

Supplementary Figures and Table for manuscript Nkabyo, Koch *et al*

Figure S1

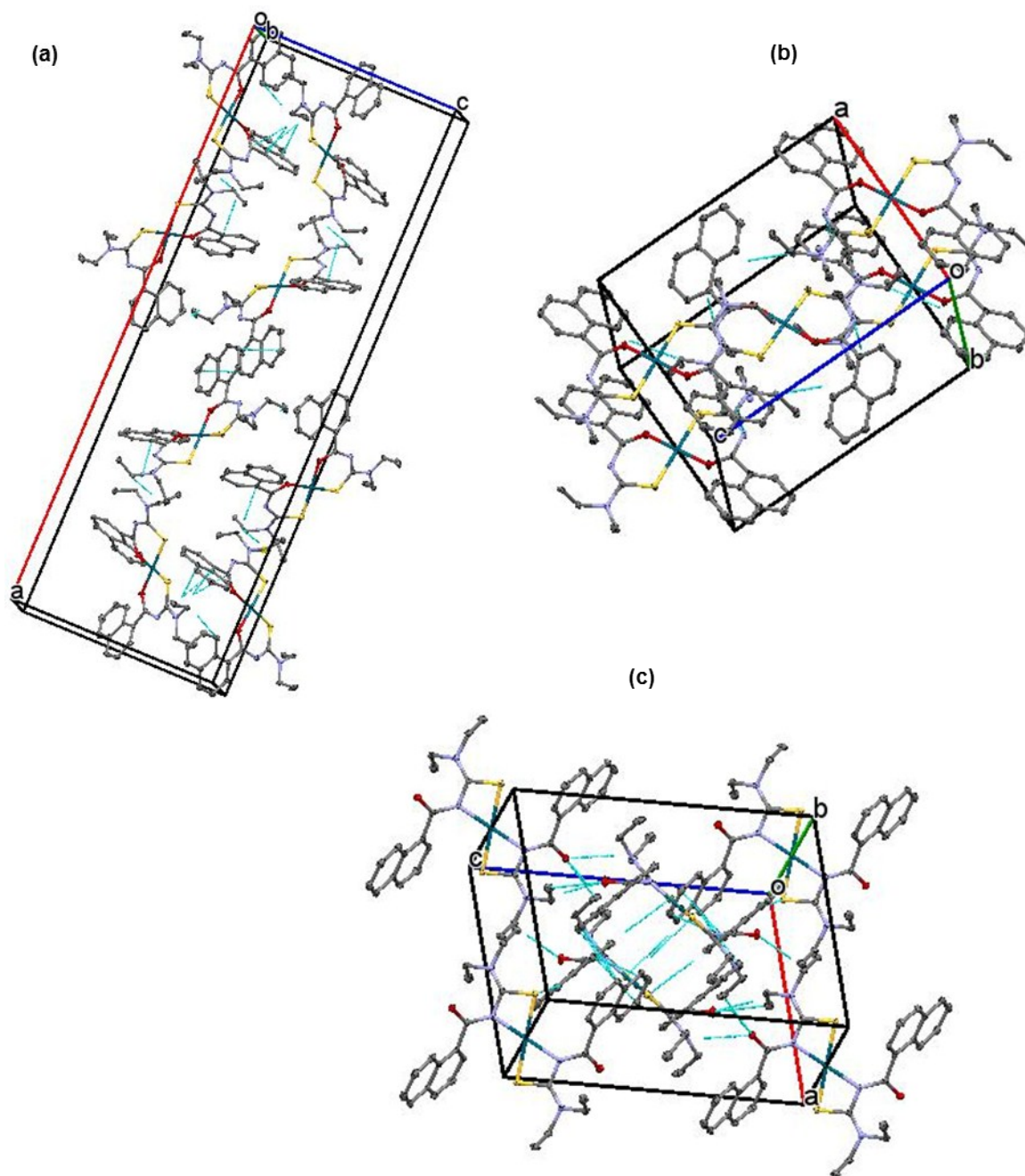


Figure S1. Crystal packing of (a) *cis*-[Pd(L-κS,O)₂], (b) *trans*-[Pd(L-κS,O)₂] and (c) *trans*-[Pd(L-κS,N)₂].

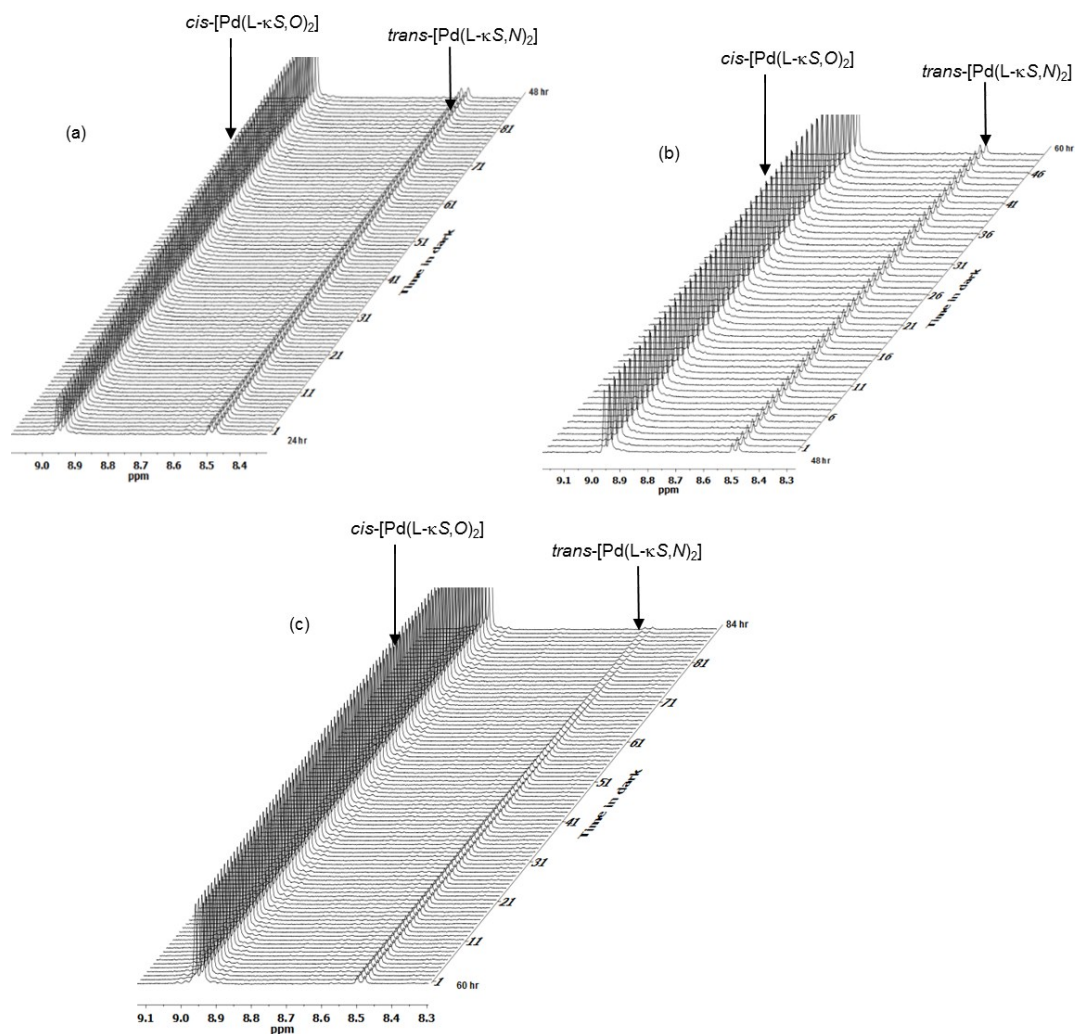
Figure S2

Figure S2. An array of ^1H NMR spectra representing spontaneous $\text{trans} \rightarrow \text{cis}$ isomerism for isolated $\text{trans-[Pd(L-}\kappa\text{S,O)}_2\text{]}$ and $\text{trans-[Pd(L-}\kappa\text{S,N)}_2\text{]}$ to $\text{cis-[Pd(L-}\kappa\text{S,O)}_2\text{]}$ after (a) 48 hr, (b) 60 hr, and (c) 80 hr in the dark in chloroform- d at 25°C .

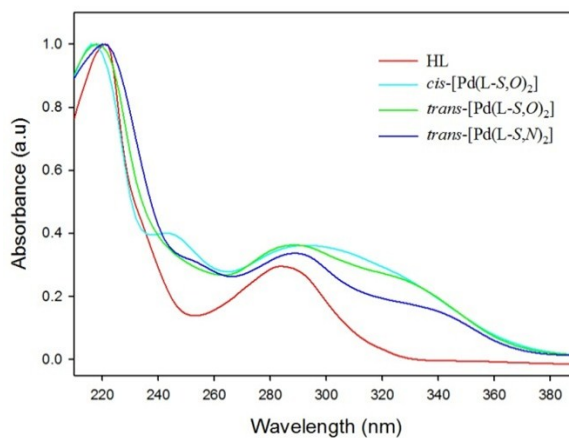
Figure S3

Figure S3. Overlaid photo-diode UV Spectra of free HL, $\text{cis-[Pd(L-}\kappa\text{S,O)}_2\text{]}$, $\text{trans-[Pd(L-}\kappa\text{S,O)}_2\text{]}$ and $\text{trans-[Pd(L-}\kappa\text{S,N)}_2\text{]}$ at 262 nm.

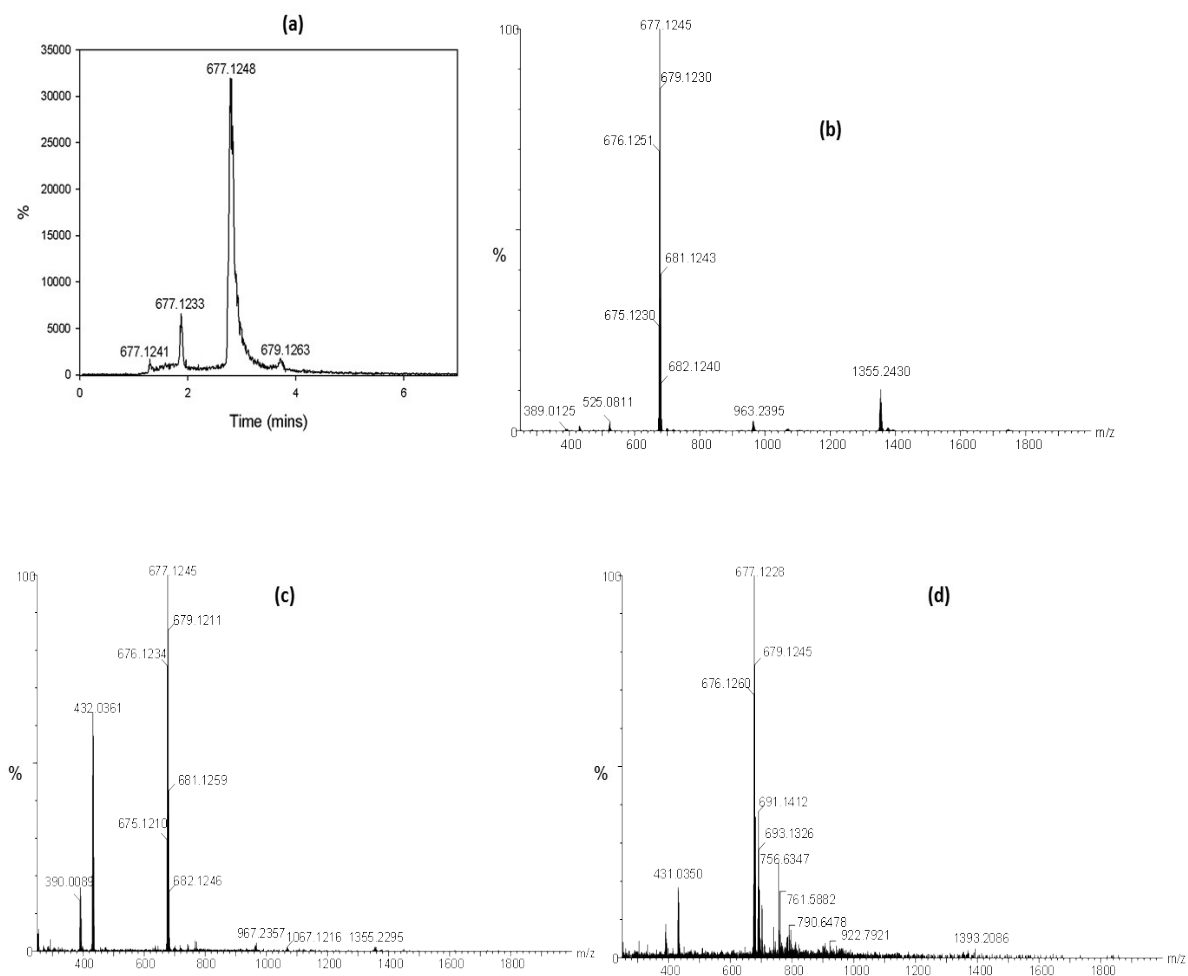
Figure S4

Figure S4. (a) Total ion chromatogram of a solution of *cis*-[Pd(L-κS,O)₂] after 30 min irradiation with a 5 Watt LED lamp; Mass spectra of (b) *cis*-[Pd(L-κS,O)₂], (c) *trans*-[Pd(L-κS,O)₂] and (d) *trans*-[Pd(L-κS,N)₂].

Table S1. Important bond lengths (Å) and angles (°) for *cis*-[Pd(L-κS,O)₂], *trans*-[Pd(L-κS,O)₂] and *trans*-[Pd(L-κS,N)₂].

	<i>cis</i> -[Pd(L-κS,O) ₂]	<i>trans</i> -[Pd(L-κS,O) ₂]	<i>trans</i> -[Pd(L-κS,N) ₂]
Pd(1)-S(1A)	2.2241(10)	2.285(12)	2.3252(10)
Pd(1)-S1(B)	2.2458(9)	2.278(4)	2.3252(10)
Pd(1)-O(1A)	2.015(2)	1.9778(13)	-
Pd(1)-O(1B)	2.032(2)	1.9778(13)	-
S(1A)-C(12A)	1.735(4)	1.70(3)	1.741(3)
S(1B)-C(12B)	1.738(3)	1.734(11)	-
O(1A)-C(11A)	1.275(4)	1.282(2)	1.225(4)
O(1B)-C(11B)	1.270(4)	-	-
N(1A)-C(11A)	1.326(4)	1.32(3)	1.384(4)
N(1A)-C(12A)	1.348(5)	1.37(5)	1.366(4)
N(1B)-C(11B)	1.326(4)	1.317(9)	-
N(1B)-C(12B)	1.350(4)	1.339(16)	-
Pd(1)-N(1)	-	-	2.050(2)
S(A1)-Pd(1)-S(1B)	86.93(3)	180.00	180.00
S(1A)-Pd(1)-O(1A)	93.98(8)	93.8(3)	-
S(1A)-Pd(1)-O(1B)	177.99(7)	86.2(3)	-
S(1B)-Pd(1)-O(1A)	179.09(8)	93.98(12)	-
S(1B)-Pd(1)-O(1B)	92.57(6)	86.02(12)	-
O(1A)-Pd(1)-O(1B)	86.53(9)	180.00	-
Pd(1)-S(1A)-C(12A)	108.14(12)	108.5(12)	79.94(9)
Pd(1)-S(1B)-C(12B)	104.66(11)	108.2(2)	-
Pd(1)-O(1A)-C(11A)	130.5(2)	130.38(12)	-
Pd(1)-O(1B)-C(11B)	128.6(2)	-	-
C(11A)-N(1A)-C(12A)	126.1(3)	126.0(2)	121.5(2)
C(11B)-N(1B)-C(12B)	125.7(3)	127.8(7)	-
S(1)-Pd(1)-N(1)	-	-	70.75(6)
S(1)-Pd(1)-N(1_a)	-	-	109.25(6)
N(1)-Pd(1)-N(1_a)	-	-	180.00
Pd(1)-N(1)-C(11)	-	-	126.09(17)
Pd(1)-N(1)-C(12)	-	-	99.81(17),