Electric supplemental Information for:

Reevaluation of Absolute Luminescence Quantum Yields of Standard Solutions Using a Spectrometer with an Integrating Sphere and a Back-Thinned CCD Detector

Kengo Suzuki,[a] Atsushi Kobayashi,[b] Shigeo Kaneko,[b] Kazuyuki Takehira,[b] Toshitada Yoshihara,[b] Hitoshi Ishida,[c] Yoshimi Shiina,[c] Shigero Oishi[c] and Seiji Tobita*[b]

[a] *Hamamatsu Photonics K. K., Joko-cho, Hamamatsu 431-3196, Japan,*

[b] *Department of Chemistry and Chemical Biology, Gunma University, Kiryu, Gunma 376-8515, Japan. Email: tobita@chem-bio.gunma-u.ac.jp*

[c] *Department of Chemistry, School of Science, Kitasato University, Kitasato, Sagamihara Kanagawa 228-8555, Japan*

Corresponding Author's Email: tobita@chem-bio.gunma-u.ac.jp

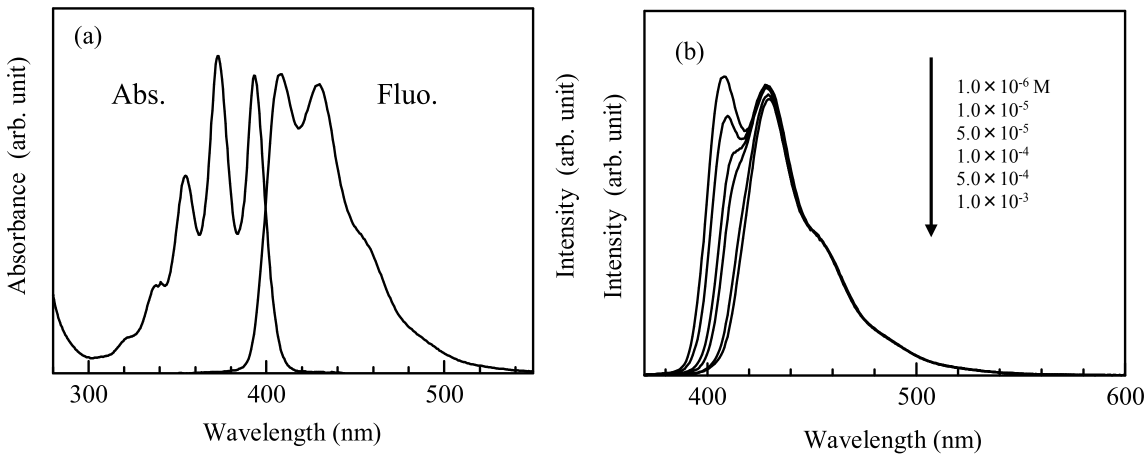

Fig. S1 (a) Absorption and fluorescence spectra of 1.0×10^{-6}M 9,10-diphenylanthracene in cyclohexane, and (b) concentration dependence of the fluorescence spectra of 9,10-diphenylanthracene in cyclohexane.

Quantum yield of intersystem crossing for 9,10-diphenylanthracence

The quantum yield of intersystem crossing (Φ_{isc}) for 9,10-diphenylanthracence (DPA) was determined by measuring transient absorption spectra. The molar absorption coefficient ($\varepsilon_{450}^{^3DPA^*}$) of triplet DPA (^{3}DPA*) at 450 nm was determined by the triplet-triplet energy transfer method (Bonneau, R.; Carmichael, I.; Hug, G. L. *Pure Appl. Chem*. 1991, *63*, 289.) using naphthalene in the excited triplet state as a reference donor. Figure S1 shows the transient absorption spectra observed after 308 nm laser photolysis of the naphthalene/DPA system in cyclohexane. From the analyses of the transient absorption spectra in Fig. S1, the molar absorption coefficient of ^{3}DPA* was determined to be 15,500 $M^{-1}cm^{-1}$ at 450 nm.

The Φ_{isc} value of DPA was determined to be 0.02 from the following equation using benzophenone triplet as an actinometer.

$$\Phi_{isc} = \frac{\Delta A_{450}^{^3DPA^*}}{\varepsilon_{450}^{^3DPA^*} I_{abs}} \tag{1}$$

where $\Delta A_{450}^{^3DPA^*}$ and I_{abs} are the initial absorbance at 450 nm due to the formation of ^{3}DPA* and the photon flux of the incident laser pulse absorbed by benzophenone at 355 nm.

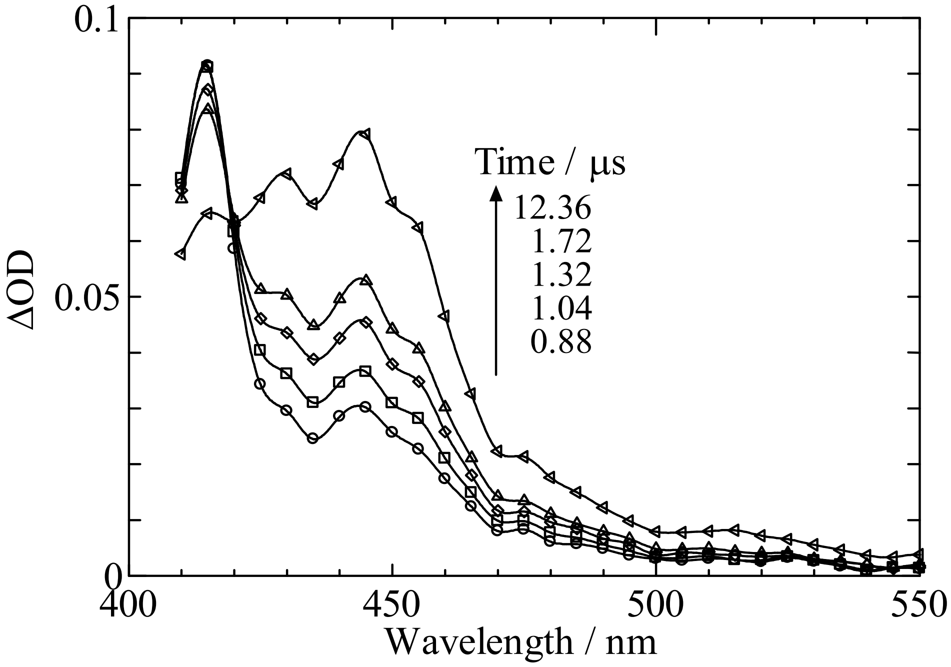

Fig. S2 Transient absorption spectra obtained by energy transfer from Np (OD_{308} = 0.5) to DPA (1 × 10^{-4} M) in CH at 293 K.

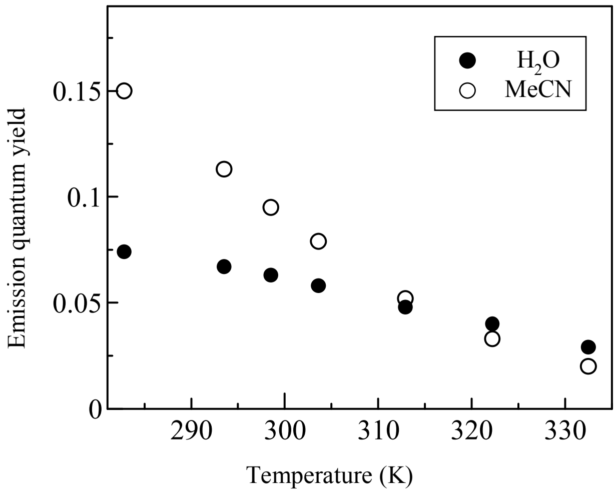

Fig. S3 Temperature dependence of emission quantum yields of $[Ru(bpy)_3](PF_6)_2$ in H_2O and CH_3CN under Ar saturated conditions.

Table S1 Corrected Fluorescence Spectra of Standard Solutions

2-APY				QBS					
this work		literature		this work				literature	
λ (nm)	$I(\lambda)$	λ (nm)	$I(\lambda)$	λ (nm)	$I(\lambda)$	λ (nm)	$I(\lambda)$	λ (nm)	$I(\lambda)$
300	1.2	322.6	4.9	380	0.8	635	1.8	384.6	1.4
305	1.0	331.7	14.9	385	1.6	640	1.7	388.3	3.5
310	2.0	346.0	66.3	390	3.0	645	1.5	392.2	5.5
315	2.2	359.7	98.1	395	6.0	650	1.3	396.0	8.7
320	4.4	367.7	100	400	11.6	655	1.0	400.0	13.8
325	10.5	375.9	91.8	405	21.4	660	1.2	404.0	19.4
330	23.9	390.6	66.0	410	33.0	665	0.8	408.2	26.6
335	41.2	404.9	37.1	415	46.2	670	0.8	412.4	36.6
340	56.5	420.2	20.2	420	59.3	675	0.7	416.7	45.5
345	73.2	434.8	9.5	425	71.2	680	0.8	421.1	54.7
350	85.9	450.5	4.9	430	80.7	685	0.5	425.5	64.6
355	95.3	465.1	2.4	435	88.9	690	0.7	430.1	74.6
360	98.9	480.8	0.6	440	93.2	695	0.4	434.8	82.5
365	98.9			445	97.7	700	0.6	439.6	90.0
370	96.3			450	99.4			444.4	95.0
375	91.1			455	99.9			449.4	98.6
380	83.4			460	98.6			454.5	100
385	73.6			465	95.5			459.8	99.2
390	65.7			470	90.9			465.1	97.5
395	56.9			475	86.8			470.6	93.8
400	48.5			480	81.9			476.2	88.3
405	41.9			485	76.1			481.9	81.7
410	35.2			490	70.0			487.8	74.9
415	29.8			495	63.8			493.8	67.9
420	24.9			500	58.1			500.0	60.3
425	20.4			505	52.4			506.3	53.4
430	16.8			510	47.1			512.8	46.9
435	13.7			515	42.1			519.5	41.0
440	10.8			520	37.4			526.3	35.0
445	9.3			525	33.3			533.3	30.0
450	7.4			530	29.5			540.5	24.9
455	6.1			535	26.0			547.9	20.0
460	5.2			540	22.8			555.6	16.4
465	4.3			545	20.2			563.4	13.6
470	3.4			550	17.5			571.4	11.6
475	2.8			555	15.3			579.7	10.0
480	2.4			560	13.5			588.2	8.5
485	1.8			565	12.0			597.0	6.8
490	1.8			570	10.3			606.1	5.5
495	1.2			575	9.0			615.4	4.2
500	1.1			580	7.9			625.0	3.2
505	1.0			585	6.9			634.9	2.4
510	0.8			590	5.9			645.2	1.5
515	0.5			595	5.4			655.7	0.7
520	0.3			600	4.6			666.7	0
525	0.6			605	3.9				
530	0.2			610	3.6				
535	0.1			615	3.2				
540	0.1			620	2.7				
545	0.4			625	2.4				
550	0.1			630	2.3				

Table S1 (Continued)

3-API						*N,N*-DMANB					
this work				literature		this work				literature	
λ (nm)	$I(\lambda)$	λ (nm)	$I(\lambda)$	λ (nm)	$I(\lambda)$	λ (nm)	$I(\lambda)$	λ (nm)	$I(\lambda)$	λ (nm)	$I(\lambda)$
420	0.4	675	3.3	434.8	1.4	425	0.3	680	16.7	444.4	2.2
425	0.5	680	3.0	439.6	2.0	430	0.8	685	15.6	449.4	2.9
430	0.8	685	2.7	444.4	4.0	435	1.3	690	14.2	454.5	4.2
435	1.5	690	2.3	449.4	7.7	440	1.5	695	12.4	459.8	8.3
440	2.6	695	2.1	454.5	13.9	445	2.0	700	11.8	465.1	14.2
445	5.1	700	1.9	459.8	21.5	450	3.9	705	10.7	470.6	21.1
450	9.2	705	1.7	465.1	33.7	455	6.7	710	9.5	476.2	30.2
455	15.5	710	1.5	470.6	46.4	460	10.3	715	8.7	481.9	40.8
460	24.3	715	1.3	476.2	60.8	465	15.2	720	8.7	487.8	50.9
465	34.9	720	1.2	481.9	74.0	470	22.4	725	7.1	493.8	61.0
470	47.0	725	1.0	487.8	84.8	475	30.7	730	6.8	500.0	71.2
475	59.5	730	1.0	493.8	93.4	480	38.8	735	6.2	506.3	81.4
480	71.5	735	0.8	500.0	98.4	485	47.9	740	5.6	512.8	88.7
485	82.1	740	0.7	506.3	100	490	57.0	745	4.8	519.5	94.1
490	90.0	745	0.7	512.8	99.0	495	64.8	750	5.2	526.3	98.5
495	95.4	750	0.6	519.5	95.0	500	72.3	755	4.3	533.3	100.0
500	99.0	755	0.4	526.3	89.2	505	79.5	760	3.5	540.5	99.3
505	99.9	760	0.5	533.3	82.3	510	85.8	765	3.6	547.9	96.7
510	99.5	765	0.5	540.5	73.5	515	89.9	770	3.1	555.6	92.2
515	97.3	770	0.3	547.9	63.3	520	93.9	775	2.9	563.4	87.3
520	93.6	775	0.3	555.6	54.8	525	96.9	780	2.9	571.4	81.8
525	89.4	780	0.4	563.4	46.3	530	99.0	785	3.0	579.7	75.5
530	84.6			571.4	39.9	535	99.4	790	2.2	588.2	69.6
535	79.1			579.7	34.1	540	99.3	795	1.9	597.0	63.8
540	73.3			588.2	29.0	545	98.1	800	2.2	606.1	58.0
545	67.1			597.0	24.5	550	95.7	805	2.2	615.4	52.4
550	61.3			606.1	20.9	555	93.4	810	0.9	625.0	45.9
555	55.9			615.4	17.5	560	90.6	815	1.7	634.9	40.2
560	50.7			625.0	14.7	565	87.3	820	1.3	645.2	35.0
565	45.8			634.9	12.3	570	82.5	825	2.3	655.7	30.5
570	40.9			645.2	10.0	575	79.1	830	0.4	666.7	26.6
575	36.6			655.7	7.9	580	75.3	835	1.7	678.0	22.5
580	32.8			666.7	5.9	585	70.7	840	1.1	689.7	19.0
585	29.1			678.0	4.2	590	66.3			701.8	16.3
590	25.8			689.7	2.7	595	62.4			714.3	13.4
595	22.9			701.8	1.6	600	58.8			727.3	11.0
600	20.4			714.3	0.8	605	54.7			740.7	9.0
605	17.9					610	50.9			754.7	6.9
610	15.9					615	47.7			769.2	5.4
615	14.2					620	44.1			784.3	4.0
620	12.5					625	40.9			800.0	2.7
625	11.1					630	37.9			816.3	1.8
630	9.8					635	35.3			833.3	0.8
635	8.7					640	32.2				
640	7.6					645	29.8				
645	6.8					650	27.3				
650	6.0					655	25.3				
655	5.3					660	23.4				
660	4.7					665	21.8				
665	4.3					670	19.4				
670	3.7					675	17.9				

Table S1 (Continued)

4,4'-DMANS					
this work				literature	
λ (nm)	$I(\lambda)$	λ (nm)	$I(\lambda)$	λ (nm)	$I(\lambda)$
550	0.3	795	51.2	555.6	2.6
555	0.5	800	48.1	563.4	3.4
560	1.0	805	45.3	571.4	4.1
565	1.4	810	41.9	579.7	6.4
570	2.1	815	39.9	588.2	9.4
575	3.3	820	36.7	597.0	13.6
580	4.9	825	34.7	606.1	19.1
585	6.6	830	32.9	615.4	24.9
590	8.8	835	30.6	625.0	33.2
595	11.6	840	28.7	634.9	42.8
600	14.8	845	26.4	645.2	53.2
605	18.4	850	24.6	655.7	64.0
610	22.7	855	23.1	666.7	74.7
615	27.0	860	20.8	678.0	84.5
620	32.0	865	18.8	689.7	91.9
625	37.6	870	17.9	701.8	96.4
630	43.2	875	16.8	714.3	99.4
635	49.0	880	15.9	727.3	100.0
640	55.2	885	14.8	740.7	98.4
645	60.8	890	13.4	754.7	93.3
650	66.6	895	12.8	769.2	86.7
655	72.1	900	11.9	784.3	78.1
660	77.1	905	10.8	800.0	67.9
665	82.1	910	10.2	816.3	57.1
670	86.4	915	9.5	833.3	46.6
675	90.3	920	8.5	851.1	37.6
680	93.6	925	8.3	869.6	29.6
685	96.1	930	7.5	888.9	22.2
690	98.8	935	6.9	909.1	16.0
695	99.4	940	6.9	930.2	11.5
700	100	945	6.2	952.4	7.4
705	99.6	950	5.7		
710	99.1				
715	98.2				
720	96.9				
725	95.0				
730	91.8				
735	89.8				
740	87.8				
745	84.9				
750	81.2				
755	78.5				
760	74.7				
765	71.2				
770	67.7				
775	64.6				
780	60.7				
785	57.9				
790	54.4				

Table S2 Concentration Dependence of Φ_f and τ_f for QBS in 1N H_2SO_4 at 295 K

conc. (M)	Φ_f	τ_{f1} (ns)	τ_{f2} (ns)	amplitude	ratio	$<\tau_f>$ (ns)
7×10^{-3}	0.497	16.8		0.104	96.7%	16.4
			3.7	0.016	3.3%	
5×10^{-3}	0.524	17.3		0.114	97.4%	16.9
			2.8	0.019	2.6%	
2×10^{-3}	0.549	18.6		0.107	97.6%	18.2
			3.3	0.015	2.4%	
1×10^{-3}	0.580	18.9		0.110	98.5%	18.6
			1.8	0.017	1.5%	
7×10^{-4}	0.588	19.1		0.106	97.8%	18.8
			3.1	0.015	2.2%	
5×10^{-4}	0.590	19.0		0.115	98.4%	18.7
			1.7	0.021	1.6%	
2×10^{-4}	0.592	19.3		0.107	98.5%	19.0
			1.7	0.019	1.5%	
1×10^{-4}	0.598	19.3		0.111	98.5%	19.0
			1.8	0.018	1.5%	
7×10^{-5}	0.596	19.4		0.113	98.4%	19.1
			2.5	0.014	1.6%	
5×10^{-5}	0.594	19.4		0.101	98.3%	19.1
			2.0	0.017	1.7%	
2×10^{-5}	0.594	19.4		0.118	98.7%	19.1
			1.5	0.020	1.3%	
1×10^{-5}	0.596	19.3		0.121	98.8%	19.1
			1.3	0.021	1.2%	