A New Charge Transporting Host Material for Short Wavelength Organic Electrophosphorescence: 2,7–Bis(diphenylphosphine oxide)–9,9–dimethylfluorene

Asanga B. Padmaperuma, Linda S. Sapochak,* and Paul E. Burrows

Materials Division, Energy Science and Technology Directorate, Pacific Northwest National Laboratory, 908 Battelle Blvd, Richland, WA 99352, USA.

Supplementary information

Crystallographic Experimental Section

Data Collection

A colorless prismatic crystal was selected under ambient conditions. The crystal was mounted and centered in the X-ray beam by using a video camera.

The crystal evaluation and data collection were performed room temperature on a Bruker CCD-1000 diffractometer with Mo K_α (λ = 0.71073 Å) radiation and the detector to crystal distance of 5.03 cm.

The initial cell constants were obtained from three series of ω scans at different starting angles. Each series consisted of 30 frames collected at intervals of 0.3º in a 10º range about ω with the exposure time of 20 seconds per frame. The obtained reflections were successfully indexed by an automated indexing routine built in the SMART program. The final cell constants were calculated from a set of strong reflections from the actual data collection.

The data were collected using the full sphere routine by collecting four sets of frames with 0.3º scans in ω with an exposure time 20 sec per frame. This dataset was corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements [1] using SADABS software [2].

Structure Solution and Refinement

The systematic absences in the diffraction data were consistent for the space groups $P1$ and $P\bar{1}$ [2]. The *E*-statistics strongly suggested the centrosymmetric space group $P\bar{1}$

yielded chemically reasonable and computationally stable results of refinement. The positions of almost all non-hydrogen atoms were found by direct methods. The remaining atoms were located in an alternating series of least-squares cycles and difference Fourier maps. All non-hydrogen atoms were refined in full-matrix anisotropic approximation. All hydrogen atoms were placed in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients.

The ORTEP diagram was drawn at 50% probability level. H-atoms were omitted for clarity.

The resulting CIF file has been tested with PLATON [3] software. The results and comments have been included to output package (Platon_Po06.doc)

References

[1] Blessing, R.H. *Acta Cryst*. **1995**, *A51*, 33-38.

[2] All software and sources of the scattering factors are contained in the SHELXTL (version 5.1) program library (G. Sheldrick, Bruker Analytical X-Ray Systems, Madison, WI).

[3] A.L.Spek, J.Appl.Cryst. 36, 7-13.

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Po06. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	12419(1)	1848(1)	4229(1)	33(1)
P(2)	3092(1)	7285(1)	1108(1)	37(1)
C(1)	13503(2)	2860(2)	2693(2)	58(1)
C(2)	14444(3)	2820(3)	1962(2)	75(1)
C(3)	15470(3)	1605(3)	1742(2)	78(1)
C(4)	15555(2)	426(3)	2232(2)	71(1)
C(5)	14599(2)	456(2)	2959(1)	50(1)
C(6)	13563(2)	1685(2)	3199(1)	38(1)
C(7)	12549(2)	210(2)	4631(1)	36(1)

C(8)	13547(2)	-630(2)	5247(2)	61(1)
C(9)	13738(3)	-1912(2)	5583(2)	73(1)
C(10)	12910(2)	-2356(2)	5324(2)	63(1)
C(11)	11906(2)	-1539(2)	4722(2)	62(1)
C(12)	11718(2)	-262(2)	4374(2)	51(1)
C(13)	10725(1)	2932(2)	3828(1)	33(1)
C(14)	10326(2)	2893(2)	2961(1)	35(1)
C(15)	9004(2)	3767(2)	2715(1)	30(1)
C(16)	8322(2)	3895(2)	1834(1)	34(1)
C(17)	9014(2)	4316(2)	947(1)	56(1)
C(18)	8308(2)	2583(2)	1739(2)	52(1)
C(19)	6885(1)	5011(2)	2034(1)	32(1)
C(20)	5767(2)	5558(2)	1493(1)	36(1)
C(21)	4529(2)	6570(2)	1830(1)	37(1)
C(22)	1607(2)	7493(2)	1876(1)	39(1)
C(23)	1231(2)	6479(2)	1984(2)	55(1)
C(24)	111(2)	6575(3)	2555(2)	69(1)
C(25)	-672(2)	7695(3)	3017(2)	67(1)
C(26)	-331(2)	8723(2)	2907(2)	62(1)
C(27)	811(2)	8624(2)	2338(1)	49(1)
C(28)	2773(2)	8983(2)	664(1)	39(1)
C(29)	1765(2)	9700(2)	29(1)	50(1)
C(30)	1501(2)	10981(2)	-377(2)	62(1)
C(31)	2232(2)	11562(2)	-154(2)	67(1)
C(32)	3210(3)	10878(3)	474(2)	84(1)
C(33)	3498(2)	9581(2)	882(2)	68(1)
C(34)	4437(2)	7006(2)	2697(1)	45(1)
C(35)	5552(2)	6470(2)	3235(1)	42(1)
C(36)	6777(2)	5466(2)	2899(1)	32(1)
C(37)	8093(1)	4691(1)	3327(1)	30(1)
C(38)	8484(2)	4743(2)	4184(1)	34(1)
C(39)	9803(2)	3847(2)	4430(1)	35(1)
O(1)	12737(1)	2389(1)	4977(1)	45(1)
O(2)	3302(1)	6456(1)	352(1)	53(1)

Table 2. Bond lengths [Å] and angles [°] for Po06.

P(1)-O(1)	1.4867(12)	C(11)-C(12)	1.379(3)	C(24)-C(25)	1.377(4)
P(1)-C(7)	1.7987(18)	C(11)-H(11)	0.9300	C(24)-H(24)	0.9300
P(1)-C(6)	1.8017(18)	C(12)-H(12)	0.9300	C(25)-C(26)	1.374(3)
P(1)-C(13)	1.8087(15)	C(13)-C(39)	1.393(2)	C(25)-H(25)	0.9300
P(2)-O(2)	1.4844(13)	C(13)-C(14)	1.399(2)	C(26)-C(27)	1.392(3)
P(2)-C(21)	1.8024(16)	C(14)-C(15)	1.385(2)	C(26)-H(26)	0.9300
P(2)-C(28)	1.8044(19)	C(14)-H(14)	0.9300	C(27)-H(27)	0.9300
P(2)-C(22)	1.8080(18)	C(15)-C(37)	1.404(2)	C(28)-C(33)	1.376(3)
C(1)-C(2)	1.379(3)	C(15)-C(16)	1.522(2)	C(28)-C(29)	1.388(2)
C(1)-C(6)	1.388(3)	C(16)-C(19)	1.526(2)	C(29)-C(30)	1.380(3)
C(1)-H(1)	0.9300	C(16)-C(18)	1.530(2)	C(29)-H(29)	0.9300
C(2)-C(3)	1.365(4)	C(16)-C(17)	1.535(2)	C(30)-C(31)	1.369(3)
C(2)-H(2)	0.9300	C(17)-H(17A)	0.9600	C(30)-H(30)	0.9300
C(3)-C(4)	1.375(4)	C(17)-H(17B)	0.9600	C(31)-C(32)	1.356(3)
C(3)-H(3)	0.9300	C(17)-H(17C)	0.9600	C(31)-H(31)	0.9300
C(4)-C(5)	1.388(3)	C(18)-H(18A)	0.9600	C(32)-C(33)	1.390(3)
C(4)-H(4)	0.9300	C(18)-H(18B)	0.9600	C(32)-H(32)	0.9300
C(5)-C(6)	1.387(2)	C(18)-H(18C)	0.9600	C(33)-H(33)	0.9300
C(5)-H(5)	0.9300	C(19)-C(20)	1.386(2)	C(34)-C(35)	1.381(2)
C(7)-C(8)	1.383(2)	C(19)-C(36)	1.401(2)	C(34)-H(34)	0.9300
C(7)-C(12)	1.389(2)	C(20)-C(21)	1.402(2)	C(35)-C(36)	1.389(2)
C(8)-C(9)	1.379(3)	C(20)-H(20)	0.9300	C(35)-H(35)	0.9300
C(8)-H(8)	0.9300	C(21)-C(34)	1.398(2)	C(36)-C(37)	1.466(2)
C(9)-C(10)	1.364(3)	C(22)-C(23)	1.386(3)	C(37)-C(38)	1.387(2)
C(9)-H(9)	0.9300	C(22)-C(27)	1.388(3)	C(38)-C(39)	1.388(2)
C(10)-C(11)	1.369(3)	C(23)-C(24)	1.374(3)	C(38)-H(38)	0.9300
C(10)-H(10)	0.9300	C(23)-H(23)	0.9300	C(39)-H(39)	0.9300
O(1)-P(1)-C(7)	111.32(8)	O(2)-P(2)-C(21)	112.59(7)	C(2)-C(1)-C(6)	121.2(2)
O(1)-P(1)-C(6)	111.76(8)	O(2)-P(2)-C(28)	113.00(8)	C(2)-C(1)-H(1)	119.4
C(7)-P(1)-C(6)	107.44(8)	C(21)-P(2)-C(28)	107.04(8)	C(6)-C(1)-H(1)	119.4
O(1)-P(1)-C(13)	112.51(7)	O(2)-P(2)-C(22)	111.65(8)	C(3)-C(2)-C(1)	119.6(2)
C(7)-P(1)-C(13)	107.74(7)	C(21)-P(2)-C(22)	107.59(8)	C(3)-C(2)-H(2)	120.2
C(6)-P(1)-C(13)	105.76(8)	C(28)-P(2)-C(22)	104.46(8)	C(1)-C(2)-H(2)	120.2

C(2)-C(3)-C(4)	120.4(2)	C(14)-C(15)-C(37)	119.86(14)	C(23)-C(24)-C(25)	120.5(2)
C(2)-C(3)-H(3)	119.8	C(14)-C(15)-C(16)	129.11(13)	C(23)-C(24)-H(24)	119.8
C(4)-C(3)-H(3)	119.8	C(37)-C(15)-C(16)	111.02(12)	C(25)-C(24)-H(24)	119.8
C(3)-C(4)-C(5)	120.4(2)	C(15)-C(16)-C(19)	101.21(12)	C(26)-C(25)-C(24)	119.9(2)
C(3)-C(4)-H(4)	119.8	C(15)-C(16)-C(18)	111.29(13)	C(26)-C(25)-H(25)	120.1
C(5)-C(4)-H(4)	119.8	C(19)-C(16)-C(18)	111.16(14)	C(24)-C(25)-H(25)	120.1
C(6)-C(5)-C(4)	119.7(2)	C(15)-C(16)-C(17)	111.42(14)	C(25)-C(26)-C(27)	119.9(2)
C(6)-C(5)-H(5)	120.2	C(19)-C(16)-C(17)	111.28(14)	C(25)-C(26)-H(26)	120.0
C(4)-C(5)-H(5)	120.2	C(18)-C(16)-C(17)	110.22(15)	C(27)-C(26)-H(26)	120.0
C(5)-C(6)-C(1)	118.70(17)	C(16)-C(17)-H(17A)	109.5	C(22)-C(27)-C(26)	120.40(19)
C(5)-C(6)-P(1)	123.23(14)	C(16)-C(17)-H(17B)	109.5	C(22)-C(27)-H(27)	119.8
C(1)-C(6)-P(1)	117.57(14)	H(17A)-C(17)-H(17B)	109.5	C(26)-C(27)-H(27)	119.8
C(8)-C(7)-C(12)	118.17(17)	C(16)-C(17)-H(17C)	109.5	C(33)-C(28)-C(29)	118.43(18)
C(8)-C(7)-P(1)	116.98(14)	H(17A)-C(17)-H(17C)	109.5	C(33)-C(28)-P(2)	124.37(14)
C(12)-C(7)-P(1)	124.84(13)	H(17B)-C(17)-H(17C)	109.5	C(29)-C(28)-P(2)	117.13(14)
C(9)-C(8)-C(7)	121.21(19)	C(16)-C(18)-H(18A)	109.5	C(30)-C(29)-C(28)	120.77(19)
C(9)-C(8)-H(8)	119.4	C(16)-C(18)-H(18B)	109.5	C(30)-C(29)-H(29)	119.6
C(7)-C(8)-H(8)	119.4	H(18A)-C(18)-H(18B)	109.5	C(28)-C(29)-H(29)	119.6
C(10)-C(9)-C(8)	119.8(2)	C(16)-C(18)-H(18C)	109.5	C(31)-C(30)-C(29)	120.10(19)
C(10)-C(9)-H(9)	120.1	H(18A)-C(18)-H(18C)	109.5	C(31)-C(30)-H(30)	120.0
C(8)-C(9)-H(9)	120.1	H(18B)-C(18)-H(18C)	109.5	C(29)-C(30)-H(30)	120.0
C(9)-C(10)-C(11)	120.1(2)	C(20)-C(19)-C(36)	120.46(13)	C(32)-C(31)-C(30)	119.7(2)
C(9)-C(10)-H(10)	120.0	C(20)-C(19)-C(16)	128.74(14)	C(32)-C(31)-H(31)	120.1
C(11)-C(10)-H(10)	120.0	C(36)-C(19)-C(16)	110.80(12)	C(30)-C(31)-H(31)	120.1
C(10)-C(11)-C(12)	120.54(19)	C(19)-C(20)-C(21)	118.71(14)	C(31)-C(32)-C(33)	120.9(2)
C(10)-C(11)-H(11)	119.7	C(19)-C(20)-H(20)	120.6	C(31)-C(32)-H(32)	119.5
C(12)-C(11)-H(11)	119.7	C(21)-C(20)-H(20)	120.6	C(33)-C(32)-H(32)	119.5
C(11)-C(12)-C(7)	120.21(17)	C(34)-C(21)-C(20)	120.06(14)	C(28)-C(33)-C(32)	120.1(2)
C(11)-C(12)-H(12)	119.9	C(34)-C(21)-P(2)	121.87(12)	C(28)-C(33)-H(33)	120.0
C(7)-C(12)-H(12)	119.9	C(20)-C(21)-P(2)	118.06(12)	C(32)-C(33)-H(33)	120.0
C(39)-C(13)-C(14)	120.13(13)	C(23)-C(22)-C(27)	118.68(17)	C(35)-C(34)-C(21)	121.33(15)
C(39)-C(13)-P(1)	116.48(11)	C(23)-C(22)-P(2)	117.73(14)	C(35)-C(34)-H(34)	119.3
C(14)-C(13)-P(1)	123.39(12)	C(27)-C(22)-P(2)	123.56(14)	C(21)-C(34)-H(34)	119.3
C(15)-C(14)-C(13)	119.20(14)	C(24)-C(23)-C(22)	120.7(2)	C(34)-C(35)-C(36)	118.42(15)
C(15)-C(14)-H(14)	120.4	C(24)-C(23)-H(23)	119.7	C(34)-C(35)-H(35)	120.8
C(13)-C(14)-H(14)	120.4	C(22)-C(23)-H(23)	119.7	C(36)-C(35)-H(35)	120.8

C(35)-C(36)-C(19)	121.02(14)
C(35)-C(36)-C(37)	130.25(14)
C(19)-C(36)-C(37)	108.71(13)
C(38)-C(37)-C(15)	121.27(13)
C(38)-C(37)-C(36)	130.46(14)
C(15)-C(37)-C(36)	108.25(13)
C(37)-C(38)-C(39)	118.30(14)
C(37)-C(38)-H(38)	120.8
C(39)-C(38)-H(38)	120.8
C(38)-C(39)-C(13)	121.21(14)
C(38)-C(39)-H(39)	119.4
C(13)-C(39)-H(39)	119.4

Table 3. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Po06. 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}
P(1)	27(1)	34(1)	36(1)	-8(1)	-7(1)	-11(1)
P(2)	29(1)	38(1)	36(1)	-7(1)	-8(1)	-7(1)
C(1)	53(1)	53(1)	63(1)	0(1)	2(1)	-24(1)
C(2)	78(2)	93(2)	66(2)	4(1)	4(1)	-56(2)
C(3)	67(2)	127(2)	56(1)	-24(2)	17(1)	-60(2)
C(4)	50(1)	92(2)	64(1)	-38(1)	13(1)	-22(1)
C(5)	43(1)	53(1)	50(1)	-18(1)	0(1)	-15(1)
C(6)	31(1)	45(1)	39(1)	-7(1)	-6(1)	-17(1)
C(7)	32(1)	39(1)	35(1)	-5(1)	-3(1)	-15(1)
C(8)	61(1)	66(1)	65(1)	17(1)	-32(1)	-38(1)
C(9)	76(2)	66(1)	78(2)	31(1)	-36(1)	-38(1)
C(10)	72(1)	52(1)	66(1)	11(1)	-4(1)	-36(1)
C(11)	67(1)	61(1)	74(2)	-3(1)	-9(1)	-43(1)
C(12)	48(1)	50(1)	60(1)	-1(1)	-17(1)	-24(1)
C(13)	27(1)	32(1)	38(1)	-6(1)	-6(1)	-11(1)
C(14)	28(1)	34(1)	36(1)	-11(1)	-2(1)	-9(1)
C(15)	30(1)	29(1)	32(1)	-6(1)	-3(1)	-12(1)
C(16)	28(1)	34(1)	33(1)	-9(1)	-4(1)	-6(1)
C(17)	44(1)	66(1)	36(1)	-2(1)	3(1)	-12(1)
C(18)	51(1)	38(1)	62(1)	-18(1)	-21(1)	-9(1)
C(19)	29(1)	29(1)	33(1)	-6(1)	-2(1)	-8(1)
C(20)	32(1)	35(1)	34(1)	-8(1)	-5(1)	-8(1)
C(21)	30(1)	37(1)	36(1)	-5(1)	-8(1)	-7(1)
C(22)	32(1)	40(1)	38(1)	2(1)	-10(1)	-12(1)
C(23)	54(1)	42(1)	63(1)	6(1)	-10(1)	-20(1)
C(24)	68(1)	68(2)	74(2)	20(1)	-9(1)	-43(1)
C(25)	48(1)	93(2)	51(1)	15(1)	-3(1)	-35(1)
C(26)	45(1)	77(2)	52(1)	-14(1)	6(1)	-20(1)
C(27)	40(1)	54(1)	52(1)	-13(1)	1(1)	-20(1)
C(28)	31(1)	43(1)	34(1)	-4(1)	-1(1)	-11(1)
C(29)	40(1)	48(1)	50(1)	-3(1)	-12(1)	-11(1)
C(30)	52(1)	52(1)	57(1)	5(1)	-14(1)	-5(1)

C(31)	68(1)	45(1)	71(2)	6(1)	-2(1)	-18(1)
C(32)	89(2)	69(2)	111(2)	13(2)	-34(2)	-50(2)
C(33)	67(1)	63(1)	79(2)	15(1)	-35(1)	-36(1)
C(34)	32(1)	41(1)	42(1)	-14(1)	-4(1)	1(1)
C(35)	36(1)	41(1)	35(1)	-14(1)	-6(1)	-4(1)
C(36)	31(1)	29(1)	33(1)	-5(1)	-4(1)	-10(1)
C(37)	28(1)	26(1)	34(1)	-5(1)	-3(1)	-11(1)
C(38)	33(1)	32(1)	35(1)	-11(1)	-2(1)	-12(1)
C(39)	36(1)	35(1)	35(1)	-8(1)	-7(1)	-15(1)
O(1)	40(1)	49(1)	49(1)	-17(1)	-10(1)	-17(1)
O(2)	48(1)	53(1)	50(1)	-21(1)	-12(1)	-10(1)

Table 4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Po06.

	x	y	z	U(eq)
H(1)	12816	3690	2850	70
H(2)	14379	3615	1621	90
H(3)	16117	1575	1257	93
H(4)	16257	-397	2077	85
H(5)	14652	-345	3283	60
H(8)	14101	-324	5437	73
H(9)	14428	-2471	5984	88
H(10)	13027	-3216	5556	75
H(11)	11346	-1848	4546	75
H(12)	11033	286	3966	61
H(14)	10940	2289	2556	42
H(17A)	8530	4439	409	83
H(17B)	9938	3626	867	83
H(17C)	9006	5146	1011	83
H(18A)	7898	2315	2305	78
H(18B)	9225	1890	1638	78
H(18C)	7792	2720	1216	78

H(20)	5837	5259	917	43
H(23)	1741	5726	1666	66
H(24)	-120	5880	2631	82
H(25)	-1429	7756	3402	80
H(26)	-863	9484	3214	74
H(27)	1041	9320	2265	59
H(29)	1261	9313	-124	59
H(30)	825	11450	-804	74
H(31)	2060	12423	-431	80
H(32)	3694	11281	633	101
H(33)	4181	9118	1303	81
H(34)	3607	7671	2917	54
H(35)	5485	6774	3807	50
H(38)	7878	5363	4584	41
H(39)	10076	3857	5008	42