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Supplementary Information **Open Access**

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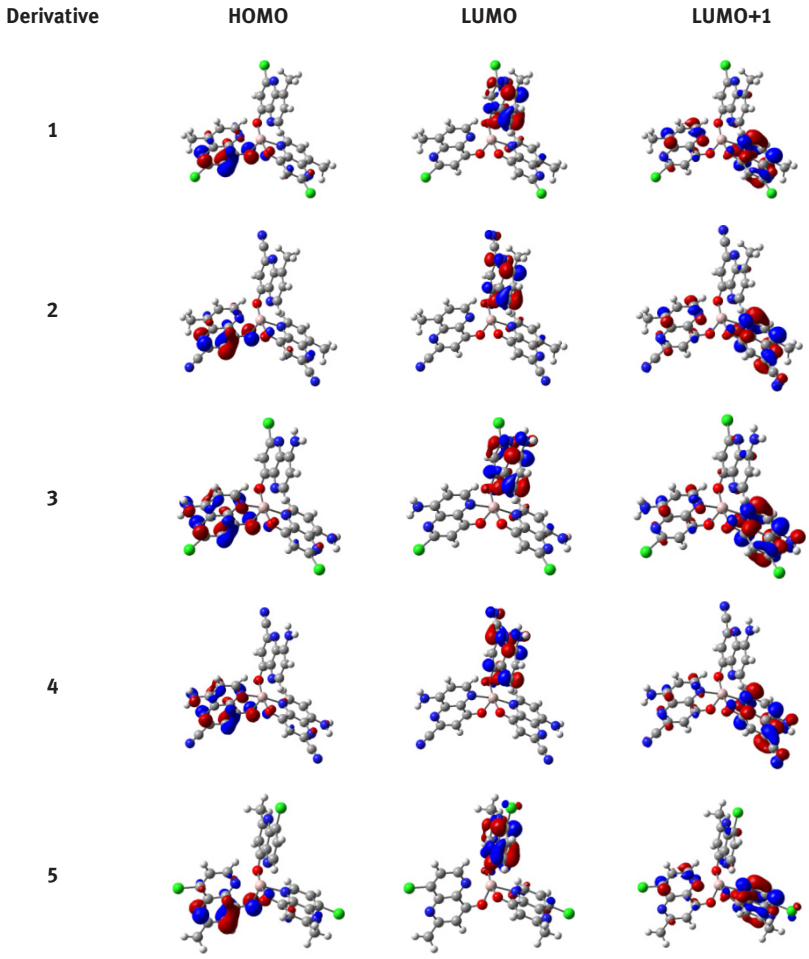
Supplement: Push-pull effect on the geometrical, optical and charge transfer properties of disubstituted derivatives of *mer*-tris(4-hydroxy-1,5-naphthyridinato) aluminum (*mer*-AlND3)



Supplementary Figure 1: Frontier molecular orbitals (FMOs) for the ground states (S_0) of disubstituted derivatives of AlND3 (1-8) computed at B3LYP/6-31G(D) method.

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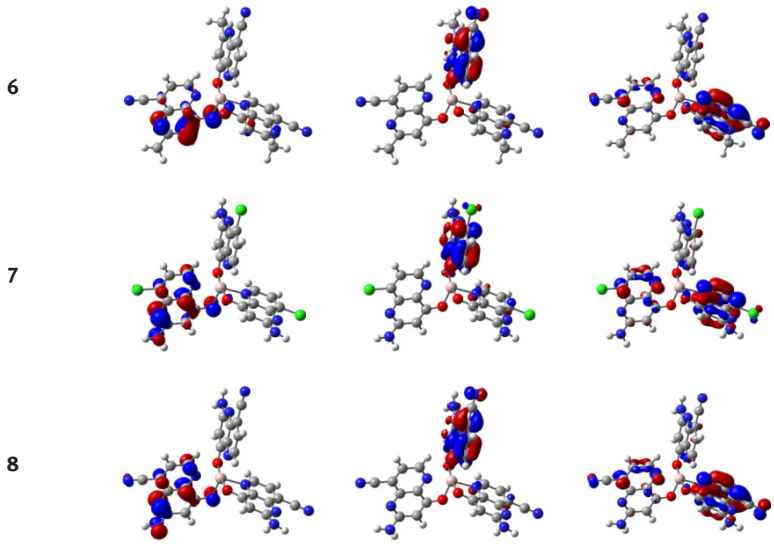
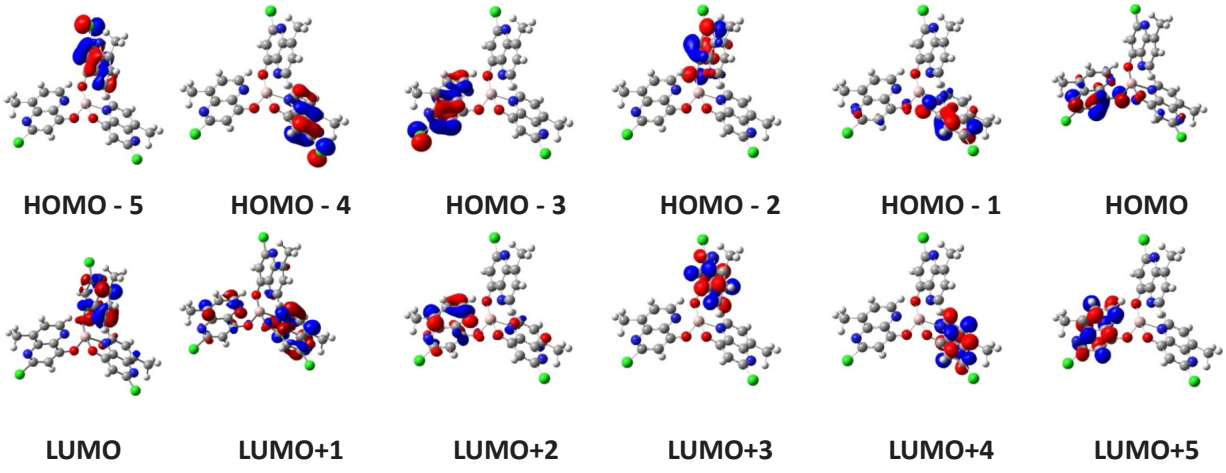
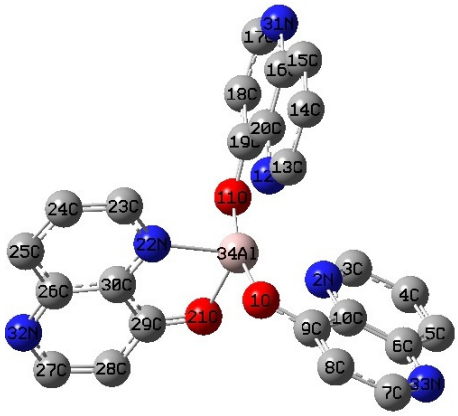


Continued **Supplementary Figure 1:** Frontier molecular orbitals (FMOs) for the ground states (S_0) of disubstituted derivatives of AlND3 (1-8) computed at B3LYP/6-31G(D) method.



Supplementary Figure 2: Frontier molecular orbitals (FMOs) (H-5 to L+5) for the ground state (S_0) of the disubstituted derivative 1, computed at B3LYP/6-31G(d) method.



Supplementary Figure 3: The ligand bond labels used in the text for the disubstituted AlND3 complexes considered in this study in Table 3 and Table S1(a-d).

Supplementary Table S1(a): Calculated geometrical parameters of (1 and 2) in their Ground (HF-S_0) and First excited state (S_1) computed at HF/6-31G(D) and CIS/6-31G(D) methods respectively, and the differences of the bond lengths (A°) between the S_1 and ground states for ligands A ($\Delta A_{E\text{-}G}$), B($\Delta B_{E\text{-}G}$) and C($\Delta C_{E\text{-}G}$).

	Derivatives	**1**			**2**		
	Ligand A	**HF-S_0**	**S_1**	**($\Delta A_{E\text{-}G}$)**	**HF-S_0**	**S_1**	**($\Delta A_{E\text{-}G}$)**
a	Al(34)-O(21)	1.842	1.900	0.059	1.842	1.895	0.053
b	Al(34)-N(22)	2.092	2.024	-0.068	2.093	2.038	-0.055
c	C(30)-N(22)	1.353	1.328	-0.025	1.356	1.318	-0.038
d	C(30)-C(29)	1.433	1.428	-0.005	1.428	1.438	0.010
e	C(30)-C(26)	1.385	1.425	0.040	1.387	1.426	0.038
f	C(29)-O(21)	1.286	1.263	-0.023	1.285	1.263	-0.022
g	C(29)-C(28)	1.374	1.428	0.054	1.378	1.419	0.041
h	C(28)-C(27)	1.407	1.359	-0.048	1.404	1.370	-0.035
i	C(26)-C(25)	1.426	1.421	-0.005	1.430	1.427	-0.003
j	C(25)-C(24)	1.368	1.413	0.045	1.366	1.404	0.039
k	C(24)-C(23)	1.406	1.365	-0.042	1.409	1.368	-0.042
l	C(23)-N(22)	1.300	1.377	0.077	1.299	1.376	0.078
m	N(32)-C(26)	1.354	1.348	-0.006	1.347	1.316	-0.031
n	N(32)-C(27)	1.288	1.321	0.032	1.303	1.362	0.059
	Ligand B	**HF-S_0**	**S_1**	**($\Delta B_{E\text{-}G}$)**	**HF-S_0**	**S_1**	**($\Delta B_{E\text{-}G}$)**
a	Al(34)-O(11)	1.866	1.870	0.005	1.866	1.868	0.003
b	Al(34)-N(12)	2.131	2.121	-0.010	2.130	2.117	-0.013
c	C(20)-N(12)	1.349	1.349	0.000	1.352	1.352	0.000
d	C(20)-C(16)	1.383	1.383	0.000	1.387	1.386	-0.001
e	C(20)-C(19)	1.431	1.431	0.000	1.426	1.427	0.000
f	C(19)-C(18)	1.374	1.374	0.000	1.378	1.378	0.000
g	C(19)-O(11)	1.286	1.287	0.000	1.286	1.287	0.001
h	C(18)-C(17)	1.409	1.409	0.000	1.407	1.407	0.000
i	C(16)-C(15)	1.426	1.426	0.000	1.431	1.431	0.000
j	C(15)-C(14)	1.369	1.370	0.000	1.367	1.368	0.000
k	C(14)-C(13)	1.408	1.407	-0.001	1.411	1.410	-0.001
l	C(13)-N(12)	1.302	1.302	0.000	1.300	1.301	0.001
m	N(31)-C(16)	1.354	1.355	0.001	1.347	1.347	0.000
n	N(31)-C(17)	1.289	1.290	0.001	1.303	1.303	0.000
	Ligand C	**HF-S_0**	**S_1**	**($\Delta C_{E\text{-}G}$)**	**HF-S_0**	**S_1**	**($\Delta C_{E\text{-}G}$)**
a	Al(34)-O(1)	1.869	1.867	-0.002	1.869	1.865	-0.004
b	Al(34)-N(2)	2.066	2.076	0.010	2.067	2.078	0.011
c	C(10)-N(2)	1.350	1.349	-0.001	1.353	1.352	0.000
d	C(10)-C(9)	1.432	1.431	-0.001	1.427	1.426	-0.001
e	C(10)-C(6)	1.382	1.382	0.000	1.385	1.385	0.000
f	C(9)-O(1)	1.373	1.374	0.001	1.376	1.376	0.000
g	C(9)-C(8)	1.290	1.291	0.001	1.290	1.290	0.000
h	C(8)-C(7)	1.410	1.410	0.000	1.408	1.408	0.000
i	C(6)-C(5)	1.427	1.426	0.000	1.431	1.431	0.000
j	C(5)-C(4)	1.369	1.369	0.000	1.367	1.367	0.000
k	C(4)-C(3)	1.408	1.408	0.000	1.411	1.410	0.000
l	C(3)-N(2)	1.300	1.301	0.000	1.299	1.299	0.000
m	N(33)-C(6)	1.355	1.355	0.000	1.348	1.348	0.000
n	N(33)-C(7)	1.287	1.287	0.000	1.302	1.302	0.000

Supplementary Table 1(b): Calculated geometrical parameters of (3 and 4) in their Ground (HF-S_0) and First excited state (S_1) computed at HF/6-31G(D) and CIS/6-31G(D) methods respectively, and the differences of the bond lengths (A°) between the S_1 and ground states for ligands A ($\Delta A_{E\text{-}G}$), B($\Delta B_{E\text{-}G}$) and C($\Delta C_{E\text{-}G}$).

	Derivatives	**3**			**4**		
	Ligand A	**HF-S_0**	**S_1**	**($\Delta A_{E\text{-}G}$)**	**HF-S_0**	**S_1**	**($\Delta A_{E\text{-}G}$)**
a	Al(34)-O(21)	1.857	1.891	0.035	1.857	1.877	0.020
b	Al(34)-N(22)	2.075	2.050	-0.025	2.075	2.078	0.003
c	C(30)-N(22)	1.355	1.329	-0.027	1.357	1.309	-0.048
d	C(30)-C(29)	1.434	1.416	-0.017	1.429	1.449	0.020
e	C(30)-C(26)	1.375	1.435	0.061	1.379	1.425	0.046
f	C(29)-O(21)	1.283	1.270	-0.012	1.282	1.273	-0.009
g	C(29)-C(28)	1.377	1.431	0.054	1.380	1.400	0.020
h	C(28)-C(27)	1.405	1.358	-0.047	1.404	1.383	-0.021
i	C(26)-C(25)	1.434	1.414	-0.020	1.438	1.449	0.011
j	C(25)-C(24)	1.387	1.430	0.043	1.386	1.402	0.015
k	C(24)-C(23)	1.392	1.356	-0.037	1.392	1.372	-0.020
l	C(23)-N(22)	1.308	1.374	0.066	1.308	1.369	0.061
m	N(32)-C(26)	1.354	1.318	-0.036	1.346	1.301	-0.045
n	N(32)-C(27)	1.288	1.351	0.063	1.303	1.375	0.072
	Ligand B	**HF-S_0**	**S_1**	**($\Delta B_{E\text{-}G}$)**	**HF-S_0**	**S_1**	**($\Delta B_{E\text{-}G}$)**
a	Al(34)-O(11)	1.883	1.884	0.001	1.883	1.880	-0.003
b	Al(34)-N(12)	2.098	2.081	-0.017	2.098	2.082	-0.016
c	C(20)-N(12)	1.352	1.352	0.000	1.353	1.353	0.000
d	C(20)-C(16)	1.378	1.378	0.000	1.378	1.378	0.000
e	C(20)-C(19)	1.433	1.433	0.000	1.428	1.428	0.000
f	C(19)-C(18)	1.377	1.377	0.000	1.380	1.380	-0.001
g	C(19)-O(11)	1.283	1.284	0.001	1.282	1.284	0.002
h	C(18)-C(17)	1.407	1.407	0.000	1.406	1.406	0.000
i	C(16)-C(15)	1.435	1.435	0.000	1.439	1.439	0.000
j	C(15)-C(14)	1.388	1.389	0.001	1.388	1.389	0.001
k	C(14)-C(13)	1.393	1.392	-0.001	1.393	1.392	-0.001
l	C(13)-N(12)	1.310	1.311	0.001	1.310	1.311	0.001
m	N(31)-C(16)	1.354	1.354	0.000	1.346	1.346	0.000
n	N(31)-C(17)	1.289	1.289	0.000	1.303	1.303	0.000
	Ligand C	**HF-S_0**	**S_1**	**($\Delta C_{E\text{-}G}$)**	**HF-S_0**	**S_1**	**($\Delta C_{E\text{-}G}$)**
a	Al(34)-O(1)	1.884	1.881	-0.003	1.884	1.879	-0.005
b	Al(34)-N(2)	2.052	2.058	0.006	2.052	2.050	-0.002
c	C(10)-N(2)	1.352	1.351	0.000	1.353	1.353	0.000
d	C(10)-C(9)	1.433	1.432	-0.001	1.429	1.428	-0.001
e	C(10)-C(6)	1.374	1.374	0.000	1.378	1.378	0.000
f	C(9)-O(1)	1.376	1.376	0.000	1.286	1.287	0.001
g	C(9)-C(8)	1.287	1.287	0.000	1.379	1.378	0.000
h	C(8)-C(7)	1.408	1.408	0.000	1.407	1.407	0.000
i	C(6)-C(5)	1.434	1.434	0.000	1.439	1.439	0.000
j	C(5)-C(4)	1.387	1.388	0.000	1.387	1.388	0.001
k	C(4)-C(3)	1.393	1.393	0.000	1.393	1.392	-0.001
l	C(3)-N(2)	1.309	1.309	0.001	1.309	1.310	0.001
m	N(33)-C(6)	1.355	1.355	0.000	1.302	1.302	0.000
n	N(33)-C(7)	1.287	1.287	0.000	1.347	1.347	0.000

Supplementary Table 1(c): Calculated geometrical parameters of (5 and 6) in their Ground (HF-S_0) and First excited state (S_1) computed at HF/6-31G(D) and CIS/6-31G(D) methods respectively, and the differences of the bond lengths (A°) between the S_1 and ground states for ligands A ($\Delta A_{E\text{-}G}$), B($\Delta B_{E\text{-}G}$) and C($\Delta C_{E\text{-}G}$).

	Derivatives	**5**			**6**		
	Ligand A	**HF-S_0**	**S_1**	**($\Delta A_{E\text{-}G}$)**	**HF-S_0**	**S_1**	**($\Delta A_{E\text{-}G}$)**
a	Al(34)-O(21)	1.835	1.902	0.067	1.831	1.910	0.079
b	Al(34)-N(22)	2.092	2.022	-0.070	2.110	2.018	-0.092
c	C(30)-N(22)	1.350	1.333	-0.016	1.347	1.334	-0.013
d	C(30)-C(29)	1.434	1.427	-0.007	1.434	1.433	-0.001
e	C(30)-C(26)	1.391	1.421	0.030	1.392	1.407	0.016
f	C(29)-O(21)	1.289	1.261	-0.028	1.289	1.256	-0.034
g	C(29)-C(28)	1.369	1.429	0.060	1.369	1.428	0.059
h	C(28)-C(27)	1.416	1.362	-0.054	1.417	1.366	-0.051
i	C(26)-C(25)	1.420	1.415	-0.005	1.419	1.425	0.006
j	C(25)-C(24)	1.365	1.412	0.047	1.368	1.419	0.050
k	C(24)-C(23)	1.404	1.362	-0.041	1.405	1.362	-0.043
l	C(23)-N(22)	1.301	1.372	0.071	1.302	1.370	0.068
m	N(32)-C(26)	1.346	1.318	-0.028	1.344	1.322	-0.022
n	N(32)-C(27)	1.305	1.365	0.060	1.307	1.361	0.053
	Ligand B	**HF-S_0**	**S_1**	**($\Delta B_{E\text{-}G}$)**	**HF-S_0**	**S_1**	**($\Delta B_{E\text{-}G}$)**
a	Al(34)-O(11)	1.858	1.863	0.005	1.852	1.857	0.005
b	Al(34)-N(12)	2.131	2.118	-0.013	2.162	2.156	-0.046
c	C(20)-N(12)	1.346	1.347	0.001	1.343	1.344	0.001
d	C(20)-C(16)	1.383	1.384	0.001	1.389	1.389	0.000
e	C(20)-C(19)	1.432	1.432	0.001	1.431	1.431	0.001
f	C(19)-C(18)	1.291	1.291	0.001	1.291	1.292	0.001
g	C(19)-O(11)	1.369	1.369	0.000	1.369	1.369	0.000
h	C(18)-C(17)	1.419	1.419	0.000	1.420	1.420	0.000
i	C(16)-C(15)	1.421	1.421	0.000	1.420	1.420	0.000
j	C(15)-C(14)	1.366	1.366	0.000	1.370	1.370	0.000
k	C(14)-C(13)	1.406	1.405	-0.001	1.407	1.407	-0.001
l	C(13)-N(12)	1.302	1.303	0.000	1.303	1.303	0.000
m	N(31)-C(16)	1.347	1.346	0.000	1.345	1.344	0.000
n	N(31)-C(17)	1.305	1.305	0.000	1.307	1.307	0.000
	Ligand C	**HF-S_0**	**S_1**	**($\Delta C_{E\text{-}G}$)**	**HF-S_0**	**S_1**	**($\Delta C_{E\text{-}G}$)**
a	Al(34)-O(1)	1.863	1.860	-0.003	1.858	1.854	-0.004
b	Al(34)-N(2)	2.066	2.076	0.010	2.108	2.109	0.001
c	C(10)-N(2)	1.347	1.346	-0.001	1.345	1.344	-0.001
d	C(10)-C(9)	1.433	1.432	-0.001	1.432	1.430	-0.001
e	C(10)-C(6)	1.388	1.388	0.000	1.388	1.388	0.000
f	C(9)-O(1)	1.368	1.368	0.000	1.368	1.368	0.000
g	C(9)-C(8)	1.294	1.294	0.000	1.295	1.295	0.000
h	C(8)-C(7)	1.419	1.420	0.000	1.421	1.421	0.000
i	C(6)-C(5)	1.422	1.421	0.000	1.421	1.420	0.000
j	C(5)-C(4)	1.365	1.366	0.000	1.369	1.369	0.000
k	C(4)-C(3)	1.405	1.406	0.000	1.407	1.407	0.000
l	C(3)-N(2)	1.301	1.301	0.000	1.301	1.302	0.000
m	N(33)-C(6)	1.347	1.348	0.000	1.345	1.346	0.000
n	N(33)-C(7)	1.304	1.304	0.000	1.306	1.306	0.000

Supplementary Table 1(d): Calculated geometrical parameters of (7 and 8) in their Ground (HF-S_0) and First excited state (S_1) computed at HF/6-31G(D) and CIS/6-31G(D) methods respectively, and the differences of the bond lengths (A°) between the S_1 and ground states for ligands A (ΔA_{E-G}), B(ΔB_{E-G}) and C(ΔC_{E-G}).

	Derivatives	**7**			**8**		
	Ligand A	**HF-S_0**	**S_1**	**(ΔA_{E-G})**	**HF-S_0**	**S_1**	**(ΔA_{E-G})**
a	Al(34)-O(21)	1.837	1.870	0.033	1.833	1.873	0.040
b	Al(34)-N(22)	2.098	2.031	-0.067	2.075	2.032	-0.043
c	C(30)-N(22)	1.344	1.344	0.000	1.339	1.343	0.004
d	C(30)-C(29)	1.442	1.426	-0.016	1.443	1.437	-0.006
e	C(30)-C(26)	1.393	1.436	0.044	1.396	1.418	0.022
f	C(29)-O(21)	1.287	1.276	-0.012	1.288	1.271	-0.017
g	C(29)-C(28)	1.364	1.400	0.035	1.363	1.394	0.031
h	C(28)-C(27)	1.423	1.380	-0.043	1.426	1.384	-0.041
i	C(26)-C(25)	1.418	1.422	0.004	1.416	1.440	0.024
j	C(25)-C(24)	1.367	1.405	0.039	1.372	1.408	0.035
k	C(24)-C(23)	1.400	1.373	-0.027	1.399	1.376	-0.024
l	C(23)-N(22)	1.304	1.359	0.055	1.307	1.357	0.050
m	N(32)-C(26)	1.343	1.304	-0.040	1.340	1.304	-0.036
n	N(32)-C(27)	1.309	1.375	0.066	1.313	1.373	0.060
	Ligand B	**S_0**	**S_1**	**(ΔB_{E-G})**	**HF-S_0**	**S_1**	**(ΔB_{E-G})**
a	Al(34)-O(11)	1.858	1.867	0.009	1.853	1.861	0.007
b	Al(34)-N(12)	2.140	2.116	-0.024	2.097	2.134	0.037
c	C(20)-N(12)	1.341	1.341	0.000	1.336	1.337	0.000
d	C(20)-C(16)	1.391	1.389	-0.002	1.378	1.393	0.015
e	C(20)-C(19)	1.439	1.440	0.001	1.439	1.440	0.001
f	C(19)-C(18)	1.289	1.288	-0.001	1.289	1.289	-0.001
g	C(19)-O(11)	1.364	1.365	0.001	1.363	1.363	0.001
h	C(18)-C(17)	1.426	1.425	-0.001	1.429	1.428	-0.001
i	C(16)-C(15)	1.419	1.419	0.000	1.418	1.418	0.000
j	C(15)-C(14)	1.368	1.368	0.000	1.374	1.374	0.000
k	C(14)-C(13)	1.402	1.402	0.000	1.402	1.401	0.000
l	C(13)-N(12)	1.305	1.305	0.000	1.308	1.308	0.000
m	N(31)-C(16)	1.344	1.344	0.000	1.340	1.340	0.000
n	N(31)-C(17)	1.309	1.309	0.000	1.313	1.313	0.000
	Ligand C	**HF-S_0**	**S_1**	**(ΔC_{E-G})**	**HF-S_0**	**S_1**	**(ΔC_{E-G})**
a	Al(34)-O(1)	1.864	1.867	0.003	1.859	1.861	0.002
b	Al(34)-N(2)	2.071	2.108	0.037	2.051	2.101	0.050
c	C(10)-N(2)	1.342	1.341	-0.001	1.338	1.337	-0.001
d	C(10)-C(9)	1.389	1.389	0.000	1.392	1.392	0.000
e	C(10)-C(6)	1.440	1.440	0.000	1.440	1.440	0.000
f	C(9)-O(1)	1.364	1.364	0.001	1.362	1.363	0.000
g	C(9)-C(8)	1.292	1.291	-0.001	1.292	1.291	-0.001
h	C(8)-C(7)	1.426	1.425	0.000	1.429	1.428	0.000
i	C(6)-C(5)	1.419	1.419	0.000	1.418	1.418	0.000
j	C(5)-C(4)	1.367	1.367	0.000	1.373	1.373	0.000
k	C(4)-C(3)	1.402	1.403	0.000	1.402	1.402	0.000
l	C(3)-N(2)	1.303	1.303	0.000	1.306	1.306	0.000
m	N(33)-C(6)	1.345	1.345	0.000	1.342	1.342	0.000
n	N(33)-C(7)	1.307	1.308	0.000	1.311	1.311	0.000

Supplementary Table 2(a): The NBO charges (Q) of the ligands for (1-2) in the optimized ground ($Q_{HF\text{-}S0}$) and first excited (Q_{S1}) states structures and the charge differences between Q_{S1} and Q_{S0} states calculated at the HF/6-31G(D) and CIS/6-31G(D) methods, respectively (Note: for EDG and EWG labels are not shown).

	Derivative-1									
		$Q_{HF\text{-}S0}$			Q_{S1}			$Q_{S1} - Q_{HF\text{-}S0}$		
Atom		**A**	**B**	**C**	**A**	**B**	**C**	**A**	**B**	**C**
O	**1**	-0.917	-0.917	-0.927	-0.882	-0.914	-0.928	0.035	0.002	-0.002
N	**2**	-0.631	-0.638	-0.642	-0.653	-0.646	-0.636	-0.022	-0.008	0.006
C	**3**	0.156	0.152	0.168	0.110	0.154	0.166	-0.046	0.002	-0.002
C	**4**	-0.308	-0.309	-0.307	-0.303	-0.310	-0.306	0.005	-0.001	0.001
C	**5**	0.086	0.083	0.084	0.100	0.086	0.083	0.014	0.003	-0.002
C	**6**	0.175	0.173	0.173	0.188	0.173	0.172	0.012	0.000	0.000
C	**7**	0.318	0.315	0.315	0.290	0.315	0.315	-0.027	0.000	-0.001
C	**8**	-0.417	-0.418	-0.419	-0.419	-0.418	-0.419	-0.003	0.001	0.000
C	**9**	0.524	0.511	0.511	0.559	0.511	0.512	0.035	-0.001	0.001
C	**10**	0.108	0.098	0.107	0.111	0.100	0.107	0.003	0.001	0.000
N	**11**	-0.582	-0.578	-0.575	-0.612	-0.579	-0.575	-0.030	0.000	0.000
C		-0.653	-0.654	-0.653	-0.660	-0.654	-0.653	-0.007	0.000	0.000
Cl		-0.021	-0.016	-0.020	-0.003	-0.016	-0.021	0.018	0.001	0.000
Al		2.139			2.135			-0.004		
	Derivative 2									
		$Q_{HF\text{-}S0}$			Q_{S1}			$Q_{S1} - Q_{HF\text{-}S0}$		
Atom		**A**	**B**	**C**	**A**	**B**	**C**	**A**	**B**	**C**
O	**1**	-0.915	-0.915	-0.925	-0.884	-0.913	-0.927	0.031	0.002	-0.002
N	**2**	-0.636	-0.643	-0.648	-0.655	-0.651	-0.643	-0.019	-0.008	0.005
C	**3**	0.169	0.165	0.181	0.122	0.167	0.180	-0.047	0.002	-0.001
C	**4**	-0.312	-0.313	-0.310	-0.309	-0.314	-0.310	0.003	-0.001	0.000
C	**5**	0.095	0.092	0.093	0.110	0.095	0.092	0.015	0.003	-0.001
C	**6**	0.171	0.167	0.167	0.179	0.167	0.167	0.008	0.000	0.000
C	**7**	0.199	0.199	0.198	0.180	0.200	0.197	-0.019	0.001	-0.001
C	**8**	-0.363	-0.366	-0.367	-0.361	-0.365	-0.366	0.003	0.001	0.001
C	**9**	0.518	0.505	0.504	0.550	0.505	0.504	0.032	-0.001	0.000
C	**10**	0.110	0.101	0.111	0.121	0.102	0.111	0.011	0.001	0.000
N	**11**	-0.527	-0.523	-0.519	-0.558	-0.523	-0.518	-0.031	0.000	0.001
C		0.313	0.310	0.312	0.315	0.309	0.312	0.002	-0.001	0.000
C		-0.655	-0.656	-0.655	-0.662	-0.656	-0.655	-0.007	0.000	0.000
N		-0.337	-0.331	-0.335	-0.331	-0.330	-0.335	0.005	0.001	0.000
Al		2.139			2.135			-0.004		

Supplementary Table 2 (b): The NBO charges (Q) of the ligands for (3-4) in the optimized ground ($Q_{HF\text{-}S0}$) and first excited (Q_{S1}) states structures and the charge differences between Q_{S1} and Q_{S0} states calculated at the HF/6-31G(D) and CIS/6-31G(D) methods, respectively (Note: for EDG and EWG labels are not shown).

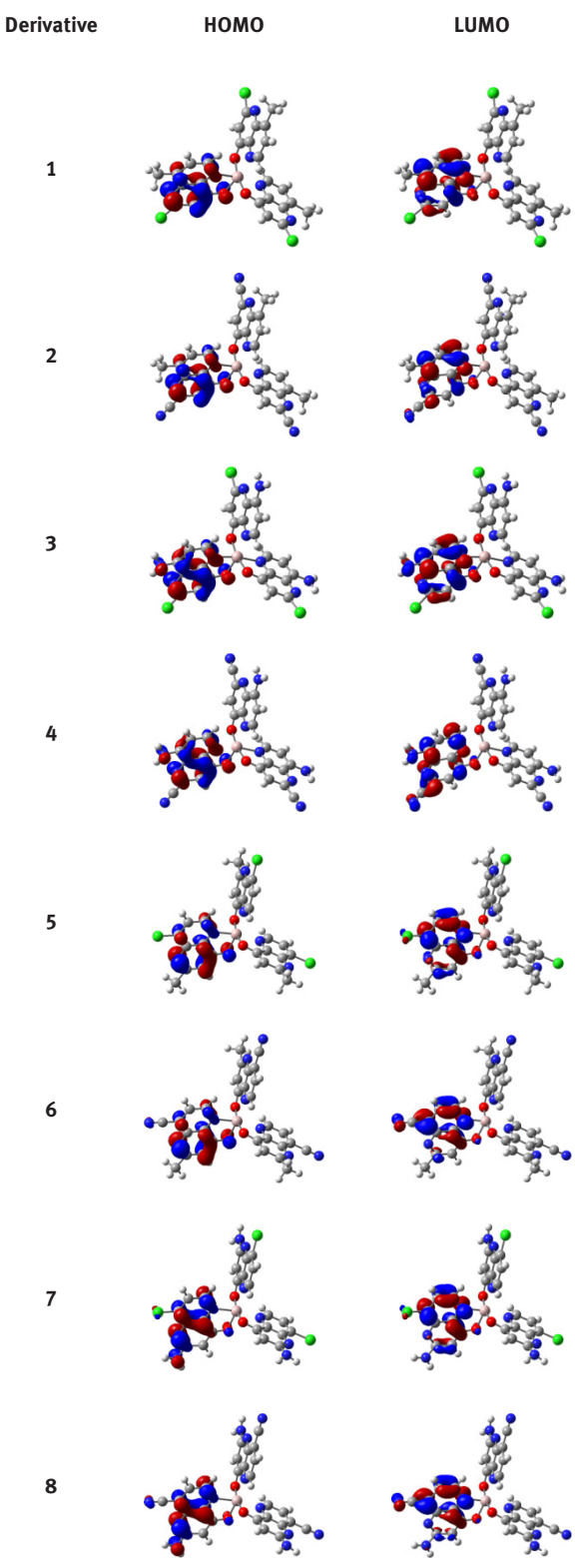
	Derivative 3									
		$Q_{HF\text{-}S0}$			Q_{S1}			$Q_{S1} - Q_{HF\text{-}S0}$		
Atom		**A**	**B**	**C**	**A**	**B**	**C**	**A**	**B**	**C**
O	**1**	-0.908	-0.907	-0.918	-0.887	-0.907	-0.919	0.022	0.001	-0.001
N	**2**	-0.692	-0.700	-0.698	-0.697	-0.704	-0.697	-0.005	-0.004	0.001
C	**3**	0.182	0.177	0.190	0.136	0.177	0.189	-0.046	0.000	-0.001
C	**4**	-0.414	-0.415	-0.411	-0.377	-0.415	-0.411	0.037	-0.001	0.000
C	**5**	0.345	0.342	0.342	0.342	0.344	0.342	-0.003	0.002	0.000
C	**6**	0.125	0.122	0.122	0.137	0.122	0.122	0.012	0.000	0.000
C	**7**	0.313	0.311	0.311	0.276	0.311	0.311	-0.037	0.000	-0.001
C	**8**	-0.418	-0.420	-0.421	-0.405	-0.420	-0.420	0.013	0.001	0.001
C	**9**	0.528	0.516	0.516	0.548	0.516	0.515	0.020	-0.001	0.000
C	**10**	0.127	0.118	0.128	0.123	0.119	0.128	-0.004	0.000	0.000
N	**11**	-0.598	-0.595	-0.591	-0.611	-0.595	-0.590	-0.014	0.000	0.001
N		-0.849	-0.849	-0.850	-0.856	-0.848	-0.850	-0.007	0.001	0.000
Cl		-0.028	-0.023	-0.027	-0.012	-0.023	-0.026	0.016	0.001	0.001
Al		2.135			2.132			-0.002		
	Derivative 4									
		$Q_{HF\text{-}S0}$			Q_{S1}			$Q_{S1} - Q_{HF\text{-}S0}$		
Atom		**A**	**B**	**C**	**A**	**B**	**C**	**A**	**B**	**C**
O	**1**	-0.906	-0.905	-0.917	-0.895	-0.905	-0.917	0.011	0.000	-0.001
N	**2**	-0.697	-0.705	-0.705	-0.702	-0.709	-0.706	-0.005	-0.004	-0.001
C	**3**	0.191	0.184	0.199	0.162	0.185	0.199	-0.028	0.000	0.000
C	**4**	-0.419	-0.420	-0.417	-0.405	-0.420	-0.417	0.014	0.000	0.000
C	**5**	0.352	0.350	0.350	0.354	0.351	0.351	0.003	0.001	0.001
C	**6**	0.122	0.119	0.118	0.135	0.118	0.118	0.013	0.000	0.000
C	**7**	0.190	0.190	0.188	0.159	0.190	0.188	-0.031	0.000	0.000
C	**8**	-0.363	-0.366	-0.367	-0.350	-0.365	-0.366	0.013	0.001	0.001
C	**9**	0.520	0.509	0.507	0.534	0.508	0.506	0.014	-0.001	-0.001
C	**10**	0.132	0.123	0.134	0.135	0.124	0.134	0.004	0.001	0.001
N	**11**	-0.539	-0.542	-0.534	-0.539	-0.554	-0.533	0.000	-0.012	0.000
N		-0.844	-0.844	-0.845	-0.843	-0.846	-0.845	0.001	-0.002	0.001
C		0.313	0.316	0.315	0.312	0.315	0.314	0.000	-0.001	0.000
N		-0.339	-0.344	-0.343	-0.338	-0.338	-0.342	0.001	0.006	0.000
Al		2.134			2.133			-0.001		

Supplementary Table 2 (c): The NBO charges (Q) of the ligands for (5-6) in the optimized ground ($Q_{HF\text{-}S0}$) and first excited (Q_{S1}) states structures and the charge differences between Q_{S1} and Q_{S0} states calculated at the HF/6-31G(D) and CIS/6-31G(D) methods, respectively (Note: for EDG and EWG labels are not shown).

	Derivative 5									
		$Q_{HF\text{-}S0}$			Q_{S1}			$Q_{S1} - Q_{HF\text{-}S0}$		
Atom		**A**	**B**	**C**	**A**	**B**	**C**	**A**	**B**	**C**
O	**1**	-0.925	-0.926	-0.936	-0.883	-0.924	-0.938	0.042	0.002	-0.002
N	**2**	-0.617	-0.624	-0.629	-0.639	-0.634	-0.621	-0.022	-0.010	0.007
C	**3**	0.140	0.136	0.153	0.093	0.139	0.151	-0.047	0.003	-0.002
C	**4**	-0.307	-0.308	-0.306	-0.298	-0.309	-0.306	0.009	-0.001	0.001
C	**5**	0.038	0.035	0.038	0.037	0.038	0.036	-0.001	0.003	-0.002
C	**6**	0.166	0.163	0.163	0.181	0.164	0.163	0.015	0.000	0.000
C	**7**	0.346	0.346	0.344	0.330	0.346	0.344	-0.016	0.001	-0.001
C	**8**	-0.405	-0.405	-0.407	-0.410	-0.405	-0.406	-0.005	0.001	0.000
C	**9**	0.513	0.499	0.500	0.561	0.498	0.500	0.047	-0.001	0.001
C	**10**	0.115	0.105	0.114	0.110	0.107	0.114	-0.006	0.002	0.000
N	**11**	-0.580	-0.576	-0.574	-0.619	-0.576	-0.573	-0.039	0.000	0.001
C		-0.661	-0.662	-0.661	-0.657	-0.662	-0.661	0.004	0.000	0.000
Cl		0.039	0.042	0.039	0.049	0.044	0.038	0.011	0.002	-0.001
Al		2.143			2.138			-0.005		
	Derivative 6									
		$Q_{HF\text{-}S0}$			Q_{S1}			$Q_{S1} - Q_{HF\text{-}S0}$		
Atom		**A**	**B**	**C**	**A**	**B**	**C**	**A**	**B**	**C**
O	**1**	-0.927	-0.928	-0.938	-0.877	-0.926	-0.941	0.049	0.003	-0.003
N	**2**	-0.592	-0.598	-0.605	-0.612	-0.611	-0.597	-0.019	-0.013	0.009
C	**3**	0.119	0.115	0.133	0.068	0.120	0.131	-0.050	0.004	-0.002
C	**4**	-0.229	-0.230	-0.228	-0.224	-0.232	-0.227	0.005	-0.002	0.001
C	**5**	-0.079	-0.080	-0.079	-0.080	-0.075	-0.081	-0.001	0.005	-0.002
C	**6**	0.221	0.217	0.217	0.241	0.218	0.217	0.020	0.000	0.000
C	**7**	0.356	0.355	0.354	0.346	0.356	0.353	-0.010	0.001	-0.001
C	**8**	-0.404	-0.404	-0.405	-0.418	-0.403	-0.404	-0.014	0.002	0.001
C	**9**	0.514	0.499	0.500	0.568	0.497	0.500	0.054	-0.002	0.000
C	**10**	0.107	0.095	0.105	0.104	0.098	0.104	-0.003	0.002	0.000
N	**11**	-0.585	-0.581	-0.579	-0.627	-0.580	-0.578	-0.042	0.000	0.001
C		-0.664	-0.665	-0.664	-0.660	-0.665	-0.664	0.004	0.000	0.000
C		0.321	0.317	0.319	0.315	0.315	0.320	-0.006	-0.002	0.001
N		-0.312	-0.306	-0.310	-0.305	-0.303	-0.311	0.008	0.003	-0.001
Al		2.146			2.140			-0.006		

Supplementary Table 2 (d): The NBO charges (Q) of the ligands for (7-8) in the optimized ground ($Q_{HF\text{-}S0}$) and first excited (Q_{S1}) states structures and the charge differences between Q_{S1} and Q_{S0} states calculated at the HF/6-31G(D) and CIS/6-31G(D) methods, respectively (Note: for EDG and EWG labels are not shown).

		Derivative 7								
		$Q_{HF\text{-}S0}$			Q_{S1}			$Q_{S1} - Q_{HF\text{-}S0}$		
Atom		**A**	**B**	**C**	**A**	**B**	**C**	**A**	**B**	**C**
O	**1**	-0.923	-0.925	-0.933	-0.901	-0.922	-0.933	0.021	0.003	0.000
N	**2**	-0.609	-0.617	-0.621	-0.624	-0.620	-0.613	-0.015	-0.003	0.007
C	**3**	0.115	0.111	0.129	0.071	0.113	0.127	-0.044	0.001	-0.002
C	**4**	-0.293	-0.295	-0.293	-0.280	-0.295	-0.293	0.013	0.000	0.001
C	**5**	0.020	0.018	0.021	0.003	0.019	0.020	-0.017	0.001	-0.001
C	**6**	0.188	0.186	0.185	0.210	0.186	0.185	0.022	0.000	0.000
C	**7**	0.564	0.564	0.562	0.557	0.563	0.561	-0.007	0.000	-0.001
C	**8**	-0.449	-0.448	-0.449	-0.462	-0.449	-0.450	-0.013	-0.001	-0.001
C	**9**	0.524	0.510	0.512	0.551	0.512	0.514	0.027	0.002	0.002
C	**10**	0.104	0.093	0.101	0.098	0.094	0.100	-0.007	0.001	-0.001
N	**11**	-0.649	-0.646	-0.643	-0.670	-0.646	-0.643	-0.021	0.000	0.000
N		-0.875	-0.874	-0.876	-0.867	-0.875	-0.877	0.008	0.000	0.000
Cl		0.030	0.033	0.031	0.038	0.033	0.029	0.009	0.000	-0.002
Al		2.143			2.141			-0.002		
		Derivative 8								
		Q_{S0}			Q_{S1}			$Q_{S1} - Q_{HF\text{-}S0}$		
Atom		**A**	**B**	**C**	**A**	**B**	**C**	**A**	**B**	**C**
O	**1**	-0.924	-0.927	-0.935	-0.898	-0.924	-0.935	0.026	0.003	0.000
N	**2**	-0.584	-0.591	-0.596	-0.596	-0.596	-0.588	-0.012	-0.005	0.008
C	**3**	0.087	0.084	0.102	0.045	0.086	0.100	-0.042	0.002	-0.002
C	**4**	-0.214	-0.215	-0.214	-0.204	-0.216	-0.213	0.009	-0.001	0.001
C	**5**	-0.107	-0.107	-0.104	-0.121	-0.105	-0.106	-0.014	0.002	-0.002
C	**6**	0.246	0.243	0.243	0.270	0.244	0.242	0.024	0.000	0.000
C	**7**	0.573	0.572	0.571	0.569	0.572	0.571	-0.004	0.000	0.000
C	**8**	-0.449	-0.448	-0.448	-0.468	-0.448	-0.449	-0.020	0.000	-0.001
C	**9**	0.524	0.510	0.511	0.557	0.510	0.513	0.033	0.000	0.002
C	**10**	0.100	0.087	0.095	0.092	0.088	0.094	-0.008	0.002	-0.001
N	**11**	-0.655	-0.652	-0.649	-0.674	-0.652	-0.650	-0.019	0.000	0.000
N		-0.869	-0.868	-0.870	-0.860	-0.868	-0.871	0.009	0.000	0.000
C		0.326	0.322	0.325	0.321	0.322	0.325	-0.005	0.000	0.001
N		-0.325	-0.318	-0.322	-0.321	-0.318	-0.323	0.004	0.001	-0.002
Al		2.146			2.143			-0.003		



Supplementary Figure 4: Frontier molecular orbitals (FMOs) for the excited state (S_1) of disubstituted derivatives of AlND3 (1-8) computed at CIS/6-31G(D) method.