

Supporting Information

Self-assembled via Metal-Ligand Coordination AzaBODIPY-Zinc Phthalocyanine and AzaBODIPY-Zinc Naphthalocyanine Conjugates: Synthesis, Structure and Photoinduced Electron Transfer

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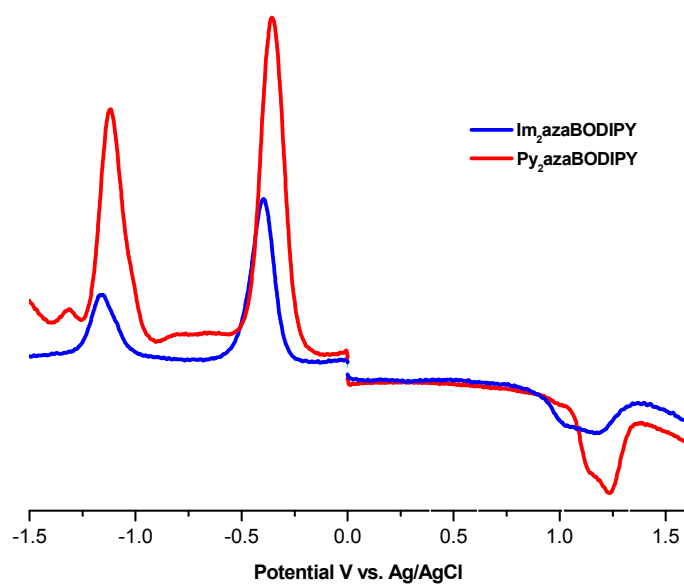


Figure S1. Differential pulse voltammograms of Im₂-azaBODIPY (blue trace) and Py₂-azaBODIPY (red trace) in DCB containing 0.1 M (TBAP)ClO₄.

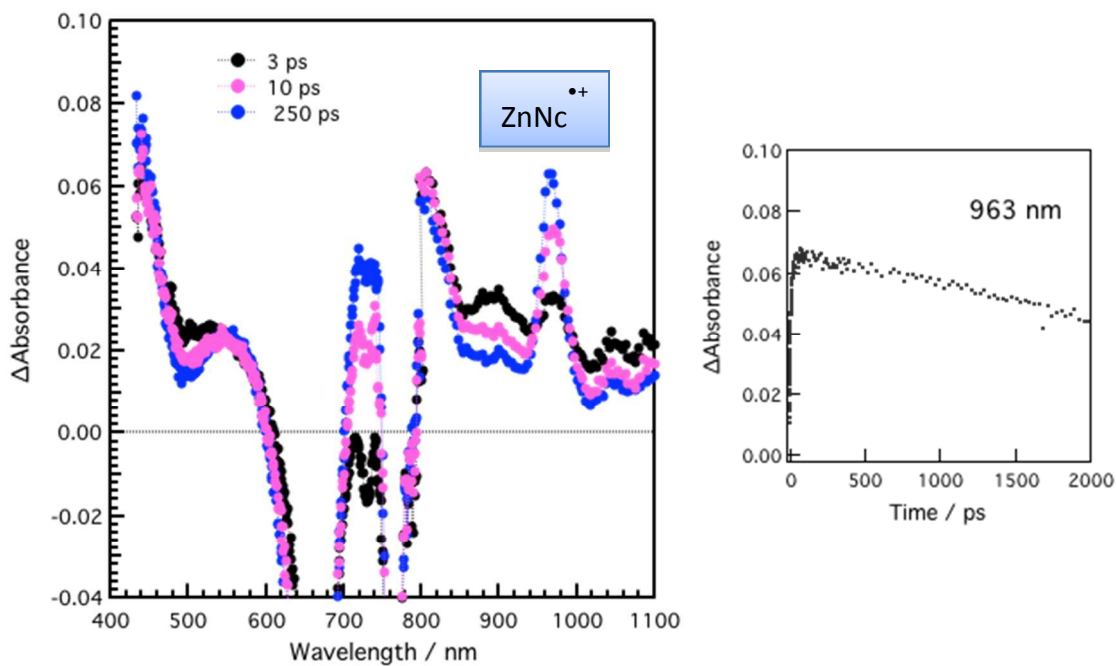


Figure S2. (a) Femtosecond transient absorption spectral trace recorded at different time intervals for $(\text{ZnNc})_2\text{:Py}_2\text{-aza(BODIPY)}$ in toluene; $\lambda_{\text{ex}} = 390$ nm. (b) The time profile of the $\text{ZnNc}^{\bullet+}$ peak at 823 nm.

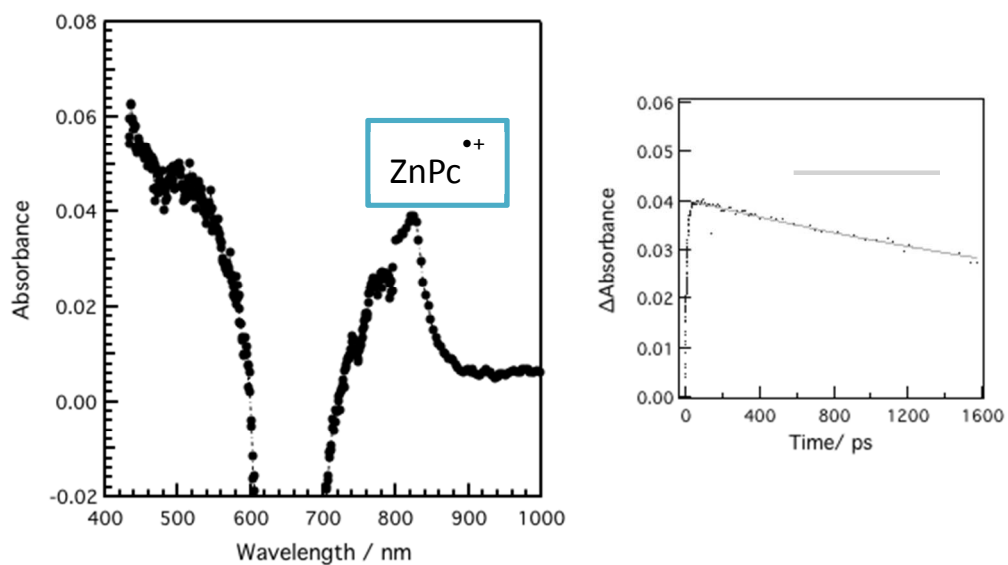


Figure S3. (a) Femtosecond transient absorption spectrum of $(\text{ZnPc})_2\text{:Im}_2\text{-aza(BODIPY)}$ in toluene; $\lambda_{\text{ex}} = 390 \text{ nm}$. (b) The time profile of the $\text{ZnPc}^{\bullet+}$ peak at 823 nm.

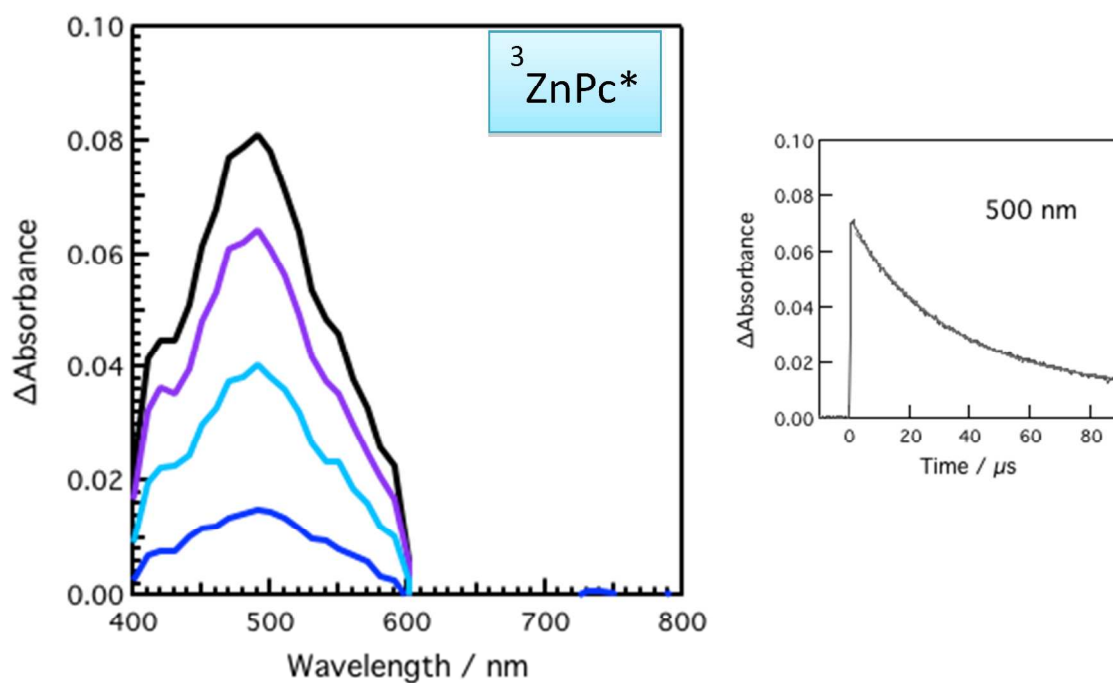


Figure S4. Nanosecond transient spectra of ZnPc in toluene, ex = 430 nm.

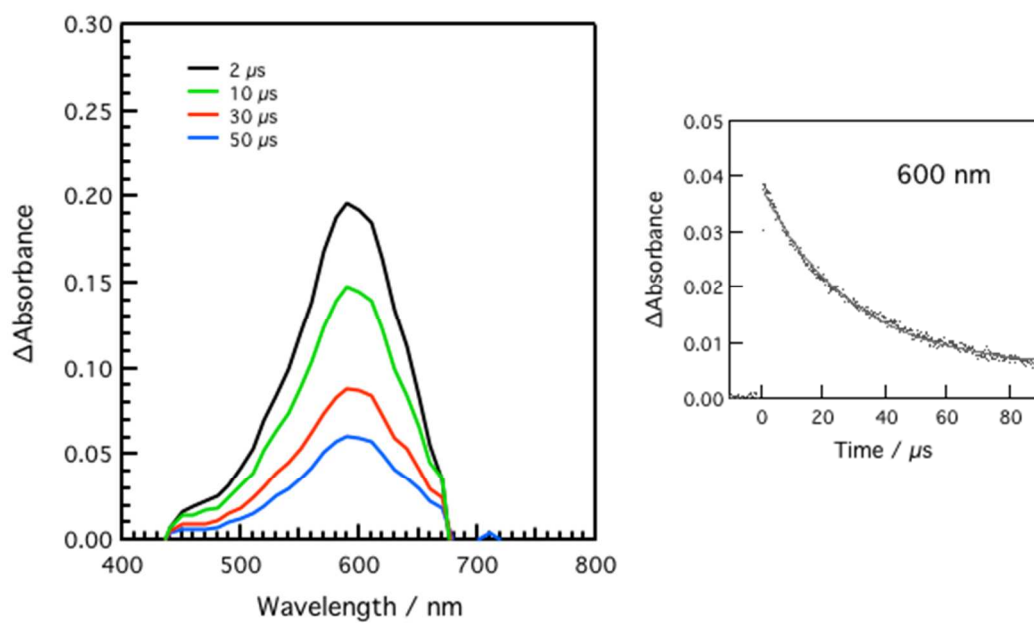


Figure S5. Nanosecond transient spectra of ZnNc in toluene, ex = 430 nm.

Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for str0473. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
F(1)	3477(1)	4448(1)	1535(1)	21(1)
F(2)	5713(1)	3794(1)	1710(1)	20(1)
O(1)	582(1)	-335(1)	1672(1)	24(1)
O(2)	1073(1)	-2105(1)	1347(1)	34(1)
O(3)	2084(1)	7322(1)	2897(1)	22(1)
O(4)	3202(1)	6006(1)	3347(1)	26(1)
N(1)	4881(1)	3760(1)	1020(1)	18(1)
N(2)	6282(1)	5349(1)	752(1)	19(1)
N(3)	5391(1)	5768(1)	1376(1)	18(1)
N(4)	-2095(1)	-3563(1)	2352(1)	29(1)
N(5)	2(1)	8597(1)	4114(1)	32(1)
C(1)	4262(1)	2684(1)	878(1)	19(1)
B(1)	4821(2)	4418(1)	1427(1)	18(1)
C(2)	4632(1)	2472(1)	492(1)	21(1)
C(3)	5518(1)	3422(1)	391(1)	20(1)
C(4)	5647(1)	4249(1)	727(1)	18(1)
C(5)	5276(1)	6825(1)	1596(1)	18(1)
C(6)	5954(1)	7829(1)	1419(1)	21(1)
C(7)	6528(1)	7376(1)	1090(1)	20(1)
C(8)	6144(1)	6080(1)	1060(1)	19(1)
C(9)	3348(1)	1877(1)	1092(1)	19(1)
C(10)	2256(2)	1240(1)	874(1)	23(1)
C(11)	1339(2)	480(1)	1058(1)	24(1)
C(12)	1526(1)	359(1)	1462(1)	21(1)
C(13)	2596(1)	961(1)	1686(1)	19(1)
C(14)	3514(1)	1712(1)	1500(1)	19(1)
C(15)	480(2)	-1584(1)	1593(1)	22(1)
C(16)	-446(1)	-2226(1)	1862(1)	22(1)
C(17)	-1002(2)	-1634(1)	2175(1)	25(1)
C(18)	-1816(2)	-2342(2)	2410(1)	28(1)
C(19)	-1570(2)	-4105(1)	2044(1)	29(1)

C(20)	-746(2)	-3482(1)	1793(1)	27(1)
C(21)	6215(1)	3541(1)	26(1)	20(1)
C(22)	6114(2)	2564(1)	-250(1)	23(1)
C(23)	6813(2)	2624(1)	-588(1)	27(1)
C(24)	7612(2)	3666(1)	-661(1)	28(1)
C(25)	7711(2)	4647(2)	-394(1)	30(1)
C(26)	7021(2)	4590(1)	-54(1)	27(1)
C(27)	4533(1)	6899(1)	1952(1)	19(1)
C(28)	4419(2)	5897(1)	2211(1)	22(1)
C(29)	3634(2)	5995(1)	2532(1)	22(1)
C(30)	2974(1)	7123(1)	2599(1)	20(1)
C(31)	3114(2)	8151(1)	2356(1)	23(1)
C(32)	3890(2)	8038(1)	2036(1)	22(1)
C(33)	2358(1)	6816(1)	3263(1)	20(1)
C(34)	1485(1)	7428(1)	3548(1)	20(1)
C(35)	1882(2)	7278(1)	3945(1)	25(1)
C(36)	1115(2)	7882(2)	4215(1)	31(1)
C(37)	-380(2)	8711(2)	3731(1)	30(1)
C(38)	319(2)	8157(1)	3437(1)	25(1)
C(39)	7242(2)	8066(1)	794(1)	23(1)
C(40)	6800(2)	9281(1)	689(1)	28(1)
C(41)	7382(2)	9917(2)	390(1)	32(1)
C(42)	8420(2)	9365(2)	196(1)	34(1)
C(43)	8904(2)	8177(2)	302(1)	34(1)
C(44)	8312(2)	7523(2)	600(1)	28(1)

Table S2. Bond lengths [Å] and angles [°] for py₂-azaBODIPY.

F(1)-B(1)	1.3730(17)
F(2)-B(1)	1.3995(17)
O(1)-C(15)	1.3588(17)
O(1)-C(12)	1.4108(16)
O(2)-C(15)	1.1918(17)
O(3)-C(33)	1.3621(16)
O(3)-C(30)	1.4012(16)
O(4)-C(33)	1.2010(16)
N(1)-C(1)	1.3599(17)
N(1)-C(4)	1.3940(16)
N(1)-B(1)	1.5602(18)
N(2)-C(4)	1.3201(17)
N(2)-C(8)	1.3231(17)
N(3)-C(5)	1.3630(17)
N(3)-C(8)	1.3885(17)
N(3)-B(1)	1.5538(18)
N(4)-C(19)	1.334(2)
N(4)-C(18)	1.340(2)
N(5)-C(37)	1.332(2)
N(5)-C(36)	1.332(2)
C(1)-C(2)	1.4114(18)
C(1)-C(9)	1.4683(18)
C(2)-C(3)	1.3835(19)
C(2)-H(2A)	0.9500
C(3)-C(4)	1.4402(18)
C(3)-C(21)	1.4709(18)
C(5)-C(6)	1.4138(18)
C(5)-C(27)	1.4645(18)
C(6)-C(7)	1.3796(19)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.4311(18)
C(7)-C(39)	1.4663(19)
C(9)-C(14)	1.3980(19)
C(9)-C(10)	1.4025(19)

C(10)-C(11)	1.3848(19)
C(10)-H(10A)	0.9500
C(11)-C(12)	1.3810(19)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.3802(19)
C(13)-C(14)	1.3844(19)
C(13)-H(13A)	0.9500
C(14)-H(14A)	0.9500
C(15)-C(16)	1.4958(19)
C(16)-C(20)	1.384(2)
C(16)-C(17)	1.388(2)
C(17)-C(18)	1.389(2)
C(17)-H(17A)	0.9500
C(18)-H(18A)	0.9500
C(19)-C(20)	1.385(2)
C(19)-H(19A)	0.9500
C(20)-H(20A)	0.9500
C(21)-C(26)	1.399(2)
C(21)-C(22)	1.4005(19)
C(22)-C(23)	1.3859(19)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.384(2)
C(23)-H(23A)	0.9500
C(24)-C(25)	1.384(2)
C(24)-H(24A)	0.9500
C(25)-C(26)	1.386(2)
C(25)-H(25A)	0.9500
C(26)-H(26A)	0.9500
C(27)-C(28)	1.3959(19)
C(27)-C(32)	1.4023(19)
C(28)-C(29)	1.3880(19)
C(28)-H(28A)	0.9500
C(29)-C(30)	1.3858(19)
C(29)-H(29A)	0.9500
C(30)-C(31)	1.3860(19)
C(31)-C(32)	1.3802(19)

C(31)-H(31A)	0.9500
C(32)-H(32A)	0.9500
C(33)-C(34)	1.4886(19)
C(34)-C(35)	1.385(2)
C(34)-C(38)	1.3860(19)
C(35)-C(36)	1.385(2)
C(35)-H(35A)	0.9500
C(36)-H(36A)	0.9500
C(37)-C(38)	1.385(2)
C(37)-H(37A)	0.9500
C(38)-H(38A)	0.9500
C(39)-C(44)	1.396(2)
C(39)-C(40)	1.400(2)
C(40)-C(41)	1.383(2)
C(40)-H(40A)	0.9500
C(41)-C(42)	1.375(2)
C(41)-H(41A)	0.9500
C(42)-C(43)	1.385(2)
C(42)-H(42A)	0.9500
C(43)-C(44)	1.393(2)
C(43)-H(43A)	0.9500
C(44)-H(44A)	0.9500
C(15)-O(1)-C(12)	116.93(10)
C(33)-O(3)-C(30)	121.62(11)
C(1)-N(1)-C(4)	107.48(11)
C(1)-N(1)-B(1)	130.32(11)
C(4)-N(1)-B(1)	122.20(11)
C(4)-N(2)-C(8)	119.75(12)
C(5)-N(3)-C(8)	107.60(11)
C(5)-N(3)-B(1)	131.03(11)
C(8)-N(3)-B(1)	121.36(11)
C(19)-N(4)-C(18)	116.90(13)
C(37)-N(5)-C(36)	116.73(13)
N(1)-C(1)-C(2)	109.27(11)
N(1)-C(1)-C(9)	125.26(12)

C(2)-C(1)-C(9)	125.47(12)
F(1)-B(1)-F(2)	110.88(11)
F(1)-B(1)-N(3)	110.93(11)
F(2)-B(1)-N(3)	108.54(11)
F(1)-B(1)-N(1)	111.04(11)
F(2)-B(1)-N(1)	109.31(11)
N(3)-B(1)-N(1)	106.00(10)
C(3)-C(2)-C(1)	108.90(12)
C(3)-C(2)-H(2A)	125.6
C(1)-C(2)-H(2A)	125.6
C(2)-C(3)-C(4)	105.26(11)
C(2)-C(3)-C(21)	127.42(12)
C(4)-C(3)-C(21)	127.30(12)
N(2)-C(4)-N(1)	123.68(12)
N(2)-C(4)-C(3)	127.04(12)
N(1)-C(4)-C(3)	109.07(11)
N(3)-C(5)-C(6)	109.14(11)
N(3)-C(5)-C(27)	124.78(12)
C(6)-C(5)-C(27)	126.06(12)
C(7)-C(6)-C(5)	108.26(12)
C(7)-C(6)-H(6A)	125.9
C(5)-C(6)-H(6A)	125.9
C(6)-C(7)-C(8)	106.11(12)
C(6)-C(7)-C(39)	128.98(13)
C(8)-C(7)-C(39)	124.53(12)
N(2)-C(8)-N(3)	124.77(12)
N(2)-C(8)-C(7)	125.58(12)
N(3)-C(8)-C(7)	108.84(11)
C(14)-C(9)-C(10)	118.59(12)
C(14)-C(9)-C(1)	123.25(12)
C(10)-C(9)-C(1)	118.16(12)
C(11)-C(10)-C(9)	121.27(13)
C(11)-C(10)-H(10A)	119.4
C(9)-C(10)-H(10A)	119.4
C(12)-C(11)-C(10)	118.29(13)
C(12)-C(11)-H(11A)	120.9

C(10)-C(11)-H(11A)	120.9
C(13)-C(12)-C(11)	122.14(12)
C(13)-C(12)-O(1)	116.31(12)
C(11)-C(12)-O(1)	121.46(12)
C(12)-C(13)-C(14)	119.20(12)
C(12)-C(13)-H(13A)	120.4
C(14)-C(13)-H(13A)	120.4
C(13)-C(14)-C(9)	120.49(13)
C(13)-C(14)-H(14A)	119.8
C(9)-C(14)-H(14A)	119.8
O(2)-C(15)-O(1)	124.27(13)
O(2)-C(15)-C(16)	124.34(13)
O(1)-C(15)-C(16)	111.38(11)
C(20)-C(16)-C(17)	118.75(13)
C(20)-C(16)-C(15)	117.69(13)
C(17)-C(16)-C(15)	123.56(13)
C(18)-C(17)-C(16)	118.07(14)
C(18)-C(17)-H(17A)	121.0
C(16)-C(17)-H(17A)	121.0
N(4)-C(18)-C(17)	123.88(14)
N(4)-C(18)-H(18A)	118.1
C(17)-C(18)-H(18A)	118.1
N(4)-C(19)-C(20)	123.62(14)
N(4)-C(19)-H(19A)	118.2
C(20)-C(19)-H(19A)	118.2
C(16)-C(20)-C(19)	118.76(14)
C(16)-C(20)-H(20A)	120.6
C(19)-C(20)-H(20A)	120.6
C(26)-C(21)-C(22)	117.94(12)
C(26)-C(21)-C(3)	122.31(12)
C(22)-C(21)-C(3)	119.72(12)
C(23)-C(22)-C(21)	121.02(13)
C(23)-C(22)-H(22A)	119.5
C(21)-C(22)-H(22A)	119.5
C(24)-C(23)-C(22)	120.17(14)
C(24)-C(23)-H(23A)	119.9

C(22)-C(23)-H(23A)	119.9
C(25)-C(24)-C(23)	119.64(13)
C(25)-C(24)-H(24A)	120.2
C(23)-C(24)-H(24A)	120.2
C(24)-C(25)-C(26)	120.45(14)
C(24)-C(25)-H(25A)	119.8
C(26)-C(25)-H(25A)	119.8
C(25)-C(26)-C(21)	120.75(14)
C(25)-C(26)-H(26A)	119.6
C(21)-C(26)-H(26A)	119.6
C(28)-C(27)-C(32)	118.19(12)
C(28)-C(27)-C(5)	123.71(12)
C(32)-C(27)-C(5)	118.10(12)
C(29)-C(28)-C(27)	121.35(13)
C(29)-C(28)-H(28A)	119.3
C(27)-C(28)-H(28A)	119.3
C(30)-C(29)-C(28)	118.79(13)
C(30)-C(29)-H(29A)	120.6
C(28)-C(29)-H(29A)	120.6
C(29)-C(30)-C(31)	121.22(12)
C(29)-C(30)-O(3)	124.48(12)
C(31)-C(30)-O(3)	114.25(12)
C(32)-C(31)-C(30)	119.38(13)
C(32)-C(31)-H(31A)	120.3
C(30)-C(31)-H(31A)	120.3
C(31)-C(32)-C(27)	120.98(13)
C(31)-C(32)-H(32A)	119.5
C(27)-C(32)-H(32A)	119.5
O(4)-C(33)-O(3)	125.12(12)
O(4)-C(33)-C(34)	124.37(12)
O(3)-C(33)-C(34)	110.50(11)
C(35)-C(34)-C(38)	118.37(13)
C(35)-C(34)-C(33)	117.89(12)
C(38)-C(34)-C(33)	123.72(13)
C(34)-C(35)-C(36)	118.76(14)
C(34)-C(35)-H(35A)	120.6

C(36)-C(35)-H(35A)	120.6
N(5)-C(36)-C(35)	123.67(14)
N(5)-C(36)-H(36A)	118.2
C(35)-C(36)-H(36A)	118.2
N(5)-C(37)-C(38)	124.19(14)
N(5)-C(37)-H(37A)	117.9
C(38)-C(37)-H(37A)	117.9
C(37)-C(38)-C(34)	118.26(14)
C(37)-C(38)-H(38A)	120.9
C(34)-C(38)-H(38A)	120.9
C(44)-C(39)-C(40)	118.66(13)
C(44)-C(39)-C(7)	121.91(13)
C(40)-C(39)-C(7)	119.35(13)
C(41)-C(40)-C(39)	120.62(15)
C(41)-C(40)-H(40A)	119.7
C(39)-C(40)-H(40A)	119.7
C(42)-C(41)-C(40)	120.14(15)
C(42)-C(41)-H(41A)	119.9
C(40)-C(41)-H(41A)	119.9
C(41)-C(42)-C(43)	120.42(14)
C(41)-C(42)-H(42A)	119.8
C(43)-C(42)-H(42A)	119.8
C(42)-C(43)-C(44)	119.83(15)
C(42)-C(43)-H(43A)	120.1
C(44)-C(43)-H(43A)	120.1
C(43)-C(44)-C(39)	120.29(15)
C(43)-C(44)-H(44A)	119.9
C(39)-C(44)-H(44A)	119.9

Symmetry transformations used to generate equivalent atoms:

Table S3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for py₂-azaBODIPY. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
F(1)	22(1)	19(1)	22(1)	-2(1)	7(1)	-2(1)
F(2)	26(1)	16(1)	19(1)	1(1)	2(1)	1(1)
O(1)	29(1)	18(1)	26(1)	-1(1)	11(1)	-5(1)
O(2)	48(1)	22(1)	35(1)	-5(1)	21(1)	-5(1)
O(3)	24(1)	24(1)	19(1)	0(1)	5(1)	3(1)
O(4)	32(1)	22(1)	25(1)	2(1)	7(1)	6(1)
N(1)	22(1)	14(1)	18(1)	0(1)	5(1)	-2(1)
N(2)	22(1)	16(1)	19(1)	1(1)	4(1)	0(1)
N(3)	22(1)	16(1)	16(1)	0(1)	4(1)	0(1)
N(4)	32(1)	29(1)	26(1)	4(1)	5(1)	-7(1)
N(5)	27(1)	34(1)	37(1)	-11(1)	9(1)	1(1)
C(1)	22(1)	16(1)	19(1)	-1(1)	4(1)	0(1)
B(1)	22(1)	15(1)	17(1)	0(1)	4(1)	0(1)
C(2)	27(1)	18(1)	18(1)	-2(1)	5(1)	-2(1)
C(3)	24(1)	17(1)	18(1)	1(1)	4(1)	1(1)
C(4)	21(1)	17(1)	17(1)	2(1)	4(1)	1(1)
C(5)	21(1)	15(1)	19(1)	-1(1)	1(1)	1(1)
C(6)	27(1)	15(1)	22(1)	0(1)	3(1)	-2(1)
C(7)	22(1)	18(1)	19(1)	0(1)	2(1)	-2(1)
C(8)	20(1)	18(1)	18(1)	2(1)	4(1)	-1(1)
C(9)	23(1)	14(1)	21(1)	0(1)	6(1)	0(1)
C(10)	30(1)	20(1)	19(1)	-1(1)	5(1)	-3(1)
C(11)	27(1)	21(1)	25(1)	-2(1)	2(1)	-6(1)
C(12)	25(1)	14(1)	24(1)	0(1)	10(1)	-1(1)
C(13)	26(1)	15(1)	18(1)	0(1)	6(1)	2(1)
C(14)	23(1)	14(1)	20(1)	-1(1)	4(1)	1(1)
C(15)	26(1)	19(1)	22(1)	-2(1)	4(1)	-3(1)
C(16)	24(1)	22(1)	21(1)	2(1)	2(1)	-3(1)
C(17)	28(1)	22(1)	26(1)	0(1)	4(1)	-4(1)
C(18)	30(1)	32(1)	25(1)	-1(1)	7(1)	-3(1)
C(19)	36(1)	23(1)	29(1)	2(1)	6(1)	-7(1)

C(20)	34(1)	23(1)	26(1)	0(1)	7(1)	-4(1)
C(21)	23(1)	20(1)	18(1)	2(1)	4(1)	2(1)
C(22)	27(1)	22(1)	21(1)	0(1)	4(1)	0(1)
C(23)	33(1)	27(1)	20(1)	-3(1)	6(1)	3(1)
C(24)	34(1)	30(1)	21(1)	4(1)	12(1)	5(1)
C(25)	39(1)	26(1)	29(1)	2(1)	16(1)	-3(1)
C(26)	38(1)	21(1)	25(1)	-1(1)	11(1)	-3(1)
C(27)	23(1)	16(1)	18(1)	-2(1)	2(1)	-1(1)
C(28)	29(1)	16(1)	21(1)	-2(1)	4(1)	1(1)
C(29)	31(1)	17(1)	20(1)	0(1)	5(1)	-2(1)
C(30)	22(1)	22(1)	17(1)	-3(1)	4(1)	-1(1)
C(31)	29(1)	19(1)	22(1)	-2(1)	4(1)	5(1)
C(32)	30(1)	17(1)	20(1)	0(1)	4(1)	1(1)
C(33)	23(1)	17(1)	21(1)	0(1)	4(1)	-2(1)
C(34)	21(1)	17(1)	24(1)	-2(1)	5(1)	-3(1)
C(35)	23(1)	28(1)	24(1)	0(1)	4(1)	2(1)
C(36)	28(1)	40(1)	24(1)	-6(1)	5(1)	-2(1)
C(37)	22(1)	28(1)	40(1)	-2(1)	6(1)	3(1)
C(38)	23(1)	24(1)	28(1)	2(1)	3(1)	0(1)
C(39)	27(1)	22(1)	20(1)	-2(1)	3(1)	-8(1)
C(40)	38(1)	21(1)	26(1)	0(1)	6(1)	-6(1)
C(41)	46(1)	24(1)	27(1)	4(1)	2(1)	-11(1)
C(42)	43(1)	38(1)	21(1)	2(1)	4(1)	-21(1)
C(43)	33(1)	43(1)	27(1)	-5(1)	11(1)	-12(1)
C(44)	30(1)	27(1)	27(1)	-2(1)	5(1)	-7(1)

Table S4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for py₂-azaBODIPY.

	x	y	z	U(eq)
H(2A)	4323	1788	327	25
H(6A)	6006	8671	1511	26
H(10A)	2144	1331	596	27
H(11A)	601	52	909	29
H(13A)	2700	861	1964	23
H(14A)	4263	2117	1651	23
H(17A)	-830	-769	2228	30
H(18A)	-2199	-1936	2624	34
H(19A)	-1773	-4966	1995	35
H(20A)	-392	-3908	1578	33
H(22A)	5557	1850	-205	28
H(23A)	6744	1948	-770	32
H(24A)	8090	3708	-893	33
H(25A)	8256	5365	-444	37
H(26A)	7096	5270	127	33
H(28A)	4888	5132	2166	26
H(29A)	3550	5302	2704	27
H(31A)	2680	8926	2410	28
H(32A)	3989	8742	1870	27
H(35A)	2664	6772	4032	30
H(36A)	1399	7779	4487	37
H(37A)	-1183	9205	3653	36
H(38A)	8	8274	3167	30
H(40A)	6093	9673	824	34
H(41A)	7063	10736	318	39
H(42A)	8808	9802	-11	41
H(43A)	9637	7808	171	41
H(44A)	8638	6705	671	34

Optimized Structure Results of (ZnPc)₂:py₂.azaBODIPY

HF=-9337.0844708 A.U.

%chk=ZnPc2-py2.chk

%nprocshared=2

OPT B3LYP/3-21G* Integral(Ultrafine) SCF(Conver=6)

ZnPc2-py2

O 1

B	0.29353500	7.26048300	0.09367300
C	2.83784600	8.00004500	-0.19120500
C	4.65107000	6.53688900	-1.01570400
C	5.33239000	5.32576700	-1.07207800
C	4.84264900	4.24512600	-0.33490900
C	3.68994300	4.37422000	0.44231200
C	3.01056600	5.58215400	0.48971600
C	6.56807800	2.56725300	-0.96611200
C	6.85689000	1.13479200	-0.68128600
C	6.05379800	0.34763600	0.14586000
C	6.40963000	-0.97961000	0.34639900
C	8.28005900	-0.76066100	-1.03334000
C	3.53346200	9.23579000	-0.31045500
C	7.98626500	0.57219400	-1.27975600
C	2.90703300	11.71608900	-0.28069200
C	4.20591400	12.18637500	0.00217700
C	4.50682500	13.54260900	-0.08058300
C	3.51814800	14.46010900	-0.44858600
C	2.22565300	14.00839700	-0.72686900
C	1.91722100	12.65233900	-0.64419500
C	-2.84398900	6.39173800	0.20650100
C	-2.17766400	5.33848900	0.85810600
C	-2.73212800	4.06263200	0.90869800
C	2.62155100	10.28256800	-0.21806800
C	-3.96491400	3.82893200	0.29792600
C	-4.64529700	4.85945200	-0.35672700
C	-4.09236300	6.12940800	-0.39772500
C	-4.18738800	1.40887700	0.83172000
C	-5.17110700	0.31919200	0.58269800
C	-4.87170500	-0.94813600	1.08709000
C	-5.76965600	-1.98307500	0.87210700
C	-7.21131000	-0.56854900	-0.29856700
C	-6.35985500	0.51416600	-0.12262000
C	-2.73814800	11.45020900	0.23334300
C	1.32998800	9.66105200	-0.04348100
C	-4.02651700	11.81426100	-0.20821900
C	-4.45090000	13.13859600	-0.15339300

C	-3.59848000	14.12901100	0.34386600
C	-2.31742100	13.78287200	0.78123600
C	-1.88655800	12.45895500	0.72867900
C	-2.32343700	7.75699600	0.17758000
C	-3.14040100	8.92200600	0.19245300
C	-2.32291400	10.04893200	0.19481400
C	-0.96976400	9.55096200	0.15713600
C	3.48279500	6.68944000	-0.24366400
F	0.25743700	6.37214800	-0.97571000
F	0.41707900	6.54712000	1.33415900
H	5.01473800	7.36769500	-1.60727600
H	6.21732900	5.21050600	-1.67418500
H	3.34220000	3.51766700	1.00386800
H	2.12072700	5.68764100	1.09142900
H	5.17703800	0.76608100	0.61550500
H	5.82408400	-1.63515100	0.97630500
H	9.14203800	-1.24546700	-1.47061500
H	8.61037500	1.17862100	-1.92173300
H	4.97208800	11.48526200	0.31098100
H	5.50905500	13.88628500	0.14708400
H	3.75367400	15.51576600	-0.51564800
H	1.45517300	14.71398200	-1.01533500
H	0.91644600	12.30380900	-0.85436200
H	-1.22603500	5.53107600	1.33027200
H	-2.22203700	3.26014200	1.41354500
H	4.59776100	9.32189100	-0.44194100
H	-5.59345200	4.64173700	-0.82920600
H	-4.61016200	6.91918700	-0.92697900
H	-3.95152400	-1.10309900	1.63358300
H	-5.58676900	-2.98315600	1.24038700
H	-8.14533500	-0.47508400	-0.83545700
H	-6.60643000	1.48666700	-0.51974700
H	-4.68369900	11.05575100	-0.61665600
H	-5.44245100	13.40116100	-0.50308800
H	-3.93026100	15.15966500	0.38876000
H	-1.65354200	14.54540200	1.17168700
H	-0.89481800	12.19276300	1.06494600
H	-4.21322000	8.90887500	0.27498000
N	1.50125600	8.25621100	-0.02099300
N	0.15024300	10.24684300	0.05935000
N	-1.00546800	8.13737300	0.16296600
N	7.50533200	-1.53428600	-0.23063700
N	-6.92864500	-1.80301900	0.18854000
O	5.42592100	2.95846700	-0.29437700
O	7.25046100	3.28333700	-1.69093300
O	-4.63908300	2.58703200	0.26721300
O	-3.13731000	1.26905000	1.44842800
N	-9.75796900	-2.53889800	-1.12708900

N	-7.66859900	-4.19236700	-1.84610800
N	-7.33031000	-4.92887600	0.79246300
N	-9.45088500	-3.31236700	1.50451100
C	-9.81533700	-2.36511200	-2.50504700
C	-8.03894300	-3.75590700	-3.11108500
C	-6.65160400	-5.12223500	-2.01361800
C	-6.37209500	-5.75557100	0.21756000
C	-7.39641600	-5.24991900	2.14341500
C	-9.18340900	-3.87149300	2.74658900
C	-10.57103500	-2.50493200	1.64975300
C	-10.83960600	-1.85902000	-0.57916100
C	-6.34358000	-5.27266600	-3.43382400
C	-7.21668400	-4.41258700	-4.12462400
C	-6.42032900	-6.29148000	2.45278600
C	-5.77630700	-6.60939800	1.24188600
C	-11.02590200	-2.52999100	3.03789700
C	-10.15244200	-3.39013400	3.72826400
C	-11.59456200	-1.19511600	-1.63840500
C	-10.95050600	-1.51329300	-2.84936400
Zn	-8.21918600	-3.34780800	-0.09630500
N	-6.03989700	-5.81870100	-1.06427800
N	-8.22482400	-4.73958000	3.04376700
N	-11.19087300	-1.81823700	0.69867700
N	-9.00576100	-2.89792100	-3.40989400
C	-6.09646400	-6.94839400	3.63684700
C	-4.79196500	-7.59231100	1.18398500
H	-6.60728000	-6.70044200	4.55878100
H	-4.31238200	-7.83321300	0.24359200
C	-7.19588600	-4.32566900	-5.51344200
C	-5.42640300	-6.06886300	-4.11322400
H	-7.87898600	-3.66487500	-6.03214500
H	-4.76584900	-6.73165400	-3.56854200
C	-12.74022400	-0.40406000	-1.61625300
C	-11.43564400	-1.04839000	-4.06891100
H	-13.23095200	-0.17642600	-0.67827000
H	-10.93579900	-1.30987300	-4.99314300
C	-12.08840400	-1.90737400	3.68625300
C	-10.31792800	-3.65046600	5.08534900
H	-12.75731100	-1.25403100	3.14030200
H	-9.64224800	-4.32059000	5.60177600
C	-6.27130400	-5.11727700	-6.19854000
C	-5.39704300	-5.97860200	-5.50671000
C	-11.37828700	-3.02115000	5.74134000
C	-12.25312600	-2.15991900	5.05001700
C	-13.22334000	0.07175900	-2.83673300
C	-12.57853400	-0.24665600	-4.04893300
C	-4.45801000	-8.24608700	2.37173600
C	-5.10270100	-7.92784400	3.58389500

N	6.51585200	-4.15779400	1.32540000
N	7.03584700	-4.51466600	-1.36165900
N	9.66806300	-3.78985500	-0.95859000
N	9.15916100	-3.47920500	1.73628600
C	5.26802000	-4.62429300	0.92857300
C	5.70629900	-4.91414200	-1.34765500
C	7.50859200	-4.70494000	-2.65298500
C	9.73989700	-4.10385100	-2.31080900
C	10.96023500	-3.50806200	-0.53043800
C	10.52539700	-3.23329100	1.74832400
C	8.72341400	-3.44382400	3.05396800
C	6.48849100	-4.02997700	2.70941100
C	6.43977900	-5.22455600	-3.50282400
C	5.30531700	-5.35605800	-2.68124700
C	11.88677900	-3.60745600	-1.65500200
C	11.11947900	-3.98208200	-2.77442500
C	9.84479200	-3.14371300	3.94101800
C	10.97902600	-3.01119700	3.11922000
C	5.16603500	-4.39063100	3.21346400
C	4.39864300	-4.76420500	2.09369100
Zn	7.97477100	-3.48467000	0.10007800
N	8.74200700	-4.49149300	-3.09292700
N	11.34532000	-3.22085900	0.70520800
N	7.49320700	-3.67068500	3.49624600
N	4.88947600	-4.93894700	-0.30246900
C	13.26361100	-3.42457100	-1.75200300
C	11.70935800	-4.18332300	-4.01944000
H	13.84230900	-3.14591800	-0.88030600
H	11.10796500	-4.48071100	-4.86930900
C	4.10320300	-5.84612700	-3.18277100
C	6.40255200	-5.57975800	-4.84789100
H	3.24025100	-5.94845700	-2.53689700
H	7.28565900	-5.47995700	-5.46634300
C	4.63343900	-4.43043800	4.49931000
C	3.07916800	-5.18692200	2.23112100
H	5.23858900	-4.14974600	5.35219200
H	2.50426900	-5.48044600	1.36178900
C	9.93406000	-3.00554400	5.32297700
C	12.23281800	-2.73696000	3.65746600
H	9.05389000	-3.11770000	5.94350400
H	13.09820200	-2.64513200	3.01324700
C	4.05955800	-6.19622800	-4.53419700
C	5.19565700	-6.06468800	-5.35689900
C	12.32506700	-2.58971100	5.04330500
C	11.18922400	-2.72241800	5.86625900
C	3.30738700	-4.84459600	4.63930900
C	2.53918800	-5.21842100	3.51834600
C	13.08849600	-3.99103700	-4.12207600

C	13.85660900	-3.61607200	-3.00148800
H	3.13945100	-6.57850400	-4.96080500
H	5.12801900	-6.34843500	-6.40076300
H	13.58172300	-4.13550800	-5.07632300
H	14.92574600	-3.47943100	-3.11558400
H	13.28476500	-2.37291400	5.49799200
H	11.29673100	-2.60518500	6.93838700
H	2.85820900	-4.88508900	5.62488000
H	1.51406700	-5.53910500	3.66342600
H	-11.53668100	-3.19774100	6.79891400
H	-13.06795200	-1.69046400	5.58893800
H	-3.69427000	-9.01510200	2.36549900
H	-4.82227500	-8.45828500	4.48651300
H	-14.11159700	0.69251500	-2.85798600
H	-12.98333000	0.13543300	-4.97894700
H	-6.22408600	-5.07392000	-7.28049400
H	-4.69391100	-6.58151900	-6.06957300

Optimized Structure Results of (ZnNc)₂:py₂-azaBODIPY

HF=-10559.4444831 A.U.

%chk=ZnNc2-py2.chk

%nprocs=8

OPT B3LYP/3-21G* Integral(Ultrafine)

ZnNc2-py2

O 1

B	0.00329800	7.58574800	-0.52418500
C	-2.58643700	8.20704900	-0.41838300
C	-4.38957600	6.66459800	0.27471700
C	-5.01066200	5.42616900	0.26230700
C	-4.43556800	4.37011400	-0.45011500
C	-3.23800800	4.54575100	-1.14446500
C	-2.61382900	5.79007500	-1.12194100
C	-4.83752200	1.97779700	-1.00415300
C	-5.86622100	0.94355900	-0.70433600
C	-6.98586900	1.19337200	0.09095700
C	-7.88957600	0.16144700	0.30621000
C	-6.62950900	-1.30890200	-0.99784700
C	-3.34460500	9.40921300	-0.34573600
C	-5.68511400	-0.32646700	-1.25594800
C	-2.83205100	11.91584800	-0.32973800
C	-4.12776600	12.32763400	-0.70351200
C	-4.49556200	13.66842900	-0.64125600
C	-3.57839300	14.62858800	-0.20357200
C	-2.28950100	14.23508800	0.16511000
C	-1.91429900	12.89479400	0.10356200
C	3.18259000	6.86725000	-0.43608200
C	2.61095500	5.78320500	-1.12619800
C	3.23309300	4.53786500	-1.14504100
C	-2.47748400	10.49703300	-0.37337500
C	4.43860200	4.36657500	-0.46329500
C	5.02394800	5.42798000	0.23270300
C	4.40437900	6.66715600	0.24212800
C	4.82756400	1.96714400	-0.99601900
C	5.85869900	0.93452700	-0.69905100
C	5.66678300	-0.34200400	-1.23166500
C	6.61318700	-1.32306800	-0.97561000
C	7.89623600	0.16122700	0.28959100
C	6.99113700	1.19209300	0.07539500
C	2.83845200	11.91424800	-0.46823700
C	-1.15033000	9.93590500	-0.45887500
C	4.07695600	12.33742100	0.05560800
C	4.44098700	13.68044900	0.02783600

C	3.57669400	14.63090700	-0.52394700
C	2.34438500	14.22592400	-1.04316000
C	1.97401800	12.88303200	-1.01805700
C	2.59490400	8.20518100	-0.43983800
C	3.35557500	9.40784500	-0.40177600
C	2.48815800	10.49481500	-0.45623400
C	1.16012000	9.93364300	-0.50579700
C	-3.17567000	6.86931000	-0.41648200
F	0.00922500	6.70270900	0.55002900
F	-0.00349900	6.86671200	-1.76655000
H	-4.82572200	7.47258700	0.84815000
H	-5.93270200	5.25262400	0.80021800
H	-2.80810000	3.72430400	-1.69182800
H	-1.68819600	5.93748600	-1.65771900
H	-7.14069300	2.16863900	0.52584500
H	-8.77405300	0.29905600	0.91290500
H	-6.53776000	-2.30817000	-1.40050400
H	-4.81856200	-0.52400300	-1.87198000
H	-4.83713500	11.59356000	-1.06669800
H	-5.49381700	13.96697900	-0.93926400
H	-3.86604100	15.67217300	-0.15270800
H	-1.57431100	14.97390700	0.50770200
H	-0.91587700	12.59145300	0.38342300
H	1.68058000	5.92829800	-1.65442600
H	2.79577400	3.71202300	-1.67979200
H	-4.41835100	9.44628500	-0.28935500
H	5.95260100	5.25765800	0.76018000
H	4.84821600	7.48038500	0.80212000
H	4.79062600	-0.54554500	-1.83195800
H	6.51299900	-2.32727300	-1.36373700
H	8.79076600	0.30509600	0.87985200
H	7.15462300	2.17252100	0.49524900
H	4.74143000	11.60957400	0.50590500
H	5.39438700	13.98852400	0.44078900
H	3.86168600	15.67617100	-0.54770500
H	1.67186100	14.95733100	-1.47605600
H	1.01977200	12.57131600	-1.41764400
H	4.43087100	9.44535000	-0.41572900
N	-1.25451100	8.52494900	-0.49471700
N	0.00536500	10.57624100	-0.48169500
N	1.26244500	8.52308100	-0.50997000
N	-7.72260400	-1.07504100	-0.22729400
N	7.71861000	-1.08174500	-0.22516600
O	-5.17405800	3.16675600	-0.38467100
O	-3.84590900	1.79020900	-1.69959900
O	5.17625200	3.16299300	-0.39661800
O	3.82551800	1.77370500	-1.67461700
N	10.51444800	-1.64394100	1.23580500

N	8.49514900	-3.44166000	1.82970100
N	8.34551100	-4.16901500	-0.83724500
N	10.39617900	-2.40437500	-1.42340500
C	10.48173000	-1.48271400	2.61643400
C	8.76969300	-2.99232200	3.11480900
C	7.53016200	-4.43487000	1.93001400
C	7.41115100	-5.05831700	-0.31850200
C	8.50387100	-4.46333000	-2.18703300
C	10.22594700	-2.96412900	-2.68243300
C	11.46406600	-1.51963200	-1.49856400
C	11.57283100	-0.88577700	0.74752900
C	7.14996000	-4.62150200	3.32774800
C	7.93775600	-3.70502900	4.08051100
C	7.61254300	-5.55692100	-2.56381000
C	6.91907800	-5.93447800	-1.37798400
C	11.99113600	-1.48904100	-2.86021900
C	11.20452400	-2.40708000	-3.61240100
C	12.22464000	-0.17899600	1.84637000
C	11.53216100	-0.55781400	3.03251200
Zn	9.08662500	-2.54361600	0.11497400
N	7.01650300	-5.15559400	0.94238100
N	9.34245700	-3.88789100	-3.03595000
N	11.98424700	-0.80608600	-0.50934900
N	9.66087900	-2.07706600	3.47005200
C	7.39644000	-6.19849200	-3.75827800
C	6.00299200	-6.95707400	-1.37551600
H	7.93780600	-5.90784000	-4.65099300
H	5.48936300	-7.24064600	-0.46436100
C	7.83967500	-3.62567600	5.44712300
C	6.25555000	-5.46787400	3.93381700
H	8.45075000	-2.92898400	6.00897600
H	5.66708600	-6.16582200	3.34986900
C	13.29417800	0.68140700	1.88211600
C	11.90261900	-0.07942000	4.26518300
H	13.81895000	0.95320100	0.97364900
H	11.37368500	-0.38359000	5.16091700
C	13.02392600	-0.78945700	-3.43269600
C	11.44248100	-2.63498400	-4.94471800
H	13.62008200	-0.09942600	-2.84706100
H	10.84099500	-3.34201300	-5.50393500
C	5.86694200	-5.28021900	8.16163500
C	6.75997900	-4.44796000	7.52794000
C	6.91857000	-4.47979200	6.11337700
C	6.11712100	-5.41147000	5.34788500
C	5.20490900	-6.25527000	6.04287400
C	5.08122300	-6.19326800	7.41131000
H	5.75873300	-5.24380200	9.23933000
H	7.36238900	-3.74988000	8.09954600

H	4.60600500	-6.95312700	5.46740700
H	4.38242900	-6.84300800	7.92508500
C	12.49831900	-1.92381100	-5.57818700
C	13.29823700	-0.99024900	-4.81336300
C	14.35004900	-0.29455500	-5.47440500
C	14.60734600	-0.49851200	-6.81004100
C	13.82330100	-1.41357400	-7.55970700
C	12.79818800	-2.10568600	-6.95814300
H	14.94902200	0.40341900	-4.89908900
H	15.41231800	0.03855300	-7.29795000
H	14.03895200	-1.56419900	-8.61101900
H	12.19827400	-2.80654200	-7.52893600
C	13.43281800	1.36323700	5.58737700
C	14.49632800	2.23268400	5.65134900
C	15.18659300	2.60973900	4.46967100
C	14.79880500	2.10954500	3.24878400
C	13.70257000	1.20719400	3.13794600
C	12.99845500	0.82241200	4.34357100
H	12.90519100	1.07194200	6.48942200
H	14.81513900	2.63410800	6.60616500
H	16.02400600	3.29435800	4.53682000
H	15.32628900	2.39458300	2.34464500
C	4.80059400	-8.70527600	-2.66736500
C	5.74281400	-7.63998700	-2.59480000
C	6.44773000	-7.25626100	-3.80016700
C	6.16808100	-7.96081900	-5.00568300
C	5.24997400	-8.98430300	-5.03357700
C	4.55905700	-9.36043900	-3.85213700
H	4.27469000	-8.99196900	-1.76288100
H	6.69829900	-7.67255300	-5.90713200
H	5.04934500	-9.51101700	-5.95917700
H	3.83935100	-10.16976100	-3.89015700
N	-10.48594000	-1.65964800	1.28697100
N	-10.43222900	-2.36417500	-1.38958500
N	-8.37399900	-4.14650600	-0.88887700
N	-8.45938200	-3.47556300	1.79546000
C	-11.55371100	-0.88930300	0.83990000
C	-11.49952900	-1.47610700	-1.42087600
C	-10.29246200	-2.89702600	-2.66397700
C	-8.56405200	-4.41093600	-2.24074600
C	-7.43153500	-5.05000500	-0.41086300
C	-7.49665400	-4.47437200	1.85255100
C	-8.70216500	-3.05238600	3.09576700
C	-10.42003700	-1.52735500	2.66943700
C	-11.29121600	-2.31842500	-3.55868900
C	-12.05835800	-1.41572300	-2.76875700
C	-6.96679400	-5.90444600	-1.50005100
C	-7.68560000	-5.49892100	-2.66130600

C	-7.85113100	-3.78845400	4.02673200
C	-7.08515400	-4.69204300	3.23683700
C	-11.45767800	-0.60895300	3.12960000
C	-12.17736800	-0.20425500	1.96847500
Zn	-9.08765400	-2.53935300	0.11459100
N	-9.41987000	-3.81489100	-3.05757000
N	-7.00869600	-5.17579400	0.83835700
N	-9.58124000	-2.14172400	3.49079500
N	-11.99461900	-0.78254400	-0.40491800
C	-6.05468200	-6.92986600	-1.54067600
C	-7.49918700	-6.11511100	-3.87395300
H	-5.52155100	-7.23494400	-0.64781000
H	-8.05960800	-5.80338700	-4.74755300
C	-13.10328000	-0.70303900	-3.30161900
C	-11.56068800	-2.51735800	-4.88967000
H	-13.68442100	-0.02512100	-2.68748100
H	-10.97366600	-3.21294500	-5.47783600
C	-11.79753200	-0.15569200	4.38041500
C	-13.24381900	0.65711400	2.04764300
H	-11.24815000	-0.47941900	5.25677300
H	-13.78946000	0.94872100	1.15780400
C	-7.72122200	-3.73851300	5.39211700
C	-6.18114400	-5.55495800	3.80404800
H	-8.31587100	-3.05126800	5.98255300
H	-5.60963800	-6.24287100	3.19200900
C	-14.76579400	-0.33877400	-6.63357000
C	-14.47676600	-0.16366500	-5.30032600
C	-13.41041800	-0.87405400	-4.67937900
C	-12.62997600	-1.79163200	-5.48272400
C	-12.96247500	-1.94354200	-6.85882300
C	-14.00066500	-1.23798600	-7.42102300
H	-15.58149600	0.20910200	-7.09067000
H	-15.06118100	0.52218700	-4.69617500
H	-12.37707700	-2.63240700	-7.45851800
H	-14.24124800	-1.36584800	-8.46993500
C	-6.01008900	-5.52932900	5.21545900
C	-6.78916400	-4.61056400	6.01871600
C	-6.59802300	-4.60950200	7.42959700
C	-5.69496900	-5.45917500	8.02482100
C	-4.93131000	-6.35969600	7.23751500
C	-5.08652100	-6.39193400	5.87125800
H	-7.18356800	-3.92095000	8.02957100
H	-5.56194100	-5.44617100	9.10027100
H	-4.22430200	-7.02346900	7.72123500
H	-4.50447400	-7.08009700	5.26748800
C	-14.71216400	2.05913600	3.47922100
C	-15.06959700	2.53447300	4.71914400
C	-14.35219700	2.13168600	5.87589800

C	-13.29245300	1.26190000	5.76848500
C	-12.88911900	0.74631100	4.50368600
C	-13.62093300	1.15736400	3.32351500
H	-15.26034600	2.36395200	2.59405600
H	-15.90358000	3.21906300	4.82049500
H	-14.64716800	2.51376200	6.84618900
H	-12.74406600	0.95102700	6.65142000
C	-6.30599000	-7.85375000	-5.18703000
C	-6.55559500	-7.17474300	-3.96043600
C	-5.82481600	-7.58686300	-2.78011200
C	-4.88835400	-8.65325300	-2.89725200
C	-4.67617400	-9.28317000	-4.10116900
C	-5.39242800	-8.87922100	-5.25808900
H	-6.85551100	-7.54426100	-6.06968000
H	-4.34304000	-8.96120200	-2.01143900
H	-3.96041900	-10.09367800	-4.17319000
H	-5.21474500	-9.38621500	-6.19925800

Optimized Structure Results of (ZnPc)₂:im₂-azaBODIPY

HF=-9752.7618495

%chk=pim2-ZnPc2.chk

%nprocshared=4

OPT B3LYP/3-21G* Integral(Ultrafine) SCF(Conver=6)

pim2-ZnPc2

O 1

B	0.06058800	8.83410600	-0.55062100
C	-2.41073300	9.72620900	-0.09973000
C	-4.30689900	8.33614500	0.66180100
C	-5.08014000	7.18076600	0.63769200
C	-4.70146100	6.13389400	-0.20726400
C	-3.56335000	6.24558300	-1.00997400
C	-2.79150500	7.39682000	-0.97738000
C	-6.54230700	4.54564000	0.33695400
C	-3.00591800	10.99405900	0.15527400
C	-2.19573900	13.41548700	0.31271300
C	-3.46486200	14.00136000	0.12781600
C	-3.65933600	15.36311200	0.33941200
C	-2.59135600	16.17099600	0.74113000
C	-1.32730500	15.60445600	0.92326200
C	-1.12546200	14.24228700	0.71168700
C	3.12133600	7.75888900	-0.87509400
C	2.35623800	6.81412100	-1.58236400
C	2.81638000	5.51367500	-1.76861600
C	-2.02168100	11.97607600	0.11515900
C	4.05377200	5.14178000	-1.23950400
C	4.82993500	6.06419800	-0.53048600
C	4.37128600	7.35955000	-0.35453500
C	4.08491500	2.76788000	-1.99633100
C	3.38879600	12.79414500	-0.46367000
C	-0.78788000	11.28129000	-0.16675900
C	4.71609200	13.02606300	-0.04926400
C	5.23532100	14.31680700	-0.00970100
C	4.44086900	15.40500000	-0.38308400
C	3.12221300	15.19001300	-0.79187500
C	2.59665600	13.90032200	-0.83361300
C	2.70307500	9.14850100	-0.70641800
C	3.60310900	10.25012100	-0.65669900
C	2.87223300	11.42759200	-0.52688700
C	1.48837300	11.02551900	-0.47365100
C	-3.15290800	8.46821000	-0.13546800
F	0.06918800	7.85763200	0.43958000
F	-0.16004100	8.23987400	-1.83942700

H	-4.58651200	9.13619300	1.33586500
H	-5.95370000	7.07967700	1.25843900
H	-3.30073800	5.41824500	-1.65542700
H	-1.91431900	7.48702200	-1.59976200
H	-4.29271500	13.38716700	-0.20593500
H	-4.64061800	15.79672900	0.18596800
H	-2.74387200	17.23079800	0.90841700
H	-0.49547200	16.22437700	1.23713300
H	-0.14679200	13.80528000	0.84736500
H	1.40251000	7.11176600	-1.99151300
H	2.23147200	4.79484700	-2.31628600
H	-4.05530300	11.14464000	0.33828200
H	5.77841500	5.74191100	-0.12274700
H	4.96509100	8.06221100	0.21625700
H	5.32983700	12.18988000	0.26406900
H	6.25601000	14.47674400	0.31754100
H	4.84625300	16.40960200	-0.35433400
H	2.50238800	16.02897400	-1.08626300
H	1.57593300	13.73539900	-1.14730000
H	4.66816200	10.16841600	-0.78664000
N	-1.06522100	9.89985900	-0.30302300
N	0.42782700	11.78819700	-0.26876200
N	1.41837000	9.61905200	-0.60211700
O	-5.38452500	4.90792100	-0.34078400
O	-7.13433800	5.25644800	1.14364600
O	4.63986900	3.86384300	-1.34700300
O	3.00179200	2.76775300	-2.57334000
C	-8.79676300	-2.53520500	-2.17203200
C	-8.26757000	-1.28575800	-2.32311300
C	-8.83667200	-1.60480800	-0.18028700
N	-9.14776700	-2.72736700	-0.82657900
H	-8.96315200	-3.30434700	-2.90353100
H	-7.91710200	-0.75812300	-3.19024000
H	-8.95381100	-1.43737300	0.87493000
N	-8.29558100	-0.68893600	-1.05059100
C	8.17919900	-2.22649800	-0.61995000
C	8.49987500	-3.70098600	-2.21900900
C	7.63515700	-2.77248500	-2.72314600
N	7.43217500	-1.82726000	-1.70242200
H	8.19614500	-1.71200300	0.32353900
H	8.91586400	-4.57629400	-2.68282400
H	7.18340300	-2.66841700	-3.69177600
N	8.83313400	-3.35247800	-0.90072700
C	5.37249000	-0.72356900	-2.43098700
C	4.57422300	0.41118000	-2.49532600
C	4.99293300	1.60163400	-1.89098000
C	6.22098700	1.65646200	-1.22436000
C	7.03040700	0.52666600	-1.17055600

C	6.60470100	-0.66537300	-1.76893400
H	5.03603600	-1.65611800	-2.86497500
H	3.61524400	0.39490200	-2.99720900
H	6.53559700	2.58362500	-0.76860900
H	7.99902800	0.57300700	-0.68955300
C	-8.56703400	1.39585900	0.20237600
C	-8.11591800	2.66734000	0.53339200
C	-6.95616700	3.17919700	-0.05843500
C	-6.23956900	2.40978500	-0.98080300
C	-6.67959500	1.13076000	-1.30381100
C	-7.84378900	0.62367800	-0.71503600
H	-9.48422400	1.01159900	0.62984700
H	-8.65518000	3.28691800	1.23843100
H	-5.34080600	2.81415700	-1.42261200
H	-6.11061000	0.51470000	-1.98796300
N	8.92154900	-5.62778900	1.37425400
N	10.74556100	-5.92743200	-0.67624400
N	11.89686300	-3.51346900	0.00923400
N	10.03115300	-3.18236000	2.01783500
C	8.55003700	-6.89208000	0.94217900
C	10.09523000	-7.14823300	-0.79123900
C	11.80353200	-5.93440000	-1.57521300
C	12.77358600	-3.88906600	-0.99739600
C	12.36372700	-2.31860300	0.53885700
C	10.78748500	-2.03940500	2.24128000
C	9.08006300	-3.25505500	3.02675800
C	8.14049400	-5.32364000	2.48063700
C	11.80975100	-7.19048500	-2.32235300
C	10.73503400	-7.95414900	-1.82910500
C	13.57714700	-1.90438200	-0.16287200
C	13.83520100	-2.89331400	-1.13002000
C	9.20514600	-2.09695500	3.90853300
C	10.27970700	-1.33213700	3.41450300
C	7.22325700	-6.42692600	2.75995900
C	7.48127400	-7.41442100	1.79154800
Zn	10.07073300	-4.32316400	0.34169100
N	12.71534700	-4.98640800	-1.74196600
N	11.83831500	-1.62848400	1.54313000
N	8.19430500	-4.22372200	3.22033300
N	9.06982900	-7.57769900	-0.06839000
C	14.41846600	-0.80613700	-0.01142500
C	14.94045700	-2.80954300	-1.97146200
H	14.21221200	-0.05724700	0.74299000
H	15.12969300	-3.58190900	-2.70633900
C	10.46985500	-9.22914000	-2.32059300
C	12.64685900	-7.68232400	-3.31978600
H	9.64555000	-9.80878100	-1.92438600
H	13.47572200	-7.08741000	-3.68243500

C	6.25783200	-6.61581200	3.74423200
C	6.78076700	-8.61674400	1.78169900
H	6.07506400	-5.84991600	4.48747800
H	6.99527500	-9.37025800	1.03430800
C	8.50394400	-1.70588300	5.04620700
C	10.68025100	-0.15795200	4.04703700
H	7.68659500	-2.30959200	5.42034800
H	11.51665500	0.41297700	3.66342400
C	11.30188000	-9.72177800	-3.32835700
C	12.37767000	-8.95737600	-3.82210500
C	9.97269000	0.24159400	5.18249200
C	8.89667700	-0.52336700	5.67620600
C	5.54757700	-7.81860500	3.73356300
C	5.80594500	-8.80728900	2.76387400
C	15.78304600	-1.70487600	-1.82746000
C	15.52517300	-0.71496900	-0.85872700
N	-8.43413000	-5.50331100	0.63365800
N	-10.20178300	-3.83209600	1.94015600
N	-11.97348800	-4.08060500	-0.16337100
N	-10.17780400	-5.69800500	-1.49786600
C	-7.72975800	-5.33089900	1.81700600
C	-9.22596400	-3.91836100	2.92427100
C	-11.25766900	-3.09902300	2.46530300
C	-12.75510400	-3.30745000	0.68348700
C	-12.74268900	-4.37716300	-1.27860900
C	-11.22601500	-5.75024100	-2.40660500
C	-9.19360400	-6.56657700	-1.94920200
C	-7.71685500	-6.39765200	-0.14678300
C	-10.93255500	-2.66616200	3.82237600
C	-9.65412400	-3.18167600	4.11113200
C	-14.06196900	-3.76103300	-1.15148400
C	-14.06977400	-3.08733700	0.08380000
C	-9.60816900	-7.17014600	-3.21395400
C	-10.88680800	-6.65650400	-3.50177200
C	-6.49949500	-6.80376300	0.55289200
C	-6.50751500	-6.13202200	1.78915700
Zn	-9.97417400	-4.35801200	-0.00481400
N	-12.41617800	-2.83349900	1.87568100
N	-12.38996400	-5.12098500	-2.31973600
N	-8.05214000	-6.86395100	-1.34327200
N	-8.07950200	-4.58236100	2.85507800
C	-15.18017000	-3.76328200	-1.97987400
C	-15.19646600	-2.39871700	0.52329700
H	-15.16149000	-4.29198600	-2.92461800
H	-15.19078100	-1.89156700	1.47998500
C	-9.05055300	-2.96406200	5.34690400
C	-11.63932100	-1.92102000	4.76271400
H	-8.07141100	-3.37525700	5.55832000

H	-12.62656800	-1.54119000	4.53098200
C	-5.46702900	-7.67114800	0.20910200
C	-5.48318900	-6.30998400	2.71418000
H	-5.47817900	-8.18664300	-0.74303600
H	-5.50637700	-5.79176300	3.66461500
C	-8.99286100	-8.08987100	-4.05843400
C	-11.58276200	-7.04936100	-4.64149900
H	-8.01324200	-8.48400100	-3.81868500
H	-12.56985600	-6.65331500	-4.84463800
C	-9.75263600	-2.20837400	6.28798000
C	-11.03231700	-1.69298000	5.99932400
C	-10.96413300	-7.96453300	-5.49600700
C	-9.68425800	-8.47877600	-5.20784600
C	-4.43338000	-7.84703200	1.13203600
C	-4.44136500	-7.17440800	2.36985600
C	-16.31859100	-2.39290900	-0.30850200
C	-16.31052300	-3.06708300	-1.54550700
H	16.65265500	-1.60514800	-2.46674500
H	16.20159100	0.12743400	-0.77077400
H	13.00662800	-9.37180200	-4.60152900
H	11.12380900	-10.70962300	-3.73735000
H	8.37219000	-0.18695100	6.56309500
H	10.25549800	1.15112600	5.69991000
H	4.78649900	-7.99999400	4.48369900
H	5.23878800	-9.73068900	2.78623900
H	-11.47494500	-8.29112900	-6.39448400
H	-9.23501900	-9.19118400	-5.89013400
H	-3.61126000	-8.51347500	0.89785200
H	-3.62518500	-7.33594600	3.06455900
H	-9.31260900	-2.01657200	7.25978900
H	-11.55199200	-1.11519800	6.75496100
H	-17.19947800	-3.04522000	-2.16529300
H	-17.21373100	-1.86531700	0.00014100

Optimized Structure Results of (ZnNc)₂:Im₂-azaBODIPY

HF=-10975.1248132

%chk=pim2-ZnNc2.chk

%NProc=4

OPT B3LYP/3-21G* Integral(Ultrafine)

pim2-ZnNc2

O 1

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C	-2.52258282	10.86887899	-0.85970473
C	-4.41917429	9.46995750	-0.10915925
C	-5.17193461	8.30031475	-0.12136706
C	-4.76844627	7.24824275	-0.94805705
C	-3.63416663	7.37276350	-1.75420087
C	-2.88342932	8.53747453	-1.73362531
C	-6.53459659	5.59959807	-0.33511128
C	-3.11399592	12.14039625	-0.61589547
C	-2.29070515	14.55669656	-0.44587419
C	-3.55352615	15.15003031	-0.64939070
C	-3.74285153	16.51307914	-0.44158605
C	-2.67591977	17.31488840	-0.02517650
C	-1.41800798	16.74093831	0.17538492
C	-1.22127759	15.37744947	-0.03234077
C	2.99090832	8.84591232	-1.49634153
C	2.22832642	7.91764636	-2.22751495
C	2.65587853	6.60277557	-2.38316538
C	-2.12238371	13.11617660	-0.64012028
C	3.85740812	6.19841118	-1.79809991
C	4.63496261	7.10606965	-1.07173465
C	4.20918670	8.41708755	-0.92707726
C	3.81658571	3.80954807	-2.49868937
C	3.31365720	13.88055192	-1.08053288
C	-0.88761316	12.41299709	-0.89901434
C	4.62924580	14.09774489	-0.62315067
C	5.16146586	15.38259614	-0.56721690
C	4.39200778	16.47939023	-0.96684647
C	3.08507967	16.27899769	-1.41850241
C	2.54661926	14.99528480	-1.47677462
C	2.59323260	10.24332941	-1.34387499
C	3.50446554	11.33363727	-1.26594132
C	2.78346285	12.52015220	-1.15994727
C	1.39349819	12.13492323	-1.14923245
C	-3.26235319	9.60980809	-0.90067765
F	-0.08154741	8.96868837	-0.29992415
F	-0.24893753	9.38816596	-2.57810376

H	-4.71465370	10.27340192	0.55414487
H	-6.04535116	8.19063827	0.49838028
H	-3.35476150	6.54199184	-2.38803824
H	-2.00640796	8.63524072	-2.35498166
H	-4.38021239	14.54056745	-0.99450201
H	-4.71922300	16.95242056	-0.60940874
H	-2.82446053	18.37572511	0.13911453
H	-0.58704108	17.35616491	0.50058827
H	-0.24730809	14.93454092	0.11745598
H	1.30055849	8.23811013	-2.67693790
H	2.07167412	5.89651720	-2.94732747
H	-4.16522223	12.29751030	-0.44915957
H	5.55618818	6.76017226	-0.62289722
H	4.80139438	9.10827734	-0.34065406
H	5.22290390	13.25488264	-0.28965205
H	6.17267967	15.53126521	-0.20690675
H	4.80757857	17.47937378	-0.92533137
H	2.48483640	17.12468432	-1.73350274
H	1.53495065	14.84154331	-1.82379722
H	4.57221531	11.23887629	-1.36076999
N	-1.17305496	11.03411078	-1.03996272
N	0.33522053	12.90863990	-0.97234948
N	1.31198770	10.72970337	-1.27970706
O	-5.41427300	6.00017810	-1.05319812
O	-7.15819578	6.31173909	0.44591283
O	4.39823343	4.89682027	-1.85848207
O	2.76752634	3.84740640	-3.13473908
C	-8.22236080	-1.80012015	-2.32419504
C	-7.84490370	-0.51382482	-2.58348304
C	-8.27122704	-0.74332719	-0.39654949
N	-8.48386221	-1.93575802	-0.95174295
H	-8.33405261	-2.63206213	-2.99483428
H	-7.59640238	-0.01252129	-3.50009227
H	-8.35415801	-0.51594476	0.65067611
N	-7.87872998	0.16275504	-1.35194311
C	7.47804660	-1.38277207	-0.69657370
C	7.75602769	-2.95429646	-2.20939692
C	7.00077851	-1.98331335	-2.80097278
N	6.82462663	-0.97695439	-1.83543939
H	7.48918155	-0.82569261	0.22253164
H	8.11803515	-3.88300308	-2.61021074
H	6.61018014	-1.88986537	-3.79685083
N	8.04804839	-2.57124839	-0.89076343
C	4.89310247	0.23031066	-2.72619763
C	4.17913151	1.41094674	-2.88151053
C	4.64380013	2.59626601	-2.30111096
C	5.83464104	2.59975545	-1.56830902
C	6.56161760	1.42234835	-1.42377032

C	6.08819594	0.23603871	-1.99698378
H	4.51690418	-0.69624948	-3.13980241
H	3.24941530	1.43590565	-3.43527843
H	6.18529235	3.52300803	-1.13104219
H	7.50310055	1.42575287	-0.88954851
C	-8.30632425	2.29815881	-0.23284565
C	-7.95647813	3.62159759	0.00586622
C	-6.85689930	4.18763366	-0.64807640
C	-6.10229233	3.42374808	-1.54460266
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C	-7.54187553	1.53185778	-1.12098157
H	-9.17493404	1.86539260	0.24665576
H	-8.52720378	4.23711457	0.68941954
H	-5.25027802	3.87123899	-2.03459613
H	-5.83987095	1.48586095	-2.43845173
N	7.74934953	-4.63493281	1.55090681
N	9.53253996	-5.37332056	-0.43583177
N	11.04677701	-3.11837123	0.09921913
N	9.22851361	-2.34654916	2.04178884
C	7.18484340	-5.85025102	1.19304499
C	8.68986181	-6.47622257	-0.48106715
C	10.58722573	-5.61046324	-1.30705800
C	11.86247368	-3.70509612	-0.85694296
C	11.68457148	-1.97080422	0.55025216
C	10.15135438	-1.31990497	2.18954665
C	8.26460651	-2.19537590	3.03074513
C	7.01816331	-4.12798208	2.61637719
C	10.40254752	-6.89917082	-1.97051335
C	9.19714022	-7.44855349	-1.44640914
C	12.95565487	-1.79964877	-0.14983196
C	13.06889356	-2.90218936	-1.04390423
C	8.55185138	-1.00316945	3.82450666
C	9.75035418	-0.44722465	3.29007674
C	5.93140967	-5.04385165	2.95479366
C	6.03479503	-6.13655560	2.04758564
Zn	9.11022355	-3.60679317	0.45300070
N	11.63903097	-4.83248271	-1.51915265
N	11.25948525	-1.13282395	1.48568263
N	7.23847652	-2.99836795	3.27499121
N	7.59940049	-6.67882046	0.24365378
C	13.93589915	-0.84342867	-0.05980254
C	14.16279406	-3.05903589	-1.85747823
H	13.84132999	-0.01354255	0.63078756
H	14.23946374	-3.90656244	-2.52853283
C	8.73109715	-8.67497664	-1.84988837
C	11.15306893	-7.57109734	-2.90296199
H	7.81774733	-9.08598331	-1.43586891
H	12.07353523	-7.14632089	-3.28620817

C	4.95739263	-5.00081828	3.92078318
C	5.16067272	-7.19375088	2.09225297
H	4.89617091	-4.16821852	4.61179466
H	5.25385653	-8.02154698	1.39903247
C	7.90792966	-0.42951542	4.89312908
C	10.31595449	0.68602861	3.82055246
H	7.00266736	-0.86794932	5.29674686
H	11.23470632	1.09123235	3.41257058
C	9.77472100	-11.36546220	-4.23112643
C	9.04633212	-10.67319449	-3.29207314
C	9.47399041	-9.39879115	-2.82243686
C	10.69919212	-8.84048031	-3.35506831
C	11.42325916	-9.59015001	-4.32526698
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H	9.43587753	-12.33498086	-4.57708170
H	8.12904156	-11.09039926	-2.89026324
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H	11.53940584	-11.37656868	-5.49138497
C	9.67400846	1.31593509	4.92126548
C	8.45540655	0.75181516	5.46355904
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C	9.57228530	3.09662298	6.58335546
C	10.20083494	2.49742550	5.51703488
H	6.92491037	0.97829782	6.97418175
H	7.89469917	3.02688192	7.95609236
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H	11.11582596	2.91620530	5.11146577
C	3.18642039	-8.24483687	3.17490942
C	2.20215397	-8.23130215	4.13610992
C	2.10998600	-7.14977281	5.05241749
C	2.99902994	-6.10163615	4.98167560
C	4.03063141	-6.07611351	3.99998376
C	4.13052943	-7.18314035	3.07216997
H	3.26483875	-9.07452245	2.48020510
H	1.49444810	-9.04900779	4.20448058
H	1.33712204	-7.16016691	5.81232129
H	2.93296902	-5.27612889	5.68258989
C	16.35932838	-2.18204851	-2.61857015
C	15.19801271	-2.08565644	-1.80052418
C	15.08338303	-0.96505537	-0.89099451
C	16.13719237	-0.00835314	-0.85384085
C	17.24328580	-0.13763024	-1.66115643
C	17.35548524	-1.23585509	-2.55289020
H	16.44374290	-3.02337820	-3.29826260
H	16.05018039	0.82940998	-0.17003234
H	18.03719831	0.59891785	-1.61961216
H	18.23360705	-1.32475770	-3.18177163

N	-7.29103224	-4.40944095	0.69357663
N	-9.28035673	-2.93412762	1.93274454
N	-11.05081944	-3.65732382	-0.07182873
N	-9.04443655	-5.08002202	-1.34234334
C	-6.59127856	-4.00738788	1.82321242
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C	-10.42970474	-2.33626357	2.43393986
C	-11.92212661	-2.94624394	0.74191054
C	-11.78734930	-4.17332722	-1.12783322
C	-10.09620221	-5.37785322	-2.19935904
C	-7.93963738	-5.81046494	-1.75810305
C	-6.45881412	-5.23998247	-0.04281602
C	-10.14519175	-1.72496634	3.72973915
C	-8.77398887	-1.99711210	4.00736207
C	-13.18620210	-3.77084203	-1.00372623
C	-13.27190098	-2.99101486	0.18487687
C	-8.27601546	-6.58173760	-2.95252901
C	-9.64536531	-6.30675932	-3.23304645
C	-5.16594912	-5.37137154	0.62580977
C	-5.24969867	-4.58596037	1.81057799
Zn	-9.02670805	-3.59546711	0.02784096
N	-11.63072151	-2.31858925	1.87331236
N	-11.34357083	-4.93896034	-2.11630283
N	-6.74863863	-5.86041229	-1.17877163
N	-7.03171988	-3.23283666	2.80525791
C	-14.29018840	-4.02409439	-1.77878433
C	-14.46274574	-2.45749871	0.61035036
H	-14.21234643	-4.62488416	-2.67740693
H	-14.51589229	-1.87240022	1.52106749
C	-8.17698412	-1.56951862	5.16765666
C	-10.93114643	-1.02364727	4.61073403
H	-7.13589678	-1.79186735	5.37098143
H	-11.97567379	-0.83330475	4.39286954
C	-4.02996163	-6.07264803	0.30720484
C	-4.19742305	-4.49134624	2.68629540
H	-3.98205836	-6.67339079	-0.59360246
H	-4.27613570	-3.89444257	3.58747711
C	-7.54101790	-7.44083533	-3.73096491
C	-10.29239134	-6.88836984	-4.29489386
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H	-11.33731818	-6.67837627	-4.49142334
C	-9.16036934	0.36225056	8.21689356
C	-8.39818328	-0.34949828	7.32047523
C	-8.95405652	-0.83046141	6.10062320
C	-10.34763475	-0.55460489	5.81905296
C	-11.10132735	0.18513766	6.77465033
C	-10.52642622	0.63229680	7.94111521
H	-8.72210971	0.72011362	9.14120158

H	-7.35454684	-0.55891323	7.53007366
H	-12.14580433	0.38830177	6.56293541
H	-11.11450164	1.19280904	8.65840635
C	-9.56328944	-7.77639705	-5.13235210
C	-8.17145147	-8.05598002	-4.84702439
C	-7.46835757	-8.95212153	-5.70162413
C	-8.08941904	-9.54323162	-6.77697956
C	-9.45362847	-9.26910134	-7.05673668
C	-10.16815661	-8.40970537	-6.25523476
H	-6.42623993	-9.16164868	-5.48463606
H	-7.54015449	-10.22400418	-7.41681418
H	-9.92955022	-9.74380292	-7.90684231
H	-11.21154603	-8.20019733	-6.46600987
C	-1.86550306	-5.13848620	3.24930124
C	-0.71308741	-5.82924237	2.95525393
C	-0.63212106	-6.61856162	1.77841006
C	-1.70310901	-6.69784470	0.91884491
C	-2.91413325	-5.99760059	1.18610427
C	-2.99838775	-5.19573085	2.38868338
H	-1.93156706	-4.53549976	4.14897947
H	0.14336378	-5.78370863	3.61685876
H	0.28400593	-7.15868559	1.57048335
H	-1.64363380	-7.30056727	0.01857714
C	-16.89733442	-2.16437561	0.21024938
C	-15.62950564	-2.69058301	-0.16820274
C	-15.54217489	-3.48282196	-1.37698684
C	-16.72781355	-3.70084970	-2.13473983
C	-17.93386147	-3.17424982	-1.73491284
C	-18.01952093	-2.39794293	-0.54990471
H	-16.96075203	-1.57263276	1.11735825
H	-16.66016364	-4.29597235	-3.03931144
H	-18.82710584	-3.35064120	-2.32273955
H	-18.97719559	-1.99092610	-0.24699787