

Supporting Information for

Z-Selective Olefin Metathesis Processes Catalyzed by a
Molybdenum Hexaisopropylterphenoxide Monopyrrolide Complex

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Experimental procedures, X-ray procedures, and crystallographic details (Tables 1-5).

Experimental Procedures.

General Details. All air-sensitive manipulations were performed under nitrogen in a drybox or using Schlenk techniques. All glassware was oven-dried and allowed to cool in a vacuum before use. Ether, pentane, and toluene were sparged with nitrogen and passed through activated alumina. All solvents were stored over molecular sieves in a nitrogen atmosphere. Deuterated solvents were degassed and passed through activated alumina before use and stored over molecular sieves. 3-Hexene and 4-octene were purchased from Aldrich, degassed, dried over sodium benzophenone ketyl, and vacuum distilled. *Cis*-cyclooctene and *cis,cis*-1,5-cyclooctadiene were purchased from Aldrich, degassed, dried over CaH₂, and vacuum distilled. Mo(NAr)(CHCMe₂Ph)(NMe₂C₄H₂)₂, Mo(NAd)(CHCMe₃Ph)(NMe₂C₄H₂)₂,ⁱ Mo(NAd)(CHCMe₂Ph)(NC₄H₄)₂,ⁱⁱ **1a**,ⁱⁱⁱ **1b**,^{iv} (1-Naphthyl)₃SiOH,^v (R)-2'-(tert-butyl)dimethylsilyloxy)-3,3'-dimethyl-5,5',6,6',7,7',8,8'-octahydro-1,1'-binaphthyl-2-ol (Me₂Bitet),^{vi} (R)-3,3'-dibenzhydryl-2'-(tert-butyl)dimethylsilyloxy)-5,5',6,6',7,7',8,8'-octahydro-1,1'-binaphthyl-2-ol (Bz₂Bitet),^{vii} DCMNBD^{viii} and DCMenNBD^{ix} were prepared according to the literature. Mono-protected phenols Me₂Bitet-TBS and Bz₂Bitet-TBS were prepared from the corresponding diols as described in the literature.^{iiib} NMR spectra were obtained on Varian spectrometers operating at 300 MHz (¹H) or 500 MHz (¹³C). NMR chemical shifts are reported as ppm relative to tetramethylsilane, and were referenced to the residual proton or ¹³C signal of the solvent (¹H C₆D₆: 7.16 ppm, ¹H CD₂Cl₂: 5.32 ppm, ¹³C C₆D₆: 128.06ppm, ¹³CDCl₃: 77.16ppm). A TA Instruments Q1000 differential scanning calorimeter (DSC) was used to determine the thermal transitions. Heating and cooling scans were performed at a rate of 10 °C/min.

In situ generation of catalysts. **1c**: Mo(NAd)(CHCMe₂Ph)(NMe₂C₄H₂)₂ was dissolved in C₆D₆ containing 1.1 mg anthracene as internal standard. Me₂Bitet-TBS was added to the stirred mixture in one portion as a solid and the solution was stirred for 5h. The entire reaction mixture was transferred to a J-young tube and the ¹H NMR spectrum recorded. The resulting mixture was used for subsequent metathesis reactions. Only the relevant diagnostic signals of *in situ* generated complexes are recorded: ¹H NMR (C₆D₆, 300 MHz) δ = 12.24 (s, 1H, Mo=CH, minor, 47%) 11.80 (s, 1H, Mo=CH, major diastereomer, 53%).

1d: Prepared from Mo(NAd)(CHCMe₂Ph)(NC₄H₄)₂ and Bz₂Bitet-TBS in the same manner as **1c**. ¹H NMR (C₆D₆, 300 MHz) δ = 12.35 (s, 1H, Mo=CH, minor, 23%), 11.53 (s, 1H, Mo=CH, major, 77%).

2a: Mo(NAd)(CHCMe₂Ph)(NC₄H₄)₂ (153 mg, 0.300 mmol) was dissolved in 20 mL of diethyl ether and the solution was chilled to -25 °C. 2,6-(Trip)₂C₆H₃OH (Trip = 2,4,6(*i*-Pr)₃C₆H₂) (150 mg, 0.300 mmol, 1eq) was added in one portion as a solid. The mixture became orange after 10 minutes, and was allowed to warm to room temperature and was stirred for 1h. All volatiles were removed *in vacuo*. The resulting solid was dissolved in 5 mL pentane and the pentane was then removed *in vacuo*. This process was repeated three times in order to remove residual pyrrole. A yellow solid was isolated after allowing a pentane solution to stand at -25 °C for 72 hours; 145 mg (45%) isolated: ¹H NMR (C₆D₆, 300 MHz) δ = 11.95 (s, 1H, Mo=CH, J_{CH} = 119.4 Hz), 7.33-6.85 (mult, 8H, Ar), 6.33 (t, 2H, NC₂H₄), 6.45 (t, 2H, NC₂H₄), 3.04 (sept, 2H, CHMe₂), 2.96 (sept, 4H, CHMe₂), 1.78, 1.60, 1.58, 1.55, 1.23, 1.38-1.34, 1.20-1.16, 1.11 (57H, Mo=CHCMe₂Ph, NAd, (CHMe₂)₆); ¹³C NMR (C₆D₆, 500 MHz) δ = 288.11, 159.34, 149.85, 147.87, 147.35, 147.28, 134.73, 133.70, 131.75, 131.32, 127.24, 126.21, 121.48, 121.45, 109.85, 76.30, 52.46, 43.92, 35.81, 34.46, 32.85, 32.06, 31.40, 31.33, 29.81, 25.01, 24.65, 24.52, 24.37, 24.27, 23.70. Anal. Calcd for C₆₀H₈₀MoN₂O: C, 76.56; H, 8.57; N, 2.98. Found: C, 76.21; H, 8.61; N; 2.92.

2b: Mo(NAd)(CHCMe₂Ph)(NMe₂C₄H₂)₂ (6.7 mg, 0.0118mmol) was dissolved in 1 mL C₆D₆, and to it was added 2,6-(Trip)₂C₆H₃OH (5.9 mg, 0.0118mmol). The entire reaction mixture was transferred to a J-Young NMR tube and heated to 60 °C over 5 days. The catalyst was used *in situ* in further reactions: ¹H NMR (C₆D₆, 300 MHz) δ = 12.16 (s, 1H, Mo=CH), 7.4-6.8 (mult, 12H, Ar), 6.13 (s, 2H, NC₄H₂Me₂), 3.05 (sept, 4H, CHMe₂), 2.93 (sept, 2H, CHMe₂), 1.94 (s, 6H, NC₄H₂Me₂), 1.76, 1.62, 1.52, 1.36-1.14 (NAd, CMe₂Ph, CHMe₂, mult, 42H).

2c: Mo(NAr)(CHCMe₂Ph)(NMe₂C₄H₂)₂ (9.2 mg, 0.0172 mmol) was dissolved in 1 mL C₆D₆ and 8.6 mg (0.0172 mmol) 2,6-(Trip)₂C₆H₃OH was added to the solution. The entire reaction

mixture was transferred to a J-young NMR tube and heated to 60 °C for 2h. The catalyst was used *in situ* for further reactions. ^1H NMR (C_6D_6 , 300 MHz) δ = 12.76 (s, 1H, Mo=CH).

3a: Mo(NAd)(CHCMe₂Ph)(NMe₂C₄H₉)₂ (0.176 g, 0.311 mmol) was dissolved in 50 mL toluene and the solution was chilled to -25 °C. Ph₄PhOH (0.1238 g, 0.311 mmol) was dissolved in 10 mL toluene and the solution was chilled to -25 °C. The alcohol solution was added to the Mo solution in one portion, and the mixture was allowed to stir overnight, during which time the color changed to slightly deeper orange. All volatiles were removed *in vacuo*. The resulting solid was dissolved in 5 mL pentane. The pentane was then removed *in vacuo*. Pentane was added and removed three times in a similar manner in order to remove residual dimethylpyrrole. Yellow crystals were obtained from pentane after sitting at -25 °C overnight; 165 mg (61%) isolated in two crops: ^1H NMR (C_6D_6 , 300 MHz) δ = 10.96 (s, 1H, Mo=CH, J_{CH} = 121.8 Hz), 7.32-6.92 (mult, 26H, Ar), 6.19 (s, 2H, NC₂H₂Me), 2.26 (s, 6H, NC₂H₂Me₂), 1.75 (s, 3H, NAd), 1.71 (br, 3H, NAd), 1.52 (6H, C=CHMe₂Ph), 1.30 (br, 6H, NAd), 1.24 (s, 3H, NAd); ^{13}C NMR (C_6D_6 , 400 MHz) δ = 284.31 (Mo=C), 160.7, 149.8, 142.9, 142.7, 138.5, 133.8, 52.1, 44.2, 36.2, 33.7, 30.3, 23.2, 18.0, 14.9. Anal. Calcd for C₅₆H₅₆MoN₂O: C, 77.40; H, 6.50; N, 3.22. Found: C, 77.37, H, 6.75, 2.95.

3b: Compound **3b** was prepared from Mo(NAd)(CHCMe₂Ph)(NC₄H₉)₂ and (1-Naphthyl)₃SiOH in the same manner as **2a**: ^1H NMR (toluene-d₈, 300 MHz) δ = 11.81 (s, 1H, Mo=CH).

Representative procedure for ROMP of cyclic olefins: 146.8 mg (0.705mmol, 50 eq) of DCMNBD was dissolved in 0.7 mL C₆D₆, and to the solution was added a 0.5 mL C₆D₆ solution of **3b** (generated *in situ* as described above) (0.0141 mmol) in one portion. The mixture immediately became deep red/brown. The mixture was stirred for 1h, then transferred to a J-young tube where the progress of the reaction was monitored by ^1H NMR. After the monomer was consumed, the reaction mixture was transferred to a vial, and 500 μL benzaldehyde was added. The reaction mixture became deep green within 5 minutes, and was stirred for 1 h. The entire mixture was added dropwise to 100 mL of vigorously stirring methanol. A fine white solid immediately formed, and the mixture was stirred for 12 h. The white or off-white polymers were isolated on a medium or fine porosity frit by filtration, rinsed with MeOH, and dried *in vacuo*.

***cis*-syndiotactic poly-DCMNBD:** ^1H NMR (C_6D_6 , 300 MHz) $\delta = 5.34$ (m, 2H, C_5H , C_6H), 3.015 (m, 2H, C_1H , C_4H), 3.73 (s, 6H, CO_2Me), 2.52 (m, 1H, C_7H), 1.46 (m, 1H, C_7H); ^{13}C NMR: (CDCl_3 , 500 MHz): $\delta = 165.37$ (CO_2CH_3), 142.29 (C_3), 131.5 (C_5), 52.06 (CO_2CH_3), 44.44 (C_4), 38.01 (C_7).

***cis*, syndiotactic-polydicarbomethoxynorbornadiene:** ^1H NMR (CDCl_3) $\delta = 5.34$ (br, 1H, C_5H or C_6H), 5.29 (br, 1H, C_5H or C_6H), 4.75, 4.68, 2.13 (br, 1H,), 2.03 (br, 1H,), 1.93, 1.67, 1.47, 1.39, 1.02 (other resonances are overlapping).

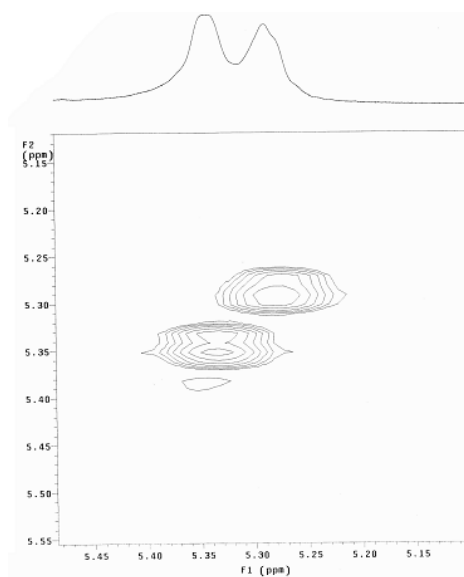


Figure 1: ^1H COSY spectrum of *cis,syndiotactic* poly-DCMenNBD in the olefinic proton region

***cis*-polycyclooctene:** ^1H NMR (CD_2Cl_2 , 500 MHz) δ = 5.38 (t, 1H, C=CH), 2.06 (m, 2H, CH_2), 1.34 (m, 4H, CH_2); ^{13}C NMR: (CDCl_3 , 500 MHz) δ = 130.02 (C=CH), 29.91, 29.29, 27.38.

***cis*-polycyclooctadiene:** ^1H NMR (CD_2Cl_2 , 500 MHz) δ = 5.42 (t, 1H, C=CH), 2.12 (m, 2H, CH_2); ^{13}C NMR (CDCl_3 , 500 MHz) δ = 129.70 (C=CH), 27.53 (CH_2).

Representative procedure for cross metathesis of *cis*-3-hexene and *cis*-4-octene: 4.4 mg (0.0046 mmol) **3c** was dissolved in 5 mL pentane, and to it was added 230 μL of a 1M (each) pentane solution of *cis*-3-hexene and *cis*-4-octene. Aliquots were taken at regular intervals by running 0.2 mL of the reaction mixture through a plug of alumina, and analyzed by gas chromatography. *Cis/trans* ratios of products were determined by comparison with authentic *cis*-3-heptene and *trans*-3-heptene.

W(NAr)(C₃H₆)(Pyr)(HIPTO). W(NAr)(CHCMe₂Ph)(Pyr)₂(DME)^x (0.718 g, 1.01 mmol) and HIPTOH (0.503 g, 1.01 mmol) were mixed as solids in a 100 mL Schlenk flask equipped with a stir bar. When benzene (~20 mL) was added, the solution turned dark brown immediately. The mixture was stirred at 60 °C for 2 days, at which time the sample taken to

dryness *in vacuo* to give a dark brown residue. Pentane (~20 mL) was added to the mixture. The solution was frozen, pumped, and thawed three times. Ethylene (1 atm) was added to the solution at room temperature. The sample was stirred for 30 minutes. A white fluffy solid precipitated out of the dark solution. Diethyl ether (~10 mL) was added, and the resulting solution was filtered through Celite to remove the dark impurities. The filtrate was concentrated to ~4 mL and left at -27 °C overnight. The off-white solid was isolated by filtration. The filtrate was degassed and exposed to 1 atm of ethylene. Another crop of off-white solid was collected, affording a total yield of 0.332 g (34%). The isolated yield is low because the compound cannot be easily separated from the dark impurities; an NMR scale (~30 mg) reaction showed that the reaction does go to completion when the sample was exposed to 1 atm of ethylene: ¹H NMR (500 MHz, C₆D₆) δ 7.38 (s, 2, PyrH), 7.27 (d, 2, *m*-ArH, *J*_{HH} = 8 Hz), 7.20 (s, 4, ArH), 6.94 (d, 2, *m*-ArH, *J*_{HH} = 8 Hz), 6.88 (t, 1, *p*-ArH, *J*_{HH} = 8 Hz), 6.79 (t, 1, *p*-ArH, *J*_{HH} = 8 Hz), 6.15 (s, 2, PyrH), 4.24 (m, 2, WCH_α), 3.64 (sept, 2, CHMe₂), 3.52 (m, 2, WCH_α), 3.42 (br s, 1, CHMe₂), 2.88 (sept, 2, CHMe₂), 2.66 (br s, 3, CHMe₂), 1.37 (br s, 12, CHMe₂), 1.31 (d, 12, CHMe₂, *J*_{HH} = 7 Hz), 1.05 (d, 12, CHMe₂, *J*_{HH} = 7 Hz), 0.94 (br s, 12, CHMe₂), -0.78 (m, 1, WCH_β), -1.11 (m, 1, WCH_β); ¹³C NMR (125 MHz, C₆D₆) δ 160.31, 149.50, 149.00 (br s), 148.78, 147.67 (br s), 147.51, 136.11, 132.34, 131.88, 131.56, 127.87, 123.28, 121.85 (br s), 120.78 (br s), 119.91, 110.52, 98.60 (WC_α, *J*_{CW} = 66 Hz), 35.15, 32.29 (br s), 31.07 (br s), 28.71, 27.40 (br s), 26.23 (br s), 24.82, 23.38, -3.73 (WC_β). A 23 mg sample of the tungstacyclobutane in C₆D₆ (~0.6 mL) was degassed and ¹³C-ethylene (~1 atm) was added: ¹³C NMR (125 MHz, C₆D₆) δ 98.60 (WC_α, *J*_{CH} = 157 Hz, *J*_{CαCβ} = 11 Hz), -3.73 (WC_β, *J*_{CH} = 153 Hz, *J*_{CαCβ} = 13 Hz). Anal. Calcd for C₅₅H₇₆N₂O_W: C, 68.45; H, 7.94; N, 2.90. Found: C, 68.52; H, 8.04; N, 2.99.

X-Ray Procedures and Crystallographic Details. Low temperature diffraction data were collected on a Siemens Platform three-circle diffractometer coupled to a Bruker-AXS Smart Apex CCD detector with graphite-monochromated Mo K α radiation ($\lambda = 0.71073 \text{ \AA}$), performing ϕ - and ω -scans. The structure was solved by direct methods using SHELXS^{xi} and refined against F^2 on all data by full-matrix least squares with SHELXL-97^{xii}, following

established refinement strategies.^{xiii} The crystal was non-merohedrally twinned. Two independent orientation matrices for the unit cell were found using the program CELL_NOW,^{xiv} and data reduction taking into account the twinning was performed with SAINT.^{xv} The program TWINABS^{xvi} was used to perform absorption correction and to set up a HKLF5 format file for structure refinement. The twin ratio was refined freely and converged at a value of 0.4417(13). As a result of the non-merohedral twinning, there are three more "observations" than "unique reflections" reported in the CIF file. This is reasonable as not all observed reflections can be merged for non-merohedral twins and was taken into account when estimating the standard uncertainties of all parameters. In order to counteract correlation effects caused by the twinning, similarity and rigid bond restraints were applied to the displacement parameters of all atoms. All non-hydrogen atoms were refined anisotropically. Coordinates for the six hydrogen atoms of the metallocyclobutane were taken from the difference Fourier synthesis. Those hydrogen atoms were subsequently refined semi-freely with the help of distance restraints while constraining the U_{iso} value of the hydrogen atoms to 1.2 times the U_{eq} value of the carbon atom the hydrogen binds to. All other hydrogen atoms were included in the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms they are linked to (1.5 times for methyl groups). A disorder of one aryl ring of the HIPTOH ligand was refined with the help of similarity restraints on 1-2 and 1-3 distances. The ratio between the two components of the disorder was refined freely and converged at 0.587(15).

Table 1. Crystal data and structure refinement for 09097.

Identification code	09097	
Empirical formula	C ₅₅ H ₇₆ N ₂ O W	
Formula weight	965.03	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 8.702(2) Å	$\alpha = 92.188(4)^\circ$
	b = 12.330(3) Å	$\beta = 91.229(4)^\circ$
	c = 23.758(6) Å	$\gamma = 101.656(4)^\circ$
Volume	2493.7(11) Å ³	
Z	2	
Density (calculated)	1.285 Mg/m ³	
Absorption coefficient	2.354 mm ⁻¹	
F(000)	1004	
Crystal size	0.45 x 0.09 x 0.04 mm ³	
Theta range for data collection	1.69 to 27.06°	
Index ranges	-11 ≤ h ≤ 10, -15 ≤ k ≤ 15, 0 ≤ l ≤ 30	
Reflections collected	10594	
Independent reflections	10597 [R(int) = 0.0985]	
Completeness to theta = 27.06°	96.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9117 and 0.4172	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	10597 / 1432 / 601	
Goodness-of-fit on F ²	1.025	
Final R indices [I > 2σ(I)]	R1 = 0.0672, wR2 = 0.1587	
R indices (all data)	R1 = 0.0822, wR2 = 0.1684	
Largest diff. peak and hole	3.581 and -4.665 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 09097. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
C(1)	1212(11)	8320(8)	2963(4)	28(2)
C(2)	708(11)	9387(9)	2678(4)	28(2)
C(3)	1588(11)	9772(8)	2118(4)	26(2)
W(1)	2692(1)	8515(1)	2305(1)	19(1)
O(1)	4131(7)	9608(5)	2804(2)	19(1)
C(31)	5404(9)	10209(6)	3068(3)	16(1)
C(32)	6208(9)	11191(6)	2830(3)	20(1)
C(37)	5621(13)	11717(8)	2330(5)	18(1)
C(38)	4447(18)	12347(13)	2418(6)	19(1)
C(43)	3820(30)	12530(20)	3002(7)	22(2)
C(44)	4760(50)	13600(40)	3289(17)	32(4)
C(45)	2070(30)	12540(40)	3004(9)	24(4)
C(39)	3930(20)	12881(19)	1964(7)	22(2)
C(40)	4460(20)	12761(16)	1423(7)	24(2)
C(46)	3910(20)	13302(13)	907(6)	32(2)
C(47)	2990(20)	14197(13)	1049(7)	38(3)
C(48)	3020(40)	12430(20)	484(12)	41(3)
C(41)	5610(20)	12142(16)	1346(6)	22(2)
C(42)	6200(20)	11597(17)	1787(6)	20(2)
C(49)	7527(19)	10972(16)	1670(9)	20(3)
C(50)	7110(30)	10130(30)	1175(14)	23(4)
C(51)	9060(20)	11790(20)	1562(17)	27(3)
C(37A)	5477(17)	11683(11)	2344(7)	18(1)
C(38A)	4340(20)	12335(17)	2461(8)	19(1)
C(43A)	3910(40)	12610(30)	3061(9)	22(2)
C(44A)	4830(80)	13750(50)	3280(30)	32(4)
C(45A)	2160(40)	12550(60)	3147(15)	24(4)
C(39A)	3670(30)	12770(30)	2006(9)	22(2)
C(40A)	4080(30)	12630(20)	1452(9)	24(2)
C(46A)	3340(30)	13148(18)	965(9)	32(2)
C(47A)	4530(30)	14126(18)	741(10)	38(3)

C(48A)	2790(60)	12300(30)	481(15)	41(3)
C(41A)	5210(30)	12010(20)	1349(9)	22(2)
C(42A)	5910(30)	11500(20)	1784(7)	20(2)
C(49A)	7180(30)	10840(20)	1642(13)	20(3)
C(50A)	6670(40)	10020(40)	1140(20)	23(4)
C(51A)	8710(30)	11650(40)	1520(30)	27(3)
C(33)	7602(10)	11782(6)	3106(3)	19(2)
C(34)	8168(10)	11421(7)	3603(3)	23(2)
C(35)	7338(9)	10487(7)	3844(3)	19(2)
C(36)	5925(9)	9871(6)	3589(3)	16(1)
C(52)	4949(8)	8933(6)	3895(2)	18(1)
C(53)	5417(9)	7905(6)	3935(3)	18(1)
C(58)	6959(9)	7684(7)	3704(3)	21(2)
C(59)	6713(12)	6613(7)	3335(4)	29(2)
C(60)	8114(10)	7600(8)	4192(4)	25(2)
C(54)	4467(9)	7061(7)	4229(3)	21(2)
C(55)	3092(9)	7214(6)	4474(3)	21(1)
C(61)	2063(11)	6265(7)	4770(4)	29(2)
C(62)	1567(16)	5235(9)	4373(5)	54(3)
C(63)	2917(13)	5969(10)	5298(4)	47(3)
C(56)	2679(9)	8238(6)	4446(3)	20(1)
C(57)	3560(9)	9109(6)	4157(3)	21(1)
C(64)	3063(9)	10234(6)	4134(3)	21(2)
C(65)	4120(11)	11108(7)	4526(4)	29(2)
C(66)	1345(9)	10186(8)	4279(4)	27(2)
N(2)	4642(9)	7938(6)	2056(3)	21(1)
C(17)	4651(11)	7134(8)	1621(4)	25(2)
C(18)	6151(12)	7008(8)	1531(4)	30(2)
C(19)	7159(11)	7732(7)	1920(4)	24(2)
C(20)	6228(10)	8266(8)	2228(4)	24(2)
N(1)	1470(9)	7553(6)	1834(3)	20(1)
C(11)	633(10)	6863(7)	1409(3)	20(2)
C(12)	832(11)	7169(8)	831(3)	23(2)
C(13)	-68(11)	6427(8)	428(4)	28(2)
C(14)	-1038(12)	5453(8)	560(4)	28(2)
C(15)	-1178(11)	5170(8)	1121(4)	25(2)

C(16)	-358(10)	5861(7)	1548(4)	22(2)
C(121)	1887(12)	8231(8)	672(4)	29(2)
C(122)	3120(14)	7980(10)	258(5)	41(2)
C(123)	950(14)	9025(9)	424(5)	40(2)
C(161)	-481(11)	5552(8)	2166(4)	26(2)
C(162)	937(13)	5109(9)	2372(4)	34(2)
C(163)	-2027(12)	4739(8)	2301(4)	31(2)

Table 3. Bond lengths [Å] and angles [°] for 09097.

C(1)-C(2)	1.635(14)	C(39)-H(39)	0.9500
C(1)-W(1)	2.037(9)	C(40)-C(41)	1.391(13)
C(1)-H(1A)	0.994(19)	C(40)-C(46)	1.528(11)
C(1)-H(1B)	0.992(19)	C(46)-C(48)	1.519(12)
C(2)-C(3)	1.588(14)	C(46)-C(47)	1.522(12)
C(2)-W(1)	2.380(9)	C(46)-H(46)	1.0000
C(2)-H(2A)	0.985(19)	C(47)-H(47A)	0.9800
C(2)-H(2B)	1.003(19)	C(47)-H(47B)	0.9800
C(3)-W(1)	2.038(10)	C(47)-H(47C)	0.9800
C(3)-H(3A)	0.985(19)	C(48)-H(48A)	0.9800
C(3)-H(3B)	0.983(19)	C(48)-H(48B)	0.9800
W(1)-N(1)	1.768(7)	C(48)-H(48C)	0.9800
W(1)-O(1)	1.980(6)	C(41)-C(42)	1.408(12)
W(1)-N(2)	2.058(8)	C(41)-H(41)	0.9500
O(1)-C(31)	1.332(10)	C(42)-C(49)	1.534(11)
C(31)-C(32)	1.414(9)	C(49)-C(50)	1.525(11)
C(31)-C(36)	1.415(9)	C(49)-C(51)	1.536(12)
C(32)-C(33)	1.415(10)	C(49)-H(49)	1.0000
C(32)-C(37)	1.503(12)	C(50)-H(50A)	0.9800
C(32)-C(37A)	1.512(13)	C(50)-H(50B)	0.9800
C(37)-C(42)	1.409(11)	C(50)-H(50C)	0.9800
C(37)-C(38)	1.417(11)	C(51)-H(51A)	0.9800
C(38)-C(39)	1.397(12)	C(51)-H(51B)	0.9800
C(38)-C(43)	1.527(11)	C(51)-H(51C)	0.9800
C(43)-C(45)	1.526(12)	C(37A)-C(42A)	1.412(12)
C(43)-C(44)	1.535(12)	C(37A)-C(38A)	1.417(12)
C(43)-H(43)	1.0000	C(38A)-C(39A)	1.397(14)
C(44)-H(44A)	0.9800	C(38A)-C(43A)	1.526(12)
C(44)-H(44B)	0.9800	C(43A)-C(45A)	1.528(13)
C(44)-H(44C)	0.9800	C(43A)-C(44A)	1.534(13)
C(45)-H(45A)	0.9800	C(43A)-H(43A)	1.0000
C(45)-H(45B)	0.9800	C(44A)-H(44D)	0.9800
C(45)-H(45C)	0.9800	C(44A)-H(44E)	0.9800
C(39)-C(40)	1.389(13)	C(44A)-H(44F)	0.9800

C(45A)-H(45D)	0.9800	C(52)-C(57)	1.423(9)
C(45A)-H(45E)	0.9800	C(53)-C(54)	1.410(10)
C(45A)-H(45F)	0.9800	C(53)-C(58)	1.531(9)
C(39A)-C(40A)	1.384(14)	C(58)-C(59)	1.532(9)
C(39A)-H(39A)	0.9500	C(58)-C(60)	1.539(9)
C(40A)-C(41A)	1.390(15)	C(58)-H(58)	1.0000
C(40A)-C(46A)	1.533(13)	C(59)-H(59A)	0.9800
C(46A)-C(48A)	1.527(13)	C(59)-H(59B)	0.9800
C(46A)-C(47A)	1.540(13)	C(59)-H(59C)	0.9800
C(46A)-H(46A)	1.0000	C(60)-H(60A)	0.9800
C(47A)-H(47D)	0.9800	C(60)-H(60B)	0.9800
C(47A)-H(47E)	0.9800	C(60)-H(60C)	0.9800
C(47A)-H(47F)	0.9800	C(54)-C(55)	1.385(11)
C(48A)-H(48D)	0.9800	C(54)-H(54)	0.9500
C(48A)-H(48E)	0.9800	C(55)-C(56)	1.384(10)
C(48A)-H(48F)	0.9800	C(55)-C(61)	1.528(9)
C(41A)-C(42A)	1.411(14)	C(61)-C(62)	1.535(10)
C(41A)-H(41A)	0.9500	C(61)-C(63)	1.538(10)
C(42A)-C(49A)	1.536(13)	C(61)-H(61)	1.0000
C(49A)-C(50A)	1.527(13)	C(62)-H(62A)	0.9800
C(49A)-C(51A)	1.535(13)	C(62)-H(62B)	0.9800
C(49A)-H(49A)	1.0000	C(62)-H(62C)	0.9800
C(50A)-H(50D)	0.9800	C(63)-H(63A)	0.9800
C(50A)-H(50E)	0.9800	C(63)-H(63B)	0.9800
C(50A)-H(50F)	0.9800	C(63)-H(63C)	0.9800
C(51A)-H(51D)	0.9800	C(56)-C(57)	1.400(10)
C(51A)-H(51E)	0.9800	C(56)-H(56)	0.9500
C(51A)-H(51F)	0.9800	C(57)-C(64)	1.536(9)
C(33)-C(34)	1.393(10)	C(64)-C(66)	1.532(9)
C(33)-H(33)	0.9500	C(64)-C(65)	1.537(9)
C(34)-C(35)	1.381(10)	C(64)-H(64)	1.0000
C(34)-H(34)	0.9500	C(65)-H(65A)	0.9800
C(35)-C(36)	1.418(10)	C(65)-H(65B)	0.9800
C(35)-H(35)	0.9500	C(65)-H(65C)	0.9800
C(36)-C(52)	1.511(10)	C(66)-H(66A)	0.9800
C(52)-C(53)	1.414(9)	C(66)-H(66B)	0.9800

C(66)-H(66C)	0.9800	C(162)-H(16C)	0.9800
N(2)-C(20)	1.404(11)	C(163)-H(16D)	0.9800
N(2)-C(17)	1.405(11)	C(163)-H(16E)	0.9800
C(17)-C(18)	1.366(14)	C(163)-H(16F)	0.9800
C(17)-H(17)	0.9500	C(2)-C(1)-W(1)	80.0(5)
C(18)-C(19)	1.417(13)	C(2)-C(1)-H(1A)	106(6)
C(18)-H(18)	0.9500	W(1)-C(1)-H(1A)	113(5)
C(19)-C(20)	1.353(12)	C(2)-C(1)-H(1B)	100(6)
C(19)-H(19)	0.9500	W(1)-C(1)-H(1B)	143(5)
C(20)-H(20)	0.9500	H(1A)-C(1)-H(1B)	103(5)
N(1)-C(11)	1.389(11)	C(3)-C(2)-C(1)	115.2(7)
C(11)-C(16)	1.411(13)	C(3)-C(2)-W(1)	57.8(4)
C(11)-C(12)	1.441(12)	C(1)-C(2)-W(1)	57.5(4)
C(12)-C(13)	1.406(12)	C(3)-C(2)-H(2A)	110(6)
C(12)-C(121)	1.506(13)	C(1)-C(2)-H(2A)	103(6)
C(13)-C(14)	1.372(15)	W(1)-C(2)-H(2A)	120(5)
C(13)-H(13)	0.9500	C(3)-C(2)-H(2B)	122(6)
C(14)-C(15)	1.394(14)	C(1)-C(2)-H(2B)	100(6)
C(14)-H(14)	0.9500	W(1)-C(2)-H(2B)	133(5)
C(15)-C(16)	1.385(12)	H(2A)-C(2)-H(2B)	104(5)
C(15)-H(15)	0.9500	C(2)-C(3)-W(1)	81.0(6)
C(16)-C(161)	1.531(12)	C(2)-C(3)-H(3A)	117(6)
C(121)-C(123)	1.522(14)	W(1)-C(3)-H(3A)	120(6)
C(121)-C(122)	1.541(13)	C(2)-C(3)-H(3B)	117(6)
C(121)-H(121)	1.0000	W(1)-C(3)-H(3B)	115(6)
C(122)-H(12A)	0.9800	H(3A)-C(3)-H(3B)	106(5)
C(122)-H(12B)	0.9800	N(1)-W(1)-O(1)	177.3(3)
C(122)-H(12C)	0.9800	N(1)-W(1)-C(1)	96.2(4)
C(123)-H(12D)	0.9800	O(1)-W(1)-C(1)	86.5(3)
C(123)-H(12E)	0.9800	N(1)-W(1)-C(3)	93.2(3)
C(123)-H(12F)	0.9800	O(1)-W(1)-C(3)	86.9(3)
C(161)-C(162)	1.526(13)	C(1)-W(1)-C(3)	83.8(4)
C(161)-C(163)	1.555(14)	N(1)-W(1)-N(2)	91.2(3)
C(161)-H(161)	1.0000	O(1)-W(1)-N(2)	86.9(3)
C(162)-H(16A)	0.9800	C(1)-W(1)-N(2)	137.2(4)
C(162)-H(16B)	0.9800	C(3)-W(1)-N(2)	137.9(4)

N(1)-W(1)-C(2)	97.5(3)	C(43)-C(45)-H(45C)	109.5
O(1)-W(1)-C(2)	84.4(3)	H(45A)-C(45)-H(45C)	109.5
C(1)-W(1)-C(2)	42.6(4)	H(45B)-C(45)-H(45C)	109.5
C(3)-W(1)-C(2)	41.2(4)	C(40)-C(39)-C(38)	122.1(12)
N(2)-W(1)-C(2)	171.3(3)	C(40)-C(39)-H(39)	118.9
C(31)-O(1)-W(1)	163.7(4)	C(38)-C(39)-H(39)	118.9
O(1)-C(31)-C(32)	119.8(6)	C(39)-C(40)-C(41)	117.9(10)
O(1)-C(31)-C(36)	119.7(6)	C(39)-C(40)-C(46)	124.7(11)
C(32)-C(31)-C(36)	120.5(7)	C(41)-C(40)-C(46)	117.4(11)
C(31)-C(32)-C(33)	118.5(7)	C(48)-C(46)-C(47)	111.6(16)
C(31)-C(32)-C(37)	124.8(6)	C(48)-C(46)-C(40)	111.0(13)
C(33)-C(32)-C(37)	116.6(6)	C(47)-C(46)-C(40)	113.9(11)
C(31)-C(32)-C(37A)	120.5(6)	C(48)-C(46)-H(46)	106.6
C(33)-C(32)-C(37A)	120.4(6)	C(47)-C(46)-H(46)	106.6
C(37)-C(32)-C(37A)	4.9(9)	C(40)-C(46)-H(46)	106.6
C(42)-C(37)-C(38)	120.1(9)	C(46)-C(47)-H(47A)	109.5
C(42)-C(37)-C(32)	122.0(10)	C(46)-C(47)-H(47B)	109.5
C(38)-C(37)-C(32)	117.9(10)	H(47A)-C(47)-H(47B)	109.5
C(39)-C(38)-C(37)	119.0(10)	C(46)-C(47)-H(47C)	109.5
C(39)-C(38)-C(43)	119.1(11)	H(47A)-C(47)-H(47C)	109.5
C(37)-C(38)-C(43)	121.8(11)	H(47B)-C(47)-H(47C)	109.5
C(45)-C(43)-C(38)	114.2(12)	C(46)-C(48)-H(48A)	109.5
C(45)-C(43)-C(44)	109.6(14)	C(46)-C(48)-H(48B)	109.5
C(38)-C(43)-C(44)	110.2(13)	H(48A)-C(48)-H(48B)	109.5
C(45)-C(43)-H(43)	107.5	C(46)-C(48)-H(48C)	109.5
C(38)-C(43)-H(43)	107.5	H(48A)-C(48)-H(48C)	109.5
C(44)-C(43)-H(43)	107.5	H(48B)-C(48)-H(48C)	109.5
C(43)-C(44)-H(44A)	109.5	C(40)-C(41)-C(42)	122.7(11)
C(43)-C(44)-H(44B)	109.5	C(40)-C(41)-H(41)	118.7
H(44A)-C(44)-H(44B)	109.5	C(42)-C(41)-H(41)	118.7
C(43)-C(44)-H(44C)	109.5	C(41)-C(42)-C(37)	118.1(10)
H(44A)-C(44)-H(44C)	109.5	C(41)-C(42)-C(49)	119.2(10)
H(44B)-C(44)-H(44C)	109.5	C(37)-C(42)-C(49)	122.6(11)
C(43)-C(45)-H(45A)	109.5	C(50)-C(49)-C(42)	111.9(12)
C(43)-C(45)-H(45B)	109.5	C(50)-C(49)-C(51)	110.0(12)
H(45A)-C(45)-H(45B)	109.5	C(42)-C(49)-C(51)	110.6(11)

C(50)-C(49)-H(49)	108.0	C(43A)-C(45A)-H(45F)	109.5
C(42)-C(49)-H(49)	108.0	H(45D)-C(45A)-H(45F)	109.5
C(51)-C(49)-H(49)	108.0	H(45E)-C(45A)-H(45F)	109.5
C(49)-C(50)-H(50A)	109.5	C(40A)-C(39A)-C(38A)	123.6(15)
C(49)-C(50)-H(50B)	109.5	C(40A)-C(39A)-H(39A)	118.2
H(50A)-C(50)-H(50B)	109.5	C(38A)-C(39A)-H(39A)	118.2
C(49)-C(50)-H(50C)	109.5	C(39A)-C(40A)-C(41A)	117.6(13)
H(50A)-C(50)-H(50C)	109.5	C(39A)-C(40A)-C(46A)	122.1(14)
H(50B)-C(50)-H(50C)	109.5	C(41A)-C(40A)-C(46A)	120.3(14)
C(49)-C(51)-H(51A)	109.5	C(48A)-C(46A)-C(40A)	111.1(16)
C(49)-C(51)-H(51B)	109.5	C(48A)-C(46A)-C(47A)	108.9(18)
H(51A)-C(51)-H(51B)	109.5	C(40A)-C(46A)-C(47A)	110.7(14)
C(49)-C(51)-H(51C)	109.5	C(48A)-C(46A)-H(46A)	108.7
H(51A)-C(51)-H(51C)	109.5	C(40A)-C(46A)-H(46A)	108.7
H(51B)-C(51)-H(51C)	109.5	C(47A)-C(46A)-H(46A)	108.7
C(42A)-C(37A)-C(38A)	120.3(12)	C(46A)-C(47A)-H(47D)	109.5
C(42A)-C(37A)-C(32)	121.1(13)	C(46A)-C(47A)-H(47E)	109.5
C(38A)-C(37A)-C(32)	118.6(12)	H(47D)-C(47A)-H(47E)	109.5
C(39A)-C(38A)-C(37A)	117.8(13)	C(46A)-C(47A)-H(47F)	109.5
C(39A)-C(38A)-C(43A)	119.9(14)	H(47D)-C(47A)-H(47F)	109.5
C(37A)-C(38A)-C(43A)	122.3(14)	H(47E)-C(47A)-H(47F)	109.5
C(38A)-C(43A)-C(45A)	115.1(15)	C(46A)-C(48A)-H(48D)	109.5
C(38A)-C(43A)-C(44A)	111.2(17)	C(46A)-C(48A)-H(48E)	109.5
C(45A)-C(43A)-C(44A)	109.2(17)	H(48D)-C(48A)-H(48E)	109.5
C(38A)-C(43A)-H(43A)	107.0	C(46A)-C(48A)-H(48F)	109.5
C(45A)-C(43A)-H(43A)	107.0	H(48D)-C(48A)-H(48F)	109.5
C(44A)-C(43A)-H(43A)	107.0	H(48E)-C(48A)-H(48F)	109.5
C(43A)-C(44A)-H(44D)	109.5	C(40A)-C(41A)-C(42A)	122.1(14)
C(43A)-C(44A)-H(44E)	109.5	C(40A)-C(41A)-H(41A)	119.0
H(44D)-C(44A)-H(44E)	109.5	C(42A)-C(41A)-H(41A)	119.0
C(43A)-C(44A)-H(44F)	109.5	C(41A)-C(42A)-C(37A)	118.6(13)
H(44D)-C(44A)-H(44F)	109.5	C(41A)-C(42A)-C(49A)	119.4(13)
H(44E)-C(44A)-H(44F)	109.5	C(37A)-C(42A)-C(49A)	121.9(13)
C(43A)-C(45A)-H(45D)	109.5	C(50A)-C(49A)-C(51A)	110.5(15)
C(43A)-C(45A)-H(45E)	109.5	C(50A)-C(49A)-C(42A)	111.9(16)
H(45D)-C(45A)-H(45E)	109.5	C(51A)-C(49A)-C(42A)	109.2(14)

C(50A)-C(49A)-H(49A)	108.4	C(53)-C(58)-H(58)	108.6
C(51A)-C(49A)-H(49A)	108.4	C(59)-C(58)-H(58)	108.6
C(42A)-C(49A)-H(49A)	108.4	C(60)-C(58)-H(58)	108.6
C(49A)-C(50A)-H(50D)	109.5	C(58)-C(59)-H(59A)	109.5
C(49A)-C(50A)-H(50E)	109.5	C(58)-C(59)-H(59B)	109.5
H(50D)-C(50A)-H(50E)	109.5	H(59A)-C(59)-H(59B)	109.5
C(49A)-C(50A)-H(50F)	109.5	C(58)-C(59)-H(59C)	109.5
H(50D)-C(50A)-H(50F)	109.5	H(59A)-C(59)-H(59C)	109.5
H(50E)-C(50A)-H(50F)	109.5	H(59B)-C(59)-H(59C)	109.5
C(49A)-C(51A)-H(51D)	109.5	C(58)-C(60)-H(60A)	109.5
C(49A)-C(51A)-H(51E)	109.5	C(58)-C(60)-H(60B)	109.5
H(51D)-C(51A)-H(51E)	109.5	H(60A)-C(60)-H(60B)	109.5
C(49A)-C(51A)-H(51F)	109.5	C(58)-C(60)-H(60C)	109.5
H(51D)-C(51A)-H(51F)	109.5	H(60A)-C(60)-H(60C)	109.5
H(51E)-C(51A)-H(51F)	109.5	H(60B)-C(60)-H(60C)	109.5
C(34)-C(33)-C(32)	121.2(7)	C(55)-C(54)-C(53)	121.7(7)
C(34)-C(33)-H(33)	119.4	C(55)-C(54)-H(54)	119.2
C(32)-C(33)-H(33)	119.4	C(53)-C(54)-H(54)	119.2
C(35)-C(34)-C(33)	119.8(8)	C(56)-C(55)-C(54)	118.8(7)
C(35)-C(34)-H(34)	120.1	C(56)-C(55)-C(61)	121.1(7)
C(33)-C(34)-H(34)	120.1	C(54)-C(55)-C(61)	120.1(7)
C(34)-C(35)-C(36)	121.2(7)	C(55)-C(61)-C(62)	111.4(7)
C(34)-C(35)-H(35)	119.4	C(55)-C(61)-C(63)	110.8(7)
C(36)-C(35)-H(35)	119.4	C(62)-C(61)-C(63)	110.0(9)
C(31)-C(36)-C(35)	118.6(7)	C(55)-C(61)-H(61)	108.2
C(31)-C(36)-C(52)	121.4(6)	C(62)-C(61)-H(61)	108.2
C(35)-C(36)-C(52)	119.9(6)	C(63)-C(61)-H(61)	108.2
C(53)-C(52)-C(57)	120.1(7)	C(61)-C(62)-H(62A)	109.5
C(53)-C(52)-C(36)	121.0(6)	C(61)-C(62)-H(62B)	109.5
C(57)-C(52)-C(36)	118.8(6)	H(62A)-C(62)-H(62B)	109.5
C(54)-C(53)-C(52)	118.7(7)	C(61)-C(62)-H(62C)	109.5
C(54)-C(53)-C(58)	118.1(7)	H(62A)-C(62)-H(62C)	109.5
C(52)-C(53)-C(58)	123.2(7)	H(62B)-C(62)-H(62C)	109.5
C(53)-C(58)-C(59)	112.2(7)	C(61)-C(63)-H(63A)	109.5
C(53)-C(58)-C(60)	110.2(6)	C(61)-C(63)-H(63B)	109.5
C(59)-C(58)-C(60)	108.6(7)	H(63A)-C(63)-H(63B)	109.5

C(61)-C(63)-H(63C)	109.5	C(20)-C(19)-C(18)	106.2(8)
H(63A)-C(63)-H(63C)	109.5	C(20)-C(19)-H(19)	126.9
H(63B)-C(63)-H(63C)	109.5	C(18)-C(19)-H(19)	126.9
C(55)-C(56)-C(57)	122.5(7)	C(19)-C(20)-N(2)	111.9(8)
C(55)-C(56)-H(56)	118.7	C(19)-C(20)-H(20)	124.1
C(57)-C(56)-H(56)	118.7	N(2)-C(20)-H(20)	124.1
C(56)-C(57)-C(52)	118.1(7)	C(11)-N(1)-W(1)	172.4(7)
C(56)-C(57)-C(64)	121.1(7)	N(1)-C(11)-C(16)	119.4(8)
C(52)-C(57)-C(64)	120.8(7)	N(1)-C(11)-C(12)	119.2(8)
C(66)-C(64)-C(57)	113.6(7)	C(16)-C(11)-C(12)	121.3(8)
C(66)-C(64)-C(65)	109.1(7)	C(13)-C(12)-C(11)	115.5(9)
C(57)-C(64)-C(65)	110.9(7)	C(13)-C(12)-C(121)	122.3(8)
C(66)-C(64)-H(64)	107.7	C(11)-C(12)-C(121)	122.2(8)
C(57)-C(64)-H(64)	107.7	C(14)-C(13)-C(12)	123.6(9)
C(65)-C(64)-H(64)	107.7	C(14)-C(13)-H(13)	118.2
C(64)-C(65)-H(65A)	109.5	C(12)-C(13)-H(13)	118.2
C(64)-C(65)-H(65B)	109.5	C(13)-C(14)-C(15)	119.4(8)
H(65A)-C(65)-H(65B)	109.5	C(13)-C(14)-H(14)	120.3
C(64)-C(65)-H(65C)	109.5	C(15)-C(14)-H(14)	120.3
H(65A)-C(65)-H(65C)	109.5	C(16)-C(15)-C(14)	120.9(9)
H(65B)-C(65)-H(65C)	109.5	C(16)-C(15)-H(15)	119.5
C(64)-C(66)-H(66A)	109.5	C(14)-C(15)-H(15)	119.5
C(64)-C(66)-H(66B)	109.5	C(15)-C(16)-C(11)	119.2(8)
H(66A)-C(66)-H(66B)	109.5	C(15)-C(16)-C(161)	121.5(9)
C(64)-C(66)-H(66C)	109.5	C(11)-C(16)-C(161)	119.3(8)
H(66A)-C(66)-H(66C)	109.5	C(12)-C(121)-C(123)	111.5(8)
H(66B)-C(66)-H(66C)	109.5	C(12)-C(121)-C(122)	110.1(8)
C(20)-N(2)-C(17)	103.9(7)	C(123)-C(121)-C(122)	110.9(8)
C(20)-N(2)-W(1)	131.0(6)	C(12)-C(121)-H(121)	108.1
C(17)-N(2)-W(1)	125.0(6)	C(123)-C(121)-H(121)	108.1
C(18)-C(17)-N(2)	110.2(8)	C(122)-C(121)-H(121)	108.1
C(18)-C(17)-H(17)	124.9	C(121)-C(122)-H(12A)	109.5
N(2)-C(17)-H(17)	124.9	C(121)-C(122)-H(12B)	109.5
C(17)-C(18)-C(19)	107.8(8)	H(12A)-C(122)-H(12B)	109.5
C(17)-C(18)-H(18)	126.1	C(121)-C(122)-H(12C)	109.5
C(19)-C(18)-H(18)	126.1	H(12A)-C(122)-H(12C)	109.5

H(12B)-C(122)-H(12C)	109.5
C(121)-C(123)-H(12D)	109.5
C(121)-C(123)-H(12E)	109.5
H(12D)-C(123)-H(12E)	109.5
C(121)-C(123)-H(12F)	109.5
H(12D)-C(123)-H(12F)	109.5
H(12E)-C(123)-H(12F)	109.5
C(162)-C(161)-C(16)	112.1(8)
C(162)-C(161)-C(163)	110.3(8)
C(16)-C(161)-C(163)	114.2(8)
C(162)-C(161)-H(161)	106.6
C(16)-C(161)-H(161)	106.6
C(163)-C(161)-H(161)	106.6
C(161)-C(162)-H(16A)	109.5
C(161)-C(162)-H(16B)	109.5
H(16A)-C(162)-H(16B)	109.5
C(161)-C(162)-H(16C)	109.5
H(16A)-C(162)-H(16C)	109.5
H(16B)-C(162)-H(16C)	109.5
C(161)-C(163)-H(16D)	109.5
C(161)-C(163)-H(16E)	109.5
H(16D)-C(163)-H(16E)	109.5
C(161)-C(163)-H(16F)	109.5
H(16D)-C(163)-H(16F)	109.5
H(16E)-C(163)-H(16F)	109.5

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 09097. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(1)	21(4)	41(5)	21(3)	-3(3)	-1(3)	1(3)
C(2)	20(3)	41(5)	23(4)	-11(3)	-5(3)	8(3)
C(3)	24(4)	34(4)	20(4)	-9(3)	-11(3)	6(3)
W(1)	17(1)	28(1)	10(1)	-2(1)	-3(1)	3(1)
O(1)	23(2)	24(3)	10(3)	3(2)	0(2)	3(2)
C(31)	12(3)	20(3)	17(3)	1(2)	0(2)	5(2)
C(32)	18(3)	30(4)	13(3)	3(2)	2(2)	5(2)
C(37)	18(3)	20(3)	14(2)	1(2)	-1(2)	2(3)
C(38)	21(3)	19(3)	15(3)	1(2)	-1(3)	1(3)
C(43)	26(4)	26(4)	15(3)	0(3)	1(3)	6(3)
C(44)	31(5)	35(10)	26(5)	-8(6)	-1(4)	0(5)
C(45)	27(4)	27(5)	17(11)	-3(11)	-2(6)	8(4)
C(39)	20(5)	34(5)	15(3)	3(3)	-1(3)	8(4)
C(40)	26(6)	32(4)	15(3)	3(3)	-2(4)	8(4)
C(46)	38(7)	42(5)	18(4)	5(3)	-9(5)	11(4)
C(47)	52(8)	41(5)	24(6)	12(4)	-10(5)	15(4)
C(48)	44(10)	51(6)	27(4)	-2(4)	-17(5)	14(5)
C(41)	21(6)	31(5)	12(3)	1(3)	-2(4)	4(5)
C(42)	20(5)	23(4)	14(2)	2(3)	-1(3)	2(4)
C(49)	20(6)	27(5)	11(4)	1(3)	1(4)	2(5)
C(50)	25(12)	31(7)	12(5)	-1(4)	-5(9)	6(9)
C(51)	23(7)	29(7)	28(7)	2(5)	4(9)	0(6)
C(37A)	18(3)	20(3)	14(2)	1(2)	-1(2)	2(3)
C(38A)	21(3)	19(3)	15(3)	1(2)	-1(3)	1(3)
C(43A)	26(4)	26(4)	15(3)	0(3)	1(3)	6(3)
C(44A)	31(5)	35(10)	26(5)	-8(6)	-1(4)	0(5)
C(45A)	27(4)	27(5)	17(11)	-3(11)	-2(6)	8(4)
C(39A)	20(5)	34(5)	15(3)	3(3)	-1(3)	8(4)
C(40A)	26(6)	32(4)	15(3)	3(3)	-2(4)	8(4)
C(46A)	38(7)	42(5)	18(4)	5(3)	-9(5)	11(4)
C(47A)	52(8)	41(5)	24(6)	12(4)	-10(5)	15(4)

C(48A)	44(10)	51(6)	27(4)	-2(4)	-17(5)	14(5)
C(41A)	21(6)	31(5)	12(3)	1(3)	-2(4)	4(5)
C(42A)	20(5)	23(4)	14(2)	2(3)	-1(3)	2(4)
C(49A)	20(6)	27(5)	11(4)	1(3)	1(4)	2(5)
C(50A)	25(12)	31(7)	12(5)	-1(4)	-5(9)	6(9)
C(51A)	23(7)	29(7)	28(7)	2(5)	4(9)	0(6)
C(33)	22(4)	16(4)	19(3)	2(3)	-2(3)	3(3)
C(34)	17(4)	25(4)	25(4)	1(3)	-5(3)	0(3)
C(35)	17(4)	28(4)	12(3)	3(3)	-1(3)	5(3)
C(36)	14(3)	25(3)	12(3)	2(2)	3(2)	8(3)
C(52)	15(3)	31(3)	7(3)	2(2)	-4(2)	2(2)
C(53)	19(3)	25(3)	10(3)	-1(3)	-3(2)	1(3)
C(58)	20(4)	24(4)	18(4)	2(3)	2(3)	0(3)
C(59)	38(6)	20(4)	26(5)	-1(3)	5(4)	2(4)
C(60)	19(4)	29(5)	27(4)	1(3)	1(3)	5(4)
C(54)	22(4)	26(4)	16(4)	3(3)	0(3)	4(3)
C(55)	21(4)	28(3)	13(3)	0(3)	-4(3)	1(3)
C(61)	26(4)	31(4)	30(5)	8(3)	5(3)	4(4)
C(62)	55(8)	36(5)	58(6)	-1(5)	14(6)	-22(5)
C(63)	34(6)	61(7)	45(6)	33(5)	3(4)	2(5)
C(56)	15(3)	31(3)	13(4)	3(3)	0(3)	3(3)
C(57)	16(3)	29(3)	18(4)	2(3)	-1(3)	2(3)
C(64)	23(4)	32(3)	9(4)	-2(3)	1(3)	7(3)
C(65)	29(4)	30(4)	26(5)	0(3)	-4(4)	2(4)
C(66)	24(4)	38(5)	19(4)	2(4)	3(3)	8(3)
N(2)	20(2)	30(4)	13(3)	-1(2)	-3(2)	5(3)
C(17)	28(3)	29(4)	15(4)	-3(3)	1(3)	1(3)
C(18)	29(4)	35(5)	26(4)	-8(3)	-3(3)	12(4)
C(19)	27(3)	22(4)	25(4)	-6(3)	-2(3)	13(3)
C(20)	15(3)	38(5)	18(4)	-6(3)	-3(3)	6(3)
N(1)	18(3)	27(3)	16(3)	2(2)	0(2)	6(3)
C(11)	18(4)	30(4)	14(3)	-4(2)	-5(3)	8(3)
C(12)	24(4)	31(4)	14(3)	-5(2)	-5(3)	10(3)
C(13)	29(5)	43(4)	12(3)	-8(3)	-10(3)	11(3)
C(14)	32(5)	32(4)	23(3)	-15(3)	-11(3)	15(3)
C(15)	21(4)	28(4)	25(3)	-10(3)	-5(3)	8(3)

C(16)	22(4)	26(4)	20(3)	-8(2)	0(3)	10(3)
C(121)	34(5)	38(4)	14(4)	2(3)	1(3)	7(3)
C(122)	47(6)	52(7)	27(5)	4(4)	14(4)	12(5)
C(123)	54(7)	38(5)	30(5)	6(4)	1(5)	15(5)
C(161)	29(4)	30(5)	19(3)	-4(3)	-2(3)	7(3)
C(162)	39(4)	39(6)	25(5)	4(4)	-1(4)	14(4)
C(163)	38(4)	22(5)	32(5)	-6(3)	7(4)	3(4)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for 09097.

	x	y	z	U(eq)
H(1A)	1750(90)	8610(80)	3330(20)	34
H(1B)	170(60)	7910(70)	3080(40)	34
H(2A)	980(100)	9970(60)	2980(30)	34
H(2B)	-460(30)	9160(80)	2690(40)	34
H(3A)	2190(100)	10540(30)	2120(40)	31
H(3B)	960(100)	9660(70)	1760(20)	31
H(43)	3989	11898	3234	27
H(44A)	4354	13701	3666	48
H(44B)	4650	14231	3063	48
H(44C)	5867	13556	3322	48
H(45A)	1751	12646	3392	35
H(45B)	1470	11840	2840	35
H(45C)	1867	13155	2781	35
H(39)	3190	13340	2028	27
H(46)	4885	13675	718	39
H(47A)	2696	14514	700	57
H(47B)	3643	14782	1290	57
H(47C)	2043	13872	1246	57
H(48A)	3661	11887	392	61
H(48B)	2784	12792	141	61
H(48C)	2038	12062	647	61
H(41)	6023	12084	981	26
H(49)	7696	10560	2013	24
H(50A)	7980	9748	1115	34
H(50B)	6929	10519	834	34
H(50C)	6160	9593	1256	34
H(51A)	9897	11376	1490	41
H(51B)	9361	12292	1893	41
H(51C)	8918	12218	1234	41
H(43A)	4235	12049	3307	27

H(44D)	4535	13902	3662	48
H(44E)	4589	14320	3032	48
H(44F)	5959	13756	3270	48
H(45D)	1993	12748	3541	35
H(45E)	1579	11797	3052	35
H(45F)	1788	13072	2902	35
H(39A)	2880	13187	2080	27
H(46A)	2413	13429	1106	39
H(47D)	4030	14455	435	57
H(47E)	5440	13860	599	57
H(47F)	4865	14686	1047	57
H(48D)	2331	12650	176	61
H(48E)	2006	11685	616	61
H(48F)	3692	12010	341	61
H(41A)	5535	11916	973	26
H(49A)	7366	10418	1979	24
H(50D)	7500	9601	1071	34
H(50E)	6487	10418	809	34
H(50F)	5702	9501	1233	34
H(51D)	9022	12164	1843	41
H(51E)	8545	12064	1186	41
H(51F)	9534	11230	1446	41
H(33)	8162	12438	2948	23
H(34)	9122	11817	3776	28
H(35)	7721	10252	4186	22
H(58)	7435	8318	3472	26
H(59A)	7726	6506	3196	43
H(59B)	6006	6666	3015	43
H(59C)	6250	5984	3558	43
H(60A)	9095	7457	4040	37
H(60B)	7652	6992	4429	37
H(60C)	8331	8298	4419	37
H(54)	4779	6370	4261	26
H(61)	1093	6515	4891	35
H(62A)	924	4639	4577	81
H(62B)	2504	4992	4237	81

H(62C)	956	5417	4051	81
H(63A)	2242	5356	5480	71
H(63B)	3162	6616	5561	71
H(63C)	3893	5746	5190	71
H(56)	1763	8353	4630	24
H(64)	3202	10486	3740	26
H(65A)	3792	11819	4500	43
H(65B)	5213	11189	4414	43
H(65C)	4029	10871	4915	43
H(66A)	1102	10925	4253	40
H(66B)	1172	9936	4664	40
H(66C)	661	9666	4014	40
H(17)	3745	6735	1420	29
H(18)	6462	6522	1256	36
H(19)	8268	7824	1957	29
H(20)	6601	8798	2524	29
H(13)	-1	6611	44	33
H(14)	-1609	4976	270	34
H(15)	-1844	4494	1213	30
H(121)	2452	8597	1022	35
H(12A)	3733	7489	431	62
H(12B)	3822	8673	167	62
H(12C)	2590	7617	-88	62
H(12D)	533	8741	49	59
H(12E)	1635	9755	394	59
H(12F)	80	9091	670	59
H(161)	-472	6255	2392	31
H(16A)	984	4422	2158	50
H(16B)	840	4960	2773	50
H(16C)	1898	5660	2317	50
H(16D)	-2928	5054	2188	47
H(16E)	-2052	4620	2706	47
H(16F)	-2076	4029	2094	47

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