## 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 $\mathbf{1}$ (a), 2 (b) and $\mathbf{3}$ (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 $\mathbf{1}$ (a, selected bond lengths: C8-C7 of 1.395(5) $\AA, \mathrm{C} 8-$ C9 of $1.386(5) \AA$, and C8-C16 of $1.487(5) \AA$; selected bond angles: C7-C8-C9 of $123.5(3)^{\circ}, \mathrm{C} 7-\mathrm{C} 8-\mathrm{C} 16$ of $119.9(3)^{\circ}$, and C9-C8-C16 of $\left.115.9(3)^{\circ}\right), \mathbf{2}(\mathrm{b}$, selected bond lengths: C8-C7 of $1.395(4) \AA, \mathrm{C} 8-\mathrm{C} 9$ of $1.387(5) \AA$, and C8-C16 of $1.487(4) \AA$; selected bond angles: C7-C8-C9 of $122.7(3)^{\circ}$, C7-C8-C16 of 119.8(3) ${ }^{\circ}$, and C9-C8-C16 of $117.2(3)^{\circ}$ ) and 3 (c, selected bond lengths: C8-C7 of 1.417(4) $\AA, \mathrm{C} 8-\mathrm{C} 9$ of $1.372(5) \AA$, and $\mathrm{C} 8-\mathrm{C} 16$ of $1.494(4) \AA$; selected bond angles: $\mathrm{C} 7-\mathrm{C} 8-\mathrm{C} 9$ of $124.0(3)^{\circ}, \mathrm{C} 7-\mathrm{C} 8-\mathrm{C} 16$ of $118.8(3)^{\circ}$, and $\mathrm{C} 9-\mathrm{C} 8-\mathrm{C} 16$ of $\left.116.8(3)^{\circ}\right)$.


Fig. S6 The PXRD patterns of $\mathbf{1}$.


Fig. S7 The PXRD patterns of $\mathbf{2}$.


Fig. $\mathbf{S 8}$ The PXRD patterns of $\mathbf{3}$.


Fig. S9 TGA curves for triarylmethyl carbocation radical salts $\mathbf{1}$ (a) and 2 (b).

