Electronic Supplementary Information

Positional isomerism in triarylmethyl carbocation radical salts:

position isomeric effects, crystal structures and properties

Guo-Ping Yong,* Chen Shen, Ya Feng, Xue-Rui Zhang and Yu-Mei Zhao

Department of Chemistry, University of Science and Technology of China, Hefei 230026, P. R. China

E-mail: gpyong@ustc.edu.cn



Scheme S1 Proposed reaction mechanism.



Fig. S1 Dihedral angles among two imidazo[1,2-*a*]pyridine rings and one pyridine ring for **1**.



Fig. S2 Dihedral angles among two imidazo[1,2-a]pyridine rings and one pyridine ring for 2.



Fig. S3 Dihedral angles among two imidazo[1,2-a]pyridine rings and one pyridine ring for 3.



Fig. S4 The space-filling representation for 1 (a), 2 (b) and 3 (c): showing the high steric shielding of the central carbon atom (green).



Fig. S5 ORTEP diagrams with ellipsoids drawn at 50% probability for triarylmethyl carbocation radical moiety in **1** (a, selected bond lengths: C8–C7 of 1.395(5) Å, C8–C9 of 1.386(5) Å, and C8–C16 of 1.487(5) Å; selected bond angles: C7–C8–C9 of 123.5(3)°, C7–C8–C16 of 119.9(3)°, and C9–C8–C16 of 115.9(3)°), **2** (b, selected bond lengths: C8–C7 of 1.395(4) Å, C8–C9 of 1.387(5) Å, and C8–C16 of 1.487(4) Å; selected bond angles: C7–C8–C9 of 122.7(3)°, C7–C8–C16 of 119.8(3)°, and C9–C8–C16 of 117.2(3)°) and **3** (c, selected bond lengths: C8–C7 of 1.417(4) Å, C8–C9 of 1.372(5) Å, and C8–C16 of 1.494(4) Å; selected bond angles: C7–C8–C9 of 1.24.0(3)°, C7–C8–C16 of 118.8(3)°, and C9–C8–C16 of 116.8(3)°).



Fig. S6 The PXRD patterns of 1.



Fig. S7 The PXRD patterns of 2.



Fig. S8 The PXRD patterns of 3.



Fig. S9 TGA curves for triarylmethyl carbocation radical salts 1 (a) and 2 (b).