Chiral Tridentate Bis(oxazol-2-yliomino) Isoindoline-based Pincer Ligands: Isolation and Characterization via Deligation from *In-Situ* Prepared Cd-Ligand Complexes.

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Electronic Supplementary Material

XRD data for Cd((*R*,*R*)-**5**)$_2$

Table 1. Crystal data and structure refinement for Cd((R,R)-**5**)$_2$.

Identification code	daley04_0m_sq	
Empirical formula	C52 H40 Cd N10 O4	
Formula weight	981.34	
Temperature	150.0 K	
Wavelength	0.71073 Å	
Crystal system	Trigonal	
Space group	P 31 2 1	
Unit cell dimensions	a = 19.2930(15) Å	α= 90°.
	b = 19.293 Å	β= 90°.
	c = 11.7970(9) Å	γ = 120°.
Volume	3802.8(7) Å^3	
Z	3	
Density (calculated)	1.286 Mg/m^3	
Absorption coefficient	0.484 mm^{-1}	
F(000)	1506	
Crystal size	0.33 x 0.1 x 0.06 mm^3	
Theta range for data collection	1.726 to 25.392°.	
Index ranges	-23<=h<=23, -22<=k<=23, -13<=l<=14	
Reflections collected	32483	
Independent reflections	4673 [R(int) = 0.0509]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.895	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4673 / 1 / 305	
Goodness-of-fit on F^2	0.989	
Final R indices [I>2sigma(I)]	R1 = 0.0309, wR2 = 0.0684	
R indices (all data)	R1 = 0.0390, wR2 = 0.0709	
Absolute structure parameter	-0.009(11)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.286 and -0.238 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Cd((R,R)-**5**)$_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4048(4)	8817(4)	6632(5)	68(2)
C(2)	3491(5)	7959(4)	6541(5)	65(2)
C(3)	3896(3)	8339(3)	8332(4)	45(1)
C(4)	4424(4)	8589(3)	10175(4)	39(1)
C(5)	4337(4)	8369(3)	11383(4)	37(1)
C(6)	3711(4)	7784(4)	11995(5)	50(2)
C(7)	3807(4)	7746(4)	13149(5)	52(2)
C(8)	4517(4)	8290(4)	13671(4)	57(2)
C(9)	5151(4)	8884(3)	13069(4)	46(1)
C(10)	5036(3)	8911(3)	11903(4)	37(1)
C(11)	5540(3)	9475(3)	11005(4)	39(1)
C(12)	6729(3)	10665(4)	10514(4)	47(1)
C(13)	7826(4)	11836(4)	10155(6)	71(2)
C(14)	7357(4)	11492(4)	9075(5)	57(2)
C(18)	2546(6)	9955(7)	5985(7)	79(4)
C(17)	2380(6)	9454(8)	6915(7)	129(9)
C(16)	2861(6)	9124(7)	7148(7)	102(5)
C(15)	3508(5)	9295(6)	6451(7)	57(2)
C(20)	3674(5)	9796(5)	5520(6)	57(2)
C(19)	3193(6)	10126(5)	5287(6)	53(4)
C(15B)	3773(7)	9374(6)	6129(8)	57(2)
C(20B)	4018(6)	9714(6)	5060(7)	57(2)
C(19B)	3704(7)	10161(6)	4595(7)	65(5)
C(18B)	3145(9)	10267(8)	5198(10)	79(4)
C(17B)	2900(8)	9927(9)	6266(9)	87(6)
C(16B)	3214(7)	9480(8)	6731(8)	102(5)
C(21)	7809(4)	11441(4)	8078(5)	60(2)
C(22)	8189(4)	11008(4)	8155(7)	74(2)
C(23)	8635(6)	10951(6)	7250(9)	101(3)
C(24)	8690(6)	11364(6)	6285(8)	94(3)
C(25)	8318(5)	11818(7)	6166(7)	92(3)
C(26)	7862(4)	11835(5)	7072(5)	75(2)
Cd(1)	5565(1)	10000	8333	45(1)
N(1)	4302(3)	8998(3)	7815(3)	51(1)
N(2)	3859(3)	8136(3)	9469(4)	44(1)
N(3)	5148(3)	9260(2)	9987(3)	38(1)
N(4)	6245(3)	10088(3)	11267(3)	44(1)
N(5)	6698(3)	10706(3)	9430(4)	50(1)
O(1)	3371(2)	7681(3)	7717(3)	53(1)
O(2)	7359(3)	11283(3)	11039(3)	66(1)

Table 3. Bond lengths [Å] and angles [°] for Cd((R,R)-**5**)$_2$.

C(1)-C(2)	1.458(9)	C(17B)-C(16B)	1.3900
C(1)-C(15)	1.717(9)	C(21)-C(22)	1.363(10)
C(1)-C(15B)	1.5364(14)	C(21)-C(26)	1.386(10)
C(1)-N(1)	1.463(7)	C(22)-C(23)	1.409(12)
C(2)-O(1)	1.464(7)	C(23)-C(24)	1.363(13)
C(3)-N(1)	1.268(7)	C(24)-C(25)	1.389(13)
C(3)-N(2)	1.389(7)	C(25)-C(26)	1.395(10)
C(3)-O(1)	1.370(7)	Cd(1)-N(1)#1	2.311(5)
C(4)-C(5)	1.472(7)	Cd(1)-N(1)	2.311(5)
C(4)-N(2)	1.301(7)	Cd(1)-N(3)#1	2.312(4)
C(4)-N(3)	1.367(7)	Cd(1)-N(3)	2.312(4)
C(5)-C(6)	1.375(8)	Cd(1)-N(5)	2.308(5)
C(5)-C(10)	1.371(8)	Cd(1)-N(5)#1	2.308(5)
C(6)-C(7)	1.382(7)		
C(7)-C(8)	1.385(9)	C(2)-C(1)-C(15)	107.4(6)
C(8)-C(9)	1.384(8)	C(2)-C(1)-C(15B)	116.6(7)
C(9)-C(10)	1.398(6)	C(2)-C(1)-N(1)	108.1(5)
C(10)-C(11)	1.481(7)	N(1)-C(1)-C(15)	102.2(6)
C(11)-N(3)	1.369(6)	N(1)-C(1)-C(15B)	113.1(6)
C(11)-N(4)	1.317(7)	C(1)-C(2)-O(1)	103.8(5)
C(12)-N(4)	1.364(8)	N(1)-C(3)-N(2)	131.8(5)
C(12)-N(5)	1.285(6)	N(1)-C(3)-O(1)	118.3(4)
C(12)-O(2)	1.354(7)	O(1)-C(3)-N(2)	109.9(5)
C(13)-C(14)	1.510(9)	N(2)-C(4)-C(5)	119.3(5)
C(13)-O(2)	1.441(8)	N(2)-C(4)-N(3)	130.4(5)
C(14)-C(21)	1.497(8)	N(3)-C(4)-C(5)	110.2(5)
C(14)-N(5)	1.470(8)	C(6)-C(5)-C(4)	132.2(5)
C(18)-C(17)	1.3900	C(10)-C(5)-C(4)	106.7(5)
C(18)-C(19)	1.3900	C(10)-C(5)-C(6)	121.1(5)
C(17)-C(16)	1.3900	C(5)-C(6)-C(7)	118.3(6)
C(16)-C(15)	1.3900	C(6)-C(7)-C(8)	120.4(5)
C(15)-C(20)	1.3900	C(9)-C(8)-C(7)	122.0(5)
C(20)-C(19)	1.3900	C(8)-C(9)-C(10)	116.4(5)
C(15B)-C(20B)	1.3900	C(5)-C(10)-C(9)	121.7(5)
C(15B)-C(16B)	1.3900	C(5)-C(10)-C(11)	105.9(4)
C(20B)-C(19B)	1.3900	C(9)-C(10)-C(11)	132.3(5)
C(19B)-C(18B)	1.3900	N(3)-C(11)-C(10)	110.2(5)
C(18B)-C(17B)	1.3900	N(4)-C(11)-C(10)	119.7(4)

N(4)-C(11)-N(3)	130.1(5)
N(5)-C(12)-N(4)	131.6(6)
N(5)-C(12)-O(2)	116.7(6)
O(2)-C(12)-N(4)	111.6(4)
O(2)-C(13)-C(14)	105.7(5)
C(21)-C(14)-C(13)	116.8(6)
N(5)-C(14)-C(13)	103.4(5)
N(5)-C(14)-C(21)	112.8(5)
C(17)-C(18)-C(19)	120.0
C(16)-C(17)-C(18)	120.0
C(15)-C(16)-C(17)	120.0
C(16)-C(15)-C(1)	120.9(5)
C(16)-C(15)-C(20)	120.0
C(20)-C(15)-C(1)	118.8(5)
C(15)-C(20)-C(19)	120.0
C(20)-C(19)-C(18)	120.0
C(20B)-C(15B)-C(1)	121.7(6)
C(20B)-C(15B)-C(16B)	120.0
C(16B)-C(15B)-C(1)	118.1(6)
C(15B)-C(20B)-C(19B)	120.0
C(18B)-C(19B)-C(20B)	120.0
C(19B)-C(18B)-C(17B)	120.0
C(18B)-C(17B)-C(16B)	120.0
C(17B)-C(16B)-C(15B)	120.0
C(22)-C(21)-C(14)	119.9(7)
C(22)-C(21)-C(26)	118.6(7)
C(26)-C(21)-C(14)	121.5(7)
C(21)-C(22)-C(23)	122.3(9)
C(24)-C(23)-C(22)	117.4(10)
C(23)-C(24)-C(25)	122.6(8)
C(24)-C(25)-C(26)	117.9(8)
C(21)-C(26)-C(25)	121.2(8)
N(1)-Cd(1)-N(1)#1	100.9(3)
N(1)-Cd(1)-N(3)	79.08(15)
N(1)-Cd(1)-N(3)#1	97.98(15)
N(1)#1-Cd(1)-N(3)	97.98(15)
N(1)#1-Cd(1)-N(3)#1	79.08(15)
N(3)#1-Cd(1)-N(3)	175.4(2)
N(5)-Cd(1)-N(1)#1	84.04(19)
N(5)#1-Cd(1)-N(1)#1	158.98(15)
N(5)-Cd(1)-N(1)	158.98(15)
N(5)#1-Cd(1)-N(1)	84.04(19)
N(5)-Cd(1)-N(3)#1	103.03(16)
N(5)#1-Cd(1)-N(3)	103.03(16)
N(5)-Cd(1)-N(3)	80.00(16)
N(5)#1-Cd(1)-N(3)#1	80.00(16)
N(5)#1-Cd(1)-N(5)	98.7(3)
C(1)-N(1)-Cd(1)	122.7(4)
C(3)-N(1)-C(1)	104.7(5)
C(3)-N(1)-Cd(1)	125.2(4)
C(4)-N(2)-C(3)	121.4(5)
C(4)-N(3)-C(11)	107.0(4)
C(4)-N(3)-Cd(1)	126.7(3)
C(11)-N(3)-Cd(1)	125.8(3)
C(11)-N(4)-C(12)	124.0(4)
C(12)-N(5)-C(14)	107.7(5)
C(12)-N(5)-Cd(1)	125.5(4)
C(14)-N(5)-Cd(1)	121.6(4)
C(3)-O(1)-C(2)	104.7(5)
C(12)-O(2)-C(13)	105.9(5)

Symmetry transformations used to generate equivalent atoms:

#1 x-y+1,-y+2,-z+5/3

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Cd((R,R)-**5**)$_2$. 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}
C(1)	70(4)	88(5)	29(3)	10(3)	-11(3)	28(4)
C(2)	98(5)	73(5)	19(3)	3(3)	-3(3)	39(4)
C(3)	48(3)	60(4)	23(2)	-3(3)	-8(3)	25(3)
C(4)	49(3)	53(3)	22(2)	-2(2)	-7(3)	30(3)
C(5)	47(3)	41(3)	28(3)	-1(2)	-1(2)	27(3)
C(6)	50(3)	66(4)	31(3)	6(3)	1(3)	26(3)
C(7)	61(4)	55(4)	31(3)	8(3)	0(3)	22(3)
C(8)	90(5)	56(4)	16(2)	7(2)	-3(3)	30(4)
C(9)	63(4)	46(3)	22(3)	3(2)	-4(2)	22(3)
C(10)	50(3)	47(3)	19(2)	0(2)	2(2)	29(3)
C(11)	50(3)	51(3)	22(2)	-6(2)	-1(2)	32(3)
C(12)	49(3)	59(4)	34(3)	-10(3)	2(2)	28(3)
C(13)	68(4)	71(4)	44(4)	-13(3)	11(3)	12(3)
C(14)	61(4)	57(4)	35(3)	2(3)	13(3)	17(3)
C(18)	132(12)	102(9)	49(6)	-15(7)	-34(7)	95(10)
C(17)	151(18)	240(20)	65(11)	81(14)	55(12)	147(19)
C(16)	127(14)	156(15)	58(9)	55(8)	18(7)	97(12)
C(15)	61(5)	57(3)	24(4)	9(3)	-5(3)	6(4)
C(20)	61(5)	57(3)	24(4)	9(3)	-5(3)	6(4)
C(19)	79(10)	39(7)	58(9)	-3(6)	-23(8)	42(7)
C(15B)	61(5)	57(3)	24(4)	9(3)	-5(3)	6(4)
C(20B)	61(5)	57(3)	24(4)	9(3)	-5(3)	6(4)
C(19B)	103(12)	33(8)	53(8)	-3(6)	-37(9)	28(8)
C(18B)	132(12)	102(9)	49(6)	-15(7)	-34(7)	95(10)
C(17B)	118(17)	124(16)	66(12)	-21(13)	-37(12)	96(15)
C(16B)	127(14)	156(15)	58(9)	55(8)	18(7)	97(12)
C(21)	44(4)	69(4)	43(3)	-12(3)	7(3)	11(3)
C(22)	59(4)	68(4)	69(5)	4(4)	18(4)	12(4)
C(23)	91(7)	100(7)	101(7)	-20(6)	21(6)	39(6)
C(24)	81(6)	103(7)	66(5)	-25(5)	29(4)	21(5)
C(25)	67(6)	136(8)	41(4)	0(4)	9(4)	26(6)
C(26)	48(4)	112(6)	38(4)	4(4)	6(3)	19(4)
Cd(1)	58(1)	56(1)	19(1)	3(1)	2(1)	28(1)
N(1)	62(3)	63(3)	23(2)	10(2)	-4(2)	27(3)
N(2)	50(3)	58(3)	23(2)	5(2)	4(2)	26(3)
N(3)	47(3)	51(2)	18(2)	-3(2)	0(2)	27(2)
N(4)	50(3)	58(3)	21(2)	-1(2)	1(2)	25(3)
N(5)	50(3)	64(4)	22(2)	-1(2)	6(2)	18(3)
O(1)	65(3)	64(3)	21(2)	1(2)	-8(2)	25(2)
O(2)	67(3)	66(3)	32(2)	-9(2)	5(2)	9(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Cd((R,R)-5)2.

	x	y	z	U(eq)
H(1A)	4509	9009	6094	81
H(1B)	4535	8922	6194	81
H(2A)	3722	7695	6082	78
H(2B)	2980	7853	6194	78
H(6)	3224	7416	11633	60
H(7)	3384	7344	13588	62
H(8)	4570	8254	14466	68
H(9)	5639	9254	13428	55
H(13A)	8360	11884	10099	85
H(13B)	7897	12373	10307	85
H(14)	7120	11830	8851	68
H(18)	2217	10181	5826	94
H(17)	1938	9338	7392	154
H(16)	2747	8782	7784	123
H(20)	4116	9913	5043	69
H(19)	3306	10468	4651	64
H(20B)	4400	9641	4648	69
H(19B)	3872	10393	3865	78
H(18B)	2931	10572	4880	94
H(17B)	2518	10000	6678	105
H(16B)	3046	9248	7461	123
H(22)	8153	10735	8842	89
H(23)	8888	10638	7310	122
H(24)	8994	11340	5669	113
H(25)	8373	12108	5489	111
H(26)	7584	12123	6998	91

XRD data for Cd((*S*,*S*)-**6**)$_2$

Table 1. Crystal data and structure refinement for Cd((S,S)-**6**)$_2$.

Identification code	daley05_sq	
Empirical formula	C40 H48 Cd N10 O4	
Formula weight	845.28	
Temperature	120.0 K	
Wavelength	0.71073 Å	
Crystal system	Trigonal	
Space group	P 32 2 1	
Unit cell dimensions	a = 19.1032(14) Å	α= 90°.
	b = 19.1032 Å	β= 90°.
	c = 11.8529(9) Å	γ = 120°.
Volume	3746.0(6) Å^3	
Z	3	
Density (calculated)	1.124 Mg/m^3	
Absorption coefficient	0.480 mm^{-1}	
F(000)	1314	
Crystal size	0.453 x 0.157 x 0.155 mm^3	
Theta range for data collection	1.231 to 27.490°.	
Index ranges	-24<=h<=24, -20<=k<=24, -15<=l<=14	
Reflections collected	25490	
Independent reflections	5594 [R(int) = 0.0285]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.477 and 0.400	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5594 / 0 / 253	
Goodness-of-fit on F^2	1.060	
Final R indices [I>2sigma(I)]	R1 = 0.0249, wR2 = 0.0629	
R indices (all data)	R1 = 0.0271, wR2 = 0.0642	
Absolute structure parameter	-0.002(7)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.639 and -0.336 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Cd((S,S)-**6**)$_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	5927(2)	1120(2)	3412(2)	34(1)
C(2)	6455(2)	2032(2)	3496(2)	38(1)
C(3)	6071(2)	1672(2)	1711(2)	27(1)
C(4)	5555(2)	1431(2)	-132(2)	26(1)
C(5)	5667(2)	1653(2)	-1340(2)	27(1)
C(6)	6320(2)	2258(2)	-1925(2)	30(1)
C(7)	6237(2)	2286(2)	-3092(2)	33(1)
C(8)	5528(2)	1738(2)	-3631(2)	35(1)
C(9)	4869(2)	1130(2)	-3047(2)	33(1)
C(10)	4963(2)	1104(1)	-1885(2)	27(1)
C(11)	4429(2)	534(2)	-1009(2)	29(1)
C(12)	3235(2)	-655(2)	-551(2)	34(1)
C(13)	2187(2)	-1910(2)	-248(3)	52(1)
C(14)	2548(2)	-1493(2)	879(3)	40(1)
C(15)	6323(3)	623(3)	3692(3)	56(1)
C(16)	7040(3)	831(4)	2966(4)	81(2)
C(17)	6519(4)	692(3)	4965(3)	72(1)
C(18)	1963(3)	-1402(3)	1655(4)	65(1)
C(19)	1339(4)	-2227(3)	2110(5)	107(2)
C(20)	1552(4)	-992(4)	1065(7)	121(3)
N(1)	5652(2)	1003(1)	2225(2)	32(1)
N(2)	6120(1)	1875(1)	585(2)	28(1)
N(3)	4809(2)	759(1)	28(2)	28(1)
N(4)	3728(2)	-80(1)	-1294(2)	33(1)
N(5)	3234(2)	-697(1)	533(2)	33(1)
O(1)	6609(1)	2310(1)	2333(2)	35(1)
O(2)	2642(2)	-1315(1)	-1099(2)	48(1)
Cd(1)	4365(1)	0	1667	28(1)

Table 3. Bond lengths [Å] and angles [°] for Cd((S,S)-**6**)$_2$.

C(1)-C(2)	1.518(4)	N(1)-C(3)-N(2)	131.7(3)
C(1)-C(15)	1.517(5)	N(1)-C(3)-O(1)	117.2(2)
C(1)-N(1)	1.480(3)	O(1)-C(3)-N(2)	111.1(2)
C(2)-O(1)	1.453(3)	N(2)-C(4)-C(5)	119.5(2)
C(3)-N(1)	1.273(4)	N(2)-C(4)-N(3)	130.9(2)
C(3)-N(2)	1.380(3)	N(3)-C(4)-C(5)	109.6(2)
C(3)-O(1)	1.354(3)	C(6)-C(5)-C(4)	131.6(3)
C(4)-C(5)	1.478(3)	C(10)-C(5)-C(4)	106.7(2)
C(4)-N(2)	1.301(3)	C(10)-C(5)-C(6)	121.7(2)
C(4)-N(3)	1.373(3)	C(5)-C(6)-C(7)	117.0(3)
C(5)-C(6)	1.389(4)	C(8)-C(7)-C(6)	121.0(3)
C(5)-C(10)	1.384(4)	C(7)-C(8)-C(9)	122.2(3)
C(6)-C(7)	1.398(4)	C(10)-C(9)-C(8)	116.2(3)
C(7)-C(8)	1.386(4)	C(5)-C(10)-C(9)	121.9(2)
C(8)-C(9)	1.395(4)	C(5)-C(10)-C(11)	106.3(2)
C(9)-C(10)	1.393(3)	C(9)-C(10)-C(11)	131.8(3)
C(10)-C(11)	1.482(4)	N(3)-C(11)-C(10)	109.4(2)
C(11)-N(3)	1.382(3)	N(4)-C(11)-C(10)	119.8(2)
C(11)-N(4)	1.309(3)	N(4)-C(11)-N(3)	130.7(2)
C(12)-N(4)	1.355(4)	N(4)-C(12)-O(2)	111.0(2)
C(12)-N(5)	1.287(3)	N(5)-C(12)-N(4)	132.8(3)
C(12)-O(2)	1.368(3)	N(5)-C(12)-O(2)	116.2(3)
C(13)-C(14)	1.530(5)	O(2)-C(13)-C(14)	105.3(2)
C(13)-O(2)	1.441(4)	C(18)-C(14)-C(13)	114.9(3)
C(14)-C(18)	1.524(5)	N(5)-C(14)-C(13)	103.3(2)
C(14)-N(5)	1.484(4)	N(5)-C(14)-C(18)	111.9(3)
C(15)-C(16)	1.494(6)	C(1)-C(15)-C(17)	109.6(3)
C(15)-C(17)	1.543(5)	C(16)-C(15)-C(1)	112.6(3)
C(18)-C(19)	1.522(6)	C(16)-C(15)-C(17)	112.9(4)
C(18)-C(20)	1.528(8)	C(14)-C(18)-C(20)	112.1(4)
N(1)-Cd(1)	2.333(3)	C(19)-C(18)-C(14)	109.6(4)
N(3)-Cd(1)	2.316(2)	C(19)-C(18)-C(20)	110.9(5)
N(5)-Cd(1)	2.317(2)	C(1)-N(1)-Cd(1)	122.85(18)
		C(3)-N(1)-C(1)	107.8(2)
C(15)-C(1)-C(2)	116.8(3)	C(3)-N(1)-Cd(1)	124.40(19)
N(1)-C(1)-C(2)	102.6(2)	C(4)-N(2)-C(3)	122.1(2)
N(1)-C(1)-C(15)	111.4(2)	C(4)-N(3)-C(11)	107.8(2)
O(1)-C(2)-C(1)	104.7(2)	C(4)-N(3)-Cd(1)	125.81(17)

C(11)-N(3)-Cd(1)	125.44(17)
C(11)-N(4)-C(12)	122.9(2)
C(12)-N(5)-C(14)	108.2(2)
C(12)-N(5)-Cd(1)	124.8(2)
C(14)-N(5)-Cd(1)	121.35(19)
C(3)-O(1)-C(2)	105.3(2)
C(12)-O(2)-C(13)	106.8(2)
N(1)-Cd(1)-N(1)#1	99.97(13)
N(3)#1-Cd(1)-N(1)#1	79.50(8)
N(3)#1-Cd(1)-N(1)	96.53(8)
N(3)-Cd(1)-N(1)	79.50(8)
N(3)-Cd(1)-N(1)#1	96.53(8)
N(3)#1-Cd(1)-N(3)	173.90(13)
N(3)#1-Cd(1)-N(5)	104.53(8)
N(3)-Cd(1)-N(5)#1	104.53(8)
N(3)-Cd(1)-N(5)	79.50(8)
N(3)#1-Cd(1)-N(5)#1	79.50(8)
N(5)-Cd(1)-N(1)#1	84.03(9)
N(5)#1-Cd(1)-N(1)#1	158.94(8)
N(5)-Cd(1)-N(1)	158.94(8)
N(5)#1-Cd(1)-N(1)	84.03(9)
N(5)#1-Cd(1)-N(5)	99.70(13)

Symmetry transformations used to generate equivalent atoms:

#1 x-y,-y,-z+1/3

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Cd((S,S)-**6**)$_2$. 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}
C(1)	45(2)	33(2)	17(1)	-1(1)	-3(1)	15(1)
C(2)	53(2)	33(2)	17(1)	3(1)	-5(1)	12(1)
C(3)	32(1)	26(1)	18(1)	-2(1)	-2(1)	11(1)
C(4)	36(2)	24(1)	15(1)	2(1)	1(1)	14(1)
C(5)	38(2)	27(1)	16(1)	2(1)	1(1)	17(1)
C(6)	37(2)	30(1)	22(1)	5(1)	5(1)	17(1)
C(7)	48(2)	33(1)	20(1)	9(1)	9(1)	22(1)
C(8)	57(2)	34(2)	14(1)	5(1)	6(1)	23(1)
C(9)	50(2)	25(1)	19(1)	-1(1)	-1(1)	15(1)
C(10)	40(2)	21(1)	18(1)	3(1)	5(1)	14(1)
C(11)	44(2)	22(1)	15(1)	1(1)	1(1)	12(1)
C(12)	41(2)	26(1)	24(1)	-4(1)	-5(1)	8(1)
C(13)	55(2)	32(2)	40(2)	-1(1)	3(2)	-1(2)
C(14)	40(2)	30(2)	31(2)	7(1)	7(1)	5(1)
C(15)	94(3)	61(2)	27(2)	0(2)	-12(2)	50(2)
C(16)	91(4)	118(4)	64(3)	6(3)	-1(3)	74(4)
C(17)	128(4)	79(3)	36(2)	-8(2)	-28(2)	72(3)
C(18)	58(2)	57(2)	66(3)	0(2)	22(2)	17(2)
C(19)	94(4)	76(4)	129(5)	38(3)	71(4)	27(3)
C(20)	89(4)	94(4)	175(8)	14(5)	48(5)	42(4)
N(1)	47(1)	29(1)	15(1)	1(1)	-3(1)	14(1)
N(2)	33(1)	27(1)	18(1)	3(1)	1(1)	11(1)
N(3)	36(1)	25(1)	14(1)	0(1)	0(1)	9(1)
N(4)	44(2)	24(1)	19(1)	0(1)	-4(1)	9(1)
N(5)	40(1)	27(1)	22(1)	3(1)	3(1)	8(1)
O(1)	42(1)	30(1)	18(1)	3(1)	-4(1)	6(1)
O(2)	52(1)	30(1)	30(1)	-3(1)	-3(1)	-2(1)
Cd(1)	42(1)	20(1)	13(1)	1(1)	1(1)	10(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Cd((S,S)-**6**)$_2$.

	x	y	z	U(eq)
H(1)	5447	943	3914	40
H(2A)	6170	2268	3906	46
H(2B)	6966	2181	3893	46
H(6)	6801	2636	-1547	36
H(7)	6672	2688	-3523	39
H(8)	5488	1777	-4425	42
H(9)	4385	756	-3421	40
H(13A)	2244	-2394	-342	62
H(13B)	1607	-2076	-291	62
H(14)	2766	-1803	1284	47
H(15)	5914	45	3539	67
H(16A)	6894	823	2171	122
H(16B)	7216	435	3087	122
H(16C)	7481	1372	3163	122
H(17A)	6695	307	5166	109
H(17B)	6035	572	5399	109
H(17C)	6951	1242	5136	109
H(18)	2277	-1056	2309	79
H(19A)	1088	-2604	1481	160
H(19B)	923	-2178	2529	160
H(19C)	1605	-2429	2614	160
H(20A)	1149	-1371	530	182
H(20B)	1958	-514	657	182
H(20C)	1285	-828	1627	182

XRD data for (*R*,*R*)-**5**H

Table 1. Crystal data and structure refinement for (R,R)-**5**H.

Identification code	daley10	
Empirical formula	C26 H21 N5 O2	
Formula weight	435.48	
Temperature	120.0 K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 6.1731(2) Å	α= 90°.
	b = 9.1085(3) Å	β= 90°.
	c = 37.2539(12) Å	γ = 90°.
Volume	2094.70(12) Å^3	
Z	4	
Density (calculated)	1.381 Mg/m^3	
Absorption coefficient	0.730 mm^{-1}	
F(000)	912	
Crystal size	0.35 x 0.25 x 0.12 mm^3	
Theta range for data collection	4.748 to 64.541°.	
Index ranges	-7<=h<=7, -10<=k<=9, -42<=l<=42	
Reflections collected	6476	
Independent reflections	3056 [R(int) = 0.0298]	
Completeness to theta = 64.541°	97.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9175 and 0.7841	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3056 / 0 / 299	
Goodness-of-fit on F^2	1.098	
Final R indices [I>2sigma(I)]	R1 = 0.0533, wR2 = 0.1262	
R indices (all data)	R1 = 0.0591, wR2 = 0.1293	
Absolute structure parameter	0.7(2)	
Extinction coefficient	0.0010(3)	
Largest diff. peak and hole	0.389 and -0.180 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for (R,R)-**5**H. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	10196(8)	2295(5)	640(1)	34(1)
C(2)	10594(8)	3753(5)	554(1)	40(1)
C(3)	9081(9)	4560(5)	370(1)	42(1)
C(4)	7143(9)	3901(5)	270(1)	42(1)
C(5)	6745(8)	2458(5)	356(1)	35(1)
C(6)	8250(7)	1638(5)	544(1)	27(1)
C(7)	7783(8)	48(5)	633(1)	31(1)
C(8)	7930(8)	-1008(5)	310(1)	36(1)
C(9)	10576(7)	-1451(5)	701(1)	30(1)
C(10)	13004(8)	-2130(4)	1133(1)	31(1)
C(11)	14906(7)	-2895(4)	1282(1)	31(1)
C(12)	16412(8)	-3788(5)	1120(1)	41(1)
C(13)	18053(9)	-4352(6)	1332(1)	45(1)
C(14)	18154(9)	-4048(6)	1696(1)	49(1)
C(15)	16630(8)	-3144(5)	1860(1)	42(1)
C(16)	15021(8)	-2581(4)	1646(1)	32(1)
C(17)	13154(8)	-1634(4)	1733(1)	30(1)
C(18)	10935(8)	-244(5)	2088(1)	33(1)
C(19)	8280(9)	763(6)	2398(1)	49(1)
C(20)	8671(8)	1564(6)	2060(1)	42(1)
C(21)	6685(7)	2074(5)	1854(1)	30(1)
C(22)	5224(8)	2974(5)	2025(1)	41(1)
C(23)	3491(9)	3505(7)	1840(2)	62(2)
C(24)	3159(10)	3129(8)	1486(2)	67(2)
C(25)	4631(9)	2212(7)	1321(1)	58(2)
C(26)	6355(8)	1685(6)	1500(1)	40(1)
N(1)	9407(6)	-566(4)	882(1)	32(1)
N(2)	12420(6)	-2205(4)	802(1)	32(1)
N(3)	12090(6)	-1388(4)	1413(1)	31(1)
N(4)	12655(6)	-1189(4)	2050(1)	35(1)
N(5)	10115(7)	583(4)	1860(1)	41(1)
O(1)	10038(5)	-1695(3)	351(1)	34(1)
O(2)	10197(7)	-147(4)	2430(1)	53(1)

Table 3. Bond lengths [Å] and angles [°] for (R,R)-**5**H.

C(1)-H(1)	0.9500	C(19)-H(19A)	0.9900
C(1)-C(2)	1.387(7)	C(19)-H(19B)	0.9900
C(1)-C(6)	1.388(6)	C(19)-C(20)	1.475(7)
C(2)-H(2)	0.9500	C(19)-O(2)	1.450(6)
C(2)-C(3)	1.373(7)	C(20)-H(20)	1.0000
C(3)-H(3)	0.9500	C(20)-C(21)	1.519(7)
C(3)-C(4)	1.390(7)	C(20)-N(5)	1.466(6)
C(4)-H(4)	0.9500	C(21)-C(22)	1.377(6)
C(4)-C(5)	1.376(7)	C(21)-C(26)	1.379(6)
C(5)-H(5)	0.9500	C(22)-H(22)	0.9500
C(5)-C(6)	1.382(6)	C(22)-C(23)	1.361(7)
C(6)-C(7)	1.513(6)	C(23)-H(23)	0.9500
C(7)-H(7)	1.0000	C(23)-C(24)	1.380(8)
C(7)-C(8)	1.544(6)	C(24)-H(24)	0.9500
C(7)-N(1)	1.475(6)	C(24)-C(25)	1.379(8)
C(8)-H(8A)	0.9900	C(25)-H(25)	0.9500
C(8)-H(8B)	0.9900	C(25)-C(26)	1.345(7)
C(8)-O(1)	1.452(6)	C(26)-H(26)	0.9500
C(9)-N(1)	1.274(5)	N(3)-H(3A)	0.8800
C(9)-N(2)	1.382(6)		
C(9)-O(1)	1.362(5)	C(2)-C(1)-H(1)	119.8
C(10)-C(11)	1.474(6)	C(2)-C(1)-C(6)	120.5(5)
C(10)-N(2)	1.285(5)	C(6)-C(1)-H(1)	119.8
C(10)-N(3)	1.366(5)	C(1)-C(2)-H(2)	119.8
C(11)-C(12)	1.376(6)	C(3)-C(2)-C(1)	120.5(5)
C(11)-C(16)	1.387(6)	C(3)-C(2)-H(2)	119.8
C(12)-H(12)	0.9500	C(2)-C(3)-H(3)	120.4
C(12)-C(13)	1.385(7)	C(2)-C(3)-C(4)	119.3(4)
C(13)-H(13)	0.9500	C(4)-C(3)-H(3)	120.4
C(13)-C(14)	1.386(7)	C(3)-C(4)-H(4)	119.9
C(14)-H(14)	0.9500	C(5)-C(4)-C(3)	120.2(5)
C(14)-C(15)	1.391(7)	C(5)-C(4)-H(4)	119.9
C(15)-H(15)	0.9500	C(4)-C(5)-H(5)	119.5
C(15)-C(16)	1.373(6)	C(4)-C(5)-C(6)	121.0(5)
C(16)-C(17)	1.476(6)	C(6)-C(5)-H(5)	119.5
C(17)-N(3)	1.380(5)	C(1)-C(6)-C(7)	121.4(4)
C(17)-N(4)	1.283(5)	C(5)-C(6)-C(1)	118.6(4)
C(18)-N(4)	1.374(6)	C(5)-C(6)-C(7)	120.0(4)
C(18)-N(5)	1.243(6)	C(6)-C(7)-H(7)	109.3
C(18)-O(2)	1.359(5)	C(6)-C(7)-C(8)	114.5(3)

C(8)-C(7)-H(7)	109.3
N(1)-C(7)-C(6)	111.7(4)
N(1)-C(7)-H(7)	109.3
N(1)-C(7)-C(8)	102.3(4)
C(7)-C(8)-H(8A)	111.0
C(7)-C(8)-H(8B)	111.0
H(8A)-C(8)-H(8B)	109.0
O(1)-C(8)-C(7)	103.8(3)
O(1)-C(8)-H(8A)	111.0
O(1)-C(8)-H(8B)	111.0
N(1)-C(9)-N(2)	129.5(4)
N(1)-C(9)-O(1)	118.1(4)
O(1)-C(9)-N(2)	112.4(4)
N(2)-C(10)-C(11)	124.1(4)
N(2)-C(10)-N(3)	130.0(4)
N(3)-C(10)-C(11)	105.9(3)
C(12)-C(11)-C(10)	130.6(4)
C(12)-C(11)-C(16)	121.2(4)
C(16)-C(11)-C(10)	108.2(4)
C(11)-C(12)-H(12)	121.2
C(11)-C(12)-C(13)	117.5(4)
C(13)-C(12)-H(12)	121.2
C(12)-C(13)-H(13)	119.4
C(12)-C(13)-C(14)	121.2(5)
C(14)-C(13)-H(13)	119.4
C(13)-C(14)-H(14)	119.4
C(13)-C(14)-C(15)	121.2(5)
C(15)-C(14)-H(14)	119.4
C(14)-C(15)-H(15)	121.5
C(16)-C(15)-C(14)	117.1(4)
C(16)-C(15)-H(15)	121.5
C(11)-C(16)-C(17)	107.2(4)
C(15)-C(16)-C(11)	121.9(4)
C(15)-C(16)-C(17)	130.9(4)
N(3)-C(17)-C(16)	106.0(3)
N(4)-C(17)-C(16)	125.1(4)
N(4)-C(17)-N(3)	128.9(4)
N(5)-C(18)-N(4)	128.6(4)
N(5)-C(18)-O(2)	117.8(4)
O(2)-C(18)-N(4)	113.3(4)
H(19A)-C(19)-H(19B)	109.1
C(20)-C(19)-H(19A)	111.2
C(20)-C(19)-H(19B)	111.2
O(2)-C(19)-H(19A)	111.2
O(2)-C(19)-H(19B)	111.2
O(2)-C(19)-C(20)	102.8(4)
C(19)-C(20)-H(20)	107.1
C(19)-C(20)-C(21)	116.8(4)
C(21)-C(20)-H(20)	107.1
N(5)-C(20)-C(19)	103.5(4)
N(5)-C(20)-H(20)	107.1
N(5)-C(20)-C(21)	114.8(4)
C(22)-C(21)-C(20)	118.4(4)
C(22)-C(21)-C(26)	120.0(4)
C(26)-C(21)-C(20)	121.6(4)
C(21)-C(22)-H(22)	120.3
C(23)-C(22)-C(21)	119.4(4)
C(23)-C(22)-H(22)	120.3
C(22)-C(23)-H(23)	119.6
C(22)-C(23)-C(24)	120.9(5)
C(24)-C(23)-H(23)	119.6
C(23)-C(24)-H(24)	120.7
C(25)-C(24)-C(23)	118.6(5)
C(25)-C(24)-H(24)	120.7
C(24)-C(25)-H(25)	119.4
C(26)-C(25)-C(24)	121.1(5)
C(26)-C(25)-H(25)	119.4
C(21)-C(26)-H(26)	120.0
C(25)-C(26)-C(21)	119.9(5)
C(25)-C(26)-H(26)	120.0
C(9)-N(1)-C(7)	107.0(3)
C(10)-N(2)-C(9)	117.8(4)
C(10)-N(3)-C(17)	112.6(4)
C(10)-N(3)-H(3A)	123.7
C(17)-N(3)-H(3A)	123.7
C(17)-N(4)-C(18)	118.5(4)
C(18)-N(5)-C(20)	105.6(4)
C(9)-O(1)-C(8)	104.5(3)
C(18)-O(2)-C(19)	103.4(3)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for (R,R)-**5**H. 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}
C(1)	34(3)	36(2)	33(2)	-2(2)	-1(2)	2(2)
C(2)	41(3)	39(3)	42(2)	-11(2)	7(2)	-5(2)
C(3)	66(4)	26(2)	32(2)	-2(2)	13(2)	1(3)
C(4)	61(3)	31(2)	32(2)	1(2)	2(2)	18(3)
C(5)	44(3)	33(2)	28(2)	-4(2)	-5(2)	7(2)
C(6)	33(2)	29(2)	18(2)	-3(2)	1(2)	2(2)
C(7)	33(2)	29(2)	30(2)	1(2)	0(2)	1(2)
C(8)	44(3)	26(2)	38(2)	1(2)	-9(2)	-3(2)
C(9)	38(3)	24(2)	26(2)	3(2)	5(2)	0(2)
C(10)	43(3)	25(2)	25(2)	0(2)	3(2)	-7(2)
C(11)	38(3)	24(2)	32(2)	4(2)	7(2)	6(2)
C(12)	47(3)	37(3)	37(2)	-1(2)	6(2)	8(3)
C(13)	45(3)	44(3)	48(3)	3(2)	6(2)	17(3)
C(14)	50(3)	46(3)	51(3)	7(2)	-3(3)	16(3)
C(15)	51(3)	42(3)	33(2)	2(2)	0(2)	6(3)
C(16)	41(3)	22(2)	35(2)	3(2)	2(2)	0(2)
C(17)	39(3)	22(2)	29(2)	4(2)	-1(2)	-2(2)
C(18)	47(3)	24(2)	26(2)	-1(2)	-1(2)	4(2)
C(19)	60(3)	60(3)	27(2)	0(2)	3(2)	27(3)
C(20)	47(3)	41(3)	39(3)	-3(2)	1(2)	9(3)
C(21)	28(2)	26(2)	34(2)	0(2)	3(2)	6(2)
C(22)	43(3)	44(3)	37(2)	-5(2)	-1(2)	3(3)
C(23)	49(3)	78(4)	59(3)	-20(3)	5(3)	19(3)
C(24)	49(3)	102(5)	51(3)	-11(3)	-10(3)	30(4)
C(25)	50(3)	84(4)	39(3)	-14(3)	-2(3)	20(3)
C(26)	45(3)	43(3)	32(2)	0(2)	6(2)	9(2)
N(1)	38(2)	30(2)	27(2)	4(2)	3(2)	2(2)
N(2)	42(2)	28(2)	27(2)	1(1)	2(2)	4(2)
N(3)	37(2)	27(2)	28(2)	4(1)	1(2)	9(2)
N(4)	45(2)	35(2)	25(2)	0(2)	-2(2)	8(2)
N(5)	49(2)	43(2)	31(2)	5(2)	-1(2)	17(2)
O(1)	46(2)	28(2)	28(1)	-5(1)	-4(1)	4(2)
O(2)	68(2)	68(2)	22(2)	1(2)	4(2)	33(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (R,R)-**5**H.

	x	y	z	U(eq)
H(1)	11262	1743	765	41
H(2)	11923	4195	624	48
H(3)	9355	5558	312	50
H(4)	6089	4450	141	50
H(5)	5416	2018	286	42
H(7)	6312	-30	744	37
H(8A)	6757	-1749	318	44
H(8B)	7840	-464	80	44
H(12)	16328	-4010	871	49
H(13)	19130	-4960	1226	54
H(14)	19285	-4463	1836	59
H(15)	16699	-2927	2109	50
H(19A)	8149	1448	2603	59
H(19B)	6952	158	2383	59
H(20)	9527	2460	2122	51
H(22)	5423	3222	2271	49
H(23)	2498	4144	1957	74
H(24)	1941	3493	1358	81
H(25)	4425	1948	1077	69
H(26)	7344	1044	1383	48
H(3A)	10948	-817	1392	37

XRD data for (*S*,*S*)-**6**H

Table 1. Crystal data and structure refinement for (S,S)-**6**H.

Identification code	daley13	
Empirical formula	C20 H25 N5 O2	
Formula weight	367.45	
Temperature	100.0 K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P 1	
Unit cell dimensions	a = 9.2785(4) Å	α= 100.313(2)°.
	b = 10.8229(4) Å	β= 109.063(2)°.
	c = 11.2472(4) Å	γ = 110.537(2)°.
Volume	943.06(7) $Å^3$	
Z	2	
Density (calculated)	1.294 Mg/m^3	
Absorption coefficient	0.697 mm^{-1}	
F(000)	392	
Crystal size	0.17 x 0.13 x 0.08 mm^3	
Theta range for data collection	4.409 to 68.099°.	
Index ranges	-11<=h<=10, -12<=k<=12, -13<=l<=13	
Reflections collected	10393	
Independent reflections	4863 [R(int) = 0.0225]	
Completeness to theta = 67.684°	94.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.744 and 0.701	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4863 / 5 / 503	
Goodness-of-fit on F^2	1.054	
Final R indices [I>2sigma(I)]	R1 = 0.0299, wR2 = 0.0730	
R indices (all data)	R1 = 0.0323, wR2 = 0.0750	
Absolute structure parameter	0.21(15)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.151 and -0.169 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for (S,S)-**6**H. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	14341(3)	3117(2)	11108(2)	29(1)
O(2)	14764(3)	-289(2)	6665(2)	26(1)
N(1)	14792(3)	2231(2)	9355(2)	24(1)
N(2)	13380(3)	745(3)	10378(2)	24(1)
N(3)	13663(3)	-529(3)	8551(2)	22(1)
N(4)	13594(3)	-2463(2)	7004(2)	23(1)
N(5)	14797(3)	-2206(3)	5487(2)	26(1)
C(1)	15811(4)	3519(3)	7494(3)	32(1)
C(2)	16115(4)	5808(3)	8848(3)	31(1)
C(3)	15257(3)	4211(3)	8454(3)	25(1)
C(4)	15615(4)	3769(3)	9682(3)	24(1)
C(5)	14925(4)	4282(3)	10640(3)	28(1)
C(6)	14177(3)	2000(3)	10202(3)	22(1)
C(7)	13180(3)	-381(3)	9581(3)	22(1)
C(8)	12379(3)	-1794(3)	9645(3)	23(1)
C(9)	11628(4)	-2259(3)	10457(3)	25(1)
C(10)	10984(4)	-3679(3)	10279(3)	28(1)
C(11)	11101(4)	-4607(3)	9314(3)	27(1)
C(12)	11859(4)	-4134(3)	8502(3)	25(1)
C(13)	12488(3)	-2719(3)	8673(3)	23(1)
C(14)	13307(3)	-1911(3)	7957(3)	22(1)
C(15)	14379(3)	-1689(3)	6344(3)	21(1)
C(16)	15509(4)	201(3)	5785(3)	26(1)
C(17)	15702(3)	-1056(3)	5083(3)	24(1)
C(18)	15047(4)	-1405(3)	3579(3)	26(1)
C(19)	15226(5)	-2679(3)	2942(3)	36(1)
C(20)	15990(4)	-151(3)	3240(3)	33(1)
O(1')	10214(3)	-3442(2)	2932(2)	33(1)
O(2')	9906(2)	-1(2)	7442(2)	25(1)
N(1')	10080(3)	-2511(2)	4835(2)	26(1)
N(2')	11019(3)	-1094(3)	3574(2)	26(1)
N(3')	10710(3)	180(3)	5392(2)	22(1)
N(4')	10765(3)	2107(3)	6933(2)	24(1)
N(5')	10124(3)	1972(2)	8756(2)	25(1)
C(1')	7855(4)	-3870(3)	6014(3)	33(1)

C(2')	7503(4)	-6205(3)	4725(3)	35(1)
C(3')	7870(4)	-4695(3)	4770(3)	27(1)
C(4')	9561(3)	-4000(3)	4698(3)	24(1)
C(5')	9555(4)	-4627(3)	3345(3)	29(1)
C(6')	10418(3)	-2318(3)	3859(3)	24(1)
C(7')	11142(3)	27(3)	4330(3)	23(1)
C(8')	11785(3)	1413(3)	4185(3)	22(1)
C(9')	12498(3)	1872(3)	3344(3)	26(1)
C(10')	13073(4)	3286(3)	3497(3)	26(1)
C(11')	12940(4)	4206(3)	4446(3)	26(1)
C(12')	12210(4)	3732(3)	5275(3)	25(1)
C(13')	11644(3)	2326(3)	5133(3)	23(1)
C(14')	10972(3)	1540(3)	5933(3)	22(1)
C(15')	10254(3)	1392(3)	7737(3)	22(1)
C(16')	9176(4)	-461(3)	8343(3)	24(1)
C(17')	9649(3)	908(3)	9393(3)	22(1)
C(18')	8240(3)	887(3)	9814(3)	24(1)
C(19')	8784(4)	2288(3)	10832(3)	30(1)
C(20')	7743(4)	-301(3)	10375(3)	32(1)

Table 3. Bond lengths [Å] and angles [°] for (S,S)-**6**H.

O(1)-C(5)	1.451(4)	C(13)-C(14)	1.475(4)
O(1)-C(6)	1.361(4)	C(16)-H(16A)	0.9900
O(2)-C(15)	1.376(3)	C(16)-H(16B)	0.9900
O(2)-C(16)	1.454(3)	C(16)-C(17)	1.543(4)
N(1)-C(4)	1.482(4)	C(17)-H(17)	1.0000
N(1)-C(6)	1.279(3)	C(17)-C(18)	1.521(4)
N(2)-C(6)	1.385(4)	C(18)-H(18)	1.0000
N(2)-C(7)	1.290(4)	C(18)-C(19)	1.526(4)
N(3)-H(3)	0.88(2)	C(18)-C(20)	1.524(4)
N(3)-C(7)	1.376(4)	C(19)-H(19A)	0.9800
N(3)-C(14)	1.394(4)	C(19)-H(19B)	0.9800
N(4)-C(14)	1.283(4)	C(19)-H(19C)	0.9800
N(4)-C(15)	1.389(3)	C(20)-H(20A)	0.9800
N(5)-C(15)	1.264(4)	C(20)-H(20B)	0.9800
N(5)-C(17)	1.476(3)	C(20)-H(20C)	0.9800
C(1)-H(1A)	0.9800	O(1')-C(5')	1.444(4)
C(1)-H(1B)	0.9800	O(1')-C(6')	1.363(4)
C(1)-H(1C)	0.9800	O(2')-C(15')	1.377(3)
C(1)-C(3)	1.528(4)	O(2')-C(16')	1.457(3)
C(2)-H(2A)	0.9800	N(1')-C(4')	1.473(4)
C(2)-H(2B)	0.9800	N(1')-C(6')	1.268(3)
C(2)-H(2C)	0.9800	N(2')-C(6')	1.385(4)
C(2)-C(3)	1.532(4)	N(2')-C(7')	1.295(4)
C(3)-H(3A)	1.0000	N(3')-H(3')	0.89(2)
C(3)-C(4)	1.516(4)	N(3')-C(7')	1.381(4)
C(4)-H(4)	1.0000	N(3')-C(14')	1.388(4)
C(4)-C(5)	1.538(4)	N(4')-C(14')	1.287(4)
C(5)-H(5A)	0.9900	N(4')-C(15')	1.384(3)
C(5)-H(5B)	0.9900	N(5')-C(15')	1.269(4)
C(7)-C(8)	1.474(4)	N(5')-C(17')	1.476(3)
C(8)-C(9)	1.381(4)	C(1')-H(1'A)	0.9800
C(8)-C(13)	1.400(4)	C(1')-H(1'B)	0.9800
C(9)-H(9)	0.9500	C(1')-H(1'C)	0.9800
C(9)-C(10)	1.388(4)	C(1')-C(3')	1.527(4)
C(10)-H(10)	0.9500	C(2')-H(2'A)	0.9800
C(10)-C(11)	1.401(4)	C(2')-H(2'B)	0.9800
C(11)-H(11)	0.9500	C(2')-H(2'C)	0.9800
C(11)-C(12)	1.387(4)	C(2')-C(3')	1.535(4)
C(12)-H(12)	0.9500	C(3')-H(3'A)	1.0000
C(12)-C(13)	1.384(4)	C(3')-C(4')	1.520(4)

C(4')-H(4')	1.0000
C(4')-C(5')	1.548(4)
C(5')-H(5'A)	0.9900
C(5')-H(5'B)	0.9900
C(7')-C(8')	1.468(4)
C(8')-C(9')	1.387(4)
C(8')-C(13')	1.391(4)
C(9')-H(9')	0.9500
C(9')-C(10')	1.390(4)
C(10')-H(10')	0.9500
C(10')-C(11')	1.392(4)
C(11')-H(11')	0.9500
C(11')-C(12')	1.390(4)
C(12')-H(12')	0.9500
C(12')-C(13')	1.384(4)
C(13')-C(14')	1.479(4)
C(16')-H(16C)	0.9900
C(16')-H(16D)	0.9900
C(16')-C(17')	1.536(4)
C(17')-H(17')	1.0000
C(17')-C(18')	1.524(3)
C(18')-H(18')	1.0000
C(18')-C(19')	1.526(4)
C(18')-C(20')	1.526(4)
C(19')-H(19D)	0.9800
C(19')-H(19E)	0.9800
C(19')-H(19F)	0.9800
C(20')-H(20D)	0.9800
C(20')-H(20E)	0.9800
C(20')-H(20F)	0.9800

C(6)-O(1)-C(5)	104.8(2)
C(15)-O(2)-C(16)	105.3(2)
C(6)-N(1)-C(4)	106.5(2)
C(7)-N(2)-C(6)	117.7(2)
C(7)-N(3)-H(3)	123(2)
C(7)-N(3)-C(14)	112.2(2)
C(14)-N(3)-H(3)	125(2)
C(14)-N(4)-C(15)	122.7(2)
C(15)-N(5)-C(17)	107.3(2)
H(1A)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(3)-C(1)-H(1A)	109.5
C(3)-C(1)-H(1B)	109.5
C(3)-C(1)-H(1C)	109.5
H(2A)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(3)-C(2)-H(2A)	109.5
C(3)-C(2)-H(2B)	109.5
C(3)-C(2)-H(2C)	109.5
C(1)-C(3)-C(2)	111.8(2)
C(1)-C(3)-H(3A)	108.0
C(2)-C(3)-H(3A)	108.0
C(4)-C(3)-C(1)	110.5(2)
C(4)-C(3)-C(2)	110.6(2)
C(4)-C(3)-H(3A)	108.0
N(1)-C(4)-C(3)	112.7(2)
N(1)-C(4)-H(4)	108.9
N(1)-C(4)-C(5)	102.9(2)
C(3)-C(4)-H(4)	108.9
C(3)-C(4)-C(5)	114.4(2)
C(5)-C(4)-H(4)	108.9
O(1)-C(5)-C(4)	103.7(2)
O(1)-C(5)-H(5A)	111.0
O(1)-C(5)-H(5B)	111.0
C(4)-C(5)-H(5A)	111.0
C(4)-C(5)-H(5B)	111.0
H(5A)-C(5)-H(5B)	109.0
O(1)-C(6)-N(2)	112.6(2)
N(1)-C(6)-O(1)	118.1(3)
N(1)-C(6)-N(2)	129.3(3)
N(2)-C(7)-N(3)	128.9(3)
N(2)-C(7)-C(8)	124.4(3)
N(3)-C(7)-C(8)	106.6(2)
C(9)-C(8)-C(7)	131.3(3)
C(9)-C(8)-C(13)	121.4(3)
C(13)-C(8)-C(7)	107.3(2)
C(8)-C(9)-H(9)	121.1
C(8)-C(9)-C(10)	117.7(3)
C(10)-C(9)-H(9)	121.1
C(9)-C(10)-H(10)	119.4
C(9)-C(10)-C(11)	121.1(3)
C(11)-C(10)-H(10)	119.4
C(10)-C(11)-H(11)	119.6

C(12)-C(11)-C(10)	120.9(3)	H(20B)-C(20)-H(20C)	109.5
C(12)-C(11)-H(11)	119.6	C(6')-O(1')-C(5')	105.5(2)
C(11)-C(12)-H(12)	121.0	C(15')-O(2')-C(16')	104.3(2)
C(13)-C(12)-C(11)	118.0(3)	C(6')-N(1')-C(4')	107.8(2)
C(13)-C(12)-H(12)	121.0	C(7')-N(2')-C(6')	117.7(3)
C(8)-C(13)-C(14)	108.2(2)	C(7')-N(3')-H(3')	119(2)
C(12)-C(13)-C(8)	120.9(3)	C(7')-N(3')-C(14')	112.0(2)
C(12)-C(13)-C(14)	130.9(3)	C(14')-N(3')-H(3')	129(2)
N(3)-C(14)-C(13)	105.6(2)	C(14')-N(4')-C(15')	123.0(2)
N(4)-C(14)-N(3)	131.1(3)	C(15')-N(5')-C(17')	107.0(2)
N(4)-C(14)-C(13)	123.3(3)	H(1'A)-C(1')-H(1'B)	109.5
O(2)-C(15)-N(4)	118.7(2)	H(1'A)-C(1')-H(1'C)	109.5
N(5)-C(15)-O(2)	118.4(2)	H(1'B)-C(1')-H(1'C)	109.5
N(5)-C(15)-N(4)	122.8(3)	C(3')-C(1')-H(1'A)	109.5
O(2)-C(16)-H(16A)	110.9	C(3')-C(1')-H(1'B)	109.5
O(2)-C(16)-H(16B)	110.9	C(3')-C(1')-H(1'C)	109.5
O(2)-C(16)-C(17)	104.2(2)	H(2'A)-C(2')-H(2'B)	109.5
H(16A)-C(16)-H(16B)	108.9	H(2'A)-C(2')-H(2'C)	109.5
C(17)-C(16)-H(16A)	110.9	H(2'B)-C(2')-H(2'C)	109.5
C(17)-C(16)-H(16B)	110.9	C(3')-C(2')-H(2'A)	109.5
N(5)-C(17)-C(16)	104.0(2)	C(3')-C(2')-H(2'B)	109.5
N(5)-C(17)-H(17)	108.5	C(3')-C(2')-H(2'C)	109.5
N(5)-C(17)-C(18)	113.2(2)	C(1')-C(3')-C(2')	111.3(2)
C(16)-C(17)-H(17)	108.5	C(1')-C(3')-H(3'A)	108.2
C(18)-C(17)-C(16)	113.9(2)	C(2')-C(3')-H(3'A)	108.2
C(18)-C(17)-H(17)	108.5	C(4')-C(3')-C(1')	111.3(2)
C(17)-C(18)-H(18)	108.4	C(4')-C(3')-C(2')	109.3(2)
C(17)-C(18)-C(19)	111.3(2)	C(4')-C(3')-H(3'A)	108.2
C(17)-C(18)-C(20)	110.2(2)	N(1')-C(4')-C(3')	113.1(2)
C(19)-C(18)-H(18)	108.4	N(1')-C(4')-H(4')	108.8
C(20)-C(18)-H(18)	108.4	N(1')-C(4')-C(5')	103.1(2)
C(20)-C(18)-C(19)	110.2(2)	C(3')-C(4')-H(4')	108.8
C(18)-C(19)-H(19A)	109.5	C(3')-C(4')-C(5')	113.9(2)
C(18)-C(19)-H(19B)	109.5	C(5')-C(4')-H(4')	108.8
C(18)-C(19)-H(19C)	109.5	O(1')-C(5')-C(4')	105.0(2)
H(19A)-C(19)-H(19B)	109.5	O(1')-C(5')-H(5'A)	110.8
H(19A)-C(19)-H(19C)	109.5	O(1')-C(5')-H(5'B)	110.8
H(19B)-C(19)-H(19C)	109.5	C(4')-C(5')-H(5'A)	110.8
C(18)-C(20)-H(20A)	109.5	C(4')-C(5')-H(5'B)	110.8
C(18)-C(20)-H(20B)	109.5	H(5'A)-C(5')-H(5'B)	108.8
C(18)-C(20)-H(20C)	109.5	O(1')-C(6')-N(2')	112.1(2)
H(20A)-C(20)-H(20B)	109.5	N(1')-C(6')-O(1')	118.3(3)
H(20A)-C(20)-H(20C)	109.5	N(1')-C(6')-N(2')	129.7(3)

N(2')-C(7')-N(3')	128.6(3)
N(2')-C(7')-C(8')	124.8(3)
N(3')-C(7')-C(8')	106.6(2)
C(9')-C(8')-C(7')	130.7(3)
C(9')-C(8')-C(13')	121.6(3)
C(13')-C(8')-C(7')	107.7(2)
C(8')-C(9')-H(9')	121.5
C(8')-C(9')-C(10')	116.9(3)
C(10')-C(9')-H(9')	121.5
C(9')-C(10')-H(10')	119.1
C(9')-C(10')-C(11')	121.9(3)
C(11')-C(10')-H(10')	119.1
C(10')-C(11')-H(11')	119.7
C(12')-C(11')-C(10')	120.7(3)
C(12')-C(11')-H(11')	119.7
C(11')-C(12')-H(12')	121.1
C(13')-C(12')-C(11')	117.8(3)
C(13')-C(12')-H(12')	121.1
C(8')-C(13')-C(14')	108.0(3)
C(12')-C(13')-C(8')	121.2(3)
C(12')-C(13')-C(14')	130.6(3)
N(3')-C(14')-C(13')	105.7(2)
N(4')-C(14')-N(3')	131.0(3)
N(4')-C(14')-C(13')	123.3(3)
O(2')-C(15')-N(4')	119.0(2)
N(5')-C(15')-O(2')	118.2(2)
N(5')-C(15')-N(4')	122.8(3)
O(2')-C(16')-H(16C)	111.0
O(2')-C(16')-H(16D)	111.0
O(2')-C(16')-C(17')	104.0(2)
H(16C)-C(16')-H(16D)	109.0
C(17')-C(16')-H(16C)	111.0
C(17')-C(16')-H(16D)	111.0
N(5')-C(17')-C(16')	103.4(2)
N(5')-C(17')-H(17')	108.7
N(5')-C(17')-C(18')	113.2(2)
C(16')-C(17')-H(17')	108.7
C(18')-C(17')-C(16')	114.0(2)
C(18')-C(17')-H(17')	108.7
C(17')-C(18')-H(18')	108.4
C(17')-C(18')-C(19')	111.0(2)
C(17')-C(18')-C(20')	109.9(2)
C(19')-C(18')-H(18')	108.4
C(20')-C(18')-H(18')	108.4
C(20')-C(18')-C(19')	110.7(2)
C(18')-C(19')-H(19D)	109.5
C(18')-C(19')-H(19E)	109.5
C(18')-C(19')-H(19F)	109.5
H(19D)-C(19')-H(19E)	109.5
H(19D)-C(19')-H(19F)	109.5
H(19E)-C(19')-H(19F)	109.5
C(18')-C(20')-H(20D)	109.5
C(18')-C(20')-H(20E)	109.5
C(18')-C(20')-H(20F)	109.5
H(20D)-C(20')-H(20E)	109.5
H(20D)-C(20')-H(20F)	109.5
H(20E)-C(20')-H(20F)	109.5

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for (S,S)-**6**H. 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}
O(1)	42(1)	23(1)	28(1)	8(1)	20(1)	17(1)
O(2)	36(1)	21(1)	26(1)	7(1)	19(1)	12(1)
N(1)	28(1)	20(1)	26(1)	8(1)	14(1)	14(1)
N(2)	28(1)	26(1)	23(1)	9(1)	13(1)	15(1)
N(3)	26(1)	20(1)	23(1)	8(1)	13(1)	11(1)
N(4)	26(1)	23(1)	21(1)	7(1)	11(1)	12(1)
N(5)	32(1)	26(1)	26(1)	10(1)	16(1)	17(1)
C(1)	41(2)	30(2)	34(2)	15(1)	22(1)	19(1)
C(2)	34(2)	24(2)	39(2)	14(1)	17(1)	14(1)
C(3)	26(1)	23(1)	29(1)	10(1)	13(1)	12(1)
C(4)	26(1)	19(1)	27(2)	6(1)	10(1)	10(1)
C(5)	37(2)	22(2)	29(2)	8(1)	17(1)	15(1)
C(6)	24(1)	22(2)	21(1)	6(1)	8(1)	12(1)
C(7)	20(1)	24(2)	23(1)	9(1)	8(1)	11(1)
C(8)	22(1)	26(2)	23(2)	9(1)	8(1)	14(1)
C(9)	27(2)	29(2)	23(1)	8(1)	12(1)	16(1)
C(10)	30(2)	30(2)	29(2)	13(1)	16(1)	14(1)
C(11)	33(2)	24(2)	26(2)	11(1)	13(1)	14(1)
C(12)	29(2)	25(2)	25(1)	7(1)	12(1)	14(1)
C(13)	21(1)	26(2)	22(1)	9(1)	9(1)	12(1)
C(14)	21(1)	24(2)	21(1)	7(1)	8(1)	12(1)
C(15)	23(1)	21(2)	21(1)	6(1)	9(1)	11(1)
C(16)	32(2)	26(2)	24(1)	10(1)	16(1)	14(1)
C(17)	25(1)	23(1)	28(1)	9(1)	14(1)	12(1)
C(18)	28(2)	27(1)	25(1)	8(1)	13(1)	14(1)
C(19)	52(2)	35(2)	32(2)	12(1)	23(2)	25(2)
C(20)	40(2)	34(2)	28(2)	12(1)	18(1)	16(1)
O(1')	49(1)	25(1)	31(1)	7(1)	24(1)	17(1)
O(2')	32(1)	21(1)	26(1)	7(1)	16(1)	13(1)
N(1')	28(1)	22(1)	27(1)	7(1)	13(1)	11(1)
N(2')	30(1)	23(1)	27(1)	8(1)	15(1)	12(1)
N(3')	27(1)	22(1)	24(1)	9(1)	14(1)	12(1)
N(4')	27(1)	22(1)	25(1)	8(1)	12(1)	12(1)
N(5')	29(1)	22(1)	26(1)	8(1)	15(1)	11(1)
C(1')	38(2)	29(2)	35(2)	11(1)	21(1)	15(1)
C(2')	37(2)	24(2)	46(2)	12(1)	20(2)	14(1)

C(3')	29(2)	23(1)	28(1)	8(1)	10(1)	12(1)
C(4')	26(1)	20(1)	24(1)	5(1)	7(1)	11(1)
C(5')	34(2)	21(2)	32(2)	7(1)	13(1)	15(1)
C(6')	25(2)	23(2)	23(1)	3(1)	9(1)	13(1)
C(7')	23(1)	25(2)	22(1)	7(1)	10(1)	13(1)
C(8')	20(1)	24(2)	20(1)	5(1)	7(1)	10(1)
C(9')	25(2)	28(2)	25(2)	8(1)	11(1)	12(1)
C(10')	27(2)	31(2)	26(1)	12(1)	15(1)	13(1)
C(11')	28(2)	24(2)	28(2)	10(1)	11(1)	13(1)
C(12')	28(2)	24(2)	23(1)	7(1)	10(1)	13(1)
C(13')	22(1)	26(2)	22(1)	7(1)	9(1)	12(1)
C(14')	21(1)	21(2)	23(1)	6(1)	9(1)	10(1)
C(15')	20(1)	21(2)	26(1)	8(1)	10(1)	8(1)
C(16')	26(2)	23(2)	26(2)	10(1)	14(1)	11(1)
C(17')	24(1)	21(1)	24(1)	9(1)	12(1)	11(1)
C(18')	24(1)	28(1)	22(1)	7(1)	10(1)	12(1)
C(19')	34(2)	30(2)	29(2)	5(1)	16(1)	18(1)
C(20')	36(2)	31(2)	31(2)	10(1)	20(1)	12(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (S,S)-**6**H.

	x	y	z	U(eq)
H(3)	14190(40)	190(30)	8340(30)	30(9)
H(1A)	17041	3831	7925	47
H(1B)	15523	3780	6688	47
H(1C)	15225	2500	7253	47
H(2A)	15712	6215	9447	47
H(2B)	15832	6077	8045	47
H(2C)	17349	6155	9303	47
H(3A)	14003	3883	7989	30
H(4)	16870	4123	10177	29
H(5A)	15829	5132	11390	34
H(5B)	13978	4490	10169	34
H(9)	11555	-1628	11115	29
H(10)	10455	-4027	10821	33
H(11)	10656	-5574	9214	32
H(12)	11942	-4761	7849	30
H(16A)	16627	1024	6301	31
H(16B)	14755	454	5129	31
H(17)	16933	-841	5459	29
H(18)	13815	-1623	3204	31
H(19A)	14770	-2893	1973	55
H(19B)	14595	-3483	3151	55
H(19C)	16429	-2481	3294	55
H(20A)	17203	82	3604	50
H(20B)	15834	652	3629	50
H(20C)	15541	-380	2269	50
H(3')	10400(40)	-540(30)	5690(30)	36(9)
H(1'A)	8690	-3881	6811	49
H(1'B)	6722	-4297	5995	49
H(1'C)	8144	-2901	6036	49
H(2'A)	7492	-6714	3906	53
H(2'B)	6395	-6666	4740	53
H(2'C)	8387	-6198	5501	53
H(3'A)	6960	-4724	3969	32
H(4')	10456	-4082	5424	29
H(5'A)	10286	-5118	3451	35
H(5'B)	8388	-5295	2684	35

H(9')	12590	1247	2694	31
H(10')	13570	3635	2939	32
H(11')	13352	5168	4528	32
H(12')	12103	4352	5917	30
H(16C)	9669	-1035	8761	28
H(16D)	7928	-1014	7863	28
H(17')	10674	1103	10200	27
H(18')	7226	712	9007	29
H(19D)	9748	2458	11646	45
H(19E)	7834	2267	11046	45
H(19F)	9118	3038	10460	45
H(20D)	8734	-163	11150	47
H(20E)	7337	-1195	9690	47
H(20F)	6839	-307	10647	47

XRD data for Pd((*S*,*S*)-**6**)$_2$

Table 1. Crystal data and structure refinement for Pd((*S*,*S*-**6**)(OAc).

Identification code	test4_c	
Empirical formula	C22 H27 N5 O4 Pd	
Formula weight	531.88	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 6.6646(5) Å	α= 90°.
	b = 12.2835(10) Å	β= 95.441(2)°.
	c = 13.5762(10) Å	γ = 90°.
Volume	1106.40(15) Å^3	
Z	2	
Density (calculated)	1.597 Mg/m^3	
Absorption coefficient	0.878 mm^{-1}	
F(000)	544	
Crystal size	0.156 x 0.105 x 0.085 mm^3	
Theta range for data collection	1.507 to 27.574°.	
Index ranges	-8<=h<=8, -15<=k<=15, -17<=l<=17	
Reflections collected	12875	
Independent reflections	5069 [R(int) = 0.0333]	
Completeness to theta = 26.000°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.0949 and 0.0690	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5069 / 1 / 294	
Goodness-of-fit on F^2	1.018	
Final R indices [I>2sigma(I)]	R1 = 0.0289, wR2 = 0.0584	
R indices (all data)	R1 = 0.0380, wR2 = 0.0608	
Absolute structure parameter	0.020(16)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.412 and -0.441 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Pd((*S*,*S*-**6**)(OAc). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	4991(1)	5057(1)	2682(1)	18(1)
O(3)	7496(4)	5002(6)	1953(2)	23(1)
O(2)	6211(5)	7911(3)	4268(2)	25(1)
O(1)	1771(5)	2218(3)	1949(2)	24(1)
N(3)	2790(5)	5104(8)	3565(2)	20(1)
N(1)	3924(6)	3623(3)	2163(3)	18(1)
N(5)	5915(6)	6508(3)	3220(3)	20(1)
O(4)	5985(5)	5201(4)	423(2)	33(1)
N(2)	1079(6)	3410(3)	3136(3)	21(1)
C(15)	6678(11)	2369(5)	1715(5)	25(2)
N(4)	3646(6)	6748(3)	4485(3)	22(1)
C(12)	5251(7)	6991(4)	3961(3)	21(1)
C(5)	-33(8)	4655(4)	4354(4)	20(1)
C(13)	7890(8)	8018(4)	3671(4)	25(1)
C(1)	4717(8)	2944(4)	1368(3)	22(1)
C(10)	726(8)	5622(4)	4761(4)	20(1)
C(21)	7476(6)	5081(9)	1015(3)	24(1)
C(14)	7429(8)	7227(4)	2810(4)	24(1)
C(6)	-1773(7)	4192(4)	4650(3)	22(1)
C(2)	2941(7)	2183(4)	1099(4)	24(1)
C(4)	1325(7)	4323(4)	3617(3)	19(1)
C(22)	9570(8)	5012(9)	657(4)	42(1)
C(3)	2351(7)	3143(4)	2430(3)	21(1)
C(9)	-188(8)	6164(4)	5486(3)	26(1)
C(7)	-2690(8)	4738(4)	5391(4)	24(1)
C(18)	6556(12)	7765(6)	1849(5)	29(2)
C(11)	2541(8)	5893(4)	4258(3)	21(1)
C(8)	-1909(9)	5692(4)	5795(4)	28(1)
C(19)	4657(9)	8413(4)	1947(4)	34(1)
C(17)	7488(9)	1818(5)	817(5)	44(2)
C(20)	8172(10)	8468(5)	1423(4)	38(2)
C(16)	6435(9)	1555(4)	2534(4)	39(1)

Table 3. Bond lengths [Å] and angles [°] for Pd((*S*,*S*-**6**)(OAc).

Pd(1)-O(3)	2.021(3)	C(21)-C(22)	1.523(6)
Pd(1)-N(3)	1.981(3)	C(14)-H(14)	1.0000
Pd(1)-N(1)	2.002(4)	C(14)-C(18)	1.528(9)
Pd(1)-N(5)	2.002(4)	C(6)-H(6)	0.9500
O(3)-C(21)	1.277(5)	C(6)-C(7)	1.397(6)
O(2)-C(12)	1.345(6)	C(2)-H(2A)	0.9900
O(2)-C(13)	1.449(6)	C(2)-H(2B)	0.9900
O(1)-C(2)	1.454(5)	C(22)-H(22A)	0.9800
O(1)-C(3)	1.348(6)	C(22)-H(22B)	0.9800
N(3)-C(4)	1.375(8)	C(22)-H(22C)	0.9800
N(3)-C(11)	1.372(9)	C(9)-H(9)	0.9500
N(1)-C(1)	1.499(6)	C(9)-C(8)	1.386(7)
N(1)-C(3)	1.285(6)	C(7)-H(7)	0.9500
N(5)-C(12)	1.281(6)	C(7)-C(8)	1.375(7)
N(5)-C(14)	1.488(6)	C(18)-H(18)	1.0000
O(4)-C(21)	1.226(5)	C(18)-C(19)	1.512(9)
N(2)-C(4)	1.300(6)	C(18)-C(20)	1.535(9)
N(2)-C(3)	1.377(6)	C(8)-H(8)	0.9500
C(15)-H(15)	1.0000	C(19)-H(19A)	0.9800
C(15)-C(1)	1.521(9)	C(19)-H(19B)	0.9800
C(15)-C(17)	1.537(9)	C(19)-H(19C)	0.9800
C(15)-C(16)	1.515(9)	C(17)-H(17A)	0.9800
N(4)-C(12)	1.373(6)	C(17)-H(17B)	0.9800
N(4)-C(11)	1.303(6)	C(17)-H(17C)	0.9800
C(5)-C(10)	1.385(6)	C(20)-H(20A)	0.9800
C(5)-C(6)	1.385(7)	C(20)-H(20B)	0.9800
C(5)-C(4)	1.470(7)	C(20)-H(20C)	0.9800
C(13)-H(13A)	0.9900	C(16)-H(16A)	0.9800
C(13)-H(13B)	0.9900	C(16)-H(16B)	0.9800
C(13)-C(14)	1.529(7)	C(16)-H(16C)	0.9800
C(1)-H(1)	1.0000		
C(1)-C(2)	1.525(7)	N(3)-Pd(1)-O(3)	172.15(13)
C(10)-C(9)	1.378(7)	N(3)-Pd(1)-N(1)	88.9(3)
C(10)-C(11)	1.482(7)	N(3)-Pd(1)-N(5)	88.4(3)

N(1)-Pd(1)-O(3)	94.6(2)	N(1)-C(1)-H(1)	109.4
N(5)-Pd(1)-O(3)	88.2(2)	N(1)-C(1)-C(2)	101.2(4)
N(5)-Pd(1)-N(1)	177.02(16)	C(15)-C(1)-H(1)	109.4
C(21)-O(3)-Pd(1)	123.7(3)	C(15)-C(1)-C(2)	114.5(4)
C(12)-O(2)-C(13)	105.9(3)	C(2)-C(1)-H(1)	109.4
C(3)-O(1)-C(2)	105.0(3)	C(5)-C(10)-C(11)	107.0(5)
C(4)-N(3)-Pd(1)	125.5(5)	C(9)-C(10)-C(5)	122.0(5)
C(11)-N(3)-Pd(1)	125.5(5)	C(9)-C(10)-C(11)	131.0(5)
C(11)-N(3)-C(4)	109.0(3)	O(3)-C(21)-C(22)	113.0(4)
C(1)-N(1)-Pd(1)	127.2(3)	O(4)-C(21)-O(3)	126.5(4)
C(3)-N(1)-Pd(1)	125.2(3)	O(4)-C(21)-C(22)	120.5(4)
C(3)-N(1)-C(1)	107.5(4)	N(5)-C(14)-C(13)	100.7(4)
C(12)-N(5)-Pd(1)	125.5(3)	N(5)-C(14)-H(14)	110.2
C(12)-N(5)-C(14)	108.4(4)	N(5)-C(14)-C(18)	111.0(5)
C(14)-N(5)-Pd(1)	126.0(3)	C(13)-C(14)-H(14)	110.2
C(4)-N(2)-C(3)	119.9(4)	C(18)-C(14)-C(13)	114.2(5)
C(1)-C(15)-H(15)	108.2	C(18)-C(14)-H(14)	110.2
C(1)-C(15)-C(17)	108.3(6)	C(5)-C(6)-H(6)	121.7
C(17)-C(15)-H(15)	108.2	C(5)-C(6)-C(7)	116.6(4)
C(16)-C(15)-H(15)	108.2	C(7)-C(6)-H(6)	121.7
C(16)-C(15)-C(1)	112.7(5)	O(1)-C(2)-C(1)	104.7(4)
C(16)-C(15)-C(17)	111.2(6)	O(1)-C(2)-H(2A)	110.8
C(11)-N(4)-C(12)	120.3(4)	O(1)-C(2)-H(2B)	110.8
O(2)-C(12)-N(4)	113.2(4)	C(1)-C(2)-H(2A)	110.8
N(5)-C(12)-O(2)	116.2(4)	C(1)-C(2)-H(2B)	110.8
N(5)-C(12)-N(4)	130.5(4)	H(2A)-C(2)-H(2B)	108.9
C(10)-C(5)-C(4)	106.5(5)	N(3)-C(4)-C(5)	109.1(4)
C(6)-C(5)-C(10)	121.4(5)	N(2)-C(4)-N(3)	129.2(5)
C(6)-C(5)-C(4)	132.1(5)	N(2)-C(4)-C(5)	121.7(4)
O(2)-C(13)-H(13A)	110.7	C(21)-C(22)-H(22A)	109.5
O(2)-C(13)-H(13B)	110.7	C(21)-C(22)-H(22B)	109.5
O(2)-C(13)-C(14)	105.1(4)	C(21)-C(22)-H(22C)	109.5
H(13A)-C(13)-H(13B)	108.8	H(22A)-C(22)-H(22B)	109.5
C(14)-C(13)-H(13A)	110.7	H(22A)-C(22)-H(22C)	109.5
C(14)-C(13)-H(13B)	110.7	H(22B)-C(22)-H(22C)	109.5
N(1)-C(1)-C(15)	112.7(4)	O(1)-C(3)-N(2)	111.7(4)

N(1)-C(3)-O(1)	117.0(4)	H(20A)-C(20)-H(20C)	109.5
N(1)-C(3)-N(2)	131.3(4)	H(20B)-C(20)-H(20C)	109.5
C(10)-C(9)-H(9)	121.7	C(15)-C(16)-H(16A)	109.5
C(10)-C(9)-C(8)	116.7(5)	C(15)-C(16)-H(16B)	109.5
C(8)-C(9)-H(9)	121.7	C(15)-C(16)-H(16C)	109.5
C(6)-C(7)-H(7)	119.3	H(16A)-C(16)-H(16B)	109.5
C(8)-C(7)-C(6)	121.5(5)	H(16A)-C(16)-H(16C)	109.5
C(8)-C(7)-H(7)	119.3	H(16B)-C(16)-H(16C)	109.5
C(14)-C(18)-H(18)	107.2		
C(14)-C(18)-C(20)	109.9(6)		
C(19)-C(18)-C(14)	114.0(5)		
C(19)-C(18)-H(18)	107.2		
C(19)-C(18)-C(20)	111.1(6)		
C(20)-C(18)-H(18)	107.2		
N(3)-C(11)-C(10)	108.3(4)		
N(4)-C(11)-N(3)	129.0(5)		
N(4)-C(11)-C(10)	122.7(4)		
C(9)-C(8)-H(8)	119.1		
C(7)-C(8)-C(9)	121.9(5)		
C(7)-C(8)-H(8)	119.1		
C(18)-C(19)-H(19A)	109.5		
C(18)-C(19)-H(19B)	109.5		
C(18)-C(19)-H(19C)	109.5		
H(19A)-C(19)-H(19B)	109.5		
H(19A)-C(19)-H(19C)	109.5		
H(19B)-C(19)-H(19C)	109.5		
C(15)-C(17)-H(17A)	109.5		
C(15)-C(17)-H(17B)	109.5		
C(15)-C(17)-H(17C)	109.5		
H(17A)-C(17)-H(17B)	109.5		
H(17A)-C(17)-H(17C)	109.5		
H(17B)-C(17)-H(17C)	109.5		
C(18)-C(20)-H(20A)	109.5		
C(18)-C(20)-H(20B)	109.5		
C(18)-C(20)-H(20C)	109.5		
H(20A)-C(20)-H(20B)	109.5		

Table 4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for Pd((*S*,*S*-**6**)(OAc). 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}
Pd(1)	20(1)	15(1)	20(1)	-1(1)	6(1)	0(1)
O(3)	25(2)	21(2)	26(1)	1(3)	9(1)	1(3)
O(2)	26(2)	22(2)	27(2)	-4(1)	8(1)	-5(1)
O(1)	28(2)	21(2)	26(2)	-7(1)	11(2)	-6(2)
N(3)	22(2)	18(2)	20(2)	5(3)	4(1)	-6(3)
N(1)	21(2)	17(2)	18(2)	-3(2)	5(2)	1(2)
N(5)	18(2)	16(2)	27(2)	-2(2)	6(2)	-4(2)
O(4)	39(2)	29(3)	32(2)	7(2)	5(1)	1(2)
N(2)	23(2)	19(2)	21(2)	-1(2)	6(2)	1(2)
C(15)	22(4)	25(4)	30(4)	-10(3)	3(3)	-6(3)
N(4)	25(2)	18(2)	23(2)	-3(2)	8(2)	-1(2)
C(12)	23(3)	14(2)	25(3)	-1(2)	1(2)	1(2)
C(5)	26(3)	21(2)	13(2)	5(2)	5(2)	6(2)
C(13)	28(3)	23(2)	26(3)	-5(2)	8(2)	-5(2)
C(1)	27(3)	23(2)	19(3)	-4(2)	8(2)	-1(2)
C(10)	22(3)	20(3)	20(3)	8(2)	6(2)	3(2)
C(21)	31(2)	15(2)	27(2)	1(5)	6(2)	4(4)
C(14)	24(3)	19(2)	30(3)	-2(2)	7(2)	-5(2)
C(6)	21(3)	21(2)	24(3)	2(2)	2(2)	-1(2)
C(2)	23(3)	24(3)	27(3)	-5(2)	9(2)	-2(2)
C(4)	20(3)	18(2)	20(2)	6(2)	2(2)	2(2)
C(22)	42(3)	49(3)	39(3)	17(5)	22(2)	16(5)
C(3)	26(3)	18(2)	19(2)	-2(2)	3(2)	1(2)
C(9)	32(3)	23(2)	24(3)	-3(2)	7(2)	0(2)
C(7)	26(3)	22(3)	26(3)	6(2)	10(2)	3(2)
C(18)	36(4)	26(4)	27(4)	-2(3)	11(3)	-11(3)
C(11)	25(3)	20(2)	19(2)	3(2)	4(2)	5(2)
C(8)	34(3)	27(3)	24(3)	-2(2)	13(2)	4(2)
C(19)	43(4)	26(3)	34(3)	4(2)	4(2)	3(2)
C(17)	28(3)	48(4)	56(4)	-29(3)	10(3)	-3(3)
C(20)	55(4)	33(3)	30(3)	1(3)	15(3)	-13(3)
C(16)	38(4)	23(3)	55(4)	-3(3)	-2(3)	5(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for Pd((*S*,*S*-**6**)(OAc).

	x	y	z	U(eq)
H(15)	7676	2932	1975	30
H(13A)	9173	7824	4059	30
H(13B)	7990	8774	3425	30
H(1)	4931	3416	787	27
H(14)	8663	6800	2695	29
H(6)	-2315	3537	4364	26
H(2A)	2128	2439	495	29
H(2B)	3415	1434	984	29
H(22A)	10496	5484	1065	63
H(22B)	9509	5248	-35	63
H(22C)	10052	4258	709	63
H(9)	335	6829	5760	31
H(7)	-3878	4444	5621	29
H(18)	6199	7168	1362	35
H(8)	-2569	6037	6301	34
H(19A)	3632	7939	2193	51
H(19B)	4153	8706	1299	51
H(19C)	4956	9014	2412	51
H(17A)	6485	1302	520	65
H(17B)	8739	1429	1030	65
H(17C)	7758	2373	327	65
H(20A)	8604	9044	1896	58
H(20B)	7612	8795	799	58
H(20C)	9332	8012	1304	58
H(16A)	6023	1937	3116	59
H(16B)	7720	1183	2709	59
H(16C)	5404	1019	2307	59