Investigation of Triphenylamine (TPA) based Metal Complexes and Their Application in Perovskite Solar Cells

Wei Zhang, ^a Peng Liu, ^a Azar Sadollahkhani, ^a Yuanyuan Li, ^b Biaobiao Zhang, ^c Fuguo Zhang, ^c Majid Safdari, ^a Yan Hao, ^{d, 1} Yong Hua, ^{a*, 2} Lars Kloo ^{a*}

a) Department of Chemistry, Applied Physical Chemistry, KTH Royal Institute of Technology, SE-10044 Stockholm, Sweden.

 b) Wallenberg Wood Science Center, Department of Fiber and Polymer Technology, KTH Royal Institute of Technology, SE-10044 Stockholm, Sweden

c) Department of Chemistry, Organic Chemistry, KTH Royal Institute of Technology, SE-10044 Stockholm, Sweden

d) Department of Chemistry – Ångström Laboratory, Physical Chemistry, Uppsala University, SE-75120 Uppsala, Swede

¹ Department of Chemistry, Applied Physical Chemistry, KTH Royal Institute of Technology, SE-10044 Stockholm, Sweden.

² School of Materials Science and Engineering, Yunnan University, Kunming 650000, P. R. China.



Figure S1. ¹H NMR of **Y1** in d6-Acetone



Figure S2. ¹³C NMR of **Y1** in d6-DMSO



Figure S3. ¹H NMR of **Y3** in CDCl₃



Figure S4. ¹³C NMR of **Y3** in CDCl₃



Figure S5. Mass Spectroscopy of Y1



Figure S6. Mass Spectroscopy of Y2



Figure S7. Mass Spectroscopy of Y3



Figure S8. changes in the UV–vis spectra of **Y3** with gradual addition of different amounts of TeCA as dopant.



Figure S9. (a) UV/vis absorption of Spiro-OMeTAD with gradual addition of different amounts of **Y1** as dopant. (b) UV/vis absorption of Spiro-OMeTAD with gradual addition of different amounts of **Y2** as dopant. (c) UV/vis absorption of Spiro-OMeTAD with gradual addition of different amounts of **Y3** as dopant.



Figure S10. Current-voltage characteristics of ligand (**4**) with doping of 10 mM LiTFSI, 100 mM TBP and 4% volume TeCA



Figure S11. Photovoltaic performance of perovskite solar cell without hole transport materials.



Figure S12. Distribution of efficiencies of PSCs based on **Y1**, **Y2** and **Y3** as hole transport materials.



Figure S13. (a) Photovoltaic performance with increased concentrations of **Y1**, (b) Photovoltaic performance with increased concentrations of **Y2**. (c) Photovoltaic performance with increased concentrations of **Y3**.