Table. Crystal data and structure refinement for Mitocene *trans*-**1**.

Identification code	nik17t	
Empirical formula	C12 H12 N2 O2	
Formula weight	216.24	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 8.2659(9) Å	α= 90°.
	b = 6.2273(6) Å	β= 90.908(2) °.
	c = 10.0103(11) Å	γ = 90°.
Volume	515.21(9) Å ^{3}	
Z	2	
Density (calculated)	1.394 Mg/m^3	
Absorption coefficient	0.097 mm^{-1}	
F(000)	228	
Crystal size	0.2 x 0.1 x 0.025 mm^3	
Theta range for data collection	2.03 to 27.76∞.	
Index ranges	-10<=h<=10, -8<=k<=4, -12<=l<=9	
Reflections collected	3366	
Independent reflections	1731 [R(int) = 0.0877]	
Completeness to theta = 27.76∞	91.6 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1731 / 1 / 145	
Goodness-of-fit on F^2	1.081	
Final R indices [I>2sigma(I)]	R1 = 0.0579, wR2 = 0.1188	
R indices (all data)	R1 = 0.0831, wR2 = 0.1269	
Absolute structure parameter	-3(2)	
Largest diff. peak and hole	0.290 and -0.315 e Å $^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3) for Mitocene *trans*-1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(2)	5088(3)	2600(4)	7364(2)	31(1)
O(1)	4758(3)	7214(4)	7851(2)	38(1)
N(1)	2191(3)	2845(5)	7004(2)	28(1)
C(6)	1929(4)	6200(6)	7987(3)	26(1)
C(7)	3627(4)	5999(6)	7616(3)	28(1)
C(1)	1135(4)	4344(5)	7547(3)	26(1)
C(2)	-529(4)	4125(7)	7710(3)	35(1)
N(2)	2667(4)	5076(6)	4705(3)	40(1)
C(8)	3789(4)	3853(6)	6869(3)	26(1)
C(9)	4024(4)	4004(6)	5385(3)	31(1)
C(5)	1115(4)	7852(6)	8615(3)	35(1)
C(4)	-534(4)	7640(7)	8793(3)	40(1)
C(10)	2767(4)	2709(7)	4710(3)	38(1)
C(12)	5036(4)	2135(6)	8762(3)	36(1)
C(3)	-1332(4)	5796(7)	8333(4)	41(1)
C(11)	1739(4)	1693(6)	5751(3)	36(1)

Table 3. Bond lengths [Å] and angles [°] for Mitocene *trans*-1.

O(2)-C(8)	1.411(4)
O(2)-C(12)	1.430(4)
O(1)-C(7)	1.222(4)
N(1)-C(1)	1.394(4)
N(1)-C(8)	1.471(4)
N(1)-C(11)	1.487(4)
C(6)-C(5)	1.386(5)
C(6)-C(1)	1.397(5)
C(6)-C(7)	1.463(4)
C(7)-C(8)	1.538(5)
C(1)-C(2)	1.395(4)
C(2)-C(3)	1.388(5)
N(2)-C(9)	1.464(4)
N(2)-C(10)	1.476(5)
C(8)-C(9)	1.504(4)
C(9)-C(10)	1.471(5)
C(5)-C(4)	1.384(5)
C(4)-C(3)	1.398(6)
C(10)-C(11)	1.495(5)
C(8)-O(2)-C(12)	114.9(2)
C(1)-N(1)-C(8)	108.6(3)
C(1)-N(1)-C(11)	120.1(3)
C(8)-N(1)-C(11)	110.0(2)
C(5)-C(6)-C(1)	121.9(3)
C(5)-C(6)-C(7)	130.8(3)
C(1)-C(6)-C(7)	107.3(3)
O(1)-C(7)-C(6)	129.2(3)
O(1)-C(7)-C(8)	124.0(3)
C(6)-C(7)-C(8)	106.8(3)
N(1)-C(1)-C(2)	127.2(3)
N(1)-C(1)-C(6)	112.5(3)
C(2)-C(1)-C(6)	120.2(3)
C(3)-C(2)-C(1)	117.3(3)

C(9)-N(2)-C(10)	60.0(2)
O(2)-C(8)-N(1)	114.3(3)
O(2)-C(8)-C(9)	105.8(2)
N(1)-C(8)-C(9)	104.3(2)
O(2)-C(8)-C(7)	112.4(3)
N(1)-C(8)-C(7)	104.0(3)
C(9)-C(8)-C(7)	116.0(3)
N(2)-C(9)-C(10)	60.4(2)
N(2)-C(9)-C(8)	112.2(3)
C(10)-C(9)-C(8)	108.5(3)
C(4)-C(5)-C(6)	118.3(4)
C(5)-C(4)-C(3)	119.8(4)
C(9)-C(10)-N(2)	59.6(2)
C(9)-C(10)-C(11)	108.5(3)
N(2)-C(10)-C(11)	113.1(3)
C(2)-C(3)-C(4)	122.5(3)
N(1)-C(11)-C(10)	104.2(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Mitocene *trans*-1. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(2)	31(1)	34(2)	27(1)	-1(1)	-1(1)	4(1)
O(1)	32(1)	34(1)	49(1)	-12(1)	4(1)	-6(1)
N(1)	28(1)	28(2)	29(1)	-3(1)	0(1)	-6(1)
C(6)	26(2)	29(2)	24(2)	-1(2)	1(1)	-3(2)
C(7)	30(2)	29(2)	25(2)	2(2)	0(1)	-2(2)
C(1)	27(2)	33(2)	19(2)	5(2)	0(1)	-2(2)
C(2)	28(2)	48(2)	30(2)	2(2)	-2(1)	-6(2)
N(2)	38(2)	45(2)	38(2)	9(2)	-6(1)	9(2)
C(8)	23(2)	26(2)	30(2)	-1(2)	1(1)	0(2)
C(9)	30(2)	36(2)	27(2)	-1(2)	3(1)	2(2)
C(5)	35(2)	35(2)	35(2)	-3(2)	2(2)	2(2)
C(4)	39(2)	48(2)	35(2)	2(2)	7(2)	11(2)
C(10)	35(2)	51(3)	29(2)	-11(2)	-6(1)	5(2)
C(12)	43(2)	35(2)	29(2)	1(2)	-5(2)	0(2)
C(3)	23(2)	68(3)	33(2)	12(2)	3(2)	0(2)
C(11)	38(2)	37(2)	35(2)	-8(2)	-6(2)	-5(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Mitocene *trans*-1.

	x	y	z	U(eq)
H(2A)	-1078	2908	7413	42
H(2B)	2172	6235	4473	48
H(9A)	5115	4089	5020	37
H(5A)	1663	9072	8910	42
H(4A)	-1110	8720	9216	49
H(10A)	3013	1930	3887	46
H(12A)	5959	1283	9014	54
H(12B)	4063	1357	8951	54
H(12C)	5050	3454	9258	54
H(3A)	-2443	5685	8450	50
H(11A)	599	1881	5538	44
H(11B)	1970	170	5829	44

Table 6. Torsion angles [°] for Mitocene *trans*-1.

C(5)-C(6)-C(7)-O(1)	4.9(6)
C(1)-C(6)-C(7)-O(1)	-176.9(3)
C(5)-C(6)-C(7)-C(8)	-176.7(3)
C(1)-C(6)-C(7)-C(8)	1.4(3)
C(8)-N(1)-C(1)-C(2)	172.8(3)
C(11)-N(1)-C(1)-C(2)	45.1(4)
C(8)-N(1)-C(1)-C(6)	-9.1(3)
C(11)-N(1)-C(1)-C(6)	-136.9(3)
C(5)-C(6)-C(1)-N(1)	-177.0(3)
C(7)-C(6)-C(1)-N(1)	4.7(3)
C(5)-C(6)-C(1)-C(2)	1.2(5)
C(7)-C(6)-C(1)-C(2)	-177.1(3)
N(1)-C(1)-C(2)-C(3)	177.1(3)
C(6)-C(1)-C(2)-C(3)	-0.8(4)
C(12)-O(2)-C(8)-N(1)	-61.8(3)
C(12)-O(2)-C(8)-C(9)	-176.0(3)
C(12)-O(2)-C(8)-C(7)	56.4(4)
C(1)-N(1)-C(8)-O(2)	132.2(3)
C(11)-N(1)-C(8)-O(2)	-94.5(3)
C(1)-N(1)-C(8)-C(9)	-112.8(3)
C(11)-N(1)-C(8)-C(9)	20.5(3)
C(1)-N(1)-C(8)-C(7)	9.2(3)
C(11)-N(1)-C(8)-C(7)	142.5(3)
O(1)-C(7)-C(8)-O(2)	47.9(4)
C(6)-C(7)-C(8)-O(2)	-130.6(3)
O(1)-C(7)-C(8)-N(1)	172.0(3)
C(6)-C(7)-C(8)-N(1)	-6.5(3)
O(1)-C(7)-C(8)-C(9)	-74.1(4)
C(6)-C(7)-C(8)-C(9)	107.5(3)
C(10)-N(2)-C(9)-C(8)	-99.4(3)
O(2)-C(8)-C(9)-N(2)	173.9(3)
N(1)-C(8)-C(9)-N(2)	53.1(4)
C(7)-C(8)-C(9)-N(2)	-60.7(4)
O(2)-C(8)-C(9)-C(10)	109.2(3)

N(1)-C(8)-C(9)-C(10)	-11.7(4)
C(7)-C(8)-C(9)-C(10)	-125.5(3)
C(1)-C(6)-C(5)-C(4)	-0.6(5)
C(7)-C(6)-C(5)-C(4)	177.3(3)
C(6)-C(5)-C(4)-C(3)	-0.4(5)
C(8)-C(9)-C(10)-N(2)	105.5(3)
N(2)-C(9)-C(10)-C(11)	-106.5(3)
C(8)-C(9)-C(10)-C(11)	-0.9(4)
C(9)-N(2)-C(10)-C(11)	98.6(3)
C(1)-C(2)-C(3)-C(4)	-0.2(5)
C(5)-C(4)-C(3)-C(2)	0.8(5)
C(1)-N(1)-C(11)-C(10)	106.0(3)
C(8)-N(1)-C(11)-C(10)	-21.1(4)
C(9)-C(10)-C(11)-N(1)	13.0(4)
N(2)-C(10)-C(11)-N(1)	-51.0(4)

Symmetry transformations used to generate equivalent atoms: