Supplementary Material (ESI) for New Journal of Chemistry

Supporting Information for

Formation of hexaarylbiimidazole heterodimers via cross recombination of two lophyl radicals

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Investigation R_f values of homo-HABI derivatives.

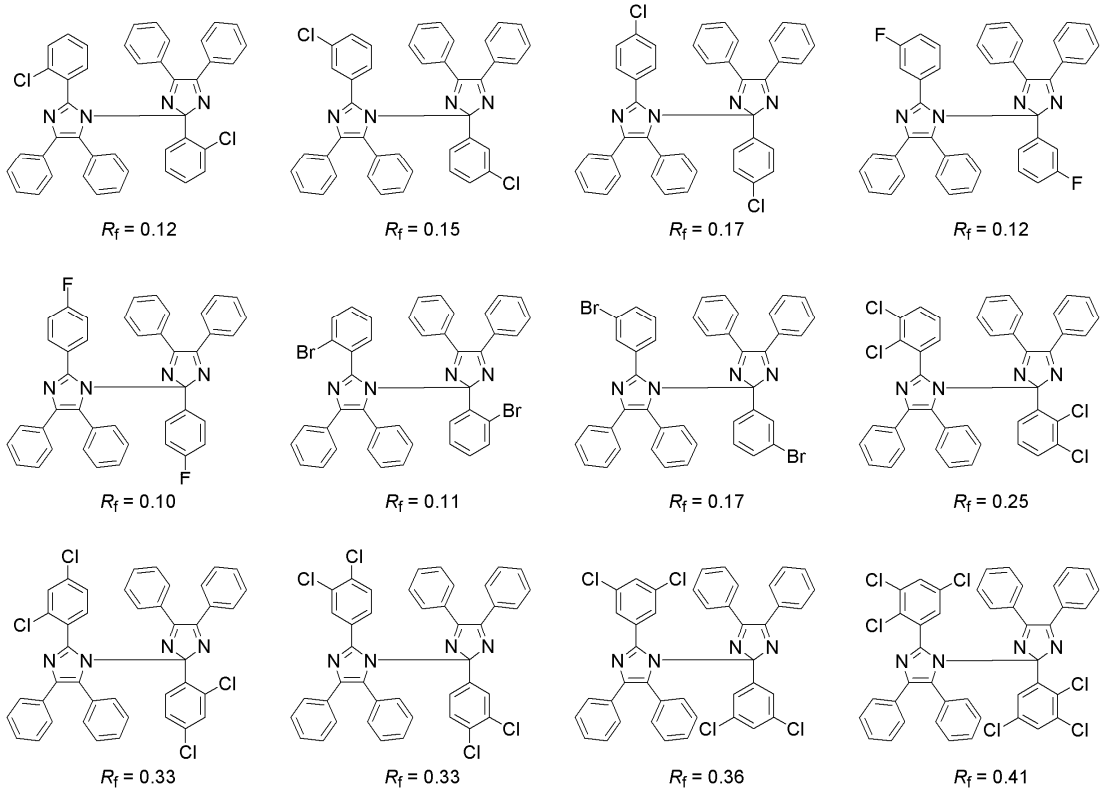

Fig. S1 Chemical structures and the R_f values (SiO_2 TLC) in chloroform of various HABI derivatives.

We checked R_f values of HABI derivatives shown above. We prepared these HABIs by a literature procedures,[1] and checked their R_f values in chloroform. We have chosen *o*-Cl-HABI (**1-1**) and 2,3,5-triCl-HABI (**2-2**) because they showed the most different R_f values in chloroform.

X-ray Crystallographic Analysis.

The diffraction data of the single crystal of HABI derivatives was collected on the Bruker APEX II CCD area detector (Mo$K\alpha$, λ = 0.71073 nm). During the data collection, the lead grass doors of the diffractometer were covered to exclude the room light. The data refinement was carried out by the Bruker APEXII software package with SHELXT program.[2] All non-hydrogen atoms were anisotropically refined.

From the X-ray crystallographic analysis (Fig. S2-S5), we found the C−N bond connecting two imidazolyl rings is formed between N1 and C2 (1,2'-isomer), which can generally be found in other HABI derivatives and The C-N bond lengths of these four HABIs are almost the same (**1-1**: 1.484 Å, **1-2**: 1.477 Å, **2-1**: 1.475 Å, and **2-2**: 1.476 Å, respectively). Crystallographic parameters of four HABI derivatives are shown in Table S1 and S2.

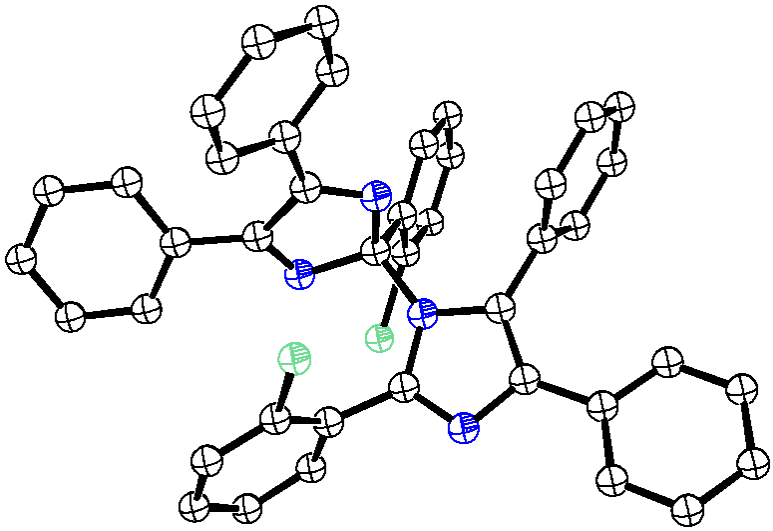

Fig. S2 Crystal structure of **1-1** (50% probability).

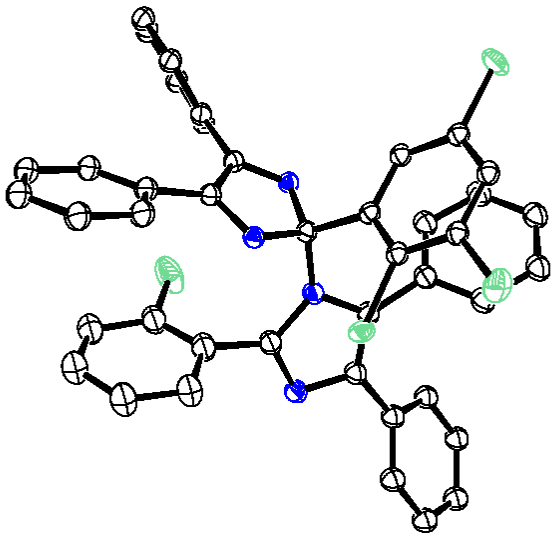

Fig. S3 Crystal structure of **1-2** (50% probability).

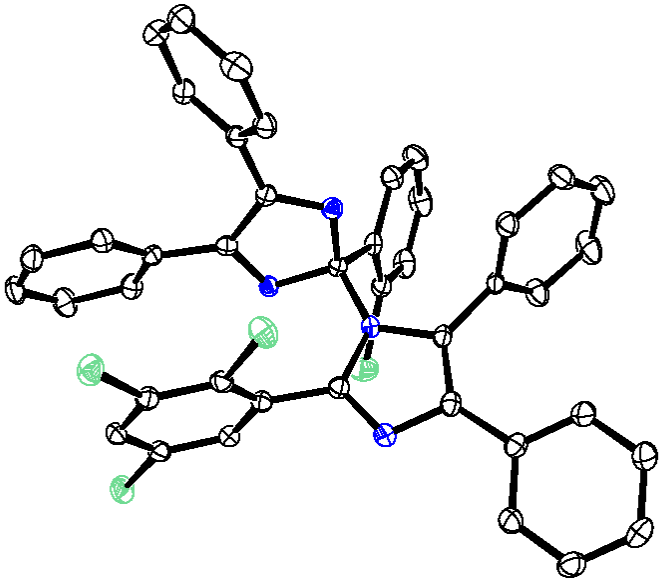

Fig. S4 Crystal structure of **2-1** (50% probability).

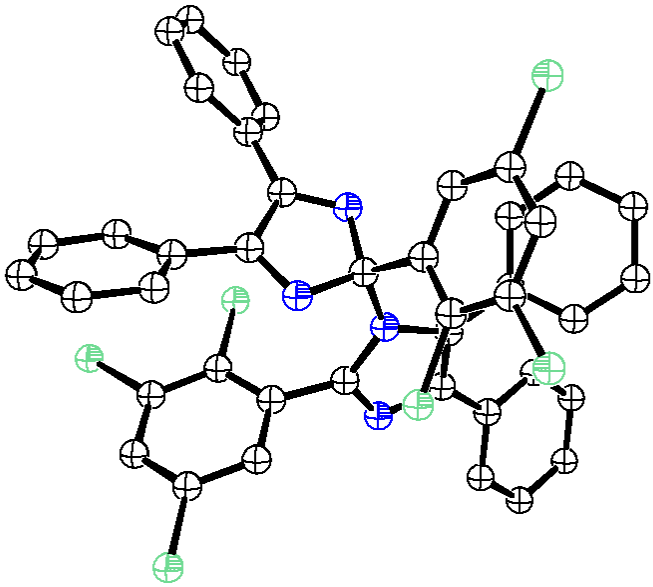

Fig. S5 Crystal structure of **2-2** (50% probability).

Table S1 Crystallographic parameters of **1-1** and **1-2**.

	1-1	**1-2**
Empirical formula	C42 H28 Cl2 N4	C42 H26 Cl4 N4
Formula weight	659.58	728.47
Temperature, K	103(2)	103
Crystal system	orthorhombic	orthorhombic
Space group	Pbca	Pbca
a, Å	16.7314(2)	16.1217(4)
b, Å	17.3877(3)	12.4587(3)
c, Å	46.0307(6)	34.4958(10)
α, degree	90.00	90
β, degree	90.00	90
γ, degree	90.00	90
Volume, Å ^{3}	13391.3(3)	6928.7(3)
Z	16	8
Density (calculated), Mg/m^3	1.309	1.397
Crystal size, mm^3	0.32 × 0.30 × 0.08	0.30 × 0.20 × 0.05
λ (Mo Kα), Å	0.71073	0.71073
Reflections collected	123308	53043
Independent reflections	19426	6337
G.O.F.	1.005	1.012
R_1	0.0409	0.0708
wR_2	0.0924	0.1555

Table S2 Crystallographic parameters of **2-1** and **2-2**.

	2-1	**2-2**
Empirical formula	C42 H26 Cl4 N4	C54 H36 Cl6 N4
Formula weight	728.47	953.57
Temperature, K	103	103(2)
Crystal system	monoclinic	monoclinic
Space group	P2(1)/n	P2(1)/n
a, Å	12.350(2)	17.8938(4)
b, Å	15.981(3)	14.1917(3)
c, Å	18.000(3)	18.1886(3)
α, degree	90	90.00
β, degree	107.400(2)	97.6160(10)
γ, degree	90	90.00
Volume, Å^3	3390.0(10)	4578.13(16)
Z	4	4
Density (calculated), Mg/m^3	1.427	1.383
Crystal size, mm^3	0.30 × 0.20 × 0.20	0.20 × 0.16 × 0.16
λ (Mo Kα), Å	0.71073	0.71073
Reflections collected	18776	81831
Independent reflections	7669	16461
G.O.F.	1.003	1.025
R_1	0.0451	0.0435
wR_2	0.1442	0.1007

References

(1) (a) K. Fujita, S. Hatano, D. Kato, J. Abe, *Org*. *Lett*. 2008, **10**, 3105. (b) S. Hatano, J. Abe, *J*. *Phys*. *Chem*. *A* 2008, **112**, 6098. (c) Y. Miyamoto, A. Kikuchi, F. Iwahori, J. Abe, *J*. *Phys*. *Chem*. *A* 2005, **109**, 10183.

(2) (a) Sheldrick GM. SHELXS-97 and SHELXL-97 1997; University of Gottingen, Germany. (b) Sheldrick GM. SADABS 1996; University of Gottingen, Germany.