

Supporting Information

Optimization of Signal Amplification by Reversible Exchange for polarization of Tridentate Chelating Bis[(2-pyridyl)alkyl]amine

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3. Structural Coordination after theoretical calculation

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1. SABRE experimental details

Preparation of *p*-H₂ gas

The *p*-H₂ generator was prepared in-house.^[1] 99.9% pure H₂ gas was passed through various area copper tubes used in the heat-exchanger design. The copper tube was sunk into liquid N₂ Dewar. The catalytic amount of FeO(OH) was used to convert *o*-H₂ into *p*-H₂ through symmetry breaking at low temperatures. This preparation designed and developed the system an H₂ enriched with 50% *para*-isomer to collect various magnetic field data. The power supply used for this application is GPS-1850D (Bench Power Supply, Linear DC). The shielding coil wound around the copper wire and the outer shielding coil consist of 20 mm diameters and 190 mm lengths. The magnetic field through the shielding coil is adjusted by setting current in the range 0-5 A.

SABRE methods in High-Field (300 MHz) NMR Detection

SABRE hyperpolarization can be successfully hyperpolarized in very different molecules. NMR data were reported as signal enhancement of concerning the signal of the thermally polarized sample in the Bruker Avance III 300 MHz (7T) magnet. Samples for these SABRE hyperpolarization experiments were conducted using a solution of [Ir(COD)(IMes)]Cl (2mg, 3.12 μmol) and Sub in CD₃OD volume of 0.9 μL. The *p*-H₂ gas was bubbled through solution 1/16 in. PTFE tubing inside the 5mm medium-wall precision NMR tube. The completion of the catalyst activation usually takes 10-20 minutes. The activation was checked by a hydride signal around -40 ~ 0 ppm. Activation by bubbling *p*-H₂ occurred outside the NMR magnet, and the signal was acquired (6 ± 2 s) after the bubbling was stopped. The pulse program was “zg30”, which is provided that the 30-degree pulse. All SABRE hyperpolarization experiments were conducted with 1 scan acquisition at 298K on 7T. The NMR data were analyzed using Mnova software (Mestrelab Research, S. L.).

Equation of enhancement factor

The polarization enhancement value of ¹H NMR signals ε was calculated according to Equation (1):

$$\varepsilon = \left(\frac{I_{HP}}{I_{therm}} \right) \cdot \left(\frac{C_{therm}}{C_{HP}} \right) \quad (1)$$

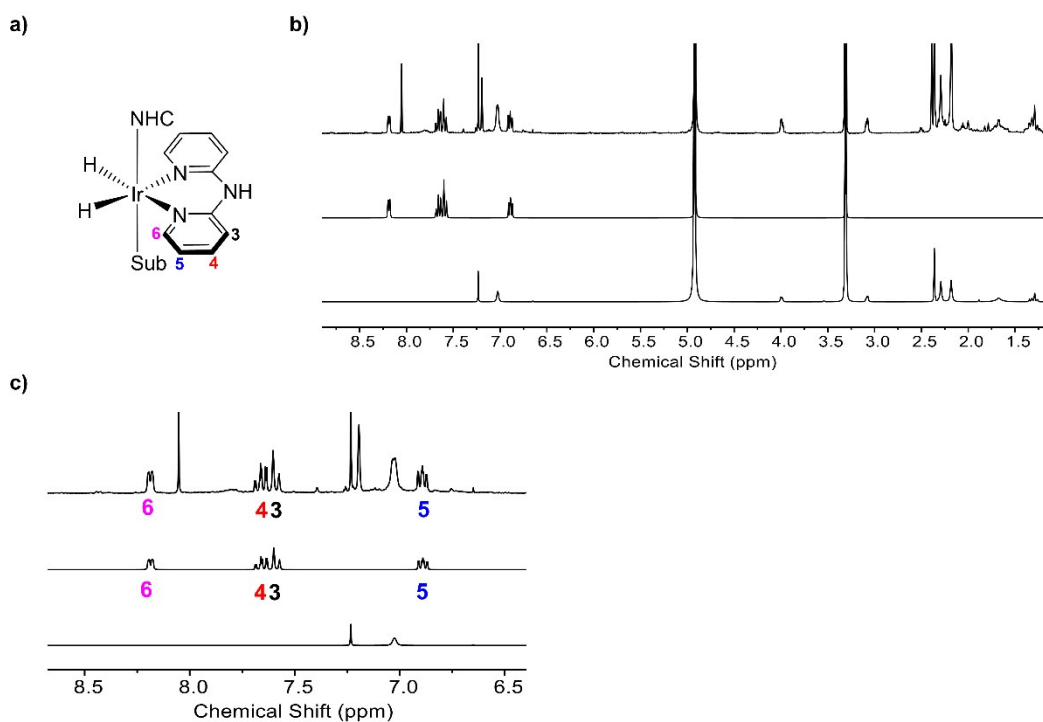
The ¹H signal enhancement ε was calculated by comparing the integral values derived from the NMR spectra of the hyperpolarization (HP) sample and the corresponding thermally polarized sample of substrates. In which I_{HP} and I_{therm} are the integrals of HP and the thermally polarized samples, respectively; C_{HP} and C_{therm} are the integrals of the HP and the thermal solvent peak of the sample, respectively. The thermally and polarized spectra were recorded using identical acquisition parameters and receiver gain.

Prediction of the coordinated structure with NMR study

We studied the possible stable structure between Ir-catalyst ([Ir(COD)(IMes)Cl]) and substrates using SABRE hyperpolarization. The two functional groups, pyridine and secondary amine, are well-known ligands forming complexes with Ir-catalysts.^[2-6] Moreover, there are three open coordination sites on the

Ir- catalyst. Therefore, it is expected that all substrates, which have three binding sites, bind with the Ir-catalysts. However, it is not obvious that a stable structure is formed with BPA and BPMA. leading to large angle strain in the structure, whereas, six- (Fig. S1(a)) and five-membered ring (Fig. S1(d)) formation within the equatorial position can result in a stable structure.

Because BPEA can form two six-membered rings after binding with the Ir-catalyst (1:1), the structure is less strained, and it would be an available structure during SABRE. This hypothesis was proven by ^1H NMR without hyperpolarization. With respect to BPA and BPMA, NMR signals of pyridine moieties were detected, which implied pyridine moieties with different chelate structures. Otherwise, split pyridine signals of the Ir-catalyst and the BPEA complex were not detected here. Figure S1(h)-(k) shows that as the amount of Ir-catalyst increased to 100 mol%, all proton signals were gradually shifted to the upfield because of the direct coordination with the iridium center.



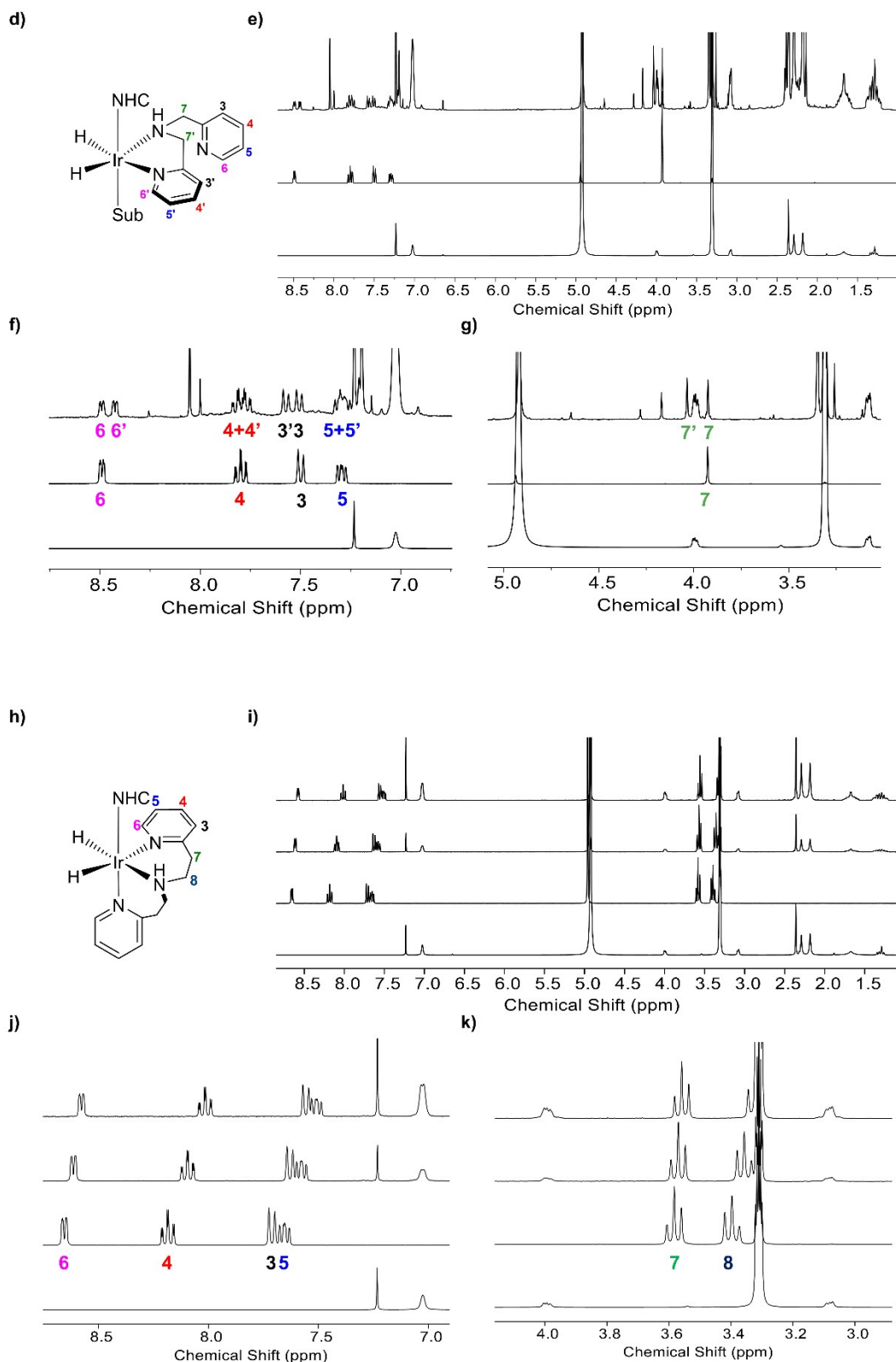


Figure S1. Prediction of coordination with catalyst and Sub (a) Proposed binding compounds (Ir-BPA) (b) ^1H NMR spectrum in CD_3OD . The lower is iridium catalyst spectrum, the middle is Sub (BPA) spectrum, and the upper is the reaction of iridium catalyst (1 eq.) and BPA (1 eq.) at 60 min. (c) ^1H NMR spectrum in CD_3OD enlarge the spectral region of δ 8.65 – 6.45 ppm (d) Proposed binding compounds (Ir-BPMA) (e) ^1H NMR spectrum in CD_3OD . The lower is iridium catalyst spectrum, the middle is Sub (BPMA) spectrum, and the upper is the reaction of iridium catalyst (1 eq.) and BPMA (1 eq.) at 30 min. (f) ^1H NMR spectrum in CD_3OD enlarge the spectral region of δ 8.70 – 6.70 ppm (g) ^1H NMR spectrum in CD_3OD

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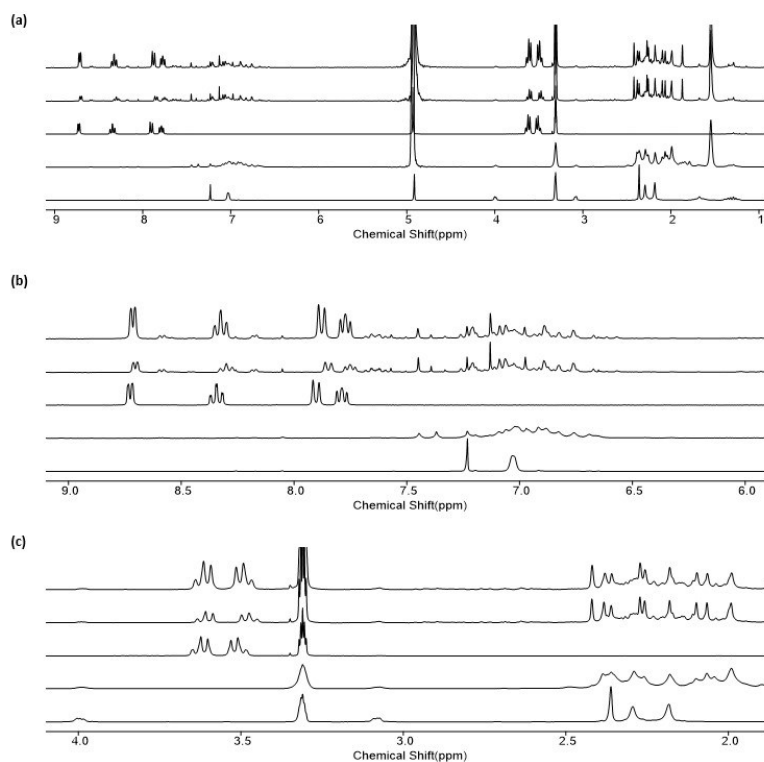


Figure S2. Fully activated iridium catalyst using 30 min. bubbling was used to see the chemical shift with different concentration of BPEA. (a) ^1H NMR spectrum in CD_3OD . The bottom spectrum corresponds to the Ir-catalyst, the second-lowest one is the activated iridium catalyst using *parahydrogen*, the third-lowest one is the Sub (BPEA) spectrum, the fourth-lowest is the reaction of Ir-catalyst (1 eq.) with BPEA (0.5 eq.), and the top spectrum is related to the reaction of Ir-catalyst (1 eq.) with BPEA (1 eq.). (b) ^1H NMR spectrum in CD_3OD with the enlarged spectral region of 9.00–6.00 ppm. (c) ^1H NMR spectrum in CD_3OD with the enlarged spectral region between 4.00–2.00 ppm

T₁ experiments

T₁ relaxation (longitudinal relaxation) is the means by which the net magnetization indicates the equilibrium over time (sec) and can be calculated mathematically, $y=A_1*\exp(-x/T_1)+y_0$

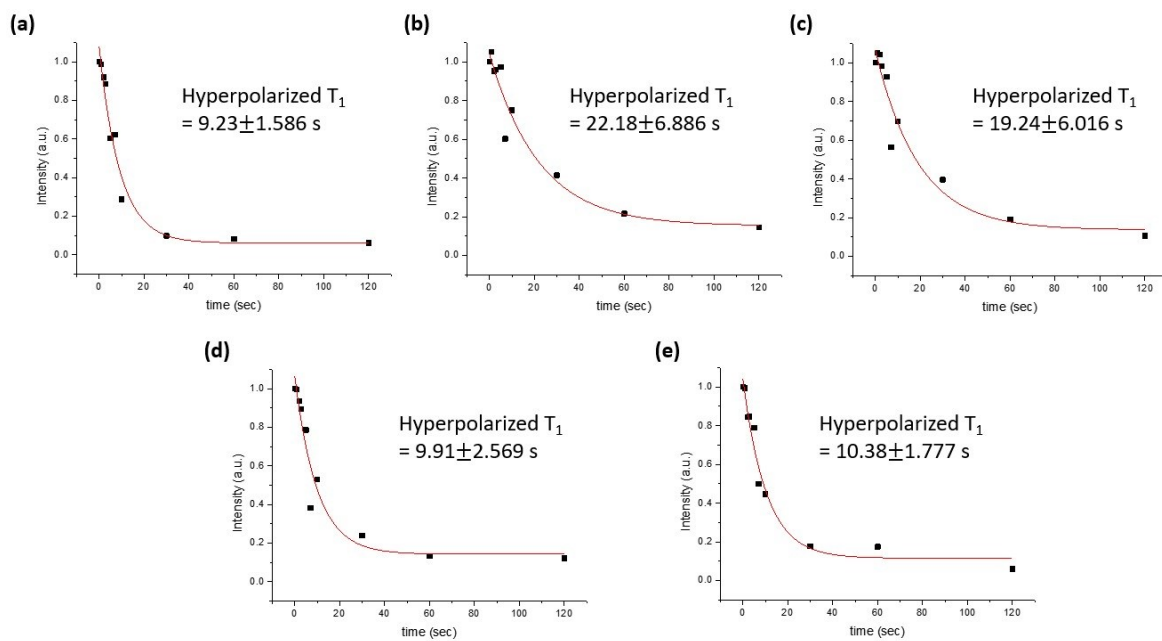
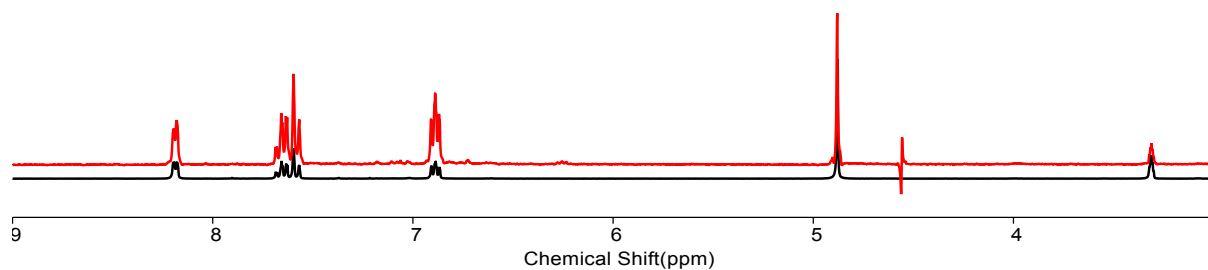


Figure S3. T_1 relaxation measurement of hyperpolarized BPEA of 70 G magnetic field. (a) H-3,5 (b) H-4, (c) H-6, (d) H-7, (e) H-8

Further spectrum with hyperpolarization

a)



b)

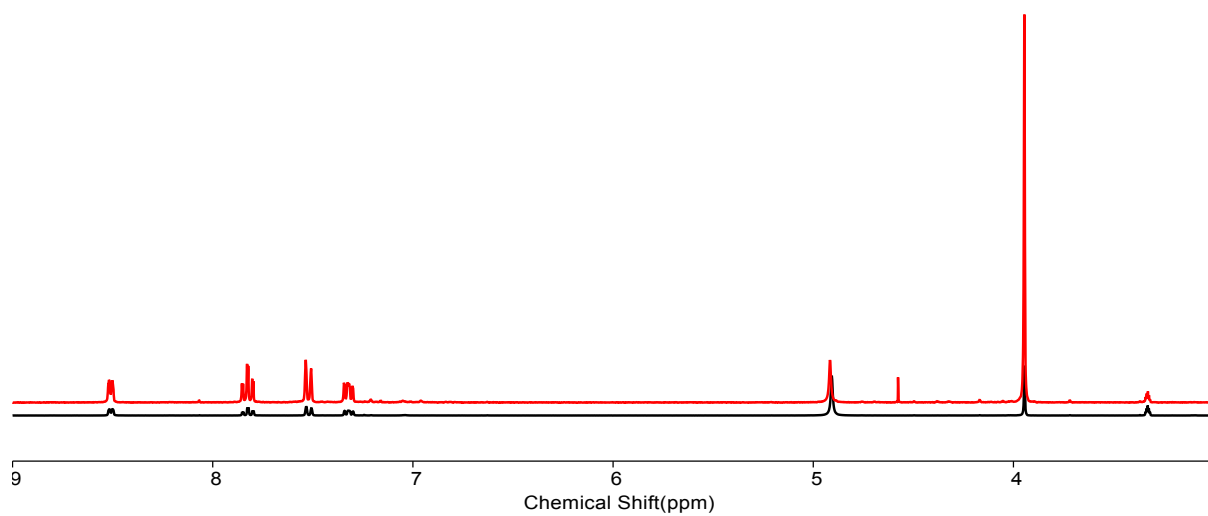
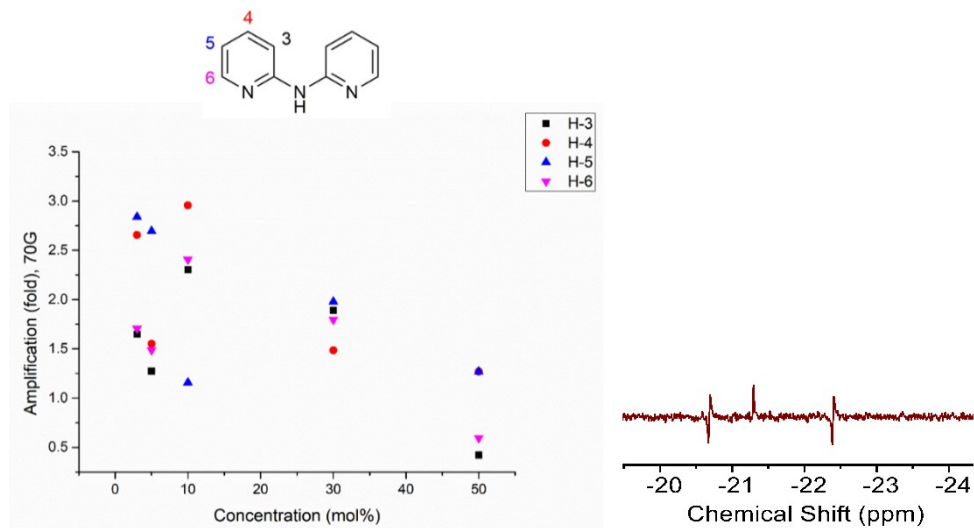


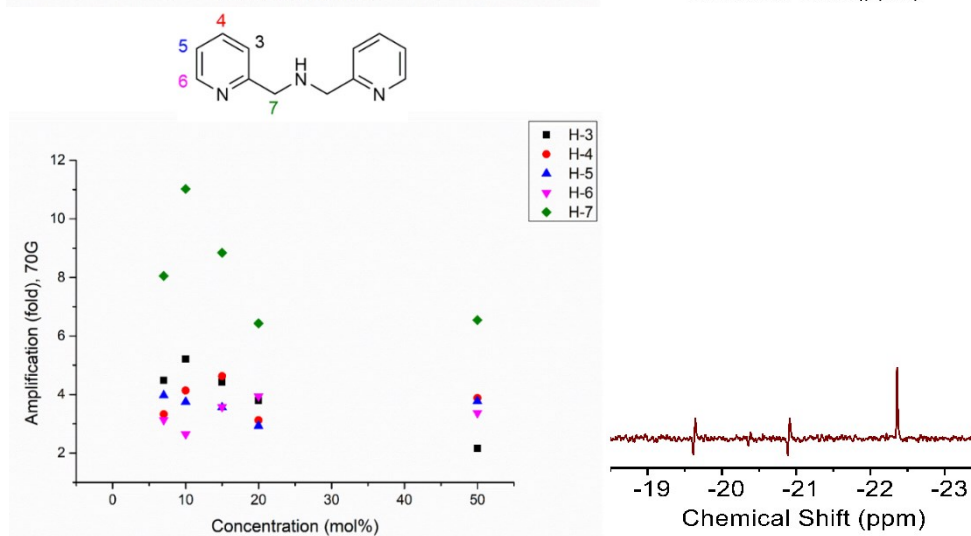
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Further SABRE experiments

a)



b)



c)

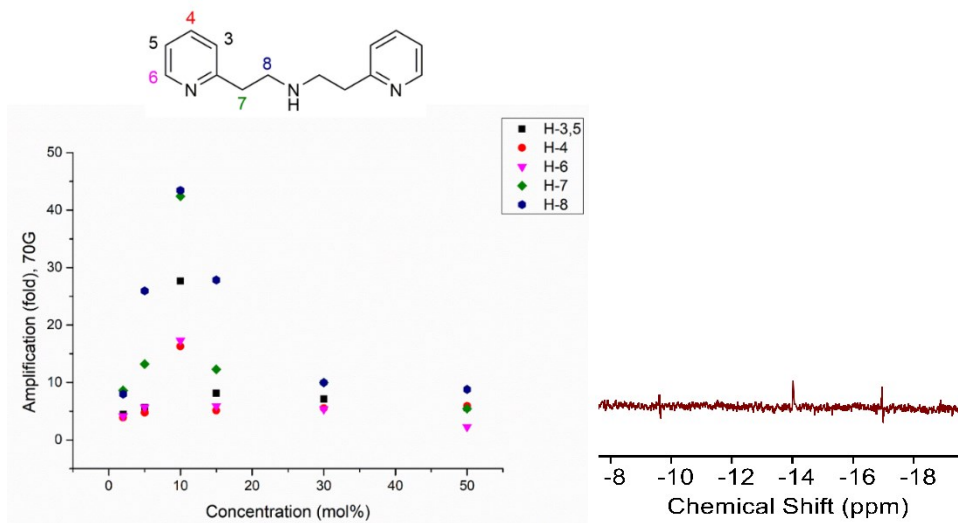


Figure S5. ^1H NMR signal enhancement and Ir-HH peaks of (a) BPA, (b) BPMA, and (c) BPEA dependence in the various concentration at 70G magnetic field. Notice the different vertical scale (fold)

2. Synthetic details

Most of the reagents used in this work were purchased from Sigma-Aldrich, Alfa aesar, Tokyo chemical industry and companies. In anhydrous conditions, the reaction glassware was flame-dried for at least 1 hour and purged with N₂. The THF solvent was distilled from Na/benzophenone under N₂ atmospheric condition. All the synthetic compounds were characterized by ¹H and ¹³C NMR spectroscopic analysis. The NMR spectra were recorded on Bruker Avance III 300 MHz. The CD₃OD was used as solvent unless otherwise stated (CD₃OD peak ¹H NMR : 3.31 (CH₃), 4.87 (OH) ppm, ¹³C NMR : 49.0 ppm). The following abbreviations are used. (brs = broad singlet, s = singlet, d = doublet, t = triplet, q = quartet, qt = quintet, st = sextet, spt = septet, and m = multiplet) Thin layer chromatography was performed with Silica gel 60 F254 and compounds were visualized under UV light at 254 nm.

Chloro(η^4 1,5-cyclooctadiene)(1,3-bis(2,4,6-trimethylphenyl)-imidazol-2-ylidene)iridium(I), [6,7]

[Ir(COD)(IMes)]Cl

1,3-bis(2,4,6-trimethylphenyl)-1,3-dihydro-2*H*-imidazol-2-ylidene (0.48 g, 1.5 mmol) in THF (3 mL) was added dropwise to a stirred solution of bis(1,5-cyclooctadiene)diiridium(I) dichloride (0.5 g, 0.72 mmol) in dry THF (2 mL) at room temperature under N₂. The mixture was stirred for 12 hours and quenched with distilled water. THF was evaporated under reduced pressure and CH₂Cl₂ (30 mL) was added to resulting mixture. The organic layer was washed with H₂O, dried over MgSO₄, and concentrated under reduced pressure to provide compound (0.95g, 98%) as a yellow solid. : ¹H NMR (300 MHz, MeOD-d₄): δ 7.23 (s, 2H), 7.02 (s, 4H), 4.00-3.98 (t, 2H, J=3 Hz), 3.09-3.07 (t, 2H, J=3 Hz), 2.36 (s, 6H), 2.26 (s, 6H), 2.18 (s, 6H), 1.77-1.42 (m, 4H), 1.39- 1.22(m, 4H), ¹³C NMR (75 MHz, MeOD-d₄): δ 140.07, 137.73, 130.48, 129.49, 125.42, 82.96, 78.37, 53.35, 34.53, 29.96, 21.33, 203.14

Bis[(2-pyridyl)ethyl]amine [8], BPEA

A solution of ammonium chloride (9.95 g, 184 mmol) in distilled water (28 mL) and methanol (4 mL) was added to 2-vinylpyridine (10 mL, 92 mmol). The solution was heated for 18 hours under reflux, and the resulting mixture was cooled at 0°C and basified with 30 % w/w aqueous NaOH solution until pH 10. CH₂Cl₂ (300 mL) was added and the organic layer was dried over MgSO₄ and concentrated under the reduced pressure to provide BPEA and PEA mixtures. The crude oily residue (10 g, 56 mmol) was dissolved in CH₂Cl₂ (20 mL) and di-*tert*-butyl dicarbonate (60 mL, 254 mmol). After stirring for 6 hours, the solution concentrated under reduced pressure to obtain protecting compounds, Boc-BPEA and Boc-PEA. The resulting residue was purified by flash column chromatography on silica gel (dichloromethane:methanol,100:0 – 30:1) as an eluent to provide Boc-BPEA as a yellow oil. Boc-BPEA (5 g) was deprotected with TFA (10 mL) in CH₂Cl₂. After stirring for 1 hour, the solution was evaporated under reduced pressure, BPEA (2.33 g, 68%)was obtained as pale-yellow oil. : ¹H NMR (300 MHz, MeOD-d₄): δ 8.77-8.75 (dt, 2H), 8.46-8.40 (t, 2H), 7.96-7.93 (d, 2H), 7.90-7.85 (t, 2H), 3.65-3.59 (td, 4H, J=6.9 Hz, 7.8 Hz, 0.9 Hz, 0.45 Hz), 3.53-3.48 (td, 4H, J=6.9 Hz, 7.8 Hz, 0.9 Hz, 0.45 Hz), ¹³C NMR (75 MHz, MeOD-d₄): δ 154.42, 146.51, 144.83, 128.39, 126.63, 47.34, 31.54

2-(Pyridin-2-yl)ethanamine, PEA

This product was prepared from 2-vinylpyridine as described above obtained. ¹H NMR (300 MHz, MeOD-d₄): δ 8.62-8.60 (d, 1H), 8.02-7.97 (t, 1H), 7.54-7.47 (m, 2H), 3.40-3.35 (t, 2H), 3.24-3.20 (t, 2H), ¹³C NMR (75 MHz, MeOD-d₄): δ 157.56, 148.80, 141.17, 126.01, 124.65, 39.85, 34.36

tert-Butyl bis[2-(pyridin-2-yl)ethyl]carbamate Boc-BPEA

This product was protected from 2-vinylpyridine as described above. ¹H NMR (300 MHz, CDCl₃): δ 8.39-8.38 (d, 2H), 7.47-7.41 (t, 2H), 7.06-7.03 (d, 2H), 6.99-6.96 (t, 2H), 3.54-3.48 (m, 4H), 2.97-2.93 (m, 4H), 1.40 (s, 9H) ¹³C NMR (75 MHz, CDCl₃): δ 159.28, 155.19, 149.25, 136.21, 123.35, 121.23, 79.17, 47.72, 37.45, 28.27

tert-Butyl 2-(pyridine-2-yl)ethylcarbamate Boc-PEA

This product was protected from 4b as described above. ¹H NMR (300 MHz, CDCl₃): δ 8.54-8.53 (d, 1H), 7.66-7.60 (t, 1H), 7.20-7.14 (m, 2H), 5.14 (brs, 1H), 3.58- 3.51 (q, 2H), 3.01-2.97 (t, 2H), 1.42 (s, 9H) ¹³C NMR (75 MHz, CDCl₃): δ 159.39, 155.95, 148.98, 136.82, 123.62, 121.58, 79.12, 39.89, 37.71, 28.42

3. Structural Coordination after theoretical calculation

Theoretical calculation

Since the BP86/LANL2DZ level of theory provided optimized structures with geometrical parameters closest to the experimental X-ray crystal structure, this level of theory was applied to obtain stable structures of Ir-catalyst complexes with BPA, BPMA, BPEA, and pyridine.^[6] A reduced catalyst model (dimethyl benzenes are omitted) was used to represent each complex in order to improve the calculation efficiency and had less of an impact on the optimized iridium complex structure. All calculations were performed using the Gaussian 16 W package. Atoms in molecule (AIM) analysis for calculating the Shannon aromaticity index was carried out using the Multiwfn program.^[9]

Pyridine-Ir-catalyst

Ir	0.25513700	0.61120800	-0.35175100
C	0.45300300	5.33168200	-1.87091000
C	0.15995900	4.27527100	-2.76732100
C	0.10329000	2.95315400	-2.28853900
N	0.32431600	2.63644000	-0.96262200
C	0.60686800	3.67045000	-0.09420200
C	0.67852400	5.01463600	-0.51143100
H	0.50311500	6.36721700	-2.22168900
H	-0.02343200	4.46619800	-3.82874300
H	0.77309300	3.38876500	0.94818900
H	0.90725200	5.79224200	0.22349500
C	-3.05513500	1.65830400	3.31263600
C	-2.99446300	2.43090500	2.12891800
C	-2.03607500	2.11723700	1.14467500
N	-1.13722200	1.08067200	1.27810000
C	-1.21842900	0.32254800	2.42748900
C	-2.14973900	0.58015200	3.45298200
H	-3.79018300	1.88081400	4.09240300
H	-3.68311800	3.26391500	1.95877700
H	-1.98083200	2.68000000	0.21082300
H	-2.16311200	-0.06071700	4.33994000
H	-0.99045400	0.40494900	-1.34400000
H	1.17439500	0.27816200	-1.63024400
C	-0.62513300	-3.53649600	0.25198600
C	0.74819800	-3.60946300	0.18271700
H	-1.36889400	-4.31929900	0.36974400
H	1.41295000	-4.46698400	0.23287400
C	0.16747800	-1.36614100	-0.03293100
N	-0.97317300	-2.17679100	0.11567500
N	1.22160300	-2.29369000	0.00527600
C	-2.37856900	-1.73445900	0.02909100
C	2.64768300	-1.98246500	-0.20210900
C	4.50901200	1.62716300	2.17793300
C	4.38579900	1.83988300	0.78397100
C	3.17207000	1.52595200	0.14153400
N	2.08084300	1.01544200	0.81336900
C	2.20924200	0.81789600	2.16849100
C	3.39404200	1.10746800	2.87660000
H	5.21669800	2.23932900	0.19473800
H	3.03914500	1.66420700	-0.93408900
H	3.43452700	0.92572200	3.95497300
H	5.44214300	1.85797200	2.70146500

H	-2.39940100	-0.70703200	-0.35971900
H	-2.92725800	-2.39248200	-0.66634100
H	-2.86629700	-1.76798300	1.01928600
H	3.14307500	-2.85413700	-0.66063700
H	2.72760100	-1.12259900	-0.88299500
H	3.15000000	-1.74332500	0.75116400
H	-0.11629700	2.10743600	-2.94227700
H	1.33440100	0.42084200	2.68543000
H	-0.53830000	-0.53118700	2.48541700

BPA-Ir-catalyst

Ir	0.23651800	0.57086200	-0.44218200
C	0.16627100	5.33573500	-1.91008300
C	0.00182100	4.32319000	-2.86447500
C	0.06472700	2.94818000	-2.47536100
N	0.24494800	2.60251600	-1.13225500
C	0.40256600	3.62370000	-0.21760700
C	0.38946800	4.98333500	-0.55300700
H	0.10566400	6.38620000	-2.21280800
H	-0.22463800	4.57607400	-3.90166900
H	0.54036700	3.30556100	0.81747200
H	0.52946200	5.73908700	0.22403400
C	-2.88593200	1.60960300	3.30131300
C	-3.25375300	1.86109100	1.95369300
C	-2.30954400	1.62137800	0.94445000
N	-1.03871300	1.14401300	1.19694400
C	-0.66202100	0.97191600	2.50699300
C	-1.57849700	1.17467600	3.57909000
H	-3.59696800	1.77172500	4.11727800
H	-4.25000700	2.22612300	1.69106900
H	-2.53860300	1.77525800	-0.11239500
H	-1.25230200	1.01604600	4.61319100
H	-1.03074500	0.24388900	-1.38823100
H	1.17750100	0.15349600	-1.68133300
C	-0.53091200	-3.53331300	0.52343400
C	0.83377400	-3.59770300	0.35216700
H	-1.25072300	-4.31202900	0.75805200
H	1.51393900	-4.44237000	0.41120000
C	0.20103600	-1.38495300	0.01519500
N	-0.90842300	-2.19161800	0.31268700
N	1.26991100	-2.29426100	0.03917700
C	-2.31452000	-1.75135100	0.34480500
C	2.67374500	-1.98544800	-0.28477700
C	4.27894500	1.27714900	2.37543900
C	4.31484200	1.50857800	0.97544500
C	3.12857000	1.36612200	0.24102300
N	1.92473100	1.00292300	0.81250100
C	1.87747100	0.85291400	2.17798700
C	3.05041700	0.96036600	2.98010100
H	5.24101900	1.78461500	0.46478600
H	3.09433400	1.50984300	-0.84112900
H	2.98328500	0.82161300	4.06506400
H	5.18492700	1.36524100	2.98294900
N	0.65496000	0.57594600	2.82736000
H	0.77026600	0.31700600	3.81052100
H	-2.44326300	-0.91911000	-0.36243300

H	-2.96216100	-2.58869000	0.03642000
H	-2.60937900	-1.42288700	1.35695900
H	3.14206000	-2.87145600	-0.74467900
H	2.69634100	-1.15300100	-1.00302900
H	3.24297100	-1.70688400	0.61953900
N	-0.09524800	1.89727300	-3.35675400
H	-0.26769200	0.97907700	-2.90683700
C	-0.12006200	1.86734300	-4.77299700
C	0.52401900	2.81121400	-5.62113900
N	-0.77850600	0.76700200	-5.25863900
C	0.43264700	2.62240400	-7.01816900
H	1.12072700	3.63239500	-5.21560400
C	-0.84231600	0.59960400	-6.60984400
C	-0.27180600	1.50778200	-7.53332100
H	0.92225400	3.33160200	-7.69428200
H	-1.37155300	-0.29722900	-6.95093200
H	-0.36179500	1.33559000	-8.60969900

BPMA-Ir-catalyst

Ir	-0.17747800	0.77390400	-0.52777500
C	-0.19778100	5.20953600	-2.85279800
C	-0.78466200	4.03826500	-3.40426100
C	-0.77921700	2.82785900	-2.68805600
N	-0.20666600	2.70099700	-1.43858700
C	0.37445100	3.83409900	-0.90358800
C	0.38965200	5.07256800	-1.56661000
H	-1.22961400	4.05460900	-4.40535800
H	-1.21447600	1.91484500	-3.09710200
H	0.84875200	3.72032800	0.07263800
H	0.86616300	5.92997600	-1.07750200
H	-1.46228600	0.42534800	-1.43639000
H	0.62857300	0.32076700	-1.83549100
C	-0.96970000	-3.27695300	0.61316900
C	0.39843600	-3.34623200	0.47135600
H	-1.69316900	-4.04672700	0.86605200
H	1.07712300	-4.18701500	0.58230000
C	-0.22430200	-1.14669800	0.02707800
N	-1.34339900	-1.94392300	0.34087300
N	0.84127100	-2.05635000	0.11539600
C	-2.75058600	-1.50775700	0.30406200
C	2.24856400	-1.74370800	-0.19028900
C	3.46414100	2.30556600	2.49611000
C	3.74669800	2.14259900	1.11850400
C	2.73125500	1.67411300	0.26157900
N	1.47272200	1.35444200	0.71561200
C	1.19173300	1.51620200	2.06213700
C	2.16575100	1.99524200	2.96504000
H	4.73319200	2.37762500	0.70807000
H	2.89331700	1.54523100	-0.81164800
H	1.90355000	2.12412800	4.02005000
H	4.23105300	2.67396400	3.18469600
C	-0.19983300	1.10583800	2.50488000
H	-0.21203100	0.01136800	2.67227800
H	-0.48946700	1.61480700	3.44337300
N	-1.21190900	1.39482800	1.40961400

H	-1.99610300	0.73194300	1.51120500
C	-1.78643100	2.80164700	1.48278600
H	-2.26068100	3.01021700	0.51002500
H	-0.93877000	3.49565500	1.60929200
C	-2.78503800	2.99859500	2.61725200
C	-4.16743900	3.18790000	2.36141100
N	-2.27259900	2.99051700	3.89500900
C	-5.05040400	3.38349800	3.45092300
H	-4.54023900	3.19665000	1.33094100
C	-3.13684000	3.17063200	4.93710900
C	-4.52745700	3.37621500	4.76482500
H	-6.11992600	3.54246000	3.27720500
H	-2.69026500	3.15794600	5.93790600
H	-5.17307300	3.52937100	5.63512400
H	-2.80029200	-0.54939300	-0.23701800
H	-3.35637300	-2.24953500	-0.24398100
H	-3.16560700	-1.40374200	1.32472100
H	2.74197800	-2.64414800	-0.59219700
H	2.27291500	-0.94809200	-0.94974100
H	2.78915100	-1.40758000	0.71154400
C	-0.27193000	6.57061600	-3.55741300
H	-0.32675600	6.42248700	-4.65351000
H	0.64795300	7.14923100	-3.35183700
N	-1.42449500	7.37579800	-3.12419300
H	-1.41506200	7.74303000	-2.16077100
C	-2.77407000	6.96615700	-3.52200600
H	-2.94093900	7.16952200	-4.60039700
H	-2.96404200	5.86992200	-3.37614700
C	-3.81373000	7.72424100	-2.69564200
C	-5.15021700	7.88190800	-3.14149600
N	-3.38367500	8.21846900	-1.49260200
C	-6.07156500	8.56759800	-2.31798900
H	-5.45509200	7.48579400	-4.11686200
C	-4.28162900	8.88290400	-0.70432900
C	-5.63198200	9.07977100	-1.07218300
H	-7.10762600	8.70955100	-2.64400100
H	-3.89234700	9.27017700	0.24441600
H	-6.31108100	9.62540800	-0.40946000

BPEA-Ir-catalyst

Ir	-0.77855700	0.12434300	-1.46069700
H	-1.97822300	-0.36817400	-2.40639100
H	0.14731900	-0.75785400	-2.43288800
C	-2.22495000	-3.34757300	0.59770300
C	-0.87322700	-3.56648600	0.73380300
H	-3.07280800	-3.94546600	0.91938000
H	-0.33531000	-4.38724300	1.19934000
C	-1.12399900	-1.55196300	-0.41688500
N	-2.37499300	-2.13171500	-0.10105300
N	-0.21693700	-2.48333300	0.11702300
C	-3.69949300	-1.64061300	-0.52087600
C	1.24790000	-2.40948100	-0.00631300
C	3.42688900	1.86795700	0.77201000
C	3.43277000	1.06554200	-0.39329400
C	2.20882000	0.59720100	-0.89537300

N	0.97741900	0.88509900	-0.33053200		
C	0.96997600	1.67776500	0.80146300		
C	2.18383600	2.16179700	1.36275600		
H	4.36341800	0.79661500	-0.90141500		
H	2.16970300	-0.04952400	-1.77338800		
H	2.13442500	2.77905900	2.26654000		
H	4.35787700	2.24712800	1.20479700		
C	-0.31786900	2.13955800	1.48146200		
H	-0.12289500	2.16084300	2.57101600		
H	-0.48082100	3.20213900	1.20687200		
C	-1.62391200	1.35103300	1.29024000		
H	-2.39120100	1.80678500	1.95413400		
H	-1.48736400	0.29892200	1.59372000		
N	-2.12637400	1.32875000	-0.13207700		
C	-2.51192400	2.68593200	-0.66086400		
H	-3.39424600	3.06942000	-0.10663200		
H	-1.67707200	3.38469100	-0.48695000		
C	-2.82196800	2.61887800	-2.17514100		
H	-3.47261100	3.46978600	-2.44377600		
H	-3.39143300	1.69229700	-2.39175800		
C	-1.58245700	2.66353200	-3.04915000		
C	-1.46939100	3.63702300	-4.07064800		
N	-0.57676100	1.73342000	-2.83517400		
C	-0.32729000	3.68455800	-4.89826300		
H	-2.28735200	4.35047100	-4.21259800		
C	0.53500300	1.78844700	-3.64991600		
C	0.69581500	2.73574900	-4.67547100		
H	-0.24196400	4.43197600	-5.69315600		
H	1.28700400	1.02009500	-3.47225100		
H	1.60071100	2.71396000	-5.28934300		
H	-3.56595500	-0.96611200	-1.38173100		
H	-4.32315600	-2.49110300	-0.84378800		
H	-4.22273600	-1.12621200	0.30839800		
H	1.50742200	-2.10569200	-1.03170300		
H	1.67395800	-1.68580500	0.70784300		
H	1.67589800	-3.40526500	0.19308100		
H		-2.98114100	0.74857000		-0.14326500

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