

# Investigation of Lewis acidic behaviour of an oxygen-bridged planarized triphenylborane toward amines and properties of their Lewis acid-base adducts

Yuichi Kitamoto,<sup>\*,a</sup> Fumiaki Kobayashi,<sup>b</sup> Takatsugu Suzuki,<sup>b</sup> Yasuo Miyata,<sup>b</sup> Hiroshi Kita,<sup>b</sup> Kenji Funaki,<sup>c</sup> Shuichi Oi<sup>\*,a</sup>

<sup>a</sup> New Industry Creation Hatchery Center, Tohoku University, 6-6-11 Aramaki-Aoba, Aoba-ku, Sendai 980-8579, Japan. E-mail: kitamoto@orgsynth.che.tohoku.ac.jp, oishu@aporg.che.tohoku.ac.jp

<sup>b</sup> Advanced Technology Center, Corporate R&D Headquarters, Konica Minolta, Inc., 2970 Ishikawa-Machi, Hachioji-shi, Tokyo 192-8505, Japan

<sup>c</sup> Department of Biomolecular Engineering, Graduate School of Engineering, Tohoku University, 6-6-11 Aramaki-Aoba, Aoba-ku, Sendai 980-8579, Japan

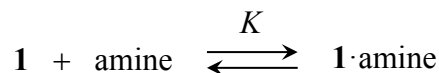
## Supplementary Information

### Contents:

1. UV-vis absorption study	.....	S2
2. <sup>1</sup> NMR spectroscopy study	.....	S6
3. X-ray crystallographic analysis	.....	S7
4. <sup>11</sup> B NMR spectroscopy study	.....	S9
5. Theoretical calculation	.....	S10
6. Transient photoluminescent decay study	.....	S31
7. References	.....	S33

## 1. UV-vis absorption study

The binding constant ( $K$ ) of oxaplanarborane **1** with pyridine, DMAP, or quinuclidine (the stoichiometry of **1**·amine is 1:1 ratio) is expressed as follow.



$$K = \frac{[\mathbf{1} \cdot \text{amine}]}{[\mathbf{1}][\text{amine}]}$$

$$\rightarrow K = \frac{[\mathbf{1} \cdot \text{amine}]}{([\mathbf{1}]_0 - [\mathbf{1} \cdot \text{amine}])([\text{amine}]_0 - [\mathbf{1} \cdot \text{amine}])}$$

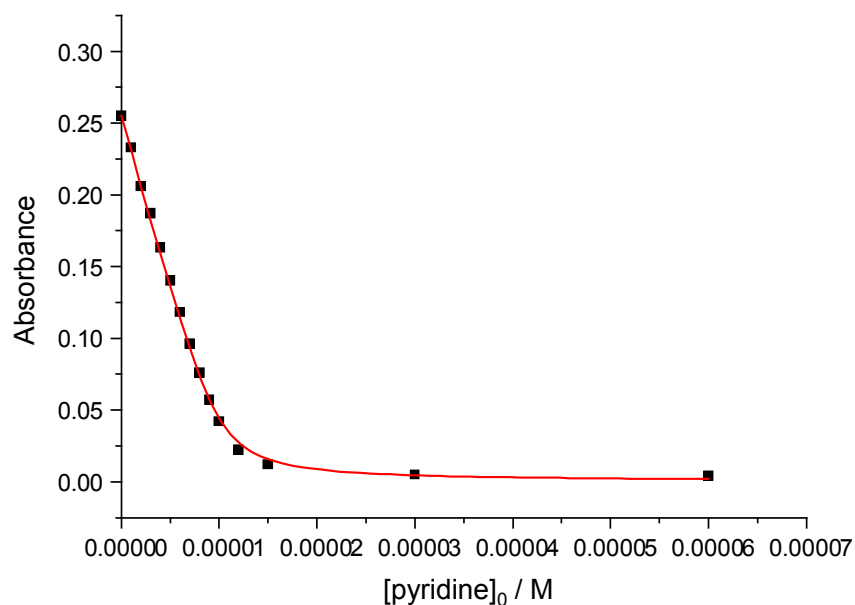
The concentration of **1**·amine is expressed as follows.

$$([\mathbf{1}]_0 - [\mathbf{1} \cdot \text{amine}])([\text{amine}]_0 - [\mathbf{1} \cdot \text{amine}])K = [\mathbf{1} \cdot \text{amine}]$$

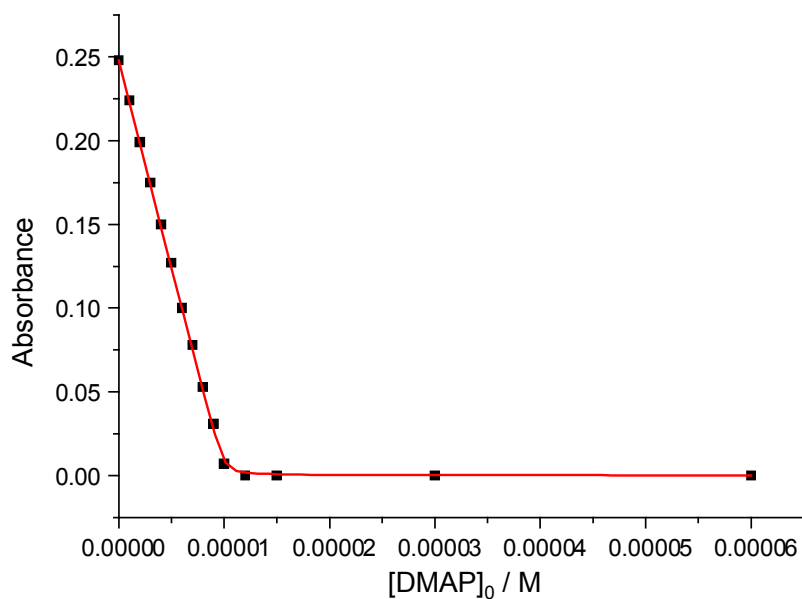
$$\rightarrow [\mathbf{1} \cdot \text{amine}]^2 - ([\mathbf{1}]_0 + [\text{amine}]_0 + 1/K)[\mathbf{1} \cdot \text{amine}] + [\mathbf{1}]_0[\text{amine}]_0 = 0$$

$$\rightarrow [\mathbf{1} \cdot \text{amine}] = \frac{([\mathbf{1}]_0 + [\text{amine}]_0 + 1/K) - \sqrt{([\mathbf{1}]_0 + [\text{amine}]_0 + 1/K)^2 - 4[\mathbf{1}]_0[\text{amine}]_0}}{2} \quad (1)$$

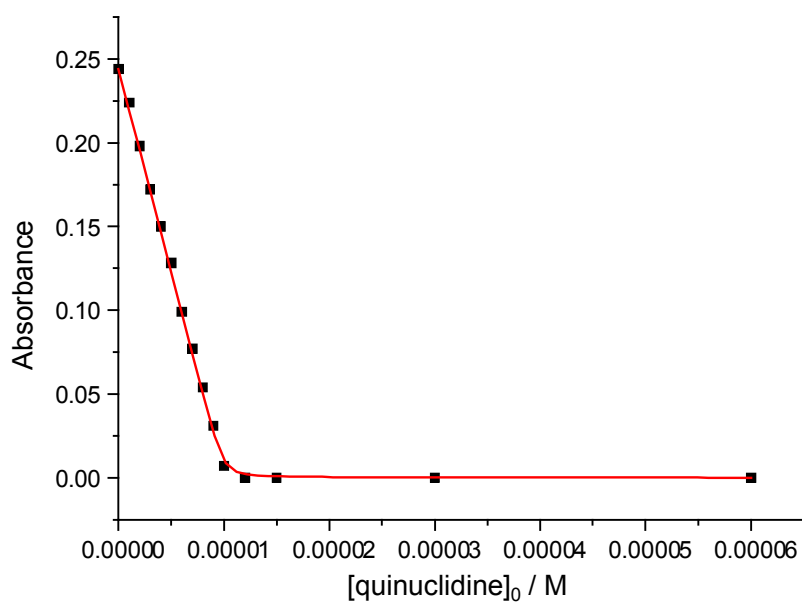
The binding constant  $K$  can be calculated by fitting the experimental data to the above 1:1 binding model according to the literature method.<sup>S1,S2</sup>



**Figure S1** The absorbance changes of **1** at 338 nm ( $1 \times 10^{-5}$  M, in cyclohexane) upon addition of pyridine at 23 °C. The fitting curve was obtained by using eq. 1. The binding constant  $K$  of **1**·pyridine was calculated to be  $2.7(\pm 0.21) \times 10^6 \text{ M}^{-1}$  ( $R^2 = 0.996$ ).

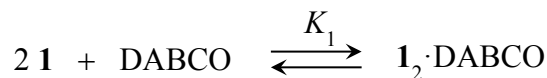


**Figure S2** The absorbance changes of **1** at 338 nm ( $1 \times 10^{-5}$  M, in cyclohexane) upon addition of DMAP at 23 °C. The fitting curve was obtained by using eq. 1. The binding constant  $K$  of **1**·DMAP was calculated to be  $6.6(\pm 1.9) \times 10^7 \text{ M}^{-1}$  ( $R^2 = 0.999$ ).



**Figure S3** The absorbance changes of **1** at 338 nm ( $1 \times 10^{-5}$  M, in cyclohexane) upon addition of quinuclidine at 23 °C. The fitting curve was obtained by using eq. 1. The binding constant  $K$  of **1**·quinuclidine was calculated to be  $5.3(\pm 2.2) \times 10^7 \text{ M}^{-1}$  ( $R^2 = 0.998$ ).

The binding constant ( $K_1$ ) of **1** with DABCO (the stoichiometry of **1**·DABCO is 2:1 ratio, i.e., **1**<sub>2</sub>·DABCO) is expressed as follow.



$$K_1 = \frac{[\mathbf{1}_2 \cdot \text{DABCO}]}{[\mathbf{1}]^2 [\text{DABCO}]}$$

$$\rightarrow K_1 = \frac{[\mathbf{1}_2 \cdot \text{DABCO}]}{([\mathbf{1}]_0 - 2[\mathbf{1}_2 \cdot \text{DABCO}])^2 ([\text{DABCO}]_0 - [\mathbf{1}_2 \cdot \text{DABCO}])}$$

$$\rightarrow \frac{1}{([\mathbf{1}]_0 - 2[\mathbf{1}_2 \cdot \text{DABCO}])^2} = K_1 \left( \frac{[\text{DABCO}]_0}{[\mathbf{1}_2 \cdot \text{DABCO}]} - 1 \right) \quad (\text{S1})$$

The concentration of **1**<sub>2</sub>·DABCO ( $[\mathbf{1}_2 \cdot \text{DABCO}]$ ) can be expressed by eq. S2, where  $Abs$  and  $Abs_0$  represent the absorbance of **1** in the presence and absence of DABCO, respectively, and  $Abs_\infty$  represents the absorbance of **1**<sub>2</sub>·DABCO.

$$2[\mathbf{1}_2 \cdot \text{DABCO}] = [\mathbf{1}]_0 \frac{Abs_0 - Abs}{Abs_0 - Abs_\infty}$$

$$\rightarrow [\mathbf{1}_2 \cdot \text{DABCO}] = \frac{[\mathbf{1}]_0 B}{2}, \text{ where } B = \frac{Abs_0 - Abs}{Abs_0 - Abs_\infty} \quad (\text{S2})$$

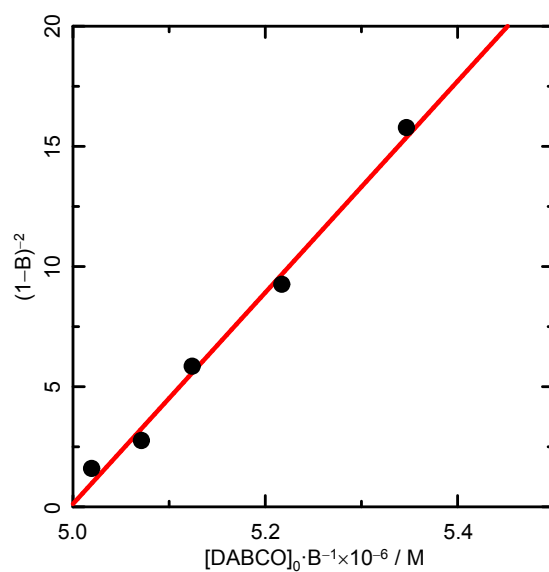
To calculate the  $K_1$  value, eq. 2 can be derived from eqs. S1 and S2 according to the literature derivation.<sup>S3,S4</sup>

$$\frac{1}{([\mathbf{1}]_0 - [\mathbf{1}]_0 B)^2} = K_1 \left( \frac{2[\text{DABCO}]_0}{[\mathbf{1}]_0 B} - 1 \right)$$

$$\rightarrow \frac{1}{(1_0 - B)^2} = K_1 \left( \frac{2[\text{DABCO}]_0}{[\mathbf{1}]_0 B} - 1 \right) [\mathbf{1}]_0^2$$

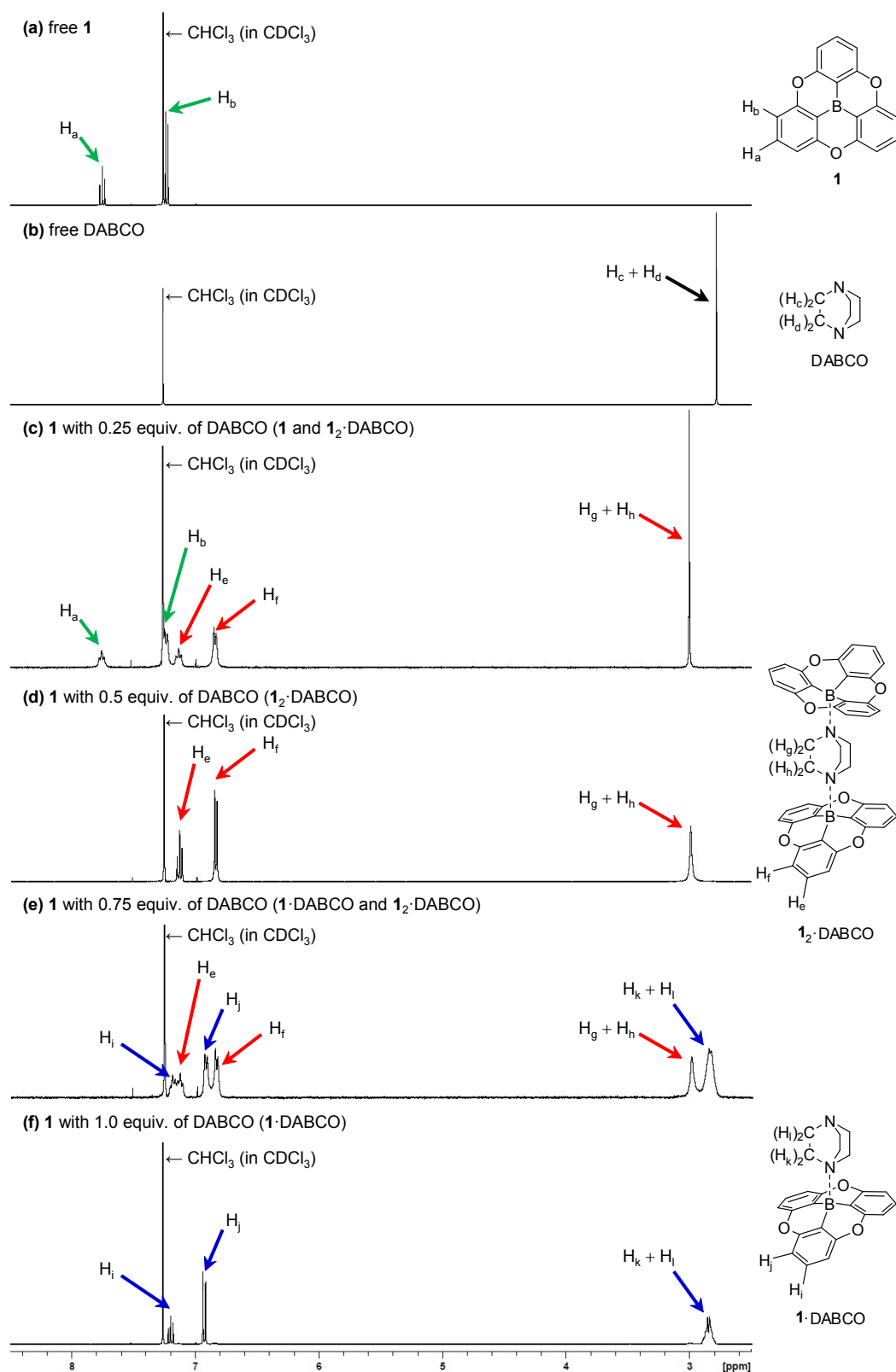
$$\rightarrow \frac{1}{(1_0 - B)^2} = K_1 [\mathbf{1}]_0 \left( \frac{2[\text{DABCO}]_0}{B} - [\mathbf{1}]_0 \right) \quad (2)$$

As shown in Figure S4, the linear plot of  $(1-B)^{-2}$  versus  $[\text{DABCO}]_0 \cdot B^{-1}$  is obtained according to the literature method.<sup>S3,S4</sup>



**Figure S4** The absorbance changes of **1** at 338 nm ( $1 \times 10^{-5}$  M, in cyclohexane) upon addition of DABCO at 23 °C. The liner plot was obtained by using eq. 2. The binding constant  $K_1$  of **1**<sub>2</sub>·DABCO was calculated to be  $2.2(\pm 0.11) \times 10^{12} \text{ M}^{-2}$  ( $R^2 = 0.992$ ).

## 2. $^1\text{H}$ NMR spectroscopy study



**Figure S5**  $^1\text{H}$  NMR spectra of a mixture of **1** ( $3.9 \times 10^{-3}$  M) and DABCO at 23 °C in  $\text{CDCl}_3$ . Tetramethylsilane was used as an internal standard (0 ppm).

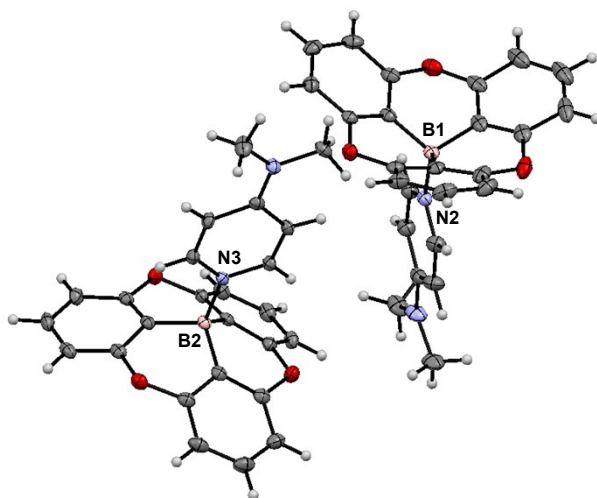
### 3. X-ray crystallographic analysis

**Table S1** Crystallographic data for **1**·DMAP, **1**·quinuclidine, and **1**<sub>2</sub>·DABCO

	<b>1</b> ·DMAP	<b>1</b> ·quinuclidine·(C <sub>6</sub> H <sub>12</sub> ) <sub>2</sub> <sup>a</sup>	<b>1</b> <sub>2</sub> ·DABCO·CHCl <sub>3</sub> <sup>b</sup>
Empirical formula	C <sub>50</sub> H <sub>38</sub> B <sub>2</sub> N <sub>4</sub> O <sub>6</sub>	C <sub>37</sub> H <sub>46</sub> BNO <sub>3</sub>	C <sub>22</sub> H <sub>16</sub> BCl <sub>3</sub> NO <sub>3</sub>
Formula weight	812.46	563.56	459.52
Crystal system	Monoclinic	Orthorhombic	Monoclinic
Space group	<i>P</i> 2 <sub>1</sub> / <i>n</i>	<i>P</i> mn2 <sub>1</sub>	<i>C</i> 2/ <i>c</i>
<i>a</i> / Å	14.9464(15)	17.996(3)	23.783(3)
<i>b</i> / Å	14.1675(14)	8.2540(16)	9.9498(10)
<i>c</i> / Å	19.4407(19)	10.502(3)	18.2611(19)
<i>α</i> / °	90	90	90
<i>β</i> / °	107.4270(10)	90	113.2150(10)
<i>γ</i> / °	90	90	90
<i>V</i> / Å <sup>3</sup>	3927.7(7)	1560.0(6)	3917.4(7)
<i>Z</i>	4	2	8
F(000)	1696	608	1880
<i>T</i> / K	100(2)	223(2)	100(2)
<i>ρ</i> <sub>calc</sub> / gcm <sup>-3</sup>	1.374	1.200	1.537
Reflections collected	22063	8774	11025
Independent reflections	8878	3565	4457
	[ <i>R</i> <sub>int</sub> = 0.0282]	[ <i>R</i> <sub>int</sub> = 0.0257]	[ <i>R</i> <sub>int</sub> = 0.0199]
<i>R</i> <sub>1</sub> , <i>wR</i> <sub>2</sub> ( <i>I</i> > 2σ( <i>I</i> ))	0.0413, 0.1226	0.0802, 0.2337	0.0444, 0.1192
<i>R</i> <sub>1</sub> , <i>wR</i> <sub>2</sub> (all data)	0.0600, 0.1400	0.0962, 0.2548	0.0474, 0.1218
Goodness-of-fit on <i>F</i> <sup>2</sup>	0.980	1.019	1.042
Largest diff. peak and hole / e·Å <sup>3</sup>	0.355 and -0.250	0.420 and -0.317	0.692 and -0.627

<sup>a</sup> Cyclohexane molecule (C<sub>6</sub>H<sub>12</sub>) was included. <sup>b</sup> Chloroform molecule (CHCl<sub>3</sub>) was included.

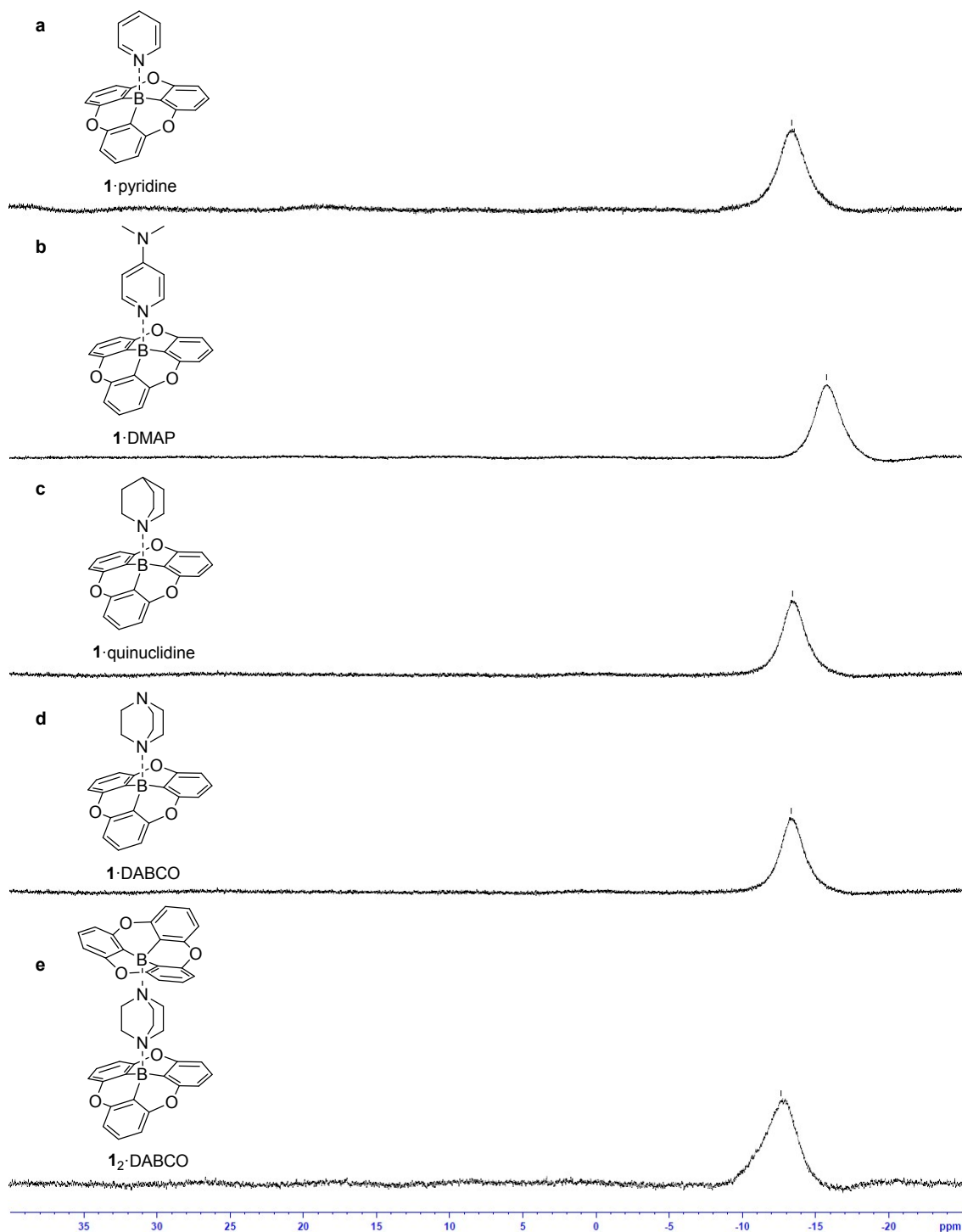
The data of **1**·quinuclidine have B Alert in the checkCIF program because the cyclohexane molecule included into the crystal shows severely disordered structure and it is also difficult to assign the hydrogen atoms of the cyclohexane molecule.



**Figure S6** Thermal ellipsoid plot drawing of **1·DMAP** (50% probability ellipsoids). Two crystallographically independent molecules were observed. Selected lengths (Å): N2–B1, 1.6195(19); N3–B2, 1.6179(19). The summation of the  $C_{\text{ipso}}\text{--B--}C_{\text{ipso}}$  angles is  $322.1^\circ$  for B1 and  $322.1^\circ$  for B2.



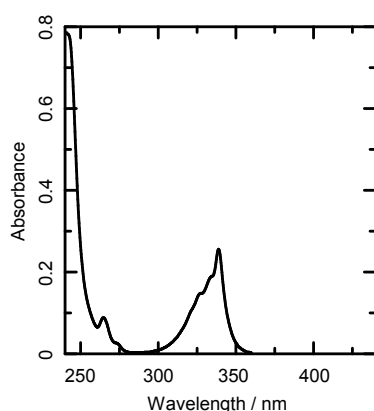
#### 4. $^{11}\text{B}$ NMR spectroscopy study



**Figure S7**  $^{11}\text{B}$  NMR spectra of  $1_n$ ·amine (DABCO:  $n = 1, 2$ ; the other amine:  $n = 1$ ) at 23 °C in  $\text{CDCl}_3$  (Table 1).  $\text{BF}_3 \cdot \text{OEt}_2$  was used as an external standard (0 ppm).

## 5. Theoretical calculation

To optimize molecular structures of **1**, **1**·pyridine, **1**·DMAP, **1**·quinuclidine, **1**<sub>2</sub>·DABCO, and **1**·DABCO at the ground state, DFT calculations were carried out using the Gaussian 09 package<sup>S5</sup> at the B3LYP/6-311G(d,p) level (in cyclohexane, PCM model). After the optimization, the TD-DFT calculations were also conducted at the B3LYP/6-311G(d,p) level (in cyclohexane, PCM model). The output views were obtained by using the GaussView version 5.0.<sup>S6</sup>



**Figure S8** Experimental UV-vis absorption spectrum of **1** ( $1 \times 10^{-5}$  M, in cyclohexane) in the absence of amine at 23 °C.

**Table S2** Calculated excitation energy ( $E$ ,  $\lambda$ ) and oscillator strength ( $f$ ) of **1** by DFT and TD-DFT at the B3LYP/6-311G(d,p) level (in cyclohexane, PCM model).

Transition	$E$ / eV	$\lambda$ / nm	$f^a$	Main CI coefficient $b$
1	3.847	322	0.1074	HOMO $\rightarrow$ LUMO 0.6939
	3.847	322	0.1077	HOMO-1 $\rightarrow$ LUMO 0.6939
2	4.661	266	0.0048	HOMO-2 $\rightarrow$ LUMO -0.2377
				HOMO-1 $\rightarrow$ LUMO+2 -0.4607
				HOMO $\rightarrow$ LUMO+2 0.4619
3	4.871	255	0.0063	HOMO-2 $\rightarrow$ LUMO 0.5344
				HOMO $\rightarrow$ LUMO+3 0.4258
	4.871	255	0.0063	HOMO-3 $\rightarrow$ LUMO 0.5344
				HOMO-1 $\rightarrow$ LUMO+3 0.4262

<sup>a</sup> Oscillator strength. <sup>b</sup> Coefficient of the wave function for each excitation.

**(Table S2 Continued)**

Transition	$E / \text{eV}$	$\lambda / \text{nm}$	$f^a$	Main CI coefficient $b$	
4	5.154	240	0.7862	HOMO-2 $\rightarrow$ LUMO	-0.3823
				HOMO-1 $\rightarrow$ LUMO+1	-0.1276
				HOMO $\rightarrow$ LUMO+2	-0.1271
				HOMO $\rightarrow$ LUMO+3	0.5401
	5.154	240	0.7859	HOMO-3 $\rightarrow$ LUMO	-0.3825
				HOMO-1 $\rightarrow$ LUMO+2	0.1281
				HOMO-1 $\rightarrow$ LUMO+3	0.5397
				HOMO $\rightarrow$ LUMO+1	-0.1276

<sup>a</sup> Oscillator strength. <sup>b</sup> Coefficient of the wave function for each excitation.

**Table S3** Calculated excitation energy of  $S_1$  ( $E_{S_1}$ ) and  $T_1$  ( $E_{T_1}$ ),  $\Delta(S_1-T_1)@S_0$ , and oscillator strength ( $f$ ) by DFT and TD-DFT at the B3LYP/6-311G(d,p) level (in cyclohexane, PCM model).<sup>a</sup>

Compound	$E_{S_1} / \text{eV}$	$E_{T_1} / \text{eV}$	$\Delta(S_1-T_1)@S_0 / \text{eV}$
	$f$	$f$	
<b>1</b>	3.847	3.292	0.554
	0.1074	0	
<b>1</b> ·pyridine	2.967	2.952	0.015
	0.0006	0	
<b>1</b> ·DMAP	3.711	3.506	0.205
	0.0010	0	
<b>1</b> ·Quinuclidine	4.584	3.601	0.984
	0.0581	0	
<b>1</b> <sub>2</sub> ·DABCO	4.537	3.597	0.940
	0.1047	0	
<b>1</b> ·DABCO	4.577	3.600	0.977
	0.0591	0	

<sup>a</sup> Based on the optimized geometry at the ground state ( $S_0$ ).

**Table S4** Calculated excitation energy ( $E$ ,  $\lambda$ ) and oscillator strength ( $f$ ) of **1**-pyridine by DFT and TD-DFT at the B3LYP/6-311G(d,p) level (in cyclohexane, PCM model).

Transition	$E$ / eV	$\lambda$ / nm	$f^a$	Main CI coefficient $b$	
1	2.967	418	0.0006	HOMO $\rightarrow$ LUMO	0.7062
2	2.984	415	0.0012	HOMO-1 $\rightarrow$ LUMO	0.7062
3	3.697	335	0.0012	HOMO $\rightarrow$ LUMO+1	0.7054
4	3.743	331	0.0019	HOMO-4 $\rightarrow$ LUMO	0.4750
				HOMO-2 $\rightarrow$ LUMO	0.4663
				HOMO-1 $\rightarrow$ LUMO+1	0.2340
5	3.847	322	0.0004	HOMO-4 $\rightarrow$ LUMO	-0.4772
				HOMO-2 $\rightarrow$ LUMO	0.5163
6	4.297	288	0.0009	HOMO-5 $\rightarrow$ LUMO	0.7061
7	4.565	272	0.0119	HOMO-3 $\rightarrow$ LUMO+1	0.6976
				HOMO-4 $\rightarrow$ LUMO+1	-0.3732
				HOMO-2 $\rightarrow$ LUMO+1	0.5163
				HOMO $\rightarrow$ LUMO+2	-0.2547
8	4.605	269	0.0527	HOMO-4 $\rightarrow$ LUMO+1	-0.2771
				HOMO $\rightarrow$ LUMO+2	0.5364
				HOMO $\rightarrow$ LUMO+3	0.1849
9	4.645	266	0.0478	HOMO-1 $\rightarrow$ LUMO+2	0.5635
				HOMO-1 $\rightarrow$ LUMO+3	-0.2630
				HOMO $\rightarrow$ LUMO+5	0.2002
10	4.836	256	0.0081	HOMO-1 $\rightarrow$ LUMO+2	0.3525
				HOMO-1 $\rightarrow$ LUMO+3	0.4404
				HOMO $\rightarrow$ LUMO+4	-0.4709
11	5.001	248	0.1644	HOMO-6 $\rightarrow$ LUMO	0.6663
				HOMO-1 $\rightarrow$ LUMO+3	-0.1520

<sup>a</sup>Oscillator strength. <sup>b</sup> Coefficient of the wave function for each excitation.

In comparison with the major excited states 7–11 having large oscillator strength, the excited states 1–6 show very smaller oscillator strength (Table S4).

**Table S5** Calculated excitation energy ( $E$ ,  $\lambda$ ) and oscillator strength ( $f$ ) of **1**-DMAP by DFT and TD-DFT at the B3LYP/6-311G(d,p) level (in cyclohexane, PCM model).

Transition	$E$ / eV	$\lambda$ / nm	$f^a$	Main CI coefficient $^b$	
1	3.711	334	0.0010	HOMO $\rightarrow$ LUMO	0.7054
2	3.724	332	0.0027	HOMO-1 $\rightarrow$ LUMO	0.7055
3	3.940	315	0.0017	HOMO $\rightarrow$ LUMO+1	0.7059
4	4.613	269	0.0489	HOMO $\rightarrow$ LUMO+2	0.5718
				HOMO $\rightarrow$ LUMO+3	0.2262
				HOMO-1 $\rightarrow$ LUMO+4	0.2117
5	4.670	265	0.0518	HOMO-1 $\rightarrow$ LUMO+2	0.5261
				HOMO-1 $\rightarrow$ LUMO+3	-0.2877
6	4.706	263	0.0119	HOMO-5 $\rightarrow$ LUMO+1	0.5957
				HOMO-3 $\rightarrow$ LUMO+1	0.3008
7	4.808	258	0.0074	HOMO-5 $\rightarrow$ LUMO+1	-0.3124
				HOMO-3 $\rightarrow$ LUMO+1	0.6266
8	4.852	256	0.0288	HOMO-1 $\rightarrow$ LUMO+2	0.3771
				HOMO-1 $\rightarrow$ LUMO+3	0.4118
				HOMO $\rightarrow$ LUMO+4	-0.3970
9	4.876	254	0.7292	HOMO-5 $\rightarrow$ LUMO+4	0.6466
				HOMO-1 $\rightarrow$ LUMO+3	0.1553
10	5.040	246	0.0045	HOMO-6 $\rightarrow$ LUMO	0.6983
11	5.113	242	0.0850	HOMO-1 $\rightarrow$ LUMO+3	0.3312
				HOMO $\rightarrow$ LUMO+4	0.4923
12	5.166	240	0.1814	HOMO-1 $\rightarrow$ LUMO+3	-0.2722
				HOMO $\rightarrow$ LUMO+5	0.5771
13	5.178	239	0.2952	HOMO-3 $\rightarrow$ LUMO+3	0.1445
				HOMO-1 $\rightarrow$ LUMO+5	0.6567
				HOMO $\rightarrow$ LUMO+2	-0.1583

<sup>a</sup> Oscillator strength. <sup>b</sup> Coefficient of the wave function for each excitation.

In comparison with the major excited states 4–13 having large oscillator strength, the excited states 1–3 show very smaller oscillator strength (Table S5).

**Table S6** Calculated excitation energy ( $E$ ,  $\lambda$ ) and oscillator strength ( $f$ ) of **1**·quinuclidine by DFT and TD-DFT at the B3LYP/6-311G(d,p) level (in cyclohexane, PCM model).

Transition	$E$ / eV	$\lambda$ / nm	$f^a$	Main CI coefficient $b$	
1	4.585	270	0.0581	HOMO $\rightarrow$ LUMO	0.5790
				HOMO-1 $\rightarrow$ LUMO	0.5789
2	4.822	257	0.0036	HOMO-1 $\rightarrow$ LUMO+2	0.4553
				HOMO $\rightarrow$ LUMO	-0.3020
				HOMO $\rightarrow$ LUMO+1	0.3826
				HOMO-1 $\rightarrow$ LUMO	-0.3029
				HOMO-1 $\rightarrow$ LUMO+1	-0.4170
				HOMO $\rightarrow$ LUMO+2	0.4235
3	5.081	244	0.0172	HOMO-1 $\rightarrow$ LUMO+1	0.4681
				HOMO $\rightarrow$ LUMO+2	0.4677
4	5.151	241	0.2503	HOMO-1 $\rightarrow$ LUMO	0.1449
				HOMO $\rightarrow$ LUMO+3	0.6600
				HOMO-1 $\rightarrow$ LUMO+3	0.6600
				HOMO $\rightarrow$ LUMO	-0.1449

<sup>a</sup>Oscillator strength. <sup>b</sup> Coefficient of the wave function for each excitation.

**Table S7** Calculated excitation energy ( $E$ ,  $\lambda$ ) and oscillator strength ( $f$ ) of  $\mathbf{1}_2\cdot\text{DABCO}$  by DFT and TD-DFT at the B3LYP/6-311G(d,p) level (in cyclohexane, PCM model).

Transition	$E$ / eV	$\lambda$ / nm	$f^a$	Main CI coefficient $b$	
1	4.534	274	0.0044	HOMO $\rightarrow$ LUMO	0.4752
				HOMO-1 $\rightarrow$ LUMO	0.4454
2	4.537	273	0.1061	HOMO-2 $\rightarrow$ LUMO	0.4457
				HOMO-3 $\rightarrow$ LUMO	0.4760
3	4.795	259	0.0008	HOMO-1 $\rightarrow$ LUMO	0.2759
				HOMO $\rightarrow$ LUMO	0.2776
4	4.797	258	0.0129	HOMO-2 $\rightarrow$ LUMO+3	0.2509
				HOMO-2 $\rightarrow$ LUMO+2	0.2749
5	4.938	251	0.0020	HOMO-2 $\rightarrow$ LUMO+1	0.5841
				HOMO-3 $\rightarrow$ LUMO+1	0.5838
6	5.067	245	0.0430	HOMO-3 $\rightarrow$ LUMO+2	0.2778
				HOMO-2 $\rightarrow$ LUMO+3	0.2395
				HOMO-1 $\rightarrow$ LUMO+3	0.2594
7	5.147	241	0.0008	HOMO $\rightarrow$ LUMO+6	0.3915
				HOMO-3 $\rightarrow$ LUMO+7	0.3423
				HOMO-1 $\rightarrow$ LUMO+6	0.3472
8	5.1545	240	0.4310	HOMO-2 $\rightarrow$ LUMO+6	0.3171
				HOMO $\rightarrow$ LUMO+7	0.3259
				HOMO-3 $\rightarrow$ LUMO+6	0.3638
				HOMO-2 $\rightarrow$ LUMO+7	-0.3004
				HOMO-1 $\rightarrow$ LUMO+7	0.3021

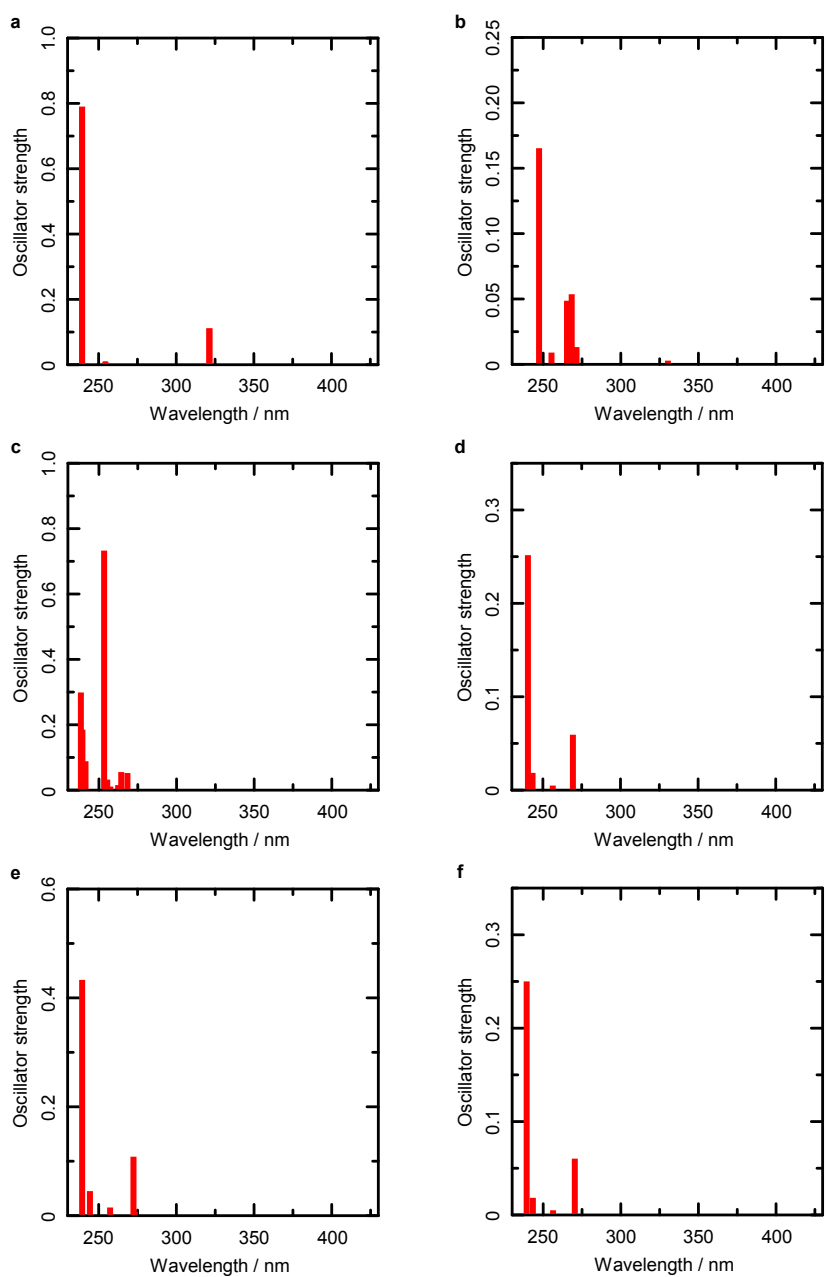
<sup>a</sup> Oscillator strength. <sup>b</sup> Coefficient of the wave function for each excitation.

**Table S8** Calculated excitation energy ( $E$ ,  $\lambda$ ) and oscillator strength ( $f$ ) of **1**-DABCO by DFT and TD-DFT at the B3LYP/6-311G(d,p) level (in cyclohexane, PCM model).

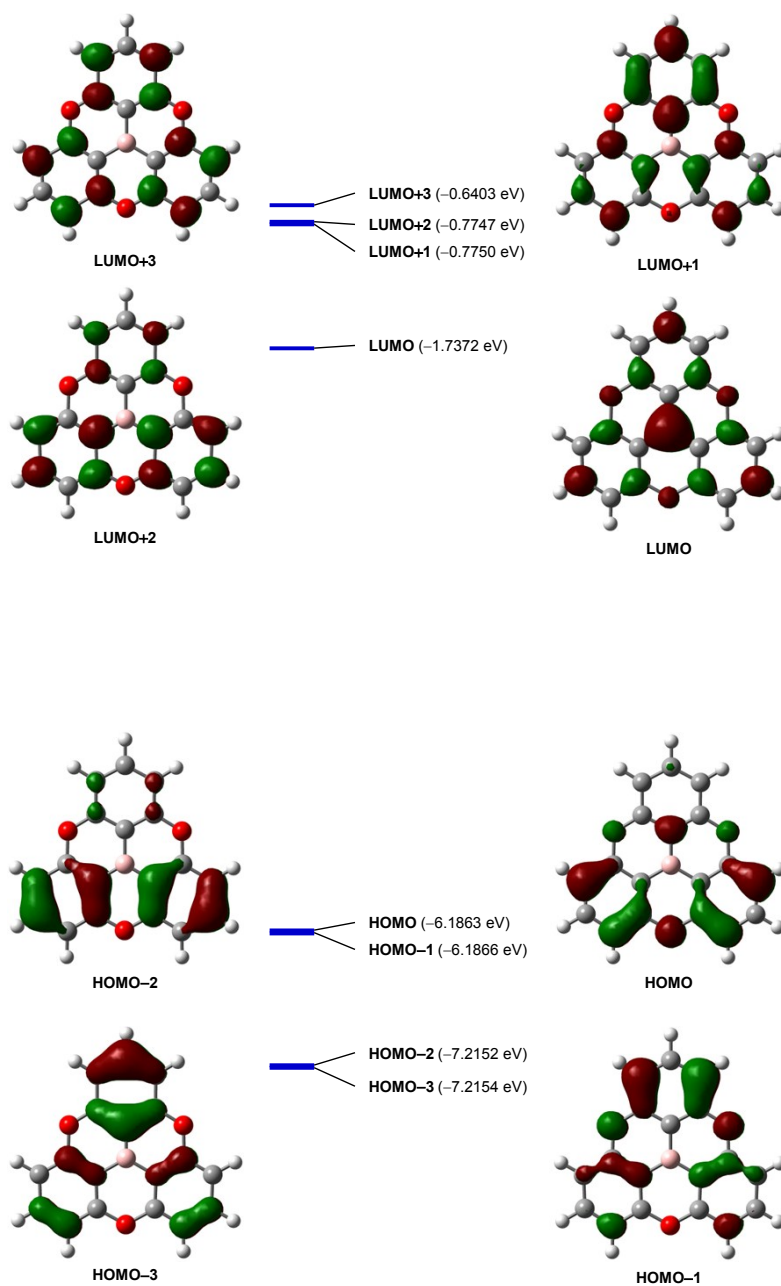
Transition	$E$ / eV	$\lambda$ / nm	$f^a$	Main CI coefficient $b$	
1	4.577	271	0.0591	HOMO $\rightarrow$ LUMO	0.5909
				HOMO-1 $\rightarrow$ LUMO	0.5906
2	4.818	257	0.0038	HOMO-1 $\rightarrow$ LUMO+1	0.4183
				HOMO $\rightarrow$ LUMO	-0.2441
				HOMO $\rightarrow$ LUMO+2	0.4149
				HOMO-1 $\rightarrow$ LUMO	0.2424
				HOMO-1 $\rightarrow$ LUMO+2	0.4666
				HOMO $\rightarrow$ LUMO+1	-0.3620
3	5.078	244	0.0170	HOMO-1 $\rightarrow$ LUMO+1	0.4580
				HOMO-1 $\rightarrow$ LUMO+2	-0.1519
				HOMO $\rightarrow$ LUMO+1	-0.1513
				HOMO $\rightarrow$ LUMO+2	-0.4573
4	5.153	240	0.2488	HOMO-1 $\rightarrow$ LUMO	0.1405
				HOMO $\rightarrow$ LUMO+3	0.6579
				HOMO-1 $\rightarrow$ LUMO+1	0.6578
				HOMO $\rightarrow$ LUMO	-0.1404

<sup>a</sup>Oscillator strength. <sup>b</sup> Coefficient of the wave function for each excitation.

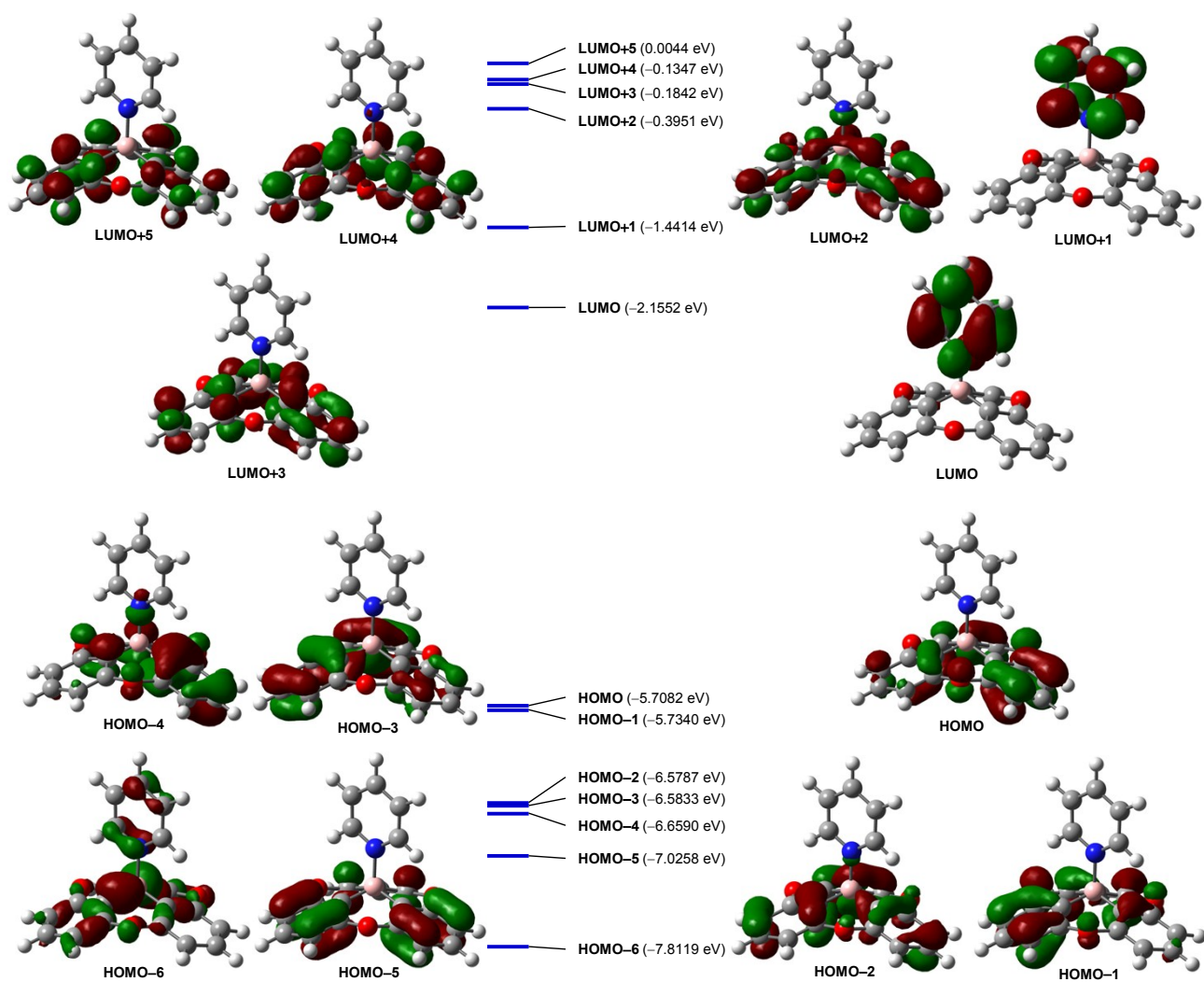




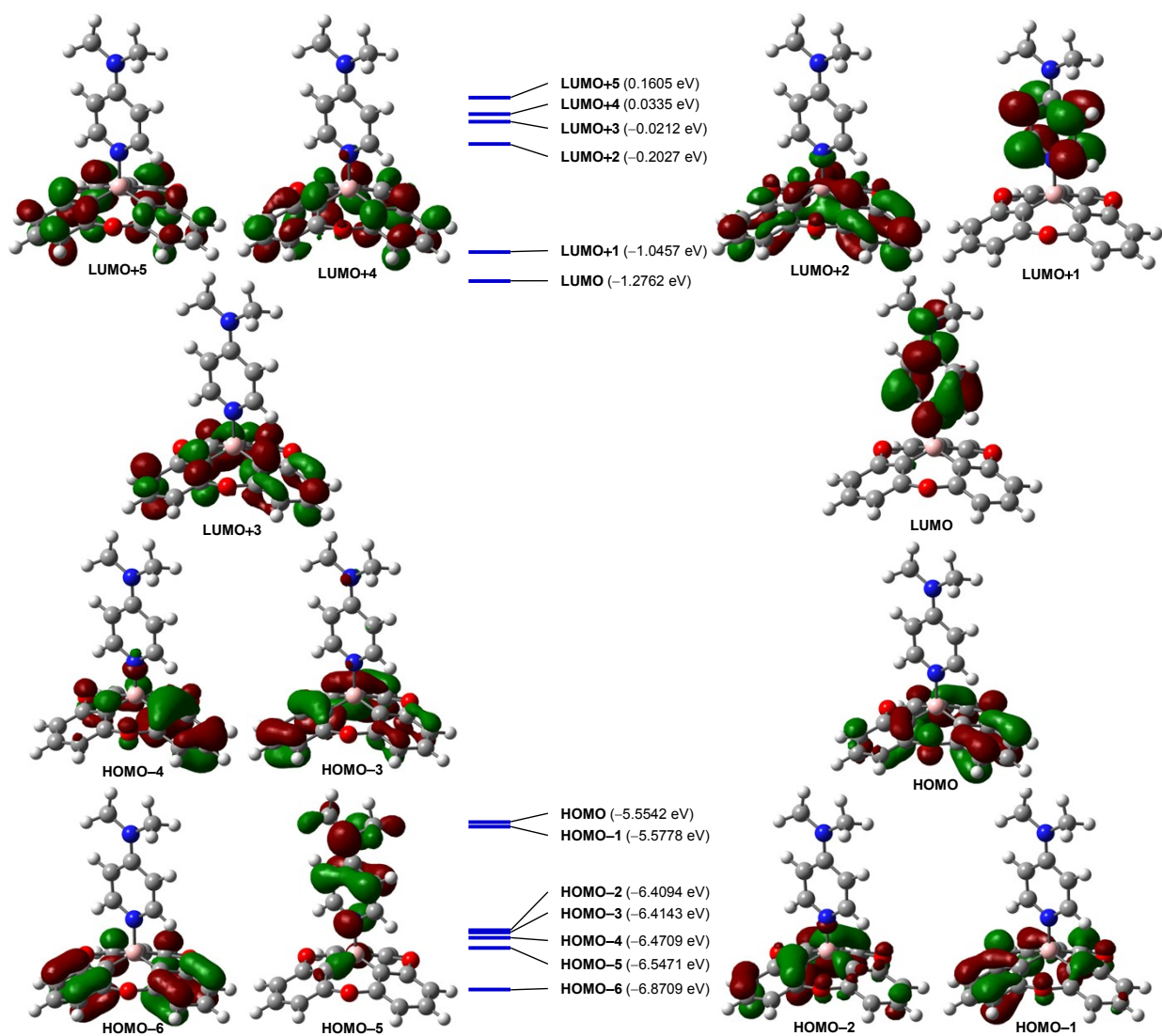
**Figure S9** Electronic transition (oscillator strength versus wavelength) obtained by TD-DFT calculation (B3LYP/6-311G(d,p), in cyclohexane (PCM model)) for (a) **1**, (b) **1**·pyridine, (c) **1**·DMAP, (d) **1**·quinuclidine, (e) **1**<sub>2</sub>·DABCO, and (f) **1**·DABCO, respectively. The values of the oscillator strength are shown in Tables 2, 4–8.



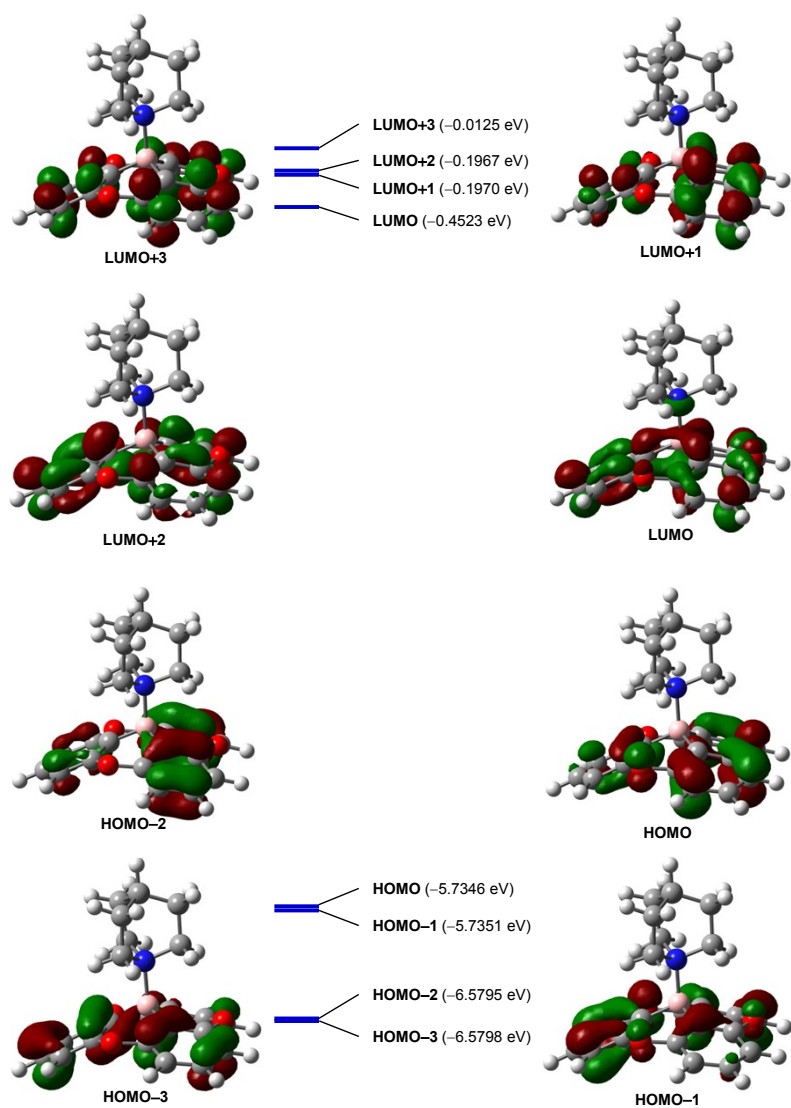
**Figure S10** HOMO and LUMO levels for **1** calculated at the B3LYP/6-311G(d,p) level (in cyclohexane, PCM model).



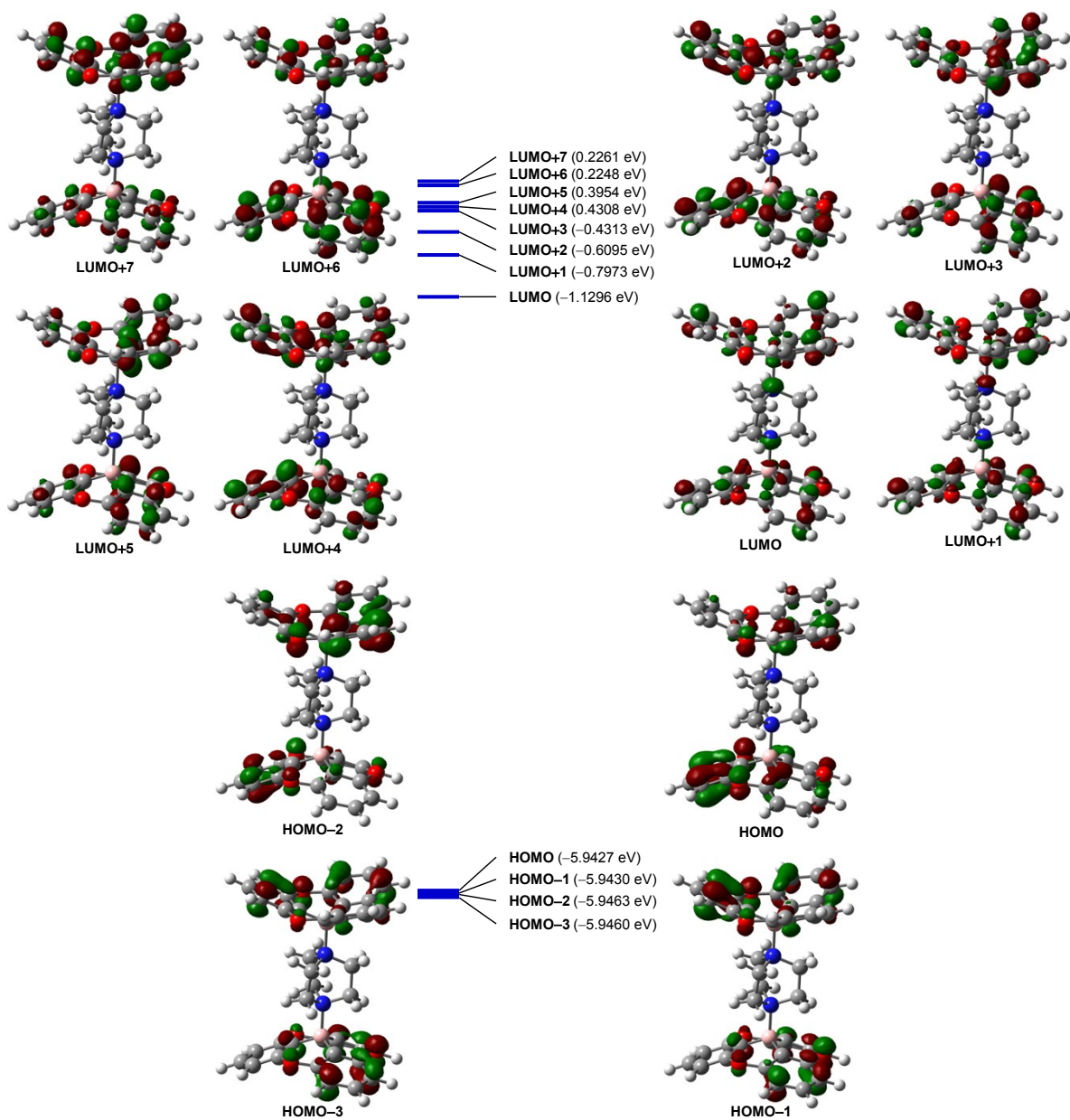
**Figure S11** HOMO and LUMO levels for **1**-pyridine calculated at the B3LYP/6-311G(d,p) level (in cyclohexane, PCM model).



**Figure S12** HOMO and LUMO levels for 1·DMAP calculated at the B3LYP/6-311G(d,p) level (in cyclohexane, PCM model).

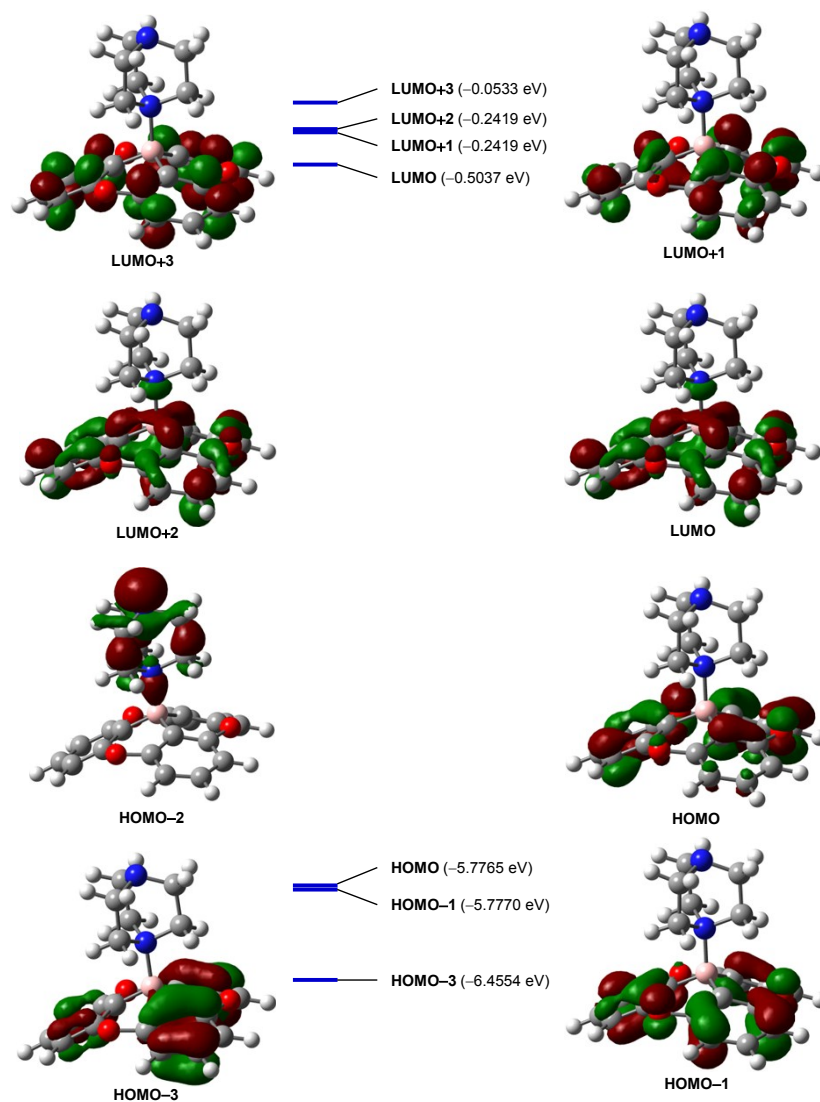


**Figure S13** HOMO and LUMO levels for 1-quinuclidine calculated at the B3LYP/6-311G(d,p) level (in cyclohexane, PCM model).



**Figure S14** HOMO and LUMO levels for  $1_2 \cdot \text{DABCO}$  calculated at the B3LYP/6-311G(d,p) level (in cyclohexane, PCM model).





**Figure S15** HOMO and LUMO levels for 1-DABCO calculated at the B3LYP/6-311G(d,p) level (in cyclohexane, PCM model).

**Table S9** The energy and coordinates of **1** at the ground state calculated at the B3LYP/6-311G(d,p) level (in cyclohexane, PCM model).

Energy = -942.1134963 Hartrees

	X	Y	Z		X	Y	Z
C	-0.000394206	-2.832618002	2.422636301	O	0.000260361	1.396514839	-2.418910264
H	-0.00073169	-3.914729624	2.445754934	B	0.000973709	3.92765×10 <sup>-5</sup>	0
C	-0.000389352	-0.681760402	3.664307267	O	0.000253306	-2.793170858	-0.0000000001
H	-0.000725672	-0.160691229	4.612990297	C	0.000203499	2.122118591	1.230557675
C	0.000650606	-0.733424866	1.270161925	C	0.000205188	0.004655919	2.452929001
C	0.000199337	-2.126768154	1.222473671	O	0.000260361	1.396514839	2.418910265
C	0.000643015	1.466749938	0.0000000001				
C	0.000650606	-0.733424866	-1.270161925				
C	0.000203499	2.122118591	-1.230557675				
C	0.000205188	0.004655919	-2.452929001				
C	0.000199337	-2.126768154	-1.222473671				
C	-0.000388182	3.514393183	1.241765908				
C	-0.000388182	3.514393184	-1.241765908				
C	-0.000389352	-0.681760402	-3.664307267				
C	-0.000394206	-2.832618002	-2.422636301				
C	-0.000626394	4.16883806	0.0000000002				
H	-0.000721677	4.075506522	2.167331762				
H	-0.000721677	4.075506522	-2.167331762				
C	-0.000628985	-2.084352677	-3.610255683				
H	-0.000725672	-0.160691229	-4.612990297				
H	-0.00073169	-3.914729623	-2.445754935				
H	-0.001101881	5.253112687	0.0000000002				
H	-0.001110136	-2.626442977	-4.549294637				
C	-0.000628985	-2.084352678	3.610255683				
H	-0.001110136	-2.626442978	4.549294637				



**Table S10** The energy and coordinates of 1-pyridine at the ground state calculated at the B3LYP/6-311G(d,p) level (in cyclohexane, PCM model).

Energy = -1190.474483 Hartrees

	X	Y	Z		X	Y	Z
C	-2.568547871	2.321184476	-1.554285133	O	1.469447115	-2.40817895	-0.464440999
H	-3.587080507	2.268677599	-1.918759409	B	0.00299714	-0.000445096	0.141048269
C	-0.465308344	3.543195715	-1.299548838	O	-2.677440923	0.003283825	-0.930894509
H	0.132407553	4.430465924	-1.468467292	C	2.167793895	1.20330845	-0.50379457
C	-0.6622806	1.267730464	-0.487978239	C	0.104241463	2.404099956	-0.734117079
C	-1.962077775	1.204585323	-0.983184628	O	1.471169758	2.409342034	-0.452004394
C	1.51502934	5.4444E-06	-0.241465932	C	-1.466839397	-0.005551363	2.295522497
C	-0.663187468	-1.264874486	-0.494512473	C	-1.717809083	-0.008918887	3.656527139
C	2.166934541	-1.20239399	-0.510003864	C	-0.643228146	-0.01142842	4.542913374
C	0.102529688	-2.400497659	-0.746541157	C	0.648068924	-0.010469684	4.028634532
C	-1.962932421	-1.198239205	-0.98939972	C	0.825847011	-0.007050841	2.65260894
C	3.51820193	1.224292689	-0.848344942	N	-0.21323229	-0.004627875	1.80159275
C	3.517327411	-1.222566807	-0.854656529	H	-0.811444917	-0.014088257	5.613082119
C	-0.467819085	-3.536238615	-1.317883368	H	-2.267125255	-0.003503434	1.568098484
C	-2.570183521	-2.3114262	-1.566301846	H	-2.740788889	-0.009543867	4.008792124
C	4.180154869	0.000984026	-0.990101906	H	1.51478813	-0.012332808	4.67633674
H	4.024598531	2.164101726	-1.030763692	H	1.806854023	-0.006168743	2.197685008
H	4.02305462	-2.161783476	-1.041918894				
C	-1.813026027	-3.47975161	-1.693767067				
H	0.12926991	-4.423044287	-1.491395121				
H	-3.588670634	-2.256302413	-1.930516256				
H	5.229276252	0.001315981	-1.264089258				
H	-2.269004849	-4.354068579	-2.144662494				
C	-1.810561107	3.489617388	-1.675696697				
H	-2.265924117	4.366587125	-2.122039899				

**Table S11** The energy and coordinates of **1**-DMAP at the ground state calculated at the B3LYP/6-311G(d,p) level (in cyclohexane, PCM model).

Energy = -1324.490195 Hartrees

	X	Y	Z		X	Y	Z
C	2.168448491	3.308929606	-1.222958833	O	1.231079023	-2.812296786	0.00022486
H	2.43495812	3.776414138	-2.16295405	B	0.592457468	0.007648006	3.12101E-05
C	2.168375962	3.309080354	1.222706704	O	1.439730429	1.356433592	-2.408739609
H	2.434829973	3.77668107	2.162659907	C	1.496886523	-0.038371947	2.400962326
C	1.232045252	1.434741823	-3.80195E-05	C	1.603239039	2.034806508	1.201743894
C	1.603310505	2.034658258	-1.201872033	O	1.439586024	1.356731849	2.408685685
C	1.124154474	-0.752309853	1.265178741	C	-1.743391587	1.231134488	-0.000110825
C	1.124231354	-0.752466228	-1.264989989	C	-3.117655095	1.294525894	-0.000157508
C	1.403093295	-2.114648233	1.200948384	C	-3.885814664	0.103422006	-0.000109262
C	1.403166565	-2.11479666	-1.200574341	C	-3.143808567	-1.107022461	-2.40303×10 <sup>-5</sup>
C	1.497031627	-0.038669133	-2.40083962	C	-1.771392688	-1.075037405	1.62982E-05
C	1.968938234	-0.692198079	3.537617421	N	-1.056422192	0.071953645	-2.37441E-05
C	1.874436188	-2.807036083	2.314661337	H	-1.143941012	2.131368367	-0.000145216
C	1.874575729	-2.807322597	-2.314173337	H	-3.584189151	2.268055414	-0.000232956
C	1.969151018	-0.692636133	-3.537385552	H	-3.633158763	-2.069290527	8.1694E-06
C	2.122813137	-2.080579379	3.482902088	H	-1.197869974	-1.992294092	8.16743E-05
H	2.236643848	-0.129744797	4.423802348	C	-5.964510335	1.386635261	-0.000292865
H	2.069002099	-3.871180558	2.259591984	H	-5.729681036	1.981172785	0.888442156
C	2.12302253	-2.081010745	-3.48248919	H	-5.729702801	1.980961364	-0.889177142
H	2.069138201	-3.871460253	-2.258960265	H	-7.033120971	1.185789473	-0.000252472
H	2.236909593	-0.130293005	-4.423624312	C	-5.993005185	-1.13544338	-0.000135081
H	2.493990811	-2.602937013	4.357702029	H	-5.772271789	-1.735011978	-0.889034469
H	2.494252554	-2.603476819	-4.357202156	H	-5.772232938	-1.735012198	0.888752314
C	2.414858438	3.940036037	-0.000157654	H	-7.05673745	-0.91011427	-0.000107417
H	2.858630605	4.929512977	-0.000205405	N	-5.241839602	0.117391946	-0.000142616

**Table S12** The energy and coordinates of 1·quinuclidine at the ground state calculated at the B3LYP/6-311G(d,p) level (in cyclohexane, PCM model).

Energy = -1271.524339 Hartrees

	X	Y	Z		X	Y	Z
C	-1.565374432	2.689233695	-2.3731759	O	-0.935838182	-1.334337236	2.434122984
H	-1.819574153	3.741395483	-2.336800626	B	-0.122185255	0.000896293	-0.001021684
C	-1.561529854	0.546819735	-3.546303022	O	-0.923954554	2.780714387	-0.067146113
H	-1.812497997	-0.051493688	-4.413487056	C	-1.04795797	-2.100679671	-1.15712756
C	-0.686348424	0.702884015	-1.285154548	C	-1.04337379	-0.053909793	-2.400599174
C	-1.047237002	2.049560994	-1.248994851	O	-0.914607844	-1.443226748	-2.380348937
C	-0.692768892	-1.459768506	0.029555002	C	2.126887942	-0.79951216	-1.153481415
C	-0.697567298	0.759966796	1.245058618	C	2.124403648	1.405581729	-0.101514747
C	-1.059567272	-2.046176041	1.240337892	C	2.115792778	-0.608829388	1.28212108
C	-1.063119019	0.054256971	2.391041023	C	3.668493444	-0.691019896	-1.247150256
C	-1.058109709	2.103252309	1.145448911	H	1.640032797	-0.428174745	-2.052955353
C	-1.570260496	-3.392439246	-1.152355363	H	1.801947644	-1.827277677	-0.997889488
C	-1.582283056	-3.337070593	1.289618548	C	3.664624755	1.43644963	0.052554325
C	-1.589684433	0.706308653	3.504095695	H	1.629764821	1.998683059	0.664985675
C	-1.584780737	2.793494141	2.235493752	H	1.806377816	1.783190755	-1.072246891
C	-1.800742363	-4.005545046	0.082207212	H	1.788889396	0.040713775	2.092891859
H	-1.819933407	-3.886263182	-2.083374068	H	1.623221793	-1.571035232	1.406608606
H	-1.840928721	-3.788067331	2.239720206	C	3.656932892	-0.752377145	1.244869055
C	-1.813959674	2.082970439	3.416636428	C	4.200316535	-0.002807977	0.019005472
H	-1.847380729	0.147792009	4.3955175	H	3.958339666	-0.119061455	-2.132893874
H	-1.838497251	3.84286667	2.149401834	H	4.104264655	-1.687693093	-1.351949336
H	-2.21193334	-5.008613932	0.102946733	H	3.944727587	1.917191992	0.993873751
H	-2.228637485	2.604039347	4.272304526	H	4.105863083	2.02767052	-0.753633747
C	-1.785848175	1.925753746	-3.522822897	H	4.089061007	-0.347215602	2.16316264
H	-2.193834156	2.407614461	-4.404296016	H	3.941392726	-1.806953108	1.193642965
N	1.590623592	-0.000218129	0.006780167	H	5.2924194	-0.003901234	0.024130454

**Table S13** The energy and coordinates of  $\mathbf{1}_2 \cdot \text{DABCO}$  at the ground state optimized at the B3LYP/6-311G(d,p) level (in cyclohexane, PCM model).

Energy = -2229.6678996 Hartrees

	X	Y	Z		X	Y	Z
C	-4.472312051	3.329753092	1.32780831	B	-3.053493262	-0.002104662	0.001871159
H	-4.721902088	3.77683186	2.282073025	O	-3.824937161	1.314354913	2.45256267
C	-4.478908291	3.403315842	-1.11586325	C	-3.960516738	0.069846453	-2.39500949
H	-4.733398891	3.906224175	-2.040532819	C	-3.962341554	2.109463347	-1.133920302
C	-3.603946389	1.459558166	0.046754343	O	-3.834485323	1.459149774	-2.36244707
C	-3.956395728	2.037265435	1.266366991	C	-0.779130556	0.641409641	-1.242922845
C	-3.603479557	-0.696056437	-1.285374254	C	-0.777148838	0.754027326	1.175654404
C	-3.598759003	-0.772045473	1.247381656	C	-0.776435821	-1.396573119	0.063620527
C	-3.955995294	-2.045018318	-1.257565764	C	0.747391098	0.836659508	-1.123438989
C	-3.950775647	-2.117368503	1.139504463	H	-1.283931359	1.595052188	-1.381304608
C	-3.952630157	-0.07465325	2.401992419	H	-1.040101629	-0.005184777	-2.079250084
C	-4.475399798	-0.525343706	-3.544321757	C	0.749436453	0.553655477	1.281187576
C	-4.471348	-2.678439584	-2.386440524	H	-1.279426036	0.395093106	2.071563508
C	-4.461929833	-2.816995835	2.230174511	H	-1.039986764	1.80129708	1.035646753
C	-4.463993896	-0.737482528	3.515736302	H	-1.036826828	-1.798190054	1.041644303
C	-4.694379096	-1.90587138	-3.529445048	H	-1.279715859	-1.993942696	-0.693783515
H	-4.728727567	0.076653656	-4.408146126	C	0.749926985	-1.387200464	-0.165627481
H	-4.721341482	-3.731737205	-2.359194542	H	1.008797047	1.871911331	-0.909737015
C	-4.682150637	-2.114463463	3.418463784	H	1.249379285	0.543373314	-2.042999564
H	-4.711269572	-3.867078884	2.141234856	H	1.011449818	-0.150151867	2.069552645
H	-4.714618165	-0.18814151	4.414719329	H	1.25253373	1.49612188	1.486364096
H	-5.100719705	-2.382484875	-4.414390011	H	1.253946392	-2.035966917	0.547515346
H	-5.084842267	-2.644159078	4.2744186	H	1.010058969	-1.718460108	-1.169713679
C	-4.697123519	4.006686949	0.125642291	N	-1.321880201	-0.000582462	-0.000669827
H	-5.104040265	5.011104331	0.156952221	N	1.293242494	0.00163739	-0.003005618
O	-3.823894624	-2.783182396	-0.08027097	C	3.572348259	1.465765414	0.055365969

(Table S13 Continued)

---

	X	Y	Z		X	Y	Z
C	3.926394335	2.128528536	-1.119798934	C	4.439857858	-0.764465827	3.500680786
C	3.925761081	2.031875391	1.279850265	C	4.444185489	-2.830803735	2.193874184
C	4.4399617	3.423058468	-1.089030597	C	4.662737664	-2.139918096	3.388906089
C	4.439050478	3.325037125	1.353904381	H	4.689194141	-0.224084436	4.405441341
C	4.659693475	4.014314172	0.158363013	H	4.696750268	-3.879098886	2.093756482
H	4.691281042	3.936304327	-2.008897941	H	5.067738278	-2.676932512	4.239197981
H	4.689666602	3.762845944	2.312188005	O	3.799172494	1.490238154	-2.354212644
H	5.064501176	5.019255397	0.198851404	O	3.800802578	-2.774821686	-0.115231445
C	3.573912219	-0.676134406	-1.29897025	O	3.79622183	1.296620223	2.458979608
C	3.927594917	-2.025297087	-1.285360157	B	3.025113259	0.003471529	-0.003628667
C	3.928595278	0.101269622	-2.401059613				
C	4.441258827	-2.64604627	-2.421607607				
C	4.442297055	-0.481253647	-3.557741414				
C	4.662206438	-1.861393683	-3.557182268				
H	4.692309599	-3.69934062	-2.405830844				
H	4.693714455	0.129870395	-4.415692694				
H	5.067542814	-2.328722451	-4.447522354				
C	3.574127547	-0.778012316	1.232818254				
C	3.926408305	-0.091161816	2.394558255				
C	3.929612285	-2.120985877	1.111023207				

---

**Table S14** The energy and coordinates of 1-DABCO at the ground state calculated at the B3LYP/6-311G(d,p) level (in cyclohexane, PCM model).

Energy = -1287.54614 Hartrees

	X	Y	Z		X	Y	Z
C	-1.577489767	3.436313734	1.002607866	B	-0.12776184	-0.000246517	0.000131633
H	-1.832117272	3.968669958	1.910770034	O	-0.928205115	1.539433174	2.313723386
C	-1.576861115	3.27995488	-1.435708743	C	-1.047755491	-0.154529579	-2.393457088
H	-1.830421053	3.69166394	-2.404818539	C	-1.053984132	1.99250774	-1.330539856
C	-0.694724986	1.4573056	-0.093976204	O	-0.922526232	1.231281799	-2.492480553
C	-1.055334444	2.145993023	1.063759058	C	2.125875615	0.592530885	-1.275805855
C	-0.689550504	-0.811797685	-1.216928019	C	2.124206301	0.815237538	1.151203395
C	-0.692314876	-0.649752639	1.309396905	C	2.129171	-1.396643343	0.130531887
C	-1.045834716	-2.151040387	-1.063607798	C	3.678466429	0.660390573	-1.211201276
C	-1.047999547	-1.997961942	1.3273652	H	1.677055694	1.57707732	-1.395829809
C	-1.053422661	0.151950796	2.391696849	H	1.776444934	-0.041380106	-2.089642393
C	-1.564465794	-0.853820546	-3.482232	C	3.677651262	0.732117964	1.17504983
C	-1.562515277	-2.887314215	-2.128040615	H	1.67859304	0.42262058	2.063660268
C	-1.566644753	-2.592332546	2.475982576	H	1.770036826	1.835650404	1.011585504
C	-1.572987482	-0.402666914	3.559717156	H	1.777811425	-1.786394397	1.085012302
C	-1.785590208	-2.226298599	-3.338871109	H	1.685011605	-1.9925641	-0.664922624
H	-1.817383353	-0.334019587	-4.398085415	C	3.681850703	-1.370281947	0.044336032
H	-1.813818412	-3.933082334	-2.001027386	H	4.019641405	1.697954911	-1.210162866
C	-1.792892166	-1.782274878	3.592225606	H	4.118173904	0.170660108	-2.082986783
H	-1.817175071	-3.645967226	2.483182808	H	4.022861629	0.215046196	2.073194088
H	-1.828510069	0.2297643	4.400932853	H	4.113382595	1.733662653	1.184985888
H	-2.192921266	-2.783558711	-4.175038826	H	4.120329441	-1.878114873	0.906237679
H	-2.201755003	-2.228622092	4.491792789	H	4.028136239	-1.888464181	-0.852736264
C	-1.801760966	3.997232051	-0.257679023	N	1.588589832	0.00276929	0.001659638
H	-2.213120651	4.998366224	-0.321876368	N	4.186218733	0.008133278	0.00281782
O	-0.918076821	-2.776437814	0.177069372				

## 6. Transient photoluminescent decay study

**Table S15** PL decay times of **1**·pyridine and **1**·DMAP in cyclohexane at 23 °C <sup>a, b</sup>

		<b>1</b> ·pyridine	<b>1</b> ·DMAP
$\tau_{\text{prompt}}$	under N <sub>2</sub>	54.7 ns (@ $\lambda_{\text{Flu}} = 420$ nm)	3.3 ns (@ $\lambda_{\text{Flu}} = 420$ nm)
	under air	5.1 ns (@ $\lambda_{\text{Flu}} = 420$ nm)	2.8 ns (@ $\lambda_{\text{Flu}} = 420$ nm)
$\tau_{\text{delayed}}$	under N <sub>2</sub>	2.95 $\mu$ s (@ $\lambda_{\text{Flu}} = 420$ nm)	–
	under air	–	–

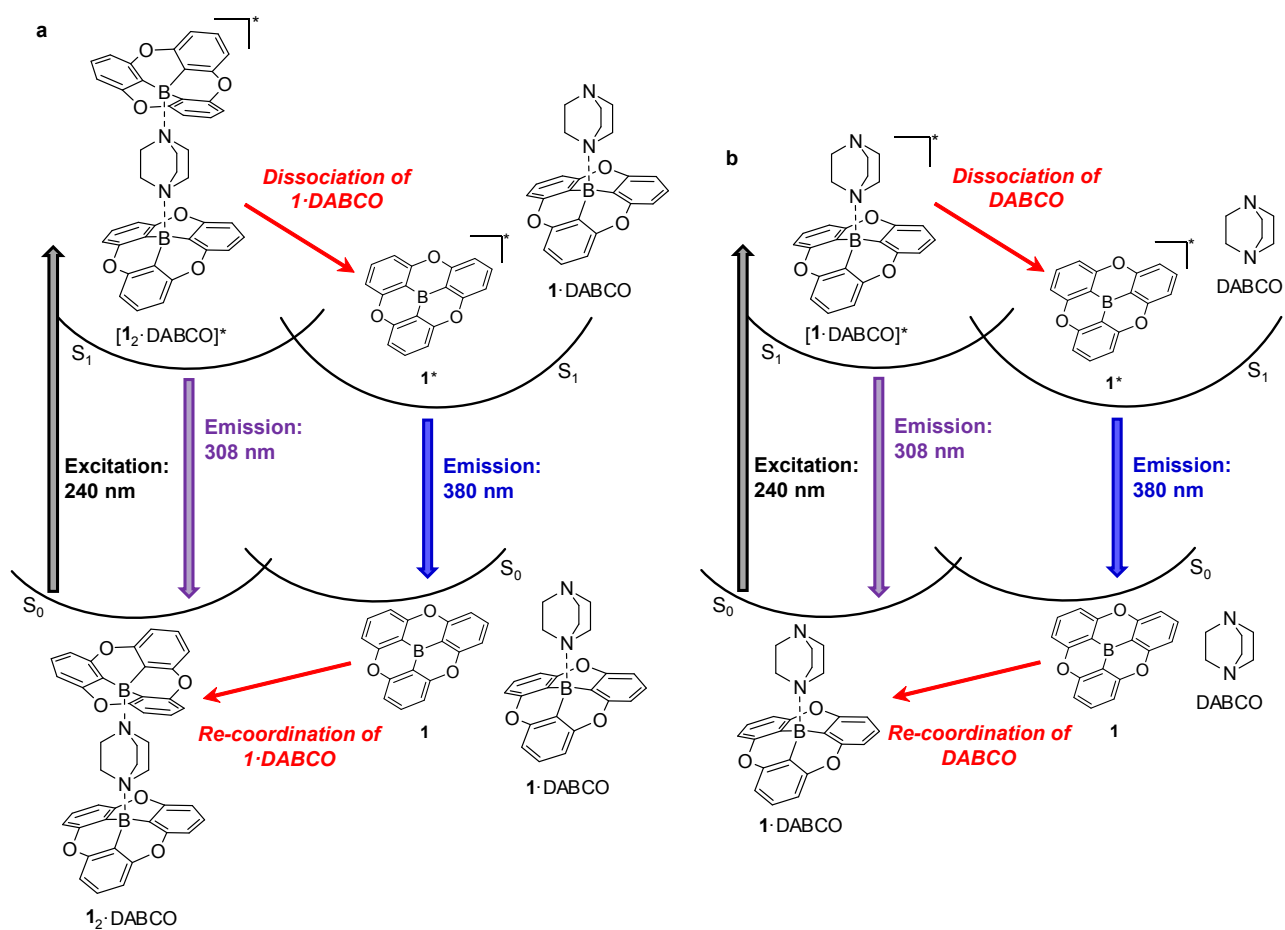
<sup>a</sup> Conditions: **1** ( $0.5 \times 10^{-5}$  mmol), pyridine (3.0 equiv. to **1**), and DMAP (1.2 equiv. to **1**).

<sup>b</sup> Excitation source: LED-laser,  $\lambda = 280$  nm.

**Table S16** PL decay times of **1**, **1**·quinuclidine, **1**<sub>2</sub>·DABCO, and **1**·DABCO in cyclohexane at 23 °C <sup>e</sup>

	<b>1</b> <sup>a</sup>	<b>1</b> ·quinuclidine <sup>b</sup>	<b>1</b> <sub>2</sub> ·DABCO <sup>c</sup>	<b>1</b> ·DABCO <sup>d</sup>
$\tau$	@ $\lambda_{\text{Flu}} = 380$ nm	@ $\lambda_{\text{Flu}} = 380$ nm	@ $\lambda_{\text{Flu}} = 380$ nm	@ $\lambda_{\text{Flu}} = 380$ nm
	4.5 ns	5.5 ns	4.5 ns	4.5 ns
		@ $\lambda_{\text{Flu}} = 308$ nm	@ $\lambda_{\text{Flu}} = 310$ nm	@ $\lambda_{\text{Flu}} = 308$ nm
		1.6 ns	0.5 ns	1.1 ns

<sup>a</sup> Conditions: **1** ( $0.5 \times 10^{-5}$  mmol). <sup>b</sup> Conditions: **1** ( $0.5 \times 10^{-5}$  mmol) and quinuclidine (1.2 equiv. to **1**). <sup>c</sup> Conditions: **1** ( $1.0 \times 10^{-5}$  mmol) and DABCO (0.5 equiv. to **1**). <sup>d</sup> Conditions: **1** ( $0.5 \times 10^{-5}$  mmol) and DABCO (1.0 equiv. to **1**). <sup>e</sup> Excitation source: LED-laser,  $\lambda = 280$  nm.



**Figure S16** Plausible mechanism and energy diagram for the dual emission behavior of (a)  $1_2 \cdot \text{DABCO}$  and (b)  $1 \cdot \text{DABCO}$ .



## 7. References

- (S1) M. Melaimi and F. P. Gabbaï, *J. Am. Chem. Soc.*, 2005, **127**, 9680.
- (S2) H. Zhao, J. H. Reibenspies and F. P. Gabbaï, *Dalton Trans.*, 2013, **42**, 608.
- (S3) J. Yuasa and S. Fukuzumi, *J. Am. Chem. Soc.*, 2006, **128**, 15976.
- (S4) J. Yuasa and S. Fukuzumi *J. Am. Chem. Soc.*, 2008, **130**, 566.
- (S5) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, M. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09 (Revision D.01), Gaussian, Inc., Wallingford CT, 2009.
- (S6) R. Dennington, T. Keith and J. Millam, Gauss View (Version 5), Semichem, Inc., Shawnee Mission, KS, 2009.