Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Synthesis and Characterization of Heterofluorenes Containing Four-Coordinated Group 13 Elements: Theoretical and Experimental Analyses and Comparison of Structures, Optical Properties and Electronic States

Takuya Matsumoto[a], Kazuo Tanaka*[a], Kazuyoshi Tanaka*[b] and Yoshiki Chujo*[a]

[a] Department of Polymer Chemistry, Graduate School of Engineering, Kyoto University, Katsura, Nishikyo-ku, Kyoto 615-8510, Japan

[b] Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, Katsura, Nishikyo-ku, Kyoto 615-8510, Japan

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General. ^{1}H (600 or 400 MHz), and ^{13}C (100 MHz) NMR spectra were recorded on JEOL JNM-ECA600, JNM-EX400 and JNM-AL400 spectrometers. ^{1}H and ^{13}C NMR spectra used tetramethylsilane (TMS) as an internal standard in $CDCl_3$ and C_6D_6. High-resolution mass spectra (HRMS) were obtained on a Thermo Fisher Scientific EXACTIVE for direct analysis in real time (DART), atomic pressure chemical ionization (APCI) and electron spray ionization (ESI). UV–vis spectra were recorded on a Shimadzu UV-3600 spectrophotometer. Fluorescence emission spectra were recorded on a HORIBA JOBIN YVON Fluoromax-4 spectrofluorometer. Photoluminescence lifetime measurement was performed on a Horiba FluoreCube spectrofluorometer system; excitation was carried out using a UV diode laser (NanoLED 290 nm). X-ray crystallographic analyses were carried out by a Rigaku R-AXIS RAPID-F graphite-monochromated Mo Kα radiation diffractometer with an imaging plate. A symmetry related absorption correction was carried out by using the program ABSCOR[1]. The analysis was carried out with direct methods (SHELX-97[2] or SIR97[3]) using Yadokari-XG[4]. The program ORTEP3[5] was used to generate the X-ray structural diagram. All reactions were performed under argon atmosphere.

Materials. All reagents were obtained from commercial sources and used without further purification. Diethyl ether (Et_2O) was purified using a two-column solid-state purification system (Glass Contour Solvent System, Joerg Meyer, Irvine, CA). 2,2'-Diiododiphenyl[6], 1-bromo-2,4-di-*t*-butyl-6-(*N*,*N*-dimethylaminomethyl)phenyl[7], [2,4-di-*t*-butyl-6-(*N*,*N*-dimethylaminomethyl)phenyl]dichloroalumane (MamxAlCl_2)[8], gallafluorene (**Gaf**)[7b] and dichloro[2,4-di-*t*-butyl-6-(*N*,*N*-dimethylaminomethyl)phenyl]dichloroindigane (MamxInCl_2)[9] were prepared according to the previous literatures.

Synthesis.

Borafluorene Bf. Dimethyldibenzosilole (2.1 g, 10 mmol) was reacted with BBr_3 (1.9 mL, 20 mmol) at 50 °C for 44 h. Excess amounts of BBr_3 and the produced dimethyldibromosilane were removed under reduced pressure. The residue containing **1** was used for the next reaction without further purification. To the solution of MamxBr (3.3 g, 10 mmol) in Et_2O (30 mL), *n*-BuLi (1.6 M in hexane, 8.0 mL, 13 mmol) was added slowly at −78 °C. After stirring for 1 h and warmed up to room temperature, the solvent was exchanged from Et_2O to toluene (20 mL). The toluene solution was added slowly at −78 °C to the solution of precursor **1** in toluene (10 mL). After warmed up to room temperature, the mixture was stirred for 40 h. After the reaction solution was quenched with water and diluted with chloroform, the solution was washed with brine and dried

over Na_2SO_4. The crude product was passed through silica gel column chromatography using hexane/ethyl acetate (20: 1 to 10 : 1). Recrystallization from hexane / chloroform gave a white solid in 47% yield (1.9 g). ^{1}H NMR (600 MHz, C_6D_6, δ, ppm): 7.78 (ddd, J = 7.6, 0.8, 0.8 Hz, 2H), 7.64 (d, J = 1.8 Hz, 1H), 7.30 (ddd, J = 7.3, 7.3, 1.4 Hz, 2H), 7.27 (ddd, J = 7.1, 1.1, 0.7 Hz, 2H), 7.14–7.11 (m, 3H), 3.51 (s, 2H), 1.73 (s, 6H), 1.44 (s, 9H), 1.24 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, δ, ppm): 154.6, 149.7, 148.3, 140.3, 132.5, 127.1, 125.7, 122.1, 119.4, 116.8, 68.3, 47.8, 37.1, 34.6, 31.6; ^{11}B NMR (128 MHz, C_6D_6, δ, ppm): 5.96; HRMS (APCI): m/z calcd. for $C_{29}H_{37}BN$ $[M+H]^+$: 410.3014; found: 410.3014.

Alumafluorene Alf. To a solution of 4,4'-diiodobiphenyl (810 mg, 2.0 mmol) and Et_2O (20 mL), 1.63 M *n*-BuLi in *n*-hexane (2.6 mL, 4.2 mmol) was added slowly at −78 °C for 2.5 h. To the solution, the mixture of $MamxAlCl_2$ (760 mg, 2.2 mmol) and Et_2O (10 mL) was added at −78 °C. After warmed up to room temperature, the mixture was stirred for 20 h. After filtration, the solution was evaporated under reduced pressure. After the solvent was removed, 4-fold-recrystallization from hexane / dichloromethane gave a white solid in 15% yield (130 mg). ^{1}H NMR (600 MHz, C_6D_6, δ, ppm): 8.07 (d, J = 7.9 Hz, 2H), 7.65 (ddd, J = 6.7, 1.5, 0.7 Hz, 2H), 7.61 (d, J = 1.7 Hz, 1H), 7.40 (ddd, J = 7.9, 7.9, 1.6 Hz, 2H), 7.28 (ddd, J = 7.9, 6.8, 1.0 Hz, 2H), 6.97 (d, J = 1.6 Hz, 1H), 3.57 (s, 2H), 1.77 (s, 6H), 1.40 (s, 9H), 1.39 (s, 9H); ^{13}C NMR (100 MHz, C_6D_6, δ, ppm): 161.8, 152.7, 151.4, 147.2, 144.9, 138.8, 136.9, 129.1, 128.5, 126.9, 121.4, 118.8, 67.4, 45.6, 37.5, 35.30, 32.8, 31.8; HRMS (DART): m/z calcd. for $C_{29}H_{37}AlN$ $[M+H]^+$: 426.2736; found: 426.2727.

Indafluorene Inf. To a solution of 4,4'-diiodobiphenyl (810 mg, 2.0 mmol) TMEDA (630 μL, 4.2 mmol) and Et_2O (20 mL), 1.63 M *n*-BuLi in *n*-hexane (2.6 mL, 4.2 mmol) was added slowly at −78 °C for 2 h. To the solution, the mixture of $MamxInCl_2$ (950 g, 2.2 mmol) and Et_2O (10 mL) was added at −78 °C. After warmed up to room temperature, the mixture was stirred for 18 h. After filtration, the solution was evaporated under reduced pressure. After the solvent was removed, 3-fold-recrystallization from hexane / dichloromethane gave a white solid **Inf** in 27% yield (140 mg). ^{1}H NMR (600 MHz, C_6D_6, δ, ppm): 8.19 (d, J = 7.8 Hz, 2H), 7.87 (d, J = 6.3, 1.9 Hz, 2H), 7.65 (d, J = 1.9 Hz, 1H), 7.41–7.34 (m, 4H), 6.99 (d, J = 1.9 Hz, 1H), 3.20 (s, 2H), 1.75 (s, 6H), 1.39 (s, 9H), 1.37 (s, 9H); ^{13}C NMR (100 MHz, C_6D_6, δ, ppm): 159.7, 151.0, 150.6, 144.2, 138.2, 128.7, 127.6, 122.8, 121.9, 120.9, 68.2, 45.7, 36.5, 35.0, 32.5, 31.8; HRMS (ESI): m/z calcd. for $C_{29}H_{37}InN$ $[M+H]^+$: 514.1959; found: 514.1956.

Computational Details. The Gaussian 09 program package[10] was used for computation.

We optimized the structures of heterofluorenes (**Bf**, **Alf**, **Gaf** and **Inf**) in the ground S_0, excited S_1 and T_1 states and calculated the electronic structures of their heterofluorenes. The density functional theory (DFT) was applied for the optimization of the structures in S_0. The time-dependent DFT (TD-DFT) was employed on the calculation of their geometry optimization in the excited states. We calculated the transition from S_0 to S_1 or T_1 of heterofluorenes with the optimized geometries in the S_0, S_1 and T_1 states by TD-DFT. The calculations were performed at the B3LYP/6-31G(d,p) levels for **Bf**, **Alf** and **Gaf** and at the B3LYP/LANL2DZ levels for **Gaf** and **Inf**.

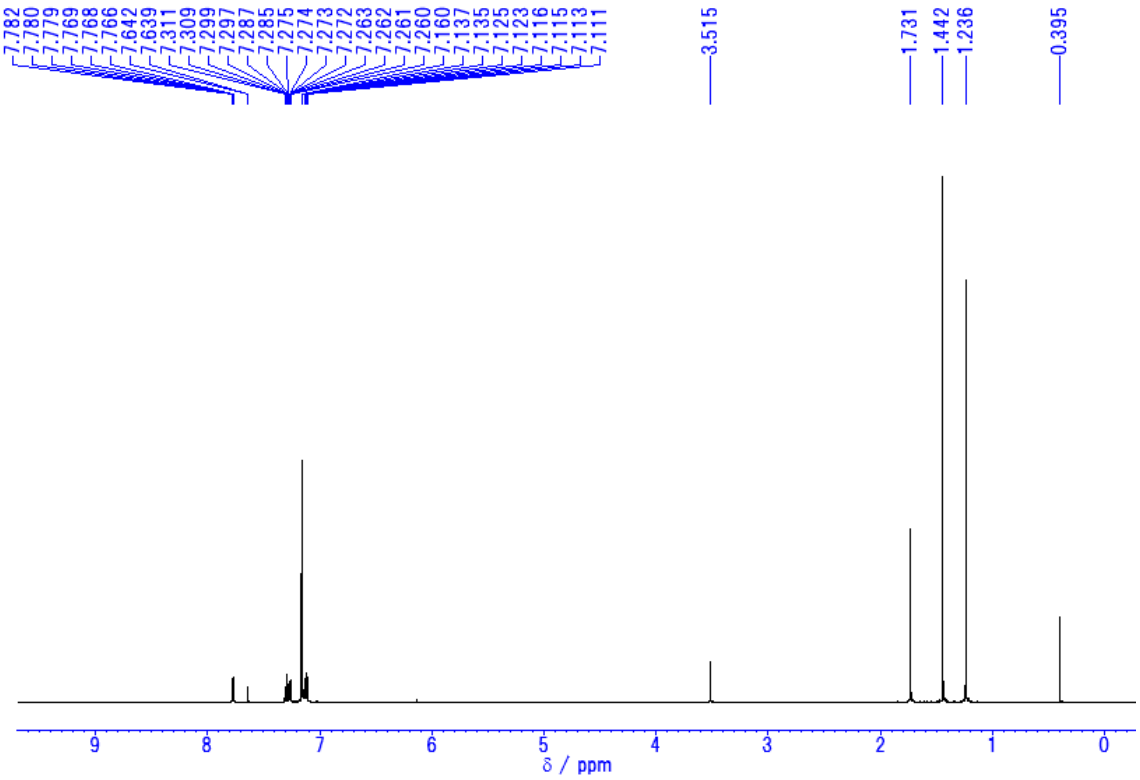

Figure S1. ^{1}H NMR spectrum of **Bf** in C_6D_6.

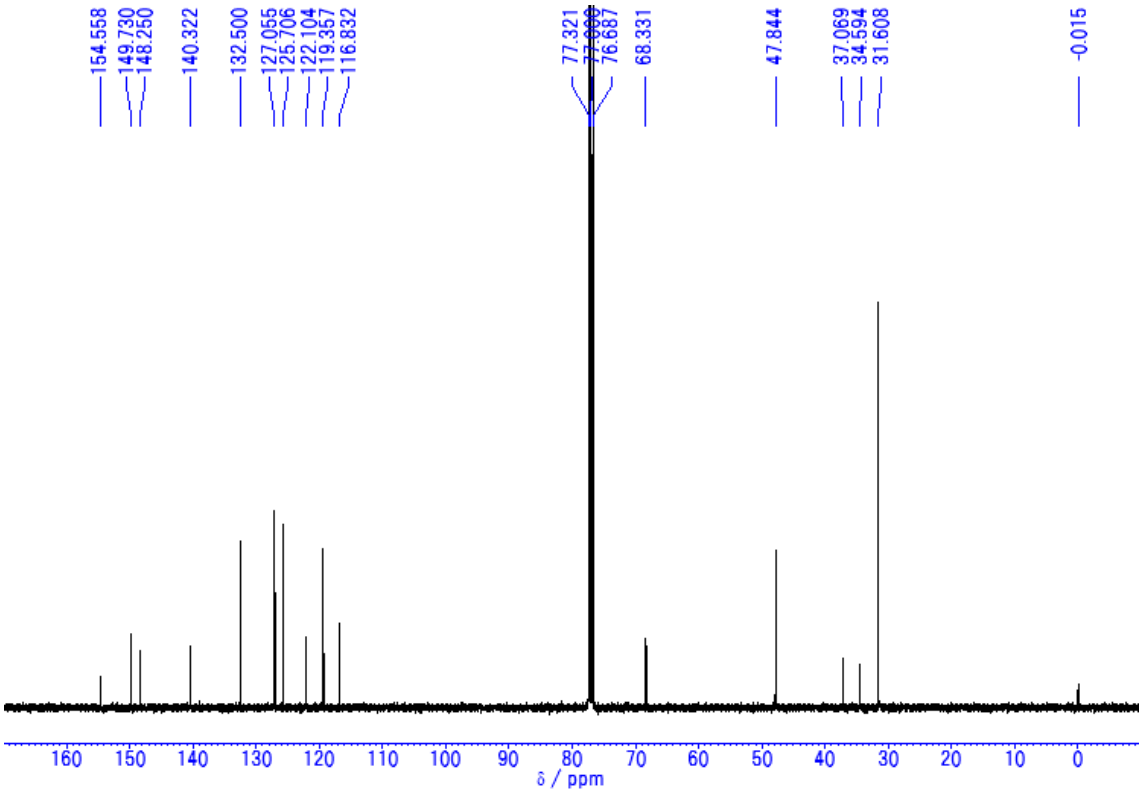

Figure S2. ^{13}C NMR spectrum of **Bf** in $CDCl_3$.

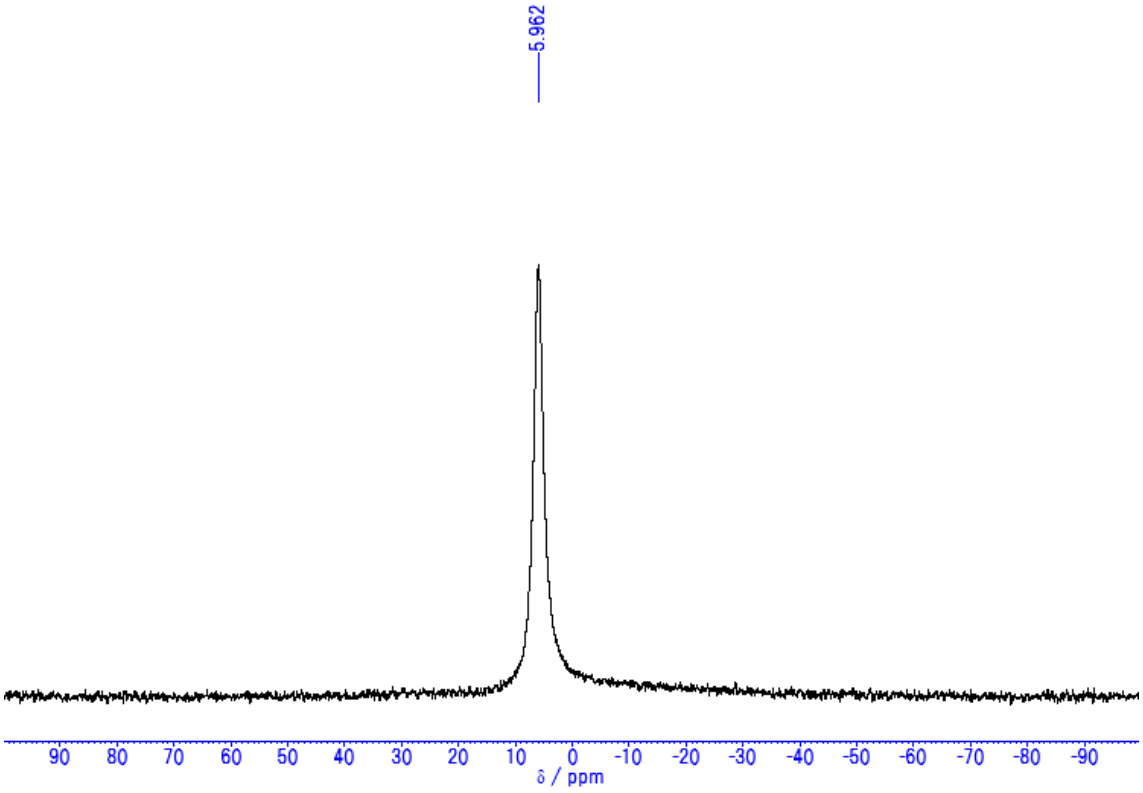

Figure S3. ^{11}B NMR spectrum of **Bf** in C_6D_6.

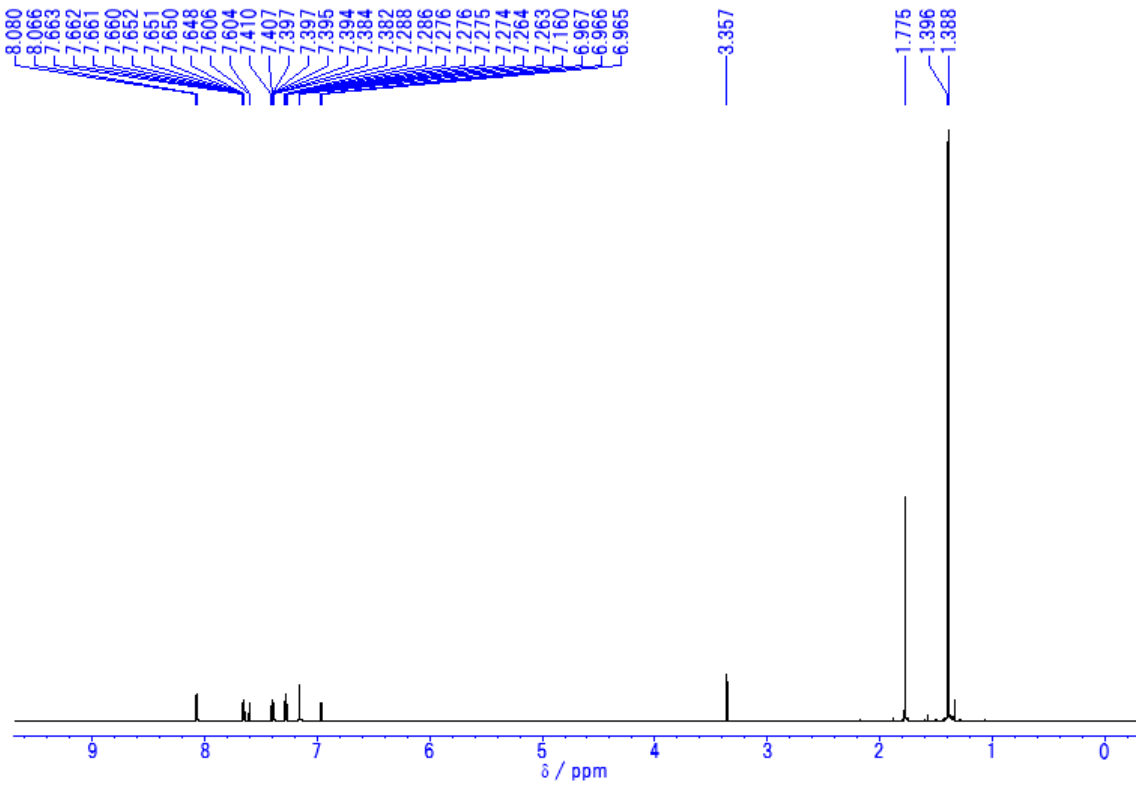

Figure S4. ^{1}H NMR spectrum of **Alf** in C_6D_6.

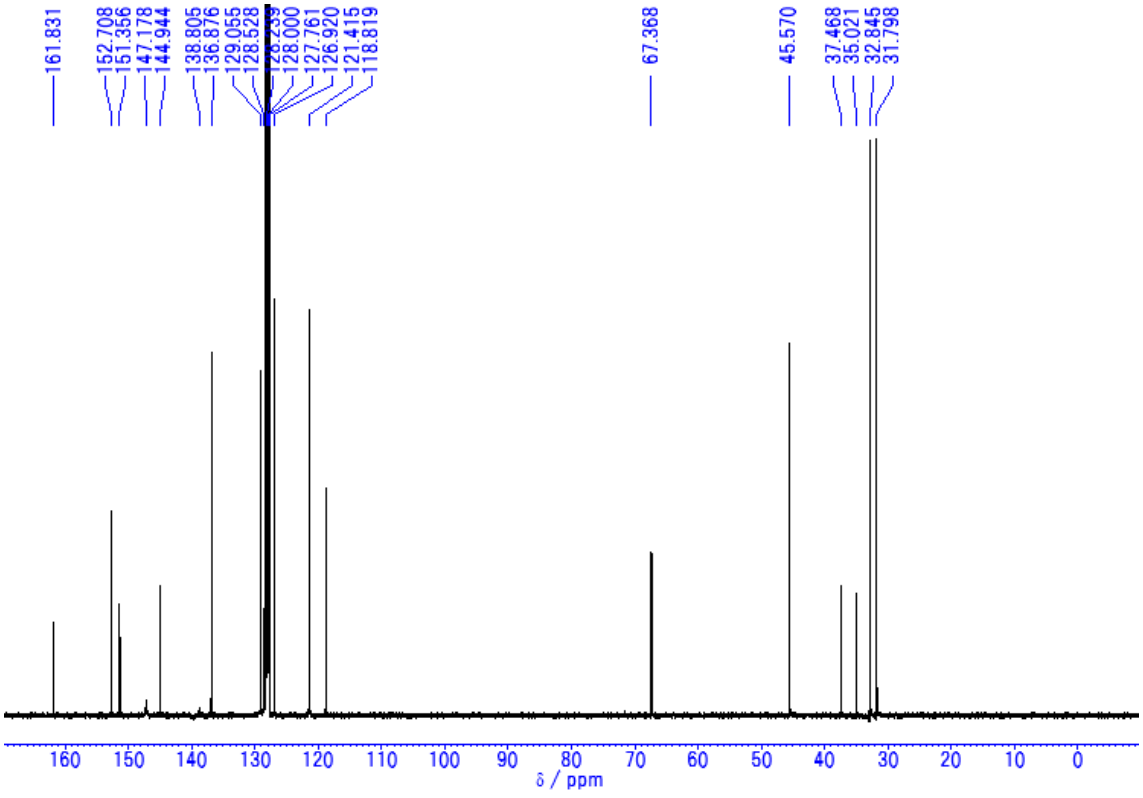

Figure S5. ^{13}C NMR spectrum of **Alf** in C_6D_6.

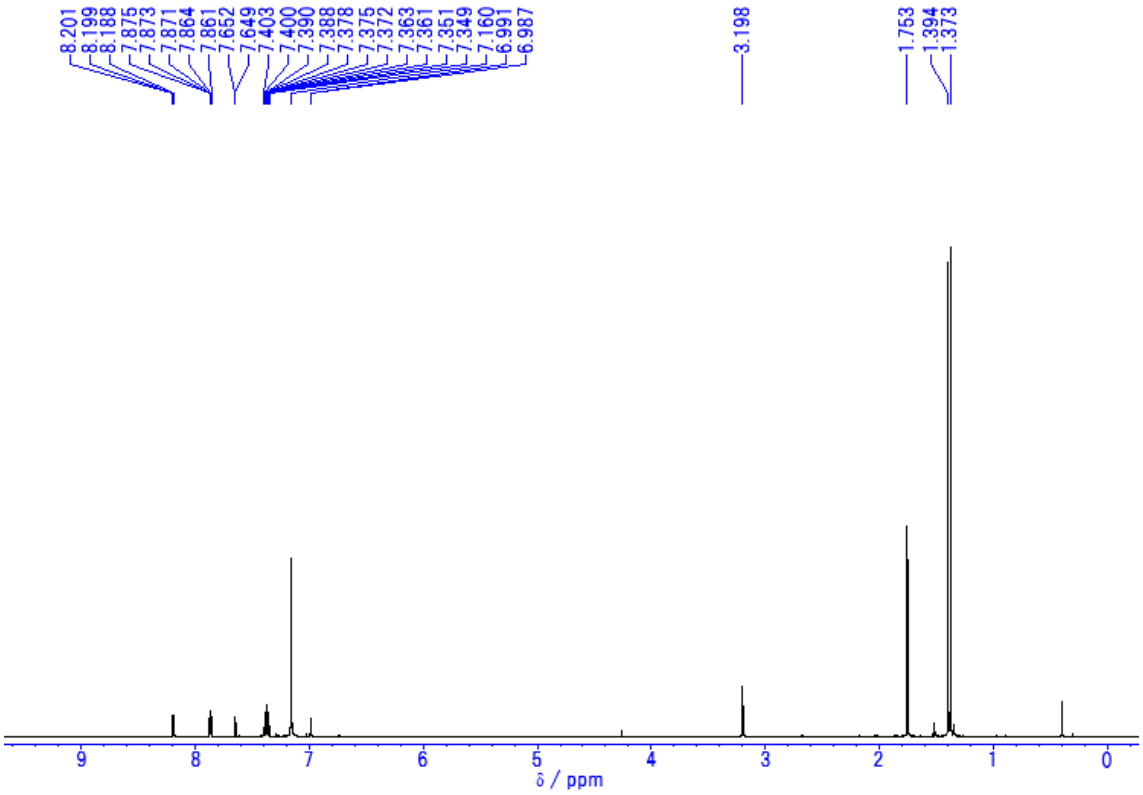

Figure S6. ^{1}H NMR spectrum of **Inf** in C_6D_6.

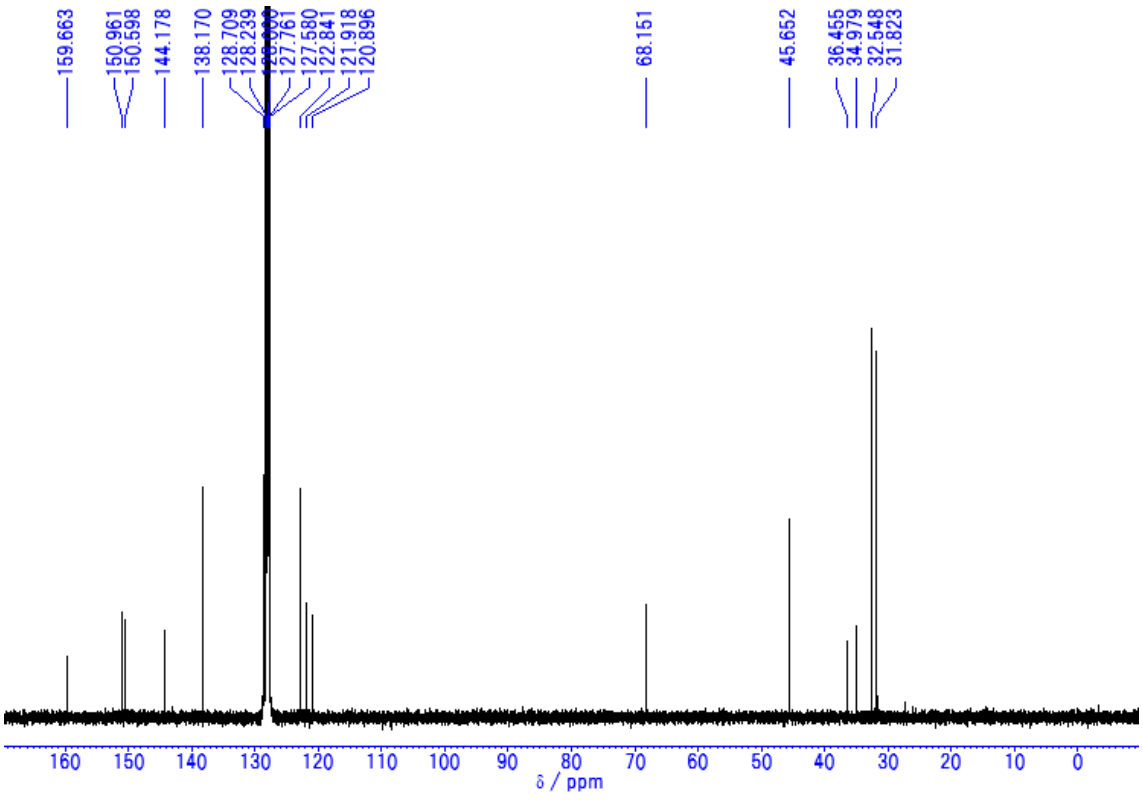

Figure S7. ^{13}C NMR spectrum of **Inf** in C_6D_6.

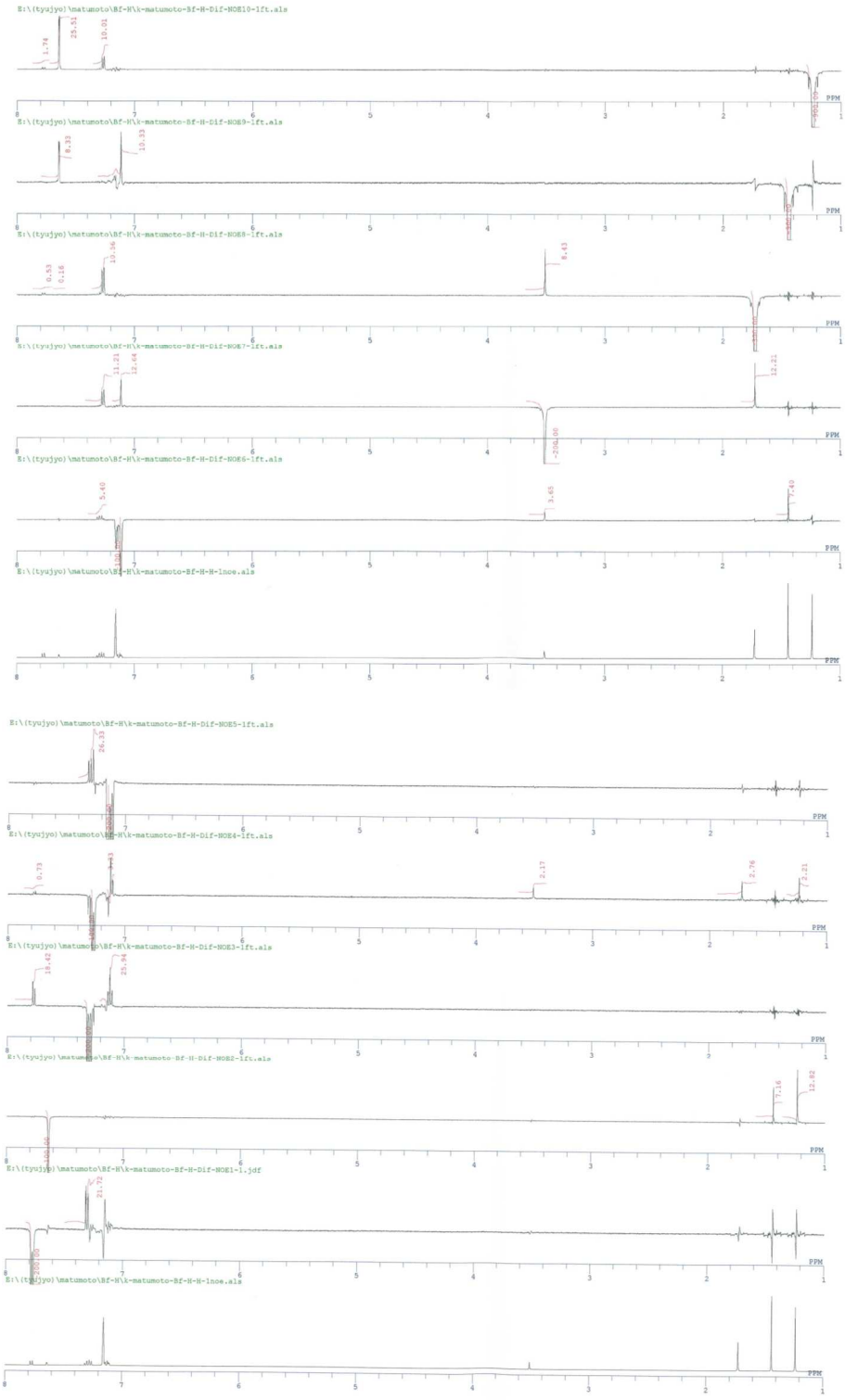

Figure S8. ^{1}H NMR NOE spectra of **Bf** in C_6D_6.

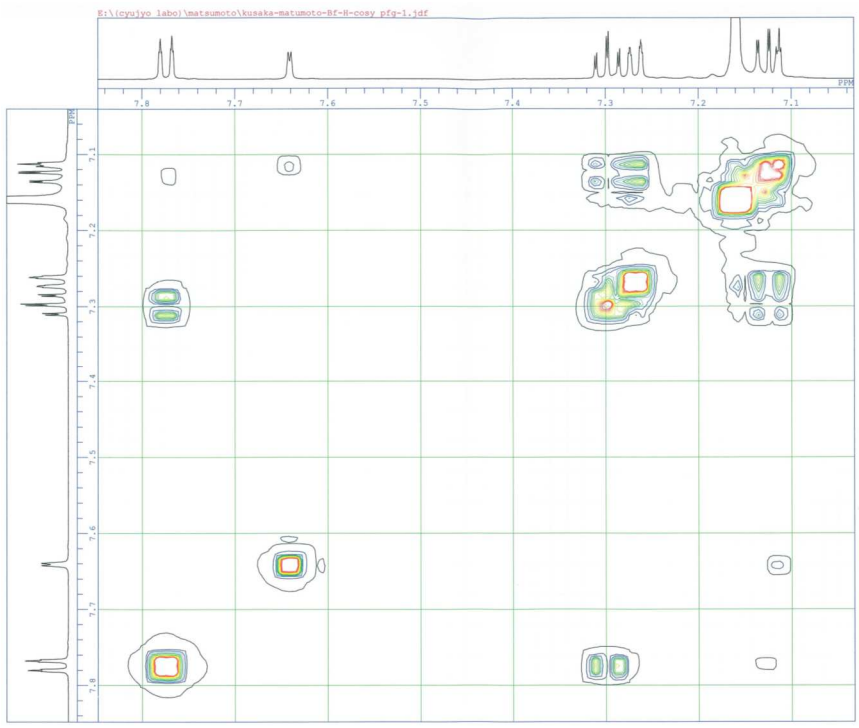

Figure S9. COSY NMR spectra of **Bf** in C_6D_6.

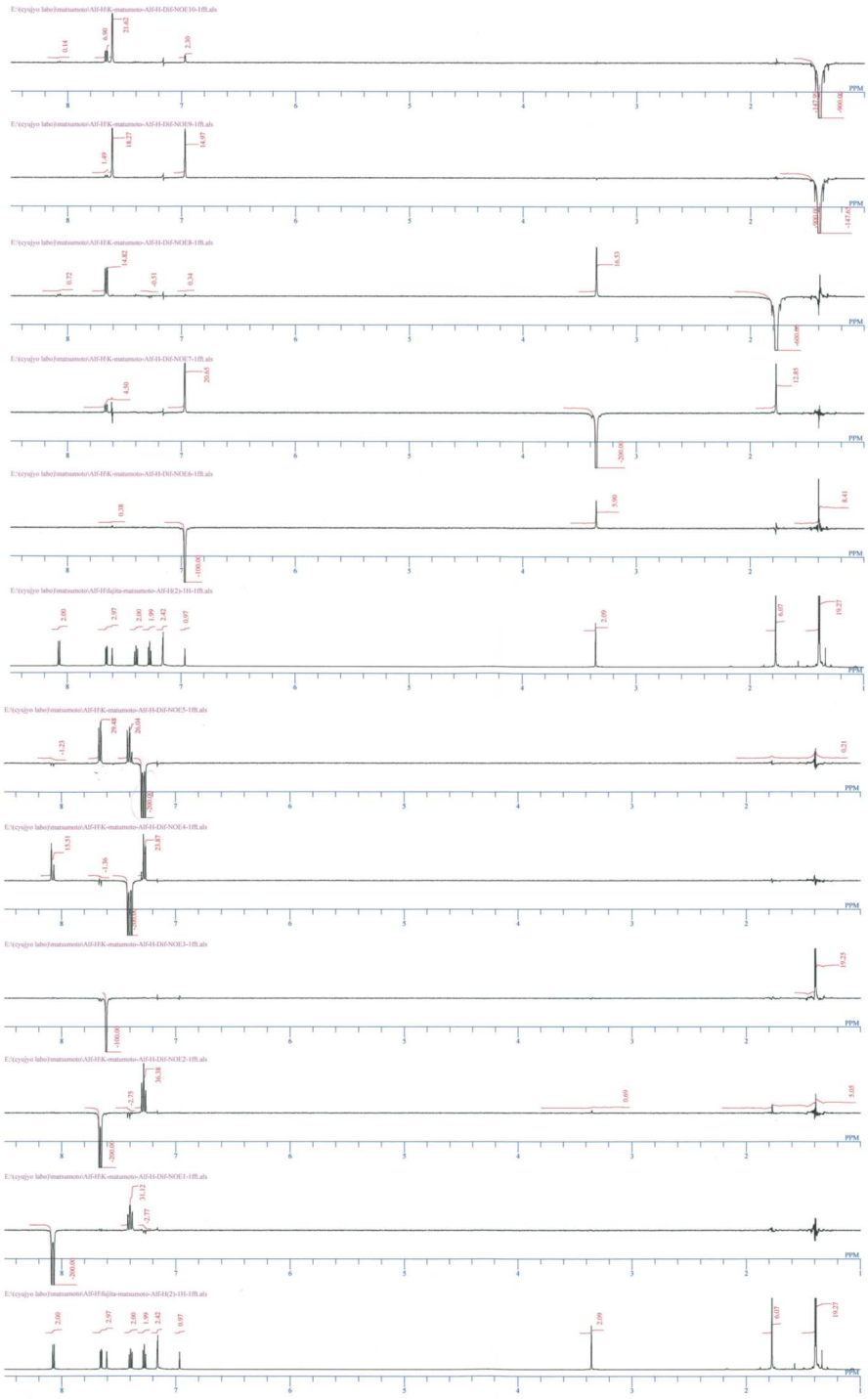

Figure S10. ^{1}H NMR NOE spectra of **Alf** in C_6D_6.

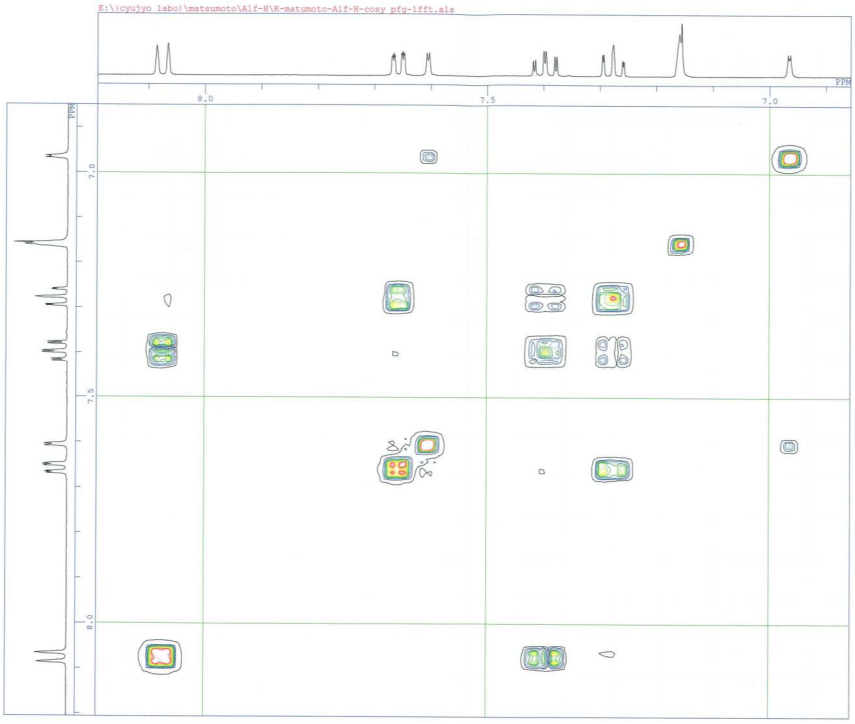

Figure S11. COSY NMR spectra of **Alf** in C_6D_6.

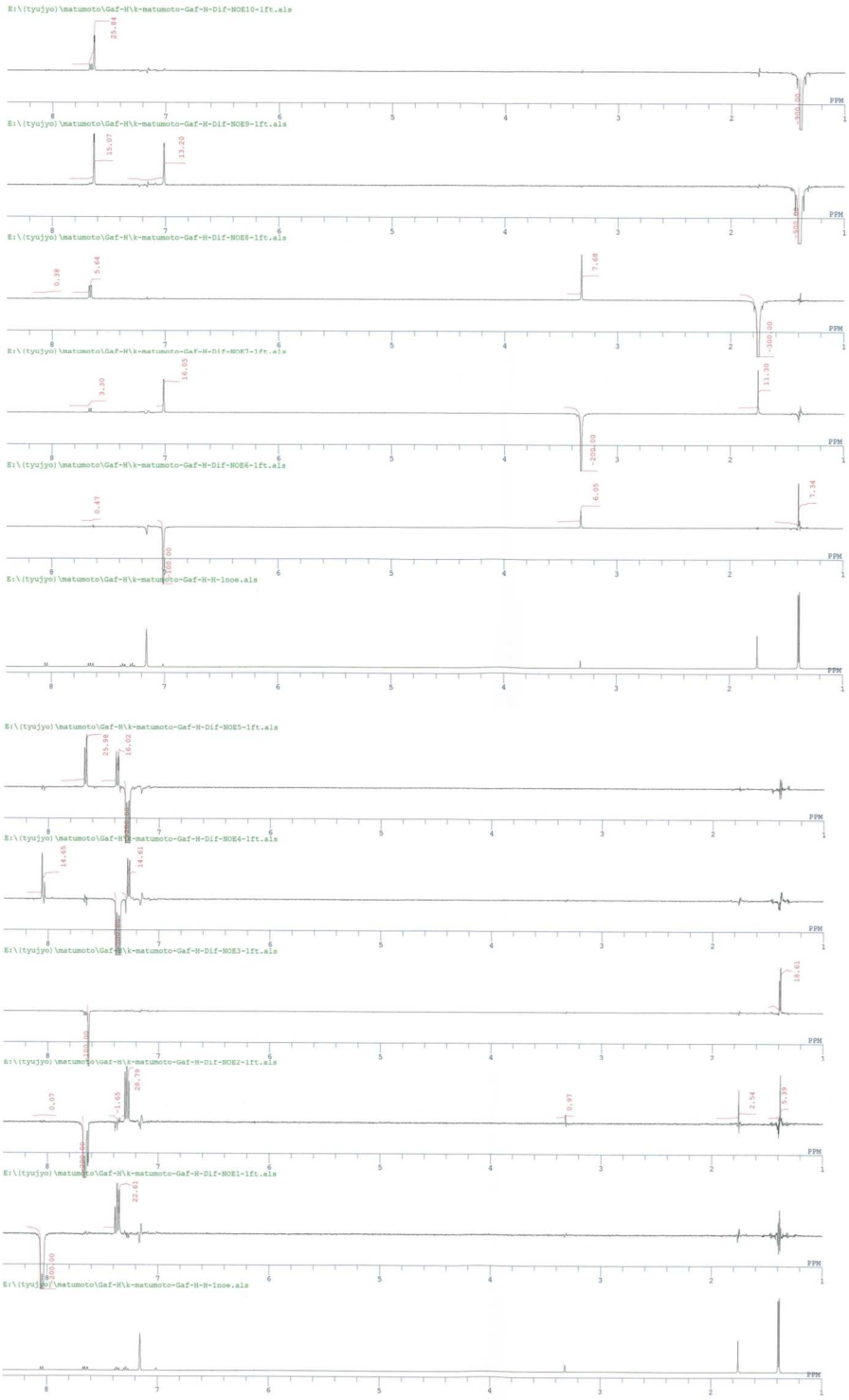

Figure S12. ^{1}H NMR NOE spectra of **Gaf** in C_6D_6.

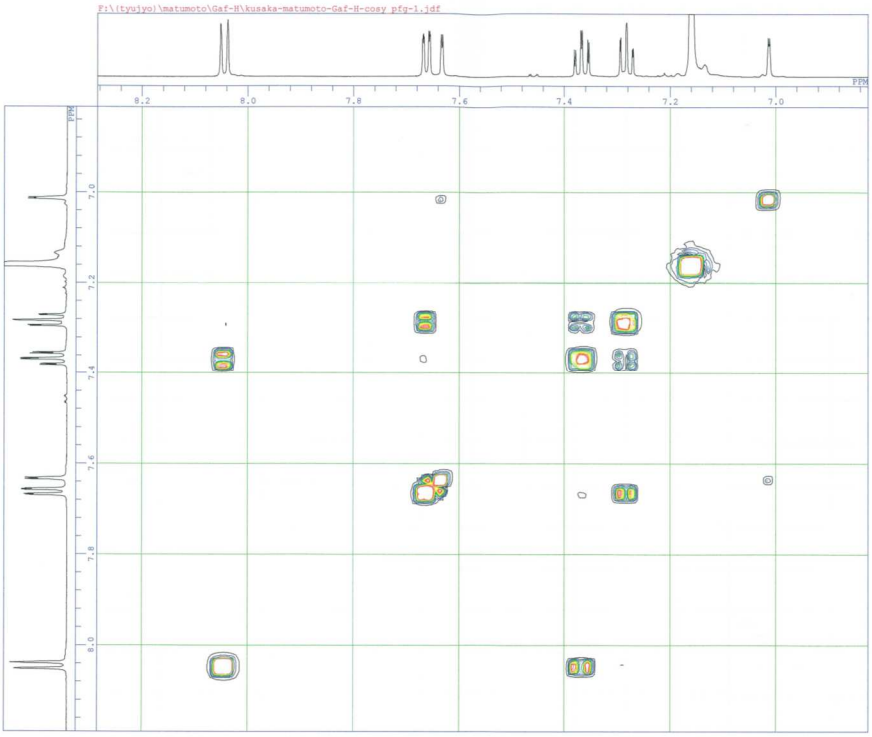

Figure S13. COSY NMR spectra of **Gaf** in C_6D_6.

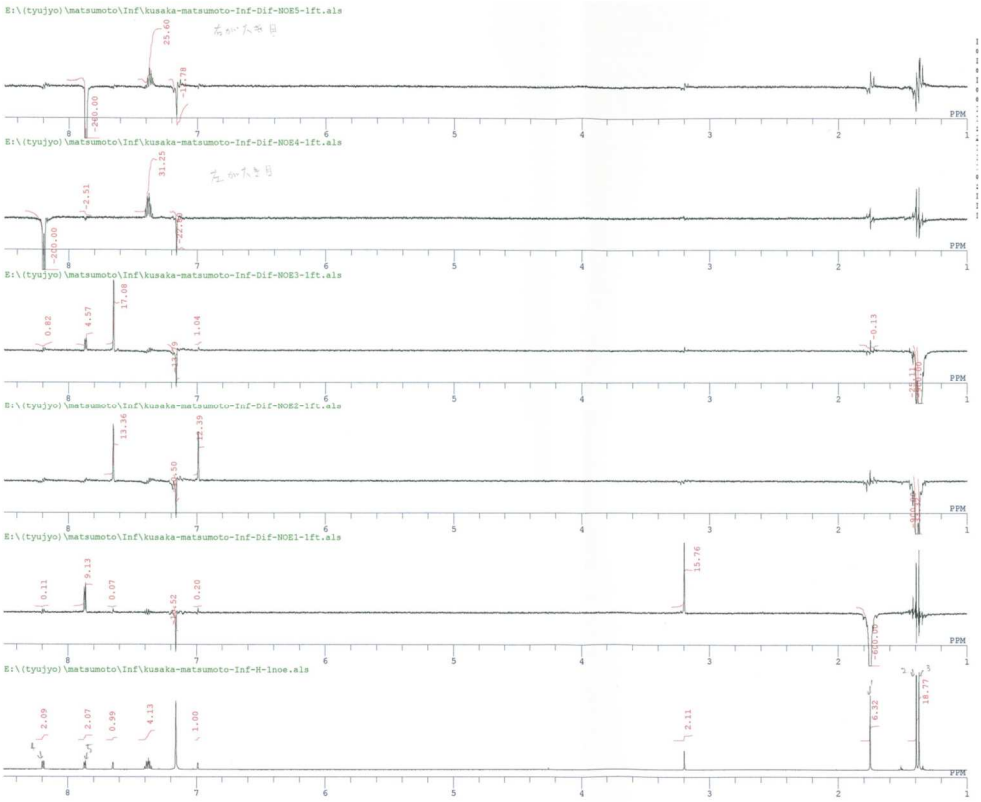

Figure S14. ^{1}H NMR NOE spectra of **Inf** in C_6D_6.

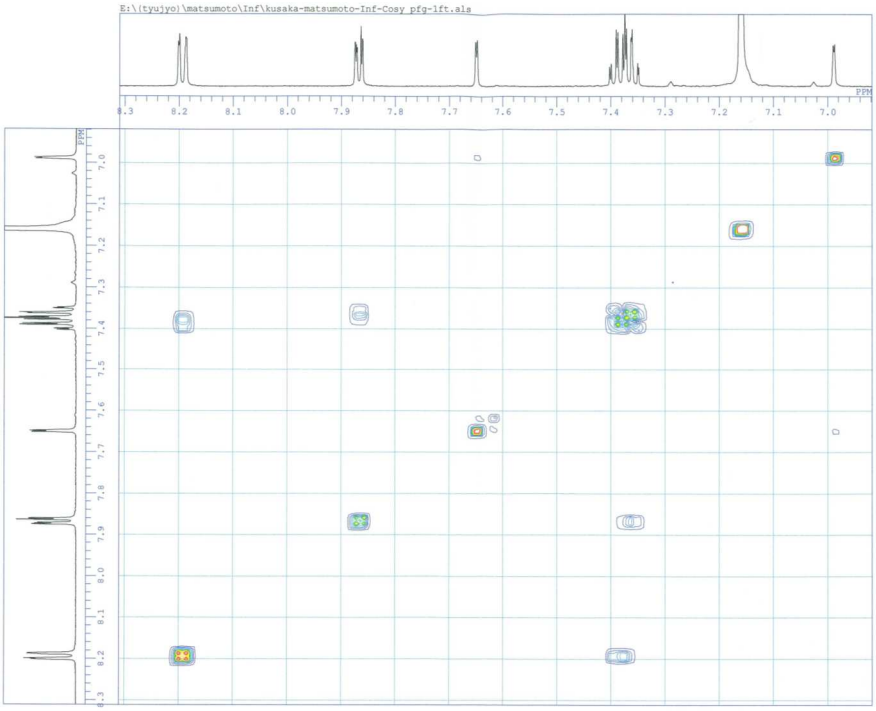

Figure S15. COSY NMR spectra of **Inf** in C_6D_6.

Preparation of Single Crystals. The single crystal of **Bf** was prepared by recrystallization from chloroform and methanol solution in the two-layer method. Those of **Alf**, **Gaf** and **Inf** were prepared by recrystallization from benzene solutions in the slow evaporation methods.

X-ray Crystal Structure Analyses. Intensity data were collected on a Rigaku R-AXIS RAPID imaging plate area detector with graphite monochromated Mo *K*α radiation at –180 °C. The structures were solved by direct method (SIR97)[9] and refined by full-matrix least-squares procedures based on F^2 (SHELX-97).[10]

Table S1. Crystallographic Data of Bf

Empirical formula	$C_{29}H_{36}BN$
Formula weight	409.40
Temperature (K)	93(2)
Wavelength (Å)	0.71075
Crystal system, space group	triclinic, *P-1*
Unit cell dimensions	a = 8.1338(11)
	b = 11.6890(15)
	c = 13.3458(18)
	α = 107.085(8)
	β = 95.758(7)
	γ = 92.208(7)
V (Å^3)	1203.7(3)
Z, calculated density (Mg m^{-3})	2, 1.130
Absorption coefficient	0.064
F(000)	444
Crystal size (mm)	0.70 × 0.60 × 0.60
θ range for data collection	3.01–25.00
Limiting indices	$-9\leq h\leq 9$, $-13\leq k\leq 13$, $-15\leq l\leq 15$
Reflections collected (unique)	8229/ 4173 [R(int) = 0.0456]
Completeness to theta = 25.00	0.983
Max. and min. transmission	0.9629 and 0.9569
Goodness-of-fit on F^2	1.070
Final R indices [$I > 2\sigma(I)$][a]	R_1 = 0.0543 wR_2 = 0.1481
R indices (all data)	R_1 = 0.0638, wR_2 = 0.1562

[a] $R_1 = \Sigma(|F_0|-|F_c|)/\Sigma|F_0|$. w$R_2 = [\Sigma w(F^2_0-F^2_c)^2/\ \Sigma w(F^2_0)^2]^{1/2}$. $w = 1/[\sigma^2(F^2_0)+[(ap)^2+bp]]$, where $p = [\max(F^2_0,0)+2F^2_c]/3$.

Table S2. Crystallographic Data of Alf

Empirical formula	$C_{29}H_{36}AlN$
Formula weight	425.57
Temperature (K)	93(2)
Wavelength (Å)	0.71075
Crystal system, space group	monoclinic, *P21/c*
Unit cell dimensions	a = 8.0433(3)
	b = 12.0138(6)
	c = 25.6152(12)
	α = 90.00
	β = 95.516(7)
	γ = 90.00
V (Å^3)	2463.75(19)
Z, calculated density (Mg m^{-3})	4, 1.147
Absorption coefficient	0.098
F(000)	920
Crystal size (mm)	0.50 × 0.50 × 0.30
θ range for data collection	3.06–25.00
Limiting indices	$-8 \le h \le 9$, $-14 \le k \le 14$, $-30 \le l \le 30$
Reflections collected (unique)	18200/ 4329 [R(int) = 0.0613]
Completeness to theta = 25.00	0.998
Max. and min. transmission	0.9712 and 0.9526
Goodness-of-fit on F^2	1.076
Final R indices [$I > 2\sigma(I)$][a]	R_1 = 0.0460, wR_2 = 0.1199
R indices (all data)	R_1 = 0.0546, wR_2 = 0.1263

[a] $R_1 = \Sigma(|F_0|-|F_c|)/\Sigma|F_0|$. w$R_2 = [\Sigma w(F^2_0-F^2_c)^2/ \Sigma w(F^2_0)^2]^{1/2}$. $w = 1/[\sigma^2(F^2_0)+[(ap)^2+bp]]$, where $p = [\max(F^2_0,0)+2F^2_c]/3$.

Table S3. Crystallographic Data of Gaf

Empirical formula	$C_{29}H_{36}GaN$
Formula weight	468.31
Temperature (K)	93(2)
Wavelength (Å)	0.71075
Crystal system, space group	monoclinic, *P21/c*
Unit cell dimensions	a = 8.0444(3)
	b = 11.9945(4)
	c = 25.5765(8)
	α = 90.00
	β = 95.569(7)
	γ = 90.00
V (Å^3)	2456.19(14)
Z, calculated density (Mg m^{-3})	4, 1.266
Absorption coefficient	1.136
F(000)	992
Crystal size (mm)	0.30 × 0.30 × 0.30
θ range for data collection	3.06–27.47
Limiting indices	$-10 \le h \le 10$, $-15 \le k \le 15$, $-33 \le l \le 33$
Reflections collected (unique)	22122/ 5611 [R(int) = 0.0692]
Completeness to theta = 27.47	0.998
Max. and min. transmission	0.7268 and 0.7268
Goodness-of-fit on F^2	1.045
Final R indices [$I > 2\sigma(I)$][a]	R_1 = 0.0438, wR_2 = 0.0807
R indices (all data)	R_1 = 0.0631, wR_2 = 0.0896

[a] $R_1 = \Sigma(|F_0|-|F_c|)/\Sigma|F_0|$. w$R_2 = [\Sigma w(F^2_0-F^2_c)^2/ \Sigma w(F^2_0)^2]^{1/2}$. $w = 1/[\sigma^2(F^2_0)+[(ap)^2+bp]]$, where $p = [\max(F^2_0,0)+2F^2_c]/3$.

Table S4. Crystallographic Data of Inf

Empirical formula	$C_{29}H_{36}InN$
Formula weight	513.41
Temperature (K)	93(2)
Wavelength (Å)	0.71075
Crystal system, space group	monoclinic, *P21/c*
Unit cell dimensions	a = 8.1017(4)
	b = 12.3146(7)
	c = 25.3088(13)
	α = 90.00
	β = 96.226(7)
	γ = 90.00
V (Å^3)	2510.1(2)
Z, calculated density (Mg m^{-3})	4, 1.359
Absorption coefficient	0.957
F(000)	1064
Crystal size (mm)	0.30 × 0.20 × 0.20
θ range for data collection	3.02–27.48
Limiting indices	$-10 \le h \le 10$, $-15 \le k \le 15$, $-32 \le l \le 28$
Reflections collected (unique)	22999/ 5725 [R(int) = 0.0475]
Completeness to theta = 27.48	0.996
Max. and min. transmission	0.8316 and 0.7622
Goodness-of-fit on F^2	1.041
Final R indices [$I > 2\sigma(I)$][a]	R_1 = 0.0523, wR_2 = 0.1442
R indices (all data)	R_1 = 0.0565, wR_2 = 0.1477

[a] $R_1 = \Sigma(|F_0|-|F_c|)/\Sigma|F_0|$. w$R_2 = [\Sigma w(F^2_0-F^2_c)^2/ \Sigma w(F^2_0)^2]^{1/2}$. $w = 1/[\sigma^2(F^2_0)+[(ap)^2+bp]]$, where $p = [\max(F^2_0,0)+2F^2_c]/3$.

UV−vis Absorption and Photoluminescence (PL) Data

Table S5. Optical Data of Heterofluorenes[a]

	Bf	Alf	Gaf	Inf
λ_{abs} (nm)[b]	281	282	282	282
ε ($\times 10^3$ $M^{-1}cm^{-1}$)	7.9	8.5	8.7	8.9
λ_{FL} (nm)[c]	345, 381	357	371	309, 330
λ_{Phos} (nm)[d]	—[j]	—[j]	488	487
Φ_{total} (%)[e]	0.011	4.5	0.11	0.077
Φ_{FL} (%)[f]	0.011	4.5	0.088	0.026
Φ_{Phos} (%)[g]	—[j]	—[j]	0.018	0.051
Φ_{Phos} / Φ_{total}	0	0	0.17	0.66
τ_{FL} (ns)[h]	0.04 (61%), 1.37 (35%), 7.20 (4.3%)	1.97	0.04	0.06 (29%), 0.94 (39%), 11.7 (7.5%), 3.30 (25%)
τ_{Phos} (μs)[i]	—[j]	—[j]	85	99

[a]Measurement in CH_2Cl_2 (1.0×10^{-4} M) under argon atmosphere at room temperature. [b]Absorption maxima. [c]Fluorescence maxima excited at 282 nm. [d]Phosphorescence maxima excited at 282 nm. [e]Relative quantum yields using 9,10-diphenylanthracene as a standard. [f]Relative quantum yields at the wavelength range from 292 nm to 445 nm. [g]Relative quantum yield at the wavelength range from 445 nm to 550 nm. [h]Fluorescence life time excited at 290 nm by a UV diode laser and detected at 360 nm. [i]Phosphorescence life time excited at 282 nm and detected at λ_{Phos}. [j]Not detected.

Table S6. Optical Data of Mf (M = B, Al, Ga) after Adding $B(C_6F_5)_3$

	$\lambda_{max,PL}$ (nm)[a, b]	$\tau_{1/2}$ [c]	χ^2 [c]
Bf	597	0.20 μs (31%), 8.95 μs (69%)	0.93
Alf	588	0.24 μs (60%), 2.14 μs (40%)	1.06
Gaf	575	0.15 μs (4%), 1.33 μs (96%)	1.17

[a]Measurement in benzene with 10 mM **Mf** (M = B, Al, Ga) after adding 1.0 eq. $B(C_6F_5)_3$ excited at 282 nm under argon atmosphere at room temperature. [b]Emission maxima excited at 282 nm. [c]Fluorescence life time excited at 290 nm by a UV diode laser and detected at $\lambda_{max,PL}$.

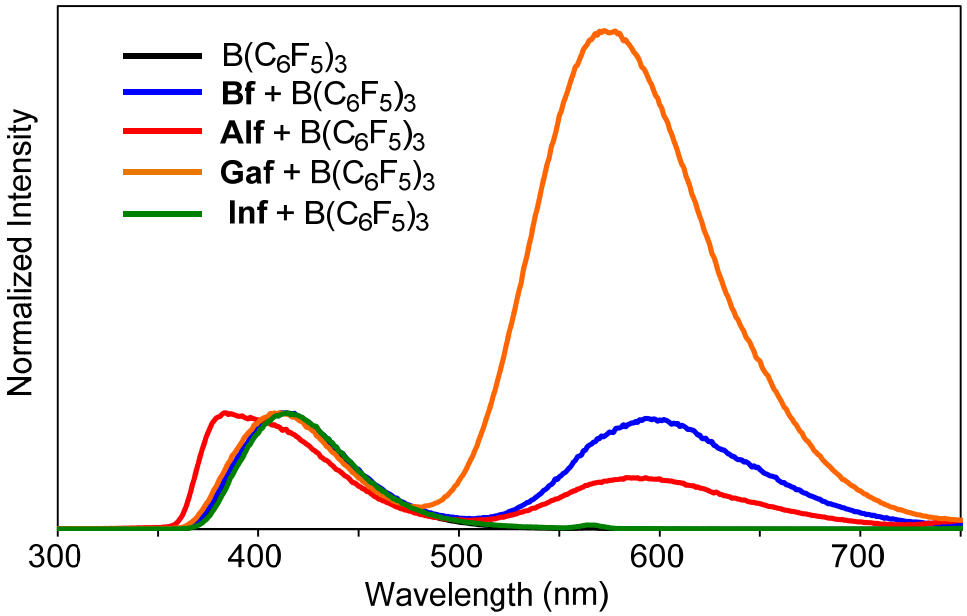

Figure S16. Photoluminescence spectra of 10 mM **Mf** (M = B (blue), Al (red), Ga (orange) In (geen)) after adding 1.0 eq. $B(C_6F_5)_3$ and 10 mM $B(C_6F_5)_3$ (black) in benzene excited at 282 nm under argon atmosphere at room temperature. The emission spectrum of $B(C_6F_5)_3$ overlapped with the spectrum of **Inf** after adding 1.0 eq. $B(C_6F_5)_3$.

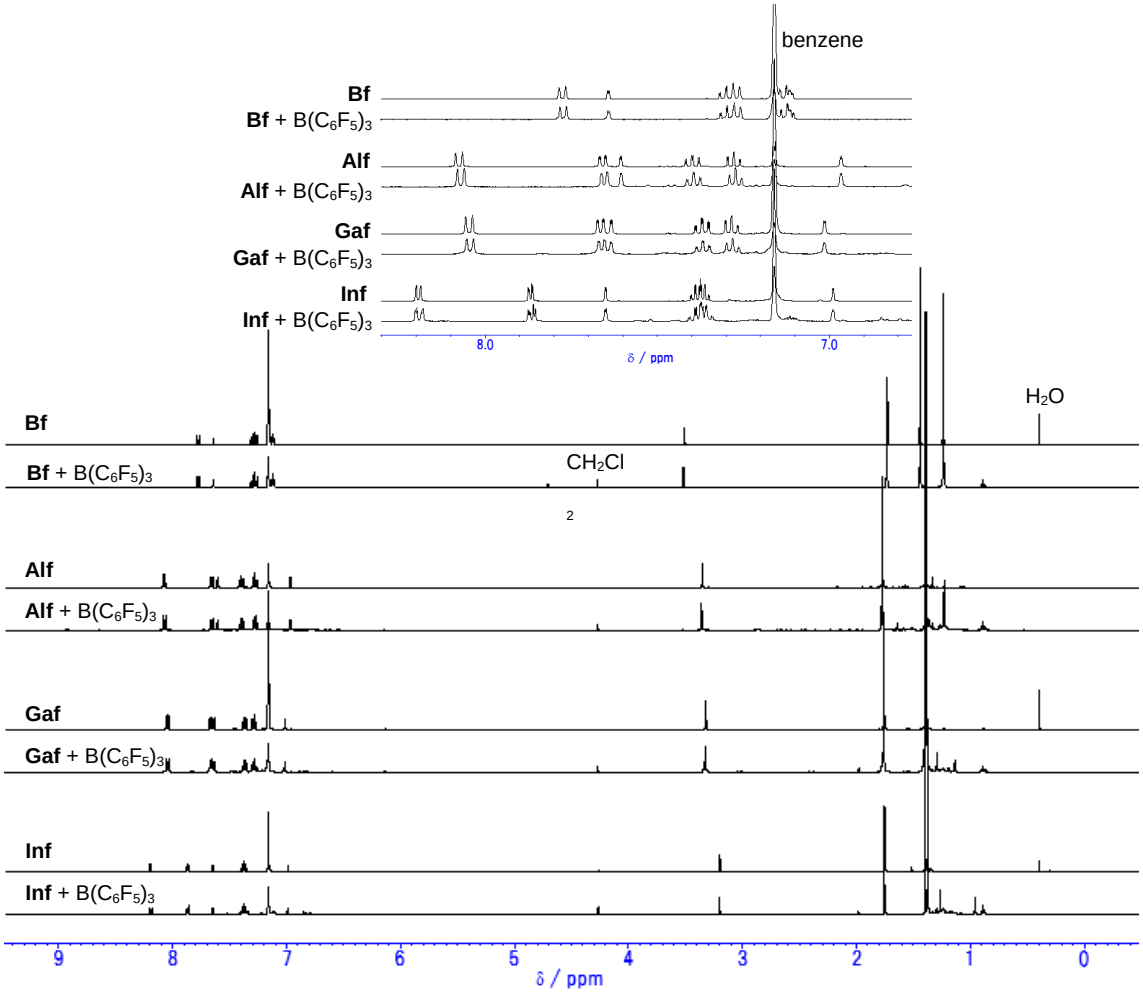

Figure S17. ^{1}H NMR spectra of **Mf** (M = B, Al, Ga and In) after adding 1.0 eq. $B(C_6F_5)_3$ in C_6D_6.

DFT Calculation by Gaussian 09 Program

Table S7. Cartesian Coordinates of the Optimized Structure of Bf in the Ground S_0 State Calculated at the B3LYP/6-31G(d,p) Level

Center Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	2.303889	1.669313	−1.815519
C	3.523101	2.330206	−2.017433
C	4.635626	1.999382	−1.242646
C	4.534850	1.012890	−0.258940
C	3.314965	0.361180	−0.060215
C	2.169349	0.675629	−0.840215
C	3.007317	−0.680380	0.943679
C	1.659686	−1.099557	0.831564
B	0.951831	−0.317805	−0.410231
C	3.850227	−1.203721	1.926775
C	3.349541	−2.154799	2.820338
C	2.016900	−2.564254	2.738803
C	1.176611	−2.032089	1.751224
C	−0.639731	0.003452	−0.210404
C	−1.370134	−1.085883	−0.739154
C	−2.753793	−1.195053	−0.709957
C	−3.512476	−0.184568	−0.111875
C	−2.805856	0.887107	0.443701
C	−1.401754	1.015919	0.432243
C	−0.791750	2.273512	1.107815
C	0.437809	1.910983	1.965626
C	−1.790146	2.981304	2.054581
C	−0.388718	3.295423	0.019427
C	−5.048907	−0.286622	−0.078353
C	−5.709524	0.924262	0.606931
C	−5.460585	−1.560429	0.697674
C	−5.591151	−0.373640	−1.524768
C	−0.496438	−2.164182	−1.325689
N	0.775120	−1.478547	−1.711055
C	1.900246	−2.439214	−1.844440
C	0.577138	−0.801475	−3.024161
H	1.452057	1.954993	−2.429026
H	3.601040	3.105106	−2.775348
H	5.580371	2.512439	−1.400651
H	5.402230	0.761902	0.346405
H	4.882360	−0.872641	2.011542
H	3.996924	−2.566320	3.590026
H	1.629848	−3.289306	3.450013
H	0.132539	−2.339165	1.722107
H	−3.233739	−2.064909	−1.152523
H	−3.380241	1.668011	0.917372
H	0.181849	1.167570	2.727140

H	1.257447	1.515620	1.370031
H	0.809200	2.806444	2.476890
H	−2.188269	2.299447	2.813438
H	−1.272149	3.792740	2.575775
H	−2.632942	3.433850	1.522763
H	0.380558	2.894590	−0.640654
H	−1.255007	3.576243	−0.589938
H	0.009190	4.207230	0.480712
H	−5.394970	1.023786	1.650648
H	−5.479086	1.861435	0.089954
H	−6.797721	0.802496	0.600537
H	−5.097435	−1.522346	1.729875
H	−6.551949	−1.658229	0.724464
H	−5.056420	−2.466254	0.235911
H	−5.322275	0.519911	−2.097719
H	−5.192602	−1.242989	−2.056195
H	−6.683923	−0.458306	−1.520510
H	−0.935807	−2.677243	−2.190066
H	−0.240804	−2.922583	−0.578446
H	1.698893	−3.139853	−2.661988
H	2.814509	−1.882720	−2.055675
H	2.025194	−2.983095	−0.909956
H	0.320329	−1.546167	−3.785140
H	1.494871	−0.289017	−3.305632
H	−0.232103	−0.077062	−2.935975

Table S8. Cartesian Coordinates of the Optimized Structure of Alf in the Ground S_0 State Calculated at the B3LYP/6-31G(d,p) Level

Center Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	2.536484	1.725899	−2.069821
C	3.763699	2.287583	−2.436858
C	4.910705	1.946532	−1.720909
C	4.831856	1.055757	−0.649884
C	3.602715	0.491278	−0.276205
C	2.421834	0.828063	−1.000715
C	3.463489	−0.469022	0.870642
C	2.164610	−0.992107	1.130919
Al	0.936743	−0.223314	−0.217511
C	4.544186	−0.853842	1.678484
C	4.358219	−1.746191	2.734996
C	3.091281	−2.264248	3.003484
C	2.010763	−1.880704	2.202541
C	−1.031429	0.031902	−0.016061
C	−1.681365	−1.108766	−0.538276
C	−3.068479	−1.246245	−0.557784
C	−3.886895	−0.240673	−0.033428
C	−3.251322	0.888947	0.499293
C	−1.855541	1.050294	0.521828
C	−1.240175	2.338449	1.121553
C	−0.214101	1.976095	2.219494
C	−2.292322	3.261096	1.772415
C	−0.542101	3.147838	0.004017
C	−5.418802	−0.402890	−0.060290
C	−6.153077	0.803070	0.555332
C	−5.815410	−1.665825	0.740977
C	−5.894646	−0.557069	−1.524448
C	−0.818561	−2.253786	−1.044187
N	0.473007	−1.736337	−1.590247
C	1.492371	−2.808030	−1.676143
C	0.259479	−1.141336	−2.934592
H	1.648043	2.009764	−2.632950
H	3.823957	2.984788	−3.268515
H	5.871690	2.374864	−1.993575
H	5.741783	0.809040	−0.110979
H	5.540809	−0.461528	1.498701
H	5.206210	−2.032575	3.351675
H	2.946764	−2.954466	3.830718
H	1.025302	−2.284217	2.432872
H	−3.508306	−2.145979	−0.982530
H	−3.870474	1.673736	0.908614
H	−0.689961	1.414183	3.030082
H	0.613231	1.366572	1.845630
H	0.223265	2.885411	2.646676

H	−2.838817	2.759028	2.577739
H	−1.790895	4.131464	2.207606
H	−3.020021	3.636281	1.045460
H	0.278402	2.591223	−0.454384
H	−1.254211	3.415561	−0.784169
H	−0.122016	4.075202	0.410217
H	−5.884582	0.951342	1.606224
H	−5.939656	1.730518	0.014194
H	−7.234398	0.637027	0.511765
H	−5.496534	−1.582006	1.784999
H	−6.902770	−1.801984	0.727492
H	−5.361655	−2.570683	0.325920
H	−5.632118	0.326139	−2.115972
H	−5.445417	−1.429024	−2.008901
H	−6.983098	−0.679576	−1.562378
H	−1.334538	−2.856242	−1.805124
H	−0.561464	−2.928526	−0.218455
H	1.157899	−3.610190	−2.346919
H	2.422938	−2.384498	−2.059036
H	1.679904	−3.212014	−0.680717
H	−0.050397	−1.914448	−3.649738
H	1.186855	−0.677734	−3.273971
H	−0.520110	−0.380428	−2.873112

Table S9. Cartesian Coordinates of the Optimized Structure of Gaf in the Ground S_0 State Calculated at the B3LYP/6-31G(d,p) Level

Center Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	2.533433	1.988525	−1.749666
C	3.781697	2.555489	−2.024335
C	4.909363	2.078426	−1.357842
C	4.788829	1.050633	−0.421735
C	3.537584	0.483949	−0.140060
C	2.383869	0.954681	−0.823884
C	3.340677	−0.605083	0.872875
C	2.017081	−1.081673	1.055519
Ga	0.838822	−0.097227	−0.191119
C	4.385286	−1.146368	1.634985
C	4.129254	−2.144603	2.576354
C	2.829166	−2.610401	2.771332
C	1.786023	−2.071037	2.011780
C	−1.123807	0.047571	−0.045985
C	−1.734809	−1.043684	−0.683483
C	−3.121373	−1.219504	−0.707684
C	−3.958677	−0.294945	−0.082690
C	−3.347236	0.800364	0.551611
C	−1.961830	0.994530	0.582786
C	−1.353781	2.238748	1.270189
C	−0.316184	1.803935	2.330672
C	−2.408734	3.109460	1.978743
C	−0.651945	3.106947	0.200645
C	−5.493058	−0.425976	−0.074518
C	−6.119944	0.799909	−0.780251
C	−5.999598	−0.489439	1.386104
C	−5.975005	−1.694958	−0.802630
C	−0.831932	−2.099570	−1.301765
N	0.441239	−1.481991	−1.762195
C	1.523031	−2.469433	−1.929494
C	0.234112	−0.730642	−3.019897
H	1.660926	2.380256	−2.269308
H	3.875331	3.360887	−2.747816
H	5.886860	2.508210	−1.559969
H	5.681776	0.702079	0.088608
H	5.405632	−0.795438	1.510601
H	4.949263	−2.553030	3.161110
H	2.633452	−3.382054	3.511281
H	0.775365	−2.441262	2.176914
H	−3.534767	−2.082426	−1.220391
H	−3.989504	1.527876	1.032022
H	−0.773270	1.159434	3.088677
H	0.513282	1.248265	1.885955
H	0.110314	2.678672	2.833525

H	−2.943395	2.554755	2.757209
H	−1.915679	3.960079	2.460086
H	−3.146554	3.514944	1.278616
H	0.144881	2.542044	−0.287019
H	−1.361295	3.435769	−0.566338
H	−0.201448	3.995538	0.656984
H	−5.848272	1.736530	−0.285197
H	−5.786694	0.864336	−1.821307
H	−7.213418	0.725269	−0.777268
H	−5.729258	0.406931	1.951680
H	−7.091615	−0.579893	1.407735
H	−5.576825	−1.353344	1.909343
H	−5.678991	−1.697159	−1.856879
H	−5.584817	−2.605243	−0.335736
H	−7.067938	−1.748828	−0.767920
H	−0.567463	−2.851300	−0.548110
H	−1.325137	−2.628351	−2.130218
H	2.447530	−1.945670	−2.183772
H	1.694976	−2.990810	−0.986933
H	1.289778	−3.195705	−2.719700
H	1.144754	−0.181285	−3.266186
H	−0.577002	−0.012750	−2.884905
H	−0.020219	−1.409854	−3.844815

Table S10. Cartesian Coordinates of the Optimized Structure of Gaf in the Ground S_0 State Calculated at the B3LYP/LANL2DZ Level

Center Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	2.440834	1.763753	−2.052162
C	3.670747	2.347766	−2.425438
C	4.835705	2.024052	−1.704742
C	4.771205	1.126995	−0.622499
C	3.541498	0.540095	−0.245774
C	2.346653	0.859999	−0.973342
C	3.411992	−0.421522	0.905633
C	2.106863	−0.954648	1.166848
Ga	0.853212	−0.201483	−0.187539
C	4.502637	−0.798013	1.722249
C	4.318068	−1.692206	2.793419
C	3.040451	−2.216737	3.065578
C	1.948597	−1.841238	2.252170
C	−1.124774	0.010648	−0.014425
C	−1.763397	−1.141122	−0.543048
C	−3.163425	−1.293431	−0.568667
C	−3.993852	−0.289727	−0.043042
C	−3.363062	0.855784	0.498458
C	−1.963163	1.035648	0.526155
C	−1.363739	2.340472	1.122720
C	−0.327890	2.003474	2.233643
C	−2.437523	3.258263	1.768249
C	−0.673828	3.158677	−0.008027
C	−5.537313	−0.390236	−0.040661
C	−6.137588	0.794596	−0.854132
C	−6.060722	−0.323327	1.424747
C	−6.045251	−1.711463	−0.671426
C	−0.887429	−2.284160	−1.053611
N	0.420022	−1.750755	−1.589345
C	1.471003	−2.816209	−1.651528
C	0.220690	−1.147909	−2.950482
H	1.545520	2.033440	−2.613303
H	3.718227	3.045606	−3.259191
H	5.789529	2.469275	−1.981138
H	5.684687	0.895057	−0.080240
H	5.497726	−0.399450	1.539242
H	5.166163	−1.972037	3.415488
H	2.895863	−2.900466	3.899981
H	0.962213	−2.243490	2.484747
H	−3.590236	−2.196037	−0.997512
H	−3.996366	1.633601	0.908682
H	−0.792516	1.415896	3.036408
H	0.527592	1.430485	1.860956
H	0.070489	2.929379	2.670460

H	−2.976539	2.752749	2.580501
H	−1.945944	4.141773	2.195287
H	−3.170918	3.615216	1.033512
H	0.151357	2.607055	−0.467825
H	−1.395847	3.415188	−0.795022
H	−0.261309	4.093169	0.396981
H	−5.849159	1.764140	−0.431025
H	−5.792220	0.766960	−1.895938
H	−7.235032	0.740065	−0.854037
H	−5.764813	0.609798	1.918473
H	−7.157925	−0.379961	1.440643
H	−5.664390	−1.157167	2.018619
H	−5.734747	−1.807820	−1.720184
H	−5.682852	−2.590220	−0.121885
H	−7.142472	−1.733167	−0.646204
H	−0.636460	−2.967427	−0.230156
H	−1.399878	−2.875716	−1.828121
H	2.403905	−2.379850	−2.020600
H	1.650791	−3.213421	−0.649416
H	1.162599	−3.631909	−2.323184
H	1.152152	−0.679758	−3.278865
H	−0.563083	−0.387449	−2.900168
H	−0.076201	−1.922252	−3.673814

Table S11. Cartesian Coordinates of the Optimized Structure of Inf in the Ground S_0 State Calculated at the B3LYP/LANL2DZ Level

Center Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	2.489047	1.752582	−2.159913
C	3.717970	2.272929	−2.619531
C	4.902978	1.928496	−1.943670
C	4.856862	1.078258	−0.824240
C	3.628078	0.552028	−0.355118
C	2.414605	0.894887	−1.041084
C	3.561973	−0.358681	0.851656
C	2.288923	−0.873224	1.269241
In	0.792317	−0.134711	−0.084326
C	4.722489	−0.709794	1.584092
C	4.643894	−1.550393	2.709071
C	3.399496	−2.054991	3.129256
C	2.237609	−1.709326	2.405836
C	−1.346554	0.048532	0.076573
C	−1.969040	−1.131338	−0.418463
C	−3.366462	−1.276064	−0.465409
C	−4.213015	−0.248735	−0.002223
C	−3.598562	0.919261	0.494919
C	−2.193547	1.095526	0.543454
C	−1.602723	2.425853	1.095950
C	−0.654575	2.139522	2.296336
C	−2.694393	3.404433	1.609817
C	−0.821117	3.165370	−0.030011
C	−5.748557	−0.433154	−0.053155
C	−6.516828	0.794409	0.497696
C	−6.148392	−1.674060	0.799514
C	−6.196837	−0.660767	−1.527377
C	−1.105999	−2.317383	−0.857348
N	0.192396	−1.876121	−1.483142
C	1.197060	−2.984277	−1.512034
C	−0.035465	−1.343077	−2.865292
H	1.576842	2.034742	−2.686852
H	3.749106	2.935010	−3.482836
H	5.859658	2.321191	−2.282890
H	5.790789	0.834883	−0.324817
H	5.698541	−0.331063	1.292634
H	5.549804	−1.804050	3.256354
H	3.333777	−2.699622	4.003784
H	1.278098	−2.097368	2.749065
H	−3.790904	−2.197854	−0.861057
H	−4.235307	1.716622	0.851981
H	−1.196578	1.638050	3.108796
H	0.195814	1.500922	2.029599
H	−0.241942	3.080093	2.685524

H	−3.287747	2.967059	2.423227
H	−2.212642	4.309769	2.001216
H	−3.377686	3.715730	0.809194
H	0.029395	2.584713	−0.403506
H	−1.481052	3.380707	−0.881041
H	−0.423940	4.118032	0.346564
H	−6.270149	0.990908	1.549152
H	−6.304025	1.702338	−0.081460
H	−7.597180	0.608498	0.439175
H	−5.852240	−1.538356	1.847761
H	−7.236036	−1.825602	0.765964
H	−5.669898	−2.589948	0.431802
H	−5.940649	0.205598	−2.151060
H	−5.717216	−1.544277	−1.966143
H	−7.284338	−0.809409	−1.576267
H	−1.657676	−2.967834	−1.555344
H	−0.840894	−2.930694	0.016019
H	0.825018	−3.843517	−2.092556
H	2.123088	−2.620476	−1.967997
H	1.422382	−3.305440	−0.490951
H	−0.385317	−2.141415	−3.538856
H	0.898647	−0.926364	−3.253827
H	−0.791328	−0.553433	−2.831908

Table S12. Cartesian Coordinates of the Optimized Structure of Bf in the Excited S_1 State Calculated at the TD-B3LYP/6-31G(d,p) Level

Center Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	−1.926467	0.916092	−2.271050
C	−3.039063	1.429411	−2.933583
C	−4.324281	1.293098	−2.374527
C	−4.492344	0.628482	−1.156495
C	−3.383329	0.109628	−0.483812
C	−2.049700	0.256209	−1.026903
C	−3.322238	−0.598245	0.791702
C	−1.948794	−0.918054	1.105966
B	−1.053658	−0.404669	−0.042761
C	−4.358394	−0.949262	1.658544
C	−4.069595	−1.613589	2.853263
C	−2.737915	−1.926030	3.185359
C	−1.696919	−1.582685	2.326926
C	0.547931	−0.267845	−0.017464
C	1.077488	0.843797	0.688352
C	2.447877	1.072236	0.841919
C	3.388041	0.213850	0.269406
C	2.877805	−0.879431	−0.437021
C	1.506566	−1.154987	−0.587641
C	1.090479	−2.439998	−1.354305
C	0.300229	−3.379170	−0.412802
C	2.300663	−3.243851	−1.879256
C	0.224826	−2.081119	−2.583768
C	4.895336	0.477805	0.445962
C	5.763785	−0.575794	−0.266689
C	5.250361	0.455193	1.951747
C	5.250393	1.865501	−0.139177
C	0.135745	1.817917	1.367630
N	−0.283261	2.986320	0.567156
C	−1.609822	3.516681	0.799740
C	0.458907	3.437601	−0.588251
H	−0.946752	0.998957	−2.742120
H	−2.921267	1.925243	−3.894289
H	−5.188387	1.692840	−2.898078
H	−5.491270	0.513699	−0.739923
H	−5.391091	−0.711164	1.410401
H	−4.875228	−1.891433	3.527357
H	−2.525449	−2.444152	4.117437
H	−0.675194	−1.843159	2.598791
H	2.780135	1.924685	1.431913
H	3.586623	−1.562162	−0.880154
H	0.913841	−3.673286	0.446173
H	−0.608870	−2.909824	−0.035482
H	0.014438	−4.291000	−0.949830

H	2.954687	−3.591854	−1.072470
H	1.934113	−4.131810	−2.403703
H	2.904708	−2.672561	−2.592767
H	−0.698147	−1.575034	−2.301196
H	0.777327	−1.431588	−3.272649
H	−0.043747	−2.993751	−3.127927
H	5.589755	−1.581452	0.128581
H	5.577454	−0.596068	−1.345219
H	6.822980	−0.341697	−0.118701
H	5.013553	−0.517623	2.393965
H	6.320214	0.644051	2.095942
H	4.700831	1.217829	2.512154
H	5.015221	1.912205	−1.207764
H	4.702975	2.670343	0.361762
H	6.320104	2.070707	−0.018967
H	0.599853	2.266610	2.257528
H	−0.782640	1.325554	1.688293
H	−1.690115	4.533886	0.418186
H	−2.311348	2.860457	0.274645
H	−1.832460	3.481477	1.867006
H	1.504442	3.156023	−0.493107
H	0.337370	4.516136	−0.699066
H	0.037607	2.935161	−1.463538

Table S13. Cartesian Coordinates of the Optimized Structure of Alf in the Excited S_1 State Calculated at the TD-B3LYP/6-31G(d,p) Level

Center Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	2.617557	1.689670	−2.049000
C	3.858943	2.155341	−2.463254
C	5.051450	1.723079	−1.810022
C	4.972422	0.851555	−0.748190
C	3.711588	0.363412	−0.289755
C	2.466555	0.755828	−1.004816
C	3.549054	−0.468740	0.853463
C	2.152145	−0.838425	1.200330
Al	0.937390	−0.183154	−0.198126
C	4.623511	−0.920682	1.679091
C	4.375772	−1.635073	2.827951
C	3.031560	−1.927342	3.211350
C	1.966690	−1.519397	2.418822
C	−1.052962	0.045176	−0.040363
C	−1.692672	−1.129747	−0.495855
C	−3.077667	−1.287280	−0.504126
C	−3.910130	−0.266864	−0.036111
C	−3.288561	0.900756	0.424728
C	−1.894833	1.084021	0.435437
C	−1.310453	2.414918	0.972555
C	−0.405297	2.133214	2.194050
C	−2.397126	3.411642	1.428841
C	−0.488269	3.114242	−0.134215
C	−5.439228	−0.453608	−0.046866
C	−6.189885	0.770107	0.511376
C	−5.812816	−1.680610	0.818783
C	−5.919442	−0.689760	−1.498676
C	−0.825655	−2.293462	−0.948789
N	0.449215	−1.795760	−1.532668
C	1.477482	−2.856067	−1.578825
C	0.224099	−1.253540	−2.893562
H	1.734995	2.041051	−2.581337
H	3.930912	2.840745	−3.303969
H	6.014786	2.097978	−2.141695
H	5.883900	0.558170	−0.235990
H	5.648539	−0.672455	1.420476
H	5.197686	−1.962449	3.457339
H	2.849695	−2.492473	4.122000
H	0.957276	−1.771996	2.739163
H	−3.504213	−2.215969	−0.877522
H	−3.918894	1.699895	0.785350
H	−0.976538	1.660266	3.000351
H	0.430780	1.472404	1.943920
H	0.015768	3.068977	2.579599

H	−3.007707	3.013096	2.245714
H	−1.917454	4.324681	1.796262
H	−3.064180	3.700285	0.609536
H	0.369502	2.514265	−0.447791
H	−1.109020	3.313366	−1.015002
H	−0.098757	4.072128	0.229582
H	−5.916917	0.976028	1.551359
H	−5.995198	1.672199	−0.077520
H	−7.268716	0.584836	0.484042
H	−5.490829	−1.539740	1.855685
H	−6.898049	−1.834084	0.817220
H	−5.346603	−2.597862	0.447078
H	−5.675858	0.167254	−2.135171
H	−5.456309	−1.576477	−1.941721
H	−7.005721	−0.833533	−1.523892
H	−1.350372	−2.940422	−1.666897
H	−0.555059	−2.920511	−0.089889
H	1.145046	−3.699590	−2.199511
H	2.397244	−2.442485	−1.997673
H	1.684802	−3.203409	−0.565048
H	−0.067724	−2.053831	−3.586960
H	1.143510	−0.781374	−3.245512
H	−0.570582	−0.506613	−2.857837

Table S14. Cartesian Coordinates of the Optimized Structure of Gaf in the Excited S_1 State Calculated at the TD-B3LYP/6-31G(d,p) Level

Center Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	2.533157	1.969068	−1.765650
C	3.780694	2.452413	−2.137656
C	4.970049	1.900035	−1.575517
C	4.881528	0.899115	−0.636072
C	3.613527	0.392009	−0.221313
C	2.378817	0.912684	−0.854842
C	3.438038	−0.568241	0.813268
C	2.041135	−0.925441	1.139013
Ga	0.834686	−0.045990	−0.133887
C	4.501456	−1.157336	1.563456
C	4.232522	−1.995415	2.619486
C	2.881384	−2.279335	2.984818
C	1.827424	−1.735600	2.262605
C	−1.139956	0.038196	−0.030469
C	−1.732992	−1.094639	−0.611699
C	−3.116699	−1.288394	−0.647734
C	−3.976932	−0.340395	−0.095194
C	−3.387567	0.794690	0.485509
C	−2.005071	1.008800	0.530783
C	−1.442857	2.298010	1.176418
C	−0.474552	1.930375	2.323884
C	−2.540512	3.208162	1.761190
C	−0.675000	3.106389	0.105832
C	−5.509515	−0.487800	−0.109165
C	−6.135002	0.691308	−0.891763
C	−6.044352	−0.478434	1.342621
C	−5.963912	−1.799566	−0.776844
C	−0.823055	−2.183115	−1.159295
N	0.434251	−1.594931	−1.668198
C	1.528974	−2.569835	−1.758433
C	0.228380	−0.920048	−2.962144
H	1.651945	2.416446	−2.220547
H	3.861574	3.236790	−2.885566
H	5.939331	2.287336	−1.873705
H	5.790879	0.514074	−0.184291
H	5.533225	−0.917525	1.324781
H	5.046221	−2.426024	3.195168
H	2.688518	−2.952731	3.815802
H	0.810810	−1.985599	2.559505
H	−3.508605	−2.185231	−1.117517
H	−4.046736	1.540018	0.911512
H	−0.978839	1.330468	3.088898
H	0.375395	1.353463	1.945965
H	−0.079647	2.835067	2.799783

H	−3.117064	2.706720	2.545884
H	−2.076133	4.092068	2.210372
H	−3.238375	3.560005	0.993911
H	0.167602	2.525186	−0.275151
H	−1.327812	3.365895	−0.734687
H	−0.275786	4.033550	0.532435
H	−5.887842	1.656119	−0.439675
H	−5.777388	0.706764	−1.926610
H	−7.227220	0.601399	−0.910732
H	−5.791195	0.448875	1.864600
H	−7.135947	−0.576739	1.348102
H	−5.625408	−1.309865	1.918866
H	−5.645614	−1.856264	−1.823003
H	−5.574383	−2.678676	−0.253102
H	−7.056835	−1.863585	−0.761336
H	−0.550667	−2.875549	−0.352878
H	−1.325905	−2.776275	−1.938212
H	2.445258	−2.050787	−2.050997
H	1.708469	−3.014293	−0.777205
H	1.316232	−3.363323	−2.489325
H	1.133248	−0.368118	−3.227188
H	−0.593543	−0.206642	−2.873320
H	−0.008254	−1.641080	−3.757766

Table S15. Cartesian Coordinates of the Optimized Structure of Gaf in the Excited S_1 State Calculated at the TD-B3LYP/LANL2DZ Level

Center Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	2.502362	1.846515	−1.940628
C	3.750053	2.311564	−2.384514
C	4.965391	1.818589	−1.789891
C	4.907568	0.894309	−0.754905
C	3.644079	0.407286	−0.269516
C	2.380766	0.853487	−0.936590
C	3.494389	−0.466338	0.854184
C	2.091805	−0.825006	1.225557
Ga	0.849952	−0.121805	−0.146492
C	4.583247	−0.970833	1.648997
C	4.338111	−1.716832	2.793942
C	2.984643	−1.987360	3.208092
C	1.902671	−1.525378	2.442390
C	−1.145074	0.029589	−0.027273
C	−1.753102	−1.150788	−0.530275
C	−3.148635	−1.338315	−0.563792
C	−4.010081	−0.342923	−0.075235
C	−3.412847	0.833400	0.436016
C	−2.018167	1.050220	0.473346
C	−1.469574	2.385025	1.054981
C	−0.552809	2.096814	2.279406
C	−2.592887	3.340874	1.542495
C	−0.664115	3.146988	−0.037272
C	−5.550101	−0.485332	−0.079197
C	−6.179633	0.664978	−0.919499
C	−6.082296	−0.402290	1.382316
C	−6.017833	−1.833055	−0.684502
C	−0.855140	−2.290510	−1.010148
N	0.434808	−1.750298	−1.560225
C	1.511675	−2.785028	−1.587999
C	0.234987	−1.171596	−2.927264
H	1.605356	2.235634	−2.422042
H	3.806452	3.031765	−3.198722
H	5.924785	2.191636	−2.140516
H	5.830641	0.564480	−0.283727
H	5.609063	−0.733198	1.377111
H	5.165541	−2.079944	3.399217
H	2.808021	−2.574918	4.107145
H	0.891182	−1.755504	2.775937
H	−3.546722	−2.263442	−0.972112
H	−4.069738	1.607170	0.814447
H	−1.109229	1.567658	3.064785
H	0.316822	1.485272	2.012390
H	−0.176705	3.039736	2.699998

H	−3.194795	2.894199	2.344754
H	−2.136300	4.255016	1.943391
H	−3.264759	3.638774	0.726573
H	0.213101	2.581720	−0.366350
H	−1.294279	3.349756	−0.914085
H	−0.305600	4.107583	0.358050
H	−5.923672	1.650934	−0.513726
H	−5.826516	0.627557	−1.958356
H	−7.274925	0.577341	−0.925018
H	−5.813385	0.548678	1.857136
H	−7.177701	−0.488204	1.395007
H	−5.666287	−1.212611	1.994998
H	−5.697144	−1.943340	−1.728820
H	−5.635380	−2.689696	−0.114083
H	−7.114285	−1.884368	−0.665800
H	−0.592451	−2.945002	−0.166848
H	−1.364115	−2.913701	−1.762898
H	2.430524	−2.336174	−1.977736
H	1.706122	−3.135610	−0.570203
H	1.227750	−3.637663	−2.225244
H	1.153589	−0.667464	−3.241138
H	−0.578267	−0.441194	−2.898762
H	−0.017353	−1.961054	−3.652431

Table S16. Cartesian Coordinates of the Optimized Structure of Inf in the Excited S_1 State Calculated at the TD-B3LYP/LANL2DZ Level

Center Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	2.864416	2.173439	−1.522994
C	4.178426	2.544309	−1.892318
C	5.274247	1.798196	−1.364125
C	5.070791	0.735290	−0.486221
C	3.746010	0.345680	−0.080122
C	2.629291	1.080314	−0.672356
C	3.470197	−0.697749	0.866434
C	2.126109	−0.957100	1.323519
In	0.791552	0.178497	−0.173528
C	4.426157	−1.621970	1.445895
C	4.054810	−2.569736	2.404215
C	2.718229	−2.711089	2.862999
C	1.729738	−1.832858	2.313285
C	−1.332402	0.139259	0.015974
C	−1.849839	−1.045760	−0.578997
C	−3.230326	−1.294891	−0.648742
C	−4.157285	−0.376565	−0.113755
C	−3.641735	0.793131	0.482837
C	−2.256586	1.077081	0.562532
C	−1.775876	2.394077	1.239584
C	−0.873421	2.068206	2.465755
C	−2.952085	3.264241	1.761435
C	−0.984735	3.266229	0.220325
C	−5.673028	−0.673463	−0.201098
C	−6.538408	0.440801	0.439076
C	−5.981772	−2.009138	0.538761
C	−6.088155	−0.808401	−1.696563
C	−0.891912	−2.116867	−1.109641
N	0.368375	−1.518230	−1.676780
C	1.476049	−2.524001	−1.763026
C	0.118305	−0.906713	−3.023682
H	2.028305	2.742563	−1.932960
H	4.347633	3.374015	−2.573791
H	6.290732	2.075890	−1.639618
H	5.932799	0.213940	−0.074041
H	5.466120	−1.547736	1.135227
H	4.825362	−3.213604	2.826831
H	2.442049	−3.449704	3.609328
H	0.699825	−1.882800	2.664035
H	−3.579080	−2.211177	−1.122177
H	−4.342580	1.505448	0.894053
H	−1.420444	1.466059	3.202776
H	0.032579	1.513875	2.191988
H	−0.547517	2.996592	2.953055

H	−3.548673	2.737390	2.517079
H	−2.549289	4.169271	2.233216
H	−3.620156	3.583824	0.951099
H	−0.056839	2.786415	−0.115988
H	−1.595507	3.483214	−0.665821
H	−0.695713	4.219603	0.682054
H	−6.317413	0.566380	1.506964
H	−6.393494	1.408020	−0.059433
H	−7.600013	0.177277	0.349106
H	−5.707330	−1.940751	1.599369
H	−7.054002	−2.238778	0.475757
H	−5.432092	−2.852404	0.103508
H	−5.892167	0.123712	−2.242326
H	−5.540830	−1.614625	−2.199922
H	−7.160858	−1.031750	−1.773967
H	−1.387384	−2.743349	−1.867885
H	−0.583011	−2.780303	−0.289977
H	1.204196	−3.352756	−2.435120
H	2.377426	−2.033244	−2.141751
H	1.693658	−2.917192	−0.766369
H	−0.131927	−1.683450	−3.762454
H	1.016753	−0.374795	−3.352780
H	−0.714860	−0.199946	−2.961663

Table S17. Cartesian Coordinates of the Optimized Structure of Bf in the Excited T_1 State Calculated at the TD-UB3LYP/6-31G(d,p) Level

Center Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	−1.880699	0.838313	−2.314539
C	−2.982041	1.333515	−3.009078
C	−4.275577	1.220201	−2.464520
C	−4.463278	0.598969	−1.226508
C	−3.365610	0.099800	−0.520961
C	−2.024395	0.220884	−1.050957
C	−3.324812	−0.564144	0.779524
C	−1.957483	−0.879996	1.122174
B	−1.044444	−0.409697	−0.031625
C	−4.373662	−0.880288	1.644333
C	−4.103448	−1.504950	2.864758
C	−2.778141	−1.812876	3.224258
C	−1.724458	−1.504289	2.367702
C	0.555984	−0.275653	0.005751
C	1.080078	0.852885	0.688595
C	2.449387	1.096744	0.826678
C	3.393204	0.234352	0.266239
C	2.888252	−0.881445	−0.407855
C	1.518433	−1.171400	−0.543813
C	1.108460	−2.481040	−1.271268
C	0.309153	−3.387508	−0.305869
C	2.322847	−3.302530	−1.757472
C	0.254436	−2.163845	−2.520370
C	4.899159	0.517400	0.423502
C	5.772152	−0.539525	−0.278588
C	5.268367	0.525877	1.926041
C	5.233580	1.897929	−0.190038
C	0.135963	1.828475	1.363586
N	−0.340097	2.954783	0.536563
C	−1.678706	3.450215	0.776467
C	0.372076	3.410140	−0.635721
H	−0.893778	0.903107	−2.772928
H	−2.848787	1.796381	−3.984101
H	−5.130685	1.604416	−3.013766
H	−5.468400	0.502046	−0.820404
H	−5.401859	−0.645698	1.375134
H	−4.919105	−1.755341	3.537541
H	−2.580267	−2.300413	4.175815
H	−0.707685	−1.761612	2.660461
H	2.778401	1.965611	1.393805
H	3.600204	−1.569376	−0.837643
H	0.916448	−3.656956	0.565601
H	−0.600197	−2.902859	0.051206
H	0.022476	−4.314462	−0.815782

H	2.972758	−3.617206	−0.933818
H	1.960551	−4.210794	−2.248925
H	2.929920	−2.758771	−2.489569
H	−0.672627	−1.651208	−2.264338
H	0.812756	−1.535320	−3.223876
H	−0.006407	−3.094004	−3.038191
H	5.614823	−1.539458	0.137665
H	5.573873	−0.582653	−1.354336
H	6.830056	−0.290184	−0.147213
H	5.046954	−0.441453	2.387890
H	6.337280	0.729450	2.056899
H	4.715148	1.292151	2.477828
H	4.987424	1.922562	−1.256873
H	4.682452	2.706012	0.301392
H	6.302133	2.116502	−0.084365
H	0.622795	2.319739	2.218837
H	−0.757549	1.327218	1.736553
H	−1.797223	4.451035	0.362529
H	−2.369963	2.756681	0.286959
H	−1.880793	3.445976	1.848574
H	1.414437	3.107568	−0.580634
H	0.269650	4.493807	−0.721665
H	−0.091878	2.937105	−1.506153

Table S18. Cartesian Coordinates of the Optimized Structure of Alf in the Excited T_1 State Calculated at the TD-UB3LYP/6-31G(d,p) Level

Center Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	2.565746	1.680305	−2.071924
C	3.804339	2.224097	−2.453852
C	4.986083	1.867774	−1.732924
C	4.924295	1.006087	−0.673014
C	3.660183	0.429795	−0.254541
C	2.428285	0.790160	−1.013475
C	3.519159	−0.445299	0.839988
C	2.148563	−0.938404	1.150050
Al	0.927904	−0.215026	−0.217982
C	4.617374	−0.873791	1.685869
C	4.394383	−1.690333	2.760006
C	3.074643	−2.140726	3.075862
C	1.993800	−1.751966	2.265632
C	−1.046731	0.039152	−0.027408
C	−1.694980	−1.118109	−0.514565
C	−3.081475	−1.262356	−0.525469
C	−3.903216	−0.246406	−0.028184
C	−3.270744	0.901058	0.468315
C	−1.875503	1.069567	0.482649
C	−1.268654	2.376311	1.051288
C	−0.294058	2.046387	2.205220
C	−2.333625	3.338834	1.618423
C	−0.515107	3.131598	−0.067861
C	−5.434297	−0.417063	−0.044769
C	−6.172724	0.800457	0.542461
C	−5.821258	−1.660995	0.790271
C	−5.915137	−0.612086	−1.502428
C	−0.832783	−2.274919	−0.993845
N	0.451624	−1.769554	−1.561347
C	1.473445	−2.838706	−1.625695
C	0.230831	−1.204733	−2.916063
H	1.683564	1.979763	−2.637466
H	3.869576	2.911040	−3.292338
H	5.940456	2.293115	−2.031563
H	5.834720	0.758913	−0.136356
H	5.627891	−0.539025	1.474148
H	5.225844	−1.999392	3.387894
H	2.915928	−2.783324	3.936807
H	1.000455	−2.111459	2.533384
H	−3.517948	−2.176220	−0.922755
H	−3.892638	1.694923	0.854971
H	−0.816956	1.541125	3.024301
H	0.526072	1.394543	1.891852
H	0.151245	2.965730	2.602026

H	−2.909114	2.884280	2.431597
H	−1.838513	4.227115	2.023925
H	−3.034630	3.679348	0.849258
H	0.322617	2.552382	−0.462669
H	−1.188673	3.367790	−0.899035
H	−0.107962	4.074080	0.316232
H	−5.900445	0.977258	1.587956
H	−5.966678	1.714743	−0.023343
H	−7.253360	0.627701	0.508010
H	−5.498994	−1.548871	1.830580
H	−6.907946	−1.803151	0.784192
H	−5.364211	−2.573760	0.396686
H	−5.660671	0.257208	−2.117633
H	−5.462284	−1.493378	−1.966279
H	−7.002955	−0.742293	−1.532391
H	−1.354034	−2.899643	−1.733160
H	−0.568790	−2.925674	−0.150992
H	1.135145	−3.664295	−2.265818
H	2.397973	−2.424621	−2.032907
H	1.673931	−3.209041	−0.619341
H	−0.070079	−1.994362	−3.617076
H	1.153445	−0.736895	−3.263556
H	−0.556927	−0.451192	−2.869052

Table S19. Cartesian Coordinates of the Optimized Structure of Gaf in the Excited T_1 State Calculated at the TD-UB3LYP/6-31G(d,p) Level

Center Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	2.528558	1.952068	−1.766923
C	3.785753	2.507375	−2.071316
C	4.953830	2.012560	−1.415975
C	4.862650	1.013674	−0.486125
C	3.577825	0.431858	−0.144875
C	2.369056	0.930289	−0.848864
C	3.398084	−0.563719	0.833414
C	2.013456	−1.029240	1.081238
Ga	0.830440	−0.091252	−0.181671
C	4.470303	−1.136695	1.625911
C	4.198618	−2.059585	2.598542
C	2.857848	−2.478620	2.857398
C	1.801977	−1.948441	2.091429
C	−1.135554	0.043597	−0.041708
C	−1.744152	−1.066313	−0.649152
C	−3.130081	−1.247027	−0.670868
C	−3.971986	−0.308299	−0.074679
C	−3.364495	0.805361	0.529877
C	−1.979614	1.005065	0.558807
C	−1.383443	2.271745	1.215866
C	−0.357854	1.871308	2.301019
C	−2.448704	3.160781	1.885621
C	−0.671563	3.110742	0.129941
C	−5.506014	−0.442689	−0.067817
C	−6.132912	0.760167	−0.812154
C	−6.018019	−0.463798	1.392066
C	−5.982455	−1.734078	−0.759366
C	−0.841719	−2.138806	−1.238781
N	0.424563	−1.533707	−1.724858
C	1.509656	−2.519608	−1.863612
C	0.212791	−0.816883	−2.999669
H	1.656846	2.357333	−2.278049
H	3.875361	3.302143	−2.805385
H	5.922768	2.441646	−1.656539
H	5.762972	0.661579	0.006998
H	5.496750	−0.827395	1.456770
H	5.009909	−2.477020	3.188970
H	2.664555	−3.208130	3.637978
H	0.790954	−2.291043	2.307074
H	−3.538811	−2.125327	−1.160685
H	−4.009992	1.544202	0.987823
H	−0.823428	1.250981	3.074015
H	0.473940	1.301446	1.879389
H	0.063280	2.761694	2.780761

H	−2.991060	2.629432	2.675030
H	−1.962105	4.026448	2.346366
H	−3.179380	3.543287	1.165291
H	0.138190	2.537096	−0.325126
H	−1.371432	3.407726	−0.658469
H	−0.236310	4.017913	0.564164
H	−5.866451	1.711730	−0.343370
H	−5.794438	0.795080	−1.852956
H	−7.226204	0.682389	−0.812605
H	−5.750723	0.449184	1.931922
H	−7.110020	−0.554977	1.412270
H	−5.596153	−1.311313	1.942157
H	−5.683021	−1.767193	−1.812098
H	−5.591306	−2.628884	−0.264192
H	−7.075393	−1.789820	−0.726396
H	−0.571512	−2.865300	−0.462582
H	−1.340499	−2.695459	−2.045656
H	2.429444	−2.000994	−2.144553
H	1.691655	−3.004271	−0.902883
H	1.276718	−3.277828	−2.623798
H	1.119063	−0.264652	−3.256966
H	−0.604291	−0.102413	−2.882824
H	−0.034531	−1.516684	−3.809683

Table S20. Cartesian Coordinates of the Optimized Structure of Gaf in the Excited T_1 State Calculated at the TD-UB3LYP/LANL2DZ Level

Center Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	2.461033	1.732443	−2.048247
C	3.705905	2.298376	−2.438770
C	4.903229	1.954882	−1.716209
C	4.855909	1.082694	−0.645883
C	3.590274	0.485638	−0.224675
C	2.345735	0.834981	−0.982416
C	3.461187	−0.400897	0.873127
C	2.089662	−0.914647	1.183074
Ga	0.844953	−0.191386	−0.184172
C	4.574521	−0.818945	1.723260
C	4.358701	−1.649988	2.805692
C	3.034547	−2.120526	3.121713
C	1.936113	−1.738187	2.301912
C	−1.137635	0.016059	−0.021498
C	−1.773545	−1.149155	−0.523738
C	−3.172979	−1.307843	−0.543621
C	−4.007297	−0.297124	−0.038871
C	−3.380299	0.862722	0.475284
C	−1.981060	1.049732	0.496779
C	−1.390603	2.370895	1.066871
C	−0.382043	2.063118	2.210934
C	−2.474944	3.311672	1.660192
C	−0.672390	3.154151	−0.070864
C	−5.550195	−0.405786	−0.029085
C	−6.160975	0.761342	−0.859991
C	−6.067556	−0.316500	1.437294
C	−6.053307	−1.740511	−0.634890
C	−0.897308	−2.301355	−1.012846
N	0.403924	−1.777719	−1.566701
C	1.457656	−2.839556	−1.609722
C	0.199356	−1.199397	−2.936114
H	1.570950	2.020542	−2.608968
H	3.758640	2.989224	−3.277309
H	5.851460	2.395139	−2.018683
H	5.770760	0.845387	−0.109156
H	5.580948	−0.467464	1.511219
H	5.193544	−1.951193	3.435743
H	2.881258	−2.765949	3.983849
H	0.944646	−2.105734	2.568535
H	−3.595787	−2.221650	−0.952278
H	−4.016328	1.646814	0.868654
H	−0.871816	1.512951	3.025313
H	0.470290	1.463145	1.875489
H	0.020129	2.999794	2.620639

H	−3.029433	2.835643	2.479745
H	−1.989417	4.208620	2.065878
H	−3.194033	3.643661	0.899939
H	0.166851	2.590829	−0.489102
H	−1.373417	3.382650	−0.885101
H	−0.273574	4.102708	0.314840
H	−5.876962	1.739758	−0.454682
H	−5.819843	0.718109	−1.902644
H	−7.258062	0.700159	−0.854216
H	−5.773970	0.626590	1.913050
H	−7.164402	−0.378553	1.459531
H	−5.663928	−1.137892	2.043469
H	−5.745173	−1.853848	−1.682655
H	−5.684979	−2.607706	−0.071100
H	−7.150354	−1.767194	−0.605954
H	−0.640757	−2.964929	−0.174961
H	−1.414265	−2.911737	−1.769834
H	2.383854	−2.411457	−2.004706
H	1.651742	−3.203276	−0.597159
H	1.145291	−3.678355	−2.250793
H	1.126139	−0.724919	−3.269617
H	−0.592735	−0.446754	−2.898554
H	−0.087396	−1.987316	−3.649125

Table S21. Cartesian Coordinates of the Optimized Structure of Inf in the Excited T_1 State Calculated at the TD-UB3LYP/LANL2DZ Level

Center Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	2.516449	1.756560	−2.122192
C	3.760895	2.276455	−2.579059
C	4.972487	1.905998	−1.899990
C	4.940636	1.056927	−0.810645
C	3.675722	0.505123	−0.315278
C	2.416707	0.884247	−1.034498
C	3.604024	−0.354331	0.814691
C	2.269638	−0.865344	1.265436
In	0.784417	−0.126851	−0.090294
C	4.788047	−0.756664	1.580661
C	4.676196	−1.565583	2.694978
C	3.391388	−2.034973	3.137359
C	2.223762	−1.668444	2.408820
C	−1.357369	0.053604	0.067832
C	−1.979960	−1.133247	−0.410462
C	−3.377132	−1.282186	−0.449349
C	−4.224621	−0.252034	0.005130
C	−3.610845	0.923432	0.484571
C	−2.205988	1.104401	0.525076
C	−1.620180	2.443873	1.061194
C	−0.681162	2.175995	2.273002
C	−2.715784	3.430022	1.551816
C	−0.830922	3.167918	−0.069405
C	−5.759802	−0.441377	−0.036565
C	−6.529196	0.789728	0.504763
C	−6.152200	−1.674223	0.831080
C	−6.214212	−0.686250	−1.506165
C	−1.117770	−2.322682	−0.841544
N	0.170790	−1.885749	−1.486067
C	1.177920	−2.990270	−1.514549
C	−0.070460	−1.362198	−2.868216
H	1.612938	2.061303	−2.651909
H	3.798755	2.948405	−3.433711
H	5.922742	2.306019	−2.248765
H	5.872627	0.803994	−0.313578
H	5.772346	−0.411124	1.278114
H	5.567674	−1.849004	3.251422
H	3.316357	−2.665922	4.020362
H	1.262385	−2.035549	2.769994
H	−3.800426	−2.209870	−0.832327
H	−4.248169	1.723510	0.834189
H	−1.231058	1.691545	3.090584
H	0.167747	1.528958	2.022238
H	−0.267767	3.122116	2.647997

H	−3.313115	3.006794	2.369752
H	−2.236579	4.342293	1.930047
H	−3.394971	3.726937	0.742187
H	0.025382	2.584543	−0.425031
H	−1.483824	3.367709	−0.929683
H	−0.440398	4.127758	0.295894
H	−6.278310	0.997898	1.552967
H	−6.321588	1.692145	−0.084796
H	−7.609292	0.600199	0.453036
H	−5.851992	−1.526338	1.876522
H	−7.239532	−1.829450	0.803720
H	−5.672403	−2.592511	0.471184
H	−5.964198	0.174369	−2.140232
H	−5.733128	−1.572502	−1.937781
H	−7.301374	−0.839511	−1.548266
H	−1.675923	−2.984677	−1.523654
H	−0.841339	−2.922741	0.037596
H	0.800592	−3.859948	−2.076233
H	2.095397	−2.630192	−1.990557
H	1.420307	−3.294364	−0.491835
H	−0.416479	−2.166389	−3.537096
H	0.857797	−0.938019	−3.263431
H	−0.833191	−0.579212	−2.834094

Table S22. Calculated Bond Lengths [Å] and Angles [°] for Gaf in S_0, S_1 and T_1 States Optimized at the B3LYP/6-31G(d,p) and B3LYP/LANL2DZ Levels

	B3LYP/6-31G(d,p)			B3LYP/LANL2DZ		
	S_0	S_1	T_1	S_0	S_1	T_1
Ga–N	2.1316	2.2167	2.1510	2.1338	2.1961	2.1500
φC1–C6–C7–C12	0.50	0.40	0.15	0.94	0.09	0.02
C12–Ga–C1	90.06	88.47	89.71	89.88	88.08	89.50
C1–Ga–C13	139.75	141.84	140.20	136.02	139.13	136.74
C12–Ga–C13	125.64	126.78	125.82	127.17	127.59	127.10
Sum of C–Ga–C	355.45	357.09	355.73	353.07	354.80	353.34
C1–Ga–N	104.83	103.30	104.65	106.24	104.75	104.65
C12–Ga–N	104.62	104.30	104.72	107.44	107.54	106.14
C13–Ga–N	85.21	83.43	84.77	86.16	84.61	85.73
Sum of C–Ga–N	294.66	291.03	294.14	299.84	296.9	296.52

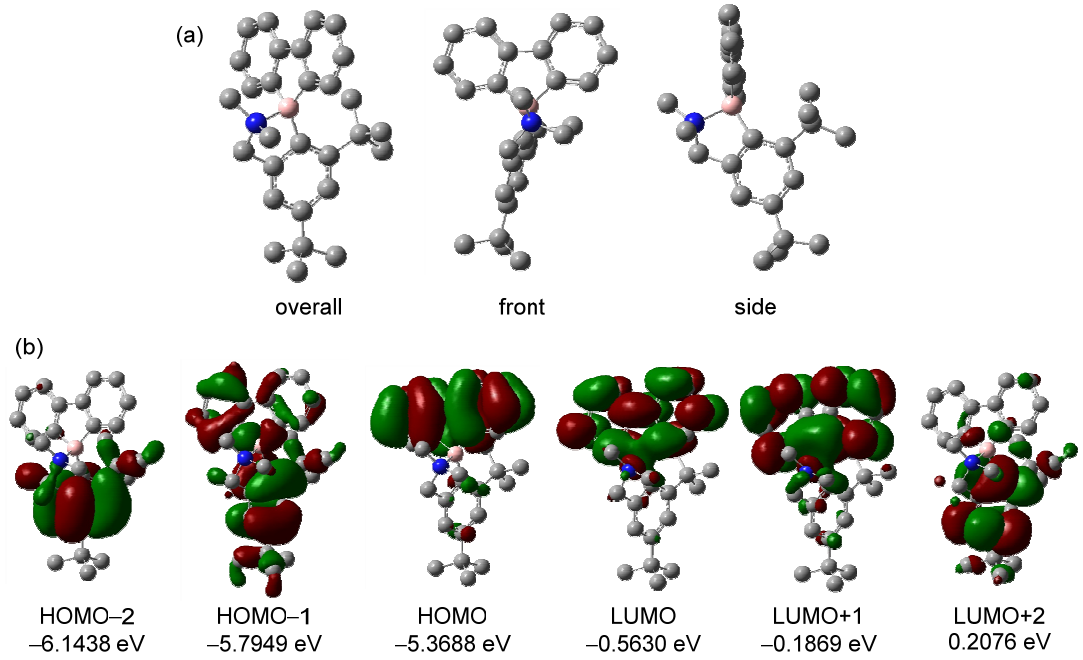

Figure S19. (a) Overall, front and side views of the optimized structure and (b) selected molecular orbitals and energy levels of **Bf** in the ground S_0 state calculated at the B3LYP/6-31G(d,p) level. Hydrogen atoms are omitted for clarity.

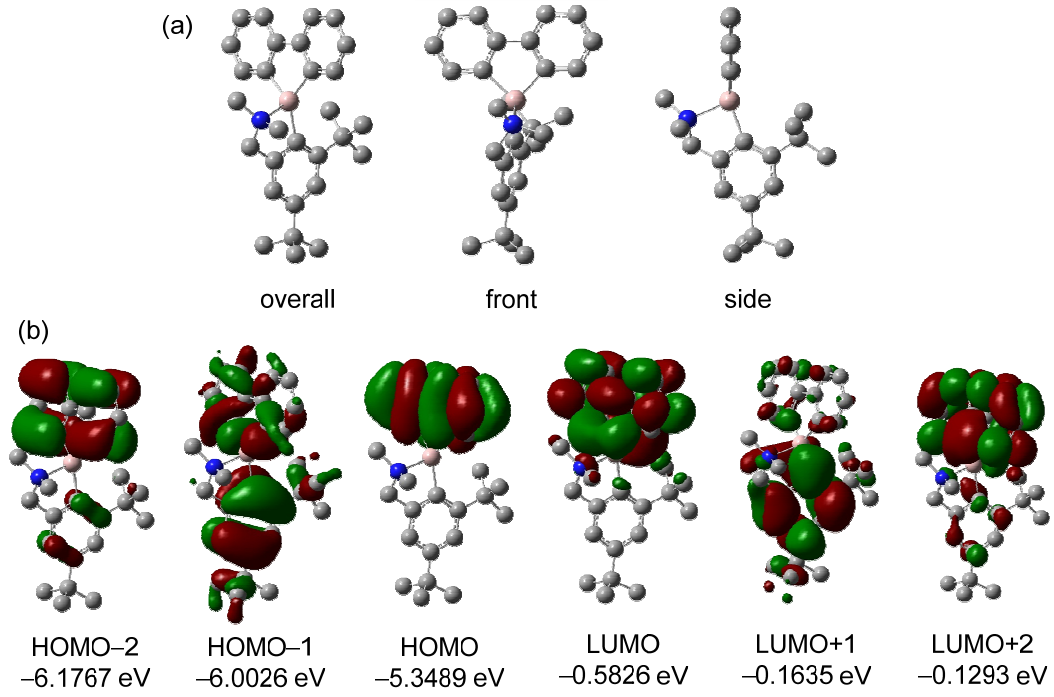

Figure S20. (a) Overall, front and side views of the optimized structure and (b) selected molecular orbitals and energy levels of **Alf** in the ground S_0 state calculated at the B3LYP/6-31G(d,p) level. Hydrogen atoms are omitted for clarity.

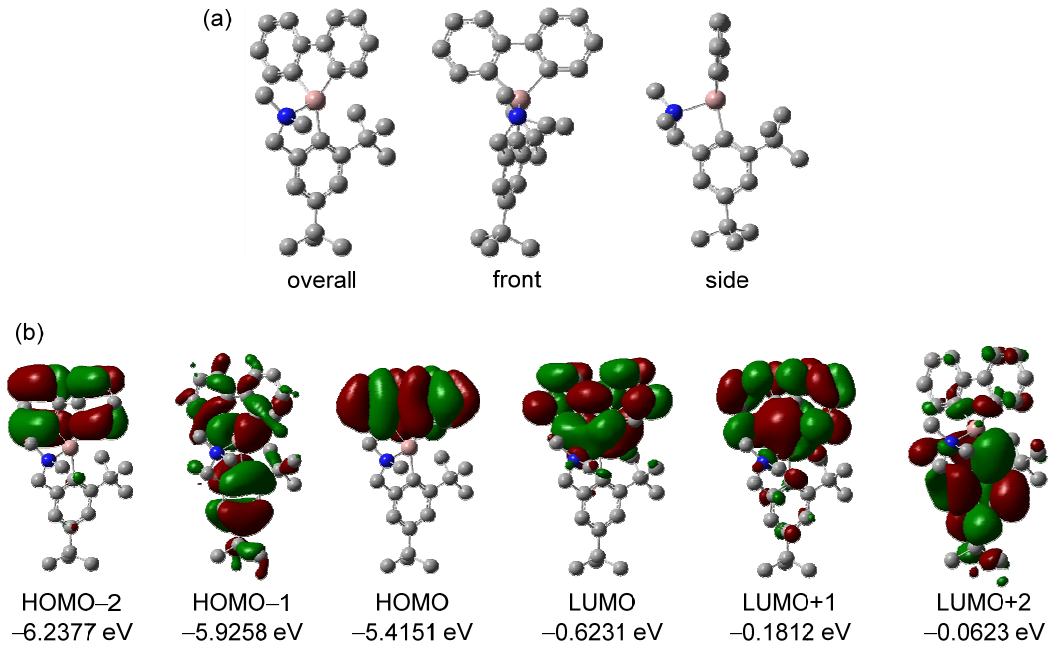

Figure S21. (a) Overall, front and side views of the optimized structure and (b) selected molecular orbitals and energy levels of **Gaf** in the ground S_0 state calculated at the B3LYP/6-31G(d,p) level. Hydrogen atoms are omitted for clarity.

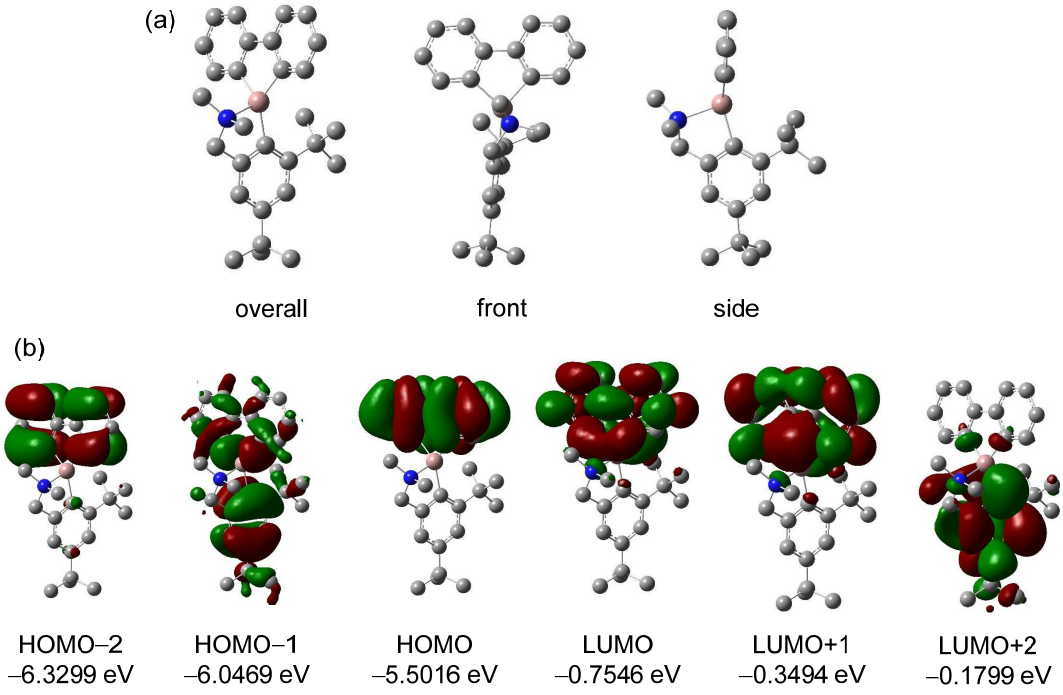

Figure S22. (a) Overall, front and side view of the optimized structure and (b) selected molecular orbitals and energy levels of **Gaf** in the ground S_0 state calculated at the B3LYP/LANL2DZ level. Hydrogen atoms are omitted for clarity.

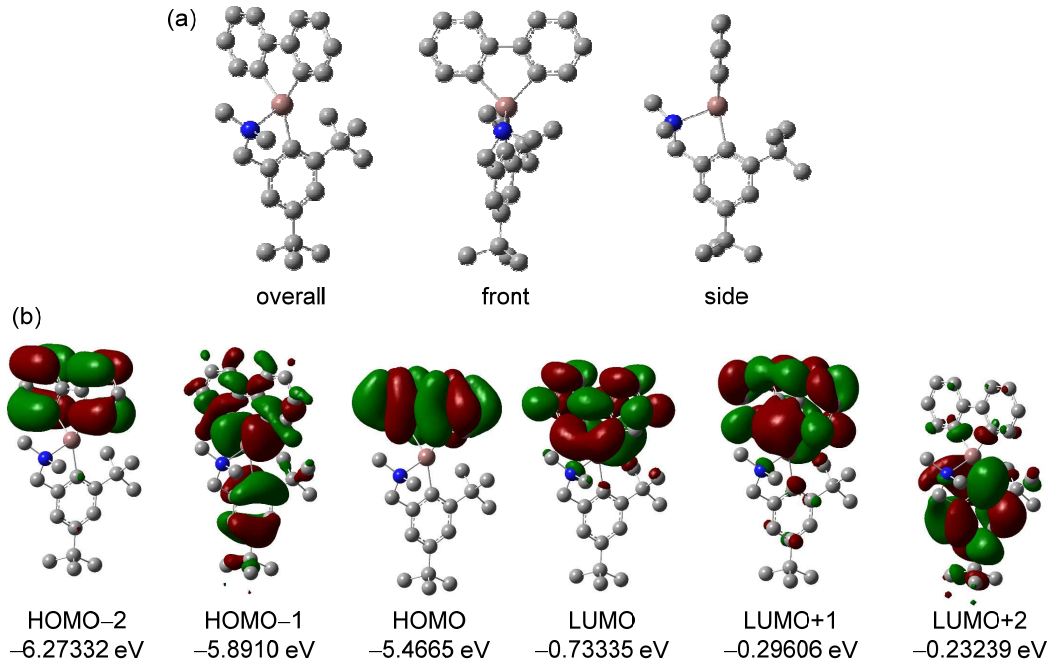

Figure S23. (a) Overall, front and side views of the optimized structure and (b) selected molecular orbitals and energy levels of **Inf** in the ground S_0 state calculated at the B3LYP/LANL2DZ level. Hydrogen atoms are omitted for clarity.

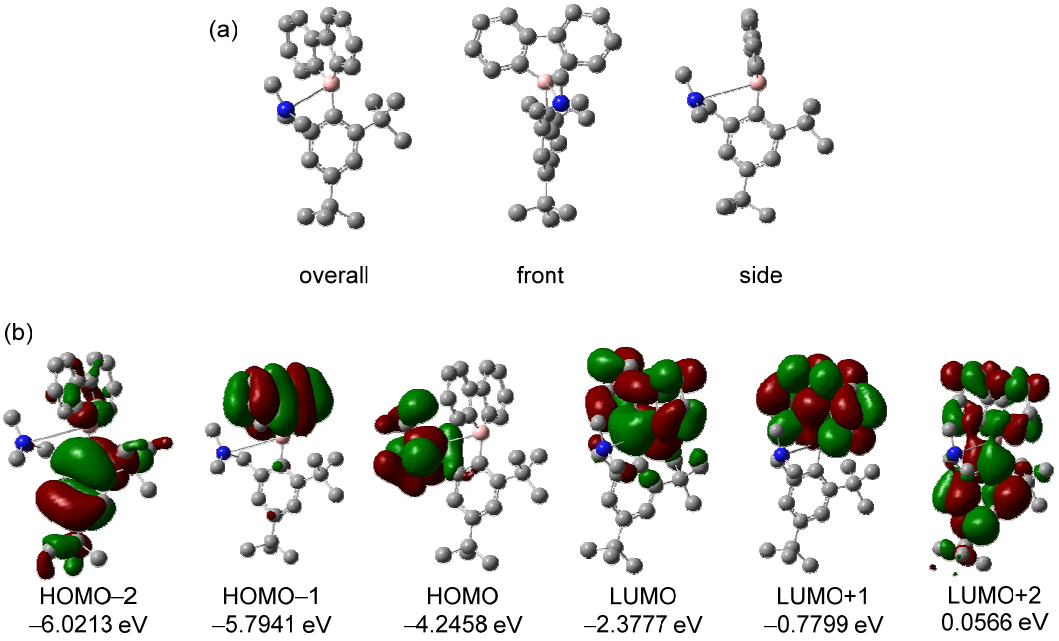

Figure S24. (a) Overall, front and side views of the optimized structure of **Bf** in the excited S_1 state and (b) selected molecular orbitals and energy levels of **Bf** for the ground state with the optimized structure in the excited S_1 state calculated at the B3LYP/6-31G(d,p) level. Hydrogen atoms are omitted for clarity.

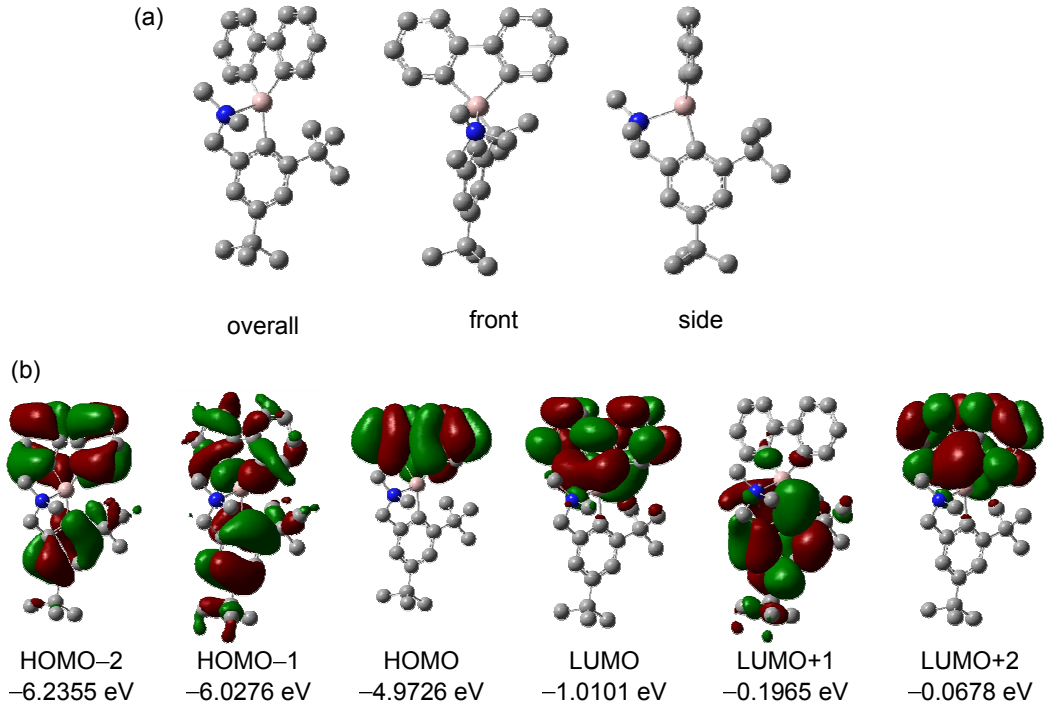

Figure S25. (a) Overall, front and side views of the optimized structure of **Alf** in the excited S_1 state and (b) selected molecular orbitals and energy levels of **Alf** for the ground state with the optimized structure in the excited S_1 state calculated at the B3LYP/6-31G(d,p) level. Hydrogen atoms are omitted for clarity.

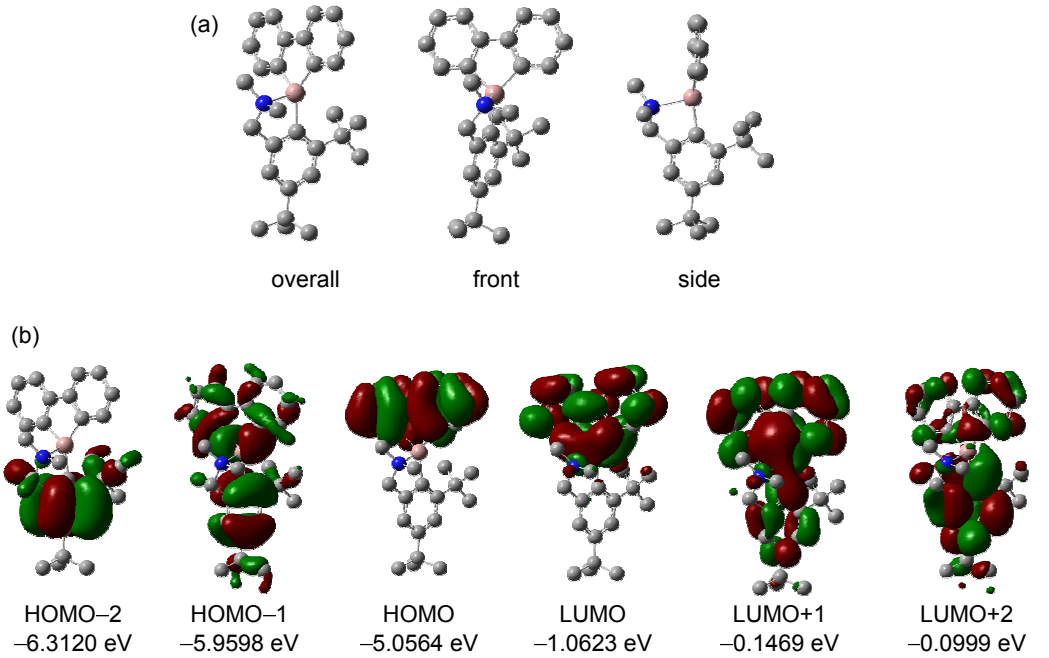

Figure S26. (a) Overall, front and side views of the optimized structure of **Gaf** in the excited S_1 state and (b) selected molecular orbitals and energy levels of **Gaf** for the ground state with the optimized structure in the excited S_1 state calculated at the B3LYP/6-31G(d,p) level. Hydrogen atoms are omitted for clarity.

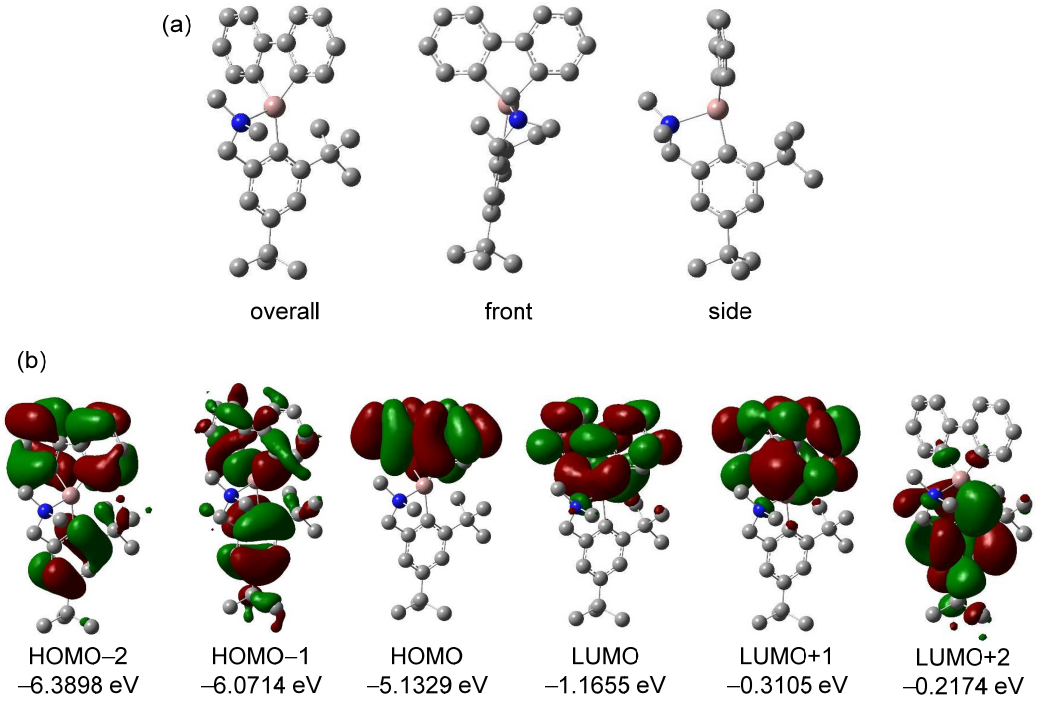

Figure S27. (a) Overall, front and side views of the optimized structure of **Gaf** in the excited S_1 state and (b) selected molecular orbitals and energy levels of **Gaf** for the ground state with the optimized structure in the excited S_1 state calculated at the B3LYP/LANL2DZ level. Hydrogen atoms are omitted for clarity.

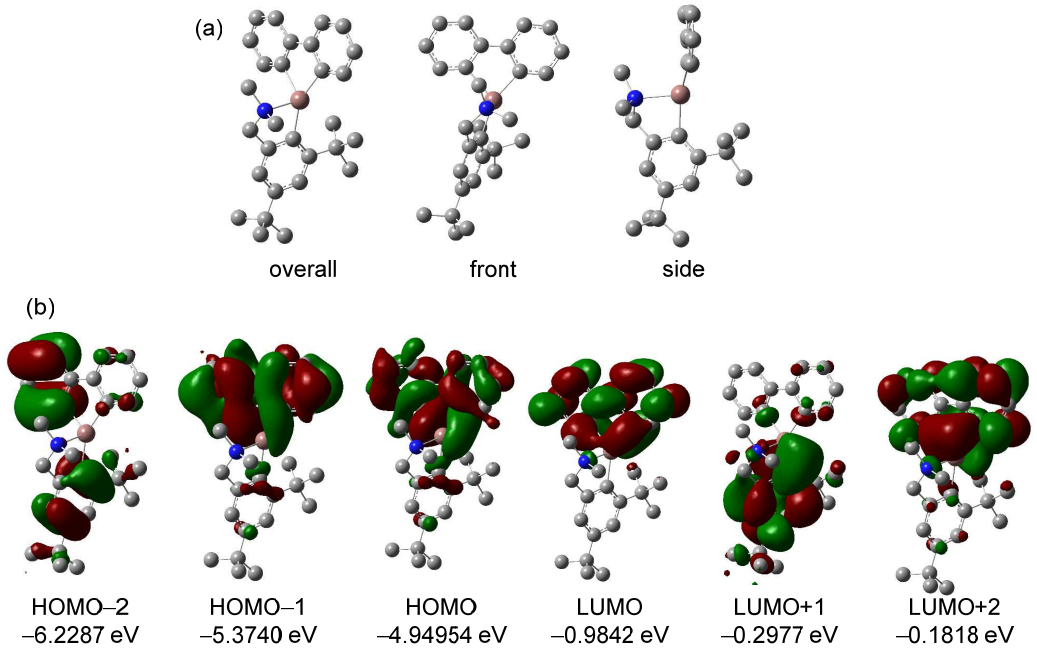

Figure S28. (a) Overall, front and side views of the optimized structure of **Inf** in the excited S_1 state and (b) selected molecular orbitals and energy levels of **Inf** for the ground state with the optimized structure in the excited S_1 state calculated at the B3LYP/LANL2DZ level. Hydrogen atoms are omitted for clarity.

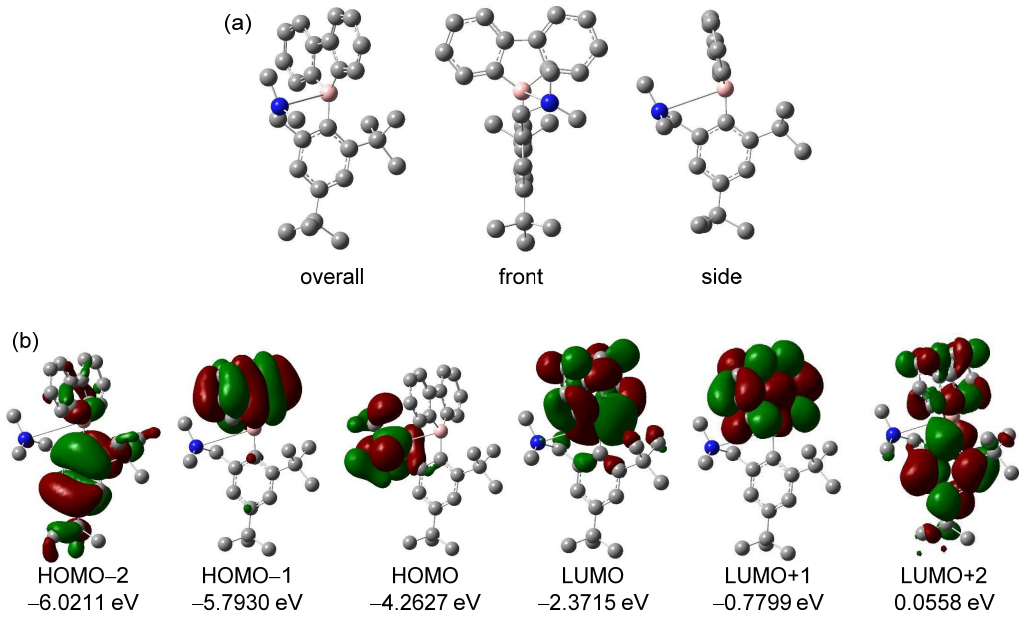

Figure S29. (a) Overall, front and side views of the optimized structure of **Bf** in the excited T_1 state and (b) selected molecular orbitals and energy levels of **Bf** for the ground state with the optimized structure in the excited T_1 state calculated at the UB3LYP/6-31G(d,p) level. Hydrogen atoms are omitted for clarity.

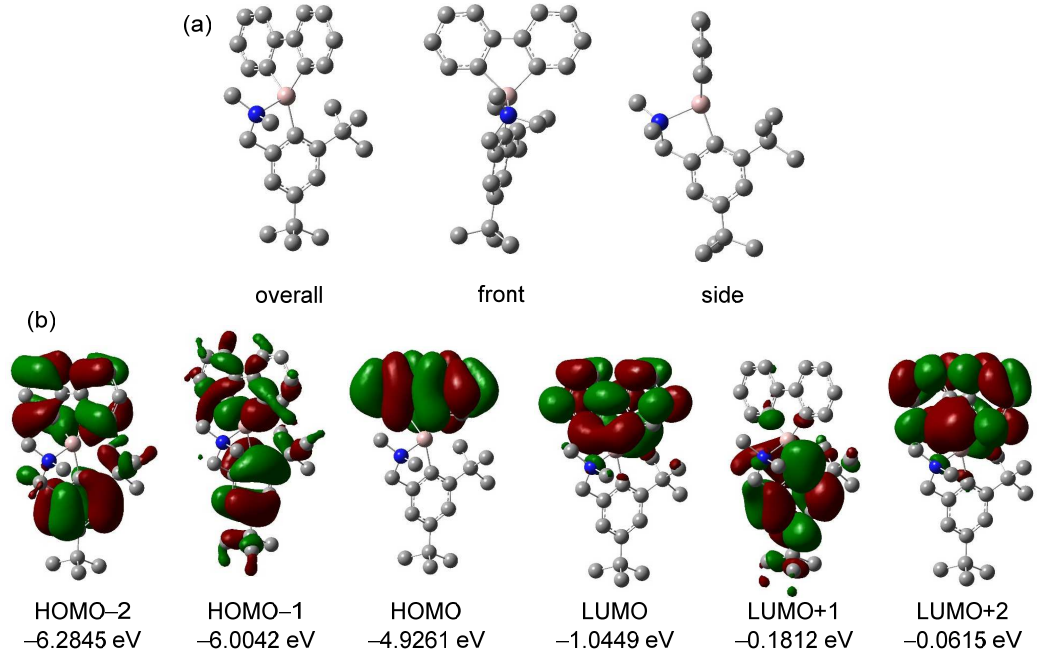

Figure S30. (a) Overall, front and side views of the optimized structure of **Alf** in the excited T_1 state and (b) selected molecular orbitals and energy levels of **Alf** for the ground state with the optimized structure in the excited T_1 state calculated at the UB3LYP/6-31G(d,p) level. Hydrogen atoms are omitted for clarity.

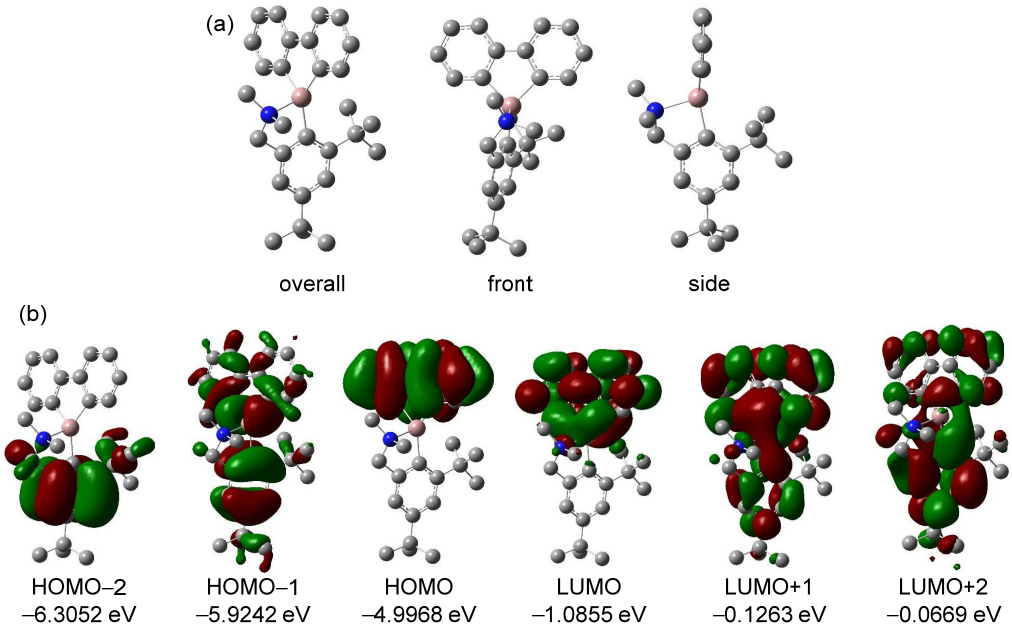

Figure S31. (a) Overall, front and side views of the optimized structure of **Gaf** in the excited T_1 state and (b) selected molecular orbitals and energy levels of **Gaf** for the ground state with the optimized structure in the excited T_1 state calculated at the UB3LYP/6-31G(d,p) level. Hydrogen atoms are omitted for clarity.

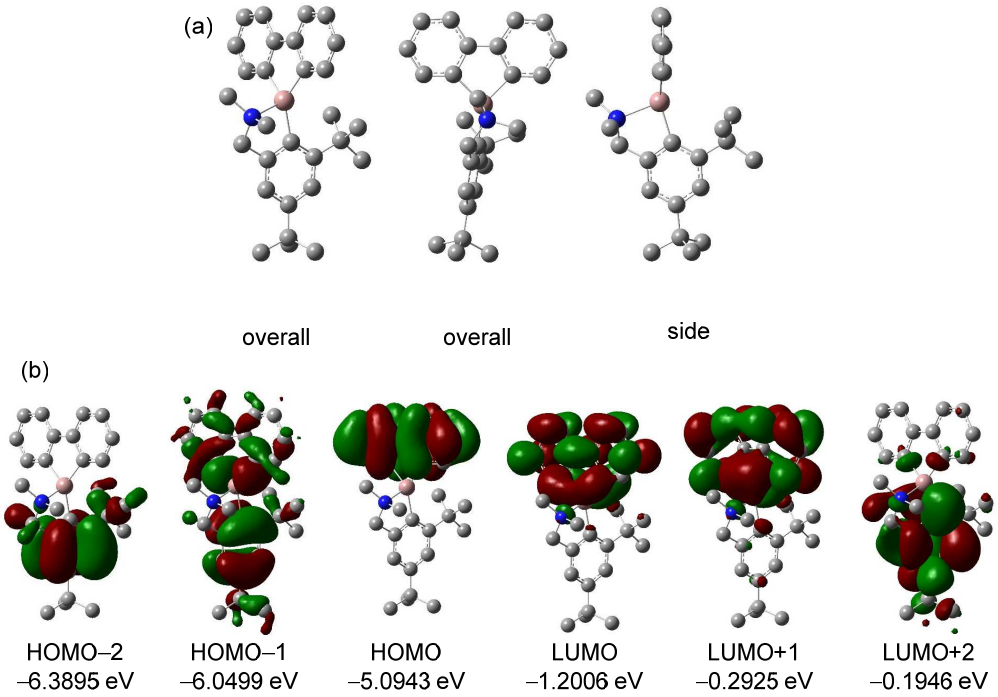

Figure S32. (a) Overall, front and side views of the optimized structure of **Gaf** in the excited T_1 state and (b) selected molecular orbitals and energy levels of **Gaf** for the ground state with the optimized structure in the excited T_1 state calculated at the UB3LYP/LANL2DZ level. Hydrogen atoms are omitted for clarity.

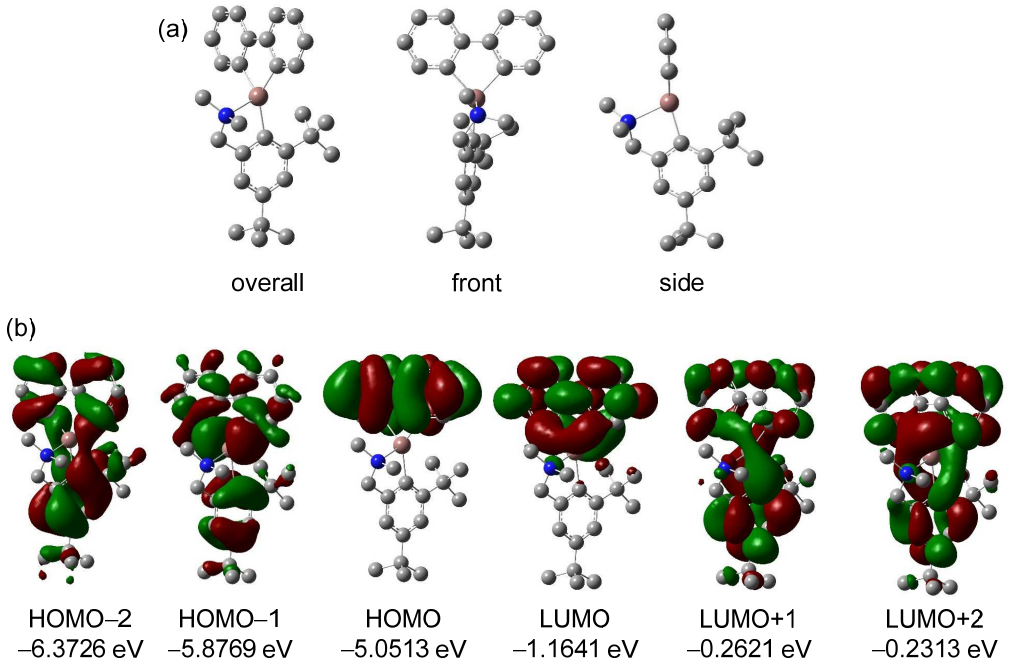

Figure S33. (a) Overall, front and side views of the optimized structure of **Inf** in the excited T_1 state and (b) selected molecular orbitals and energy levels of **Inf** for the ground state with the optimized structure in the excited T_1 state calculated at the UB3LYP/LANL2DZ level. Hydrogen atoms are omitted for clarity.

Table S23. TD-DFT Calculation Result of Bf with Optimized Structure in the Ground S_0 State Calculated at the B3LYP/6-31G(d,p) Level

Transition Energy (Wave Length)	Assignment with Contribution	Oscillator Strength *f*
4.2732 eV (290.14 nm)	HOMO→LUMO (77.78%) HOMO→LUMO+1 (22.22%)	0.0760
4.3971 eV (281.97 nm)	HOMO−3→LUMO (12.80%) HOMO−1→LUMO (24.55%) HOMO→LUMO (12.53%) HOMO→LUMO+1 (50.12%)	0.0551
4.6468 eV (266.82 nm)	HOMO−4→LUMO (2.15%) HOMO−3→LUMO (8.13%) HOMO−1→LUMO (72.85%) HOMO→LUMO (7.96%) HOMO→LUMO+2 (8.91%)	0.0957
4.8720 eV (254.48 nm)	HOMO−4→LUMO (50.05%) HOMO−3→LUMO (2.67%) HOMO−1→LUMO+1 (3.10%) HOMO→LUMO+2 (2.40%) HOMO→LUMO+3 (25.02%) HOMO→LUMO+4 (16.76%)	0.0031
4.9519 eV (250.38 nm)	HOMO−4→LUMO (2.43%) HOMO−3→LUMO (3.83%) HOMO−2→LUMO (2.36%) HOMO−2→LUMO+2 (2.81%) HOMO−1→LUMO+1 (79.75%) HOMO−1→LUMO+2 (2.21%) HOMO−1→LUMO+3 (2.44%) HOMO→LUMO+2 (4.16%)	0.0064
4.9852 eV (248.70 nm)	HOMO−2→LUMO (34.59%) HOMO−2→LUMO+1 (2.96%) HOMO−2→LUMO+2 (5.12%) HOMO−2→LUMO+3 (3.51%) HOMO−1→LUMO+1 (13.99%) HOMO−1→LUMO+2 (5.13%) HOMO−1→LUMO+3 (8.76%) HOMO→LUMO+2 (2.34%) HOMO→LUMO+3 (2.57%)	0.0112

Table S24. TD-DFT Calculation Result of Alf with Optimized Structure in the Ground S_0 State Calculated at the B3LYP/6-31G(d,p) Level

Transition Energy (Wave Length)	Assignment with Contribution	Oscillator Strength *f*
4.1684 eV (297.44 nm)	HOMO→LUMO (84.10%) HOMO→LUMO+2 (15.91%)	0.0604
4.4744 eV (277.10 nm)	HOMO−2→LUMO (24.28%) HOMO−1→LUMO (14.36%) HOMO→LUMO (12.82%) HOMO→LUMO+1 (3.72%) HOMO→LUMO+2 (44.83%)	0.0758
4.6210 eV (268.31 nm)	HOMO−5→LUMO (19.01%) HOMO−3→LUMO (5.56%) HOMO−2→LUMO (7.37%) HOMO−1→LUMO (61.04%) HOMO→LUMO (2.70%) HOMO→LUMO+2 (4.32%)	0.0246
4.6655 eV (265.75 nm)	HOMO→LUMO+1 (92.42%) HOMO→LUMO+2 (7.58%)	0.0021
4.9111 eV (252.46 nm)	HOMO−4→LUMO (65.88%) HOMO→LUMO+3 (3.03%) HOMO→LUMO+4 (31.09%)	0.0153

Table S25. TD-DFT Calculation Result of Gaf with Optimized Structure in the Ground S_0 State Calculated at the B3LYP/6-31G(d,p) Level

Transition Energy (Wave Length)	Assignment with Contribution	Oscillator Strength *f*
4.2037 eV (294.94 nm)	HOMO→LUMO (82.62%) HOMO→LUMO+1 (17.38%)	0.0641
4.4419 eV (279.12 nm)	HOMO−5→LUMO (6.43%) HOMO−2→LUMO (9.35%) HOMO−1→LUMO (59.10%) HOMO→LUMO (2.64%) HOMO→LUMO+1 (22.48%)	0.0186
4.5331 eV (273.51 nm)	HOMO−5→LUMO (4.86%) HOMO−2→LUMO (21.00%) HOMO−1→LUMO (30.01%) HOMO→LUMO (13.78%) HOMO→LUMO+1 (30.35%)	0.0824
4.8287 eV (256.77 nm)	HOMO→LUMO+1 (2.99%) HOMO→LUMO+2 (97.01%)	0.0011
4.9315 eV (251.41 nm)	HOMO−5→LUMO+1 (2.39%) HOMO−4→LUMO (49.93%) HOMO−2→LUMO (4.72%) HOMO−1→LUMO+1 (19.14%) HOMO→LUMO+4 (23.81%)	0.0180
4.9349 eV (251.24 nm)	HOMO−5→LUMO+1 (9.07%) HOMO−4→LUMO (11.64%) HOMO−2→LUMO (2.59%) HOMO−1→LUMO+1 (71.20%) HOMO→LUMO+4 (5.49%)	0.0190

Table S26. TD-DFT Calculation Result of Gaf with Optimized Structure in the Ground S_0 State Calculated at the B3LYP/LANL2DZ Level

Transition Energy (Wave Length)	Assignment with Contribution	Oscillator Strength *f*
4.2084 eV (294.61 nm)	HOMO−2→LUMO (2.92%) HOMO→LUMO (68.79%) HOMO→LUMO+1 (28.30%)	0.0664
4.4032 eV (281.58 nm)	HOMO−2→LUMO (19.90%) HOMO−1→LUMO (17.89%) HOMO→LUMO (21.63%) HOMO→LUMO+1 (40.58%)	0.0942
4.5138 eV (274.68 nm)	HOMO−5→LUMO (13.74%) HOMO−2→LUMO (5.72%) HOMO−1→LUMO (67.09%) HOMO→LUMO (6.81%) HOMO→LUMO+1 (6.64%)	0.0417
4.8063 eV (257.96 nm)	HOMO−4→LUMO (8.84%) HOMO→LUMO+2 (87.02%) HOMO→LUMO+4 (4.14%)	0.0001
4.8662 eV (254.79 nm)	HOMO−7→LUMO+1 (2.13%) HOMO−4→LUMO (53.58%) HOMO−2→LUMO (2.28%) HOMO→LUMO+2 (13.90%) HOMO→LUMO+4 (28.11%)	0.0249
4.9274 eV (251.62 nm)	HOMO−5→LUMO+1 (14.84%) HOMO−1→LUMO+1 (85.16%)	0.0043

Table S27. TD-DFT Calculation Result of Inf with Optimized Structure in the Ground S_0 State Calculated at the B3LYP/LANL2DZ Level

Transition Energy (Wave Length)	Assignment with Contribution	Oscillator Strength *f*
4.1757 eV (296.92 nm)	HOMO−1→LUMO (2.92%) HOMO→LUMO (68.79%) HOMO→LUMO+1 (28.30%)	0.0668
4.2503 eV (291.70 nm)	HOMO−3→LUMO (19.90%) HOMO−1→LUMO (17.89%) HOMO→LUMO (21.63%) HOMO→LUMO+1 (40.58%)	0.0083
4.4296 eV (279.90 nm)	HOMO−2→LUMO (13.74%) HOMO−1→LUMO (5.72%) HOMO→LUMO (67.09%) HOMO→LUMO+1 (6.81%)	0.1120
4.7062 eV (263.45 nm)	HOMO−5→LUMO+1 (8.84%) HOMO−3→LUMO+1 (87.02%) HOMO−1→LUMO+1 (4.14%)	0.0038
4.7444 eV (261.33 nm)	HOMO→LUMO+1 (2.13%) HOMO→LUMO+2 (53.58%)	0.0009
4.8495 eV (255.67 nm)	HOMO−7→LUMO+1 (14.84%) HOMO−4→LUMO (85.16%) HOMO→LUMO+4 (85.16%)	0.0263

Table S28. TD-DFT Calculation Result of Bf with Optimized Structure in the Excited S_1 State Calculated at the TD-B3LYP/6-31G(d,p) Level

Transition Energy (Wave Length)	Assignment with Contribution	Oscillator Strength *f*
1.1827 eV (1048.36 nm)	HOMO→LUMO (100%)	0.0001
2.5772 eV (481.08 nm)	HOMO−1→LUMO (100%)	0.0007
2.8688 eV (432.17 nm)	HOMO−2→LUMO (14.12%) HOMO→LUMO+1 (85.88%)	0.0002
2.8756 eV (431.15 nm)	HOMO−2→LUMO (85.36%) HOMO→LUMO+1 (14.64%)	0.0021
3.1674 eV (391.43 nm)	HOMO−3→LUMO (100%)	0.0013
3.5904 eV (345.32 nm)	HOMO→LUMO+2 (76.68%) HOMO→LUMO+3 (15.52%) HOMO→LUMO+4 (7.80%)	0.0000
3.6908 eV (335.93 nm)	HOMO−4→LUMO (75.75%) HOMO−1→LUMO+1 (16.89%) HOMO→LUMO+4 (7.36%)	0.0310
3.7034 eV (334.78 nm)	HOMO−4→LUMO (6.99%) HOMO→LUMO+2 (13.65%) HOMO→LUMO+3 (3.72%) HOMO→LUMO+4 (75.64%)	0.0147
3.7874 eV (327.36 nm)	HOMO→LUMO+2 (8.91%) HOMO→LUMO+3 (80.36%) HOMO→LUMO+4 (10.73%)	0.0040
4.1889 eV (295.98 nm)	HOMO−7→LUMO (2.15%) HOMO−5→LUMO (94.19%) HOMO−1→LUMO+3 (3.66%)	0.0752

Table S29. TD-DFT Calculation Result of Alf with Optimized Structure in the Excited S_1 State Calculated at the TD-B3LYP/6-31G(d,p) Level

Transition Energy (Wave Length)	Assignment with Contribution	Oscillator Strength *f*
3.4269 eV	HOMO→LUMO (95.67%)	0.0960
(361.80 nm)	HOMO→LUMO+2 (4.33%)	
4.0808 eV	HOMO−2→LUMO (20.80%)	0.0158
(303.82 nm)	HOMO−1→LUMO (32.72%)	
	HOMO→LUMO+2 (46.48%)	

Table S30. TD-DFT Calculation Result of Gaf with Optimized Structure in the Excited S_1 State Calculated at the TD-B3LYP/6-31G(d,p) Level

Transition Energy (Wave Length)	Assignment with Contribution	Oscillator Strength *f*
3.4485 eV	HOMO→LUMO (96.28%)	0.0915
(359.53 nm)	HOMO→LUMO+1 (3.72%)	
4.0376 eV	HOMO−5→LUMO (4.57%)	0.0009
(307.07 nm)	HOMO−3→LUMO (8.51%)	
	HOMO−1→LUMO (64.24%)	
	HOMO→LUMO+1 (18.79%)	
	HOMO→LUMO+2 (3.88%)	

Table S31. TD-DFT Calculation Result of Gaf with Optimized Structure in the Excited S_1 State Calculated at the TD-B3LYP/LANL2DZ Level

Transition Energy (Wave Length)	Assignment with Contribution	Oscillator Strength *f*
3.4729 eV	HOMO→LUMO (95.37%)	0.1143
(357.00 nm)	HOMO→LUMO+1 (4.63%)	
3.9981 eV	HOMO−2→LUMO (16.27%)	0.0114
(310.10 nm)	HOMO−1→LUMO (34.30%)	
	HOMO→LUMO+1 (49.44%)	

Table S32. TD-DFT Calculation Result of Inf with Optimized Structure in the Excited S_1 State Calculated at the TD-B3LYP/LANL2DZ Level

Transition Energy (Wave Length)	Assignment with Contribution	Oscillator Strength *f*
3.0595 eV (405.25 nm)	HOMO−1→LUMO (8.87%) HOMO→LUMO (91.13%)	0.0111
3.8331 eV (323.46 nm)	HOMO−1→LUMO (28.99%) HOMO→LUMO (2.46%) HOMO→LUMO+1 (8.07%) HOMO→LUMO+2 (60.48%)	0.0309
4.0274 eV (307.86 nm)	HOMO−2→LUMO (2.87%) HOMO−1→LUMO (46.28%) HOMO−1→LUMO+2 (3.43%) HOMO→LUMO (4.71%) HOMO→LUMO+1 (6.94%) HOMO→LUMO+2 (35.76%)	0.1954
4.1215 eV (300.82 nm)	HOMO−1→LUMO (12.07%) HOMO→LUMO+1 (87.93%)	0.1422

Table S33. TD-DFT Calculation Result of Bf with Optimized Structure in the Excited T_1 State Calculated at the TD-UB3LYP/6-31G(d,p) Level

State	Transition Energy (Wave Length)	Assignment with Contribution	Oscillator Strength *f*
triplet	1.1778 eV (1052.71 nm)	HOMO(α)→LUMO(α) (50.00%) HOMO(β)→LUMO(β) (50.00%)	0.0000
singlet	1.2210 eV (1015.39 nm)	HOMO(α)→LUMO(α) (50.00%) HOMO(β)→LUMO(β) (50.00%)	0.0019
triplet	2.0833 eV (595.15 nm)	HOMO−1(α)→LUMO(α) (50.00%) HOMO−1(β)→LUMO(β) (50.00%)	0.0000
singlet	2.6589 eV (466.30 nm)	HOMO−1(α)→LUMO(α) (50.00%) HOMO−1(β)→LUMO(β) (50.00%)	0.0012
triplet	2.8251 eV (438.87 nm)	HOMO−2(α)→LUMO(α) (50.00%) HOMO-2(β)→LUMO(β) (50.00%)	0.0000
triplet	2.8740 eV (431.41 nm)	HOMO(α)→LUMO+1(α) (50.00%) HOMO(β)→LUMO+1(β) (50.00%)	0.0000
singlet	2.8793 eV (430.61 nm)	HOMO−2(α)→LUMO(α) (11.01%) HOMO(α)→LUMO+1(α) (38.99%) HOMO-2(β)→LUMO(β) (11.01%) HOMO(β)→LUMO+1(β) (38.99%)	0.0006
singlet	2.8874 eV (429.40 nm)	HOMO−2(α)→LUMO(α) (38.68%) HOMO(α)→LUMO+1(α) (11.32%) HOMO-2(β)→LUMO(β) (38.68%) HOMO(β)→LUMO+1(β) (11.32%)	0.0031
triplet	3.1302 eV (396.09 nm)	HOMO−4(α)→LUMO(α) (35.15%) HOMO−3(α)→LUMO(α) (14.85%) HOMO−4(β)→LUMO(β) (35.15%) HOMO−3(β)→LUMO(β) (14.85%)	0.0000
triplet	3.1670 eV (391.49 nm)	HOMO−4(α)→LUMO(α) (14.48%) HOMO−3(α)→LUMO(α) (35.52%) HOMO−4(β)→LUMO(β) (14.48%) HOMO−3(β)→LUMO(β) (35.52%)	0.0000
singlet	3.1785 eV (390.07 nm)	HOMO−3(α)→LUMO(α) (50.00%) HOMO−3(β)→LUMO(β) (50.00%)	0.0018
triplet	3.4018 eV (364.47 nm)	HOMO−5(α)→LUMO(α) (47.11%) HOMO−4(α)→LUMO+3(α) (1.75%) HOMO−1(α)→LUMO+3(α) (1.14%)	0.0000

		HOMO−5(β)→LUMO(β) (47.11%) HOMO−4(β)→LUMO+3(β) (1.75%) HOMO−1(β)→LUMO+3(β) (1.14%)	
triplet	3.5169 eV (352.54 nm)	HOMO(α)→LUMO+2(α) (21.18%) HOMO(α)→LUMO+3(α) (7.94%) HOMO(α)→LUMO+4(α) (20.88%) HOMO(β)→LUMO+2(β) (21.18%) HOMO(β)→LUMO+3(β) (7.94%) HOMO(β)→LUMO+4(β) (20.88%)	0.0000
triplet	3.6055 eV (343.87 nm)	HOMO−4(α)→LUMO+1(α) (2.46%) HOMO−1(α)→LUMO+1(α) (47.54%) HOMO−4(β)→LUMO+1(β) (2.46%) HOMO−1(β)→LUMO+1(β) (47.54%)	0.0000
singlet	3.6073 eV (343.71 nm)	HOMO(α)→LUMO+2(α) (40.42%) HOMO(α)→LUMO+3(α) (6.15%) HOMO(α)→LUMO+4(α) (3.42%) HOMO(β)→LUMO+2(β) (40.42%) HOMO(β)→LUMO+3(β) (6.15%) HOMO(β)→LUMO+4(β) (3.42%)	0.0001
triplet	3.6411 eV (340.51 nm)	HOMO(α)→LUMO+2(α) (25.90%) HOMO(α)→LUMO+4(α) (24.10%) HOMO(β)→LUMO+2(β) (25.90%) HOMO(β)→LUMO+4(β) (24.10%)	0.0000
singlet	3.7445 eV (331.11 nm)	HOMO−4(α)→LUMO(α) (33.41%) HOMO−1(α)→LUMO+1(α) (9.88%) HOMO(α)→LUMO+4(α) (6.71%) HOMO−4(β)→LUMO(β) (33.41%) HOMO−1(β)→LUMO+1(β) (9.88%) HOMO(β)→LUMO+4(β) (6.71%)	0.0275
singlet	3.7536 eV (330.31 nm)	HOMO−4(α)→LUMO(α) (5.29%) HOMO−1(α)→LUMO+1(α) (1.73%) HOMO(α)→LUMO+2(α) (4.66%) HOMO(α)→LUMO+4(α) (38.32%) HOMO−4(β)→LUMO(β) (5.29%) HOMO−1(β)→LUMO+1(β) (1.73%) HOMO(β)→LUMO+2(β) (4.66%) HOMO(β)→LUMO+4(β) (38.32%)	0.0202
triplet	3.7838 eV (327.67 nm)	HOMO(α)→LUMO+2(α) (3.14%) HOMO(α)→LUMO+3(α) (41.72%) HOMO(α)→LUMO+4(α) (5.14%) HOMO(β)→LUMO+2(β) (3.14%)	0.0000

		HOMO(β)→LUMO+3(β) (41.72%) HOMO(β)→LUMO+4(β) (5.14%)	
singlet	3.8036 eV (325.97 nm)	HOMO(α)→LUMO+2(α) (4.49%) HOMO(α)→LUMO+3(α) (43.21%) HOMO(α)→LUMO+4(α) (2.31%) HOMO(β)→LUMO+2(β) (4.49%) HOMO(β)→LUMO+3(β) (43.21%) HOMO(β)→LUMO+4(β) (2.31%)	0.0055
triplet	3.9334 eV (315.21 nm)	HOMO−7(α)→LUMO(α) (7.91%) HOMO−6(α)→LUMO(α) (28.56%) HOMO−5(α)→LUMO(α) (3.03%) HOMO−1(α)→LUMO+2(α) (2.39%) HOMO−1(α)→LUMO+3(α) (5.53%) HOMO−1(α)→LUMO+5(α) (2.57%) HOMO−7(β)→LUMO(β) (7.91%) HOMO−6(β)→LUMO(β) (28.56%) HOMO−5(β)→LUMO(β) (3.03%) HOMO−1(β)→LUMO+2(β) (2.39%) HOMO−1(β)→LUMO+3(β) (5.53%) HOMO−1(β)→LUMO+5(β) (2.57%)	0.0000
triplet	3.9511 eV (313.80 nm)	HOMO−3(α)→LUMO+4(α) (14.71%) HOMO−2(α)→LUMO+2(α) (27.09%) HOMO−2(α)→LUMO+3(α) (8.20%) HOMO−3(β)→LUMO+4(β) (14.71%) HOMO−2(β)→LUMO+2(β) (27.09%) HOMO−2(β)→LUMO+3(β) (8.20%)	0.0000

Table S34. TD-DFT Calculation Result of Alf with Optimized Structure in the Excited T_1 State Calculated at the TD-UB3LYP/6-31G(d,p) Level

State	Transition Energy (Wave Length)	Assignment with Contribution	Oscillator Strength *f*
triplet	2.3444 eV (528.85 nm)	HOMO(α)→LUMO(α) (50.00%) HOMO(β)→LUMO(β) (50.00%)	0.0000
triplet	3.5832 eV (346.02 nm)	HOMO−3(α)→LUMO(α) (2.12%) HOMO−2(α)→LUMO(α) (2.60%) HOMO(α)→LUMO+2(α) (45.28%) HOMO−3(β)→LUMO(β) (2.12%) HOMO−2(β)→LUMO(β) (2.60%) HOMO(β)→LUMO+2(β) (45.28%)	0.0000
singlet	3.6386 eV (340.75 nm)	HOMO(α)→LUMO(α) (43.13%) HOMO(α)→LUMO+2(α) (6.87%) HOMO(β)→LUMO(β) (43.13%) HOMO(β)→LUMO+2(β) (6.87%)	0.1920
triplet	3.8429 eV (322.63 nm)	HOMO−5(α)→LUMO(α) (12.24%) HOMO−2(α)→LUMO(α) (4.31%) HOMO−1(α)→LUMO(α) (32.25%) HOMO(α)→LUMO+2(α) (1.20%) HOMO−5(β)→LUMO(β) (12.24%) HOMO−2(β)→LUMO(β) (4.31%) HOMO−1(β)→LUMO(β) (32.25%) HOMO(β)→LUMO+2(β) (1.20%)	0.0000
triplet	3.8764 eV (319.84 nm)	HOMO−5(α)→LUMO+1(α) (6.52%) HOMO−3(α)→LUMO+3(α) (5.30%) HOMO−2(α)→LUMO+1(α) (2.27%) HOMO−2(α)→LUMO+3(α) (5.94%) HOMO−1(α)→LUMO+1(α) (29.97%) HOMO−5(β)→LUMO+1(β) (6.52%) HOMO−3(β)→LUMO+3(β) (5.30%) HOMO−2(β)→LUMO+1(β) (2.27%) HOMO−2(β)→LUMO+3(β) (5.94%) HOMO−1(β)→LUMO+1(β) (29.97%)	0.0000
triplet	3.9646 eV (312.73 nm)	HOMO−7(α)→LUMO(α) (9.34eV) HOMO−4(α)→LUMO(α) (21.46%) HOMO−4(α)→LUMO+2(α)(1.75%) HOMO−3(α)→LUMO+4(α) (1.11%) HOMO(α)→LUMO+4(α) (13.12%) HOMO(α)→LUMO+5(α) (3.21%) HOMO−7(β)→LUMO(β) (9.34eV) HOMO−4(β)→LUMO(β) (21.46%) HOMO−4(β)→LUMO+2(β)(1.75%)	0.0000

		HOMO−3(β)→LUMO+4(β) (1.11%) HOMO(β)→LUMO+4(β) (13.12%) HOMO(β)→LUMO+5(β) (3.21%)	
triplet	4.0521 eV (305.97 nm)	HOMO−5(α)→LUMO(α) (3.47%) HOMO−3(α)→LUMO(α) (25.18%) HOMO−2(α)→LUMO(α) (17.23%) HOMO(α)→LUMO+2(α) (4.12%) HOMO−5(β)→LUMO(β) (3.47%) HOMO−3(β)→LUMO(β) (25.18%) HOMO−2(β)→LUMO(β) (17.24%) HOMO(β)→LUMO+2(β) (4.12%)	0.0000
singlet	4.0862 eV (303.42 nm)	HOMO−5(α)→LUMO(α) (4.56%) HOMO−2(α)→LUMO(α) (6.87%) HOMO−1(α)→LUMO(α) (27.52%) HOMO(α)→LUMO+2(α) (11.04%) HOMO−5(β)→LUMO(β) (4.56%) HOMO−2(β)→LUMO(β) (6.87%) HOMO−1(β)→LUMO(β) (27.52%) HOMO(β)→LUMO+2(β) (11.04%)	0.0148

Table S35. TD-DFT Calculation Result of Gaf with Optimized Structure in the Excited T_1 State Calculated at the TD-UB3LYP/6-31G(d,p) Level

State	Transition Energy (Wave Length)	Assignment with Contribution	Oscillator Strength *f*
triplet	2.3700 eV (523.13 nm)	HOMO(α)→LUMO(α) (50.00%) HOMO(β)→LUMO(β) (50.00%)	0.0000
triplet	3.6103 eV (343.42 nm)	HOMO−3(α)→LUMO(α) (4.59%) HOMO−1(α)→LUMO(α) (1.15%) HOMO(α)→LUMO+1(α) (34.34%) HOMO(α)→LUMO+2(α) (9.92%) HOMO−3(β)→LUMO(β) (4.59%) HOMO−1(β)→LUMO(β) (1.15%) HOMO(β)→LUMO+1(β) (34.34%) HOMO(β)→LUMO+2(β) (9.92%)	0.0000
singlet	3.6754 eV (337.33 nm)	HOMO−1(α)→LUMO(α) (1.37%) HOMO(α)→LUMO(α) (41.72%) HOMO(α)→LUMO+1(α) (5.59%) HOMO(α)→LUMO+2(α) (1.32%) HOMO−1(β)→LUMO(β) (1.37%) HOMO(β)→LUMO(β) (41.72%) HOMO(β)→LUMO+1(β) (5.59%) HOMO(β)→LUMO+2(β) (1.32%)	0.1923
triplet	3.7607 eV (329.69 nm)	HOMO−5(α)→LUMO(α) (7.87%) HOMO−1(α)→LUMO(α) (40.95%) HOMO(α)→LUMO+1(α) (1.18%) HOMO−5(β)→LUMO(β) (7.87%) HOMO−1(β)→LUMO(β) (40.95%) HOMO(β)→LUMO+1(β) (1.18%)	0.0000
triplet	3.9315 eV (315.36 nm)	HOMO−5(α)→LUMO+1(α) (2.04%) HOMO−5(α)→LUMO+2(α) (5.91%) HOMO−2(α)→LUMO+3(α) (14.04%) HOMO−1(α)→LUMO+1(α) (7.27%) HOMO−1(α)→LUMO+2(α) (20.73%) HOMO−5(β)→LUMO+1(β) (2.04%) HOMO−5(β)→LUMO+2(β) (5.91%) HOMO−2(β)→LUMO+3(β) (14.04%) HOMO−1(β)→LUMO+1(β) (7.27%) HOMO−1(β)→LUMO+2(β) (20.73%)	0.0000
singlet	4.0005 eV (309.92 nm)	HOMO−5(α)→LUMO(α) (4.19%) HOMO−3(α)→LUMO(α) (1.51%) HOMO−1(α)→LUMO(α) (40.97%) HOMO(α)→LUMO+1(α) (3.33%) HOMO−5(β)→LUMO(β) (4.19%)	0.0016

		HOMO−3(β)→LUMO(β) (1.51%) HOMO−1(β)→LUMO(β) (40.97%) HOMO(β)→LUMO+1(β) (3.33%)	
triplet	4.0037 eV (309.67 nm)	HOMO−7(α)→LUMO(α) (9.05%) HOMO−5(α)→LUMO(α) (3.24%) HOMO−4(α)→LUMO(α) (16.05%) HOMO−3(α)→LUMO(α) (4.80%) HOMO−3(α)→LUMO+4(α) (1.87%) HOMO(α)→LUMO+4(α) (10.93%) HOMO(α)→LUMO+5(α) (4.05%) HOMO−7(β)→LUMO(β) (9.05%) HOMO−5(β)→LUMO(β) (3.24%) HOMO−4(β)→LUMO(β) (16.05%) HOMO−3(β)→LUMO(β) (4.80%) HOMO−3(β)→LUMO+4(β) (1.87%) HOMO(β)→LUMO+4(β) (10.93%) HOMO(β)→LUMO+5(β) (4.05%)	0.0000
triplet	4.0815 eV (303.77 nm)	HOMO−7(α)→LUMO(α) (1.31%) HOMO−4(α)→LUMO(α) (4.15%) HOMO−3(α)→LUMO(α) (40.75%) HOMO(α)→LUMO+1(α) (3.79%) HOMO−7(β)→LUMO(β) (1.31%) HOMO−4(β)→LUMO(β) (4.15%) HOMO−3(β)→LUMO(β) (40.75%) HOMO(β)→LUMO+1(β) (3.79%)	0.0000

Table S36. TD-DFT Calculation Result of Gaf with Optimized Structure in the Excited T_1 State Calculated at the TD-UB3LYP/LANL2DZ Level

State	Transition Energy (Wave Length)	Assignment with Contribution	Oscillator Strength *f*
triplet	2.3541 eV (526.68 nm)	HOMO(α)→LUMO(α) (50.00%) HOMO(β)→LUMO(β) (50.00%)	0.0000
triplet	3.5646 eV (347.82 nm)	HOMO−3(α)→LUMO(α) (4.87%) HOMO(α)→LUMO+1(α) (45.13%) HOMO−3(β)→LUMO(β) (4.87%) HOMO(β)→LUMO+1(β) (45.13%)	0.0000
singlet	3.7223 eV (333.08 nm)	HOMO(α)→LUMO(α) (41.47%) HOMO(α)→LUMO+1(α) (8.53%) HOMO(β)→LUMO(β) (41.47%) HOMO(β)→LUMO+1(β) (8.53%)	0.2300
triplet	3.7955 eV (326.66 nm)	HOMO−5(α)→LUMO(α) (10.77%) HOMO−4(α)→LUMO(α) (1.12%) HOMO−1(α)→LUMO(α) (38.11%) HOMO−5(β)→LUMO(β) (10.77%) HOMO−4(β)→LUMO(β) (1.12%) HOMO−1(β)→LUMO(β) (38.11%)	0.0000
triplet	3.8855 eV (319.09 nm)	HOMO−5(α)→LUMO+2(α) (7.09%) HOMO−2(α)→LUMO+3(α) (14.45%) HOMO−1(α)→LUMO+2(α) (28.45%) HOMO−5(β)→LUMO+2(β) (7.09%) HOMO−2(β)→LUMO+3(β) (14.45%) HOMO−1(β)→LUMO+2(β) (28.45%)	0.0000
triplet	3.9499 eV (313.89 nm)	HOMO−7(α)→LUMO(α) (9.96%) HOMO−5(α)→LUMO(α) (1.94%) HOMO−4(α)→LUMO(α) (16.28%) HOMO−4(α)→LUMO+1(α) (2.32%) HOMO−3(α)→LUMO+4(α) (2.16%) HOMO(α)→LUMO+4(α) (12.00%) HOMO(α)→LUMO+5(α) (5.34%) HOMO−7(β)→LUMO(β) (9.96%) HOMO−5(β)→LUMO(β) (1.94%) HOMO−4(β)→LUMO(β) (16.28%) HOMO−4(β)→LUMO+1(β) (2.32%) HOMO−3(β)→LUMO+4(β) (2.16%) HOMO(β)→LUMO+4(β) (12.00%) HOMO(β)→LUMO+5(β) (5.34%)	0.0000
singlet	4.0156 eV (308.76 nm)	HOMO−5(α)→LUMO(α) (3.94%) HOMO−3(α)→LUMO(α) (4.97%)	0.0102

		HOMO−1(α)→LUMO(α) (30.90%) HOMO(α)→LUMO+1(α) (10.19%) HOMO−5(β)→LUMO(β) (3.94%) HOMO−3(β)→LUMO(β) (4.97%) HOMO−1(β)→LUMO(β) (30.90%) HOMO(β)→LUMO+1(β) (10.19%)	
triplet	4.0820 eV (303.74 nm)	HOMO−5(α)→LUMO(α) (2.69%) HOMO−3(α)→LUMO(α) (42.60%) HOMO(α)→LUMO+1(α) (4.71%) HOMO−5(β)→LUMO(β) (2.69%) HOMO−3(β)→LUMO(β) (42.60%) HOMO(β)→LUMO+1(β) (4.71%)	0.0000
singlet	4.1313 eV (300.11 nm)	HOMO−5(α)→LUMO(α) (3.73%) HOMO−3(α)→LUMO(α) (10.72%) HOMO−1(α)→LUMO(α) (11.30%) HOMO(α)→LUMO(α) (6.52%) HOMO(α)→LUMO+1(α) (17.74%) HOMO−5(β)→LUMO(β) (3.73%) HOMO−3(β)→LUMO(β) (10.72%) HOMO−1(β)→LUMO(β) (11.30%) HOMO(β)→LUMO(β) (6.52%) HOMO(β)→LUMO+1(β) (17.74%)	0.1391

Table S37. TD-DFT Calculation Result of Inf with Optimized Structure in the Excited T_1 State Calculated at the TD-UB3LYP/LANL2DZ Level

State	Transition Energy (Wave Length)	Assignment with Contribution	Oscillator Strength *f*
triplet	2.3577 eV (525.87 nm)	HOMO(α)→LUMO(α) (50.00%) HOMO(β)→LUMO(β) (50.00%)	0.0000
triplet	3.5252 eV (351.71 nm)	HOMO−4(α)→LUMO(α) (1.14%) HOMO−2(α)→LUMO(α) (3.35%) HOMO−1(α)→LUMO(α) (42.47%) HOMO(α)→LUMO+1(α) (1.10%) HOMO(α)→LUMO+2(α) (1.94%) HOMO−4(β)→LUMO(β) (1.14%) HOMO−2(β)→LUMO(β) (3.35%) HOMO−1(β)→LUMO(β) (42.47%) HOMO(β)→LUMO+1(β) (1.10%) HOMO(β)→LUMO+2(β) (1.94%)	0.0000
triplet	3.5909 eV (345.27 nm)	HOMO−3(α)→LUMO(α) (4.54%) HOMO−1(α)→LUMO(α) (2.99%) HOMO(α)→LUMO+1(α) (15.88%) HOMO(α)→LUMO+2(α) (26.59%) HOMO−3(β)→LUMO(β) (4.54%) HOMO−1(β)→LUMO(β) (2.99%) HOMO(β)→LUMO+1(β) (15.88%) HOMO(β)→LUMO+2(β) (26.59%)	0.0000
singlet	3.6837 eV (336.57 nm)	HOMO−1(α)→LUMO(α) (8.48%) HOMO(α)→LUMO(α) (35.54%) HOMO(α)→LUMO+1(α) (2.47%) HOMO(α)→LUMO+2(α) (3.51%) HOMO−1(β)→LUMO(β) (8.48%) HOMO(β)→LUMO(β) (35.54%) HOMO(β)→LUMO+1(β) (2.47%) HOMO(β)→LUMO+2(β) (3.51%)	0.1950
singlet	3.8166 eV (324.86 nm)	HOMO−2(α)→LUMO(α) (1.95%) HOMO−1(α)→LUMO(α) (39.02%) HOMO(α)→LUMO(α) (5.15%) HOMO(α)→LUMO+1(α) (1.52%) HOMO(α)→LUMO+2(α) (2.37%) HOMO−2(β)→LUMO(β) (1.95%) HOMO−1(β)→LUMO(β) (39.02%) HOMO(β)→LUMO(β) (5.15%) HOMO(β)→LUMO+1(β) (1.52%) HOMO(β)→LUMO+2(β) (2.37%)	0.0384
triplet	3.8655 eV	HOMO−4(α)→LUMO+1(α) (2.94%)	0.0000

	(320.74 nm)	HOMO−4(α)→LUMO+2(α) (1.79%) HOMO−4(α)→LUMO+3(α) (6.88%) HOMO−3(α)→LUMO+1(α) (2.06%) HOMO−3(α)→LUMO+3(α) (2.25%) HOMO−2(α)→LUMO+1(α) (8.69%) HOMO−2(α)→LUMO+2(α) (4.16%) HOMO−2(α)→LUMO+3(α) (3.77%) HOMO−1(α)→LUMO+1(α) (11.47%) HOMO−1(α)→LUMO+2(α) (5.99%) HOMO−4(β)→LUMO+1(β) (2.94%) HOMO−4(β)→LUMO+2(β) (1.79%) HOMO−4(β)→LUMO+3(β) (6.88%) HOMO−3(β)→LUMO+1(β) (2.06%) HOMO−3(β)→LUMO+3(β) (2.25%) HOMO−2(β)→LUMO+1(β) (8.69%) HOMO−2(β)→LUMO+2(β) (4.16%) HOMO−2(β)→LUMO+3(β) (3.77%) HOMO−1(β)→LUMO+1(β) (11.47%) HOMO−1(β)→LUMO+2(β) (5.99%)	
triplet	3.9672 eV (312.53 nm)	HOMO−7(α)→LUMO(α) (11.33%) HOMO−5(α)→LUMO(α) (18.91%) HOMO−5(α)→LUMO+2(α) (1.43%) HOMO−3(α)→LUMO+4(α) (1.59%) HOMO(α)→LUMO+4(α) (10.27%) HOMO(α)→LUMO+5(α) (6.48%) HOMO−7(β)→LUMO(β) (11.33%) HOMO−5(β)→LUMO(β) (18.91%) HOMO−5(β)→LUMO+2(β) (1.43%) HOMO−3(β)→LUMO+4(β) (1.59%) HOMO(β)→LUMO+4(β) (10.27%) HOMO(β)→LUMO+5(β) (6.48%)	0.0000
triplet	4.0642 eV (305.06 nm)	HOMO−3(α)→LUMO(α) (32.10%) HOMO−2(α)→LUMO(α) (12.35%) HOMO(α)→LUMO+1(α) (2.21%) HOMO(α)→LUMO+2(α) (3.34%) HOMO−3(β)→LUMO(β) (32.10%) HOMO−2(β)→LUMO(β) (12.35%) HOMO(β)→LUMO+1(β) (2.21%) HOMO(β)→LUMO+2(β) (3.34%)	0.0000
singlet	4.1024 eV (302.23 nm)	HOMO−3(α)→LUMO(α) (12.52%) HOMO−2(α)→LUMO(α) (4.22%) HOMO(α)→LUMO(α) (6.27%) HOMO(α)→LUMO+1(α) (10.53%) HOMO(α)→LUMO+2(α) (16.46%) HOMO−3(β)→LUMO(β) (12.52%)	0.1356

		HOMO−2(β)→LUMO(β) (4.22%) HOMO(β)→LUMO(β) (6.27%) HOMO(β)→LUMO+1(β) (10.53%) HOMO(β)→LUMO+2(β) (16.46%)	
triplet	4.1537 eV (298.49 nm)	HOMO−7(α)→LUMO(α) (14.48%) HOMO−6(α)→LUMO(α) (2.32%) HOMO−5(α)→LUMO(α) (19.86%) HOMO−5(α)→LUMO+2(α) (1.39%) HOMO(α)→LUMO+4(α) (2.06%) HOMO(α)→LUMO+5(α) (9.89%) HOMO−7(β)→LUMO(β) (14.48%) HOMO−6(β)→LUMO(β) (2.32%) HOMO−5(β)→LUMO(β) (19.86%) HOMO−5(β)→LUMO+2(β) (1.39%) HOMO(β)→LUMO+4(β) (2.06%) HOMO(β)→LUMO+5(β) (9.89%)	0.0000

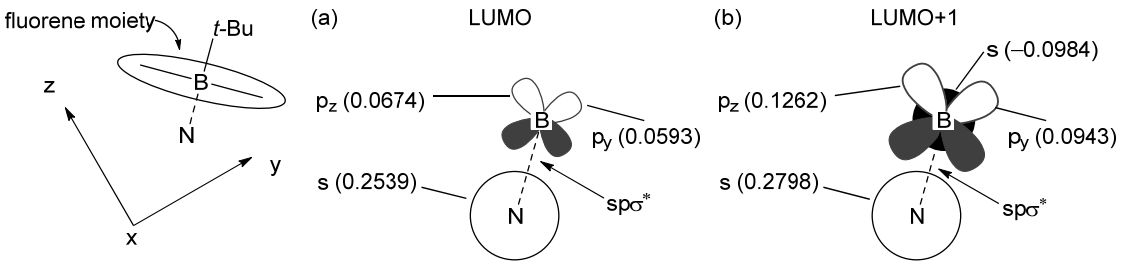

Figure S34. Molecular orbital coefficients on boron and nitrogen atoms of (a) LUMO and (b) LUMO+1 of **Bf** in the ground S_0 state calculated at the B3LYP/6-31G(d,p) level.

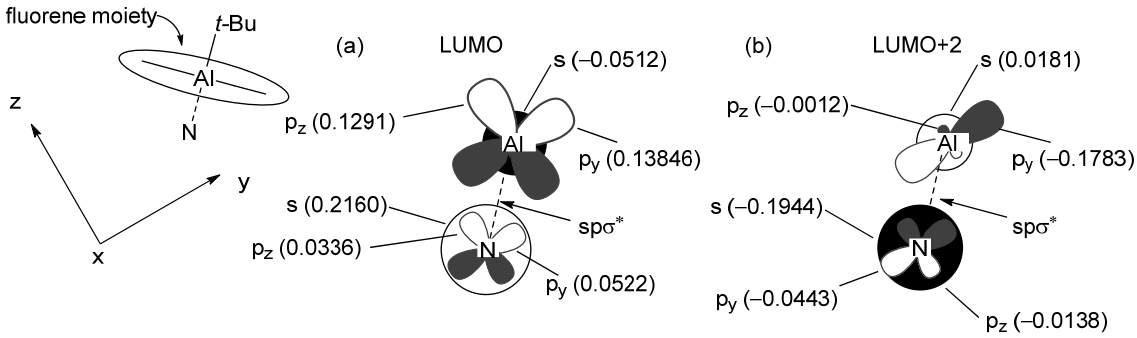

Figure S35. Molecular orbital coefficients on aluminum and nitrogen atoms of (a) LUMO and (b) LUMO+2 of **Alf** in the ground S_0 state calculated at the B3LYP/6-31G(d,p) level.

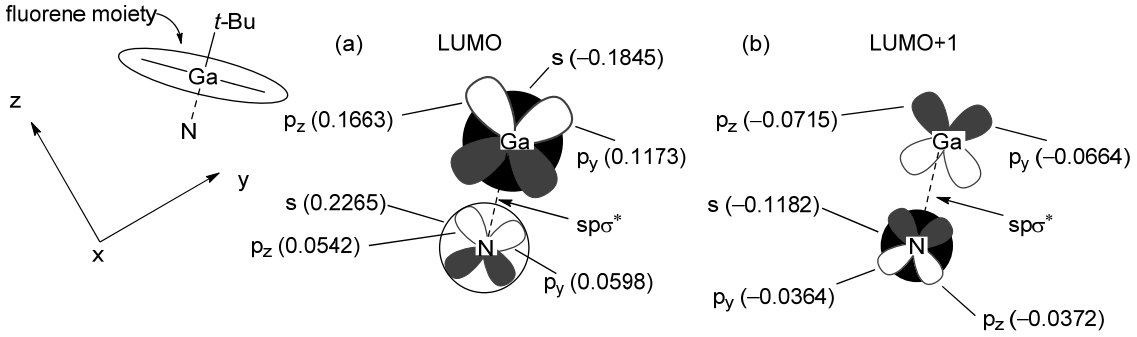

Figure S36. Molecular orbital coefficients on gallium and nitrogen atoms of (a) LUMO and (b) LUMO+1 of **Gaf** in the ground S_0 state calculated at the B3LYP/6-31G(d,p) level.

Mixing of the Wavefunction through the Spin–Orbit Interaction.

The Hamiltonian which represents the spin–orbit interaction is

$$\mathrm{H_{SO}} = \frac{e^2}{2m^2c^2}\sum_{i=1}^{2n}\sum_{N}\frac{Z_N \mathbf{L}_{Ni}}{r_{Ni}^{\ 3}}\cdot\mathbf{S}_i \qquad (1)$$

where Z_N is the atomic number of nucleus N, r_{Ni} the distance from nucleus N to electron i, $\mathbf{L}_{Ni}$ the orbital angular momentum operator for electron i with the origin at the nucleus N, and $\mathbf{S}_i$ the spin angular momentum operator for electron i.

The wavefunction for the ground S_0 state is

$$^1\Phi_0 = \left\|\varphi_1\alpha\varphi_1\beta\cdots\cdots\varphi_n\alpha\varphi_n\beta\right\| \qquad (2)$$

and those for the triplet excited T_i state are

$$^3\Phi_{ik:1} = \left\|\varphi_1\alpha\varphi_1\beta\cdots\varphi_i\alpha\varphi_k\alpha\cdots\varphi_n\alpha\varphi_n\beta\right\| \qquad (3\text{-a})$$

$$^3\Phi_{ik:0} = \left\|\varphi_1\alpha\varphi_1\beta\cdots\varphi_i\varphi_k\frac{1}{\sqrt{2}}(\alpha\beta+\beta\alpha)\cdots\varphi_n\alpha\varphi_n\beta\right\| \qquad (3\text{-b})$$

$$^3\Phi_{ik:-1} = \left\|\varphi_1\alpha\varphi_1\beta\cdots\varphi_i\beta\varphi_k\beta\cdots\varphi_n\alpha\varphi_n\beta\right\| \qquad (3\text{-c})$$

where e.g., φ_i stands for the occupied i-th MO and α and β for spin parts. The subscript ik stands for the triplet excitation from the i-th MO to the k-th one. These spin sublevels of the triplet states are degenerate, as a matter of course.

Considering the first-order perturbation correction, the wavefunction for the T_1 state is described by

$$\Psi_{\mathrm{T_1}} = {}^3\Phi_{\mathrm{T_1}} + \sum_k \frac{\left\langle {}^1\Phi_k \left| \hat{\mathrm{H}}_{\mathrm{SO}} \right| {}^3\Phi_{\mathrm{T_1}} \right\rangle}{\Delta {}^3E_{k,\mathrm{T_1}}} {}^1\Phi_k = {}^3\Phi_{\mathrm{T_1}} + \alpha\,{}^1\Phi_k \qquad (4)$$

where $\Delta^3E_{k,\mathrm{T_1}}$ is the energy difference between the S_k to the T_1 sates, and α the mixing coefficient.

Herein we confine ourselves to the vertical electronic transition from the S_0 to the T_1 state (namely $k = 0$ in equation (4)), and hence the HOMO and the LUMO of the ground S_0 state with the optimized structure in the excited T_1 state were adopted for calculation of the matrix element in α. Only one-center terms as to the group 13 elements was considered as usual.

The α_p values (p = 1, 0, −1) are given for the three kind of ${}^3\Phi_{T_1:p}$ (p = 1, 0, −1; see equations (3-a)-(3-c)) respectively, as shown in Table S38. In Table 8 of the main text, we omitted the complex α_1 and α_{-1} values.

Table S38. Mixing Coefficients α_p Values (p = 1, 0, −1) of Bf, Alf, Gaf and Inf

	α_1 ($\times 10^{-6}$)	α_0 ($\times 10^{-6}$)	α_{-1} ($\times 10^{-6}$)
Bf[a]	−5.21−5.21i	7.34	5.21−5.21i
Alf[a]	−2.99−2.99i	4.23	2.99−2.99i
Gaf[a]	45.4+45.4i (−15.7−15.7i)[b]	−64.2 (22.2)[b]	−45.4+45.4i (15.7−15.7i)[b]
Inf[b]	−64.4−64.4i	91.1	64.4−64.4i

[a]Calculated at the TD-UB3LYP/6-31G(d,p) level. [b]Calculated at the TD-UB3LYP/LANL2DZ level.

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