Supplementary Information

for

Vibrational Circular Dichroism and Single Crystal X-Ray Diffraction Analyses of $[Ir(bzq)_2(phen)]^+$ (bzq = benzo[h]quinoline; phen = 1,10-phenanthroline): Absolute Configuration and Role of CH-π Interaction in Molecular Packing

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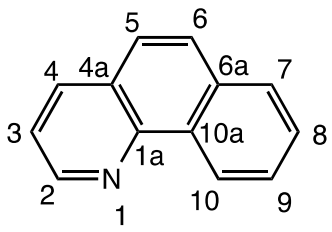
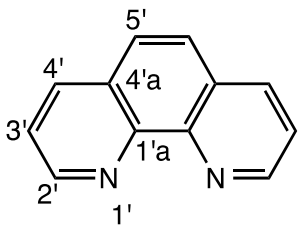
Contents:

S1. ^{1}H NMR, ^{13}C NMR, MS data and elemental analysis of [Ir(bzq)$_2$(phen)]ClO$_4$

δH (500 MHz; CD_3CN) 6.42 (2H, d, *J*=7.5 Hz, H7), 7.23 (2H, t, *J* =7.5 Hz, H8), 7.32 (2H, dd, *J* =8.0 and 5.0 Hz, H3), 7.58 (2H, d, *J* =7.5 Hz, H9), 7.75 (2H, dd, *J* =8.5 and 5.0 Hz, H3'), 7.81 (2H, d, *J* =7.5 Hz, H5), 7.87 (2H, dd, *J* =5.0 and 1.0 Hz, H4), 7.96 (2H, d, *J* =7.5 Hz, H6), 8.26 (2H, s, H5'), 8.27 (2H, dd, *J* =5.0 and 1.0 Hz, H4'), 8.38 (2H, dd, *J* =8.0 and 1.0 Hz, H2), 8.68 (2H, dd, *J* =8.0 and 1.0 Hz, H2'); δC (125 Hz, CD_3CN) 121.5 (C9), 123.2 (C3), 125.1 (C5), 127.6 (C3'), 128.2 (C4a), 129.2 (C5'), 130.0 (C7), 130.6 (C6), 130.7 (C8), 132.6 (C4'a), 135.3 (C6a), 138. 3(C2), 139.5 (C2'), 141.8 (C10a), 147.5 (C1a), 148.2 (C1'a), 149.8 (C4), 152.7 (C4'), 158.0 (C10); LRMS(FAB$^+$, 3-NBA), *m*/*z* = 729 (M+1); Anal. Found: C, 54.21; H, 3.46; N, 6.80. Calc. for $IrC_{38}H_{24}N_4ClO_4 \cdot H_2O$ ([Ir(bzq)$_2$(phen)]ClO$_4$): C, 53.93; H, 3.10; N, 6.62 %.



Bzq



Phen

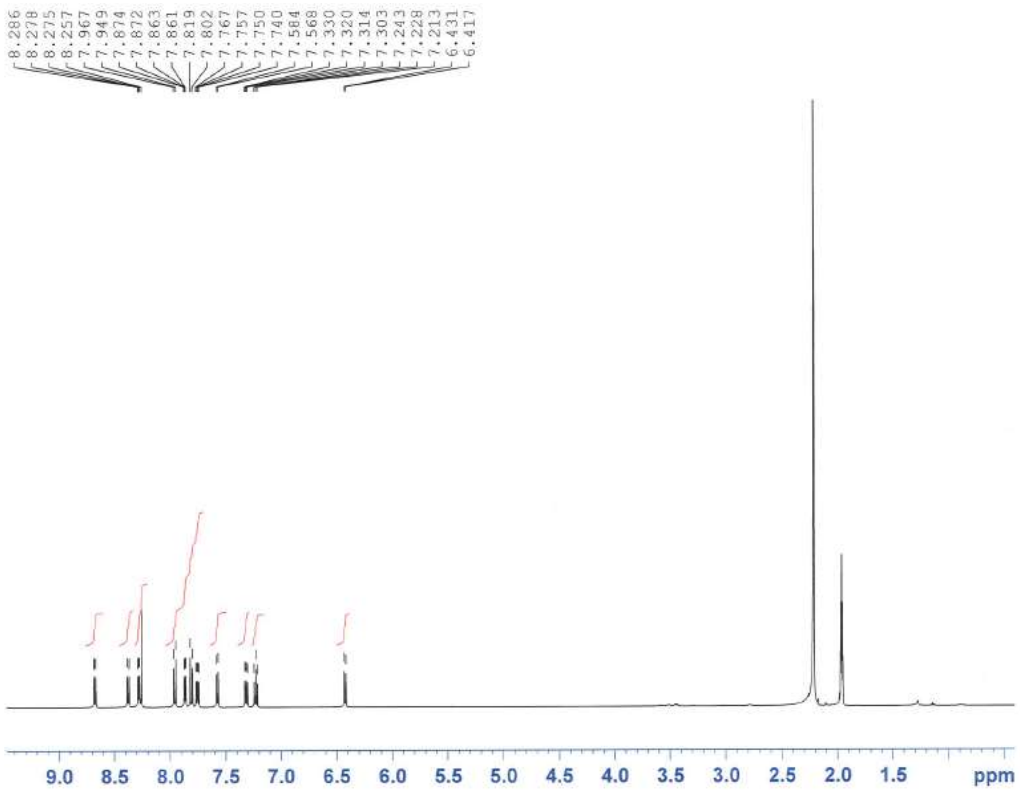


Figure S1-1 ^{1}H NMR spectrum of $[Ir(bzq)_2(phen)]ClO_4$ in CD_3CN.

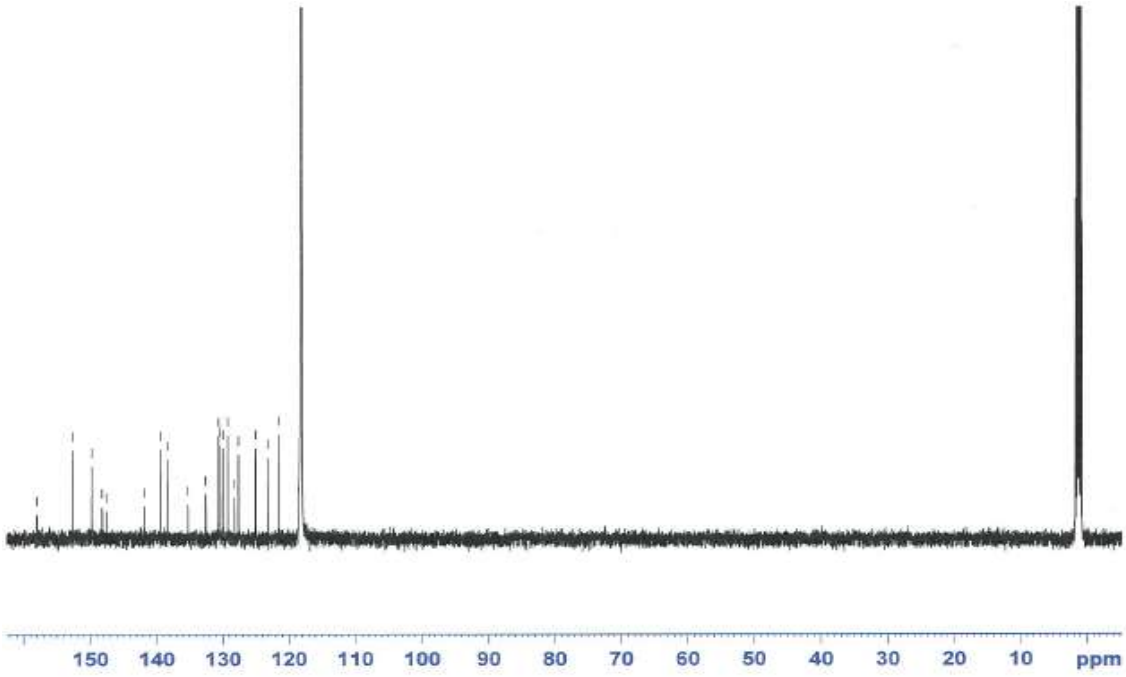


Figure S1-2 ^{13}C NMR spectrum of $[Ir(bzq)_2(phen)]ClO_4$ in CD_3CN.

S2. Optical resolution of $[Ir(bzq)_2(phen)]ClO_4$

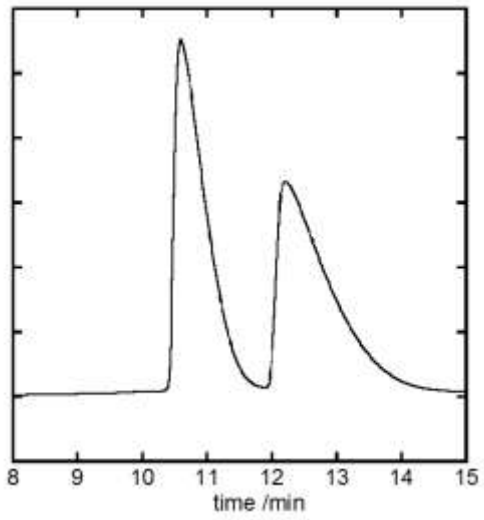


Figure S2 Chromatogram for optical resolution of $[Ir(bzq)_2(phen)]ClO_4$. An eluting solvent was $CH_3CN/CF_3COOH/NH(CH_2CH_3)_2$ = 100/0.1/0.1 (V/V/V). A flow rate was 2.5 $mLmin^{-1}$ and the monitoring wavelength was 430 nm. The used column was a CHIRALPACK IA (Daicel, Japan).

S3. X-Ray analysis of racemic [Ir(bzq)$_2$(phen)]ClO$_4$ and Δ-[Ir(bzq)$_2$(phen)]OCOCF$_3$

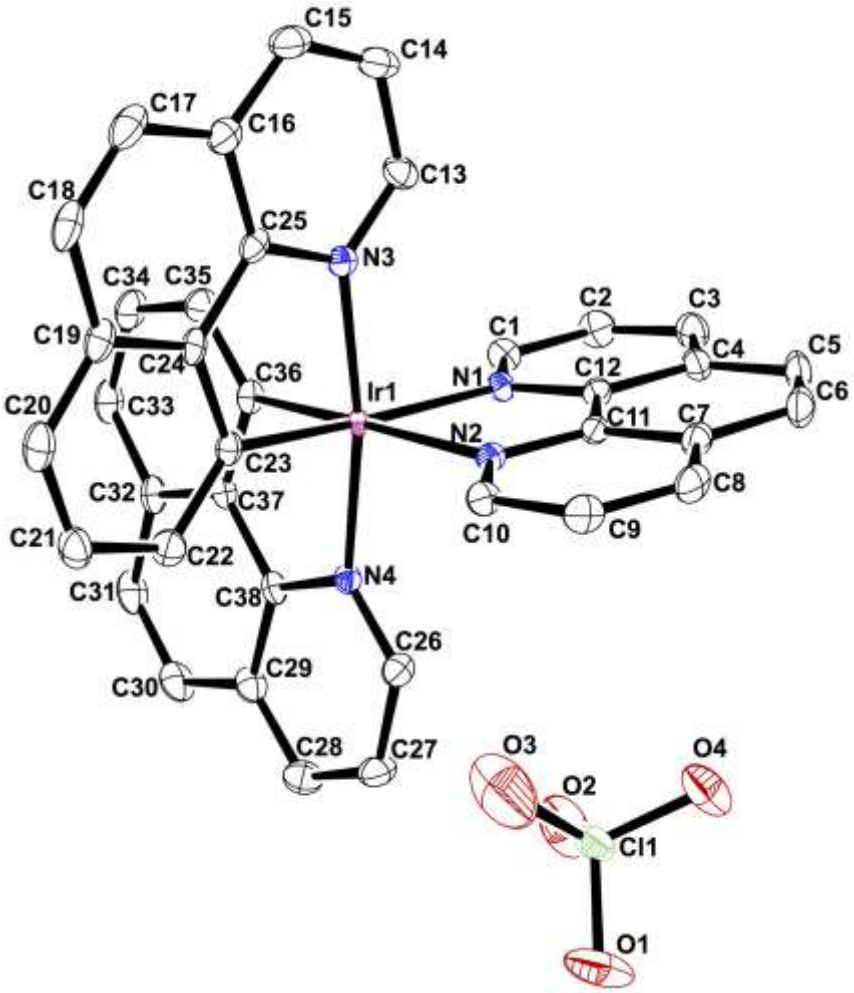


Figure S3-1 An ORTEP drawing of racemic [Ir(bzq)$_2$(phen)]·ClO$_4$ with a numbering scheme of atoms. The thermal ellipsoids are scaled to the 50% probability level. Hydrogen atoms and solvent molecules are omitted for clarity.

Table S3-1 Selected bond distances (Å) and angles (deg) of racemic $[Ir(bzq)_2(phen)]\cdot ClO_4$.

Distances (Å)			
Ir1 – N1	2.144(2)	Ir1 – N2	2.143(2)
Ir1 – N3	2.061(2)	Ir1 – N4	2.054(2)
Ir1 – C23	2.017(3)	Ir1 – C36	2.017(2)

Angles (deg)			
N1 – Ir1 – N2	77.84(8)	N1 – Ir1 – N3	93.40(9)
N1 – Ir1 – N4	93.91(8)	N1 – Ir1 – C23	171.71(8)
N1 – Ir1 – C36	97.84(9)	N2 – Ir1 – N3	91.08(8)
N2 – Ir1 – N4	95.81(8)	N2 – Ir1 – C23	95.64(9)
N2 – Ir1 – C36	174.84(9)	N3 – Ir1 – N4	170.87(8)
N3 – Ir1 – C23	81.52(10)	N3 – Ir1 – C36	92.00(9)
N4 – Ir1 – C23	91.82(10)	N4 – Ir1 – C36	81.58(10)
C23 – Ir1 – C36	88.91(10)		

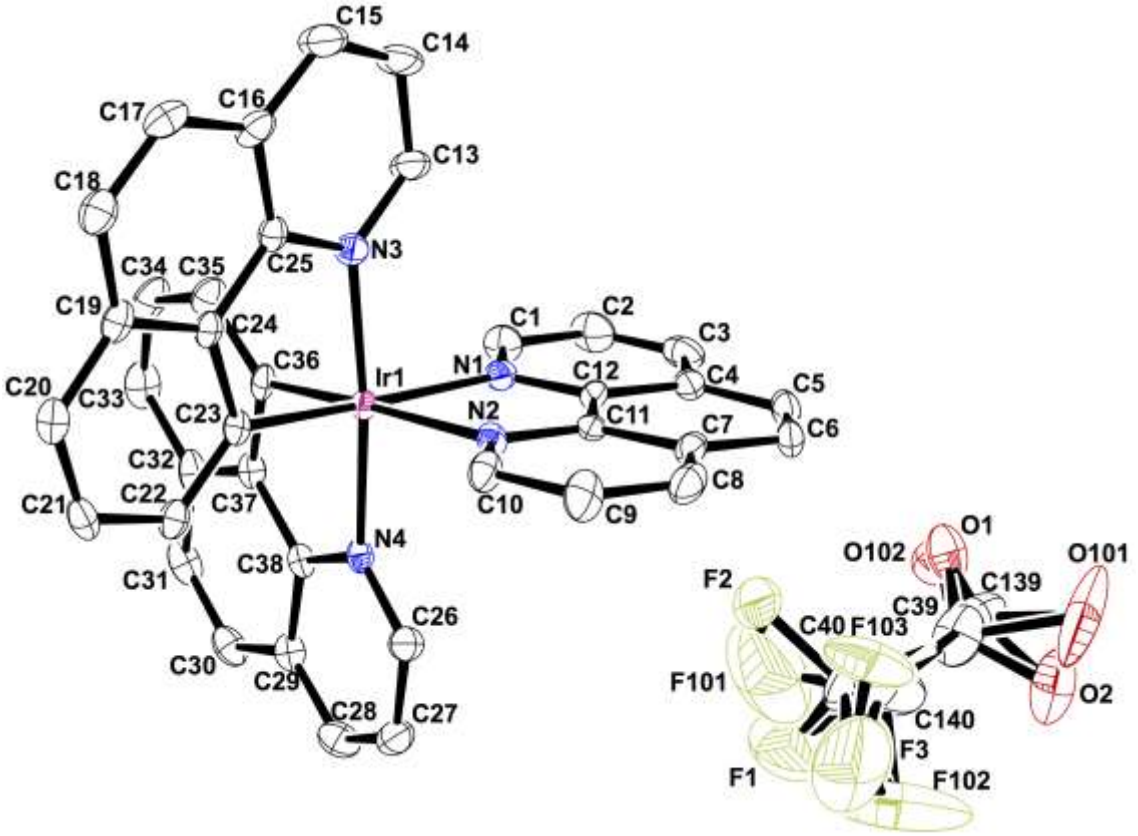


Figure S3-2 An ORTEP drawing of Δ-[Ir(bzq)$_2$(phen)]·OCOCF$_3$ with a numbering scheme of atoms. The thermal ellipsoids are scaled to the 50% probability level. Hydrogen atoms and solvent molecules are omitted for clarity. The counter anion of trifluoroacetate was disordered over two positions with an occupancy ratio of 0.505(10) : 0.495(10).

Table S3-2 Selected bond distances (Å) and angles (deg) of Δ-[Ir(bzq)$_2$(phen)]·OCOCF$_3$.

Distances (Å)			
Ir1 – N1	2.141(5)	Ir1 – N2	2.139(5)
Ir1 – N3	2.055(5)	Ir1 – N4	2.070(5)
Ir1 – C23	2.020(5)	Ir1 – C36	2.019(6)

Angles (deg)			
N1 – Ir1 – N2	77.91(18)	N1 – Ir1 – N3	95.00(19)
N1 – Ir1 – N4	89.44(18)	N1 – Ir1 – C23	173.57(19)
N1 – Ir1 – C36	95.8(2)	N2 – Ir1 – N3	90.13(18)
N2 – Ir1 – N4	94.03(18)	N2 – Ir1 – C23	96.81(19)
N2 – Ir1 – C36	172.2(2)	N3 – Ir1 – N4	174.48(19)
N3 – Ir1 – C23	81.2(2)	N3 – Ir1 – C36	95.0(2)
N4 – Ir1 – C23	94.6(2)	N4 – Ir1 – C36	81.3(2)
C23 – Ir1 – C36	89.8(2)		