Supporting Information

## 1,2,4-Diazaphospholide Complexes of Barium: Mechanism of Formation and Crystallographic Characterization

Chengfu Pi, <sup>†,§</sup>Li Wan, <sup>†</sup> Weiping Liu, <sup> $\perp$ </sup> Zaifu Pan, <sup> $\perp$ </sup>

Haoyu Wu,<sup>†</sup> Yunhua Wang,<sup>†</sup> Wenjun Zheng,<sup>†,\*</sup> Linhong Weng,<sup>†</sup> Zhenxia Chen,<sup>†</sup> and

Limin Wu<sup>§,\*</sup>

Department of Chemistry,<sup>†</sup> Laboratory of Advanced Materials,<sup>§</sup> Fudan University,

Handan Road 220, Shanghai 200433, China; Kunming Institute of Precious Metals,  $^{\perp}$ 

Kunming 650106, Yunnan, China

Department of Chemistry,<sup>†</sup> Laboratory of Advanced Materials,<sup>§</sup> Fudan University, Handan Road 220, Shanghai 200433, China





**Figure S2.** The <sup>31</sup>P NMR spectrum of complex **4** in DMSO- $d_6$  at 23 °C.



**Figure S3.** The <sup>31</sup>P NMR spectrum of complex **7** in DMSO- $d_6$  at 23 °C.



**Figure S4.** The <sup>1</sup>H NMR spectrum of H[3,5- $tBu_2dp$ ] in DMSO- $d_6$  at 23 °C.



**Figure S5.** The <sup>1</sup>H NMR spectrum of H[3,5-Ph<sub>2</sub>dp] in DMSO- $d_6$  at 23 °C.



**Figure S6.** The <sup>1</sup>H NMR spectrum of **1** in DMSO- $d_6$  at 23 °C.



**Figure S7.** The <sup>1</sup>H NMR spectrum of **2** in DMSO- $d_6$  at 23 °C.



**Figure S8.** The <sup>1</sup>H NMR spectrum of **3** in DMSO- $d_6$  at 23 °C.



**Figure S9.** The <sup>1</sup>H NMR spectrum of **4** in DMSO- $d_6$  at 23 °C.



**Figure S10.** The <sup>1</sup>H NMR spectrum of **6** in DMSO- $d_6$  at 23 °C.



**Figure S11.** The <sup>1</sup>H NMR spectrum of **7** in DMSO- $d_6$  at 23 °C.