Electronic Supplementary Information

Xanthene-anchored salen-based open- and closed-dinuclear indium complexes: synthesis and photophysical properties

Yoseph Kim,[1,2†] Ji Hye Lee,[3†] Hyeongkwon Moon,[2] Himchan Mo,[4] Hyonseok Hwang,[3] Junseong Lee,[4] Jun Hui Park,[2] Youngjo Kim,[2,*] and Myung Hwan Park,[1,*]

[1] Department of Chemistry Education, Chungbuk National University, Chungbuk 28644, Republic of Korea

[2] Department of Chemistry, Chungbuk National University, Chungbuk 28644, Republic of Korea

[3] Department of Chemistry, Institute for Molecular Science and Fusion Technology, Kangwon National University, Gangwon 24341, Republic of Korea

[4] Department of Chemistry, Chonnam National University, Gwangju 61186, Republic of Korea

[†]Y. Kim and J. H. Lee contributed equally to this work.

Contents

^{1}H and ^{13}C NMR Spectra

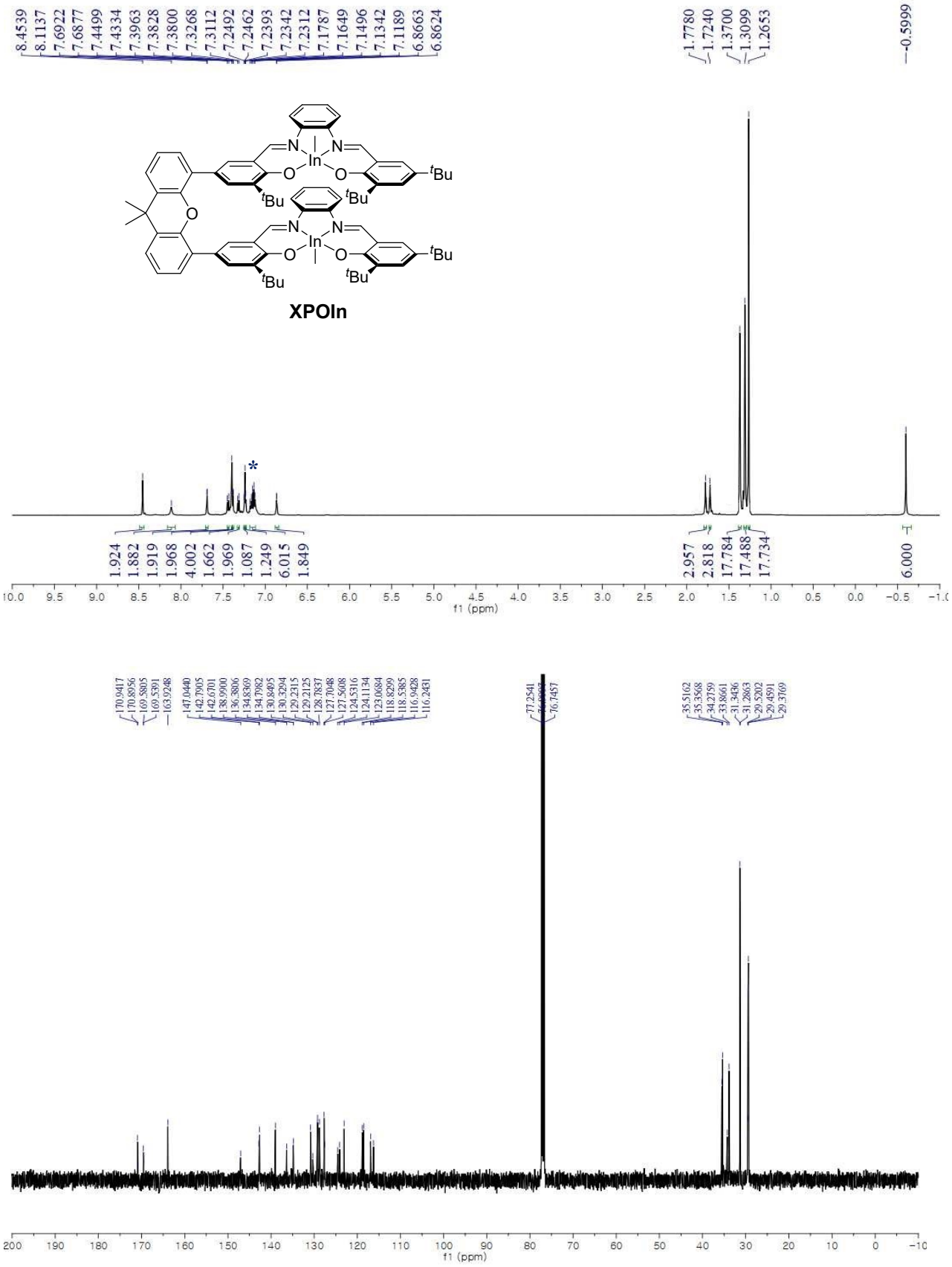

Fig. S1 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **XPOIn** (*from residual $CHCl_3$ in $CDCl_3$).

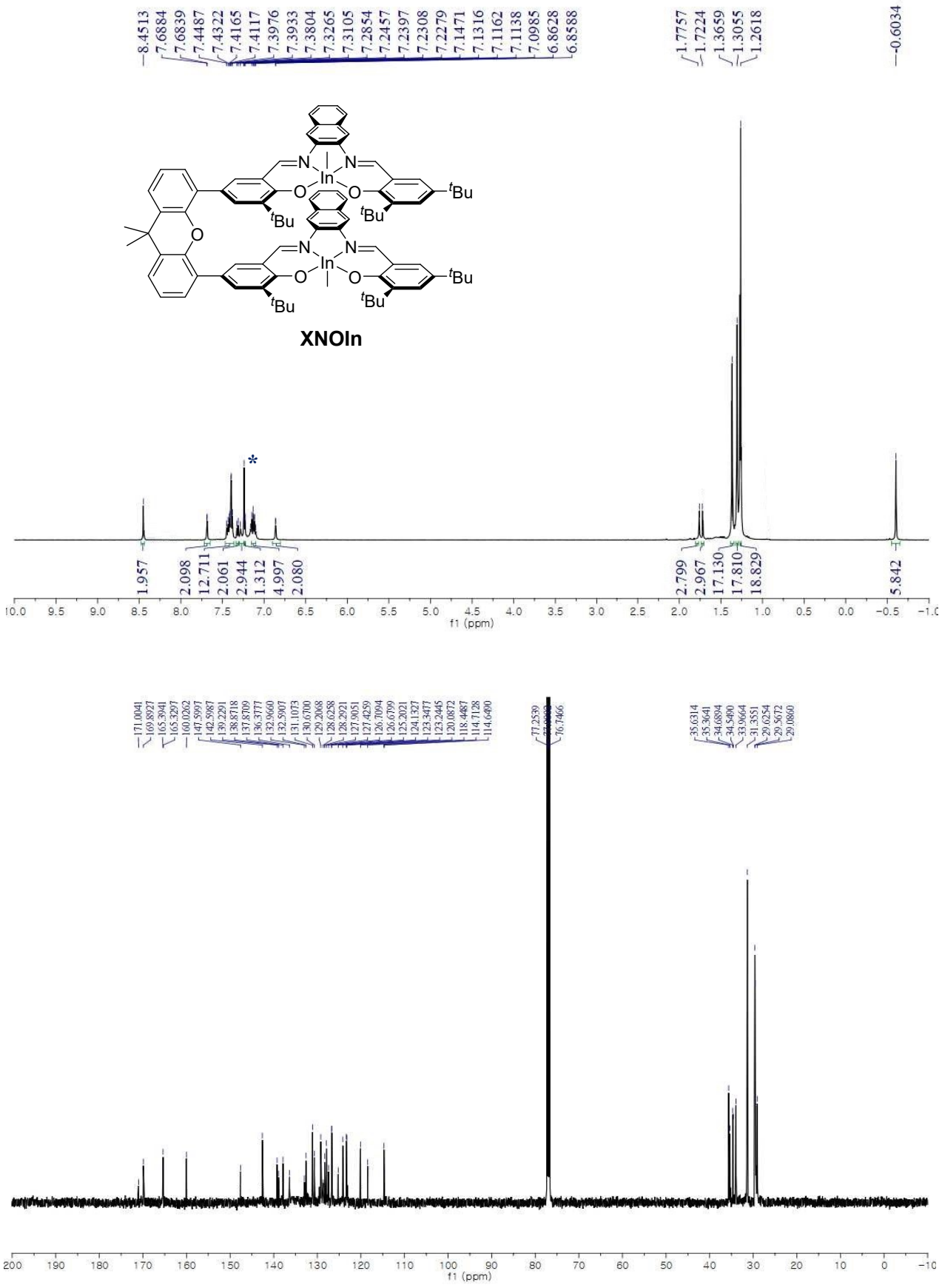

Fig. S2 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **XNOIn** (*from residual $CHCl_3$ in $CDCl_3$).

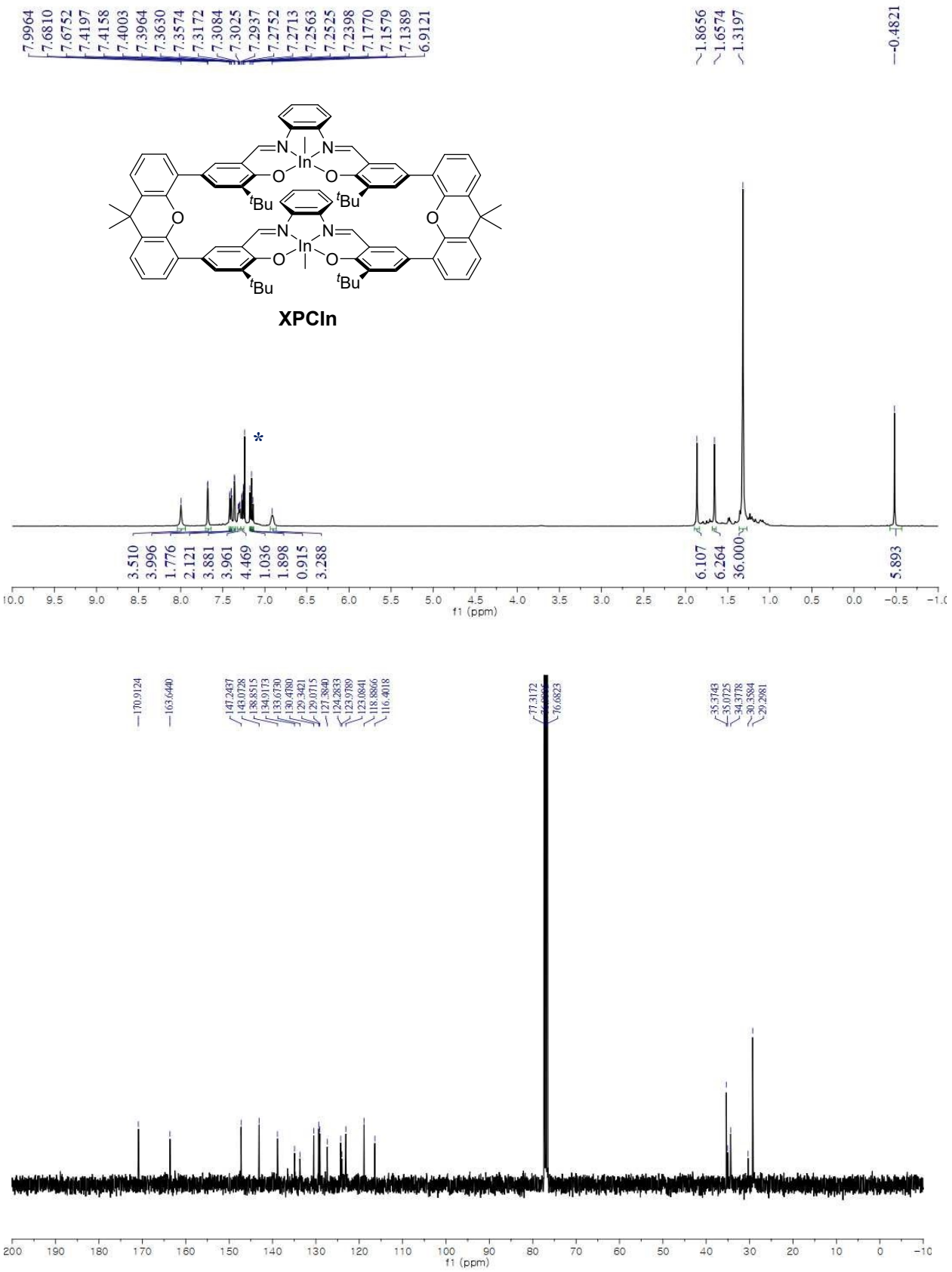

Fig. S3. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **XPCIn** (*from residual $CHCl_3$ in $CDCl_3$).

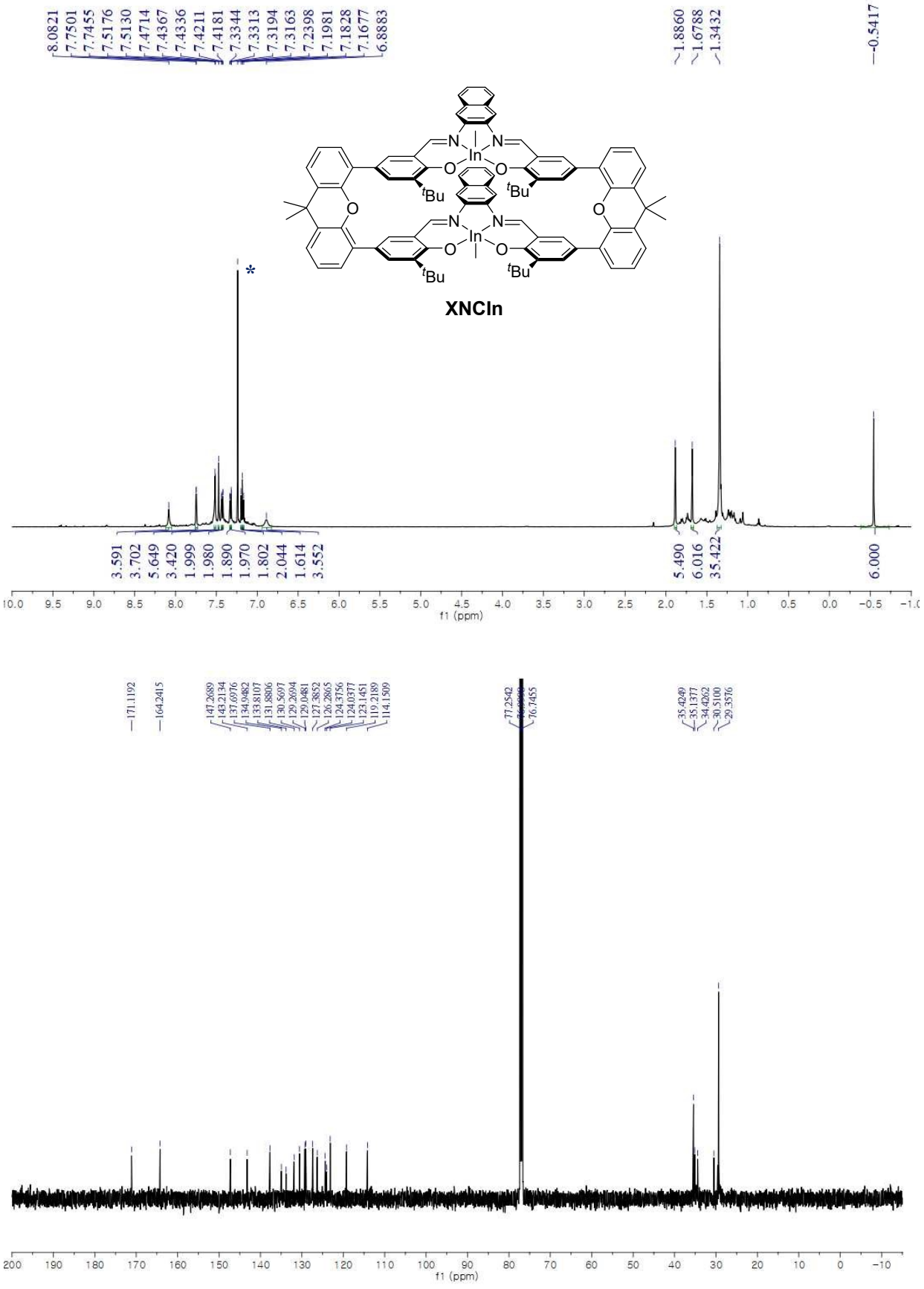

Fig. S4 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **XNCIn** (*from residual $CHCl_3$ in $CDCl_3$).

Table S1. Crystallographic data and parameters for **XNOIn**

Compound	**XNOIn2**·3.083($CHCl_3$)
Formula	$C_{92.09}H_{99.09}Cl_{9.25}In_2N_4O_5$
Formula weight	1899.41
Crystal system	Triclinic
Space group	P_{-1}
a (Å)	15.4731(4)
b (Å)	17.4895(4)
c (Å)	19.7349(5)
α (°)	110.1661(12)
β (°)	111.6006(12)
γ (°)	92.7788(12)
V (Å^3)	4566.0(2)
Z	2
ρ_{calc}(g cm^{-3})	1.382
μ (mm^{-1})	0.828
F(000)	1950
T (K)	100
Scan mode	*multi-scan*
hkl range	$-16 \le h \le 18$, $-20 \le k \le 21$, $-24 \le l \le 24$
Measurement reflns	17413
Unique reflns [R_{sigma}]	14062 [0.0594]
Reflns used for refinement	17413
Refined parameters	1202
R_1[a] (I > 2σ(I))	0.0438
wR_2[b] all data	0.1170
GOF on F^2	1.049
ρ_{fin} (max/min) (e Å^{-3})	1.609, −0.617

[a] $R_1 = \sum||Fo| - |Fc||/\sum|Fo|$. [b] $wR_2 = \{[\sum w(Fo^2 - Fc^2)^2]/[\sum w(Fo^2)^2]\}^{1/2}$.

Table S2. Selected bond lengths (Å) and angles (°) for **XNOIn**

Compound	**XNOIn**
	lengths
In–O1	2.083(15)
In–O2	2.090(15)
In–N1	2.23(2)
In–N2	2.24(2)
In–C65	2.14(3)
	Angles
O1–In–O2	85.0(6)
O1–In–N1	82.1(8)
O1–In–N2	130.9(8)
O1–In–C65	111.5(10)
O2–In–N1	131.3(8)
O2–In–N2	80.8(7)
O2–In–C65	110.1(12)
N1–In–N2	73.2(6)
C65–In–N1	118.4(12)
C65–In–N2	117.5(11)

Table S3. Crystallographic data and parameters for **XNCIn**

Compound	**XNCIn2**·2(C_6H_{14})
Formula	$C_{108}H_{118}In_2N_4O_6$
Formula weight	1797.70
Crystal system	Triclinic
Space group	P_{-1}
a (Å)	15.0203(6)
b (Å)	15.3837(7)
c (Å)	20.1621(9)
α (°)	88.505(2)
β (°)	86.216(2)
γ (°)	75.336(2)
V (Å^3)	4497.0(3)
Z	2
ρ_{calc}(g cm^{-3})	1.328
μ (mm^{-1})	0.571
F(000)	1880
T (K)	100
Scan mode	*multi-scan*
hkl range	$-18 \le h \le 18$, $-18 \le k \le 18$, $-24 \le l \le 24$
Measurement reflns	17040
Unique reflns [R_{sigma}]	10941 [0.1161]
Reflns used for refinement	17040
Refined parameters	1103
R_1[a] (I > 2σ(I))	0.0653
wR_2[b] all data	0.1899
GOF on F^2	1.029
ρ_{fin} (max/min) (e Å^{-3})	1.749, −1.082

[a] $R_1 = \sum||Fo| - |Fc||/\sum|Fo|$. [b] $wR_2 = \{[\sum w(Fo^2 - Fc^2)^2]/[\sum w(Fo^2)^2]\}^{1/2}$.

Table S4. Selected bond lengths (Å) and angles (°) for **XNCIn**

Compound	**XNCIn**
	lengths
In–O1	2.087(4)
In–O2	2.087(4)
In–N1	2.267(5)
In–N2	2.228(5)
In–C33	2.135(6)
	Angles
O1–In–O2	92.72(16)
O1–In–N1	80.02(16)
O1–In–N2	129.02(17)
O1–In–C33	108.6(2)
O2–In–N1	141.98(17)
O2–In–N2	83.61(16)
O2–In–C33	108.6(2)
N1–In–N2	73.06(17)
C33–In–N1	108.3(2)
C33–In–N2	115.1(3)

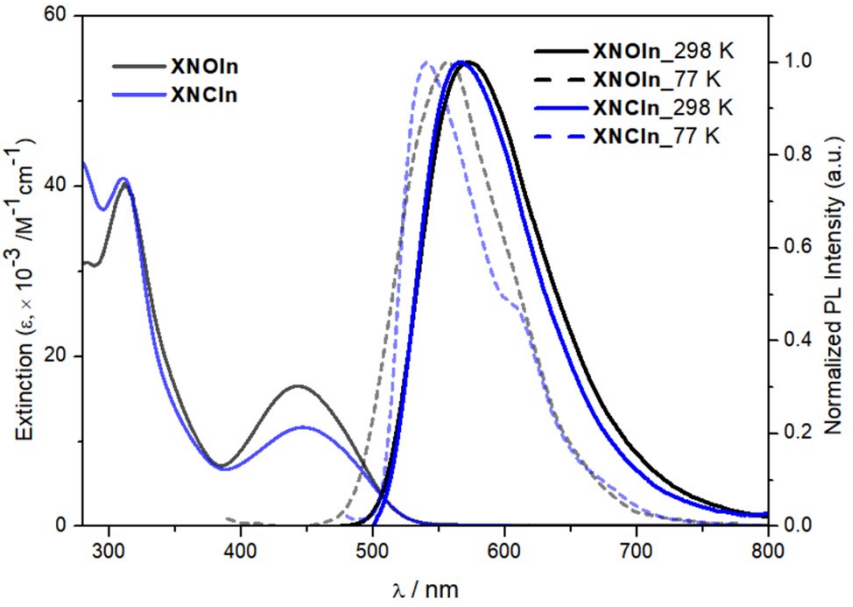

Fig. S5 UV–vis absorption (left, solid line) and PL spectra (right, solid and dash lines) of **XNOIn** and **XNCIn** in THF (20 μM).

Table S5. Photophysical data of **XNOIn** and **XNCIn**

Compd	λ_{abs}[a]/nm ($\varepsilon \times 10^{-3}$ M^{-1} cm^{-1})	λ_{ex}[a]/nm	λ_{em}/nm			Φ_{PL}[b]/%		
			298 K[a]	77 K[a]	solid	298 K[a]	77 K[a]	solid
XNOIn	312 (40.28) 444 (16.50)	443	573	557	577	4.7	25.5	24.8
XNCIn	311 (40.92) 447 (11.65)	453	567	542 607	577	3.3	15.6	16.0

[a]In deoxygenated THF (20 μM). [b]Absolute photoluminescence quantum yield (PLQY).

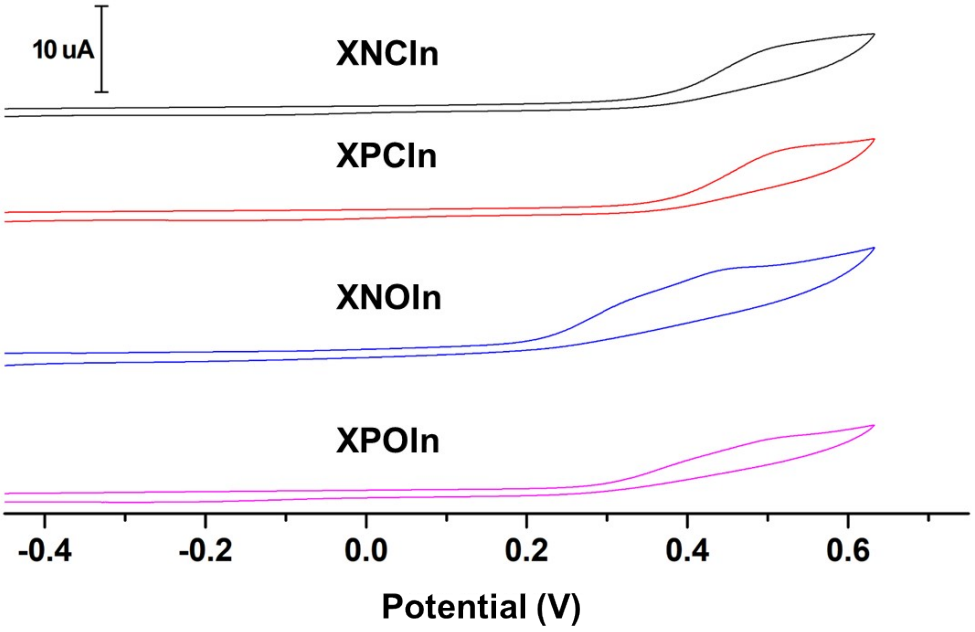

Fig. S6 Cyclic voltammograms (CV) for **XPOIn**, **XNOIn**, **XPCIn**, and **XNCIn** showing oxidation (1 mM in THF, scan rate = 100 mV/s).

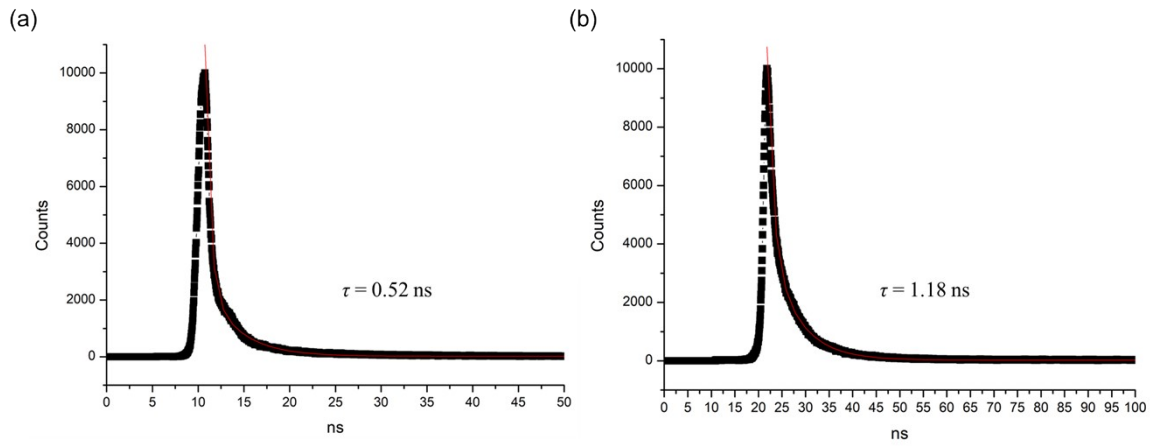

Fig. S7 Emission decay curves of **XPOIn** (a) in toluene (20 μM) solutions at 298 K (R^2 = 0.99506), (b) a PMMA film doped with 5 wt% compound (R^2 = 0.99841). Each red-line is its single exponential fitting curve.

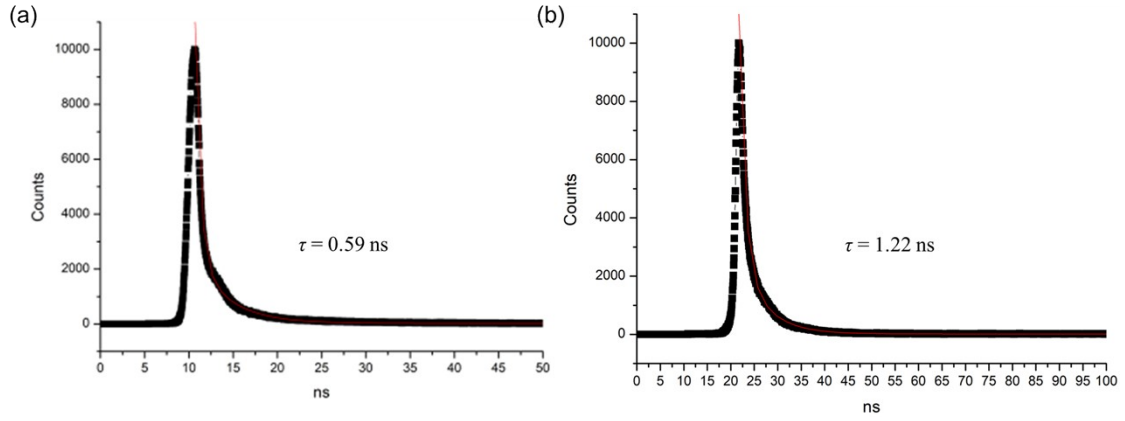

Fig. S8 Emission decay curves of **XNOIn** (a) in toluene (20 μM) solutions at 298 K (R^2 = 0.99352), (b) a PMMA film doped with 5 wt% compound (R^2 = 0.99663). Each red-line is its single exponential fitting curve.

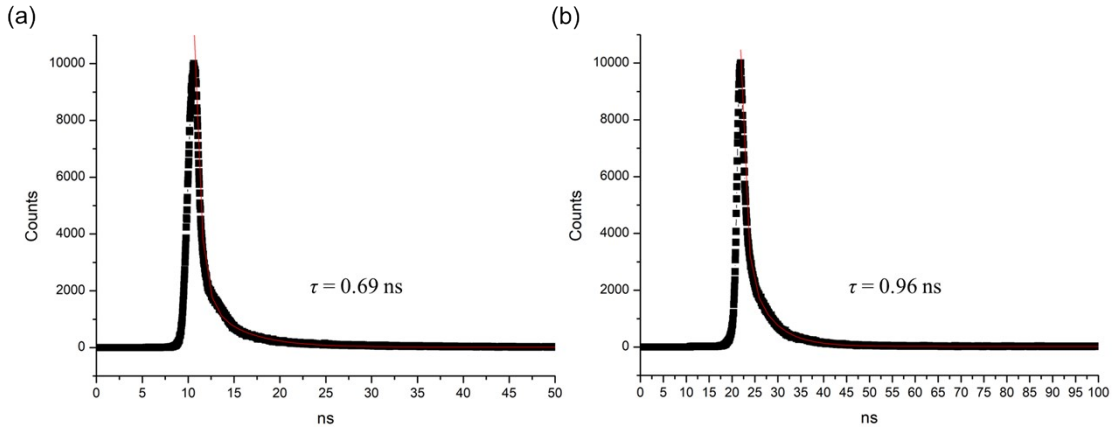

Fig. S9 Emission decay curves of **XPCIn** (a) in toluene (20 μM) solutions at 298 K (R^2 = 0.99023), (b) a PMMA film doped with 5 wt% compound (R^2 = 0.99864). Each red-line is its single exponential fitting curve.

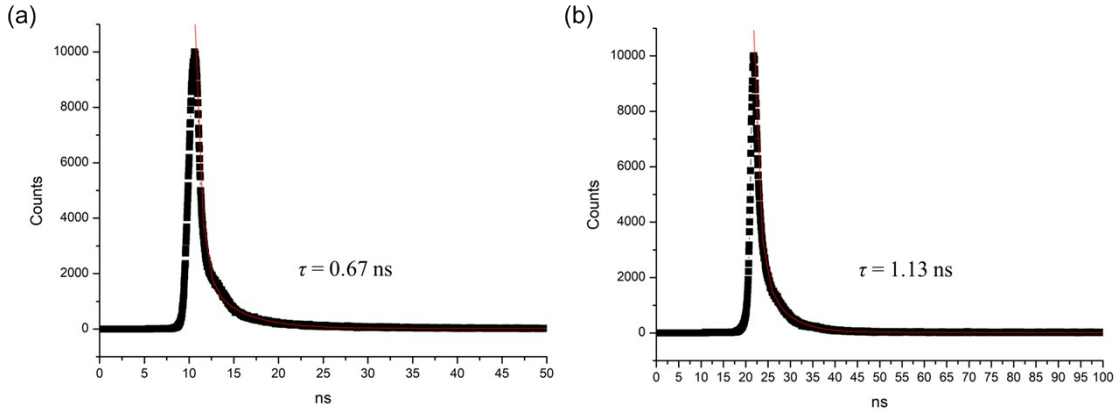

Fig. S10 Emission decay curves of **XNCIn** (a) in toluene (20 μM) solutions at 298 K (R^2 = 0.99069), (b) a PMMA film doped with 5 wt% compound (R^2 = 0.9978). Each red-line is its single exponential fitting curve.

Table S6. Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **XPOIn** from TD-B3LYP calculations using the B3LYP geometries at the ground state (S_0) optimized geometries in gas

state	λ_{calc} (nm)	f_{calc}	major contribution
1	488.45	0.0406	HOMO → LUMO (85.9%)
2	470.40	0.0595	HOMO−1 → LUMO (50.5%)
3	457.99	0.1173	HOMO → LUMO+2 (90.6%)
4	452.72	0.0062	HOMO → LUMO+1 (61.9%)
			HOMO−2 → LUMO (28.0%)
5	446.59	0.0096	HOMO−1 → LUMO (27.8%)
			HOMO → LUMO+1 (24.3%)

Table S7. Molecular orbital energies (in eV) and molecular orbital distributions (in %) of **XPOIn** at the ground state (S_0) optimized geometries in gas

	E (eV)	In–Me	imine	Phenoxy	Xanthene	In–Me	imine	Phenoxy
		I				II		
LUMO+3	−1.68	0.1	0.0	0.2	0.2	0.5	38.3	60.7
LUMO+2	−1.85	0.0	0.0	0.2	0.2	0.2	31.4	67.8
LUMO+1	−1.96	0.8	40.6	58.0	0.2	0.0	0.3	0.1
LUMO	−2.14	0.2	30.9	68.3	0.3	0.0	0.2	0.1
HOMO	−5.07	0.2	0.8	5.8	19.1	3.1	10.4	60.5
HOMO−1	−5.22	1.1	3.8	19.9	8.9	1.5	8.9	55.9
HOMO−2	−5.30	2.8	8.7	39.7	8.7	0.1	3.0	36.9
HOMO−3	−5.47	1.3	9.0	81.2	6.0	0.0	0.3	2.1

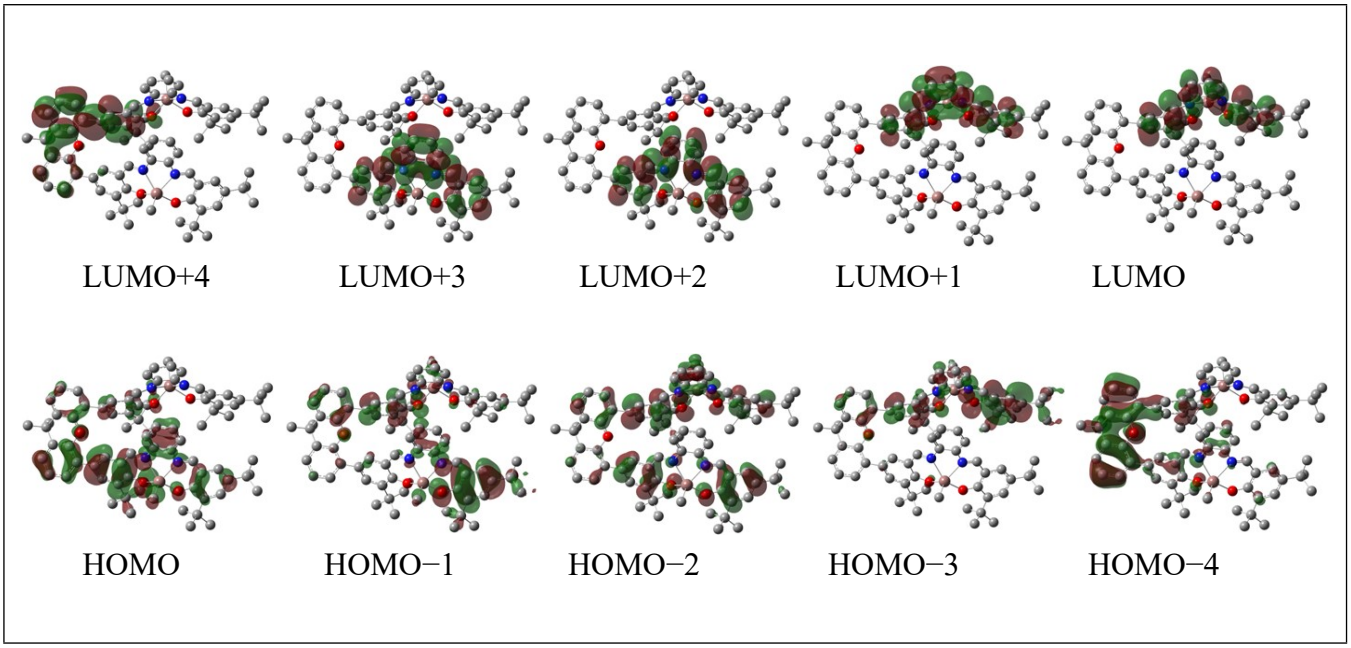

Fig. S11 The selected frontier orbitals of **XPOIn** from TD-B3LYP calculations (Isovalue = 0.04 a.u.) at the ground state (S_0) in gas.

Table S8. Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **XNOIn** from TD-B3LYP calculations using the B3LYP geometries at the ground state (S_0) optimized geometries in gas

state	λ_{calc} (nm)	f_{calc}	major contribution
1	480.03	0.0398	HOMO → LUMO (88.2%)
2	464.74	0.0335	HOMO → LUMO+1 (54.7%)
3	461.26	0.0793	HOMO−2 → LUMO (54.4%)
4	453.68	0.0393	HOMO → LUMO+2 (33.8%)
5	448.69	0.0186	HOMO−1 → LUMO (54.0%)

Table S9. Molecular orbital energies (in eV) and molecular orbital distributions (in %) of **XNOIn** at the ground state (S_0) optimized geometries in gas

	E (eV)	In–Me	imine	Phenoxy	Xanthene	In–Me	imine	Phenoxy
		I				II		
LUMO+3	−1.82	0.0	0.3	0.6	0.2	0.2	32.3	66.4
LUMO+2	−1.98	0.1	19.3	40.0	0.2	0.2	20.0	20.1
LUMO+1	−2.00	0.1	13.2	26.6	0.2	0.2	31.8	27.9
LUMO	−2.17	0.4	50.4	48.5	0.2	0.0	0.2	0.2
HOMO	−5.11	0.4	1.5	9.5	21.9	2.6	8.9	55.3
HOMO−1	−5.24	0.3	1.3	8.6	4.2	2.1	13.5	69.9
HOMO−2	−5.30	2.7	9.2	46.2	12.1	0.2	4.8	24.9
HOMO−3	−5.42	1.9	15.1	79.6	2.1	0.0	0.2	1.1

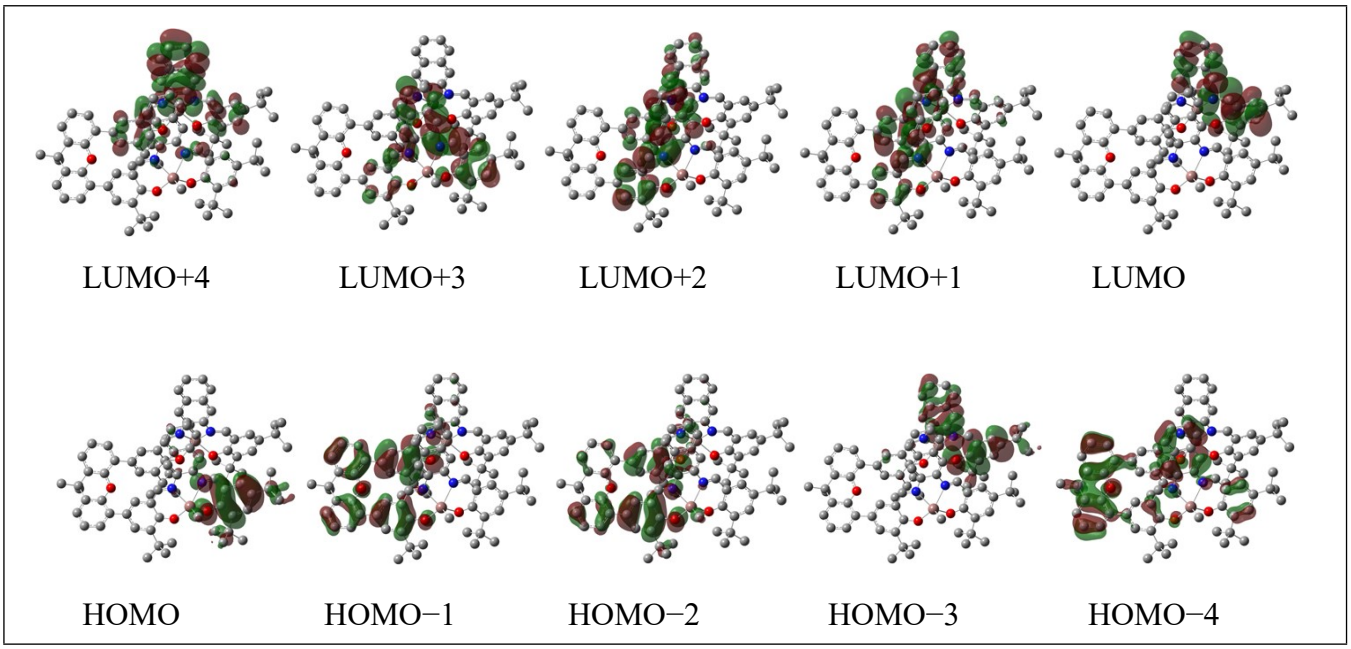

Fig. S12 The selected frontier orbitals of **XNOIn** from TD-B3LYP calculations (Isovalue = 0.04 a.u.) at the ground state (S_0) optimized geometries in gas.

Table S10. Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **XPCIn** from TD-B3LYP calculations using the B3LYP geometries at the ground state (S_0) optimized geometries in gas

state	λ_{calc} (nm)	f_{calc}	major contribution
1	486.38	0.0730	HOMO → LUMO (89.7%)
2	477.73	0.0353	HOMO → LUMO+1 (82.6%)
3	467.65	0.0486	HOMO−1 → LUMO (67.1%)
4	462.36	0.0784	HOMO−2 → LUMO (67.7%)
5	451.37	0.0028	HOMO → LUMO+2 (56.3%)

Table S11. Molecular orbital energies (in eV) and molecular orbital distributions (in %) of **XPCIn** at the ground state (S_0) optimized geometries in gas

	E (eV)	In–Me	imine	Phenoxy	Xanthene	In–Me	imine	Phenoxy	Xanthene
		I				II			
LUMO+3	−1.76	0.1	0.1	0.3	0.2	0.8	40.7	57.7	0.2
LUMO+2	−1.93	0.6	39.0	58.8	0.2	0.0	0.5	0.7	0.2
LUMO+1	−1.94	0.1	1.4	3.1	0.3	0.1	30.0	64.7	0.3
LUMO	−2.09	0.2	30.4	65.0	0.3	0.0	1.3	2.5	0.3
HOMO	−5.04	0.3	0.9	5.1	17.7	3.4	9.7	57.2	5.7
HOMO−1	−5.14	0.1	0.9	9.8	9.9	0.3	3.9	56.1	18.9
HOMO−2	−5.26	3.7	12.3	55.4	6.7	0.8	3.6	9.2	8.3
HOMO−3	−5.40	0.3	4.8	59.7	10.0	0.0	1.3	15.8	8.1

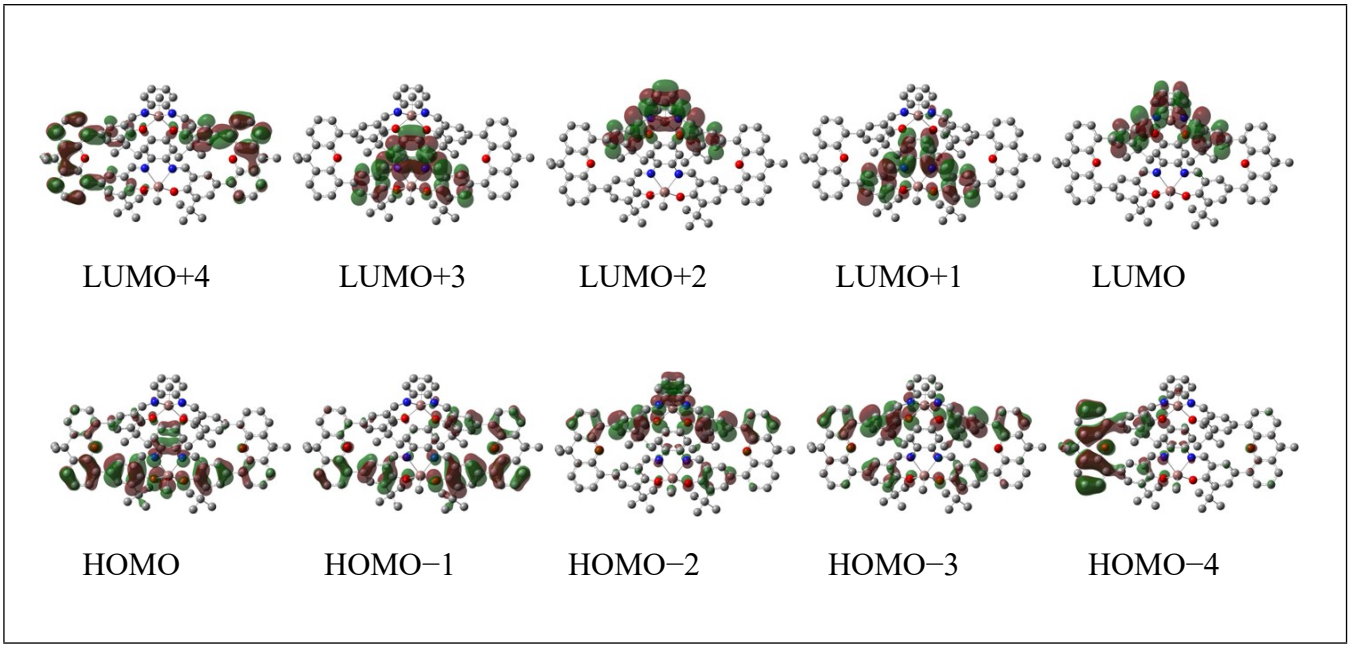

Fig. S13 The selected frontier orbitals of **XPCIn** from TD-B3LYP calculations (Isovalue = 0.04 a.u.) at the ground state (S_0) optimized geometries in gas.

Table S12. Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **XNCIn** from TD-B3LYP calculations using the B3LYP geometries at the ground state (S_0) optimized geometries in gas

state	λ_{calc} (nm)	f_{calc}	major contribution
1	487.84	0.0361	HOMO → LUMO (92.0%)
2	483.31	0.0381	HOMO−1 → LUMO (36.1%) LUMO+1 (40.1%)
3	480.94	0.0529	HOMO → LUMO (42.2%) LUMO+1 (45.5%)
4	475.89	0.0178	HOMO−1 → LUMO+1 (72.0%)
5	460.63	0.0470	HOMO → LUMO+2 (60.2%)

Table S13. Molecular orbital energies (in eV) and molecular orbital distributions (in %) of **XNCIn** at the ground state (S_0) optimized geometries in gas

	E (eV)	In–Me	imine	Phenoxy	Xanthene	In–Me	imine	Phenoxy	Xanthene
		I				II			
LUMO+3	−1.87	0.0	3.0	6.1	0.2	0.1	29.7	60.5	0.3
LUMO+2	−1.99	0.1	29.6	60.5	0.3	0.0	3.1	6.1	0.3
LUMO+1	−2.06	0.1	1.3	1.2	0.2	0.5	51.6	44.9	0.1
LUMO	−2.16	0.4	48.9	47.7	0.2	0.0	1.4	1.3	0.2
HOMO	−5.07	0.3	1.1	6.5	22.3	2.9	8.6	54.7	3.6
HOMO−1	−5.12	0.2	1.4	11.5	5.6	0.6	6.2	53.0	21.5
HOMO−2	−5.28	3.5	11.1	53.2	5.4	1.0	3.9	12.6	9.4
HOMO−3	−5.35	0.4	9.2	56.6	10.1	0.1	3.1	14.5	6.1

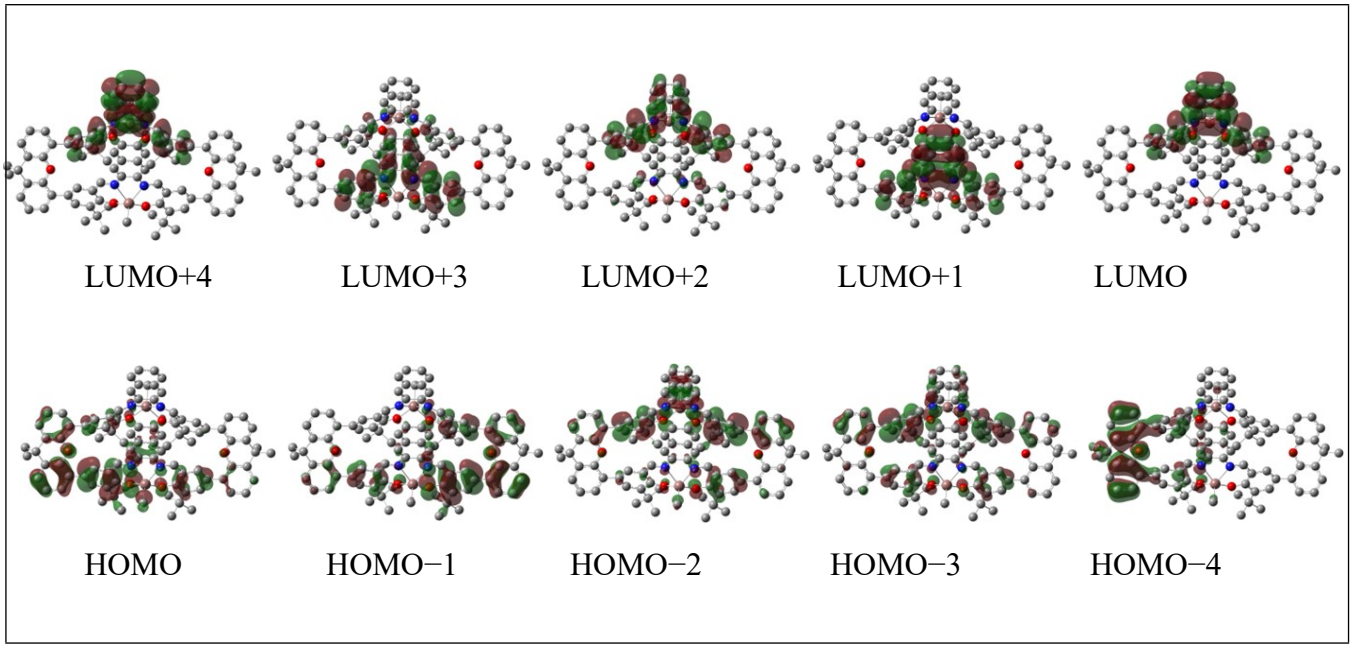

Fig. S14 The selected frontier orbitals of **XNCIn** from TD-B3LYP calculations (Isovalue = 0.04 a.u.) at the ground state (S_0) optimized geometries in gas.

Table S14. Cartesian coordinates of the ground state (S_0) fully optimized geometry of **XPOIn** in gas from B3LYP calculations (in Å)

Atom	X	Y	Z
In	-0.003258	3.173100	2.031209
In	-1.185258	-3.926145	-0.842339
C	0.566553	-1.023208	3.259449
H	1.631230	-1.216049	3.340976
O	1.449962	3.526271	0.638513
O	-1.369374	4.313968	1.011903
N	0.952205	1.103172	2.017836
O	-2.695267	-2.633085	-1.339998
N	0.086096	-4.376877	0.984450
O	6.421350	-0.492057	-0.655102
O	0.244559	-2.481432	-1.144564
N	-1.641577	1.632852	1.952294
C	8.191843	-2.136373	-0.583422
C	-2.615014	4.201145	0.647071
C	3.624057	3.826724	-0.267805
C	3.497593	-3.217894	0.404670
H	3.894752	-3.816811	1.220908
C	3.052447	1.751957	0.943496
C	-6.210477	-1.840367	-1.674283
H	-6.865060	-1.281047	-2.331478
C	-0.344058	-1.908086	3.832815
C	5.336939	2.076282	0.153340
C	4.362427	-2.531492	-0.426586
C	0.119657	0.133745	2.607586
C	-1.972327	-5.226325	1.875032
C	-2.581146	6.686913	-0.098493
C	-0.552644	-5.201468	1.931564
C	4.378738	1.287449	0.760763
H	4.641373	0.305378	1.140907
C	-2.173220	-0.477568	3.156637
H	-3.233038	-0.244756	3.165540
C	1.335221	-4.018810	1.101369
H	1.895473	-4.359889	1.977248
C	-4.285726	-1.044298	-3.158361
N	-2.568724	-4.421401	0.883088
C	-5.970897	-3.226241	0.240290
H	-6.359000	-3.770142	1.095914
C	7.605934	-4.447034	-0.129064
H	7.907318	-5.477763	0.031523
C	-1.271993	0.414208	2.559454
C	3.776358	-1.720872	-1.435419
H	4.452423	-1.151545	-2.058265
C	1.525517	-2.458281	-0.891086
C	-2.004328	-6.840086	3.692022
C	-5.387834	-0.294707	-3.934765
H	-6.133099	-0.975115	-4.361504
H	-4.930577	0.250823	-4.766240
H	-5.908604	0.440096	-3.310684
C	-3.297149	5.328799	0.062134
C	0.109179	-6.009755	2.868773
H	1.193322	-6.037163	2.891892
C	-4.569534	-3.294888	0.006890
C	1.858737	-0.737486	-2.806294
C	-1.713820	-1.636992	3.777875
C	-4.611833	5.155683	-0.340685
H	-5.120960	6.004993	-0.779328
C	8.700037	0.273345	-0.378220
C	6.785784	1.745118	0.103237
C	-1.350133	6.530937	-1.023212
H	-0.638777	5.812682	-0.617899
H	-0.843328	7.496461	-1.138000
H	-1.655392	6.192030	-2.019581
C	-3.349782	2.973659	0.797307
C	-5.351212	3.948985	-0.225623
C	4.912352	3.324530	-0.369259
H	5.658653	3.908999	-0.893137
C	9.075969	2.527019	0.439749
H	9.759614	3.313289	0.745379
C	-3.827345	-4.072699	0.947364
H	-4.407022	-4.399046	1.816091
C	-2.677212	-6.063433	2.753673
H	-3.757411	-6.133879	2.684243
C	5.825737	-2.787418	-0.358717
C	-7.652146	4.953386	0.030185

H	-7.274429	5.968429	-0.125131	H	-3.478635	0.920857	1.356781	C	-8.818187	-1.025577	-0.238313
H	-7.650788	4.758678	1.107776	C	-4.695157	2.879970	0.342010	H	-8.361756	-0.567979	0.645583
H	-8.690973	4.930233	-0.318823	H	-5.197081	1.925935	0.470257	H	-9.906758	-0.987137	-0.116725
C	7.318336	0.504523	-0.300114	C	-3.497062	7.757559	-0.726576	H	-8.561066	-0.407650	-1.103341
C	8.566102	-3.463979	-0.354198	H	-3.827857	7.481106	-1.733697	C	-8.345378	-2.487749	-0.410929
H	9.613728	-3.740537	-0.370965	H	-2.941570	8.696963	-0.812754	C	4.424250	5.818870	-1.662222
C	1.175968	-1.602873	-3.893746	H	-4.383524	7.957233	-0.114399	H	5.255647	6.060313	-0.990713
H	0.327115	-2.154051	-3.489183	C	7.703131	2.745039	0.468663	H	4.091052	6.756687	-2.118258
H	1.885106	-2.319941	-4.322549	H	7.315059	3.699781	0.809076	H	4.805278	5.180906	-2.466907
H	0.813897	-0.962371	-4.706179	C	2.411690	-1.638212	-1.680323	C	-3.266374	0.011549	-2.665109
C	-0.608355	-6.812420	3.750549	C	3.238042	5.172829	-0.916637	H	-2.859504	0.565433	-3.518912
C	6.257566	-4.111109	-0.162337	C	2.657018	3.053354	0.464826	H	-2.437997	-0.455380	-2.132820
H	5.507249	-4.888642	-0.062311	C	9.181910	-1.043322	-0.988753	H	-3.747274	0.736238	-1.998460
C	2.150399	0.834337	1.581200	C	-6.818180	-2.529700	-0.590756	C	-3.602127	-2.013039	-4.154743
H	2.525297	-0.190013	1.671664	C	9.569181	1.296806	0.014215	H	-4.318438	-2.751739	-4.531714
C	0.842127	0.274325	-2.222959	H	10.640684	1.138745	-0.021348	H	-2.772179	-2.542802	-3.687853
H	0.429403	0.892239	-3.028563	C	2.974137	0.076774	-3.493954	H	-3.213824	-1.453026	-5.013110
H	1.328761	0.944174	-1.506705	H	3.703306	-0.563557	-4.002624	C	-6.805450	3.898923	-0.722378
H	0.017180	-0.233621	-1.723199	H	3.510615	0.719351	-2.788178	C	2.113004	4.939610	-1.954488
C	-7.446104	2.519061	-0.489050	H	2.524949	0.724139	-4.253947	H	2.460691	4.277843	-2.755708
H	-8.476954	2.520402	-0.858144	C	2.097049	-3.217047	0.192548	H	1.817734	5.892080	-2.409703
H	-7.477321	2.260377	0.574789	C	-2.137384	7.218345	1.286902	H	1.233645	4.490528	-1.493001
H	-6.906576	1.725401	-1.016192	H	-3.004391	7.369314	1.939921	C	0.337647	3.990991	3.981758
C	6.827330	-1.809239	-0.532574	H	-1.631189	8.183991	1.172698	H	1.325022	3.715695	4.364936
C	-3.978997	-2.601350	-1.105625	H	-1.452474	6.526488	1.776904	H	-0.410373	3.633665	4.696865
C	-2.814271	1.789936	1.391977	C	-4.851783	-1.831886	-1.957072	H	0.278881	5.083416	3.959173
C	2.770529	6.181502	0.160703	H	1.889990	5.819315	0.689728	H	2.521652	7.140475	-0.308354

H	3.566164	6.362813	0.892326	H	11.316175	-0.604686	-0.907813	H	9.813023	-0.107313	-2.868050
C	-6.846013	4.199510	-2.239854	H	10.955608	-2.309895	-1.050065	C	-9.026336	-3.098927	-1.659306
H	-6.432029	5.185699	-2.471064	H	10.723077	-1.493327	0.508758	H	-8.768107	-2.553258	-2.571944
H	-7.878250	4.178420	-2.608279	C	-8.803943	-3.286660	0.823731	H	-10.116946	-3.071243	-1.553479
H	-6.268489	3.456916	-2.800286	H	-8.533351	-4.345140	0.747544	H	-8.723995	-4.142122	-1.798075
C	-1.033376	-5.581856	-2.195373	H	-9.893397	-3.231728	0.916578	H	0.014007	-2.797340	4.342215
H	-1.203034	-5.255987	-3.226052	H	-8.374292	-2.887986	1.749110	H	-2.421746	-2.313790	4.246235
H	-1.773420	-6.354614	-1.964395	C	9.137311	-0.903949	-2.539167	H	-0.078020	-7.436630	4.463040
H	-0.041904	-6.043153	-2.150517	H	8.129487	-0.658646	-2.884645	H	-2.567065	-7.486874	4.358017
C	10.624566	-1.382694	-0.575387	H	9.442638	-1.841896	-3.015210				

Table S15. Cartesian coordinates of the ground state (S_0) fully optimized geometry of **XNOIn** in gas from TD B3LYP calculations (in Å)

Atom	X	Y	Z	C	-3.838407	-4.118846	0.193369	C	2.416027	0.213760	2.606239
In	-0.040509	-3.369518	2.139291	C	-3.542464	3.059696	-0.277214	H	3.457673	-0.092306	2.601999
In	1.118811	3.429068	-1.839165	H	-3.899694	3.810648	0.423343	C	-1.363666	4.005091	0.101792
C	-0.281654	0.971041	2.760991	C	-3.075193	-1.925866	1.037047	H	-1.877485	4.536320	0.909803
H	-1.324522	1.253646	2.867838	C	6.019946	0.856388	-1.835579	C	4.179846	0.038944	-3.413146
O	-1.588468	-3.816481	0.884711	H	6.663586	0.125358	-2.309657	N	2.504102	4.251325	-0.245203
O	1.182282	-4.745383	1.234670	C	0.713919	1.888481	3.181611	C	5.765029	2.586947	-0.228250
N	-0.868844	-1.261918	1.861572	C	-5.430956	-2.233589	0.488368	H	6.132663	3.241169	0.556135
O	2.601107	2.026233	-2.030521	C	-4.446558	2.228568	-0.911629	C	-7.655132	4.218476	-0.807754
N	-0.133639	4.340587	-0.169183	C	0.049804	-0.273359	2.261319	H	-7.938406	5.266457	-0.830660
O	-6.532811	0.210627	-0.650292	C	1.957410	5.339587	0.463456	C	1.436145	-0.663979	2.184991
O	-0.364567	2.004964	-1.799023	C	2.167619	-7.339362	0.441059	C	-3.909701	1.236590	-1.774436
N	1.679658	-1.980917	1.741295	C	0.519615	5.389418	0.506759	H	-4.614460	0.563587	-2.243119
C	-8.283141	1.875316	-0.775153	C	-4.391029	-1.417162	0.889538	C	-1.634184	2.048165	-1.493385
C	2.409975	-4.780602	0.801703	H	-4.577611	-0.376958	1.138240	C	2.065059	7.430704	1.719527

C	5.265107	-0.916356	-3.950084	H	-5.921538	-4.176392	-0.246627	H	-0.637329	-1.641485	-3.043380
H	6.122094	-0.378886	-4.370850	C	-9.133376	-2.487198	1.175664	H	-1.472340	-1.433599	-1.499121
H	4.837957	-1.528310	-4.750808	H	-9.800148	-3.182349	1.676793	H	-0.175820	-0.312771	-1.964632
H	5.632223	-1.602194	-3.178640	C	3.698939	3.799239	0.030433	C	0.750962	9.565079	3.011614
C	2.982386	-6.030414	0.366783	H	4.232741	4.257020	0.868602	H	0.257133	10.392414	3.512569
C	-0.108101	6.449216	1.132558	C	2.693493	6.353525	1.045245	C	7.286651	-3.660274	-0.763940
H	-1.191192	6.525736	1.123878	H	3.776314	6.354517	0.965211	H	8.297869	-3.798825	-1.160316
C	4.414456	2.758898	-0.637318	C	-5.903646	2.511582	-0.819136	H	7.380532	-3.244052	0.244512
C	-2.063032	0.006363	-3.039386	C	7.341188	-5.995882	0.116572	H	6.783439	-2.919167	-1.393961
C	2.092058	1.502892	3.099133	H	6.885244	-6.990287	0.133293	C	-6.920424	1.536245	-0.748215
C	3.087470	2.413159	3.546232	H	7.404314	-5.640820	1.150512	C	3.849255	1.925895	-1.663307
H	4.131112	2.114427	3.489346	H	8.361420	-6.106589	-0.268544	C	2.805245	-2.305613	1.154845
C	4.283520	-6.017835	-0.109171	C	-7.412287	-0.685266	-0.060729	H	3.518856	-1.500366	0.954203
H	4.711138	-6.958815	-0.432514	C	-8.633717	3.228711	-0.780750	C	4.554735	-3.677043	0.209121
C	2.740066	3.649247	4.045992	H	-9.678531	3.515932	-0.785356	H	5.125171	-2.754218	0.167417
H	3.509931	4.335438	4.386663	C	-1.436612	0.657850	-4.296816	C	2.974618	-8.556489	-0.056016
C	-8.793846	-0.437795	-0.078622	H	-0.570054	1.267212	-4.040388	H	3.272902	-8.455648	-1.105300
C	-6.868489	-1.850698	0.513986	H	-2.167665	1.291353	-4.811689	H	2.351811	-9.453528	0.020654
C	0.905123	-7.227498	-0.446937	H	-1.114111	-0.120448	-4.997955	H	3.874644	-8.731572	0.543775
H	0.267596	-6.404195	-0.127550	C	0.632971	7.479147	1.764810	C	1.377979	4.030769	4.127861
H	0.326306	-8.157189	-0.393582	C	-6.314433	3.856353	-0.855552	H	1.116776	5.008066	4.521939
H	1.182558	-7.064975	-1.494511	H	-5.554296	4.624696	-0.950635	C	-7.766844	-2.738179	1.131250
C	3.230510	-3.600841	0.727580	C	-2.079776	-0.983747	1.465503	H	-7.365274	-3.628272	1.605098
C	5.108371	-4.866121	-0.209086	H	-2.390352	0.065143	1.423897	C	-2.558071	1.100973	-2.068518
C	-5.106933	-3.565479	0.122378	C	-1.018532	-0.895126	-2.337115	C	-3.568210	-5.563013	-0.278966
C	-2.781666	-3.304398	0.730570	C	-9.306675	0.746523	-0.898009	C	0.390013	3.167934	3.708388

H	-0.656197	3.454835	3.777705
C	6.594504	1.656572	-0.812049
C	0.003127	8.570705	2.421195
H	-1.082825	8.607599	2.451075
C	-9.642228	-1.344575	0.565002
H	-10.710899	-1.165806	0.581241
C	-3.211431	-0.907467	-3.515022
H	-3.965523	-0.361338	-4.092495
H	-3.711251	-1.410313	-2.680679
H	-2.800675	-1.683291	-4.169120
C	-2.156364	3.013241	-0.559549
C	1.759415	-7.627467	1.906988
H	2.646072	-7.745020	2.540192
H	1.184200	-8.559217	1.958867
H	1.148309	-6.822500	2.314881
C	4.707200	0.943271	-2.278090
C	8.309695	0.027593	0.068965
H	7.701118	-0.186004	0.954323
H	9.362127	-0.118629	0.337797
H	8.058371	-0.712776	-0.695659
C	8.072664	1.472777	-0.428104
C	-4.839012	-6.237782	-0.835735
H	-5.623786	-6.336333	-0.077584
H	-4.587087	-7.247116	-1.176666
H	-5.253858	-5.696523	-1.692830
C	3.007828	-0.831987	-2.899704
H	2.623912	-1.459366	-3.712386
H	2.190761	-0.216168	-2.525280
H	3.341155	-1.498966	-2.096640
C	2.166198	9.517657	2.966071
H	2.745251	10.309258	3.432349
C	3.708631	0.908986	-4.605049
H	4.536786	1.509210	-4.998387
H	2.902604	1.581694	-4.313019
H	3.345097	0.266510	-5.415165
C	6.537615	-5.004791	-0.759448
C	-2.519259	-5.544381	-1.417664
H	-2.897577	-4.983103	-2.279423
H	-2.306795	-6.567159	-1.749847
H	-1.585618	-5.086964	-1.090464
C	-0.316528	-3.866770	4.204533
H	-1.260802	-3.469950	4.589669
H	0.492690	-3.461887	4.820795
H	-0.326981	-4.952163	4.342891
C	-3.064317	-6.434491	0.897169
H	-2.126785	-6.054576	1.301013
H	-2.901581	-7.463602	0.556568
H	-3.805445	-6.461861	1.704110
C	2.806788	8.476606	2.331503
H	3.892453	8.440842	2.291864
C	6.485647	-5.533214	-2.212980
H	5.992175	-6.507913	-2.274708
H	7.498458	-5.648099	-2.616269
H	5.937408	-4.841025	-2.860435
C	1.016819	4.724241	-3.542141
H	1.163013	4.158414	-4.467208
H	1.789715	5.498154	-3.499938
H	0.045154	5.223535	-3.606442
C	-10.715851	1.187609	-0.465812
H	-11.433300	0.373656	-0.595790
H	-11.071955	2.011930	-1.088888
H	-10.740664	1.507413	0.580347
C	8.504043	2.439799	0.690693
H	8.393785	3.486771	0.388881
H	9.558794	2.276972	0.934703
H	7.926429	2.284486	1.608373
C	-9.367866	0.311239	-2.392085
H	-8.387309	-0.015070	-2.748802
H	-9.698530	1.146360	-3.018835
H	-10.069478	-0.520378	-2.516691
C	8.965699	1.739447	-1.663675
H	8.735476	1.057858	-2.488045
H	10.023219	1.605632	-1.408557
H	8.830496	2.762510	-2.029693

Table S16. Cartesian coordinates of the ground state (S_0) fully optimized geometry of **XPCIn** in gas from B3LYP calculations (in Å)

Atom	X	Y	Z
In	-0.019889	-2.619725	-1.852097
In	0.051302	3.687050	1.298804
O	1.363077	-3.222610	-0.467112
O	-1.542806	-3.307734	-0.671622
O	-1.417018	2.268432	1.512739
O	1.551387	2.320404	1.602455
O	7.137100	-0.305252	0.041255
O	-7.196695	-0.234583	0.312232
N	1.322422	-0.797492	-1.949779
N	-1.346061	-0.795180	-2.003473
N	-1.245109	4.326562	-0.457879
N	1.397602	4.337250	-0.411483
C	2.647459	-3.015506	-0.360965
C	3.288032	-1.857372	-0.932814
C	4.693536	-1.693882	-0.848555
H	5.140008	-0.819908	-1.310164
C	5.494208	-2.639710	-0.234739
C	4.832630	-3.723018	0.403128
H	5.457096	-4.422062	0.945173
C	3.463089	-3.936613	0.387080
C	2.829712	-5.129828	1.134012
C	1.822950	-4.607881	2.187587
H	2.333170	-3.993076	2.937217
H	-4.965065	3.485747	-1.066893
H	1.352518	-5.450665	2.707285
H	1.039682	-4.007986	1.724366
C	2.111657	-6.071608	0.136528
H	1.299133	-5.559561	-0.377660
H	1.693743	-6.932431	0.671279
H	2.814538	-6.451773	-0.613513
C	3.884127	-5.971905	1.881483
H	4.612946	-6.425650	1.200692
H	3.380344	-6.787710	2.409739
H	4.428902	-5.385165	2.628945
C	2.574410	-0.793434	-1.577449
H	3.168097	0.109707	-1.744219
C	0.715485	0.304021	-2.586041
C	1.411731	1.342106	-3.224168
H	2.495917	1.327998	-3.250171
C	-1.377403	1.340292	-3.281425
H	-2.459279	1.320212	-3.356040
C	-0.706424	0.305024	-2.612401
C	-2.601698	-0.752397	-1.640851
H	-3.147278	0.186030	-1.772717
C	-2.820195	-3.055135	-0.601998
C	-3.709317	-4.020038	-0.009216
C	-5.065311	-3.733063	-0.005772
H	-5.749707	-4.460175	0.413961
C	-5.455653	2.057124	0.450067
C	-5.641237	-2.536700	-0.507468
C	-4.776821	-1.574559	-0.991903
H	-5.164244	-0.630575	-1.361849
C	-3.380359	-1.811825	-1.070874
C	-3.168332	-5.338773	0.582533
C	-2.163256	-5.030626	1.718482
H	-1.322055	-4.441982	1.354045
H	-1.776101	-5.965889	2.139550
H	-2.652254	-4.475696	2.526856
C	-4.291882	-6.207886	1.184300
H	-4.822078	-5.695751	1.994485
H	-3.852768	-7.118410	1.604464
H	-5.026768	-6.517532	0.433004
C	-2.478425	-6.177411	-0.521176
H	-3.185878	-6.423258	-1.321230
H	-2.108381	-7.119047	-0.099263
H	-1.635419	-5.642220	-0.957527
C	0.099714	-3.646034	-3.731265
H	1.108060	-3.588747	-4.153032
H	-0.593945	-3.219263	-4.462768
H	-0.152669	-4.704103	-3.612033
C	-2.674986	2.193076	1.172939
C	-3.218768	2.978630	0.093721
C	-4.589923	2.874815	-0.248978
C	-4.897675	1.263648	1.487241

H	-5.576060	0.613324	2.021549	C	3.362495	2.988447	0.176774	H	7.024137	-4.764426	-0.628197
C	-3.562212	1.288475	1.863092	C	4.732722	2.856894	-0.165135	C	9.014253	-3.962582	-0.609619
C	-3.048280	0.403297	3.018999	H	5.125652	3.463542	-0.978133	H	9.488296	-4.925687	-0.772155
C	-1.936883	-0.542357	2.505045	C	5.574747	2.011143	0.525490	C	9.781421	-2.808479	-0.521262
H	-2.331293	-1.228019	1.748754	C	5.005171	1.234580	1.568458	H	10.860736	-2.878769	-0.612009
H	-1.547459	-1.145857	3.332839	H	5.671758	0.566845	2.097630	C	9.190457	-1.552447	-0.324570
H	-1.109170	0.016757	2.070104	C	3.676324	1.304305	1.960451	C	7.796601	-1.492182	-0.201328
C	-2.502700	1.290173	4.165040	C	3.153385	0.466909	3.147388	C	10.072913	-0.303479	-0.255006
H	-1.662860	1.900217	3.832751	C	4.248770	-0.444514	3.738526	C	11.038696	-0.420972	0.954622
H	-2.162113	0.659147	4.993906	H	3.821281	-1.025415	4.562105	H	10.479106	-0.503161	1.890789
H	-3.285072	1.954738	4.548823	H	5.091019	0.125865	4.145682	H	11.688458	0.456965	1.022943
C	-4.165426	-0.480541	3.611512	H	4.635012	-1.155129	3.000316	H	11.677722	-1.304340	0.861966
H	-4.973130	0.111695	4.055894	C	1.991910	-0.445855	2.689697	C	10.898393	-0.192122	-1.564710
H	-3.742124	-1.102223	4.406974	H	2.333275	-1.155248	1.929882	H	11.531401	-1.072346	-1.707354
H	-4.599187	-1.152891	2.864015	H	1.168386	0.135746	2.277980	H	11.553565	0.683493	-1.545318
C	-2.459626	3.908248	-0.684857	H	1.614612	-1.023606	3.541309	H	10.238100	-0.104429	-2.432258
H	-2.984172	4.300882	-1.561810	C	2.671517	1.408326	4.278770	C	9.215737	0.951506	-0.085584
C	-0.623027	5.282664	-1.284023	H	2.314733	0.816448	5.129468	C	9.817416	2.218404	-0.077098
C	-1.300200	6.228456	-2.066609	H	1.856349	2.050005	3.943421	H	10.893433	2.293679	-0.198804
H	-2.384544	6.265477	-2.051088	H	3.491372	2.043832	4.632228	C	9.070497	3.378054	0.088931
C	1.492668	6.241261	-2.015024	C	-0.005654	5.198764	2.814775	H	9.558266	4.347992	0.095634
H	2.575289	6.288351	-1.958913	H	-0.944913	5.759633	2.784757	C	7.693271	3.281896	0.275036
C	0.795804	5.288966	-1.257986	H	0.815815	5.912261	2.696302	H	7.102553	4.175887	0.449305
C	2.618661	3.920503	-0.611013	H	0.083423	4.750968	3.809174				
H	3.158988	4.313327	-1.478232	C	6.980322	-2.644722	-0.304378				
C	2.805910	2.219118	1.260971	C	7.628980	-3.871221	-0.512671				

C	7.041844	2.042114	0.282448	H	-10.758086	-1.241112	2.050421	H	-6.877486	4.272693	0.071734
C	7.827812	0.884524	0.082240	H	-10.673132	0.515601	2.322939	C	-6.921514	2.132698	0.218466
C	-7.123739	-2.442248	-0.591687	H	-9.192449	-0.458559	2.324115	C	-7.781149	1.014698	0.210623
C	-7.828603	-3.546382	-1.099690	C	-11.443056	0.048819	-0.276953	C	0.804923	7.157007	-2.807780
H	-7.262416	-4.409754	-1.434562	H	-11.412011	0.211891	-1.358474	H	1.358424	7.894266	-3.381115
C	-9.214154	-3.539437	-1.218110	H	-11.968165	0.888540	0.185308	C	-0.592201	7.150553	-2.833684
H	-9.730301	-4.401082	-1.630607	H	-12.049845	-0.837972	-0.078312	H	-1.130878	7.882648	-3.427386
C	-9.936017	-2.422409	-0.806799	C	-9.174639	1.140374	0.103972	C	0.727946	2.374038	-3.859715
H	-11.016357	-2.429127	-0.892047	C	-9.709495	2.417166	-0.096960	H	1.283325	3.164586	-4.354757
C	-9.285484	-1.303599	-0.275263	H	-10.780981	2.544050	-0.198272	C	-0.669409	2.372664	-3.889369
C	-7.884949	-1.324331	-0.195830	C	-8.884567	3.538472	-0.145261	H	-1.204775	3.160847	-4.409640
C	-10.032994	-0.107979	0.319342	H	-9.314528	4.525346	-0.287585				
C	-10.171739	-0.337384	1.853256	C	-7.513720	3.393927	0.038695				

Table S17. Cartesian coordinates of the ground state (S_0) partially optimized geometry of **XNCIn** in gas from B3LYP calculations (in Å)

0°

Atom	X	Y	Z	N	1.302052	-0.940538	-1.877853	C	4.786982	-4.204908	0.022999
In	-0.042244	-2.755424	-2.069440	N	-1.363559	-0.926560	-1.943033	H	5.406381	-4.982261	0.452494
In	0.068722	2.988244	2.159129	N	-1.217600	3.957126	0.550026	C	3.416485	-4.406702	-0.028126
O	1.323088	-3.560880	-0.772341	N	1.418967	3.952756	0.608905	C	2.775349	-5.697909	0.523677
O	-1.578876	-3.619833	-1.030332	C	2.607528	-3.378390	-0.629179	C	1.763427	-5.340614	1.639209
O	-1.398370	1.554444	2.079176	C	3.254809	-2.148409	-1.012274	H	2.270492	-4.850823	2.477776
O	1.573079	1.593259	2.205554	C	4.660629	-2.006146	-0.900224	H	1.287241	-6.251733	2.019668
O	7.115203	-0.779600	0.160042	H	5.112050	-1.073851	-1.221160	H	0.984847	-4.673388	1.269571
O	-7.193837	-0.681991	0.444768	C	5.455684	-3.040259	-0.440886	C	2.060932	-6.472774	-0.610673
H	1.253341	-5.884638	-1.045050	H	1.636797	-7.403609	-0.216629	H	2.767500	-6.736429	-1.405885

C	3.823131	-6.648429	1.138837	C	-3.751456	-4.414012	-0.492002	C	-3.182147	2.508992	0.786406
H	4.554266	-6.995777	0.400353	C	-5.104161	-4.117799	-0.434523	C	-4.547429	2.467643	0.410014
H	3.314081	-7.533521	1.533633	H	-5.794909	-4.898177	-0.139432	H	-4.911108	3.215006	-0.291398
H	4.365686	-6.184934	1.969848	C	-5.668962	-2.848271	-0.726006	C	-5.423518	1.542652	0.944385
C	2.548543	-0.996306	-1.491068	C	-4.795554	-1.827180	-1.045201	C	-4.878181	0.576748	1.831352
H	3.142787	-0.078217	-1.508510	H	-5.173524	-0.830919	-1.250983	H	-5.562865	-0.155879	2.234819
C	0.711630	0.246656	-2.356543	C	-3.401987	-2.062285	-1.168983	C	-3.546997	0.530864	2.220815
C	1.405819	1.341320	-2.838214	C	-3.222940	-5.819408	-0.135128	C	-3.047248	-0.546328	3.207797
H	2.490837	1.330280	-2.865013	C	-2.212277	-5.719509	1.032793	C	-1.925916	-1.385545	2.550288
C	0.738067	2.483292	-3.344600	H	-1.365136	-5.086675	0.770376	H	-2.306893	-1.925199	1.677747
C	1.440935	3.614581	-3.840623	H	-1.835053	-6.716901	1.287369	H	-1.547894	-2.127370	3.262945
H	2.527831	3.606235	-3.818105	H	-2.693310	-5.304697	1.925574	H	-1.093091	-0.757914	2.235094
C	0.762256	4.702274	-4.342944	C	-4.354391	-6.767228	0.313333	C	-2.520118	0.122277	4.501194
H	1.310450	5.563429	-4.712820	H	-4.877597	-6.395830	1.201090	H	-1.678140	0.782945	4.294973
C	-0.654155	4.705076	-4.382427	H	-3.924302	-7.740662	0.569943	H	-2.188331	-0.646193	5.208724
H	-1.177339	5.568132	-4.782944	H	-5.093844	-6.936270	-0.477241	H	-3.309957	0.706687	4.986622
C	-1.364236	3.620433	-3.918122	C	-2.543950	-6.464074	-1.368464	C	-4.170402	-1.521467	3.617549
H	-2.450772	3.616320	-3.955949	H	-3.255858	-6.563893	-2.195654	H	-4.985501	-1.017696	4.148965
C	-0.694396	2.486905	-3.383200	H	-2.181730	-7.467015	-1.114479	H	-3.756687	-2.274852	4.295540
C	-1.393766	1.349337	-2.910643	H	-1.697095	-5.870067	-1.711321	H	-4.592336	-2.049804	2.756300
H	-2.475582	1.339798	-2.998451	C	0.101932	-3.486357	-4.079870	C	-2.418396	3.575048	0.213545
C	-0.731242	0.252943	-2.390064	H	1.105305	-3.331510	-4.488711	H	-2.924440	4.123397	-0.587760
C	-2.615404	-0.932477	-1.563830	H	-0.610135	-2.980530	-4.739738	C	-0.604105	5.077079	-0.044805
H	-3.149546	0.021446	-1.536461	H	-0.112838	-4.558625	-4.118934	C	-1.273250	6.159942	-0.580664
C	-2.853485	-3.371753	-0.916630	C	-2.651730	1.542582	1.714853	H	-2.358317	6.195030	-0.560381
C	-0.572380	7.262667	-1.130714	C	-1.244189	8.380585	-1.694067	H	-2.330976	8.381950	-1.715130

C	-0.535619	9.444558	-2.206714	C	2.008408	-1.318544	2.806392	H	11.666469	-1.900832	0.761563
H	-1.061536	10.291828	-2.636754	H	2.331034	-1.890455	1.931145	C	10.849515	-0.448635	-1.465092
C	0.880654	9.443027	-2.172394	H	1.181910	-0.672284	2.514503	H	11.475367	-1.300781	-1.744455
H	1.428602	10.289145	-2.576414	H	1.642276	-2.030605	3.554980	H	11.509087	0.413696	-1.331791
C	1.561377	8.377575	-1.626101	C	2.728998	0.240706	4.670522	H	10.174363	-0.235497	-2.298804
H	2.647912	8.376686	-1.594561	H	2.378850	-0.482865	5.415621	C	9.199159	0.473708	0.194214
C	0.860736	7.261108	-1.096049	H	1.915656	0.935877	4.460945	C	9.808604	1.722958	0.381125
C	1.531666	6.156536	-0.513127	H	3.560465	0.801620	5.112096	H	10.883165	1.811382	0.255480
H	2.614544	6.188777	-0.439247	C	-0.005073	4.173783	3.940513	C	9.071044	2.847609	0.729533
C	0.834604	5.075237	-0.010753	H	-0.959813	4.701237	4.029010	H	9.564580	3.803913	0.873260
C	2.625604	3.559402	0.302625	H	0.794367	4.921150	3.955049	C	7.696488	2.729591	0.921970
H	3.151910	4.102469	-0.489156	H	0.111637	3.544297	4.827845	H	7.114854	3.589509	1.239298
C	2.821066	1.544954	1.830925	C	6.941407	-3.044098	-0.517375	C	7.036887	1.505350	0.754026
C	3.367410	2.486029	0.885929	C	7.581413	-4.231015	-0.904937	C	7.813256	0.388019	0.370063
C	4.728492	2.401516	0.496543	H	6.970943	-5.095740	-1.142588	C	-7.150175	-2.725292	-0.788288
H	5.112790	3.135245	-0.208631	C	8.965237	-4.313629	-1.027075	C	-7.870071	-3.728761	-1.458371
C	5.574113	1.444002	1.016565	H	9.432228	-5.245680	-1.330220	H	-7.315896	-4.536884	-1.925137
C	5.015551	0.507903	1.926180	C	9.739651	-3.187052	-0.783512	C	-9.255542	-3.686313	-1.569695
H	5.684797	-0.243150	2.323719	H	10.817533	-3.247769	-0.895661	H	-9.783167	-4.467470	-2.108569
C	3.694716	0.519827	2.349913	C	9.157486	-1.969554	-0.403631	C	-9.962468	-2.637028	-0.988976
C	3.184584	-0.501180	3.389676	C	7.765414	-1.921989	-0.257775	H	-11.042883	-2.616693	-1.070945
C	4.281989	-1.504177	3.801529	C	10.046896	-0.745733	-0.170218	C	-9.296645	-1.621725	-0.293825
H	3.863939	-2.210329	4.526149	C	11.033254	-1.038782	0.992107	C	-7.896522	-1.672030	-0.222802
H	5.136315	-1.013644	4.281085	H	10.489671	-1.254039	1.916485	C	-10.026911	-0.521768	0.479406
H	4.648647	-2.085722	2.949203	H	11.688499	-0.181560	1.174822	C	-10.163802	-0.980241	1.961298
H	-10.761600	-1.895874	2.021776	H	-10.652141	-0.202233	2.557766	H	-9.184743	-1.184159	2.403156

C	-11.436752	-0.258870	-0.078673	C	-9.672170	2.032753	0.449167	H	-6.820073	3.805065	0.907582
H	-11.407409	0.066894	-1.122836	H	-10.741838	2.186873	0.368652	C	-6.887231	1.668543	0.719227
H	-11.949593	0.506669	0.509115	C	-8.833327	3.137646	0.574007	C	-7.761098	0.576102	0.537632
H	-12.053889	-1.158343	-0.014332	H	-9.250631	4.140040	0.585115				
C	-9.152964	0.734044	0.452843	C	-7.465203	2.949346	0.735994				