31.0, δ 31.1, δ 32.6, δ 37.2, δ 37.8, δ 38.2, δ 64.5, δ 121.8, δ 125.2, δ 127.2, δ 137.5, δ 146.1 (carbene carbon not detected).



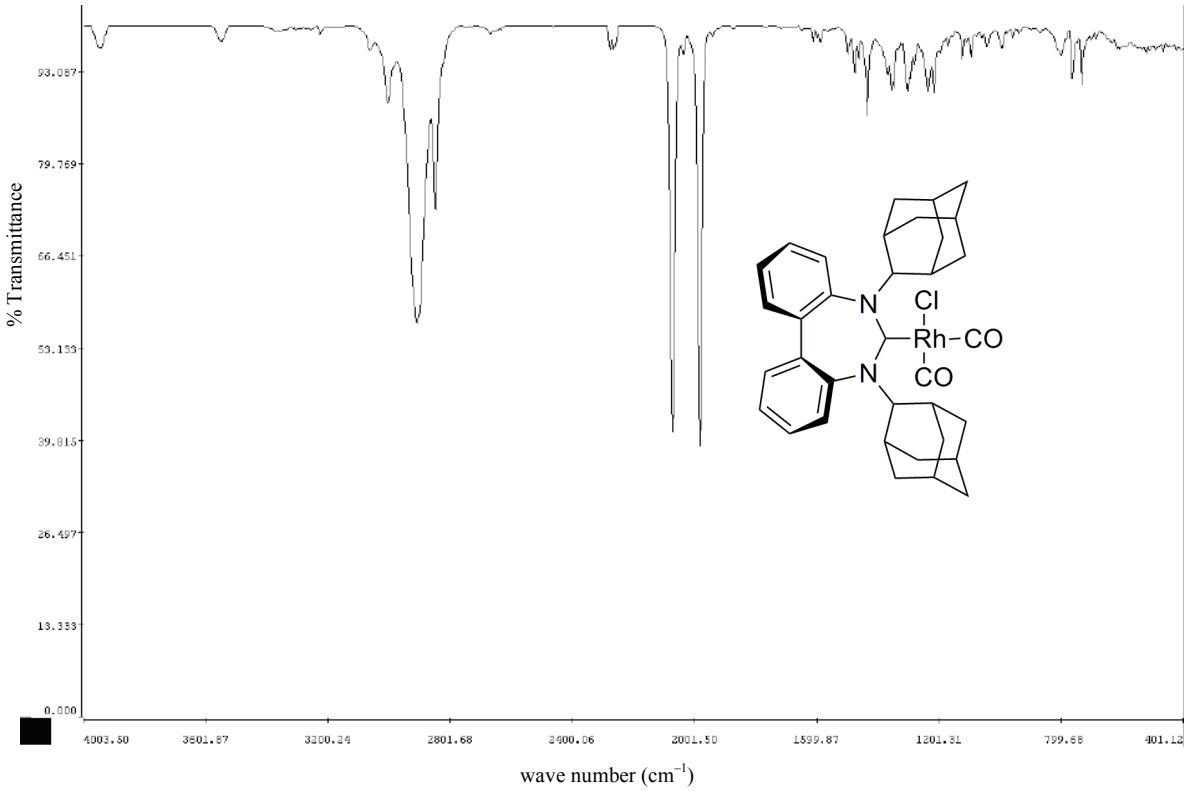
5. Free NHC **4** (179 mg, 0.387 mmol) and $[Rh(COD)Cl]_2$ (83.3 mg, 0.44 equiv) were combined in dry THF in a glove box. The deep orange solution was stirred at room temperature for 5 h, after which time the reaction mixture was removed from the glove box. Removal of solvent on a rotary evaporator followed by purification of product by column chromatography (SiO_2, 20% to 50% (gradient) Et_2O in hexanes) afforded **5** as a bright yellow solid in 70% yield. NMR (C_6D_6, 297K, 300 MHz): δ 0.66 (d, J = 12.1 Hz, 1H), δ 0.98 - 1.88 (m, 24H), δ 1.96 - 2.12 (m, 2H), δ 2.12 - 2.36 (m, 6H), δ 2.54 - 2.74 (m, 3H), δ 3.56 (m, 1H), δ 3.86 (m, 1H), δ 4.90 (s, 1H), δ 4.95 (s, 1H), δ 5.59 (m, 2H), δ 6.97 - 7.33 (m, 7H), δ 7.93 (dd, J = 7.5, 1.7 Hz, 1H). ^{13}C NMR (C_6D_6, 297K, 75 MHz): δ 20.9, δ 25.6, δ 27.4, δ 27.7, δ 27.9, δ 28.5, δ 28.8, δ 30.8, δ 31.1, δ 31.2, δ 31.4, δ 31.9, δ 32.0, δ 33.2, δ 33.8, δ 35.6, δ 37.8, δ 38.09, δ 38.14, δ 38.6, δ 38.8, δ 39.2, δ 66.0 (d, J = 14.9 Hz), δ 66.9, δ 68.8 (d, J = 15.8 Hz,) δ 71.4, δ 100.6 (d, J = 5.6 Hz), δ 102.6 (d, J = 5.4 Hz), δ 116.2, δ 124.9, δ 126.4, δ 127.27, δ 127.32, δ 127.5, δ 129.7, δ 127.3 (d, J = 15.4 Hz), δ 147.2 (d, J = 9.8 Hz), δ 158.0. HRMS (ESI-EMM): m/z = ([M - Cl]$^+$) 673.3020, Δ < 1 ppm.

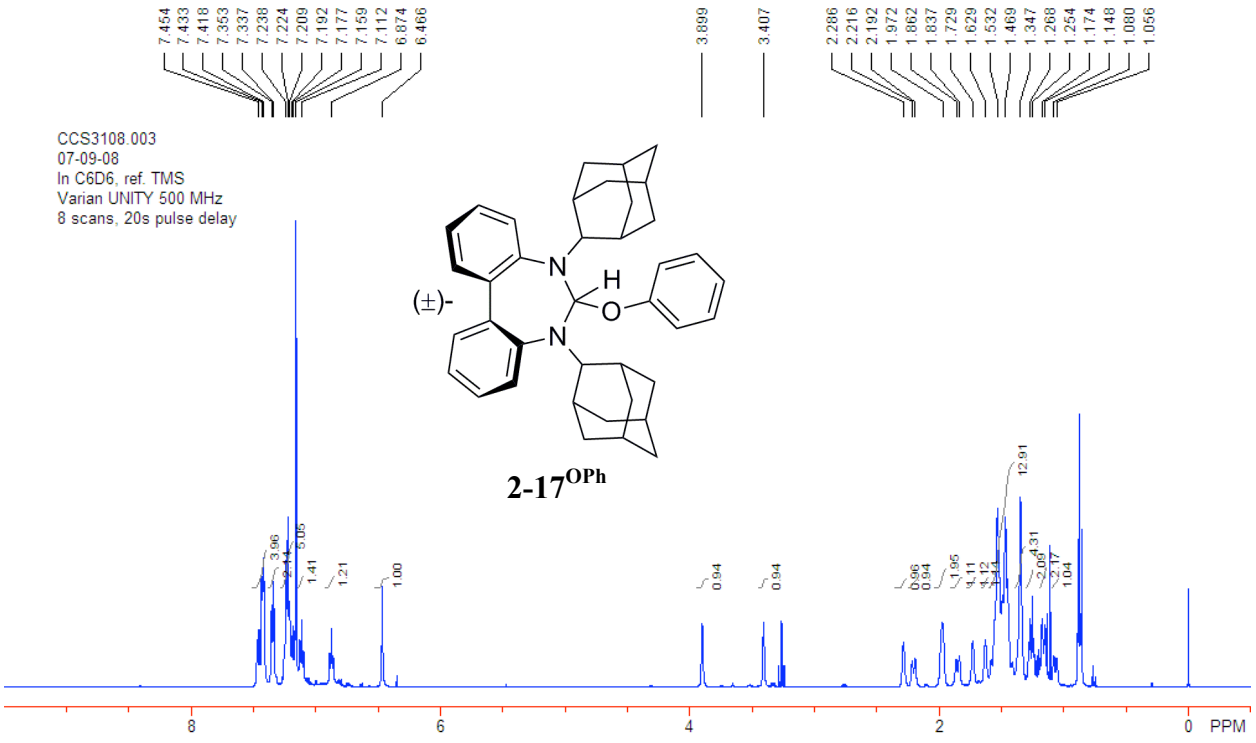


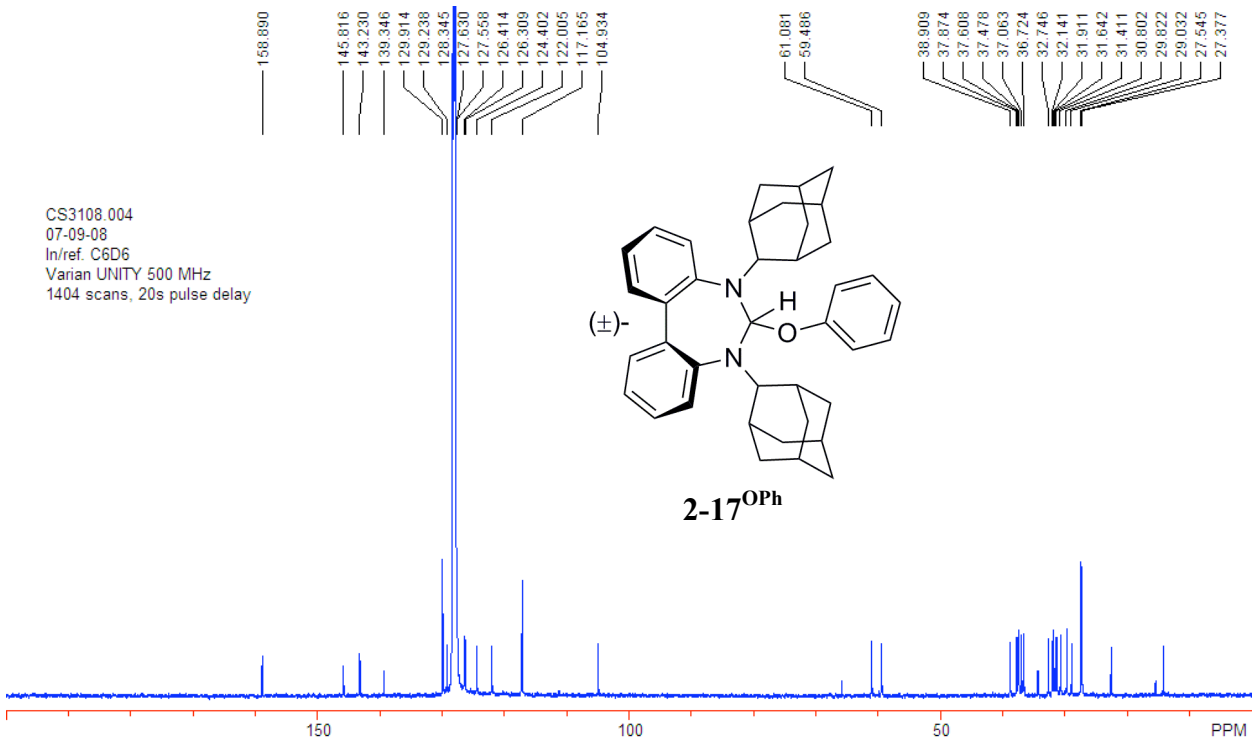
6. The NHC-Rh complex **5** was dissolved in benzene-d_6 (0.025 M solution) in a thick-walled glass pressure vessel. The vessel was purged with CO gas and pressurized to 60 psi with CO gas. This solution was vigorously stirred for 2h under 60 psi CO pressure, after which time the

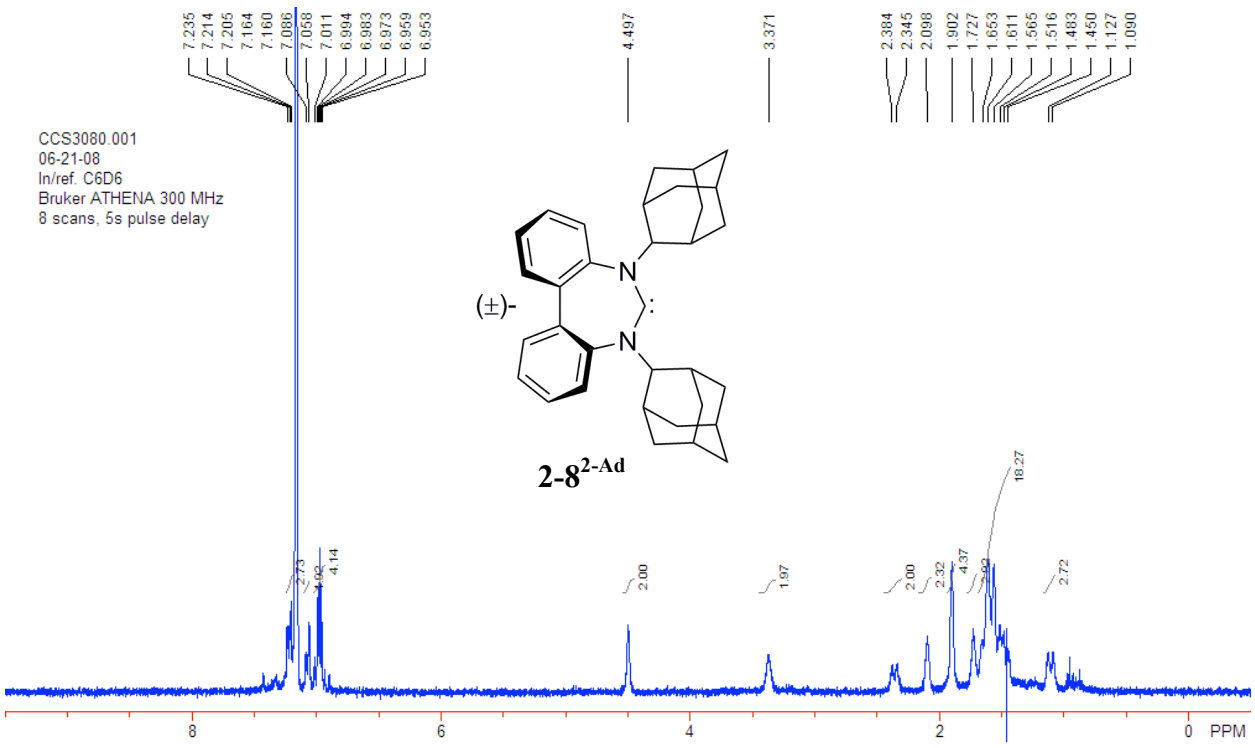
sample was removed from the CO atmosphere and ^{1}H and ^{13}C NMR and IR spectra were quickly obtained of the crude reaction mixture. The NMR spectra revealed complete conversion of **5** into the Rh-dicarbonyl complex **6** together with the release of free COD. The instability of complex **6** in the absence of a CO atmosphere prevented isolation. ^{1}H NMR (C_6D_6, 297K, 300 MHz): δ 1.06 - 2.15 (m, 26H), δ 2.21 (8H, free COD), δ 3.81 (s, 1H), δ 4.23 (s, 1H), δ 4.64 (s, 1H), δ 5.58 (s, 4H, free COD), δ 5.61 (s, 1H), δ 6.68 - 6.71 (m, 1H), δ 6.86 - 7.08 (m, 5H), δ 7.22 (dd, J = 7.6, 1.4 Hz, 1H), δ 7.75 (dd, J = 7.6, 1.8 Hz, 1H). ^{13}C NMR (C_6D_6, 297K, 75 MHz): δ 21.4, δ 27.0, δ 27.1, δ 27.2, δ 28.4, δ 30.4, δ 30.5, δ 30.7, δ 31.4, δ 31.5, δ 36.9, δ 37.1, δ 37.4, δ 37.48, δ 37.52, δ 68.0, δ 68.3, δ 115.6, δ 120.6, δ 125.4, δ 126.4, δ 126.9, δ 127.2 (d, J = 7.1 Hz), δ 127.5 (d, J = 8.2 Hz), δ 127.7 (d, J = 10.4 Hz), δ 128.8, δ 130.0 (d, J = 57.8 Hz), δ 136.8 (d, J = 90.3 Hz), δ 137.8, δ 147.2 (d, J = 46.3 Hz), δ 184.2 (d, J = 77.1 Hz), δ 187.4 (d, J = 52.9 Hz).

Infrared spectrum (FTIR) of **6** (0.025 M in C_6D_6): (carbonyl stretching frequencies 1988.25 cm^{-1} and 2077.92 cm^{-1}):





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06-21-08
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Bruker ATHENA 300 MHz
8 scans, 5s pulse delay
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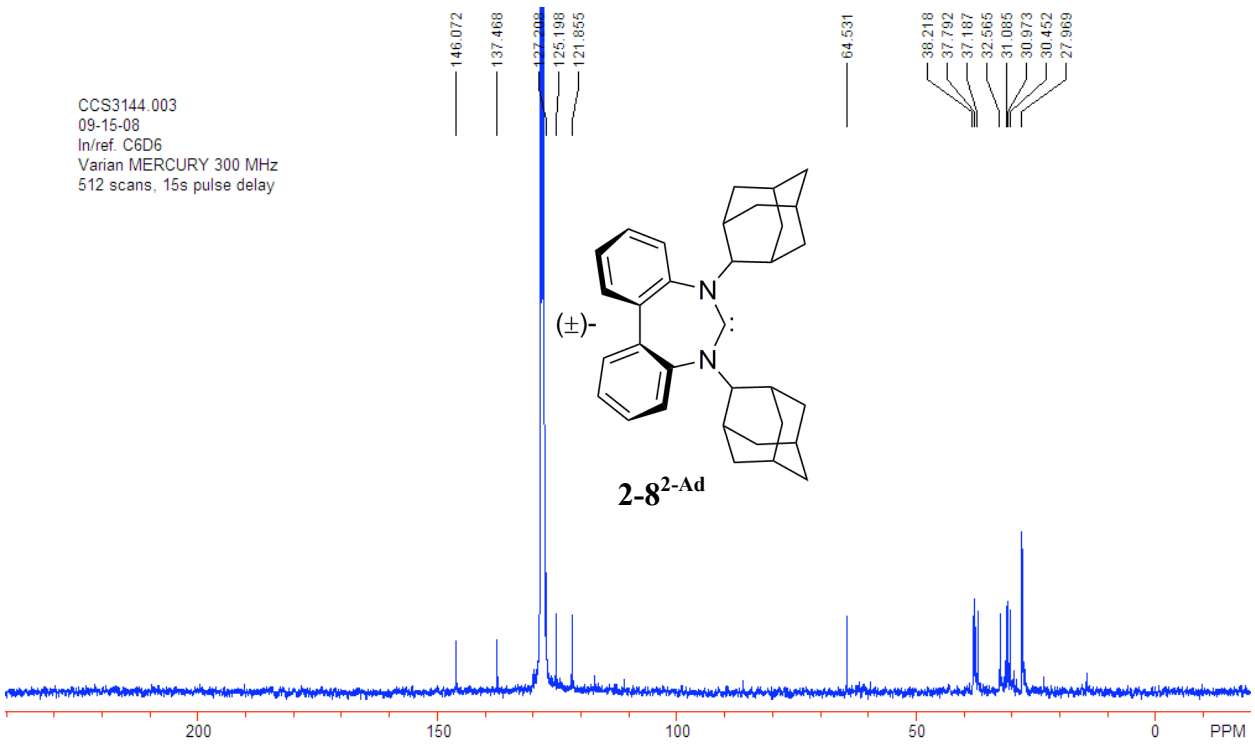
7.214
7.205
7.164
7.160
7.086
7.058
7.011
6.994
6.983
6.973
6.959
6.953
4.497
3.371
2.384
2.345
2.098
1.902
1.727
1.653
1.611
1.565
1.516
1.483
1.450
1.127
1.090
(±)-
N
N
2-8^2-Ad
18.27
2.73
2.92
4.14
2.00
1.97
2.00
2.32
4.37
2.72
8
6
4
2
0
PPM


CCS3144.003
09-15-08
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Varian MERCURY 300 MHz
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121.855
64.531
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37.792
37.187
32.565
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(±)-
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50
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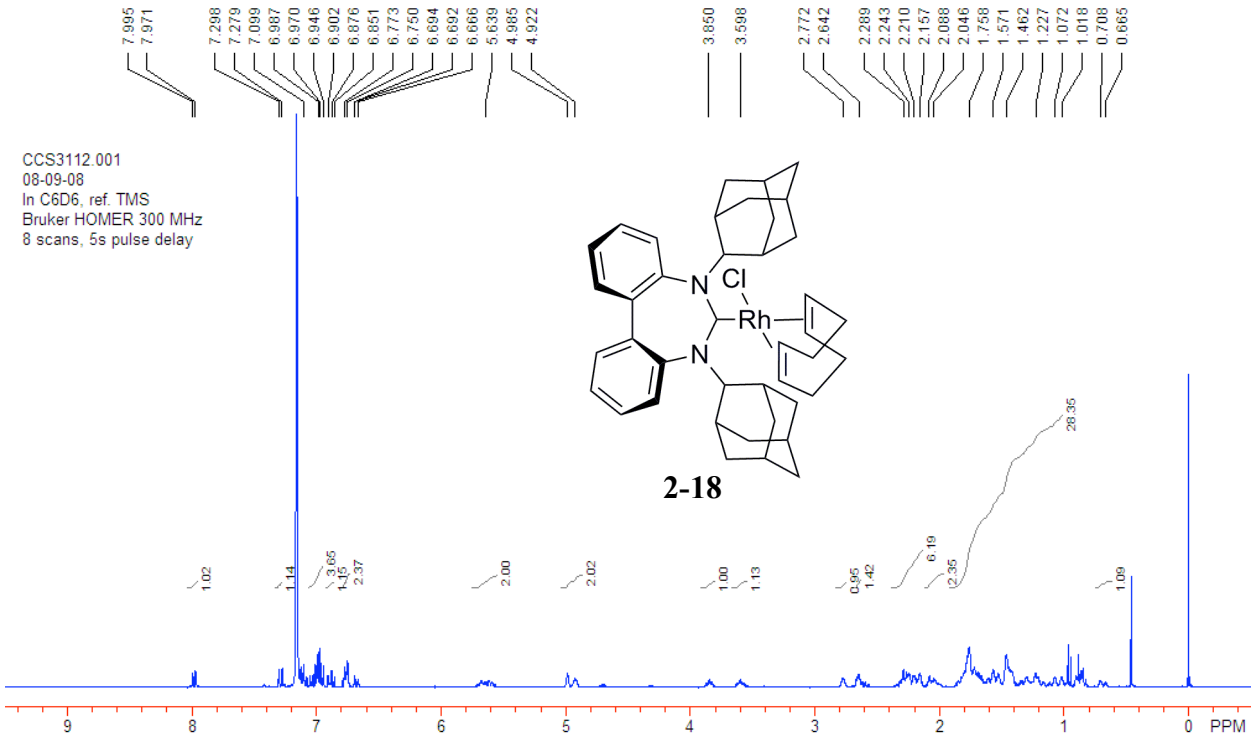
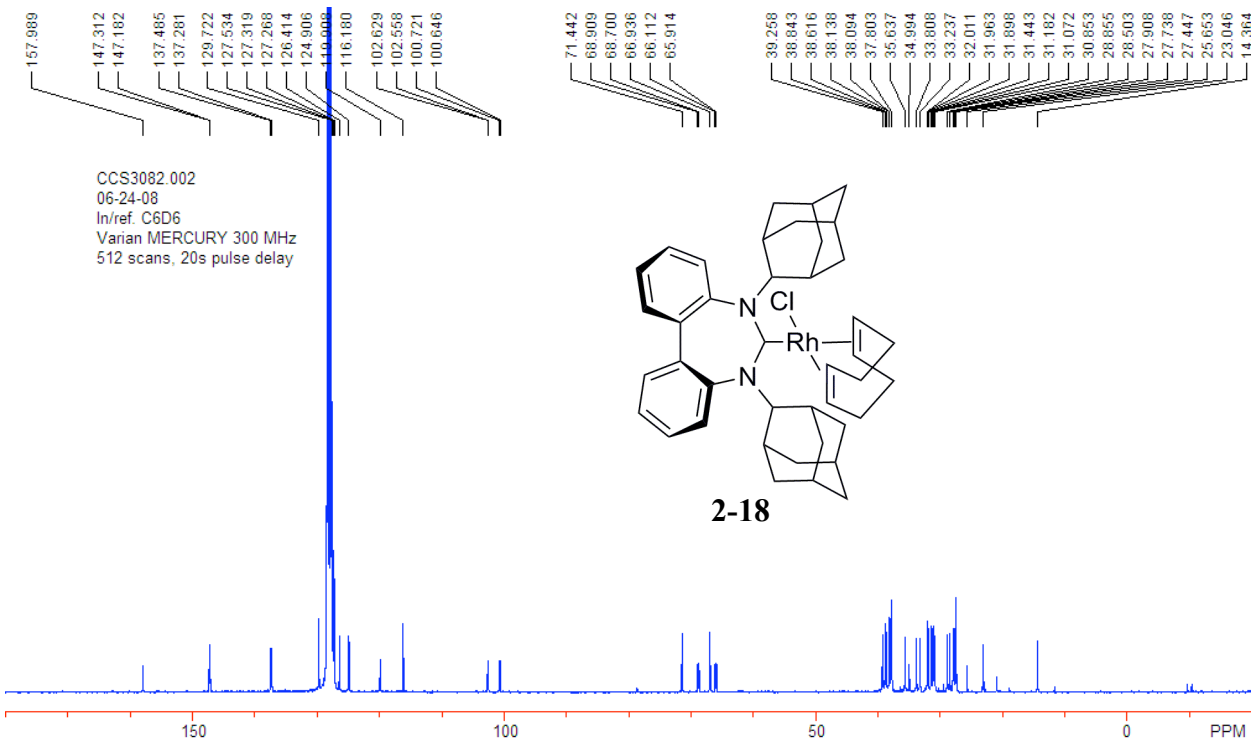
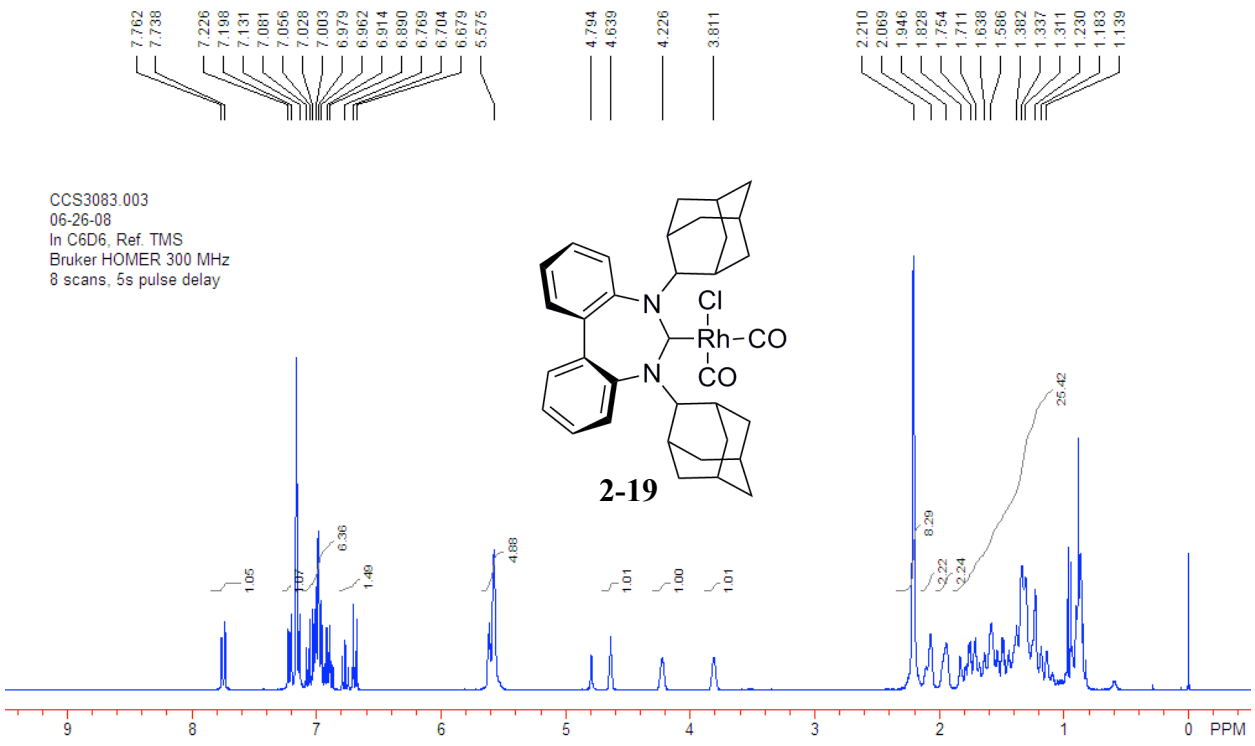
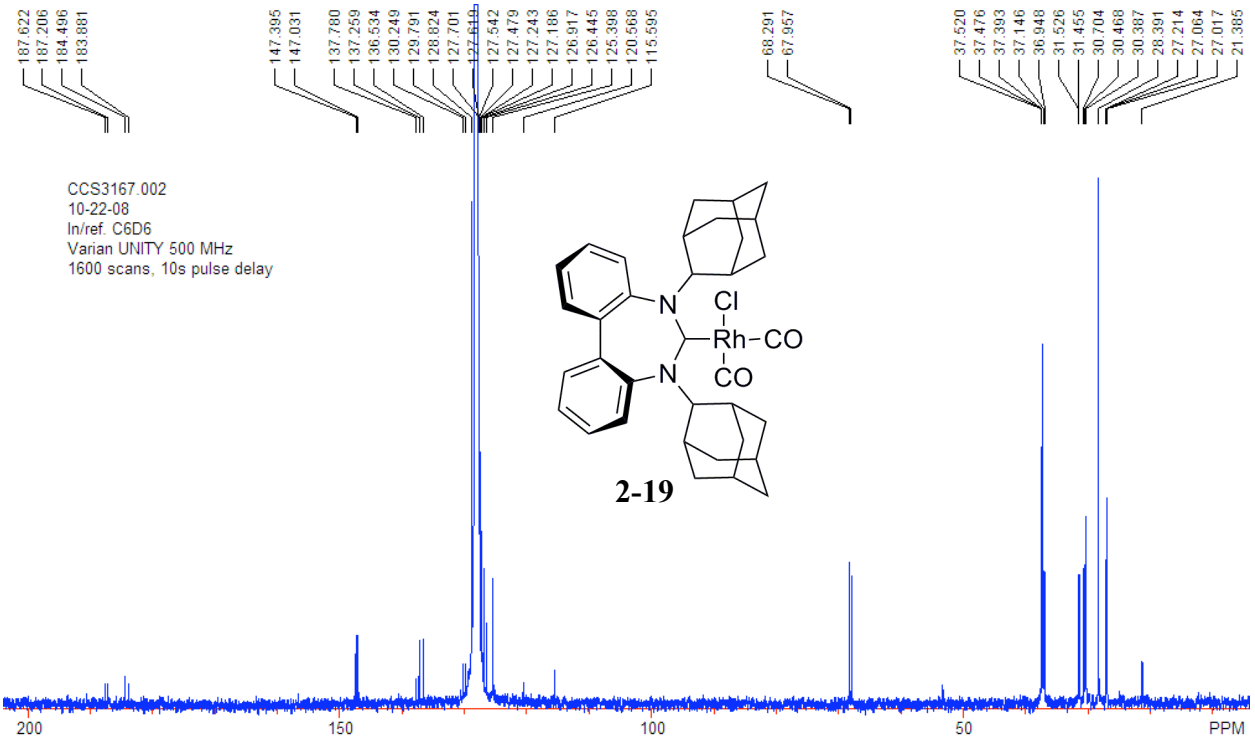
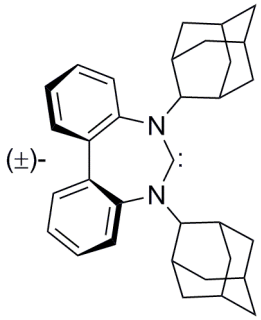
PPM











4.

Data Collection

A colorless crystal with approximate dimensions 0.38 x 0.10 x 0.10 mm3 was selected under oil under ambient conditions and attached to the tip of a MiTeGen MicroMount©. The crystal was mounted in a stream of cold nitrogen at 100(2) K and centered in the X-ray beam by using a video camera.

The crystal evaluation and data collection were performed on a Bruker SMART APEXII diffractometer with Cu Kα (λ = 1.54178 Å) radiation and the diffractometer to crystal distance of 4.03 cm.

The initial cell constants were obtained from three series of ω scans at different starting angles. Each series consisted of 50 frames collected at intervals of 0.5º in a 25º range about with the exposure time of 60 seconds per frame. The reflections were successfully indexed by an automated indexing routine built in the SMART program. The final cell constants were calculated from a set of 7705 strong reflections from the actual data collection.

The data were collected by using the full sphere data collection routine to survey the reciprocal space to the extent of a full sphere to a resolution of 0.83 Å. A total of 22130 data were harvested by collecting 15 sets of frames with 0.5º scans in with an exposure time 60-90 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements.[1]

Structure Solution and Refinement

The systematic absences in the diffraction data were consistent for the space groups $P\bar{1}$ and $P1$. The *E*-statistics strongly suggested the centrosymmetric space group $P\bar{1}$ that yielded chemically reasonable and computationally stable results of refinement.[2]

A successful solution by the direct methods provided most non-hydrogen atoms from the *E*-map. The remaining non-hydrogen atoms were located in an alternating series of least-squares cycles and difference Fourier maps. All non-hydrogen atoms were refined with anisotropic 3 displacement coefficients. All hydrogen atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients.

There is also one molecule of solvate benzene per two molecules of carbene in the asymmetric unit. The two carbenes are enantiomers.

The only crystal large enough for the single-crystal X-ray diffraction experiment proved to be a non-merohedral twin with a 35.7(2)% second component contribution. The twin components are related by a 179.7° rotation about reciprocal axis [101].

The final least-squares refinement of 685 parameters against 9780 data resulted in residuals *R* (based on *F*2 for $I \geqslant 2\sigma$) and *wR* (based on *F*2 for all data) of 0.0586 and 0.1399, respectively. The final difference Fourier map was featureless.

The molecular diagram is drawn with 40% probability ellipsoids.

References

(1) Bruker-AXS. (2007) APEX2, SADABS, and SAINT Software Reference Manuals. Bruker-AXS, Madison, Wisconsin, USA.
(2) Sheldrick, G. M. (2008) SHELXL. *Acta Cryst.* **A64**, 112-122.

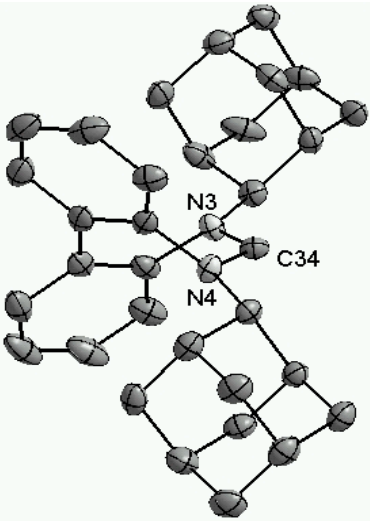


Figure S1. Solid-state structure of free NHC **4** (only one of two independent NHC molecules is shown). Hydrogen atoms and solvent molecule (C_6H_6) are omitted for clarity. Thermal ellipsoids are shown at 40% probability.

Table S1. Crystal data and structure refinement for **4**.

Identification code	**4**	
Empirical formula	$C_{72}\ H_{82}\ N_4$	
Formula weight	1003.42	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 11.1433(5) Å	α = 99.512(3)°.
	b = 13.6753(5) Å	β = 91.001(3)°.
	c = 19.3610(8) Å	γ = 109.659(3)°.
Volume	2731.72(19) $Å^3$	
Z	2	
Density (calculated)	1.220 Mg/m^3	

Absorption coefficient	0.528 mm^{-1}
F(000)	1084
Crystal size	0.14 x 0.03 x 0.03 mm^3
Theta range for data collection	3.49 to 68.03°.
Index ranges	-13<=h<=13, -16<=k<=16, 0<=l<=23
Reflections collected	9780
Independent reflections	9780 [R(int) = 0.0000]
Completeness to theta = 68.03°	98.0 %
Absorption correction	Empirical with SADABS
Max. and min. transmission	0.9843 and 0.9297
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9780 / 0 / 685
Twin component ratio	35.7(2)%
Goodness-of-fit on F^2	1.006
Final R indices [I>2sigma(I)]	R1 = 0.0586, wR2 = 0.1225
R indices (all data)	R1 = 0.1093, wR2 = 0.1399
Largest diff. peak and hole	0.222 and -0.225 e.$Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	8953(2)	7511(1)	4886(1)	23(1)
N(2)	10598(2)	7236(2)	5435(1)	25(1)
N(3)	3905(2)	1733(1)	-57(1)	23(1)
N(4)	5586(2)	3140(1)	483(1)	22(1)
C(1)	10148(2)	7428(2)	4844(1)	22(1)
C(2)	8770(2)	8205(2)	5492(1)	23(1)
C(3)	8713(2)	9187(2)	5422(1)	26(1)
C(4)	8579(2)	9870(2)	6002(1)	31(1)
C(5)	8504(2)	9584(2)	6658(1)	31(1)
C(6)	8569(2)	8611(2)	6728(1)	27(1)
C(7)	8709(2)	7912(2)	6149(1)	23(1)
C(8)	8800(2)	6874(2)	6204(1)	22(1)
C(9)	7968(2)	6188(2)	6586(1)	28(1)
C(10)	8063(3)	5209(2)	6615(1)	33(1)
C(11)	8982(2)	4906(2)	6262(1)	33(1)
C(12)	9817(2)	5579(2)	5887(1)	28(1)
C(13)	9738(2)	6567(2)	5858(1)	24(1)
C(14)	8267(2)	7460(2)	4207(1)	21(1)
C(15)	6850(2)	7330(2)	4291(1)	23(1)
C(16)	6135(2)	6277(2)	4514(1)	29(1)

C(17)	6186(2)	5363(2)	3952(1)	32(1)
C(18)	7598(2)	5473(2)	3895(1)	28(1)
C(19)	8322(2)	6520(2)	3664(1)	22(1)
C(20)	7722(2)	6559(2)	2960(1)	27(1)
C(21)	6323(2)	6452(2)	3022(1)	28(1)
C(22)	6249(2)	7360(2)	3581(1)	26(1)
C(23)	5599(2)	5404(2)	3244(2)	37(1)
C(24)	11965(2)	7303(2)	5495(1)	23(1)
C(25)	12501(2)	7538(2)	6262(1)	28(1)
C(26)	12566(3)	8634(2)	6625(1)	37(1)
C(27)	13446(3)	9465(2)	6245(2)	37(1)
C(28)	12879(3)	9258(2)	5494(2)	36(1)
C(29)	12813(2)	8163(2)	5122(1)	28(1)
C(30)	14154(2)	8096(2)	5130(2)	37(1)
C(31)	14719(3)	8299(2)	5887(2)	37(1)
C(32)	13845(3)	7474(2)	6272(2)	42(1)
C(33)	14790(3)	9399(2)	6247(2)	37(1)
C(34)	5069(2)	2442(2)	-130(1)	23(1)
C(35)	3724(2)	1288(2)	575(1)	25(1)
C(36)	3686(2)	253(2)	546(1)	34(1)
C(37)	3579(3)	-175(2)	1148(2)	44(1)
C(38)	3505(3)	420(2)	1785(2)	44(1)
C(39)	3553(2)	1450(2)	1816(1)	37(1)
C(40)	3668(2)	1902(2)	1213(1)	27(1)
C(41)	3799(2)	3019(2)	1230(1)	26(1)
C(42)	2997(2)	3492(2)	1582(1)	36(1)
C(43)	3155(3)	4538(2)	1574(1)	40(1)
C(44)	4119(3)	5123(2)	1210(1)	37(1)
C(45)	4921(2)	4665(2)	860(1)	29(1)
C(46)	4766(2)	3615(2)	872(1)	22(1)
C(47)	3147(2)	1058(2)	-714(1)	24(1)
C(48)	1736(2)	527(2)	-586(1)	31(1)
C(49)	1101(2)	1358(2)	-382(1)	36(1)
C(50)	1156(2)	1974(2)	-976(1)	33(1)
C(51)	2559(2)	2530(2)	-1089(1)	29(1)
C(52)	3207(2)	1712(2)	-1290(1)	25(1)
C(53)	2520(2)	965(2)	-1966(1)	32(1)
C(54)	1122(2)	401(2)	-1858(1)	32(1)
C(55)	1054(3)	-224(2)	-1265(2)	40(1)
C(56)	475(2)	1221(2)	-1650(1)	32(1)
C(57)	6972(2)	3752(2)	522(1)	22(1)
C(58)	7501(2)	4338(2)	1273(1)	25(1)
C(59)	7358(2)	3555(2)	1772(1)	29(1)
C(60)	8114(2)	2825(2)	1529(1)	31(1)
C(61)	7573(2)	2219(2)	790(1)	28(1)
C(62)	7708(2)	2993(2)	283(1)	24(1)

C(63)	9124(2)	3643(2)	273(1)	29(1)
C(64)	9671(2)	4258(2)	1010(1)	30(1)
C(65)	8912(2)	4984(2)	1255(1)	30(1)
C(66)	9531(2)	3479(2)	1514(1)	34(1)
C(67)	3150(2)	7460(2)	1838(1)	25(1)
C(68)	3849(2)	7790(2)	2478(1)	28(1)
C(69)	3238(2)	7868(2)	3095(1)	29(1)
C(70)	1928(2)	7608(2)	3067(1)	23(1)
C(71)	1227(2)	7280(2)	2427(1)	27(1)
C(72)	1836(2)	7200(2)	1809(1)	27(1)

Table S3. Bond lengths [Å] and angles [°] for **4**.

N(1)-C(1)	1.377(3)	C(11)-H(11)	0.9500	C(24)-C(25)	1.531(3)
N(1)-C(2)	1.444(3)	C(12)-C(13)	1.393(3)	C(24)-C(29)	1.534(3)
N(1)-C(14)	1.489(3)	C(12)-H(12)	0.9500	C(24)-H(24)	1.0000
N(2)-C(1)	1.342(3)	C(14)-C(19)	1.540(3)	C(25)-C(26)	1.525(3)
N(2)-C(13)	1.452(3)	C(14)-C(15)	1.542(3)	C(25)-C(32)	1.529(4)
N(2)-C(24)	1.496(3)	C(14)-H(14)	1.0000	C(25)-H(25)	1.0000
N(3)-C(34)	1.359(3)	C(15)-C(16)	1.529(3)	C(26)-C(27)	1.531(4)
N(3)-C(35)	1.442(3)	C(15)-C(22)	1.532(3)	C(26)-H(26A)	0.9900
N(3)-C(47)	1.494(3)	C(15)-H(15)	1.0000	C(26)-H(26B)	0.9900
N(4)-C(34)	1.372(3)	C(16)-C(17)	1.533(3)	C(27)-C(28)	1.519(4)
N(4)-C(46)	1.444(3)	C(16)-H(16A)	0.9900	C(27)-C(33)	1.531(4)
N(4)-C(57)	1.483(3)	C(16)-H(16B)	0.9900	C(27)-H(27)	1.0000
C(2)-C(7)	1.392(3)	C(17)-C(23)	1.527(4)	C(28)-C(29)	1.528(3)
C(2)-C(3)	1.394(3)	C(17)-C(18)	1.537(3)	C(28)-H(28A)	0.9900
C(3)-C(4)	1.382(3)	C(17)-H(17)	1.0000	C(28)-H(28B)	0.9900
C(3)-H(3)	0.9500	C(18)-C(19)	1.532(3)	C(29)-C(30)	1.527(3)
C(4)-C(5)	1.384(4)	C(18)-H(18A)	0.9900	C(29)-H(29)	1.0000
C(4)-H(4)	0.9500	C(18)-H(18B)	0.9900	C(30)-C(31)	1.530(4)
C(5)-C(6)	1.384(3)	C(19)-C(20)	1.525(3)	C(30)-H(30A)	0.9900
C(5)-H(5)	0.9500	C(19)-H(19)	1.0000	C(30)-H(30B)	0.9900
C(6)-C(7)	1.394(3)	C(20)-C(21)	1.525(3)	C(31)-C(33)	1.525(3)
C(6)-H(6)	0.9500	C(20)-H(20A)	0.9900	C(31)-C(32)	1.529(4)
C(7)-C(8)	1.478(3)	C(20)-H(20B)	0.9900	C(31)-H(31)	1.0000
C(8)-C(13)	1.394(3)	C(21)-C(23)	1.525(4)	C(32)-H(32A)	0.9900
C(8)-C(9)	1.398(3)	C(21)-C(22)	1.531(3)	C(32)-H(32B)	0.9900
C(9)-C(10)	1.389(3)	C(21)-H(21)	1.0000	C(33)-H(33A)	0.9900
C(9)-H(9)	0.9500	C(22)-H(22A)	0.9900	C(33)-H(33B)	0.9900
C(10)-C(11)	1.380(4)	C(22)-H(22B)	0.9900	C(35)-C(40)	1.390(3)
C(10)-H(10)	0.9500	C(23)-H(23A)	0.9900	C(35)-C(36)	1.393(3)
C(11)-C(12)	1.381(3)	C(23)-H(23B)	0.9900	C(36)-C(37)	1.378(4)

C(36)-H(36)	0.9500	C(50)-C(56)	1.530(4)	C(60)-H(60)	1.0000
C(37)-C(38)	1.380(4)	C(50)-H(50)	1.0000	C(61)-C(62)	1.533(3)
C(37)-H(37)	0.9500	C(51)-C(52)	1.529(3)	C(61)-H(61A)	0.9900
C(38)-C(39)	1.383(4)	C(51)-H(51A)	0.9900	C(61)-H(61B)	0.9900
C(38)-H(38)	0.9500	C(51)-H(51B)	0.9900	C(62)-C(63)	1.531(3)
C(39)-C(40)	1.398(3)	C(52)-C(53)	1.529(3)	C(62)-H(62)	1.0000
C(39)-H(39)	0.9500	C(52)-H(52)	1.0000	C(63)-C(64)	1.531(3)
C(40)-C(41)	1.479(3)	C(53)-C(54)	1.524(4)	C(63)-H(63A)	0.9900
C(41)-C(46)	1.389(3)	C(53)-H(53A)	0.9900	C(63)-H(63B)	0.9900
C(41)-C(42)	1.394(3)	C(53)-H(53B)	0.9900	C(64)-C(65)	1.532(3)
C(42)-C(43)	1.384(4)	C(54)-C(55)	1.528(3)	C(64)-C(66)	1.532(3)
C(42)-H(42)	0.9500	C(54)-C(56)	1.532(3)	C(64)-H(64)	1.0000
C(43)-C(44)	1.388(4)	C(54)-H(54)	1.0000	C(65)-H(65A)	0.9900
C(43)-H(43)	0.9500	C(55)-H(55A)	0.9900	C(65)-H(65B)	0.9900
C(44)-C(45)	1.380(3)	C(55)-H(55B)	0.9900	C(66)-H(66A)	0.9900
C(44)-H(44)	0.9500	C(56)-H(56A)	0.9900	C(66)-H(66B)	0.9900
C(45)-C(46)	1.392(3)	C(56)-H(56B)	0.9900	C(67)-C(68)	1.375(3)
C(45)-H(45)	0.9500	C(57)-C(58)	1.540(3)	C(67)-C(72)	1.383(3)
C(47)-C(52)	1.530(3)	C(57)-C(62)	1.545(3)	C(67)-H(67)	0.9500
C(47)-C(48)	1.538(3)	C(57)-H(57)	1.0000	C(68)-C(69)	1.393(3)
C(47)-H(47)	1.0000	C(58)-C(65)	1.527(3)	C(68)-H(68)	0.9500
C(48)-C(49)	1.534(4)	C(58)-C(59)	1.529(3)	C(69)-C(70)	1.379(3)
C(48)-C(55)	1.536(4)	C(58)-H(58)	1.0000	C(69)-H(69)	0.9500
C(48)-H(48)	1.0000	C(59)-C(60)	1.533(3)	C(70)-C(71)	1.376(3)
C(49)-C(50)	1.525(4)	C(59)-H(59A)	0.9900	C(70)-H(70)	0.9500
C(49)-H(49A)	0.9900	C(59)-H(59B)	0.9900	C(71)-C(72)	1.392(3)
C(49)-H(49B)	0.9900	C(60)-C(61)	1.529(3)	C(71)-H(71)	0.9500
C(50)-C(51)	1.529(3)	C(60)-C(66)	1.534(3)	C(72)-H(72)	0.9500

C(1)-N(1)-C(2)	116.92(19)	C(4)-C(3)-H(3)	119.9
C(1)-N(1)-C(14)	115.94(18)	C(2)-C(3)-H(3)	119.9
C(2)-N(1)-C(14)	117.18(17)	C(3)-C(4)-C(5)	120.2(2)
C(1)-N(2)-C(13)	120.40(19)	C(3)-C(4)-H(4)	119.9
C(1)-N(2)-C(24)	118.18(19)	C(5)-C(4)-H(4)	119.9
C(13)-N(2)-C(24)	116.39(18)	C(4)-C(5)-C(6)	119.5(2)
C(34)-N(3)-C(35)	118.35(19)	C(4)-C(5)-H(5)	120.3
C(34)-N(3)-C(47)	117.11(19)	C(6)-C(5)-H(5)	120.3
C(35)-N(3)-C(47)	117.23(17)	C(5)-C(6)-C(7)	121.2(2)
C(34)-N(4)-C(46)	117.65(19)	C(5)-C(6)-H(6)	119.4
C(34)-N(4)-C(57)	116.63(18)	C(7)-C(6)-H(6)	119.4
C(46)-N(4)-C(57)	118.51(17)	C(2)-C(7)-C(6)	118.7(2)
N(2)-C(1)-N(1)	113.4(2)	C(2)-C(7)-C(8)	118.4(2)
C(7)-C(2)-C(3)	120.1(2)	C(6)-C(7)-C(8)	122.8(2)
C(7)-C(2)-N(1)	120.01(19)	C(13)-C(8)-C(9)	119.2(2)
C(3)-C(2)-N(1)	119.8(2)	C(13)-C(8)-C(7)	118.9(2)
C(4)-C(3)-C(2)	120.2(2)	C(9)-C(8)-C(7)	122.0(2)

C(10)-C(9)-C(8)	120.6(2)	C(20)-C(19)-C(14)	108.41(18)
C(10)-C(9)-H(9)	119.7	C(18)-C(19)-C(14)	110.68(18)
C(8)-C(9)-H(9)	119.7	C(20)-C(19)-H(19)	109.3
C(11)-C(10)-C(9)	119.8(2)	C(18)-C(19)-H(19)	109.3
C(11)-C(10)-H(10)	120.1	C(14)-C(19)-H(19)	109.3
C(9)-C(10)-H(10)	120.1	C(19)-C(20)-C(21)	109.99(19)
C(10)-C(11)-C(12)	120.2(2)	C(19)-C(20)-H(20A)	109.7
C(10)-C(11)-H(11)	119.9	C(21)-C(20)-H(20A)	109.7
C(12)-C(11)-H(11)	119.9	C(19)-C(20)-H(20B)	109.7
C(11)-C(12)-C(13)	120.6(2)	C(21)-C(20)-H(20B)	109.7
C(11)-C(12)-H(12)	119.7	H(20A)-C(20)-H(20B)	108.2
C(13)-C(12)-H(12)	119.7	C(23)-C(21)-C(20)	109.6(2)
C(12)-C(13)-C(8)	119.7(2)	C(23)-C(21)-C(22)	109.2(2)
C(12)-C(13)-N(2)	119.0(2)	C(20)-C(21)-C(22)	108.9(2)
C(8)-C(13)-N(2)	121.3(2)	C(23)-C(21)-H(21)	109.7
N(1)-C(14)-C(19)	110.17(17)	C(20)-C(21)-H(21)	109.7
N(1)-C(14)-C(15)	111.77(18)	C(22)-C(21)-H(21)	109.7
C(19)-C(14)-C(15)	108.24(18)	C(21)-C(22)-C(15)	110.31(18)
N(1)-C(14)-H(14)	108.9	C(21)-C(22)-H(22A)	109.6
C(19)-C(14)-H(14)	108.9	C(15)-C(22)-H(22A)	109.6
C(15)-C(14)-H(14)	108.9	C(21)-C(22)-H(22B)	109.6
C(16)-C(15)-C(22)	109.4(2)	C(15)-C(22)-H(22B)	109.6
C(16)-C(15)-C(14)	110.83(18)	H(22A)-C(22)-H(22B)	108.1
C(22)-C(15)-C(14)	108.02(18)	C(21)-C(23)-C(17)	109.7(2)
C(16)-C(15)-H(15)	109.5	C(21)-C(23)-H(23A)	109.7
C(22)-C(15)-H(15)	109.5	C(17)-C(23)-H(23A)	109.7
C(14)-C(15)-H(15)	109.5	C(21)-C(23)-H(23B)	109.7
C(15)-C(16)-C(17)	109.70(19)	C(17)-C(23)-H(23B)	109.7
C(15)-C(16)-H(16A)	109.7	H(23A)-C(23)-H(23B)	108.2
C(17)-C(16)-H(16A)	109.7	N(2)-C(24)-C(25)	112.00(19)
C(15)-C(16)-H(16B)	109.7	N(2)-C(24)-C(29)	111.41(18)
C(17)-C(16)-H(16B)	109.7	C(25)-C(24)-C(29)	108.23(19)
H(16A)-C(16)-H(16B)	108.2	N(2)-C(24)-H(24)	108.4
C(23)-C(17)-C(16)	110.7(2)	C(25)-C(24)-H(24)	108.4
C(23)-C(17)-C(18)	109.7(2)	C(29)-C(24)-H(24)	108.4
C(16)-C(17)-C(18)	107.7(2)	C(26)-C(25)-C(32)	109.4(2)
C(23)-C(17)-H(17)	109.6	C(26)-C(25)-C(24)	111.20(19)
C(16)-C(17)-H(17)	109.6	C(32)-C(25)-C(24)	108.2(2)
C(18)-C(17)-H(17)	109.6	C(26)-C(25)-H(25)	109.3
C(19)-C(18)-C(17)	109.51(19)	C(32)-C(25)-H(25)	109.3
C(19)-C(18)-H(18A)	109.8	C(24)-C(25)-H(25)	109.3
C(17)-C(18)-H(18A)	109.8	C(25)-C(26)-C(27)	109.4(2)
C(19)-C(18)-H(18B)	109.8	C(25)-C(26)-H(26A)	109.8
C(17)-C(18)-H(18B)	109.8	C(27)-C(26)-H(26A)	109.8
H(18A)-C(18)-H(18B)	108.2	C(25)-C(26)-H(26B)	109.8
C(20)-C(19)-C(18)	109.9(2)	C(27)-C(26)-H(26B)	109.8

H(26A)-C(26)-H(26B)	108.3	C(36)-C(35)-N(3)	119.2(2)
C(28)-C(27)-C(33)	109.8(2)	C(37)-C(36)-C(35)	120.4(3)
C(28)-C(27)-C(26)	108.0(2)	C(37)-C(36)-H(36)	119.8
C(33)-C(27)-C(26)	110.7(2)	C(35)-C(36)-H(36)	119.8
C(28)-C(27)-H(27)	109.4	C(36)-C(37)-C(38)	120.1(3)
C(33)-C(27)-H(27)	109.4	C(36)-C(37)-H(37)	120.0
C(26)-C(27)-H(27)	109.4	C(38)-C(37)-H(37)	120.0
C(27)-C(28)-C(29)	109.8(2)	C(37)-C(38)-C(39)	119.7(3)
C(27)-C(28)-H(28A)	109.7	C(37)-C(38)-H(38)	120.1
C(29)-C(28)-H(28A)	109.7	C(39)-C(38)-H(38)	120.1
C(27)-C(28)-H(28B)	109.7	C(38)-C(39)-C(40)	121.2(3)
C(29)-C(28)-H(28B)	109.7	C(38)-C(39)-H(39)	119.4
H(28A)-C(28)-H(28B)	108.2	C(40)-C(39)-H(39)	119.4
C(30)-C(29)-C(28)	109.5(2)	C(35)-C(40)-C(39)	118.4(2)
C(30)-C(29)-C(24)	108.4(2)	C(35)-C(40)-C(41)	118.7(2)
C(28)-C(29)-C(24)	110.83(19)	C(39)-C(40)-C(41)	122.9(2)
C(30)-C(29)-H(29)	109.4	C(46)-C(41)-C(42)	119.1(2)
C(28)-C(29)-H(29)	109.4	C(46)-C(41)-C(40)	117.7(2)
C(24)-C(29)-H(29)	109.4	C(42)-C(41)-C(40)	123.2(2)
C(29)-C(30)-C(31)	110.0(2)	C(43)-C(42)-C(41)	120.8(3)
C(29)-C(30)-H(30A)	109.7	C(43)-C(42)-H(42)	119.6
C(31)-C(30)-H(30A)	109.7	C(41)-C(42)-H(42)	119.6
C(29)-C(30)-H(30B)	109.7	C(42)-C(43)-C(44)	119.7(2)
C(31)-C(30)-H(30B)	109.7	C(42)-C(43)-H(43)	120.2
H(30A)-C(30)-H(30B)	108.2	C(44)-C(43)-H(43)	120.2
C(33)-C(31)-C(32)	109.5(2)	C(45)-C(44)-C(43)	120.2(2)
C(33)-C(31)-C(30)	109.0(2)	C(45)-C(44)-H(44)	119.9
C(32)-C(31)-C(30)	108.7(2)	C(43)-C(44)-H(44)	119.9
C(33)-C(31)-H(31)	109.9	C(44)-C(45)-C(46)	120.1(2)
C(32)-C(31)-H(31)	109.9	C(44)-C(45)-H(45)	120.0
C(30)-C(31)-H(31)	109.9	C(46)-C(45)-H(45)	120.0
C(31)-C(32)-C(25)	110.3(2)	C(41)-C(46)-C(45)	120.2(2)
C(31)-C(32)-H(32A)	109.6	C(41)-C(46)-N(4)	120.4(2)
C(25)-C(32)-H(32A)	109.6	C(45)-C(46)-N(4)	119.3(2)
C(31)-C(32)-H(32B)	109.6	N(3)-C(47)-C(52)	110.83(18)
C(25)-C(32)-H(32B)	109.6	N(3)-C(47)-C(48)	111.52(19)
H(32A)-C(32)-H(32B)	108.1	C(52)-C(47)-C(48)	108.4(2)
C(31)-C(33)-C(27)	109.5(2)	N(3)-C(47)-H(47)	108.7
C(31)-C(33)-H(33A)	109.8	C(52)-C(47)-H(47)	108.7
C(27)-C(33)-H(33A)	109.8	C(48)-C(47)-H(47)	108.7
C(31)-C(33)-H(33B)	109.8	C(49)-C(48)-C(55)	109.8(2)
C(27)-C(33)-H(33B)	109.8	C(49)-C(48)-C(47)	110.60(19)
H(33A)-C(33)-H(33B)	108.2	C(55)-C(48)-C(47)	108.2(2)
N(3)-C(34)-N(4)	112.3(2)	C(49)-C(48)-H(48)	109.4
C(40)-C(35)-C(36)	120.2(2)	C(55)-C(48)-H(48)	109.4
C(40)-C(35)-N(3)	120.5(2)	C(47)-C(48)-H(48)	109.4

C(50)-C(49)-C(48) 109.6(2)
C(50)-C(49)-H(49A) 109.8
C(48)-C(49)-H(49A) 109.8
C(50)-C(49)-H(49B) 109.8
C(48)-C(49)-H(49B) 109.8
H(49A)-C(49)-H(49B)108.2
C(49)-C(50)-C(51) 108.5(2)
C(49)-C(50)-C(56) 110.0(2)
C(51)-C(50)-C(56) 109.7(2)
C(49)-C(50)-H(50) 109.6
C(51)-C(50)-H(50) 109.6
C(56)-C(50)-H(50) 109.6
C(52)-C(51)-C(50) 109.75(19)
C(52)-C(51)-H(51A) 109.7
C(50)-C(51)-H(51A) 109.7
C(52)-C(51)-H(51B) 109.7
C(50)-C(51)-H(51B) 109.7
H(51A)-C(51)-H(51B)108.2
C(51)-C(52)-C(53) 109.0(2)
C(51)-C(52)-C(47) 111.21(19)
C(53)-C(52)-C(47) 108.48(19)
C(51)-C(52)-H(52) 109.4
C(53)-C(52)-H(52) 109.4
C(47)-C(52)-H(52) 109.4
C(54)-C(53)-C(52) 110.3(2)
C(54)-C(53)-H(53A) 109.6
C(52)-C(53)-H(53A) 109.6
C(54)-C(53)-H(53B) 109.6
C(52)-C(53)-H(53B) 109.6
H(53A)-C(53)-H(53B)108.1
C(53)-C(54)-C(55) 109.0(2)
C(53)-C(54)-C(56) 109.2(2)
C(55)-C(54)-C(56) 109.1(2)
C(53)-C(54)-H(54) 109.9
C(55)-C(54)-H(54) 109.9
C(56)-C(54)-H(54) 109.9
C(54)-C(55)-C(48) 109.8(2)
C(54)-C(55)-H(55A) 109.7
C(48)-C(55)-H(55A) 109.7
C(54)-C(55)-H(55B) 109.7
C(48)-C(55)-H(55B) 109.7
H(55A)-C(55)-H(55B)108.2
C(50)-C(56)-C(54) 109.9(2)
C(50)-C(56)-H(56A) 109.7
C(54)-C(56)-H(56A) 109.7
C(50)-C(56)-H(56B) 109.7
C(54)-C(56)-H(56B) 109.7
H(56A)-C(56)-H(56B)108.2
N(4)-C(57)-C(58) 112.05(18)
N(4)-C(57)-C(62) 109.37(17)
C(58)-C(57)-C(62) 108.22(19)
N(4)-C(57)-H(57) 109.0
C(58)-C(57)-H(57) 109.0
C(62)-C(57)-H(57) 109.0
C(65)-C(58)-C(59) 109.8(2)
C(65)-C(58)-C(57) 108.24(19)
C(59)-C(58)-C(57) 110.64(19)
C(65)-C(58)-H(58) 109.4
C(59)-C(58)-H(58) 109.4
C(57)-C(58)-H(58) 109.4
C(58)-C(59)-C(60) 109.75(19)
C(58)-C(59)-H(59A) 109.7
C(60)-C(59)-H(59A) 109.7
C(58)-C(59)-H(59B) 109.7
C(60)-C(59)-H(59B) 109.7
H(59A)-C(59)-H(59B)108.2
C(61)-C(60)-C(59) 108.4(2)
C(61)-C(60)-C(66) 109.5(2)
C(59)-C(60)-C(66) 110.0(2)
C(61)-C(60)-H(60) 109.6
C(59)-C(60)-H(60) 109.6
C(66)-C(60)-H(60) 109.6
C(60)-C(61)-C(62) 110.05(19)
C(60)-C(61)-H(61A) 109.7
C(62)-C(61)-H(61A) 109.7
C(60)-C(61)-H(61B) 109.7
C(62)-C(61)-H(61B) 109.7
H(61A)-C(61)-H(61B)108.2
C(63)-C(62)-C(61) 109.0(2)
C(63)-C(62)-C(57) 108.85(18)
C(61)-C(62)-C(57) 110.53(18)
C(63)-C(62)-H(62) 109.5
C(61)-C(62)-H(62) 109.5
C(57)-C(62)-H(62) 109.5
C(62)-C(63)-C(64) 110.1(2)
C(62)-C(63)-H(63A) 109.6
C(64)-C(63)-H(63A) 109.6
C(62)-C(63)-H(63B) 109.6
C(64)-C(63)-H(63B) 109.6
H(63A)-C(63)-H(63B)108.2
C(63)-C(64)-C(65) 108.6(2)
C(63)-C(64)-C(66) 109.3(2)

C(65)-C(64)-C(66)	109.3(2)	C(68)-C(67)-H(67)	120.1
C(63)-C(64)-H(64)	109.9	C(72)-C(67)-H(67)	120.1
C(65)-C(64)-H(64)	109.9	C(67)-C(68)-C(69)	120.2(2)
C(66)-C(64)-H(64)	109.9	C(67)-C(68)-H(68)	119.9
C(58)-C(65)-C(64)	110.55(19)	C(69)-C(68)-H(68)	119.9
C(58)-C(65)-H(65A)	109.5	C(70)-C(69)-C(68)	120.1(2)
C(64)-C(65)-H(65A)	109.5	C(70)-C(69)-H(69)	120.0
C(58)-C(65)-H(65B)	109.5	C(68)-C(69)-H(69)	120.0
C(64)-C(65)-H(65B)	109.5	C(71)-C(70)-C(69)	119.8(2)
H(65A)-C(65)-H(65B)	108.1	C(71)-C(70)-H(70)	120.1
C(64)-C(66)-C(60)	109.7(2)	C(69)-C(70)-H(70)	120.1
C(64)-C(66)-H(66A)	109.7	C(70)-C(71)-C(72)	120.2(2)
C(60)-C(66)-H(66A)	109.7	C(70)-C(71)-H(71)	119.9
C(64)-C(66)-H(66B)	109.7	C(72)-C(71)-H(71)	119.9
C(60)-C(66)-H(66B)	109.7	C(67)-C(72)-C(71)	120.0(2)
H(66A)-C(66)-H(66B)	108.2	C(67)-C(72)-H(72)	120.0
C(68)-C(67)-C(72)	119.8(2)	C(71)-C(72)-H(72)	120.0

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	23(1)	30(1)	21(1)	3(1)	1(1)	14(1)
N(2)	20(1)	33(1)	26(1)	9(1)	4(1)	13(1)
N(3)	23(1)	22(1)	20(1)	3(1)	0(1)	3(1)
N(4)	20(1)	21(1)	23(1)	-1(1)	3(1)	5(1)
C(1)	21(1)	21(1)	22(1)	1(1)	-2(1)	6(1)
C(2)	20(1)	27(1)	22(1)	1(1)	1(1)	10(1)
C(3)	24(1)	27(1)	28(1)	4(1)	-3(1)	11(1)
C(4)	31(2)	26(1)	37(2)	-1(1)	-6(1)	14(1)
C(5)	27(2)	35(2)	29(2)	-9(1)	-2(1)	16(1)
C(6)	22(1)	39(2)	22(1)	2(1)	2(1)	13(1)
C(7)	16(1)	30(1)	23(1)	1(1)	-1(1)	10(1)
C(8)	20(1)	29(1)	18(1)	4(1)	-2(1)	10(1)
C(9)	22(1)	40(2)	24(1)	9(1)	4(1)	13(1)
C(10)	30(2)	37(2)	34(2)	17(1)	3(1)	8(1)
C(11)	33(2)	30(1)	40(2)	14(1)	-2(1)	13(1)
C(12)	27(1)	35(1)	29(1)	7(1)	-1(1)	16(1)
C(13)	22(1)	30(1)	20(1)	6(1)	0(1)	10(1)
C(14)	22(1)	21(1)	21(1)	5(1)	2(1)	9(1)
C(15)	20(1)	27(1)	23(1)	3(1)	1(1)	11(1)
C(16)	20(1)	36(1)	34(2)	12(1)	11(1)	12(1)

C(17)	25(2)	22(1)	48(2)	8(1)	6(1)	5(1)
C(18)	26(1)	24(1)	34(1)	1(1)	3(1)	12(1)
C(19)	17(1)	28(1)	21(1)	0(1)	1(1)	9(1)
C(20)	26(1)	31(1)	23(1)	1(1)	-1(1)	11(1)
C(21)	24(1)	38(2)	23(1)	-1(1)	-9(1)	14(1)
C(22)	22(1)	31(1)	27(1)	4(1)	-1(1)	13(1)
C(23)	24(2)	35(2)	49(2)	-4(1)	-3(1)	10(1)
C(24)	16(1)	23(1)	30(1)	-1(1)	-2(1)	9(1)
C(25)	26(1)	28(1)	29(1)	12(1)	-5(1)	4(1)
C(26)	43(2)	39(2)	23(1)	-2(1)	1(1)	8(1)
C(27)	43(2)	22(1)	43(2)	0(1)	0(1)	10(1)
C(28)	29(2)	33(2)	51(2)	23(1)	6(1)	11(1)
C(29)	17(1)	45(2)	21(1)	6(1)	2(1)	10(1)
C(30)	17(1)	46(2)	42(2)	-3(1)	2(1)	8(1)
C(31)	24(1)	30(1)	56(2)	7(1)	-7(1)	9(1)
C(32)	32(2)	30(2)	62(2)	17(1)	-21(2)	5(1)
C(33)	33(2)	32(2)	36(2)	6(1)	-9(1)	-1(1)
C(34)	20(1)	24(1)	25(1)	4(1)	-1(1)	8(1)
C(35)	19(1)	27(1)	25(1)	8(1)	-3(1)	2(1)
C(36)	29(2)	25(1)	39(2)	8(1)	-9(1)	0(1)
C(37)	40(2)	36(2)	49(2)	22(1)	-10(2)	-1(1)
C(38)	29(2)	55(2)	41(2)	30(2)	-5(1)	-3(1)
C(39)	25(2)	56(2)	24(1)	11(1)	1(1)	4(1)
C(40)	14(1)	36(1)	27(1)	10(1)	2(1)	2(1)
C(41)	21(1)	37(1)	16(1)	-1(1)	-3(1)	8(1)
C(42)	25(2)	56(2)	25(2)	0(1)	2(1)	16(1)
C(43)	31(2)	56(2)	33(2)	-13(1)	-6(1)	25(1)
C(44)	35(2)	35(2)	40(2)	-10(1)	-11(1)	19(1)
C(45)	28(1)	26(1)	30(1)	-3(1)	-7(1)	9(1)
C(46)	17(1)	28(1)	18(1)	-2(1)	-3(1)	6(1)
C(47)	25(1)	21(1)	24(1)	-1(1)	-1(1)	6(1)
C(48)	26(2)	30(1)	32(1)	14(1)	-4(1)	1(1)
C(49)	19(1)	55(2)	32(2)	12(1)	6(1)	10(1)
C(50)	31(2)	35(2)	36(2)	4(1)	1(1)	18(1)
C(51)	36(2)	24(1)	25(1)	7(1)	-4(1)	6(1)
C(52)	20(1)	31(1)	20(1)	4(1)	1(1)	4(1)
C(53)	32(2)	42(2)	22(1)	-1(1)	-2(1)	15(1)
C(54)	30(2)	28(1)	32(2)	-2(1)	-14(1)	7(1)
C(55)	33(2)	26(1)	51(2)	12(1)	-20(1)	-1(1)
C(56)	24(1)	37(2)	36(2)	13(1)	0(1)	8(1)
C(57)	18(1)	22(1)	24(1)	4(1)	2(1)	4(1)
C(58)	22(1)	23(1)	28(1)	0(1)	3(1)	6(1)
C(59)	23(1)	36(1)	20(1)	-2(1)	0(1)	4(1)
C(60)	32(2)	33(1)	30(1)	10(1)	-2(1)	11(1)
C(61)	25(1)	25(1)	32(1)	2(1)	0(1)	10(1)
C(62)	22(1)	27(1)	22(1)	1(1)	0(1)	9(1)

C(63)	22(1)	31(1)	32(1)	2(1)	5(1)	9(1)
C(64)	19(1)	30(1)	36(2)	2(1)	2(1)	5(1)
C(65)	24(1)	27(1)	32(2)	-3(1)	-3(1)	6(1)
C(66)	28(2)	39(2)	32(2)	-1(1)	-8(1)	10(1)
C(67)	27(1)	25(1)	26(1)	8(1)	7(1)	12(1)
C(68)	21(1)	34(1)	30(1)	6(1)	1(1)	10(1)
C(69)	29(2)	33(1)	24(1)	2(1)	-3(1)	11(1)
C(70)	25(1)	20(1)	25(1)	5(1)	7(1)	9(1)
C(71)	20(1)	26(1)	32(2)	2(1)	1(1)	5(1)
C(72)	28(2)	29(1)	23(1)	2(1)	-3(1)	8(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **4**.

	x	y	z	U(eq)					
H(3)	8767	9388	4973	31	H(27)	13492	10185	6484	45
H(4)	8538	10537	5951	37	H(28A)	13414	9800	5240	43
H(5)	8409	10052	7057	38	H(28B)	12010	9302	5493	43
H(6)	8517	8416	7178	33	H(29)	12457	8038	4625	33
H(9)	7333	6394	6827	33	H(30A)	14709	8626	4874	45
H(10)	7496	4748	6877	40	H(30B)	14115	7387	4888	45
H(11)	9041	4232	6276	40	H(31)	15593	8248	5891	44
H(12)	10450	5367	5647	34	H(32A)	14199	7598	6764	50
H(14)	8691	8128	4026	25	H(32B)	13805	6760	6042	50
H(15)	6792	7924	4651	27	H(33A)	15346	9936	5997	44
H(16A)	5234	6215	4577	35	H(33B)	15165	9544	6737	44
H(16B)	6531	6247	4969	35	H(36)	3735	-160	109	40
H(17)	5710	4676	4097	39	H(37)	3555	-881	1125	52
H(18A)	7980	5453	4356	33	H(38)	3421	123	2199	53
H(18B)	7663	4877	3549	33	H(39)	3507	1858	2256	45
H(19)	9235	6580	3615	27	H(42)	2335	3091	1830	43
H(20A)	7783	5979	2598	32	H(43)	2606	4854	1817	49
H(20B)	8191	7237	2813	32	H(44)	4228	5840	1201	44
H(21)	5934	6482	2560	34	H(45)	5580	5068	611	35
H(22A)	5344	7300	3625	31	H(47)	3516	495	-881	29
H(22B)	6705	8042	3436	31	H(48)	1682	113	-200	37
H(23A)	5645	4813	2886	45	H(49A)	199	1007	-291	43
H(23B)	4689	5329	3280	45	H(49B)	1548	1847	53	43
H(24)	12017	6608	5267	28	H(50)	735	2512	-844	39
H(25)	11943	6997	6517	34	H(51A)	2616	2946	-1468	35
H(26A)	12899	8763	7121	45	H(51B)	3000	3021	-654	35
H(26B)	11699	8683	6616	45	H(52)	4121	2079	-1370	30

H(53A)	2573	1373	-2349	38
H(53B)	2941	439	-2105	38
H(54)	680	-89	-2301	38
H(55A)	1464	-761	-1396	47
H(55B)	149	-595	-1191	47
H(56A)	506	1626	-2033	39
H(56B)	-433	861	-1577	39
H(57)	7121	4278	202	26
H(58)	7024	4823	1441	30
H(59A)	6444	3129	1778	34
H(59B)	7680	3943	2255	34
H(60)	8023	2316	1857	37
H(61A)	6660	1793	799	33
H(61B)	8038	1732	627	33
H(62)	7362	2590	-200	28
H(63A)	9222	4142	-56	34
H(63B)	9602	3167	107	34
H(64)	10593	4688	1001	36
H(65A)	9261	5393	1730	36
H(65B)	9001	5489	931	36
H(66A)	9885	3871	1992	41
H(66B)	10015	3004	1358	41
H(67)	3567	7410	1416	30
H(68)	4751	7965	2499	33
H(69)	3724	8100	3537	35
H(70)	1510	7656	3488	28
H(71)	326	7108	2406	33
H(72)	1350	6967	1368	3

Table S6. Torsion angles [°] for **4**.

C(13)-N(2)-C(1)-N(1)	35.7(3)
C(24)-N(2)-C(1)-N(1)	-170.25(19)
C(2)-N(1)-C(1)-N(2)	49.6(3)
C(14)-N(1)-C(1)-N(2)	-165.62(18)
C(1)-N(1)-C(2)-C(7)	-72.3(3)
C(14)-N(1)-C(2)-C(7)	143.3(2)
C(1)-N(1)-C(2)-C(3)	104.8(3)
C(14)-N(1)-C(2)-C(3)	-39.5(3)
C(7)-C(2)-C(3)-C(4)	-0.8(4)
N(1)-C(2)-C(3)-C(4)	-178.0(2)
C(2)-C(3)-C(4)-C(5)	0.2(4)
C(3)-C(4)-C(5)-C(6)	0.2(4)
C(4)-C(5)-C(6)-C(7)	0.0(4)
C(3)-C(2)-C(7)-C(6)	1.0(3)
N(1)-C(2)-C(7)-C(6)	178.2(2)
C(3)-C(2)-C(7)-C(8)	-178.7(2)
N(1)-C(2)-C(7)-C(8)	-1.5(3)
C(5)-C(6)-C(7)-C(2)	-0.6(4)
C(5)-C(6)-C(7)-C(8)	179.1(2)
C(2)-C(7)-C(8)-C(13)	45.2(3)
C(6)-C(7)-C(8)-C(13)	-134.5(2)
C(2)-C(7)-C(8)-C(9)	-134.1(2)
C(6)-C(7)-C(8)-C(9)	46.2(3)
C(13)-C(8)-C(9)-C(10)	-0.7(4)
C(7)-C(8)-C(9)-C(10)	178.7(2)
C(8)-C(9)-C(10)-C(11)	-0.3(4)
C(9)-C(10)-C(11)-C(12)	0.8(4)
C(10)-C(11)-C(12)-C(13)	-0.3(4)
C(11)-C(12)-C(13)-C(8)	-0.7(4)
C(11)-C(12)-C(13)-N(2)	-177.6(2)
C(9)-C(8)-C(13)-C(12)	1.2(4)
C(7)-C(8)-C(13)-C(12)	-178.2(2)
C(9)-C(8)-C(13)-N(2)	178.0(2)
C(7)-C(8)-C(13)-N(2)	-1.4(3)
C(1)-N(2)-C(13)-C(12)	110.6(3)
C(24)-N(2)-C(13)-C(12)	-43.8(3)
C(1)-N(2)-C(13)-C(8)	-66.2(3)
C(24)-N(2)-C(13)-C(8)	139.3(2)
C(1)-N(1)-C(14)-C(19)	47.9(3)
C(2)-N(1)-C(14)-C(19)	-167.47(18)
C(1)-N(1)-C(14)-C(15)	168.25(19)
C(2)-N(1)-C(14)-C(15)	-47.1(3)
N(1)-C(14)-C(15)-C(16)	-63.9(2)
C(19)-C(14)-C(15)-C(16)	57.6(2)
N(1)-C(14)-C(15)-C(22)	176.27(17)
C(19)-C(14)-C(15)-C(22)	-62.2(2)
C(22)-C(15)-C(16)-C(17)	58.2(2)
C(14)-C(15)-C(16)-C(17)	-60.8(3)
C(15)-C(16)-C(17)-C(23)	-58.5(3)
C(15)-C(16)-C(17)-C(18)	61.5(3)
C(23)-C(17)-C(18)-C(19)	58.9(3)
C(16)-C(17)-C(18)-C(19)	-61.6(3)
C(17)-C(18)-C(19)-C(20)	-58.6(2)
C(17)-C(18)-C(19)-C(14)	61.1(3)
N(1)-C(14)-C(19)-C(20)	-174.66(18)
C(15)-C(14)-C(19)-C(20)	62.8(2)
N(1)-C(14)-C(19)-C(18)	64.8(2)
C(15)-C(14)-C(19)-C(18)	-57.7(2)
C(18)-C(19)-C(20)-C(21)	59.2(2)
C(14)-C(19)-C(20)-C(21)	-61.8(2)
C(19)-C(20)-C(21)-C(23)	-59.8(3)
C(19)-C(20)-C(21)-C(22)	59.6(2)
C(23)-C(21)-C(22)-C(15)	60.1(3)
C(20)-C(21)-C(22)-C(15)	-59.5(3)
C(16)-C(15)-C(22)-C(21)	-59.7(2)
C(14)-C(15)-C(22)-C(21)	61.0(2)
C(20)-C(21)-C(23)-C(17)	60.0(3)
C(22)-C(21)-C(23)-C(17)	-59.2(3)
C(16)-C(17)-C(23)-C(21)	59.0(3)
C(18)-C(17)-C(23)-C(21)	-59.7(2)
C(1)-N(2)-C(24)-C(25)	155.6(2)
C(13)-N(2)-C(24)-C(25)	-49.4(3)
C(1)-N(2)-C(24)-C(29)	34.2(3)
C(13)-N(2)-C(24)-C(29)	-170.77(19)
N(2)-C(24)-C(25)-C(26)	-65.8(3)
C(29)-C(24)-C(25)-C(26)	57.4(3)
N(2)-C(24)-C(25)-C(32)	174.04(18)
C(29)-C(24)-C(25)-C(32)	-62.8(2)
C(32)-C(25)-C(26)-C(27)	58.9(3)
C(24)-C(25)-C(26)-C(27)	-60.5(3)
C(25)-C(26)-C(27)-C(28)	61.2(3)
C(25)-C(26)-C(27)-C(33)	-59.1(3)
C(33)-C(27)-C(28)-C(29)	59.4(3)
C(26)-C(27)-C(28)-C(29)	-61.4(3)
C(27)-C(28)-C(29)-C(30)	-58.9(3)
C(27)-C(28)-C(29)-C(24)	60.6(3)
N(2)-C(24)-C(29)-C(30)	-173.34(19)
C(25)-C(24)-C(29)-C(30)	63.1(2)
N(2)-C(24)-C(29)-C(28)	66.5(3)
C(25)-C(24)-C(29)-C(28)	-57.1(2)
C(28)-C(29)-C(30)-C(31)	59.4(3)

C(24)-C(29)-C(30)-C(31)	-61.6(3)	C(36)-C(35)-C(40)-C(39)	-1.0(4)
C(29)-C(30)-C(31)-C(33)	-60.1(3)	N(3)-C(35)-C(40)-C(39)	-177.0(2)
C(29)-C(30)-C(31)-C(32)	59.1(3)	C(36)-C(35)-C(40)-C(41)	175.9(2)
C(33)-C(31)-C(32)-C(25)	59.8(3)	N(3)-C(35)-C(40)-C(41)	-0.1(3)
C(30)-C(31)-C(32)-C(25)	-59.1(3)	C(38)-C(39)-C(40)-C(35)	0.5(4)
C(26)-C(25)-C(32)-C(31)	-60.0(3)	C(38)-C(39)-C(40)-C(41)	-176.3(2)
C(24)-C(25)-C(32)-C(31)	61.3(3)	C(35)-C(40)-C(41)-C(46)	-45.4(3)
C(32)-C(31)-C(33)-C(27)	-58.7(3)	C(39)-C(40)-C(41)-C(46)	131.4(3)
C(30)-C(31)-C(33)-C(27)	60.1(3)	C(35)-C(40)-C(41)-C(42)	134.2(3)
C(28)-C(27)-C(33)-C(31)	-60.2(3)	C(39)-C(40)-C(41)-C(42)	-49.1(4)
C(26)-C(27)-C(33)-C(31)	58.9(3)	C(46)-C(41)-C(42)-C(43)	0.3(4)
C(35)-N(3)-C(34)-N(4)	-41.1(3)	C(40)-C(41)-C(42)-C(43)	-179.3(2)
C(47)-N(3)-C(34)-N(4)	169.52(19)	C(41)-C(42)-C(43)-C(44)	0.2(4)
C(46)-N(4)-C(34)-N(3)	-46.1(3)	C(42)-C(43)-C(44)-C(45)	-0.3(4)
C(57)-N(4)-C(34)-N(3)	163.97(18)	C(43)-C(44)-C(45)-C(46)	-0.1(4)
C(34)-N(3)-C(35)-C(40)	71.1(3)	C(42)-C(41)-C(46)-C(45)	-0.7(3)
C(47)-N(3)-C(35)-C(40)	-139.5(2)	C(40)-C(41)-C(46)-C(45)	178.9(2)
C(34)-N(3)-C(35)-C(36)	-104.9(3)	C(42)-C(41)-C(46)-N(4)	-177.9(2)
C(47)-N(3)-C(35)-C(36)	44.4(3)	C(40)-C(41)-C(46)-N(4)	1.6(3)
C(40)-C(35)-C(36)-C(37)	0.7(4)	C(44)-C(45)-C(46)-C(41)	0.6(4)
N(3)-C(35)-C(36)-C(37)	176.8(2)	C(44)-C(45)-C(46)-N(4)	177.9(2)
C(35)-C(36)-C(37)-C(38)	0.1(4)	C(34)-N(4)-C(46)-C(41)	71.9(3)
C(36)-C(37)-C(38)-C(39)	-0.7(4)	C(57)-N(4)-C(46)-C(41)	-138.8(2)
C(37)-C(38)-C(39)-C(40)	0.4(4)		
C(34)-N(4)-C(46)-C(45)	-105.4(2)	C(51)-C(52)-C(53)-C(54)	-60.1(3)
C(57)-N(4)-C(46)-C(45)	43.9(3)	C(47)-C(52)-C(53)-C(54)	61.1(3)
C(34)-N(3)-C(47)-C(52)	-43.2(3)	C(52)-C(53)-C(54)-C(55)	-59.3(3)
C(35)-N(3)-C(47)-C(52)	167.11(19)	C(52)-C(53)-C(54)-C(56)	59.8(3)
C(34)-N(3)-C(47)-C(48)	-164.06(19)	C(53)-C(54)-C(55)-C(48)	59.4(3)
C(35)-N(3)-C(47)-C(48)	46.2(3)	C(56)-C(54)-C(55)-C(48)	-59.7(3)
N(3)-C(47)-C(48)-C(49)	64.5(3)	C(49)-C(48)-C(55)-C(54)	59.5(3)
C(52)-C(47)-C(48)-C(49)	-57.7(3)	C(47)-C(48)-C(55)-C(54)	-61.3(3)
N(3)-C(47)-C(48)-C(55)	-175.11(18)	C(49)-C(50)-C(56)-C(54)	-59.9(3)
C(52)-C(47)-C(48)-C(55)	62.6(2)	C(51)-C(50)-C(56)-C(54)	59.3(3)
C(55)-C(48)-C(49)-C(50)	-58.7(3)	C(53)-C(54)-C(56)-C(50)	-59.1(3)
C(47)-C(48)-C(49)-C(50)	60.6(3)	C(55)-C(54)-C(56)-C(50)	59.9(3)
C(48)-C(49)-C(50)-C(51)	-60.9(3)	C(34)-N(4)-C(57)-C(58)	-168.73(19)
C(48)-C(49)-C(50)-C(56)	59.0(3)	C(46)-N(4)-C(57)-C(58)	41.6(3)
C(49)-C(50)-C(51)-C(52)	60.4(3)	C(34)-N(4)-C(57)-C(62)	-48.7(3)
C(56)-C(50)-C(51)-C(52)	-59.7(3)	C(46)-N(4)-C(57)-C(62)	161.60(19)
C(50)-C(51)-C(52)-C(53)	59.7(3)	N(4)-C(57)-C(58)-C(65)	-177.38(18)
C(50)-C(51)-C(52)-C(47)	-59.8(3)	C(62)-C(57)-C(58)-C(65)	61.9(2)
N(3)-C(47)-C(52)-C(51)	-65.2(2)	N(4)-C(57)-C(58)-C(59)	62.3(2)
C(48)-C(47)-C(52)-C(51)	57.5(2)	C(62)-C(57)-C(58)-C(59)	-58.4(2)
N(3)-C(47)-C(52)-C(53)	174.94(19)	C(65)-C(58)-C(59)-C(60)	-58.5(3)
C(48)-C(47)-C(52)-C(53)	-62.4(2)	C(57)-C(58)-C(59)-C(60)	60.9(3)

C(58)-C(59)-C(60)-C(61)	-60.7(3)	C(57)-C(58)-C(65)-C(64)	-61.7(3)
C(58)-C(59)-C(60)-C(66)	59.1(3)	C(63)-C(64)-C(65)-C(58)	59.8(3)
C(59)-C(60)-C(61)-C(62)	60.4(3)	C(66)-C(64)-C(65)-C(58)	-59.3(3)
C(66)-C(60)-C(61)-C(62)	-59.7(3)	C(63)-C(64)-C(66)-C(60)	-59.6(3)
C(60)-C(61)-C(62)-C(63)	59.5(2)	C(65)-C(64)-C(66)-C(60)	59.1(3)
C(60)-C(61)-C(62)-C(57)	-60.1(3)	C(61)-C(60)-C(66)-C(64)	59.5(3)
N(4)-C(57)-C(62)-C(63)	175.80(19)	C(59)-C(60)-C(66)-C(64)	-59.5(3)
C(58)-C(57)-C(62)-C(63)	-61.9(2)	C(72)-C(67)-C(68)-C(69)	-0.3(3)
N(4)-C(57)-C(62)-C(61)	-64.5(2)	C(67)-C(68)-C(69)-C(70)	0.4(3)
C(58)-C(57)-C(62)-C(61)	57.8(2)	C(68)-C(69)-C(70)-C(71)	-0.5(3)
C(61)-C(62)-C(63)-C(64)	-59.7(2)	C(69)-C(70)-C(71)-C(72)	0.6(3)
C(57)-C(62)-C(63)-C(64)	60.9(2)	C(68)-C(67)-C(72)-C(71)	0.4(3)
C(62)-C(63)-C(64)-C(65)	-59.1(3)	C(70)-C(71)-C(72)-C(67)	-0.6(3)
C(62)-C(63)-C(64)-C(66)	60.0(3)		
C(59)-C(58)-C(65)-C(64)	59.1(3)		