

Electronic Supplementary Information for MS:

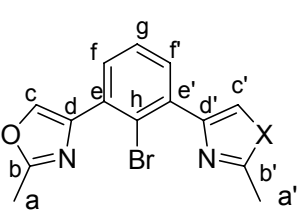
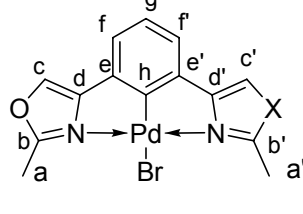
Novel bis(azole) pincer palladium complexes: synthesis, structures and application in Mizoroki - Heck reactions

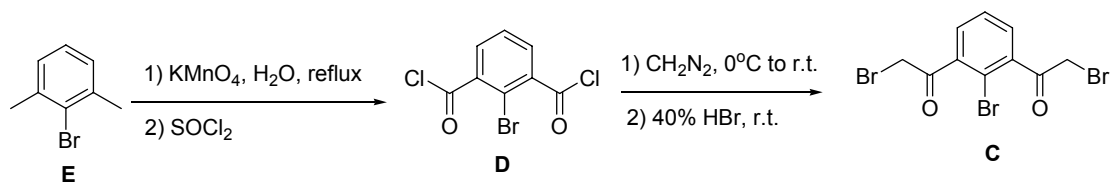
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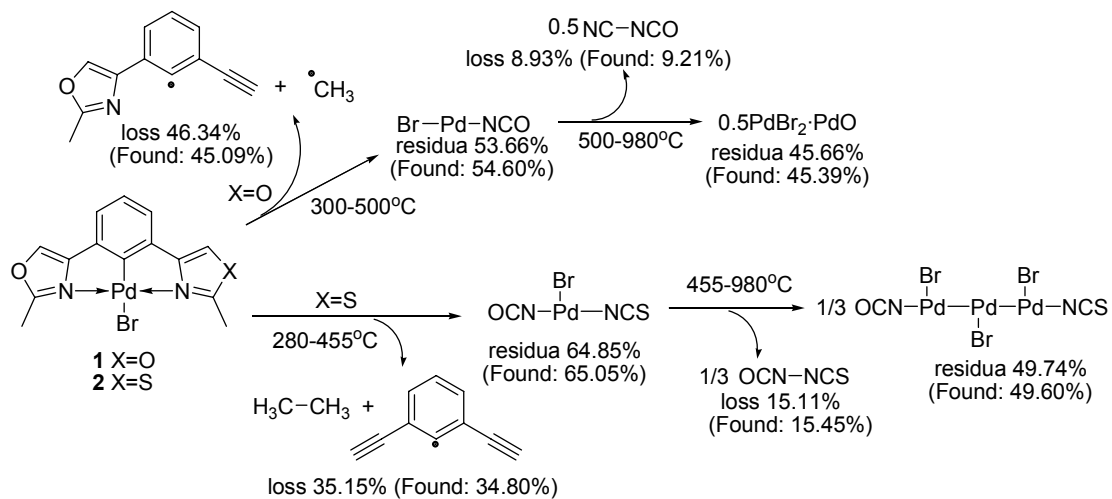
400715, China

Table S1. NMR spectral data of the proligands and the complexes in CDCl₃

 A X=O B X=S							 1 X=O 2 X=S						
¹ H NMR / δ (ppm)							¹³ C NMR / δ (ppm)						
	A	1	Δδ	B	2	Δδ	A	1	Δδ	B	2	Δδ	
a				2.54	3.02	0.48	13.8	15.3	1.5	13.8	15.6	1.8	
a'	2.54	3.01	0.47	2.79	3.24	0.45				19.2	22.1	2.9	
b	—	—	—	—	—	—	160.5	167.0	6.5	160.5	167.3	6.8	
b'	—	—	—	—	—	—				164.8	174.5	9.7	
c	8.20	7.70	−0.50	8.26	7.70	−0.56	137.9	130.2	−7.7	137.0	130.2	−6.8	
c'				7.36	7.18	−0.18				117.3	108.1	−9.2	
d	—	—	—	—	—	—	138.6	147.6	9.0	138.4	147.2	8.8	
d'	—	—	—	—	—	—				154.0	161.6	7.6	
e	—	—	—	—	—	—	133.4	134.4	1.0	133.4	134.3	0.9	
e'	—	—	—	—	—	—				137.5	137.3	−0.2	
f	7.85	7.13	−0.72	7.93	7.15	−0.78	130.2	120.7	−9.5	130.4	120.7	−9.7	
f'				7.52	7.15	−0.37				130.9	120.7	−10.2	
g	7.44	7.13	−0.31	7.42	7.15	−0.27	127.4	127.2	−0.2	127.2	125.5	−1.7	
h	—	—	—	—	—	—	120.7	158.5	37.8	121.6	157.1	35.5	



Scheme S1. Synthesis of α -bromoketone **C**.



Scheme S2. The proposal thermal decomposition pathway of the complexes.

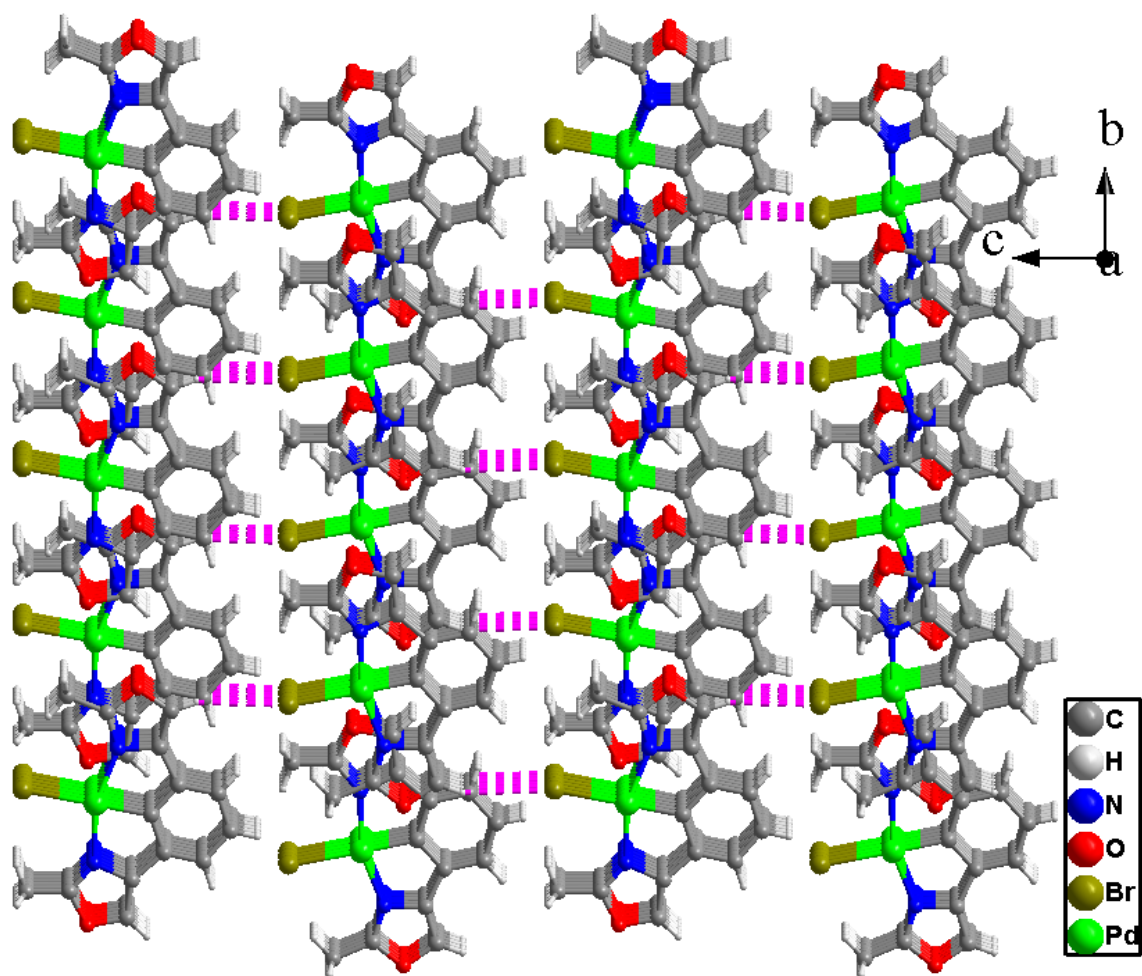
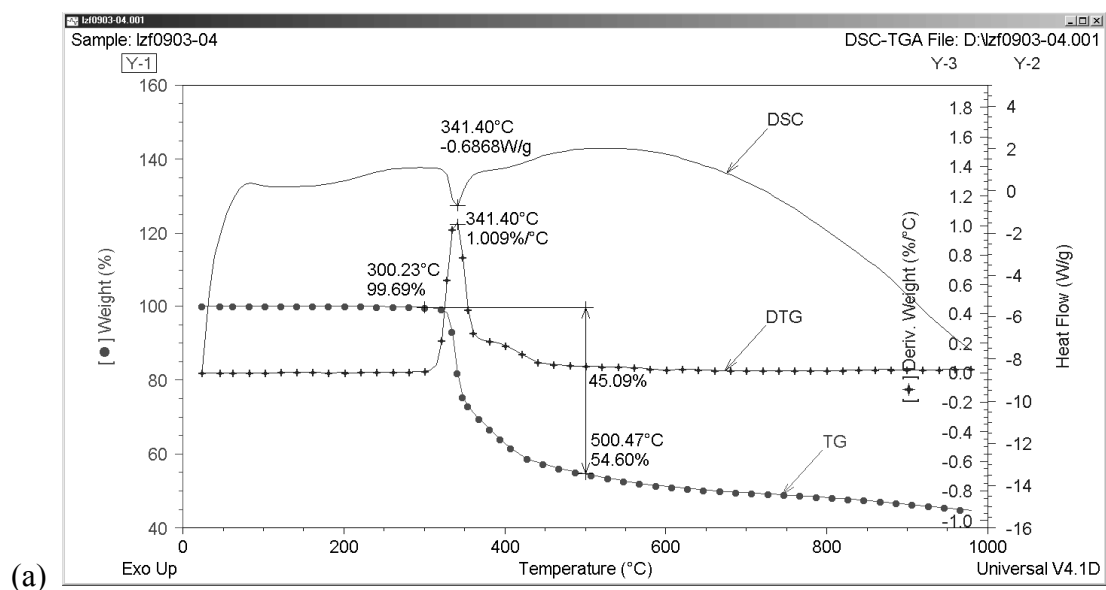


Fig. S1 Three-dimension supramolecular structures of compound 1.



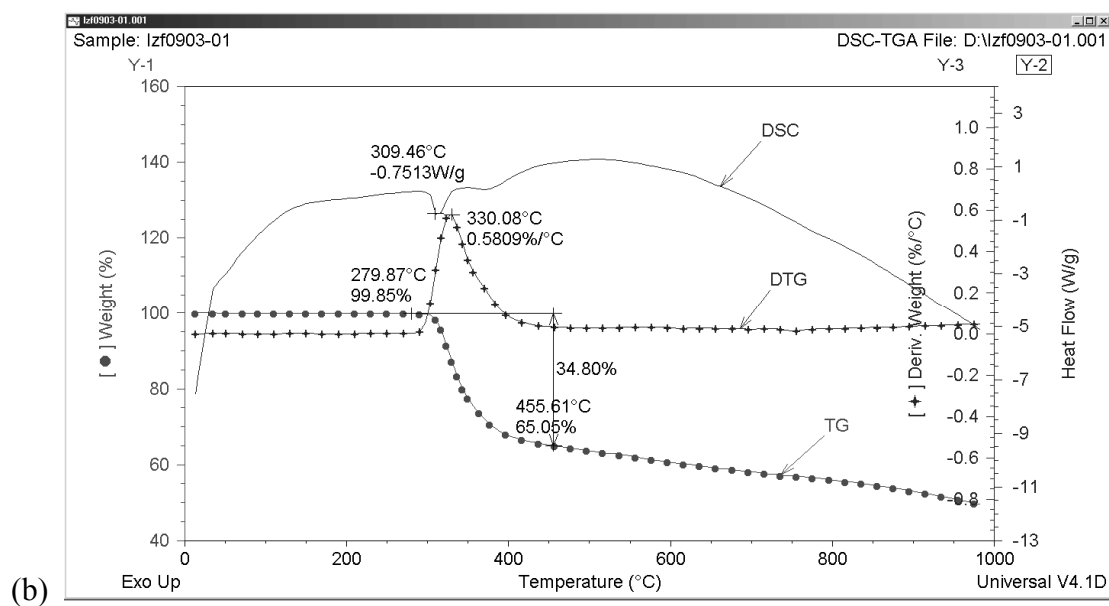


Fig. S2 TG–DTG–DSC thermograms of complex **1** (a) and **2** (b) under nitrogen atmosphere.

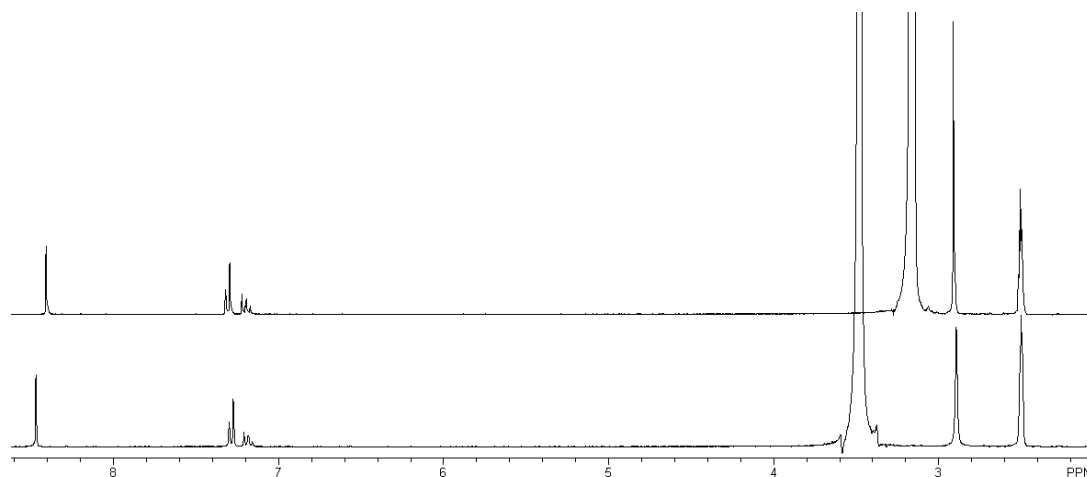


Fig. S3 ^1H NMR spectra of complex **1** recorded at 343 K (up) and 293 K (down) in DMSO- d_6 .

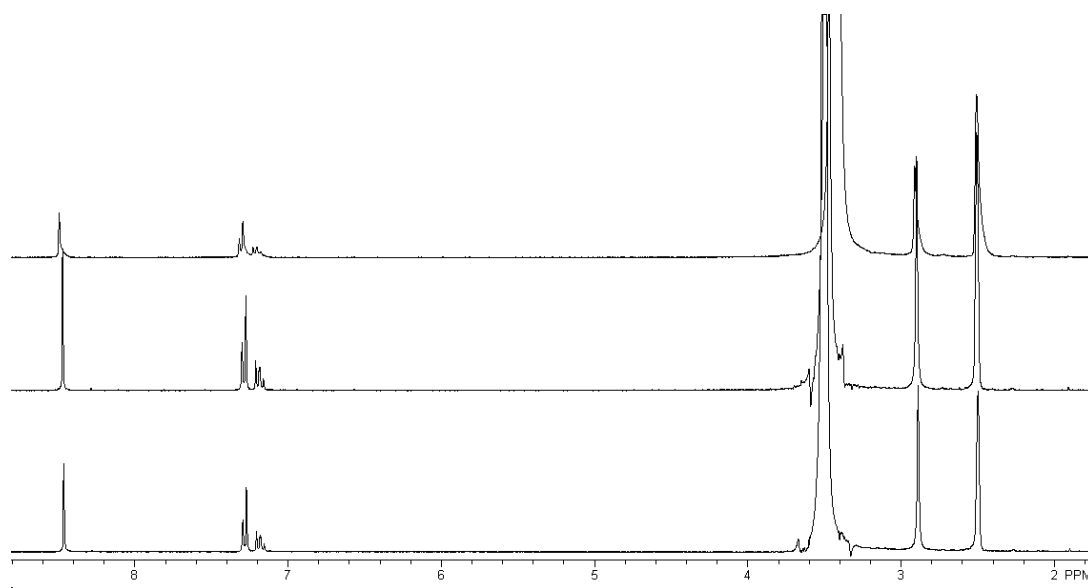


Fig. S4 ¹H NMR spectra of complex **1** recorded at 293K after heating at various temperatures in DMSO-d₆.

up: heating at 70°C for 3 hours, 20 days later; middle: heating at 70°C for 3 hours, 30 days later, then heating at 110° for 10 hours; down: heating at 70°C for 3 hours, 30 days later, then heating at 110° for 10 hours, another 5 days later, heating at 150°C for 8 hours.