

Supporting Information for:

**Palladium Pincer-type Complexes and Zwitterionic Sulfur
Adducts of Pyridine-bridged bis(1,2,3-triazolin-5-ylidenes):
Syntheses, Characterizations and Catalytic Applications**

X-ray Diffraction Studies. X-ray data for complex **8** was collected with SuperNova, Dual, Cu at zero, AtlasS2 diffractometer using Cu-K α radiation. The crystal was kept at 100.02(10) K during data collection. Using Olex2 [1], the structure was solved with the ShelXT [2] structure solution program using Direct Methods and refined with the ShelXL [3] refinement package using Least Squares minimization. All non-hydrogen atoms were generally given anisotropic displacement parameters in the final model. All H-atoms were put at calculated positions. A summary of selected important crystallographic data is given in Table SI-1. CCDC-1574476 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table SI-1. Selected X-ray Crystallographic Data for Compound **8**

Comp.	8
Formula	C ₂₅ H ₂₃ BClF ₄ N ₇ Pd
Formula weight	650.16
Color, habit	Colorless, Block
Crystal size [mm]	0.25 × 0.2 × 0.2
Temperature [K]	100.02(10)
Crystal system	Monoclinic
Space group	P2 ₁ /c
<i>a</i> [Å]	17.8856(10)
<i>b</i> [Å]	5.7367(3)
<i>c</i> [Å]	25.7084(15)
α [°]	90
β [°]	101.715(5)
γ [°]	90
<i>V</i> [Å ³]	2582.8(3)

<i>Z</i>	4
<i>D_c</i> [g·cm ⁻³]	1.672
Radiation used	Cu-Kα
<i>μ</i> [mm ⁻¹]	7.271
<i>θ</i> range [°]	4.6800–72.9790
Reflections collected	5117
max, min transmission	1.00000, 0.25776
Final R indices (<i>I</i> > 2σ(<i>I</i>))	<i>R</i> ₁ = 0.1111, <i>wR</i> ₂ = 0.2589
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.1268, <i>wR</i> ₂ = 0.2683
goodness of fit on <i>F</i> ²	1.159
Peak/hole [e·Å ⁻³]	2.21 / -1.75

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- (1) O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, *J. Appl. Cryst.* 2009, **42**, 339.
- (2) G. M. Sheldrick, *Acta Cryst.* 2015, **A71**, 3-8.
- (3) G. M. Sheldrick, *Acta Cryst.* 2015, **C71**, 3-8.