Electronic Supplementary Information (ESI)

Axially Phenoxylated Aluminum Phthalocyanines and Their Application in Organic Photovoltaic Cells.

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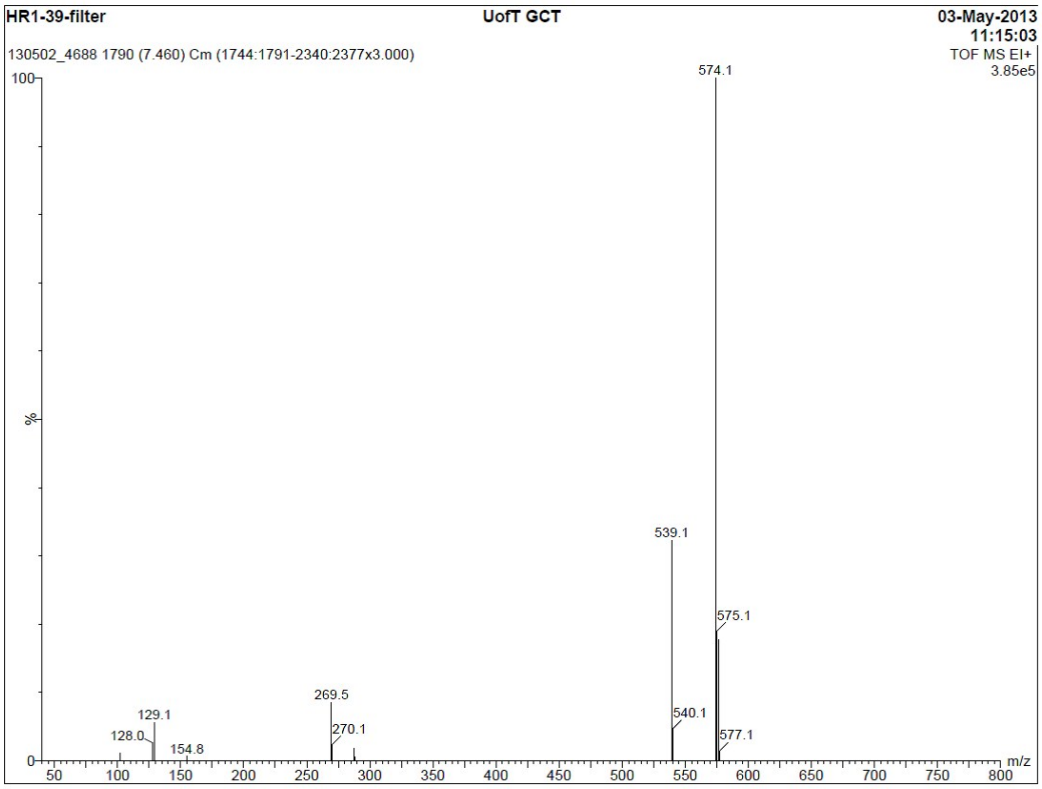
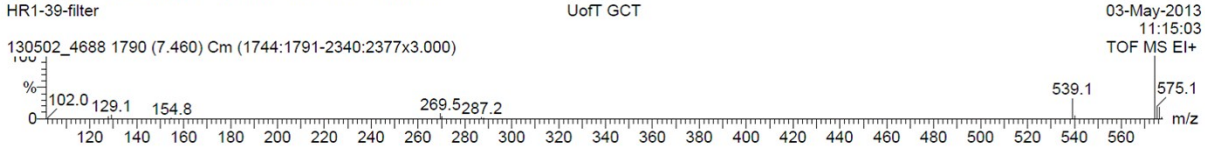


Elemental Composition Report **Page 1**

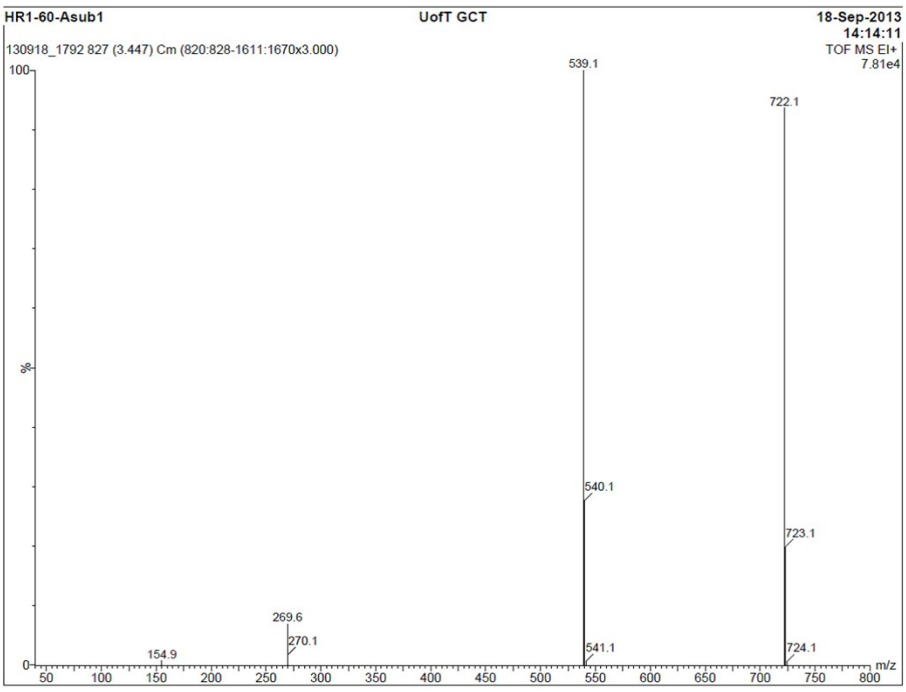
Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
254 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-8 Al: 0-1 Cl: 0-1



Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
574.1006	574.1002	0.4	0.7	29.0	33854.9	C32 H16 N8 Al Cl
	574.0985	2.1	3.7	34.0	43184.8	C39 H15 N4 Cl
	574.0967	3.9	6.8	39.0	48067.6	C40 H10 N6
	574.1051	-4.5	-7.8	37.0	49092.1	C42 H15 N2 Al

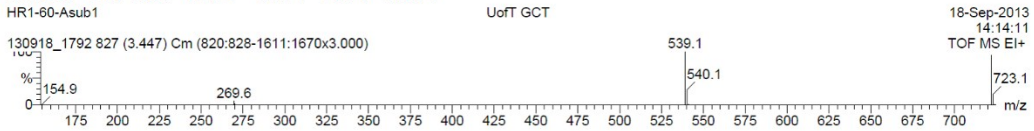
Figure S1. Low resolution (top) and high-resolution (bottom) mass spectrum (TOF-EI) of Cl-AlPc.



Elemental Composition Report **Page 1**

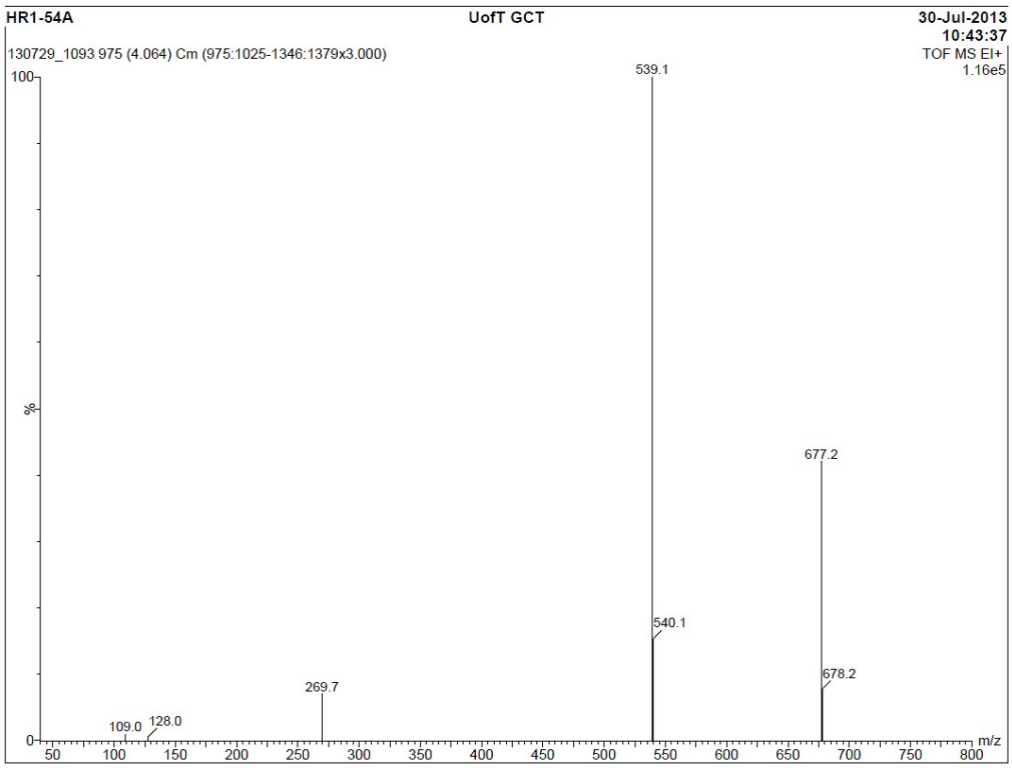
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
2291 formula(e) evaluated with 22 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-8 O: 0-1 F: 0-7 Al: 0-1



Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
722.1185	722.1185	0.0	0.0	36.5	24833.6	C43 H17 N5 O F4 Al
	722.1184	0.1	0.1	44.0	27678.1	C46 H15 N8 O Al
	722.1183	0.2	0.3	33.0	21471.4	C38 H16 N8 O F5 Al
	722.1187	-0.2	-0.3	40.0	27705.6	C48 H18 N2 O F3 Al
	722.1175	1.0	1.4	44.0	29315.5	C51 H17 N2 F2 Al
	722.1174	1.1	1.5	33.0	23701.3	C43 H18 N2 F7 Al
	722.1173	1.2	1.7	40.5	26733.8	C46 H16 N5 F3 Al
	722.1171	1.4	1.9	37.0	23670.6	C41 H15 N8 F4 Al
	722.1168	1.7	2.4	49.0	30961.6	C53 H14 N4 O
	722.1168	1.7	2.4	41.5	28746.0	C50 H16 N O F4
	722.1166	1.9	2.6	38.0	26070.5	C45 H15 N4 O F5
	722.1166	1.9	2.6	45.5	28721.4	C48 H13 N7 O F
	722.1164	2.1	2.9	34.5	22910.2	C40 H14 N7 O F6
	722.1157	2.8	3.9	45.5	30252.8	C53 H15 N F3
	722.1215	-3.0	-4.2	42.0	26697.1	C45 H13 N8 F3
	722.1155	3.0	4.2	42.0	27852.5	C48 H14 N4 F4
	722.1154	3.1	4.3	49.5	30228.3	C51 H12 N7
	722.1216	-3.1	-4.3	34.5	23663.1	C42 H15 N5 F7
	722.1153	3.2	4.4	38.5	24990.0	C43 H13 N7 F5
	722.1217	-3.2	-4.4	45.5	29287.5	C50 H14 N5 F2
	722.1218	-3.3	-4.6	38.0	26729.6	C47 H16 N2 F6
	722.1219	-3.4	-4.7	49.0	31439.8	C55 H15 N2 F

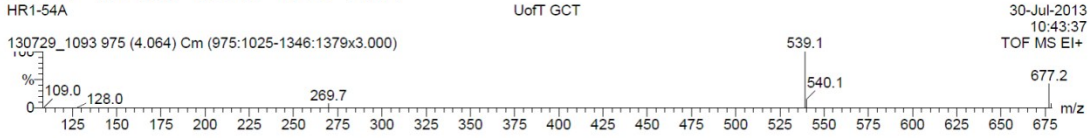
Figure S2. Low resolution (top) and high-resolution (bottom) mass spectrum (TOF-EI) of F_5PhO-AlPc.



Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
1056 formula(e) evaluated with 11 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 O: 0-5 Al: 0-1



Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
677.1503	677.1505	-0.2	-0.3	34.0	2801772.5	C38 H20 N9 O3 Al
	677.1501	0.2	0.3	38.5	2801810.5	C47 H21 N2 O4
	677.1515	-1.2	-1.8	43.5	2801812.8	C48 H17 N6
	677.1488	1.5	2.2	39.0	2801806.0	C45 H19 N5 O3
	677.1518	-1.5	-2.2	33.5	2801783.0	C40 H22 N6 O4 Al
	677.1486	1.7	2.5	41.5	2801819.3	C51 H22 O Al
	677.1528	-2.5	-3.7	43.0	2801819.0	C50 H19 N3 O
	677.1531	-2.8	-4.1	33.0	2801793.5	C42 H24 N3 O5 Al
	677.1531	-2.8	-4.1	38.5	2801786.5	C41 H18 N10 Al
	677.1474	2.9	4.3	39.5	2801801.5	C43 H17 N8 O2
	677.1473	3.0	4.4	42.0	2801817.0	C49 H20 N3 Al

Figure S3. Low resolution (top) and high-resolution (bottom) mass spectrum (TOF-EI) of NO_2PhO-AlPc.

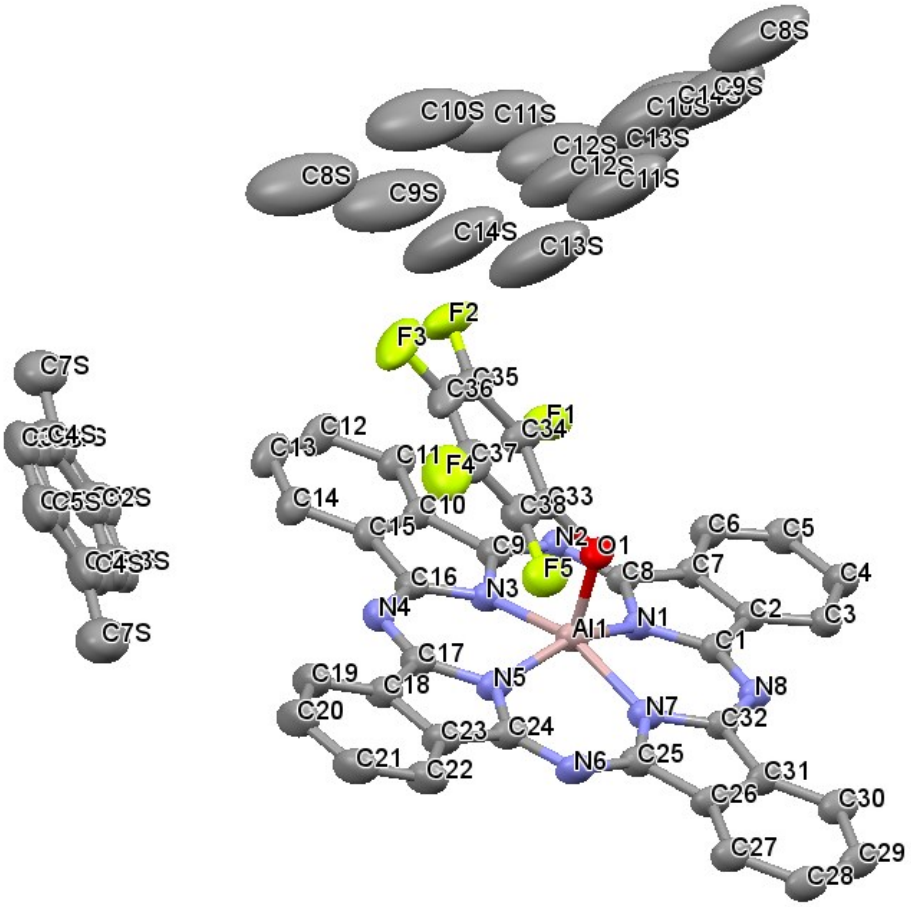


Figure S4. Molecular structure of F_5PhO-AlPc including toluene and heptane solvate molecules. Eliposoids shown at 50% probability level. Carbon – grey; nitrogben – blue; aluminum – pink; oxygen – red; fluorine – yellow. Hydrogen atoms are omitted for clarity. CCDC deposition number 1061523.

Table S1. Crystal data and structure refinement for F_5PhO-AlPc.

CCDC Deposition Number	1061523	
Identification code	F_5PhO-AlPc	
Empirical formula	C45 H28 Al F5 N8 O	
Formula weight	818.73	
Temperature	147(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 2/n	
Unit cell dimensions	a = 10.3131(6) Å	a= 90°.
	b = 14.4067(7) Å	b= 99.572(4)°.
	c = 24.7771(11) Å	g = 90°.
Volume	3630.1(3) $Å^3$	
Z	4	
Density (calculated)	1.498 Mg/m^3	
Absorption coefficient	1.153 mm^{-1}	
F(000)	1680	
Crystal size	0.120 x 0.120 x 0.020 mm^3	
Theta range for data collection	3.067 to 67.249°.	
Index ranges	-12<=h<=11, -17<=k<=17, -29<=l<=29	
Reflections collected	45324	
Independent reflections	6430 [R(int) = 0.1586]	
Completeness to theta = 67.679°	97.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7529 and 0.6166	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6430 / 14 / 526	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R1 = 0.0878, wR2 = 0.2248	
R indices (all data)	R1 = 0.1402, wR2 = 0.2660	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.898 and -0.613 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for F_5PhO-AlPc. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	6704(2)	4030(1)	5261(1)	32(1)
F(1)	6945(4)	2304(2)	4162(1)	57(1)
F(2)	6253(4)	493(3)	4057(2)	82(1)
F(3)	6316(4)	-594(3)	4949(2)	87(1)
F(4)	7094(4)	142(3)	5965(2)	79(1)
F(5)	7799(4)	1940(2)	6083(1)	55(1)
O(1)	7723(3)	3071(2)	5181(1)	36(1)
N(1)	7163(4)	4903(3)	4722(1)	30(1)
N(2)	5683(4)	4420(3)	3902(1)	32(1)
N(3)	5155(4)	3721(3)	4732(2)	33(1)
N(4)	4005(4)	2710(3)	5282(2)	34(1)
N(5)	5775(4)	3568(3)	5831(1)	34(1)
N(6)	7209(5)	4083(3)	6653(2)	37(1)
N(7)	7789(4)	4756(3)	5822(2)	35(1)
N(8)	8963(4)	5740(3)	5273(1)	32(1)
C(1)	8219(5)	5515(3)	4802(2)	30(1)
C(2)	8421(5)	5905(3)	4292(2)	32(1)
C(3)	9365(5)	6523(3)	4167(2)	35(1)
C(4)	9328(6)	6736(4)	3621(2)	40(1)
C(5)	8371(6)	6351(4)	3212(2)	41(1)
C(6)	7424(5)	5749(4)	3337(2)	36(1)
C(7)	7465(5)	5526(3)	3884(2)	31(1)
C(8)	6687(5)	4905(3)	4159(2)	30(1)
C(9)	4975(5)	3866(3)	4168(2)	32(1)
C(10)	3890(5)	3301(3)	3890(2)	32(1)
C(11)	3349(6)	3195(4)	3341(2)	40(1)
C(12)	2311(6)	2563(4)	3223(2)	47(1)
C(13)	1859(6)	2062(4)	3638(2)	49(2)

C(14)	2398(6)	2181(4)	4182(2)	42(1)
C(15)	3417(5)	2808(4)	4297(2)	34(1)
C(16)	4210(5)	3070(3)	4812(2)	32(1)
C(17)	4744(5)	2939(3)	5752(2)	35(1)
C(18)	4558(6)	2537(4)	6265(2)	39(1)
C(19)	3716(6)	1845(4)	6392(2)	48(2)
C(20)	3815(7)	1591(4)	6938(2)	54(2)
C(21)	4740(7)	2023(4)	7348(2)	51(2)
C(22)	5568(6)	2707(4)	7223(2)	46(1)
C(23)	5477(6)	2959(4)	6672(2)	38(1)
C(24)	6218(6)	3590(3)	6394(2)	37(1)
C(25)	7918(5)	4635(3)	6389(2)	35(1)
C(26)	8977(5)	5206(4)	6665(2)	37(1)
C(27)	9471(6)	5336(4)	7223(2)	42(1)
C(28)	10496(6)	5957(4)	7348(2)	44(1)
C(29)	11018(6)	6429(4)	6943(2)	45(1)
C(30)	10526(6)	6291(4)	6386(2)	41(1)
C(31)	9507(5)	5680(3)	6263(2)	35(1)
C(32)	8735(5)	5394(3)	5742(2)	30(1)
C(33)	7351(5)	2182(3)	5128(2)	38(1)
C(34)	6959(6)	1776(4)	4615(2)	45(1)
C(35)	6610(6)	862(4)	4560(3)	57(2)
C(36)	6646(6)	312(4)	5009(3)	59(2)
C(37)	7035(7)	681(4)	5519(3)	56(2)
C(38)	7386(6)	1601(4)	5573(2)	46(1)
C(1S)	10380(20)	10125(9)	5627(6)	79(4)
C(2S)	10110(20)	9196(9)	5504(6)	79(4)
C(3S)	9760(20)	8917(9)	4963(6)	79(4)
C(4S)	9670(20)	9567(10)	4544(6)	79(4)
C(5S)	9930(20)	10497(10)	4666(6)	79(4)
C(6S)	10290(20)	10776(8)	5208(6)	79(4)
C(7S)	10719(18)	10438(10)	6227(6)	95(5)
C(8S)	8300(20)	10009(15)	7409(10)	202(7)
C(9S)	9520(20)	9390(14)	7451(8)	202(7)
C(10S)	10302(18)	9907(12)	7092(8)	202(7)
C(11S)	11175(19)	9278(15)	6911(6)	202(7)

C(12S)	12292(18)	9103(14)	7358(6)	202(7)
C(13S)	13150(20)	8477(12)	7087(9)	202(7)
C(14S)	14440(20)	8981(17)	7190(10)	202(7)

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Table S3. Bond lengths [Å] and angles [°] for F_5PhO-AlPc.

Al(1)-O(1)	1.766(4)
Al(1)-N(7)	1.940(4)
Al(1)-N(3)	1.942(4)
Al(1)-N(1)	1.948(4)
Al(1)-N(5)	1.952(4)
F(1)-C(34)	1.353(6)
F(2)-C(35)	1.348(7)
F(3)-C(36)	1.350(7)
F(4)-C(37)	1.343(7)
F(5)-C(38)	1.355(6)
O(1)-C(33)	1.338(6)
N(1)-C(1)	1.390(6)
N(1)-C(8)	1.399(5)
N(2)-C(8)	1.322(6)
N(2)-C(9)	1.328(6)
N(3)-C(16)	1.391(6)
N(3)-C(9)	1.396(6)
N(4)-C(17)	1.321(6)
N(4)-C(16)	1.323(6)
N(5)-C(17)	1.386(7)
N(5)-C(24)	1.393(6)
N(6)-C(24)	1.321(7)
N(6)-C(25)	1.324(6)
N(7)-C(32)	1.379(6)
N(7)-C(25)	1.399(6)
N(8)-C(32)	1.323(6)
N(8)-C(1)	1.325(6)
C(1)-C(2)	1.430(6)
C(2)-C(3)	1.391(7)
C(2)-C(7)	1.400(6)
C(3)-C(4)	1.381(7)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.406(7)
C(4)-H(4A)	0.9500

C(5)-C(6)	1.378(7)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.388(6)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.445(7)
C(9)-C(10)	1.460(7)
C(10)-C(15)	1.387(7)
C(10)-C(11)	1.390(7)
C(11)-C(12)	1.399(8)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.397(8)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.380(7)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.379(7)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.448(7)
C(17)-C(18)	1.439(7)
C(18)-C(19)	1.392(8)
C(18)-C(23)	1.403(7)
C(19)-C(20)	1.389(7)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.416(9)
C(20)-H(20A)	0.9500
C(21)-C(22)	1.374(8)
C(21)-H(21A)	0.9500
C(22)-C(23)	1.399(7)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.436(7)
C(25)-C(26)	1.444(7)
C(26)-C(31)	1.390(7)
C(26)-C(27)	1.405(6)
C(27)-C(28)	1.380(8)
C(27)-H(27A)	0.9500
C(28)-C(29)	1.393(8)
C(28)-H(28A)	0.9500

C(29)-C(30)	1.404(7)
C(29)-H(29A)	0.9500
C(30)-C(31)	1.366(8)
C(30)-H(30A)	0.9500
C(31)-C(32)	1.458(6)
C(33)-C(38)	1.380(7)
C(33)-C(34)	1.395(7)
C(34)-C(35)	1.366(8)
C(35)-C(36)	1.363(10)
C(36)-C(37)	1.368(9)
C(37)-C(38)	1.375(8)
C(1S)-C(2S)	1.3900
C(1S)-C(6S)	1.3900
C(1S)-C(7S)	1.539(10)
C(2S)-C(3S)	1.3900
C(2S)-H(2SA)	0.9500
C(3S)-C(4S)	1.3900
C(3S)-H(3SA)	0.9500
C(4S)-C(5S)	1.3900
C(4S)-H(4SA)	0.9500
C(5S)-C(6S)	1.3900
C(5S)-H(5SA)	0.9500
C(6S)-H(6SA)	0.9500
C(7S)-H(7SA)	0.9800
C(7S)-H(7SB)	0.9800
C(7S)-H(7SC)	0.9800
C(8S)-C(9S)	1.528(10)
C(8S)-H(8SA)	0.9800
C(8S)-H(8SB)	0.9800
C(8S)-H(8SC)	0.9800
C(9S)-C(10S)	1.494(10)
C(9S)-H(9SA)	0.9900
C(9S)-H(9SB)	0.9900
C(10S)-C(11S)	1.404(9)
C(10S)-H(10A)	0.9900
C(10S)-H(10B)	0.9900

C(11S)-C(12S)	1.481(10)
C(11S)-H(11B)	0.9900
C(11S)-H(11C)	0.9900
C(12S)-C(13S)	1.501(10)
C(12S)-H(12B)	0.9900
C(12S)-H(12C)	0.9900
C(13S)-C(14S)	1.497(10)
C(13S)-H(13B)	0.9900
C(13S)-H(13C)	0.9900
C(14S)-H(14B)	0.9800
C(14S)-H(14C)	0.9800
C(14S)-H(14D)	0.9800

O(1)-Al(1)-N(7)	102.66(18)
O(1)-Al(1)-N(3)	100.58(17)
N(7)-Al(1)-N(3)	156.76(19)
O(1)-Al(1)-N(1)	102.25(18)
N(7)-Al(1)-N(1)	88.10(17)
N(3)-Al(1)-N(1)	87.28(17)
O(1)-Al(1)-N(5)	100.76(18)
N(7)-Al(1)-N(5)	87.59(17)
N(3)-Al(1)-N(5)	87.82(18)
N(1)-Al(1)-N(5)	156.98(19)
C(33)-O(1)-Al(1)	126.5(3)
C(1)-N(1)-C(8)	106.1(4)
C(1)-N(1)-Al(1)	125.9(3)
C(8)-N(1)-Al(1)	126.8(3)
C(8)-N(2)-C(9)	122.0(4)
C(16)-N(3)-C(9)	105.4(4)
C(16)-N(3)-Al(1)	125.1(3)
C(9)-N(3)-Al(1)	126.8(3)
C(17)-N(4)-C(16)	121.5(4)
C(17)-N(5)-C(24)	105.9(4)
C(17)-N(5)-Al(1)	125.2(3)
C(24)-N(5)-Al(1)	126.7(4)
C(24)-N(6)-C(25)	121.9(4)

C(32)-N(7)-C(25)	106.0(4)
C(32)-N(7)-Al(1)	126.4(3)
C(25)-N(7)-Al(1)	126.9(3)
C(32)-N(8)-C(1)	121.4(4)
N(8)-C(1)-N(1)	127.2(4)
N(8)-C(1)-C(2)	122.3(4)
N(1)-C(1)-C(2)	110.5(4)
C(3)-C(2)-C(7)	121.6(4)
C(3)-C(2)-C(1)	131.1(4)
C(7)-C(2)-C(1)	107.2(4)
C(4)-C(3)-C(2)	117.0(5)
C(4)-C(3)-H(3A)	121.5
C(2)-C(3)-H(3A)	121.5
C(3)-C(4)-C(5)	121.3(5)
C(3)-C(4)-H(4A)	119.3
C(5)-C(4)-H(4A)	119.3
C(6)-C(5)-C(4)	121.7(5)
C(6)-C(5)-H(5A)	119.2
C(4)-C(5)-H(5A)	119.2
C(5)-C(6)-C(7)	117.2(5)
C(5)-C(6)-H(6A)	121.4
C(7)-C(6)-H(6A)	121.4
C(6)-C(7)-C(2)	121.1(5)
C(6)-C(7)-C(8)	132.5(4)
C(2)-C(7)-C(8)	106.3(4)
N(2)-C(8)-N(1)	126.6(4)
N(2)-C(8)-C(7)	123.4(4)
N(1)-C(8)-C(7)	110.0(4)
N(2)-C(9)-N(3)	126.4(4)
N(2)-C(9)-C(10)	122.9(4)
N(3)-C(9)-C(10)	110.7(4)
C(15)-C(10)-C(11)	121.5(5)
C(15)-C(10)-C(9)	106.1(4)
C(11)-C(10)-C(9)	132.4(5)
C(10)-C(11)-C(12)	116.4(5)
C(10)-C(11)-H(11A)	121.8

C(12)-C(11)-H(11A)	121.8
C(13)-C(12)-C(11)	121.4(5)
C(13)-C(12)-H(12A)	119.3
C(11)-C(12)-H(12A)	119.3
C(14)-C(13)-C(12)	121.6(5)
C(14)-C(13)-H(13A)	119.2
C(12)-C(13)-H(13A)	119.2
C(15)-C(14)-C(13)	116.9(5)
C(15)-C(14)-H(14A)	121.5
C(13)-C(14)-H(14A)	121.5
C(14)-C(15)-C(10)	122.2(4)
C(14)-C(15)-C(16)	130.7(5)
C(10)-C(15)-C(16)	107.1(4)
N(4)-C(16)-N(3)	127.5(4)
N(4)-C(16)-C(15)	121.7(5)
N(3)-C(16)-C(15)	110.8(4)
N(4)-C(17)-N(5)	127.2(4)
N(4)-C(17)-C(18)	122.3(5)
N(5)-C(17)-C(18)	110.5(4)
C(19)-C(18)-C(23)	121.3(5)
C(19)-C(18)-C(17)	131.9(5)
C(23)-C(18)-C(17)	106.7(5)
C(20)-C(19)-C(18)	117.5(5)
C(20)-C(19)-H(19A)	121.3
C(18)-C(19)-H(19A)	121.3
C(19)-C(20)-C(21)	121.0(6)
C(19)-C(20)-H(20A)	119.5
C(21)-C(20)-H(20A)	119.5
C(22)-C(21)-C(20)	121.5(5)
C(22)-C(21)-H(21A)	119.2
C(20)-C(21)-H(21A)	119.2
C(21)-C(22)-C(23)	117.6(5)
C(21)-C(22)-H(22A)	121.2
C(23)-C(22)-H(22A)	121.2
C(22)-C(23)-C(18)	121.1(5)
C(22)-C(23)-C(24)	132.6(5)

C(18)-C(23)-C(24)	106.2(4)
N(6)-C(24)-N(5)	126.7(5)
N(6)-C(24)-C(23)	122.5(4)
N(5)-C(24)-C(23)	110.7(4)
N(6)-C(25)-N(7)	127.0(5)
N(6)-C(25)-C(26)	123.0(4)
N(7)-C(25)-C(26)	110.0(4)
C(31)-C(26)-C(27)	121.1(5)
C(31)-C(26)-C(25)	107.3(4)
C(27)-C(26)-C(25)	131.5(5)
C(28)-C(27)-C(26)	116.6(5)
C(28)-C(27)-H(27A)	121.7
C(26)-C(27)-H(27A)	121.7
C(27)-C(28)-C(29)	121.8(5)
C(27)-C(28)-H(28A)	119.1
C(29)-C(28)-H(28A)	119.1
C(28)-C(29)-C(30)	121.3(5)
C(28)-C(29)-H(29A)	119.4
C(30)-C(29)-H(29A)	119.4
C(31)-C(30)-C(29)	116.7(5)
C(31)-C(30)-H(30A)	121.7
C(29)-C(30)-H(30A)	121.7
C(30)-C(31)-C(26)	122.5(4)
C(30)-C(31)-C(32)	131.7(5)
C(26)-C(31)-C(32)	105.8(4)
N(8)-C(32)-N(7)	127.7(4)
N(8)-C(32)-C(31)	121.4(5)
N(7)-C(32)-C(31)	110.9(4)
O(1)-C(33)-C(38)	122.1(5)
O(1)-C(33)-C(34)	121.8(5)
C(38)-C(33)-C(34)	116.1(5)
F(1)-C(34)-C(35)	119.5(5)
F(1)-C(34)-C(33)	118.7(5)
C(35)-C(34)-C(33)	121.8(5)
F(2)-C(35)-C(36)	119.4(6)
F(2)-C(35)-C(34)	120.0(6)

C(36)-C(35)-C(34)	120.5(5)
F(3)-C(36)-C(35)	120.0(6)
F(3)-C(36)-C(37)	120.5(6)
C(35)-C(36)-C(37)	119.5(5)
F(4)-C(37)-C(36)	120.1(6)
F(4)-C(37)-C(38)	120.2(6)
C(36)-C(37)-C(38)	119.8(6)
F(5)-C(38)-C(37)	118.3(5)
F(5)-C(38)-C(33)	119.3(5)
C(37)-C(38)-C(33)	122.4(5)
C(2S)-C(1S)-C(6S)	120.0
C(2S)-C(1S)-C(7S)	119.9(4)
C(6S)-C(1S)-C(7S)	120.1(4)
C(1S)-C(2S)-C(3S)	120.0
C(1S)-C(2S)-H(2SA)	120.0
C(3S)-C(2S)-H(2SA)	120.0
C(4S)-C(3S)-C(2S)	120.0
C(4S)-C(3S)-H(3SA)	120.0
C(2S)-C(3S)-H(3SA)	120.0
C(3S)-C(4S)-C(5S)	120.0
C(3S)-C(4S)-H(4SA)	120.0
C(5S)-C(4S)-H(4SA)	120.0
C(6S)-C(5S)-C(4S)	120.0
C(6S)-C(5S)-H(5SA)	120.0
C(4S)-C(5S)-H(5SA)	120.0
C(5S)-C(6S)-C(1S)	120.0
C(5S)-C(6S)-H(6SA)	120.0
C(1S)-C(6S)-H(6SA)	120.0
C(1S)-C(7S)-H(7SA)	109.5
C(1S)-C(7S)-H(7SB)	109.5
H(7SA)-C(7S)-H(7SB)	109.5
C(1S)-C(7S)-H(7SC)	109.5
H(7SA)-C(7S)-H(7SC)	109.5
H(7SB)-C(7S)-H(7SC)	109.5
C(9S)-C(8S)-H(8SA)	109.5
C(9S)-C(8S)-H(8SB)	109.5

H(8SA)-C(8S)-H(8SB)	109.5
C(9S)-C(8S)-H(8SC)	109.5
H(8SA)-C(8S)-H(8SC)	109.5
H(8SB)-C(8S)-H(8SC)	109.5
C(10S)-C(9S)-C(8S)	100.8(7)
C(10S)-C(9S)-H(9SA)	111.6
C(8S)-C(9S)-H(9SA)	111.6
C(10S)-C(9S)-H(9SB)	111.6
C(8S)-C(9S)-H(9SB)	111.6
H(9SA)-C(9S)-H(9SB)	109.4
C(11S)-C(10S)-C(9S)	107.9(8)
C(11S)-C(10S)-H(10A)	110.1
C(9S)-C(10S)-H(10A)	110.1
C(11S)-C(10S)-H(10B)	110.1
C(9S)-C(10S)-H(10B)	110.1
H(10A)-C(10S)-H(10B)	108.4
C(10S)-C(11S)-C(12S)	109.3(8)
C(10S)-C(11S)-H(11B)	109.8
C(12S)-C(11S)-H(11B)	109.8
C(10S)-C(11S)-H(11C)	109.8
C(12S)-C(11S)-H(11C)	109.8
H(11B)-C(11S)-H(11C)	108.3
C(11S)-C(12S)-C(13S)	102.2(7)
C(11S)-C(12S)-H(12B)	111.3
C(13S)-C(12S)-H(12B)	111.3
C(11S)-C(12S)-H(12C)	111.3
C(13S)-C(12S)-H(12C)	111.3
H(12B)-C(12S)-H(12C)	109.2
C(14S)-C(13S)-C(12S)	102.0(7)
C(14S)-C(13S)-H(13B)	111.4
C(12S)-C(13S)-H(13B)	111.4
C(14S)-C(13S)-H(13C)	111.4
C(12S)-C(13S)-H(13C)	111.4
H(13B)-C(13S)-H(13C)	109.2
C(13S)-C(14S)-H(14B)	109.5
C(13S)-C(14S)-H(14C)	109.5

H(14B)-C(14S)-H(14C)	109.5
C(13S)-C(14S)-H(14D)	109.5
H(14B)-C(14S)-H(14D)	109.5
H(14C)-C(14S)-H(14D)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for F_5PhO-AlPc. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Al(1)	38(1)	36(1)	20(1)	-1(1)	3(1)	1(1)
F(1)	69(2)	60(2)	39(2)	-9(2)	2(2)	10(2)
F(2)	87(3)	66(3)	83(3)	-39(2)	-16(2)	6(2)
F(3)	73(3)	36(2)	144(4)	-12(2)	-2(3)	-7(2)
F(4)	90(3)	50(2)	99(3)	27(2)	18(2)	2(2)
F(5)	66(2)	54(2)	43(2)	6(2)	1(2)	5(2)
O(1)	36(2)	32(2)	40(2)	-4(1)	4(2)	1(2)
N(1)	29(2)	38(2)	22(2)	-4(2)	-1(2)	-1(2)
N(2)	35(2)	36(2)	24(2)	-2(2)	3(2)	-4(2)
N(3)	39(2)	36(2)	24(2)	-3(2)	6(2)	-1(2)
N(4)	35(2)	39(2)	29(2)	0(2)	8(2)	-3(2)
N(5)	45(3)	34(2)	21(2)	-2(2)	0(2)	0(2)
N(6)	53(3)	38(2)	20(2)	-3(2)	6(2)	-2(2)
N(7)	43(3)	37(2)	24(2)	0(2)	5(2)	2(2)
N(8)	35(2)	37(2)	22(2)	-2(2)	1(2)	-1(2)
C(1)	32(3)	35(3)	21(2)	-1(2)	1(2)	0(2)
C(2)	29(3)	42(3)	23(2)	-4(2)	2(2)	-2(2)
C(3)	36(3)	41(3)	28(2)	-5(2)	7(2)	-2(2)
C(4)	48(3)	45(3)	26(2)	-1(2)	8(2)	-6(3)
C(5)	47(3)	49(3)	28(2)	2(2)	4(2)	2(3)
C(6)	44(3)	43(3)	21(2)	2(2)	3(2)	-3(2)
C(7)	35(3)	37(3)	21(2)	-1(2)	4(2)	-1(2)
C(8)	32(3)	35(3)	20(2)	-2(2)	0(2)	1(2)
C(9)	37(3)	33(3)	27(2)	1(2)	9(2)	0(2)
C(10)	31(3)	36(3)	27(2)	-2(2)	-2(2)	0(2)
C(11)	46(3)	38(3)	32(3)	1(2)	-4(2)	-1(2)
C(12)	51(4)	48(3)	35(3)	1(2)	-14(3)	-7(3)
C(13)	50(4)	43(3)	45(3)	7(2)	-15(3)	-9(3)
C(14)	45(3)	38(3)	40(3)	4(2)	1(2)	-7(3)
C(15)	29(3)	39(3)	31(2)	1(2)	0(2)	-1(2)
C(16)	38(3)	31(3)	29(2)	-3(2)	9(2)	0(2)

C(17)	44(3)	34(3)	29(2)	-2(2)	9(2)	-1(2)
C(18)	53(3)	36(3)	29(2)	-1(2)	13(2)	-4(2)
C(19)	61(4)	48(3)	39(3)	-5(2)	21(3)	-10(3)
C(20)	77(5)	51(3)	39(3)	1(3)	28(3)	-10(3)
C(21)	76(5)	49(3)	34(3)	3(2)	23(3)	2(3)
C(22)	63(4)	48(3)	29(3)	0(2)	16(3)	1(3)
C(23)	54(3)	39(3)	22(2)	1(2)	10(2)	-1(3)
C(24)	50(3)	36(3)	24(2)	-2(2)	4(2)	2(2)
C(25)	45(3)	36(3)	23(2)	0(2)	4(2)	3(2)
C(26)	48(3)	39(3)	21(2)	-4(2)	-2(2)	3(2)
C(27)	51(4)	45(3)	26(3)	-1(2)	-2(2)	3(3)
C(28)	52(4)	49(3)	27(2)	-4(2)	-11(2)	6(3)
C(29)	51(4)	45(3)	32(3)	-5(2)	-13(2)	1(3)
C(30)	49(3)	41(3)	30(3)	0(2)	-4(2)	4(3)
C(31)	42(3)	38(3)	22(2)	-1(2)	-5(2)	-3(2)
C(32)	33(3)	36(3)	21(2)	-2(2)	1(2)	2(2)
C(33)	38(3)	31(3)	42(3)	-3(2)	2(2)	5(2)
C(34)	51(4)	43(3)	39(3)	-9(2)	-2(3)	1(3)
C(35)	53(4)	49(4)	63(4)	-22(3)	-7(3)	8(3)
C(36)	47(4)	30(3)	94(5)	-6(3)	0(3)	-1(3)
C(37)	56(4)	40(3)	70(4)	12(3)	10(3)	5(3)
C(38)	49(4)	45(3)	42(3)	2(2)	4(3)	2(3)
C(1S)	58(3)	71(10)	117(10)	-13(7)	43(8)	-16(8)
C(2S)	58(3)	71(10)	117(10)	-13(7)	43(8)	-16(8)
C(3S)	58(3)	71(10)	117(10)	-13(7)	43(8)	-16(8)
C(4S)	58(3)	71(10)	117(10)	-13(7)	43(8)	-16(8)
C(5S)	58(3)	71(10)	117(10)	-13(7)	43(8)	-16(8)
C(6S)	58(3)	71(10)	117(10)	-13(7)	43(8)	-16(8)
C(7S)	92(14)	90(12)	108(13)	-28(10)	26(11)	0(10)
C(8S)	400(20)	96(7)	103(8)	-17(6)	12(9)	-53(10)
C(9S)	400(20)	96(7)	103(8)	-17(6)	12(9)	-53(10)
C(10S)	400(20)	96(7)	103(8)	-17(6)	12(9)	-53(10)
C(11S)	400(20)	96(7)	103(8)	-17(6)	12(9)	-53(10)
C(12S)	400(20)	96(7)	103(8)	-17(6)	12(9)	-53(10)
C(13S)	400(20)	96(7)	103(8)	-17(6)	12(9)	-53(10)
C(14S)	400(20)	96(7)	103(8)	-17(6)	12(9)	-53(10)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) For F_5PhO-AlPc.

	x	y	z	U(eq)
H(3A)	10006	6786	4444	42
H(4A)	9962	7151	3520	48
H(5A)	8377	6509	2840	50
H(6A)	6771	5498	3059	43
H(11A)	3667	3533	3061	48
H(12A)	1904	2472	2854	56
H(13A)	1163	1630	3543	59
H(14A)	2082	1846	4464	50
H(19A)	3097	1557	6115	57
H(20A)	3254	1121	7038	64
H(21A)	4788	1834	7718	62
H(22A)	6180	2999	7500	55
H(27A)	9118	5013	7499	50
H(28A)	10856	6065	7721	53
H(29A)	11722	6853	7046	54
H(30A)	10883	6607	6107	49
H(2SA)	10175	8751	5790	94
H(3SA)	9576	8282	4879	94
H(4SA)	9423	9377	4174	94
H(5SA)	9869	10942	4380	94
H(6SA)	10467	11411	5291	94
H(7SA)	10743	9896	6468	143
H(7SB)	10050	10875	6310	143
H(7SC)	11581	10742	6287	143
H(8SA)	7833	9869	7712	303
H(8SB)	7725	9894	7060	303
H(8SC)	8574	10662	7429	303
H(9SA)	9993	9348	7832	242

H(9SB)	9291	8758	7309	242
H(10A)	9710	10177	6776	242
H(10B)	10797	10418	7300	242
H(11B)	11504	9536	6589	242
H(11C)	10714	8688	6800	242
H(12B)	11996	8791	7673	242
H(12C)	12751	9686	7485	242
H(13B)	13228	7853	7256	242
H(13C)	12821	8416	6690	242
H(14B)	15132	8581	7088	303
H(14C)	14659	9141	7579	303
H(14D)	14377	9549	6970	303

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Table S6. Torsion angles [°] for F_5PhO-AlPc.

N(7)-Al(1)-O(1)-C(33)	137.5(4)
N(3)-Al(1)-O(1)-C(33)	-42.2(4)
N(1)-Al(1)-O(1)-C(33)	-131.7(4)
N(5)-Al(1)-O(1)-C(33)	47.6(4)
C(32)-N(8)-C(1)-N(1)	-1.6(8)
C(32)-N(8)-C(1)-C(2)	177.8(5)
C(8)-N(1)-C(1)-N(8)	179.3(5)
Al(1)-N(1)-C(1)-N(8)	-12.7(7)
C(8)-N(1)-C(1)-C(2)	-0.3(5)
Al(1)-N(1)-C(1)-C(2)	167.8(3)
N(8)-C(1)-C(2)-C(3)	2.4(9)
N(1)-C(1)-C(2)-C(3)	-178.1(5)
N(8)-C(1)-C(2)-C(7)	-179.5(4)
N(1)-C(1)-C(2)-C(7)	0.1(6)
C(7)-C(2)-C(3)-C(4)	-0.8(7)
C(1)-C(2)-C(3)-C(4)	177.1(5)
C(2)-C(3)-C(4)-C(5)	0.5(8)
C(3)-C(4)-C(5)-C(6)	0.4(9)
C(4)-C(5)-C(6)-C(7)	-1.0(8)
C(5)-C(6)-C(7)-C(2)	0.7(8)
C(5)-C(6)-C(7)-C(8)	-177.1(5)
C(3)-C(2)-C(7)-C(6)	0.2(8)
C(1)-C(2)-C(7)-C(6)	-178.1(5)
C(3)-C(2)-C(7)-C(8)	178.5(5)
C(1)-C(2)-C(7)-C(8)	0.1(5)
C(9)-N(2)-C(8)-N(1)	1.3(8)
C(9)-N(2)-C(8)-C(7)	-179.0(5)
C(1)-N(1)-C(8)-N(2)	-179.9(5)
Al(1)-N(1)-C(8)-N(2)	12.2(7)
C(1)-N(1)-C(8)-C(7)	0.3(5)
Al(1)-N(1)-C(8)-C(7)	-167.5(3)
C(6)-C(7)-C(8)-N(2)	-2.0(9)
C(2)-C(7)-C(8)-N(2)	180.0(5)
C(6)-C(7)-C(8)-N(1)	177.7(5)

C(2)-C(7)-C(8)-N(1)	-0.3(6)
C(8)-N(2)-C(9)-N(3)	0.8(8)
C(8)-N(2)-C(9)-C(10)	-178.0(5)
C(16)-N(3)-C(9)-N(2)	-178.3(5)
Al(1)-N(3)-C(9)-N(2)	-16.4(7)
C(16)-N(3)-C(9)-C(10)	0.5(5)
Al(1)-N(3)-C(9)-C(10)	162.5(3)
N(2)-C(9)-C(10)-C(15)	178.7(5)
N(3)-C(9)-C(10)-C(15)	-0.2(6)
N(2)-C(9)-C(10)-C(11)	-0.2(9)
N(3)-C(9)-C(10)-C(11)	-179.2(5)
C(15)-C(10)-C(11)-C(12)	-0.2(8)
C(9)-C(10)-C(11)-C(12)	178.6(5)
C(10)-C(11)-C(12)-C(13)	-0.7(9)
C(11)-C(12)-C(13)-C(14)	1.2(9)
C(12)-C(13)-C(14)-C(15)	-0.8(9)
C(13)-C(14)-C(15)-C(10)	0.0(8)
C(13)-C(14)-C(15)-C(16)	-177.9(5)
C(11)-C(10)-C(15)-C(14)	0.6(8)
C(9)-C(10)-C(15)-C(14)	-178.5(5)
C(11)-C(10)-C(15)-C(16)	178.9(5)
C(9)-C(10)-C(15)-C(16)	-0.2(6)
C(17)-N(4)-C(16)-N(3)	-1.2(8)
C(17)-N(4)-C(16)-C(15)	178.9(5)
C(9)-N(3)-C(16)-N(4)	179.5(5)
Al(1)-N(3)-C(16)-N(4)	17.1(7)
C(9)-N(3)-C(16)-C(15)	-0.6(5)
Al(1)-N(3)-C(16)-C(15)	-163.0(3)
C(14)-C(15)-C(16)-N(4)	-1.4(9)
C(10)-C(15)-C(16)-N(4)	-179.6(5)
C(14)-C(15)-C(16)-N(3)	178.7(5)
C(10)-C(15)-C(16)-N(3)	0.5(6)
C(16)-N(4)-C(17)-N(5)	1.4(8)
C(16)-N(4)-C(17)-C(18)	-178.4(5)
C(24)-N(5)-C(17)-N(4)	178.4(5)
Al(1)-N(5)-C(17)-N(4)	-17.5(7)

C(24)-N(5)-C(17)-C(18)	-1.8(6)
Al(1)-N(5)-C(17)-C(18)	162.4(4)
N(4)-C(17)-C(18)-C(19)	4.1(10)
N(5)-C(17)-C(18)-C(19)	-175.8(6)
N(4)-C(17)-C(18)-C(23)	-178.2(5)
N(5)-C(17)-C(18)-C(23)	2.0(6)
C(23)-C(18)-C(19)-C(20)	0.3(9)
C(17)-C(18)-C(19)-C(20)	177.9(6)
C(18)-C(19)-C(20)-C(21)	0.0(9)
C(19)-C(20)-C(21)-C(22)	0.2(10)
C(20)-C(21)-C(22)-C(23)	-0.7(9)
C(21)-C(22)-C(23)-C(18)	1.0(8)
C(21)-C(22)-C(23)-C(24)	-175.8(6)
C(19)-C(18)-C(23)-C(22)	-0.8(9)
C(17)-C(18)-C(23)-C(22)	-178.9(5)
C(19)-C(18)-C(23)-C(24)	176.7(5)
C(17)-C(18)-C(23)-C(24)	-1.4(6)
C(25)-N(6)-C(24)-N(5)	-0.2(8)
C(25)-N(6)-C(24)-C(23)	177.3(5)
C(17)-N(5)-C(24)-N(6)	178.6(5)
Al(1)-N(5)-C(24)-N(6)	14.8(7)
C(17)-N(5)-C(24)-C(23)	0.9(6)
Al(1)-N(5)-C(24)-C(23)	-162.9(4)
C(22)-C(23)-C(24)-N(6)	-0.3(10)
C(18)-C(23)-C(24)-N(6)	-177.5(5)
C(22)-C(23)-C(24)-N(5)	177.5(6)
C(18)-C(23)-C(24)-N(5)	0.4(6)
C(24)-N(6)-C(25)-N(7)	-2.8(8)
C(24)-N(6)-C(25)-C(26)	177.8(5)
C(32)-N(7)-C(25)-N(6)	180.0(5)
Al(1)-N(7)-C(25)-N(6)	-9.1(8)
C(32)-N(7)-C(25)-C(26)	-0.5(6)
Al(1)-N(7)-C(25)-C(26)	170.4(3)
N(6)-C(25)-C(26)-C(31)	179.3(5)
N(7)-C(25)-C(26)-C(31)	-0.3(6)
N(6)-C(25)-C(26)-C(27)	-1.4(9)

N(7)-C(25)-C(26)-C(27)	179.0(5)
C(31)-C(26)-C(27)-C(28)	0.3(8)
C(25)-C(26)-C(27)-C(28)	-178.9(5)
C(26)-C(27)-C(28)-C(29)	-0.2(8)
C(27)-C(28)-C(29)-C(30)	-0.3(9)
C(28)-C(29)-C(30)-C(31)	0.6(8)
C(29)-C(30)-C(31)-C(26)	-0.5(8)
C(29)-C(30)-C(31)-C(32)	177.6(5)
C(27)-C(26)-C(31)-C(30)	0.0(8)
C(25)-C(26)-C(31)-C(30)	179.4(5)
C(27)-C(26)-C(31)-C(32)	-178.5(5)
C(25)-C(26)-C(31)-C(32)	0.9(6)
C(1)-N(8)-C(32)-N(7)	2.7(8)
C(1)-N(8)-C(32)-C(31)	-176.6(5)
C(25)-N(7)-C(32)-N(8)	-178.2(5)
Al(1)-N(7)-C(32)-N(8)	10.8(7)
C(25)-N(7)-C(32)-C(31)	1.1(5)
Al(1)-N(7)-C(32)-C(31)	-169.9(3)
C(30)-C(31)-C(32)-N(8)	-0.2(9)
C(26)-C(31)-C(32)-N(8)	178.1(5)
C(30)-C(31)-C(32)-N(7)	-179.5(6)
C(26)-C(31)-C(32)-N(7)	-1.2(6)
Al(1)-O(1)-C(33)-C(38)	-90.5(6)
Al(1)-O(1)-C(33)-C(34)	92.4(6)
O(1)-C(33)-C(34)-F(1)	-0.7(8)
C(38)-C(33)-C(34)-F(1)	-178.0(5)
O(1)-C(33)-C(34)-C(35)	178.4(6)
C(38)-C(33)-C(34)-C(35)	1.1(9)
F(1)-C(34)-C(35)-F(2)	-0.1(9)
C(33)-C(34)-C(35)-F(2)	-179.2(6)
F(1)-C(34)-C(35)-C(36)	178.5(6)
C(33)-C(34)-C(35)-C(36)	-0.5(10)
F(2)-C(35)-C(36)-F(3)	-0.5(10)
C(34)-C(35)-C(36)-F(3)	-179.1(6)
F(2)-C(35)-C(36)-C(37)	178.6(6)
C(34)-C(35)-C(36)-C(37)	0.0(10)

F(3)-C(36)-C(37)-F(4)	0.2(10)
C(35)-C(36)-C(37)-F(4)	-178.9(6)
F(3)-C(36)-C(37)-C(38)	179.1(6)
C(35)-C(36)-C(37)-C(38)	0.0(10)
F(4)-C(37)-C(38)-F(5)	0.6(9)
C(36)-C(37)-C(38)-F(5)	-178.3(6)
F(4)-C(37)-C(38)-C(33)	179.5(6)
C(36)-C(37)-C(38)-C(33)	0.6(10)
O(1)-C(33)-C(38)-F(5)	0.5(9)
C(34)-C(33)-C(38)-F(5)	177.8(5)
O(1)-C(33)-C(38)-C(37)	-178.4(6)
C(34)-C(33)-C(38)-C(37)	-1.1(9)
C(6S)-C(1S)-C(2S)-C(3S)	0.0
C(7S)-C(1S)-C(2S)-C(3S)	177.7(14)
C(1S)-C(2S)-C(3S)-C(4S)	0.0
C(2S)-C(3S)-C(4S)-C(5S)	0.0
C(3S)-C(4S)-C(5S)-C(6S)	0.0
C(4S)-C(5S)-C(6S)-C(1S)	0.0
C(2S)-C(1S)-C(6S)-C(5S)	0.0
C(7S)-C(1S)-C(6S)-C(5S)	-177.6(14)
C(8S)-C(9S)-C(10S)-C(11S)	-157.1(16)
C(9S)-C(10S)-C(11S)-C(12S)	-77.0(13)
C(10S)-C(11S)-C(12S)-C(13S)	-176.5(14)
C(11S)-C(12S)-C(13S)-C(14S)	125.7(18)

Symmetry transformations used to generate equivalent atoms:

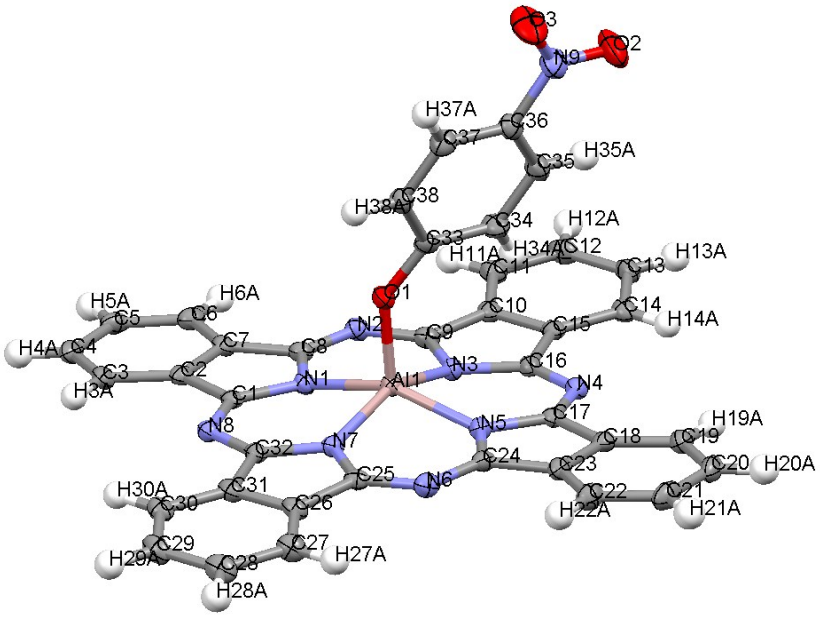

Figure S5. Molecular structure of NO_2PhO-AlPc. Eliposoids shown at 50% probability level. Carbon – grey; nitrogben – blue; aluminum – pink; oxygen – red; hydrogen – white. CCDC deposition number 1052023.

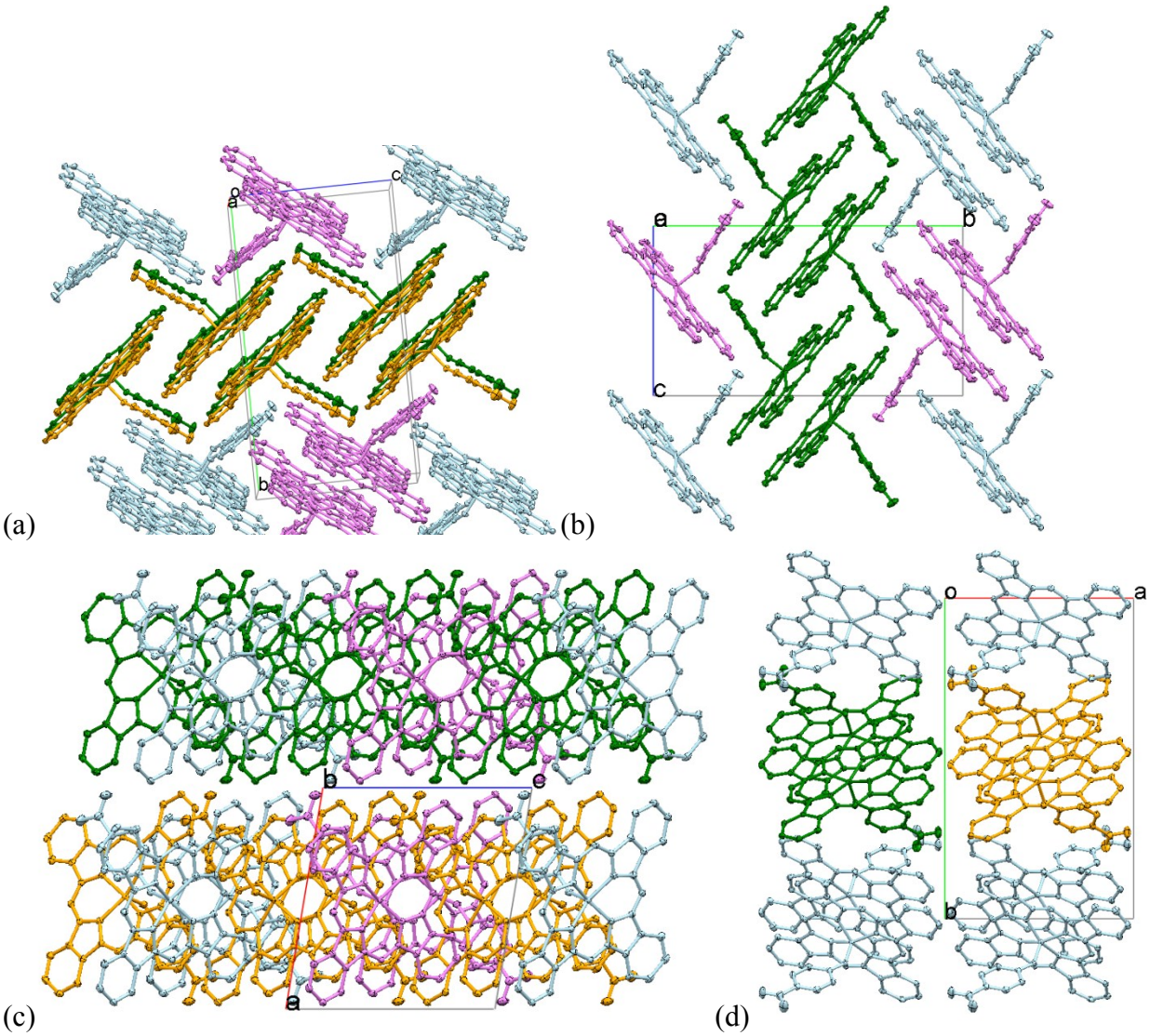

Figure S6. Solid state arrangement of NO_2PhO-AlPc as determined by x-ray diffraction of a single crystal grown by sublimation. (a) General solid state arrangement; (b) Solid-state arrangement along the b-c plane; (c) Solid-state arrangement along the a-c plane; (d) Solid-state arrangement along the a-b plane.

Table S7. Crystal data and structure refinement for NO_2PhO-AlPc.

CCDC Deposition Number	1052023	
Identification code	NO2PhO-AlPc	
Empirical formula	C38 H20 Al N9 O3	
Formula weight	677.61	
Temperature	147(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 12.4623(6) Å	□= 90°.
	b = 20.8620(11) Å	□= 99.518(2)°.
	c = 11.6002(6) Å	□ = 90°.
Volume	2974.4(3) $Å^3$	
Z	4	
Density (calculated)	1.513 Mg/m^3	
Absorption coefficient	0.128 mm^{-1}	
F(000)	1392	
Crystal size	0.160 x 0.120 x 0.080 mm^3	
Theta range for data collection	1.657 to 27.582°.	
Index ranges	-16<=h<=16, -27<=k<=26, -15<=l<=13	
Reflections collected	24158	
Independent reflections	6837 [R(int) = 0.0814]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6904	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6837 / 0 / 460	
Goodness-of-fit on F^2	1.002	
Final R indices [I>2sigma(I)]	R1 = 0.0507, wR2 = 0.0972	
R indices (all data)	R1 = 0.1093, wR2 = 0.1175	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.283 and -0.314 $e.Å^{-3}$	

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for NO2PhO-AlPc. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	4918(1)	5734(1)	1428(1)	16(1)
O(1)	5278(1)	6391(1)	2367(1)	22(1)
O(2)	9652(1)	7303(1)	5313(2)	49(1)
O(3)	8520(2)	7731(1)	6289(2)	50(1)
N(1)	3958(1)	6155(1)	150(2)	17(1)
N(2)	5246(1)	6469(1)	-1106(2)	19(1)
N(3)	6016(1)	5707(1)	393(2)	17(1)
N(4)	7390(1)	5027(1)	1521(2)	19(1)
N(5)	5685(1)	5017(1)	2276(2)	17(1)
N(6)	4378(1)	4689(1)	3498(2)	20(1)
N(7)	3609(1)	5440(1)	1995(2)	17(1)
N(8)	2223(1)	6091(1)	833(2)	18(1)
N(9)	8718(2)	7395(1)	5482(2)	31(1)
C(1)	2873(2)	6302(1)	123(2)	16(1)
C(2)	2500(2)	6740(1)	-818(2)	18(1)
C(3)	1487(2)	7029(1)	-1178(2)	21(1)
C(4)	1387(2)	7413(1)	-2152(2)	24(1)
C(5)	2265(2)	7518(1)	-2748(2)	24(1)
C(6)	3273(2)	7246(1)	-2372(2)	23(1)
C(7)	3374(2)	6851(1)	-1394(2)	18(1)
C(8)	4280(2)	6478(1)	-781(2)	18(1)
C(9)	6045(2)	6113(1)	-549(2)	19(1)
C(10)	7123(2)	6108(1)	-869(2)	19(1)
C(11)	7579(2)	6457(1)	-1689(2)	22(1)
C(12)	8673(2)	6361(1)	-1720(2)	25(1)
C(13)	9291(2)	5923(1)	-971(2)	25(1)
C(14)	8835(2)	5574(1)	-164(2)	21(1)
C(15)	7739(2)	5678(1)	-116(2)	19(1)

C(16)	7041(2)	5433(1)	662(2)	18(1)
C(17)	6755(2)	4837(1)	2264(2)	18(1)
C(18)	7123(2)	4397(1)	3218(2)	20(1)
C(19)	8108(2)	4088(1)	3590(2)	23(1)
C(20)	8174(2)	3700(1)	4566(2)	27(1)
C(21)	7289(2)	3616(1)	5150(2)	29(1)
C(22)	6302(2)	3915(1)	4777(2)	25(1)
C(23)	6240(2)	4308(1)	3798(2)	21(1)
C(24)	5357(2)	4690(1)	3192(2)	18(1)
C(25)	3565(2)	5028(1)	2922(2)	18(1)
C(26)	2479(2)	5010(1)	3213(2)	20(1)
C(27)	2027(2)	4660(1)	4026(2)	25(1)
C(28)	927(2)	4754(1)	4049(2)	27(1)
C(29)	308(2)	5190(1)	3302(2)	26(1)
C(30)	766(2)	5545(1)	2500(2)	22(1)
C(31)	1859(2)	5436(1)	2454(2)	20(1)
C(32)	2571(2)	5688(1)	1694(2)	18(1)
C(33)	6116(2)	6606(1)	3121(2)	19(1)
C(34)	7194(2)	6503(1)	2976(2)	26(1)
C(35)	8045(2)	6754(1)	3761(2)	26(1)
C(36)	7823(2)	7108(1)	4697(2)	22(1)
C(37)	6766(2)	7219(1)	4869(2)	23(1)
C(38)	5921(2)	6970(1)	4083(2)	22(1)

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Table S9. Bond lengths [Å] and angles [°] for NO2PhO-AlPc.

Al(1)-O(1)	1.7615(17)
Al(1)-N(1)	1.9520(18)
Al(1)-N(5)	1.9520(19)
Al(1)-N(7)	1.9559(19)
Al(1)-N(3)	1.965(2)
O(1)-C(33)	1.326(2)
O(2)-N(9)	1.226(3)
O(3)-N(9)	1.228(3)
N(1)-C(1)	1.381(3)
N(1)-C(8)	1.388(3)
N(2)-C(8)	1.321(3)
N(2)-C(9)	1.321(3)
N(3)-C(16)	1.387(3)
N(3)-C(9)	1.387(3)
N(4)-C(17)	1.324(3)
N(4)-C(16)	1.325(3)
N(5)-C(24)	1.381(3)
N(5)-C(17)	1.388(3)
N(6)-C(25)	1.322(3)
N(6)-C(24)	1.325(3)
N(7)-C(32)	1.384(3)
N(7)-C(25)	1.385(3)
N(8)-C(32)	1.322(3)
N(8)-C(1)	1.324(3)
N(9)-C(36)	1.447(3)
C(1)-C(2)	1.441(3)
C(2)-C(7)	1.389(3)
C(2)-C(3)	1.399(3)
C(3)-C(4)	1.374(3)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.406(3)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.381(3)
C(5)-H(5A)	0.9500

C(6)-C(7)	1.392(3)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.455(3)
C(9)-C(10)	1.452(3)
C(10)-C(15)	1.391(3)
C(10)-C(11)	1.392(3)
C(11)-C(12)	1.384(3)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.401(3)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.380(3)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.393(3)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.447(3)
C(17)-C(18)	1.452(3)
C(18)-C(19)	1.391(3)
C(18)-C(23)	1.393(3)
C(19)-C(20)	1.382(3)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.398(4)
C(20)-H(20A)	0.9500
C(21)-C(22)	1.383(3)
C(21)-H(21A)	0.9500
C(22)-C(23)	1.393(3)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.443(3)
C(25)-C(26)	1.449(3)
C(26)-C(27)	1.383(3)
C(26)-C(31)	1.393(3)
C(27)-C(28)	1.389(3)
C(27)-H(27A)	0.9500
C(28)-C(29)	1.397(3)
C(28)-H(28A)	0.9500
C(29)-C(30)	1.384(3)
C(29)-H(29A)	0.9500

C(30)-C(31)	1.390(3)
C(30)-H(30A)	0.9500
C(31)-C(32)	1.449(3)
C(33)-C(34)	1.398(3)
C(33)-C(38)	1.402(3)
C(34)-C(35)	1.382(3)
C(34)-H(34A)	0.9500
C(35)-C(36)	1.379(3)
C(35)-H(35A)	0.9500
C(36)-C(37)	1.384(3)
C(37)-C(38)	1.376(3)
C(37)-H(37A)	0.9500
C(38)-H(38A)	0.9500

O(1)-Al(1)-N(1)	100.45(8)
O(1)-Al(1)-N(5)	103.41(8)
N(1)-Al(1)-N(5)	156.12(8)
O(1)-Al(1)-N(7)	100.24(8)
N(1)-Al(1)-N(7)	87.49(8)
N(5)-Al(1)-N(7)	87.46(8)
O(1)-Al(1)-N(3)	105.54(8)
N(1)-Al(1)-N(3)	87.15(8)
N(5)-Al(1)-N(3)	87.32(8)
N(7)-Al(1)-N(3)	154.21(9)
C(33)-O(1)-Al(1)	139.85(15)
C(1)-N(1)-C(8)	106.33(17)
C(1)-N(1)-Al(1)	126.28(15)
C(8)-N(1)-Al(1)	126.16(14)
C(8)-N(2)-C(9)	121.2(2)
C(16)-N(3)-C(9)	106.63(18)
C(16)-N(3)-Al(1)	125.67(16)
C(9)-N(3)-Al(1)	125.11(15)
C(17)-N(4)-C(16)	121.60(19)
C(24)-N(5)-C(17)	106.31(17)
C(24)-N(5)-Al(1)	125.75(15)
C(17)-N(5)-Al(1)	126.44(15)

C(25)-N(6)-C(24)	121.7(2)
C(32)-N(7)-C(25)	105.87(18)
C(32)-N(7)-Al(1)	126.45(16)
C(25)-N(7)-Al(1)	126.75(14)
C(32)-N(8)-C(1)	121.57(19)
O(2)-N(9)-O(3)	121.8(2)
O(2)-N(9)-C(36)	119.3(2)
O(3)-N(9)-C(36)	119.0(2)
N(8)-C(1)-N(1)	127.6(2)
N(8)-C(1)-C(2)	121.88(19)
N(1)-C(1)-C(2)	110.55(19)
C(7)-C(2)-C(3)	121.8(2)
C(7)-C(2)-C(1)	106.79(19)
C(3)-C(2)-C(1)	131.4(2)
C(4)-C(3)-C(2)	116.8(2)
C(4)-C(3)-H(3A)	121.6
C(2)-C(3)-H(3A)	121.6
C(3)-C(4)-C(5)	121.6(2)
C(3)-C(4)-H(4A)	119.2
C(5)-C(4)-H(4A)	119.2
C(6)-C(5)-C(4)	121.4(2)
C(6)-C(5)-H(5A)	119.3
C(4)-C(5)-H(5A)	119.3
C(5)-C(6)-C(7)	117.2(2)
C(5)-C(6)-H(6A)	121.4
C(7)-C(6)-H(6A)	121.4
C(2)-C(7)-C(6)	121.2(2)
C(2)-C(7)-C(8)	106.4(2)
C(6)-C(7)-C(8)	132.4(2)
N(2)-C(8)-N(1)	127.5(2)
N(2)-C(8)-C(7)	122.6(2)
N(1)-C(8)-C(7)	109.88(19)
N(2)-C(9)-N(3)	127.8(2)
N(2)-C(9)-C(10)	122.2(2)
N(3)-C(9)-C(10)	110.03(19)
C(15)-C(10)-C(11)	121.4(2)

C(15)-C(10)-C(9)	106.4(2)
C(11)-C(10)-C(9)	132.2(2)
C(12)-C(11)-C(10)	117.2(2)
C(12)-C(11)-H(11A)	121.4
C(10)-C(11)-H(11A)	121.4
C(11)-C(12)-C(13)	121.4(2)
C(11)-C(12)-H(12A)	119.3
C(13)-C(12)-H(12A)	119.3
C(14)-C(13)-C(12)	121.3(2)
C(14)-C(13)-H(13A)	119.4
C(12)-C(13)-H(13A)	119.4
C(13)-C(14)-C(15)	117.5(2)
C(13)-C(14)-H(14A)	121.3
C(15)-C(14)-H(14A)	121.3
C(10)-C(15)-C(14)	121.3(2)
C(10)-C(15)-C(16)	107.02(19)
C(14)-C(15)-C(16)	131.6(2)
N(4)-C(16)-N(3)	127.5(2)
N(4)-C(16)-C(15)	122.58(19)
N(3)-C(16)-C(15)	109.9(2)
N(4)-C(17)-N(5)	127.2(2)
N(4)-C(17)-C(18)	122.6(2)
N(5)-C(17)-C(18)	110.3(2)
C(19)-C(18)-C(23)	121.0(2)
C(19)-C(18)-C(17)	132.9(2)
C(23)-C(18)-C(17)	106.10(19)
C(20)-C(19)-C(18)	117.1(2)
C(20)-C(19)-H(19A)	121.4
C(18)-C(19)-H(19A)	121.4
C(19)-C(20)-C(21)	121.7(2)
C(19)-C(20)-H(20A)	119.2
C(21)-C(20)-H(20A)	119.2
C(22)-C(21)-C(20)	121.6(2)
C(22)-C(21)-H(21A)	119.2
C(20)-C(21)-H(21A)	119.2
C(21)-C(22)-C(23)	116.6(2)

C(21)-C(22)-H(22A)	121.7
C(23)-C(22)-H(22A)	121.7
C(22)-C(23)-C(18)	122.0(2)
C(22)-C(23)-C(24)	131.0(2)
C(18)-C(23)-C(24)	106.9(2)
N(6)-C(24)-N(5)	127.54(19)
N(6)-C(24)-C(23)	122.0(2)
N(5)-C(24)-C(23)	110.38(19)
N(6)-C(25)-N(7)	126.8(2)
N(6)-C(25)-C(26)	122.4(2)
N(7)-C(25)-C(26)	110.82(19)
C(27)-C(26)-C(31)	121.4(2)
C(27)-C(26)-C(25)	132.4(2)
C(31)-C(26)-C(25)	106.2(2)
C(26)-C(27)-C(28)	117.0(2)
C(26)-C(27)-H(27A)	121.5
C(28)-C(27)-H(27A)	121.5
C(27)-C(28)-C(29)	121.7(2)
C(27)-C(28)-H(28A)	119.2
C(29)-C(28)-H(28A)	119.2
C(30)-C(29)-C(28)	121.2(2)
C(30)-C(29)-H(29A)	119.4
C(28)-C(29)-H(29A)	119.4
C(29)-C(30)-C(31)	117.0(2)
C(29)-C(30)-H(30A)	121.5
C(31)-C(30)-H(30A)	121.5
C(30)-C(31)-C(26)	121.7(2)
C(30)-C(31)-C(32)	131.7(2)
C(26)-C(31)-C(32)	106.56(19)
N(8)-C(32)-N(7)	127.2(2)
N(8)-C(32)-C(31)	122.21(19)
N(7)-C(32)-C(31)	110.6(2)
O(1)-C(33)-C(34)	122.4(2)
O(1)-C(33)-C(38)	119.2(2)
C(34)-C(33)-C(38)	118.4(2)
C(35)-C(34)-C(33)	120.6(2)

C(35)-C(34)-H(34A)	119.7
C(33)-C(34)-H(34A)	119.7
C(36)-C(35)-C(34)	119.4(2)
C(36)-C(35)-H(35A)	120.3
C(34)-C(35)-H(35A)	120.3
C(35)-C(36)-C(37)	121.5(2)
C(35)-C(36)-N(9)	118.8(2)
C(37)-C(36)-N(9)	119.6(2)
C(38)-C(37)-C(36)	119.0(2)
C(38)-C(37)-H(37A)	120.5
C(36)-C(37)-H(37A)	120.5
C(37)-C(38)-C(33)	121.1(2)
C(37)-C(38)-H(38A)	119.4
C(33)-C(38)-H(38A)	119.4

Symmetry transformations used to generate equivalent atoms:

Table S10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for NO2PhO-AlPc. The anisotropic
displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Al(1)	14(1)	17(1)	18(1)	0(1)	2(1)	-1(1)
O(1)	17(1)	23(1)	24(1)	-5(1)	-1(1)	0(1)
O(2)	22(1)	68(2)	53(1)	-20(1)	-3(1)	0(1)
O(3)	39(1)	69(2)	39(1)	-29(1)	-2(1)	0(1)
N(1)	15(1)	18(1)	18(1)	-1(1)	3(1)	-1(1)
N(2)	18(1)	20(1)	19(1)	2(1)	2(1)	-2(1)
N(3)	15(1)	17(1)	18(1)	0(1)	1(1)	0(1)
N(4)	17(1)	18(1)	20(1)	-2(1)	1(1)	0(1)
N(5)	16(1)	17(1)	18(1)	0(1)	2(1)	0(1)
N(6)	22(1)	21(1)	18(1)	2(1)	3(1)	-1(1)
N(7)	17(1)	16(1)	18(1)	1(1)	1(1)	-2(1)
N(8)	17(1)	18(1)	18(1)	-1(1)	2(1)	-1(1)
N(9)	28(1)	35(1)	29(1)	-4(1)	-2(1)	2(1)
C(1)	16(1)	15(1)	17(1)	-5(1)	1(1)	-3(1)
C(2)	20(1)	16(1)	16(1)	-2(1)	0(1)	-2(1)
C(3)	18(1)	20(1)	23(1)	-2(1)	-2(1)	-2(1)
C(4)	24(1)	19(1)	25(1)	0(1)	-7(1)	1(1)
C(5)	31(1)	16(1)	22(1)	3(1)	-3(1)	-4(1)
C(6)	27(1)	19(1)	22(1)	-2(1)	2(1)	-4(1)
C(7)	17(1)	18(1)	19(1)	-3(1)	-1(1)	-3(1)
C(8)	19(1)	17(1)	18(1)	-2(1)	2(1)	-3(1)
C(9)	20(1)	18(1)	18(1)	-1(1)	4(1)	-4(1)
C(10)	19(1)	18(1)	21(1)	-5(1)	4(1)	-2(1)
C(11)	22(1)	24(1)	22(1)	-3(1)	6(1)	-4(1)
C(12)	26(1)	28(1)	25(1)	-2(1)	11(1)	-7(1)
C(13)	17(1)	26(1)	32(2)	-7(1)	6(1)	-3(1)
C(14)	19(1)	23(1)	21(1)	-6(1)	4(1)	-1(1)
C(15)	19(1)	17(1)	21(1)	-7(1)	3(1)	-3(1)
C(16)	16(1)	17(1)	19(1)	-4(1)	3(1)	0(1)
C(17)	17(1)	17(1)	18(1)	-4(1)	0(1)	-2(1)

C(18)	22(1)	15(1)	22(1)	-2(1)	-2(1)	-1(1)
C(19)	21(1)	20(1)	25(1)	-2(1)	-1(1)	1(1)
C(20)	26(1)	22(1)	28(2)	-2(1)	-8(1)	7(1)
C(21)	39(2)	22(1)	24(2)	4(1)	-4(1)	5(1)
C(22)	30(1)	23(1)	22(1)	2(1)	2(1)	1(1)
C(23)	22(1)	18(1)	21(1)	-1(1)	-1(1)	1(1)
C(24)	22(1)	14(1)	17(1)	0(1)	1(1)	-1(1)
C(25)	21(1)	18(1)	14(1)	-2(1)	3(1)	-4(1)
C(26)	19(1)	23(1)	17(1)	-3(1)	3(1)	-5(1)
C(27)	26(1)	29(2)	19(1)	1(1)	5(1)	-4(1)
C(28)	29(1)	35(2)	20(1)	-5(1)	10(1)	-6(1)
C(29)	19(1)	37(2)	23(1)	-7(1)	9(1)	-4(1)
C(30)	21(1)	27(1)	18(1)	-6(1)	3(1)	-3(1)
C(31)	19(1)	23(1)	18(1)	-4(1)	4(1)	-4(1)
C(32)	15(1)	18(1)	20(1)	-5(1)	3(1)	-2(1)
C(33)	21(1)	15(1)	21(1)	2(1)	4(1)	-3(1)
C(34)	26(1)	26(1)	28(2)	-10(1)	6(1)	-2(1)
C(35)	18(1)	29(1)	29(2)	-2(1)	5(1)	-1(1)
C(36)	21(1)	24(1)	19(1)	2(1)	-1(1)	-1(1)
C(37)	27(1)	25(1)	19(1)	-2(1)	3(1)	2(1)
C(38)	18(1)	23(1)	25(1)	-2(1)	6(1)	-1(1)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for NO2PhO-AlPc.

	x	y	z	U(eq)
H(3A)	896	6962	-768	25
H(4A)	708	7612	-2430	29
H(5A)	2164	7783	-3424	29
H(6A)	3871	7325	-2765	27
H(11A)	7158	6749	-2206	27
H(12A)	9012	6597	-2261	30
H(13A)	10038	5864	-1019	30
H(14A)	9252	5274	340	25
H(19A)	8709	4140	3191	27
H(20A)	8838	3485	4846	32
H(21A)	7367	3347	5820	35
H(22A)	5698	3856	5169	30
H(27A)	2449	4370	4544	30
H(28A)	587	4516	4586	33
H(29A)	-442	5244	3345	31
H(30A)	353	5850	2004	26
H(34A)	7342	6257	2331	31
H(35A)	8776	6684	3656	31
H(37A)	6626	7464	5519	28
H(38A)	5193	7045	4193	26

Table S12. Torsion angles [°] for NO2PhO-AlPc.

N(1)-Al(1)-O(1)-C(33)	-146.3(2)
N(5)-Al(1)-O(1)-C(33)	34.6(2)
N(7)-Al(1)-O(1)-C(33)	124.4(2)
N(3)-Al(1)-O(1)-C(33)	-56.4(2)
C(32)-N(8)-C(1)-N(1)	-0.3(3)
C(32)-N(8)-C(1)-C(2)	180.0(2)
C(8)-N(1)-C(1)-N(8)	178.6(2)
Al(1)-N(1)-C(1)-N(8)	-13.5(3)
C(8)-N(1)-C(1)-C(2)	-1.6(2)
Al(1)-N(1)-C(1)-C(2)	166.27(15)
N(8)-C(1)-C(2)-C(7)	-178.9(2)
N(1)-C(1)-C(2)-C(7)	1.3(2)
N(8)-C(1)-C(2)-C(3)	0.8(4)
N(1)-C(1)-C(2)-C(3)	-178.9(2)
C(7)-C(2)-C(3)-C(4)	2.0(3)
C(1)-C(2)-C(3)-C(4)	-177.8(2)
C(2)-C(3)-C(4)-C(5)	-0.9(3)
C(3)-C(4)-C(5)-C(6)	-0.7(4)
C(4)-C(5)-C(6)-C(7)	1.4(3)
C(3)-C(2)-C(7)-C(6)	-1.3(3)
C(1)-C(2)-C(7)-C(6)	178.5(2)
C(3)-C(2)-C(7)-C(8)	179.8(2)
C(1)-C(2)-C(7)-C(8)	-0.4(2)
C(5)-C(6)-C(7)-C(2)	-0.4(3)
C(5)-C(6)-C(7)-C(8)	178.2(2)
C(9)-N(2)-C(8)-N(1)	1.7(4)
C(9)-N(2)-C(8)-C(7)	-178.3(2)
C(1)-N(1)-C(8)-N(2)	-178.7(2)
Al(1)-N(1)-C(8)-N(2)	13.4(3)
C(1)-N(1)-C(8)-C(7)	1.3(2)
Al(1)-N(1)-C(8)-C(7)	-166.58(15)
C(2)-C(7)-C(8)-N(2)	179.5(2)
C(6)-C(7)-C(8)-N(2)	0.8(4)
C(2)-C(7)-C(8)-N(1)	-0.6(3)

C(6)-C(7)-C(8)-N(1)	-179.3(2)
C(8)-N(2)-C(9)-N(3)	1.0(4)
C(8)-N(2)-C(9)-C(10)	-178.3(2)
C(16)-N(3)-C(9)-N(2)	179.2(2)
Al(1)-N(3)-C(9)-N(2)	-18.3(3)
C(16)-N(3)-C(9)-C(10)	-1.5(2)
Al(1)-N(3)-C(9)-C(10)	161.05(15)
N(2)-C(9)-C(10)-C(15)	-179.2(2)
N(3)-C(9)-C(10)-C(15)	1.4(3)
N(2)-C(9)-C(10)-C(11)	4.1(4)
N(3)-C(9)-C(10)-C(11)	-175.3(2)
C(15)-C(10)-C(11)-C(12)	-0.4(3)
C(9)-C(10)-C(11)-C(12)	176.0(2)
C(10)-C(11)-C(12)-C(13)	1.0(3)
C(11)-C(12)-C(13)-C(14)	-0.6(4)
C(12)-C(13)-C(14)-C(15)	-0.5(3)
C(11)-C(10)-C(15)-C(14)	-0.8(3)
C(9)-C(10)-C(15)-C(14)	-177.9(2)
C(11)-C(10)-C(15)-C(16)	176.4(2)
C(9)-C(10)-C(15)-C(16)	-0.8(2)
C(13)-C(14)-C(15)-C(10)	1.2(3)
C(13)-C(14)-C(15)-C(16)	-175.2(2)
C(17)-N(4)-C(16)-N(3)	-0.8(4)
C(17)-N(4)-C(16)-C(15)	176.0(2)
C(9)-N(3)-C(16)-N(4)	178.1(2)
Al(1)-N(3)-C(16)-N(4)	15.7(3)
C(9)-N(3)-C(16)-C(15)	1.0(2)
Al(1)-N(3)-C(16)-C(15)	-161.42(15)
C(10)-C(15)-C(16)-N(4)	-177.4(2)
C(14)-C(15)-C(16)-N(4)	-0.7(4)
C(10)-C(15)-C(16)-N(3)	-0.1(3)
C(14)-C(15)-C(16)-N(3)	176.6(2)
C(16)-N(4)-C(17)-N(5)	0.0(3)
C(16)-N(4)-C(17)-C(18)	-179.5(2)
C(24)-N(5)-C(17)-N(4)	179.0(2)
Al(1)-N(5)-C(17)-N(4)	-14.5(3)

C(24)-N(5)-C(17)-C(18)	-1.5(2)
Al(1)-N(5)-C(17)-C(18)	165.05(15)
N(4)-C(17)-C(18)-C(19)	0.2(4)
N(5)-C(17)-C(18)-C(19)	-179.4(2)
N(4)-C(17)-C(18)-C(23)	-179.6(2)
N(5)-C(17)-C(18)-C(23)	0.8(3)
C(23)-C(18)-C(19)-C(20)	-1.1(3)
C(17)-C(18)-C(19)-C(20)	179.1(2)
C(18)-C(19)-C(20)-C(21)	0.6(3)
C(19)-C(20)-C(21)-C(22)	0.2(4)
C(20)-C(21)-C(22)-C(23)	-0.6(4)
C(21)-C(22)-C(23)-C(18)	0.1(4)
C(21)-C(22)-C(23)-C(24)	-179.4(2)
C(19)-C(18)-C(23)-C(22)	0.8(4)
C(17)-C(18)-C(23)-C(22)	-179.4(2)
C(19)-C(18)-C(23)-C(24)	-179.7(2)
C(17)-C(18)-C(23)-C(24)	0.2(2)
C(25)-N(6)-C(24)-N(5)	-0.6(4)
C(25)-N(6)-C(24)-C(23)	-178.4(2)
C(17)-N(5)-C(24)-N(6)	-176.4(2)
Al(1)-N(5)-C(24)-N(6)	16.9(3)
C(17)-N(5)-C(24)-C(23)	1.6(2)
Al(1)-N(5)-C(24)-C(23)	-165.06(15)
C(22)-C(23)-C(24)-N(6)	-3.5(4)
C(18)-C(23)-C(24)-N(6)	177.0(2)
C(22)-C(23)-C(24)-N(5)	178.4(2)
C(18)-C(23)-C(24)-N(5)	-1.1(3)
C(24)-N(6)-C(25)-N(7)	-3.2(4)
C(24)-N(6)-C(25)-C(26)	177.2(2)
C(32)-N(7)-C(25)-N(6)	-179.3(2)
Al(1)-N(7)-C(25)-N(6)	-9.8(3)
C(32)-N(7)-C(25)-C(26)	0.4(2)
Al(1)-N(7)-C(25)-C(26)	169.82(15)
N(6)-C(25)-C(26)-C(27)	-3.1(4)
N(7)-C(25)-C(26)-C(27)	177.3(2)
N(6)-C(25)-C(26)-C(31)	178.3(2)

N(7)-C(25)-C(26)-C(31)	-1.4(3)
C(31)-C(26)-C(27)-C(28)	0.0(3)
C(25)-C(26)-C(27)-C(28)	-178.4(2)
C(26)-C(27)-C(28)-C(29)	-1.2(4)
C(27)-C(28)-C(29)-C(30)	0.4(4)
C(28)-C(29)-C(30)-C(31)	1.6(4)
C(29)-C(30)-C(31)-C(26)	-2.8(3)
C(29)-C(30)-C(31)-C(32)	176.1(2)
C(27)-C(26)-C(31)-C(30)	2.0(4)
C(25)-C(26)-C(31)-C(30)	-179.2(2)
C(27)-C(26)-C(31)-C(32)	-177.1(2)
C(25)-C(26)-C(31)-C(32)	1.7(2)
C(1)-N(8)-C(32)-N(7)	0.9(3)
C(1)-N(8)-C(32)-C(31)	-177.8(2)
C(25)-N(7)-C(32)-N(8)	-178.0(2)
Al(1)-N(7)-C(32)-N(8)	12.5(3)
C(25)-N(7)-C(32)-C(31)	0.8(2)
Al(1)-N(7)-C(32)-C(31)	-168.74(15)
C(30)-C(31)-C(32)-N(8)	-1.7(4)
C(26)-C(31)-C(32)-N(8)	177.2(2)
C(30)-C(31)-C(32)-N(7)	179.4(2)
C(26)-C(31)-C(32)-N(7)	-1.6(3)
Al(1)-O(1)-C(33)-C(34)	33.7(4)
Al(1)-O(1)-C(33)-C(38)	-148.4(2)
O(1)-C(33)-C(34)-C(35)	177.7(2)
C(38)-C(33)-C(34)-C(35)	-0.1(4)
C(33)-C(34)-C(35)-C(36)	0.2(4)
C(34)-C(35)-C(36)-C(37)	-0.1(4)
C(34)-C(35)-C(36)-N(9)	-177.1(2)
O(2)-N(9)-C(36)-C(35)	-1.8(4)
O(3)-N(9)-C(36)-C(35)	177.1(2)
O(2)-N(9)-C(36)-C(37)	-178.8(2)
O(3)-N(9)-C(36)-C(37)	0.1(4)
C(35)-C(36)-C(37)-C(38)	-0.1(4)
N(9)-C(36)-C(37)-C(38)	176.9(2)
C(36)-C(37)-C(38)-C(33)	0.2(4)

O(1)-C(33)-C(38)-C(37)	-178.0(2)
C(34)-C(33)-C(38)-C(37)	-0.1(4)

Symmetry transformations used to generate equivalent atoms:

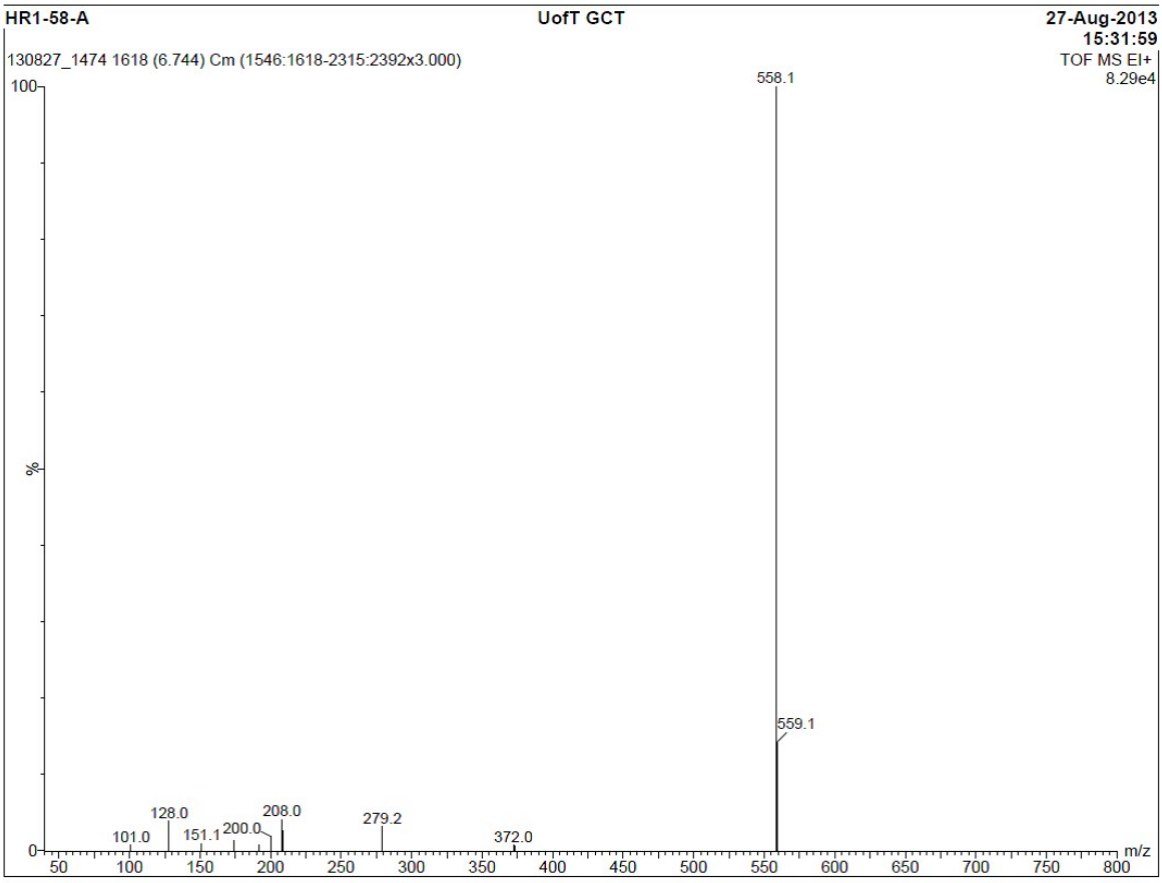

Figure S7. Mass spectrum (TOF-EI) of F-AlPc produced from the decomposition of F_5PhO-AlPc.