Supporting Information

Acid-Stimuli-Luminescence and Carbonyl-Proton Interaction Dependent Emission Property of 2,6- Biphenyl-4-pyrone Crystals

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Table S1. Bond lengths [Å] and angles [°] for **BPP**.

C1-O1	1.245(2)	C18-O3	1.240(2)
C1-C10	1.434(3)	C18-C27	1.441(3)
C1-C2	1.438(3)	C18-C19	1.445(3)
C2-C3	1.344(3)	C19-C20	1.340(3)
C3-O2	1.369(2)	C20-O4	1.362(2)
C3-C4	1.469(3)	C20-C21	1.477(3)
C4-C9	1.391(3)	C21-C26	1.389(3)
C4-C5	1.393(3)	C21-C22	1.391(3)
C5-C6	1.383(3)	C22-C23	1.373(3)
C6-C7	1.373(3)	C23-C24	1.379(3)
C7-C8	1.373(4)	C24-C25	1.371(3)
C8-C9	1.383(3)	C25-C26	1.385(3)
C10-C11	1.339(3)	C27-C28	1.335(3)
C11-O2	1.367(2)	C28-O4	1.365(2)
C11-C12	1.470(3)	C28-C29	1.473(3)
C12-C13	1.387(3)	C29-C30	1.382(3)
C12-C17	1.391(3)	C29-C34	1.389(3)
C13-C14	1.375(3)	C30-C31	1.385(3)
C14-C15	1.375(4)	C31-C32	1.375(3)
C15-C16	1.369(4)	C32-C33	1.372(4)
C16-C17	1.384(3)	C33-C34	1.383(3)
O1-C1-C10	122.32(19)	O3-C18-C19	123.2(2)
O1-C1-C2	123.0(2)	C27-C18-C19	114.42(18)
C10-C1-C2	114.67(17)	C20-C19-C18	121.2(2)
C3-C2-C1	121.2(2)	C19-C20-O4	121.3(2)
C2-C3-O2	121.11(19)	C19-C20-C21	127.4(2)
C2-C3-C4	127.0(2)	O4-C20-C21	111.33(16)
O2-C3-C4	111.91(16)	C26-C21-C22	118.0(2)
C9-C4-C5	118.3(2)	C26-C21-C20	121.18(19)
C9-C4-C3	121.6(2)	C22-C21-C20	120.73(18)
C5-C4-C3	119.99(18)	C23-C22-C21	120.8(2)
C6-C5-C4	120.3(2)	C22-C23-C24	120.7(2)
C7-C6-C5	120.7(3)	C25-C24-C23	119.3(2)
C6-C7-C8	119.6(2)	C24-C25-C26	120.3(2)
C7-C8-C9	120.3(2)	C25-C26-C21	120.9(2)
C8-C9-C4	120.7(2)	C28-C27-C18	121.8(2)
C11-C10-C1	122.2(2)	C27-C28-O4	120.97(19)
C10-C11-O2	120.50(19)	C27-C28-C29	127.8(2)
C10-C11-C12	127.0(2)	O4-C28-C29	111.23(16)
O2-C11-C12	112.51(16)	C30-C29-C34	118.3(2)
C13-C12-C17	118.2(2)	C30-C29-C28	120.97(19)

C13-C12-C11	120.42(18)	C34-C29-C28	120.7(2)
C17-C12-C11	121.4(2)	C29-C30-C31	120.4(2)
C14-C13-C12	121.3(2)	C32-C31-C30	120.6(2)
C13-C14-C15	120.0(2)	C33-C32-C31	119.6(2)
C16-C15-C14	119.4(2)	C32-C33-C34	120.1(2)
C15-C16-C17	121.1(2)	C33-C34-C29	121.0(2)
C16-C17-C12	119.9(2)	C11-02-C3	120.29(15)
03-C18-C27	122.3(2)	C20-04-C28	120.31(15)

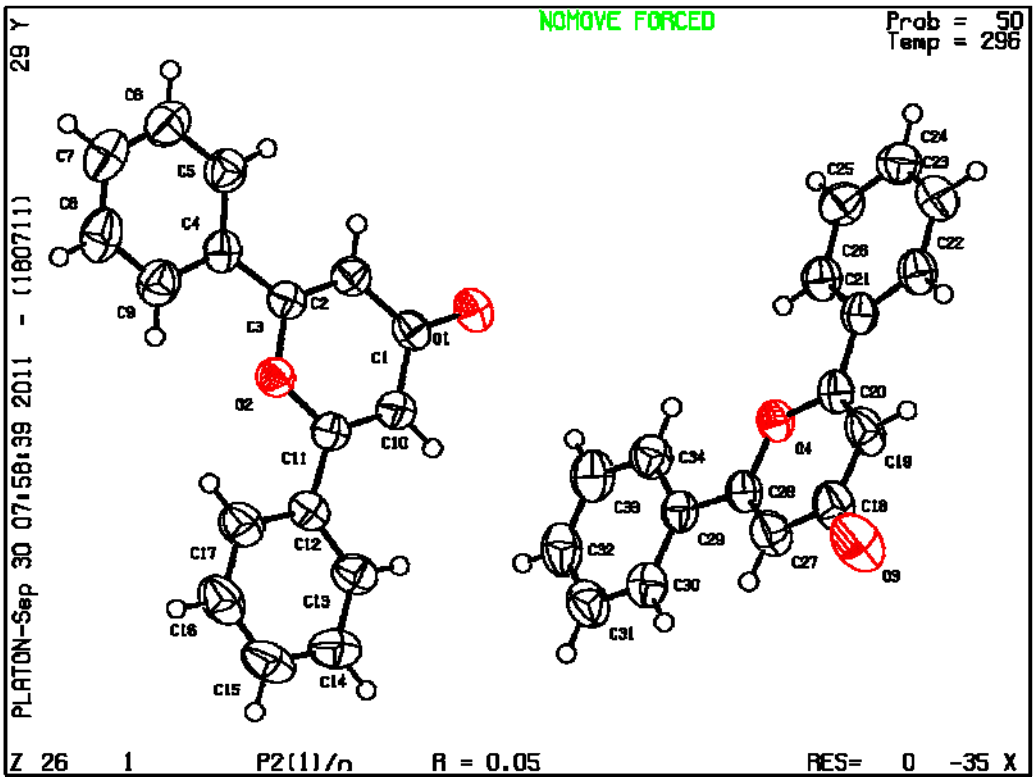

Figure S1. Labeled molecular structure of **BPP**.

Table S2. Bond lengths [Å] and angles [°] for **BPP-HCl**.

C1-O1	1.300(3)	C10-C11	1.353(3)
C1-C2	1.403(4)	C11-O2	1.352(3)
C1-C10	1.408(3)	C11-C12	1.464(3)
C2-C3	1.351(4)	C12-C13	1.384(4)
C3-O2	1.357(3)	C12-C17	1.395(4)
C3-C4	1.462(4)	C13-C14	1.383(4)
C4-C5	1.378(4)	C14-C15	1.377(5)
C4-C9	1.392(4)	C15-C16	1.369(5)
C5-C6	1.382(5)	C16-C17	1.388(4)
C6-C7	1.363(6)	C18-CL2	1.711(5)
C7-C8	1.373(6)	C18-CL3	1.729(5)
C8-C9	1.384(5)		
O1-C1-C2	118.9(2)	C11-C10-C1	120.1(3)
O1-C1-C10	123.1(2)	O2-C11-C10	119.9(2)
C2-C1-C10	118.0(2)	O2-C11-C12	113.0(2)
C3-C2-C1	120.2(2)	C10-C11-C12	127.0(2)
C2-C3-O2	119.9(2)	C13-C12-C17	118.7(2)
C2-C3-C4	127.1(2)	C13-C12-C11	120.5(2)
O2-C3-C4	112.9(2)	C17-C12-C11	120.8(2)
C5-C4-C9	119.1(3)	C14-C13-C12	121.0(3)
C5-C4-C3	120.5(3)	C15-C14-C13	119.6(3)
C9-C4-C3	120.4(3)	C16-C15-C14	120.4(3)
C4-C5-C6	120.4(4)	C15-C16-C17	120.2(3)
C7-C6-C5	120.2(4)	C16-C17-C12	120.1(3)
C6-C7-C8	120.2(4)	C12-C18-C13	113.4(3)
C7-C8-C9	120.2(4)	C11-O2-C3	121.9(2)
C8-C9-C4	119.8(4)		

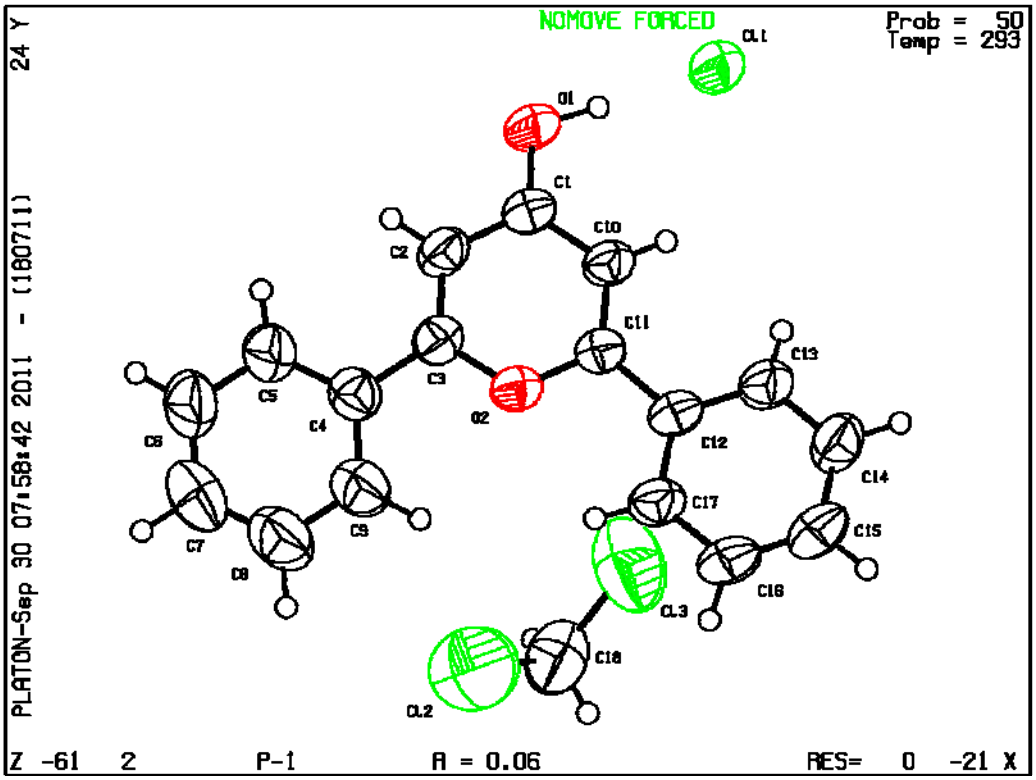

Figure S2. Labeled molecular structure of **BPP-HCl**.

Table S3. Bond lengths [Å] and angles [°] for **BPP-TFA**.

C1–O1	1.278(3)	C11–C12	1.469(3)
C1–C2	1.420(3)	C12–C17	1.391(3)
C1–C10	1.422(3)	C12–C13	1.393(3)
C2–C3	1.355(3)	C13–C14	1.387(3)
C3–O2	1.359(2)	C14–C15	1.378(4)
C3–C4	1.467(3)	C15–C16	1.367(4)
C4–C9	1.383(3)	C16–C17	1.391(3)
C4–C5	1.392(3)	C18–O4	1.211(3)
C5–C6	1.382(4)	C18–O3	1.267(3)
C6–C7	1.372(4)	C18–C19	1.534(3)
C7–C8	1.377(4)	C19–F1	1.268(4)
C8–C9	1.385(4)	C19–F2	1.278(4)
C10–C11	1.350(3)	C19–F3	1.287(4)
C11–O2	1.354(2)		
O1–C1–C2	120.64(18)	C17–C12–C13	119.3(2)
O1–C1–C10	122.54(19)	C17–C12–C11	120.6(2)
C2–C1–C10	116.82(18)	C13–C12–C11	120.1(2)

C3-C2-C1	120.25(19)	C14-C13-C12	120.2(2)
C2-C3-02	120.58(19)	C15-C14-C13	119.9(3)
C2-C3-C4	127.34(19)	C16-C15-C14	120.4(2)
02-C3-C4	112.07(17)	C15-C16-C17	120.5(3)
C9-C4-C5	118.8(2)	C12-C17-C16	119.7(2)
C9-C4-C3	121.1(2)	04-C18-03	129.8(2)
C5-C4-C3	120.17(19)	04-C18-C19	118.6(2)
C6-C5-C4	120.4(2)	03-C18-C19	111.6(2)
C7-C6-C5	120.3(2)	F1-C19-F2	107.1(3)
C6-C7-C8	119.8(2)	F1-C19-F3	105.8(3)
C7-C8-C9	120.2(3)	F2-C19-F3	104.6(3)
C4-C9-C8	120.4(2)	F1-C19-C18	112.7(2)
C11-C10-C1	120.39(19)	F2-C19-C18	111.6(2)
C10-C11-02	120.74(18)	F3-C19-C18	114.3(2)
C10-C11-C12	126.56(19)	C11-02-C3	121.13(16)
02-C11-C12	112.70(17)		

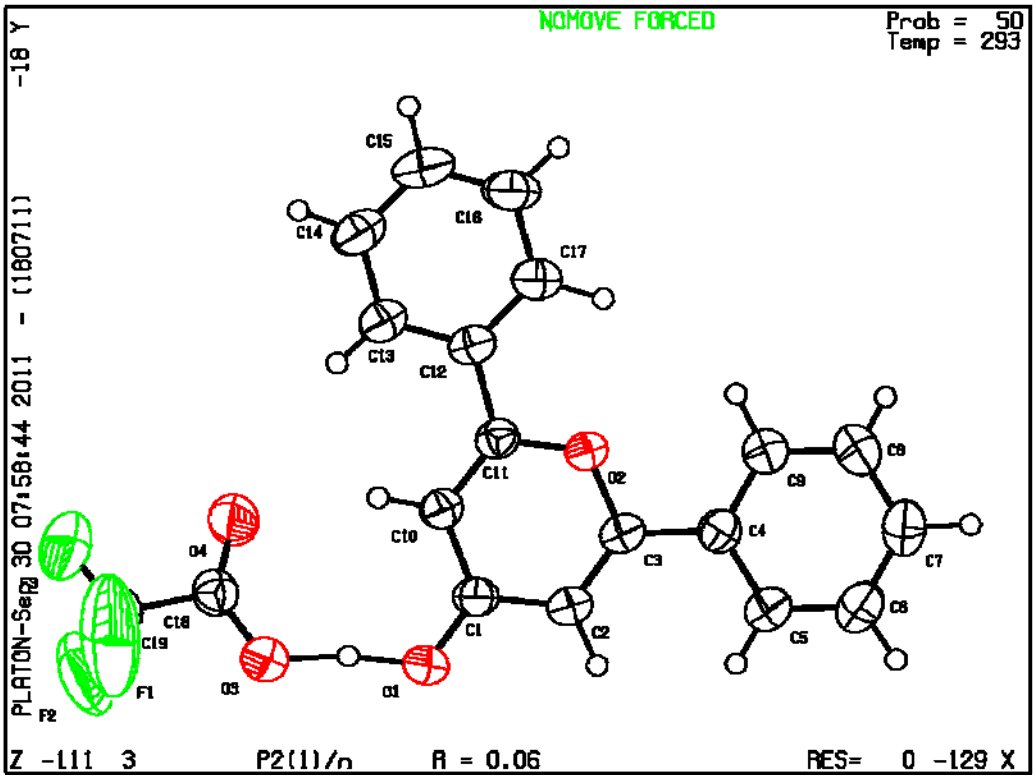

Figure S3. Labeled molecular structure of **BPP-TFA**.

Table S4. Bond lengths [Å] and angles [°] for **BPP-AcOH**.

C1-O1	1.253(2)	C10-C11	1.341(3)
C1-C10	1.433(3)	C11-O2	1.3709(19)
C1-C2	1.435(3)	C11-C12	1.467(3)
C2-C3	1.336(3)	C12-C17	1.387(3)
C3-O2	1.359(2)	C12-C13	1.393(2)
C3-C4	1.477(2)	C13-C14	1.378(3)
C4-C9	1.382(3)	C14-C15	1.369(3)
C4-C5	1.395(3)	C15-C16	1.371(3)
C5-C6	1.379(3)	C16-C17	1.378(3)
C6-C7	1.368(3)	C18-O4	1.200(3)
C7-C8	1.380(3)	C18-O3	1.309(2)
C8-C9	1.387(3)	C18-C19	1.488(3)
O1-C1-C10	122.87(17)	C10-C11-C12	127.57(16)
O1-C1-C2	122.21(18)	O2-C11-C12	111.63(16)
C10-C1-C2	114.91(18)	C17-C12-C13	118.16(18)
C3-C2-C1	121.51(18)	C17-C12-C11	120.89(16)
C3-C2-H2	119.2	C13-C12-C11	120.93(17)
C1-C2-H2	119.2	C14-C13-C12	120.75(18)
C2-C3-O2	121.16(16)	C14-C13-H13	119.6
C2-C3-C4	126.31(17)	C12-C13-H13	119.6
O2-C3-C4	112.51(16)	C15-C14-C13	120.16(18)
C9-C4-C5	118.44(17)	C15-C14-H14	119.9
C9-C4-C3	121.71(17)	C13-C14-H14	119.9
C5-C4-C3	119.82(18)	C14-C15-C16	119.9(2)
C6-C5-C4	120.7(2)	C14-C15-H15	120
C6-C5-H5	119.7	C16-C15-H15	120
C4-C5-H5	119.7	C15-C16-C17	120.4(2)
C7-C6-C5	120.3(2)	C15-C16-H16	119.8
C7-C6-H6	119.9	C17-C16-H16	119.8
C5-C6-H6	119.9	C16-C17-C12	120.57(18)
C6-C7-C8	120.11(19)	C16-C17-H17	119.7
C6-C7-H7	119.9	C12-C17-H17	119.7
C8-C7-H7	119.9	O4-C18-O3	123.6(2)
C7-C8-C9	119.8(2)	O4-C18-C19	123.8(2)
C7-C8-H8	120.1	O3-C18-C19	112.59(19)
C9-C8-H8	120.1	C18-C19-H19A	109.5
C4-C9-C8	120.7(2)	C18-C19-H19B	109.5
C4-C9-H9	119.7	H19A-C19-H19B	109.5
C8-C9-H9	119.7	C18-C19-H19C	109.5

C11-C10-C1	121.38(17)	H19A-C19-H19C	109.5
C11-C10-H10	119.3	H19B-C19-H19C	109.5
C1-C10-H10	119.3	C3-O2-C11	120.21(15)
C10-C11-O2	120.80(17)	C18-O3-H1	115.8

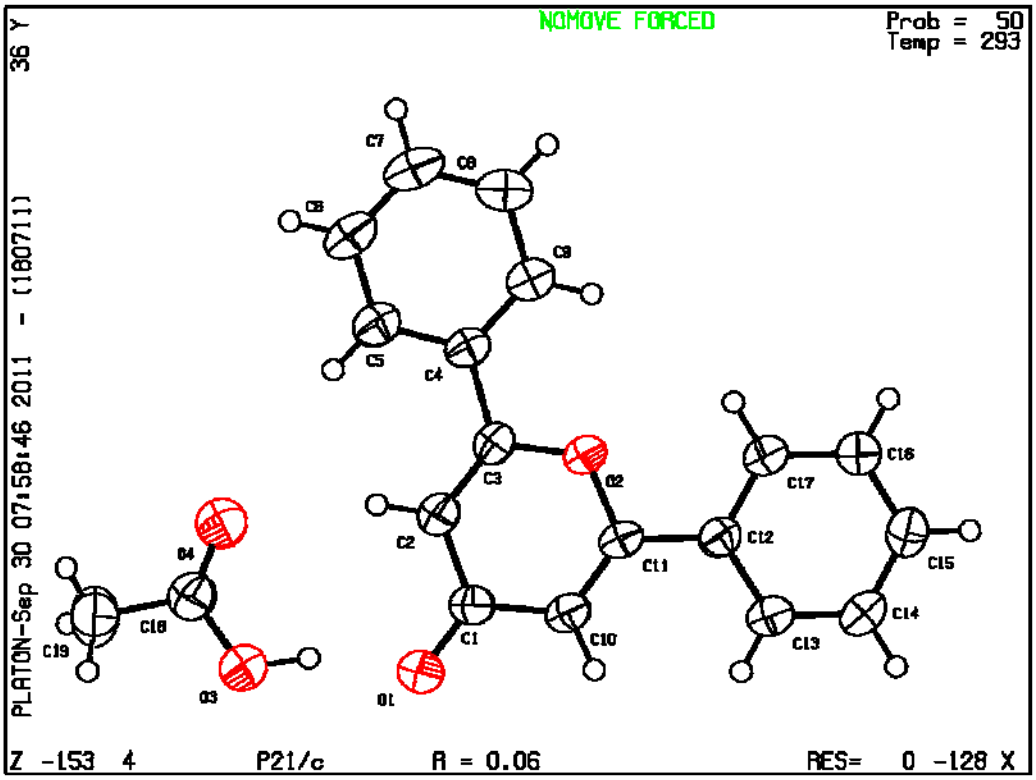

Figure S4. Labeled molecular structure of **BPP-AcOH**.