Electronic Supporting Information

Platinum(II) bis(arylacetylide) complexes bearing diarylamino-substituted bipyridine ligands for solution-processable phosphorescent OLED applications

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Experimental

General information

All reactions were carried out under an inert nitrogen atmosphere. Analytical grade solvents were purified by distillation over appropriate drying agents prior to use. All reagents and chemicals, unless otherwise stated, were purchased from commercial sources and used without further purification. All reactions were monitored by thin-layer chromatography (TLC) with Merck pre-coated aluminium plates. Flash column chromatography and preparative TLC were carried out using silica gel from Merck (230–400 mesh).The positive-ion fast atom bombardment (FAB) mass spectra were recorded in *m*-nitrobenzyl alcohol matrices on a Finngin-MAT SSQ710 mass spectrometer. Infrared spectra were recorded as CH_2C1_2 solutions on the Nicolet Magna 550 Series II FT1R spectrometer, using CaF_2 cells with a 0.5 mm path length or KBr pellets for solid state spectroscopy. NMR spectra were measured in deuterated solvent ($CDCl_3$) as the lock and reference on a Bruker Ultrashield 400 Plus spectrometer, with chemical shifts of ^{1}H NMR and ^{13}C NMR quoted relative to TMS standard ($\delta = 0.00$).

Physical measurements

Electronic absorption spectra were obtained with a Hewlett Packard 8453 spectrometer. The photoluminescent properties of the compounds were examined by using a Photon Technology International (PTI) Fluorescence QuantaMaster Series QM1 system. The phosphorescent quantum yields were determined in CH_2C1_2 solution at 293 K against $Ru(bpy)_3Cl_2$ standard ($\Phi_p = 0.062$).[1] The phosphorescent lifetimes were measured by a single photon counting spectrometer from Edinburgh Instruments (FLS920) with a hydrogen-filled pulse lamp as the excitation source. The

data analysis was conducted by iterative convolution of the luminescence decay profile with the instrument response function using the software package provided by Edinburgh Instruments. Electrochemical measurements were made using a Princeton Applied Research model 2273A potentiostat at a scan rate of 100 mV s^{-1}. A conventional three-electrode configuration consisting of a glassy carbon working electrode, a Pt-sheet counter electrode, and a Pt-wire reference electrode was used. The supporting electrolyte was 0.1 M $[Bu_4N]PF_6$ in CH_3CN. Ferrocene was added as a calibrant after each set of measurements, and all potentials reported are quoted with reference to the ferrocene–ferrocenium (Fc/Fc^+) couple. The oxidation (E_{ox}) and reduction (E_{red}) potentials were used to determine the HOMO and LUMO energy levels using the equations $E_{HOMO} = -(E_{ox} + 4.8)$ eV and $E_{LUMO} = -(E_{red} + 4.8)$ eV which were calculated using the internal standard ferrocene value of –4.8 eV with respect to the vacuum level.[2] Thermal analyses were performed with Perkin-Elmer TGA6 thermal analyzers.

Synthetic details

Synthesis of 2,2'-bipyridine *N,N'*-dioxide. A solution of 35% H_2O_2 (25 mL) was added to 2,2'-bipyridine (6.00 g, 38.42 mmol) in glacial acetic acid (40 mL). This mixture was stirred at 75 °C for an additional 8 h. The colorless solution was then cooled to room temperature. A copious amount of acetone was added to precipitate the product as a white solid, which was then collected by filtration. The crude product was further recrystallized from hot water and dried in a vacuum oven to give the product (6.51 g, 34.59 mmol, 90%) as white crystals. *Spectral Data*: ^{1}H NMR (400 MHz, d_6-DMSO): δ = 8.34 (d, J = 5.9 Hz, 2H, Ar), 7.64–7.62 (m, 2H, Ar), 7.54–7.50 (m, 2H, Ar), 7.44–7.40 (m, 2H, Ar) ppm.

Synthesis of 4,4'-dinitro-2,2'-bipyridine *N,N'*-dioxide. A mixture of fuming nitric acid (12

mL) and concentrated sulfuric acid (31.2 mL) was added to 2,2'-bipyridine *N*,*N*'-dioxide (6.51 g, 34.59 mmol) in concentrated sulfuric acid (30 mL) in an ice bath. The resulting mixture was heated to 100 °C for an additional 24 h. The acidic mixture was cooled to room temperature and poured into ice (under –40 °C), which was prepared by the addition of an excessive amount of liquid nitrogen onto water (100 mL) with constant stirring, a bright yellow precipitate was formed. The solution was subsequently filtered and a yellow product was collected. The crude product was washed with water and air-dried to give the product (3.80 g, 13.66 mmol, 40%) as a yellow powder. *Spectral Data*: ^{1}H NMR (400 MHz, d_6-DMSO): δ = 8.73 (d, *J* = 3.2 Hz, 2H, Ar), 8.63 (d, *J* = 3.2 Hz, 2H, Ar), 8.43–8.40 (m, 2H, Ar) ppm.

Synthesis of 4,4'-diamino-2,2'-bipyridine. A mixture of 4,4'-dinitro-2,2'-bipyridine *N*,*N*'-dioxide (1.50 g, 5.39 mmol) and 10% Pd/C (1.00 g) in ethanol (150 mL) was heated to reflux under a nitrogen atmosphere. After the complex was completely dissolved, a solution of hydrazine hydrate (15 mL) in ethanol (30 mL) was added dropwise over a period of 1 h. The resulting mixture was refluxed for an additional 15 h. Upon completion, the hot mixture was immediately filtered hot through a bed of celite, and washed with hot ethanol. After removal of solvent, water (120 mL) was added and the mixture was left at 2 °C overnight. The precipitate was collected by filtration and dried in the vacuum oven to give 4,4'-diamino-2,2'-bipyridine (754 mg, 4.05 mmol, 75%) as a pale yellow solid. *Spectral Data*: ^{1}H NMR (400 MHz, d_6-DMSO): δ = 8.05 (d, *J* = 5.1 Hz, 2H, Ar), 7.55 (d, *J* = 2.0 Hz, 2H, Ar), 6.49–6.47 (m, 2H, Ar), 6.08 (s, 4H, NH_2) ppm. ^{13}C NMR (100 MHz, d_6-DMSO): δ = 156.06, 154.84, 148.82, 108.53, 105.49 (Ar) ppm.

Synthesis of L1. A mixture of 4,4'-diamino-2,2'-bipyridine (104 mg, 0.58 mmol), 4-iodotoluene (630 mg, 2.90 mmol), 1.10-phenanthroline (104 mg, 0.58 mmol), CuI (110 mg, 0.58

mmol) and KOH (488 mg, 8.70 mmol) in *p*-xylene (3 mL) was heated to 125 °C for 36 h under a nitrogen atmosphere. After the mixture was cooled to room temperature, water (30 mL) was added and the mixture was stirred for 30 min. The mixture was extracted with CH_2Cl_2 (30 mL) three times. The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4. The solvent was removed on a rotary evaporator *in vacuo*. The residue was purified by a short column chromatography on silica gel eluting with hexane/CH_2Cl_2 (1:4, v/v) to remove the excess 4-iodotoluene. Then by using CH_2Cl_2/methanol (20:1, v/v) as eluent, the product band was collected. After removal of the solvent, the crude product was recrystallized from a mixture of CH_2Cl_2 and ethanol to afford **L1** (180 mg, 0.33 mmol, 56%) as a pale yellow solid. *Spectral Data*: FAB-MS (*m/z*)*:* 547.4 $[M+1]^+$. ^1H NMR (400 MHz, $CDCl_3$): δ = 8.16 (d, *J* = 5.8 Hz, 2H, Ar), 7.73 (d, *J* = 2.4 Hz, 2H, Ar), 7.14 (d, *J* = 8.3 Hz, 8H, Ar), 7.07 (d, *J* = 8.4 Hz, 8H, Ar), 6.64–6.62 (m, 2H, Ar), 2.34 (s, 12H, CH_3) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 157.43, 154.78, 149.38, 142.96, 134.97, 130.31, 126.48, 112.38, 109.97 (Ar), 20.99 (CH_3) ppm.

Synthesis of L2. This ligand was prepared by the same procedures as described above for **L1** but 1-iodo-4-methoxybenzene (678 mg, 2.90 mmol) was used. Elution using CH_2Cl_2/methanol (20:1, v/v) afforded product **L2** as a pale yellow solid. (45%, 159 mg). *Spectral Data*: FAB-MS (*m/z*): 611.3 $[M+1]^+$.^1H NMR (400 MHz, $CDCl_3$): δ = 8.14 (d, *J* = 5.8 Hz, 2H, Ar), 7.64 (d, *J* = 2.4 Hz, 2H, Ar), 7.14–7.12 (m, 8H, Ar), 6.89–6.87 (m, 8H, Ar), 6.56–6.54 (m, 2H, Ar), 3.81 (s, 12H, OCH_3) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 157.49, 157.18, 149.34, 138.38, 128.09, 114.97, 111.20, 108.79 (Ar), 55.46 (OCH_3) ppm.

Synthesis of Pt(II) precursors Pt-1 and Pt-2

Pt-1. A suspension of K_2PtCl_4 (132 mg, 0,32 mmol) in dilute hydrochloric acid was mixed with **L1** (174 mg, 0.32 mmol). The reaction mixture was refluxed overnight under N_2. Upon cooling, the precipitated solid was purified with silica column and collected as a bright yellow solid (90%, 233 mg). *Spectral data*: MS (FAB): *m/z* 812.8 (M^+). ^{1}H NMR ($CDCl_3$): δ (ppm) 8.94 (d, J = 7.0 Hz, 2H, Py), 7.07–7.73 (m, 16H, Ar), 6.79 (d, J = 2.7 Hz, 2H, Py), 6.60 (d, J = 2.7 Hz, 2 H, Py), 2.30 (s, 12H, CH_3). ^{13}C NMR ($CDCl_3$): δ (ppm) 157.07, 154.6, 148.0, 140.6, 137.0, 130.7, 126.7, 111.4, 109.0 (Ar), 21.2 (CH_3).

Pt-2. Similar synthetic procedure as for **Pt-1** was employed but now **L2** (194 mg, 0.32 mmol) was used instead to afford a yellow powder product in moderate yield (58%, 164 mg). *Spectral data*: MS (FAB): *m/z* 876.7 (M^+). ^{1}H NMR ($CDCl_3$): δ (ppm) 8.73 (d, J = 7.00 Hz, 2H, Py), 6.88–7.21 (m, 16H, Ar), 6.75 (d, J = 2.76 Hz, 2H, Py), 6.43 (q, J = 2.76 Hz, 2H, Py), 3.84 (s, 12H, OCH_3). ^{13}C NMR ($CDCl_3$): δ (ppm) 158.40, 157.07, 154.94, 147.24, 135.86, 128.45, 115.21, 110.13, 107.64 (Ar), 55.45 (OCH_3), 21.1 (CH_3).

OLED fabrication and measurements

The pre-cleaned ITO glass substrates were treated with ozone for 20 min. Then, PEDOT was deposited on the surface of ITO glass by spin-coating method to form a 40 nm-thick hole-injection layer after being cured at 120 °C for 30 min in air. The EML consisting of PVK blended with Pt(II) complexes was spin-coated from toluene solution at various concentrations. The sample was dried in a vacuum oven at 50 °C for 15 min and it was transferred to the deposition system for organic

and metal deposition. PBD (40 nm), LiF (1 nm) and Al cathode (100 nm) were successively evaporated at a base pressure less than 10^{-6} Torr. *J–L–V* characteristics and EL spectra of the devices were measured with a Keithley 2400 source meter and a coupled PR650 spectroscan photometer. All measurements were carried out at room temperature under ambient conditions. EQEs of the devices were calculated from the luminance, current density and EL spectrum, assuming a Lambertian distribution.

Computational details

Density functional theory (DFT) calculations using B3LYP were performed. The basis set used for C, H, N and O atoms was 6-31G while effective core potentials with a LanL2DZ basis set were employed for Pt atom.[3] All calculations were carried out using the Gaussian 03 program.[4] Mulliken population analyses were done using MullPop.[5] Frontier molecular orbitals obtained from the DFT calculations were plotted using the Molden 3.7 program written by Schaftenaar.[6]

X-ray crystallography

Crystallographic data collected at room temperature and the refinement results are described in **Table S1**. All cif files were checked using IUCr's checkcif algorithm. Due to the unsatisfactory data-quality (weak diffraction intensity, poor resolution and severe disorder) of the single crystals of **2b** and **2d**, a number of A- and B-level Alerts were generated in the Checkcif files. **Fig S10** indicates the electron residuals in **1a**, **2a** and **2d** resulting from the heavy metal atoms and disordered ligands. We have tried to solve the crystal structures and remove the Alerts as far as possible. These remaining alerts are inherent to the data and cannot be removed by the refinement procedures. They are listed below and the corresponding responses have been made. CheckCIF

validations have been made to these cif files, which have been deposited in the Cambridge Crystallographic Data Centre (CCDC).

CheckCIF validation of **2a**:

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.89Ang From Pt1 -2.95 eA-3

Author Response: We have noted the residual density around the Pt atoms with the presence of Q peaks. In this sense, we tried to treat the Pt atoms as disordered atoms to model them. However, upon splitting each Pt atom into two parts, the coordination geometry of the Pt with the donor atoms is unnormal and the resulting molecular structure collapsed upon refinement. Thus, the residual density around the Pt atoms is not chemically sensible to be assigned as any other elements and atoms. In fact, the appearance of residual density has been normally observed for heavy metal atoms.

CheckCIF validation of **2b**:

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low. 0.931 Why?

Author Response: This alert is generated from the weak reflections at higher theta area because the crystal quality is not satisfactory. Thus, only 93.1% overall completeness is acquired, but mass spectrum and NMR have confirmed the X-ray structural analysis.

PLAT601_ALERT_2_A Unit Cell Contains Solvent Accessible VOIDS of 230 Ang**3

Author Response: The crystal lattice indeed shows accessible voids. We have assigned several Q peaks from the electron residues trying to model some solvent molecules. However, no chemically reasonable species can be modelled after refinement. Thus, the structure did show voids but without the presence of solvent molecules.

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 13 Note

Author Response: The theta values of these missing reflections are lower than the Theta min and thus were omitted.

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.595 616 Report

Author Response: We did not omit these reflections during refinement. This is probably due to the unsatisfactory completeness where some expected reflections are too weak to be measured.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.89Ang From Pt1 3.17 eA-3

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.91Ang From Pt1 2.96 eA-3

PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on Pt1 1.71 eA-3

Author Response: We have noted the residual density around the Pt atoms with the presence of Q peaks. In this sense, we tried to treat the Pt atoms as disordered atoms to model them. However, upon splitting each Pt atom into two parts, the coordination geometry of the Pt with the donor atoms is unnormal and the resulting molecular structure collapsed upon refinement. Thus, the residual density around the Pt atoms is not chemically sensible to be assigned as any other elements and atoms. In fact, the appearance of residual density has been normally observed for heavy metal atoms.

CheckCIF validation of **2d**:

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low. 0.927 Why?

Author Response: This alert is generated from the weak reflections at higher theta area because the crystal quality is not satisfactory. Thus, only 92.7% overall completeness is acquired, but mass spectrum and NMR have confirmed the X-ray structural analysis.

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 1201 Report

Author Response: We did not omit these reflections during refinement. This is probably due to the unsatisfactory completeness where some expected reflections are too weak to be measured.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.15Ang From Pt1 3.12 eA-3

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.18Ang From Pt1 3.10 eA-3

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.36Ang From Pt2 3.03 eA-3

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.33Ang From Pt2 3.01 eA-3

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.95Ang From Pt1 -2.82 eA-3

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.03Ang From Pt2 -2.65 eA-3

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.04Ang From Pt2 -2.58 eA-3

Author Response: We have noted the residual density around the Pt atoms with the presence of Q peaks. In this sense, we tried to treat the Pt atoms as disordered atoms to model them. However, upon splitting each Pt atom into two parts, the coordination geometry of the Pt with the donor atoms

is unnormal and the resulting molecular structure collapsed upon refinement. Thus, the residual density around the Pt atoms is not chemically sensible to be assigned as any other elements and atoms. In fact, the appearance of residual density has been normally observed for heavy metal atoms.

References

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Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, *Gaussian 03*, revision B05, Gaussian, Inc., Pittsburgh, PA, 2003.

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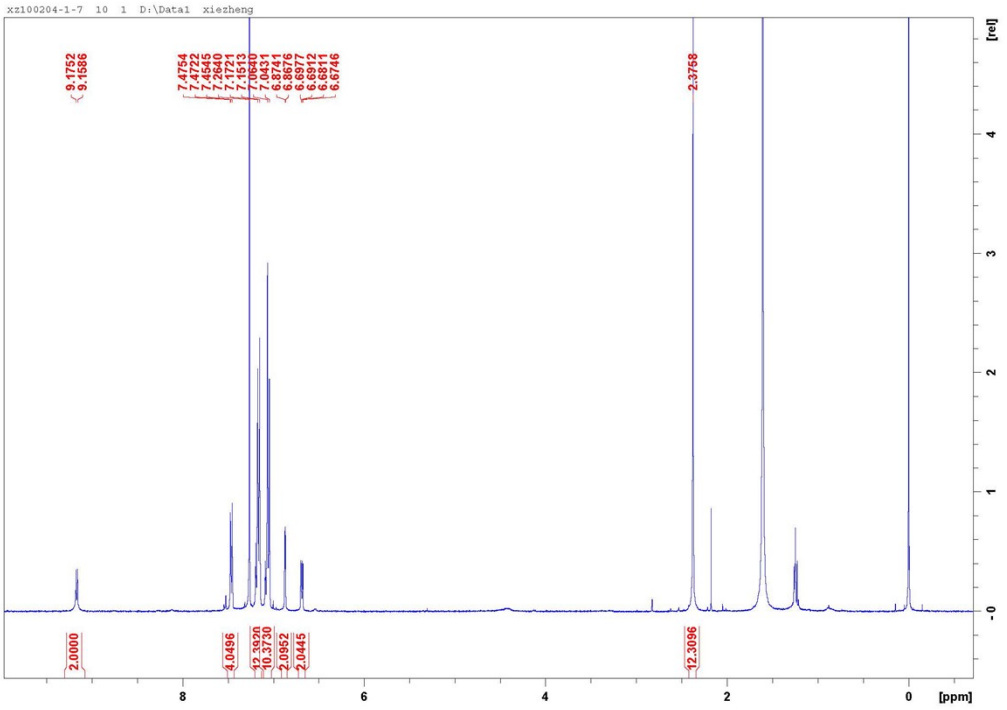

Figure S1. ^{1}H NMR spectrum of **1a**

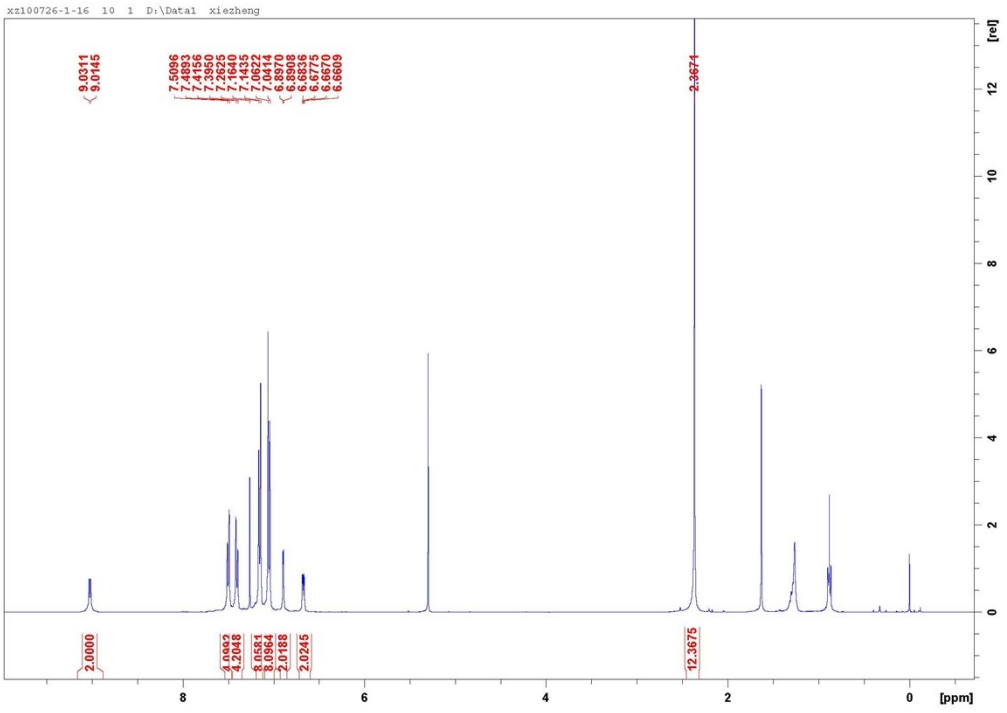

Figure S2. ^{1}H NMR spectrum of **1b**

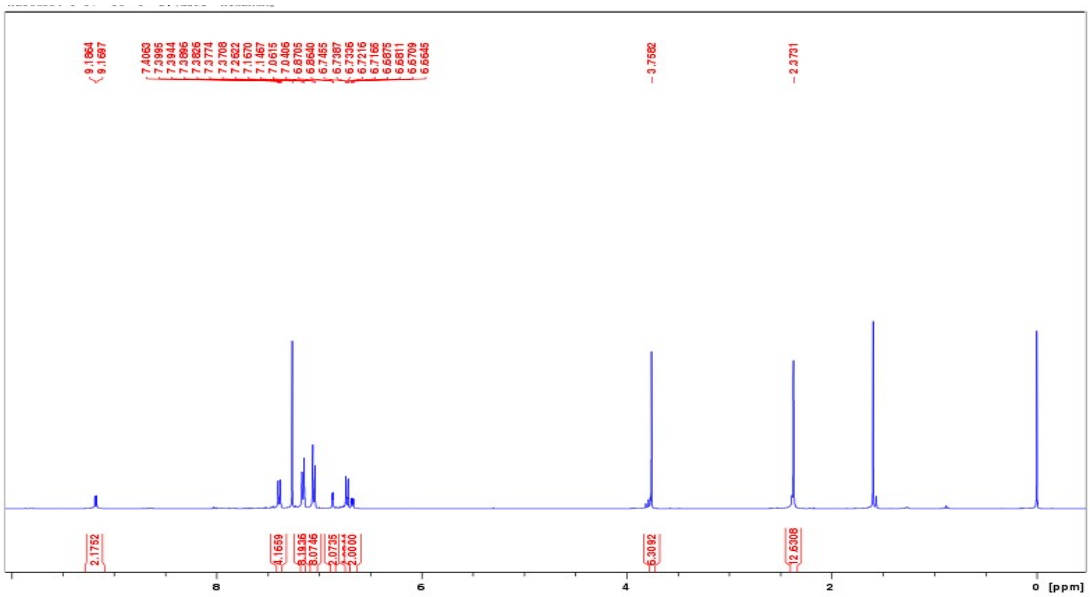

Figure S3. [1]H NMR spectrum of **1c**

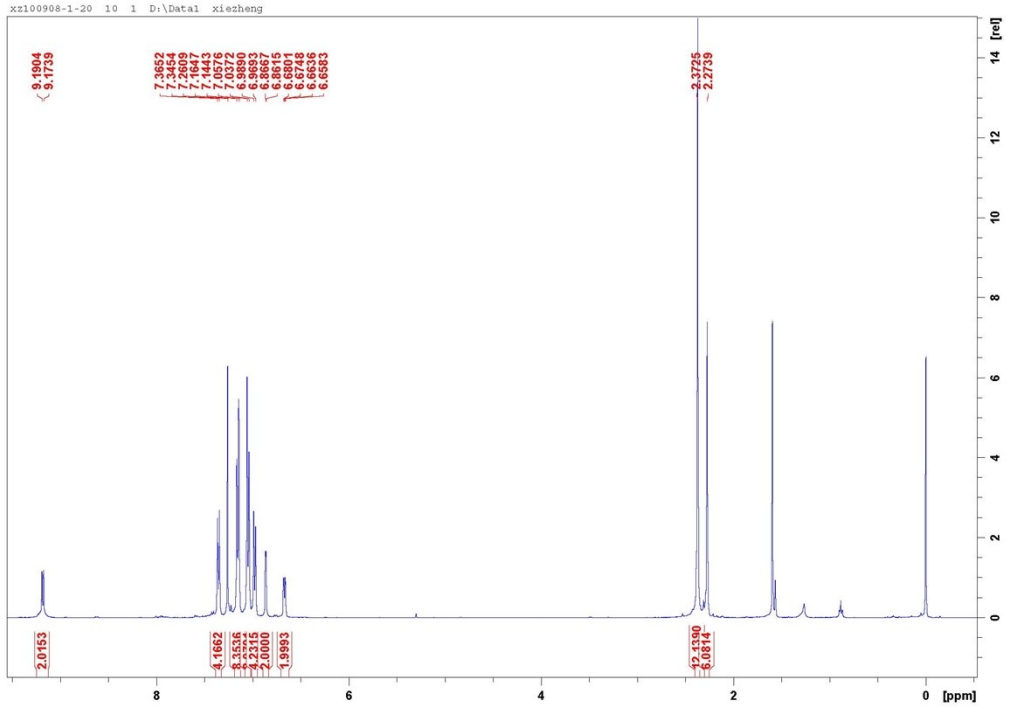

Figure S4. [1]H NMR spectrum of **1d**

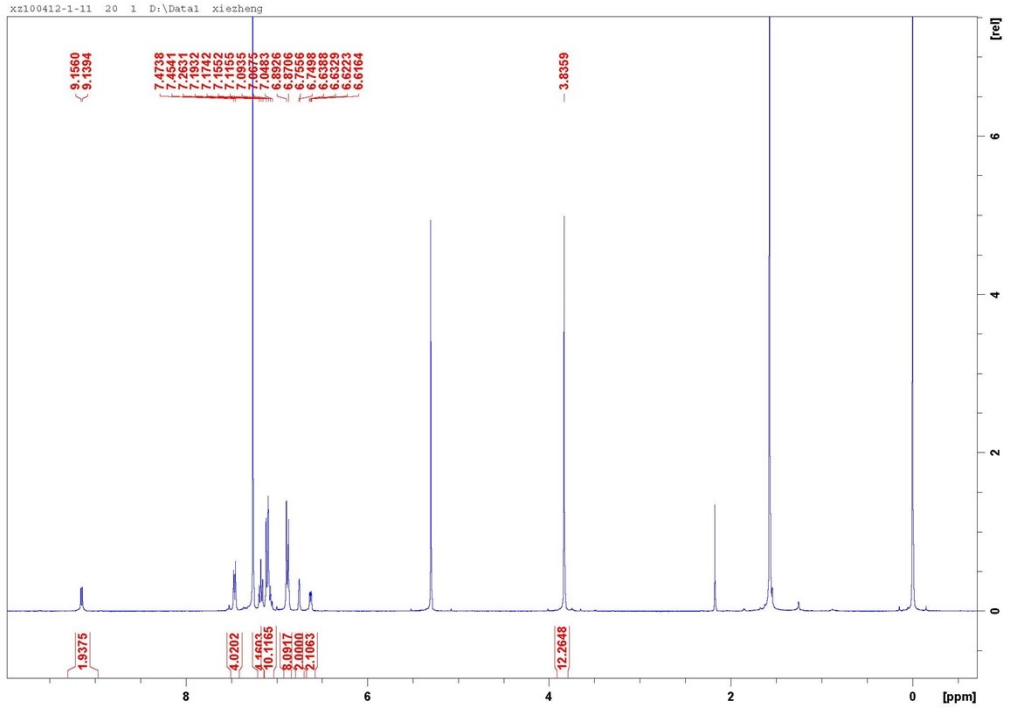

Figure S5. [1]H NMR spectrum of **2a**

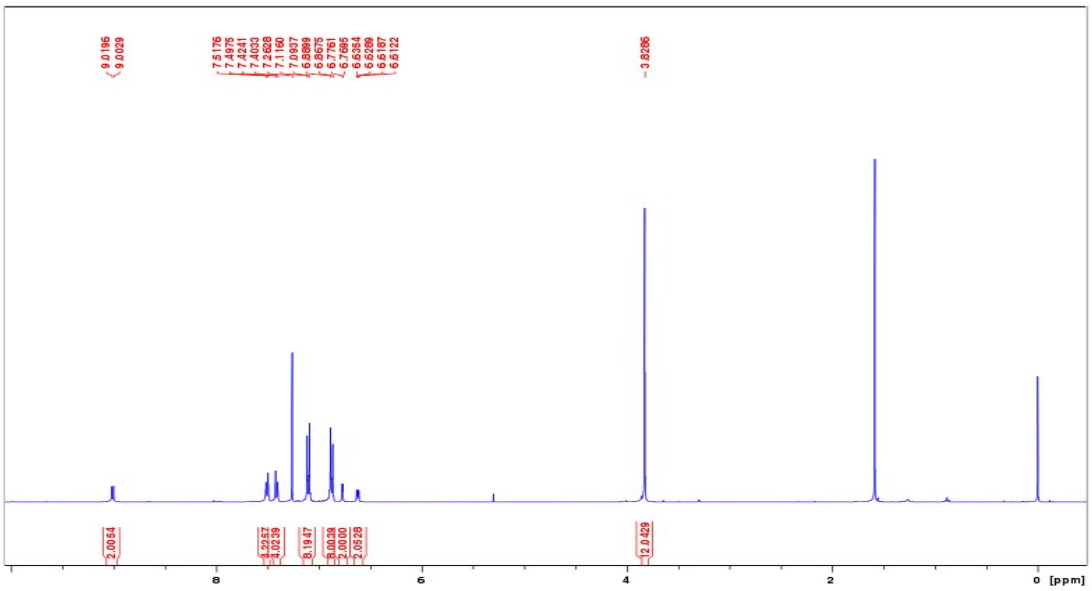

Figure S6. ^{1}H NMR spectrum of **2b**

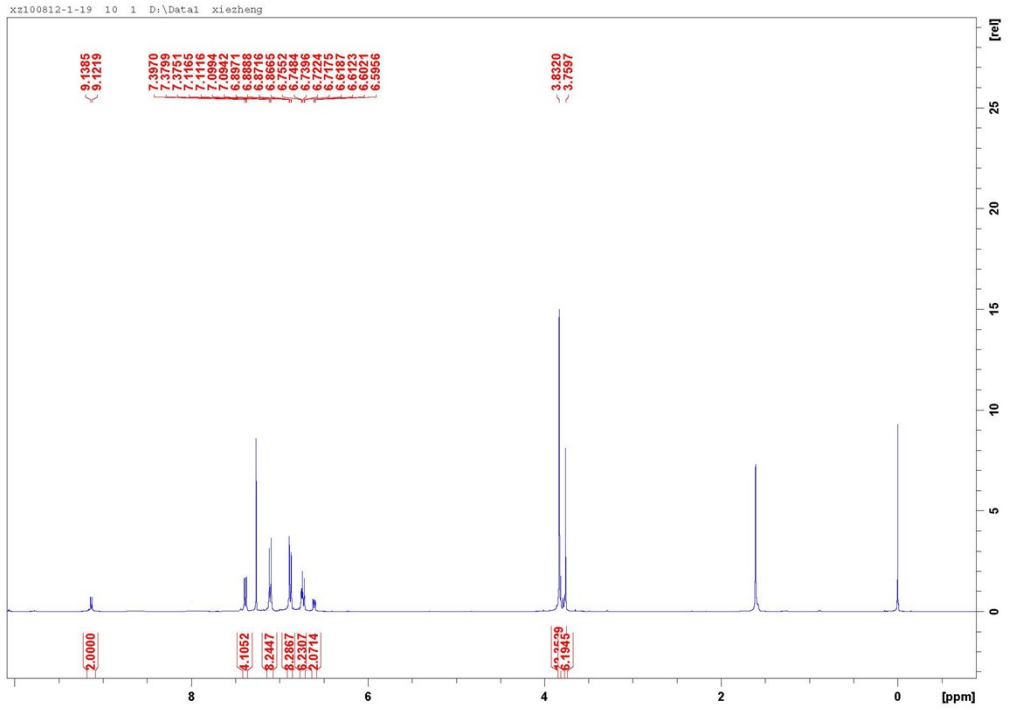

Figure S7. ^{1}H NMR spectrum of **2c**

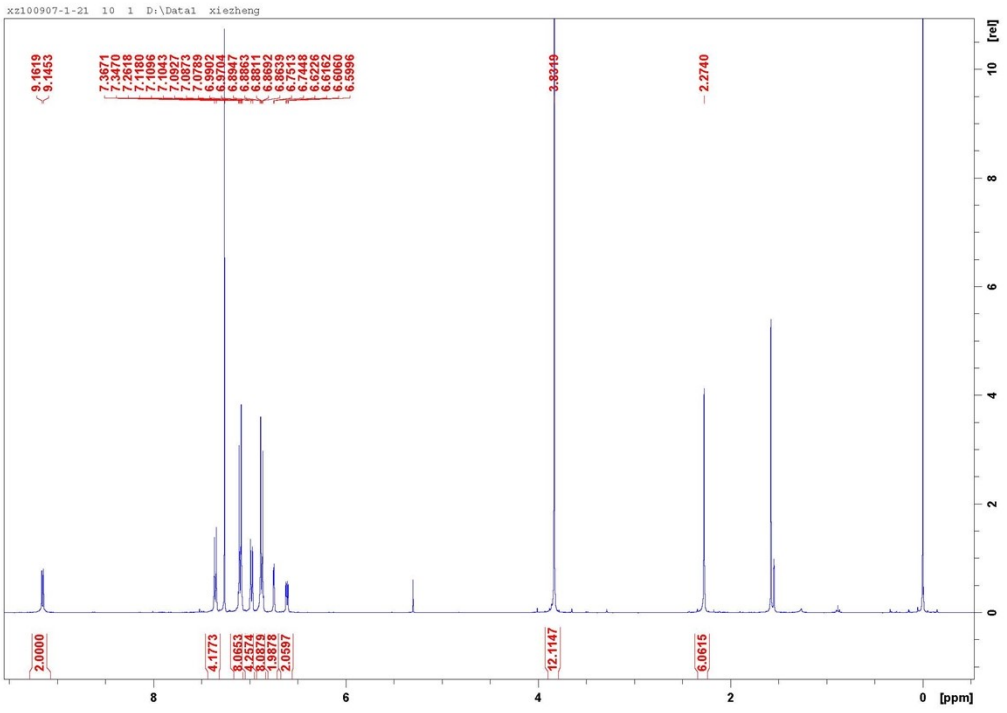

Figure S8. ^{1}H NMR spectrum of **2d**

Cartesian coordinates of DFT-computed structures

Complex 1a:

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-0.09320518	3.47524038	0.24751431
C	-1.39161146	2.92652497	0.19489480
C	-1.48641781	1.52439886	0.09153586
C	-0.33701553	0.74117104	0.05286705
C	1.00419584	2.63569735	0.19987842
C	-0.36242935	-0.73853354	-0.06129084
C	-1.53794678	-1.48215994	-0.09798874
C	-1.49128403	-2.88676736	-0.20075306
C	-0.21247904	-3.47945329	-0.25518712
C	0.91292349	-2.67768853	-0.20975486
H	0.05715823	4.54399227	0.33338367
H	2.01988379	3.01515740	0.24504553
H	-0.09885168	-4.55279848	-0.34053841
H	1.91515146	-3.09120728	-0.25643501
N	0.85740530	-1.33678456	-0.11599273
N	0.90271845	1.29729676	0.10588393
Pt	2.53949500	-0.04820108	-0.00566998
H	-2.49731288	-0.98726515	-0.03304523
H	-2.46217243	1.06241567	0.02806553
C	3.93591481	1.31017273	0.12378819
C	3.89139759	-1.45081345	-0.13354800
N	-2.52712457	3.73075706	0.23666407
N	-2.65348997	-3.65194892	-0.23978407
C	-2.63464312	-5.03607504	0.13469169
C	-2.12226458	-5.43237377	1.37686835
C	-3.15921499	-6.00544956	-0.72801805
C	-2.12050346	-6.77896514	1.73486607
H	-1.72743603	-4.68490517	2.05862820
C	-3.16625474	-7.34688600	-0.35021771
H	-3.56452014	-5.70391949	-1.68908980
C	-2.64092350	-7.76178514	0.88120726
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C	-3.90004170	-3.09366088	-0.66923448
C	-5.05093051	-3.26217214	0.11169648
C	-3.99712372	-2.40321560	-1.88433536
C	-6.27154829	-2.74981261	-0.32092198
H	-4.98295796	-3.79739267	1.05383259

C	-5.22214446	-1.88076468	-2.29674571
H	-3.11377846	-2.27675524	-2.50326517
C	-6.38284305	-2.04873092	-1.53028508
H	-7.15399962	-2.89017117	0.29928267
H	-5.27724465	-1.34513415	-3.24152048
C	-2.46205153	5.11349477	-0.13755465
C	-2.95101618	6.10011323	0.72643602
C	-1.93884637	5.49237940	-1.38073052
C	-2.91226744	7.44119835	0.34913594
H	-3.36438684	5.81257133	1.68836151
C	-1.89102836	6.83818579	-1.73818242
H	-1.57148189	4.73199159	-2.06354965
C	-2.37514362	7.83818225	-0.88300448
H	-3.29897865	8.19438394	1.03158674
H	-1.48116544	7.11417702	-2.70689800
C	-3.79065824	3.21502860	0.66963653
C	-4.93726316	3.42164028	-0.10853132
C	-3.90755449	2.52864509	1.88523349
C	-6.17316260	2.95026816	0.32725673
H	-4.85377742	3.95399951	-1.05104175
C	-5.14825252	2.04729237	2.30080430
H	-3.02724277	2.37311485	2.50182999
C	-6.30455673	2.25342852	1.53708997
H	-7.05205875	3.11959467	-0.29076022
H	-5.21897136	1.51403757	3.24587235
C	4.68515710	-2.38060464	-0.21851769
C	4.75333270	2.21867383	0.21298104
C	5.63899659	-3.43777080	-0.29683159
C	5.36511498	-4.62258756	-1.01338270
C	6.89177599	-3.32739860	0.34520527
C	6.30246389	-5.65072850	-1.08270821
H	4.40845239	-4.71950498	-1.51924199
C	7.82413154	-4.35944028	0.27352412
H	7.11578344	-2.41973120	0.89728661
C	7.53671103	-5.52696802	-0.43932617
H	6.06932083	-6.55324241	-1.64306929
H	8.78233458	-4.25163200	0.77625240
H	8.26701125	-6.33017007	-0.49428271
C	5.71921303	3.26449863	0.30179570
C	5.61997007	4.26779779	1.28974134
C	6.80448360	3.32700619	-0.59884454
C	6.56490823	5.28802127	1.37117424
H	4.79416024	4.22806235	1.99450954
C	7.74495424	4.35090389	-0.51335625

H	6.89398758	2.55894876	-1.36110852
C	7.63207120	5.33744715	0.47030953
H	6.46926437	6.04819009	2.14310469
H	8.57282378	4.37813433	-1.21794777
H	8.36862058	6.13417033	0.53538926
C	-2.29764925	9.29674440	-1.26855386
H	-3.08390783	9.88298902	-0.78154929
H	-1.33453749	9.73429852	-0.97346053
H	-2.39546266	9.43093740	-2.35118075
C	-7.65359099	1.76579473	2.01121036
H	-8.22020816	2.57086473	2.49794599
H	-8.26408595	1.40159397	1.17722493
H	-7.55328036	0.95268917	2.73742101
C	-7.71632008	-1.51728454	-2.00126146
H	-8.30581592	-2.30113794	-2.49541532
H	-8.31665575	-1.14254805	-1.16462040
H	-7.59144822	-0.70126599	-2.72037255
C	-2.61384627	-9.22209998	1.26701335
H	-3.42867951	-9.77800671	0.79147596
H	-1.67251114	-9.69645288	0.95876265
H	-2.70163593	-9.35204919	2.35097206

Complex 1b:

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	1.20720944	-3.47936826	0.15007803
C	2.49917620	-2.91236466	0.12743146
C	2.57454466	-1.50590101	0.05859615
C	1.41551372	-0.73815104	0.02413458
C	0.09959670	-2.65357105	0.11152775
C	1.42209467	0.74440570	-0.05541414
C	2.58771031	1.50270296	-0.07430620
C	2.52470670	2.90976865	-0.14280178
C	1.23783792	3.48729126	-0.18165761
C	0.12315972	2.67041300	-0.15810064
H	1.07002519	-4.55167323	0.20760733
H	-0.91005944	-3.04961171	0.13765481
H	1.11037104	4.56077840	-0.23966944
H	-0.88312868	3.07402156	-0.19602048

N	0.19461225	1.32829721	-0.09810629
N	0.18276129	-1.31191290	0.05127991
Pt	-1.46960349	0.01498144	-0.03244949
H	3.55290948	1.01790591	-0.02292647
H	3.54424997	-1.02898702	0.01964265
C	-2.85265938	-1.35939852	0.05087695
C	-2.84307158	1.39847912	-0.12486160
N	3.64317713	-3.70036502	0.16508964
N	3.67545405	3.68855558	-0.16461846
C	3.63535911	5.07125618	0.21759475
C	3.12830853	5.45095440	1.46681059
C	4.13408525	6.05366909	-0.64526000
C	3.10593626	6.79548732	1.83221521
H	2.75400556	4.69265116	2.14829113
C	4.12032107	7.39306830	-0.26048839
H	4.53571862	5.76425014	-1.61161229
C	3.59974255	7.79184230	0.97838184
H	2.70876312	7.07298025	2.80570436
H	4.51427993	8.14358055	-0.94165394
C	4.93448061	3.15140627	-0.58756804
C	6.07285859	3.32087908	0.21089312
C	5.05466021	2.48401548	-1.81319072
C	7.30488271	2.83033497	-0.21470117
H	5.98654936	3.83976973	1.16063649
C	6.29096905	1.98314704	-2.21877390
H	4.18078388	2.35870758	-2.44569807
C	7.43953075	2.15124373	-1.43427093
H	8.17790388	2.97089399	0.41856125
H	6.36477911	1.46516165	-3.17202543
C	3.59691052	-5.08339875	-0.21523696
C	4.07699310	-6.06821289	0.65543033
C	3.10232213	-5.46134681	-1.46994452
C	4.05705226	-7.40816334	0.27291801
H	4.46896764	-5.78033147	1.62619486
C	3.07343858	-6.80634821	-1.83316146
H	2.74263334	-4.70131820	-2.15734199
C	3.54845026	-7.80508750	-0.97149937
H	4.43643472	-8.16053036	0.96028875
H	2.68595310	-7.08242469	-2.81094476
C	4.90071811	-3.17297709	0.60448815
C	6.04811722	-3.35175838	-0.17898589
C	5.01017540	-2.50628129	1.83142076
C	7.27830515	-2.87106811	0.26260800
H	5.97008729	-3.87024468	-1.12967091

C	6.24515537	-2.01535049	2.25315700
H	4.12919235	-2.37375170	2.45250349
C	7.40246744	-2.19285480	1.48387579
H	8.15838714	-3.01885435	-0.35914547
H	6.31059893	-1.49787923	3.20729108
C	-3.65797156	2.31215075	-0.18246266
C	-3.66791185	-2.27250134	0.11051691
C	-4.63463699	3.34589505	-0.22733927
C	-4.37472915	4.57669945	-0.86816376
C	-5.90224025	3.16766427	0.37193144
C	-5.33179268	5.58469649	-0.90288713
H	-3.41112428	4.72738364	-1.34543122
C	-6.85757167	4.17527126	0.33622204
H	-6.12033590	2.22414716	0.86170019
C	-6.57858455	5.39075832	-0.30048356
H	-5.11622330	6.52236355	-1.40490051
H	-7.82841692	4.01856624	0.79645968
C	-4.62805448	-3.32150286	0.16774367
C	-4.53783652	-4.34149023	1.14090243
C	-5.69879526	-3.37761687	-0.75138243
C	-5.47313889	-5.36770699	1.19221130
H	-3.72257256	-4.31219246	1.85733213
C	-6.63330968	-4.40546791	-0.69930073
H	-5.78131420	-2.60197310	-1.50594519
C	-6.52566318	-5.40777867	0.27077379
H	-5.38524477	-6.14625949	1.94376492
H	-7.44623654	-4.43604846	-1.41776551
C	3.49164643	-9.26294569	-1.36293077
H	4.28522069	-9.84015900	-0.87704903
H	2.53438261	-9.71459588	-1.07023333
H	3.59244411	-9.39151825	-2.44583343
C	8.74586231	-1.69518608	1.96331550
H	9.32866993	-2.50350101	2.42472283
H	9.34504600	-1.29870703	1.13583938
H	8.63647280	-0.90370940	2.71164184
C	8.78493840	1.64309267	-1.89681607
H	9.37213062	2.44249224	-2.36815148
H	9.37809154	1.25939877	-1.05912869
H	8.67870744	0.83951298	-2.63267311
C	3.55028076	9.24937774	1.37205219
H	4.35363109	9.82117292	0.89594076
H	2.59987210	9.70927071	1.06998258
H	3.64038193	9.37508459	2.45623568
C	-7.56275560	-6.48682368	0.36627923

C	-7.59633502	6.49184314	-0.27898235
F	-8.55422596	-6.16840106	1.23573461
F	-7.03732508	-7.65814557	0.80037213
F	-8.15856933	-6.73061929	-0.82435977
F	-8.85856939	6.01868994	-0.40749204
F	-7.56808415	7.18883821	0.88570185
F	-7.40063807	7.39191019	-1.27096994

Complex 1c:

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	0.74559573	-3.47891477	0.23333723
C	2.03436008	-2.90758140	0.18554916
C	2.10501017	-1.50396641	0.08836540
C	0.94227700	-0.73997576	0.05283486
C	-0.36599086	-2.65805112	0.18794421
C	0.94234766	0.73998082	-0.05278426
C	2.10515872	1.50385177	-0.08837910
C	2.03465138	2.90747556	-0.18557063
C	0.74593614	3.47893513	-0.23328639
C	-0.36572858	2.65818394	-0.18783435
H	0.61353038	-4.55050216	0.31417179
H	-1.37533325	-3.05459468	0.22897220
H	0.61397001	4.55053477	-0.31411784
H	-1.37503284	3.05482995	-0.22880651
N	-0.28773391	1.31768288	-0.10175357
N	-0.28786219	-1.31755761	0.10186399
Pt	-1.94722966	0.00014546	0.00009465
H	3.07277011	1.02482063	-0.02823885
H	3.07267246	-1.02503983	0.02818611
C	-3.32316906	-1.38015368	0.11878381
C	-3.32304438	1.38057103	-0.11853933
N	3.18469898	-3.69164718	0.22786518
N	3.18506031	3.69142397	-0.22797960
C	3.14912079	5.07246129	0.15466557
C	2.62685031	5.45694818	1.39670646
C	3.66748794	6.05246145	-0.69993731
C	2.60894594	6.80151555	1.76160488
H	2.23712567	4.70205469	2.07317605
C	3.65881616	7.39180468	-0.31488766
H	4.08076003	5.76074942	-1.66061200

C	3.12312593	7.79458402	0.91594912
H	2.19910876	7.08163759	2.72915242
H	4.06823840	8.13932766	-0.99027780
C	4.43746307	3.15173035	-0.66375527
C	5.58834030	3.33020400	0.11335373
C	4.53850508	2.46682374	-1.88274075
C	6.81392301	2.83240444	-0.32552067
H	5.51814452	3.86065011	1.05802376
C	5.76682962	1.95952238	-2.30080729
H	3.65407295	2.33317747	-2.49858193
C	6.92887994	2.13696103	-1.53647800
H	7.69689727	2.98024926	0.29197661
H	5.82453777	1.42803454	-3.24793053
C	3.14855460	-5.07265612	-0.15487783
C	3.66666050	-6.05281616	0.69966083
C	2.62628310	-5.45693204	-1.39700879
C	3.65775656	-7.39214399	0.31447541
H	4.07991401	-5.76128712	1.66039883
C	2.60814541	-6.80143776	-1.76203250
H	2.23674129	-4.70188549	-2.07341312
C	3.12209340	-7.79469811	-0.91641799
H	4.06697070	-8.13980698	0.98983235
H	2.19831532	-7.08139920	-2.72963223
C	4.43713663	-3.15215718	0.66375395
C	5.58809180	-3.33094805	-0.11317742
C	4.53815418	-2.46710547	1.88265977
C	6.81370986	-2.83333748	0.32579972
H	5.51792311	-3.86148826	-1.05779612
C	5.76652534	-1.95999591	2.30082814
H	3.65367269	-2.33319927	2.49837293
C	6.92864583	-2.13776794	1.53668969
H	7.69673550	-2.98142865	-0.29156599
H	5.82420328	-1.42839124	3.24788770
C	-4.13273279	2.29714403	-0.19886223
C	-4.13291446	-2.29667538	0.19911439
C	-5.10542424	3.33717571	-0.27341995
C	-4.83177370	4.56435854	-0.91973062
C	-6.38277781	3.18065284	0.29713089
C	-5.78091616	5.57379094	-0.98855834
H	-3.85686094	4.71157744	-1.37583726
C	-7.34400367	4.19031749	0.23451090
H	-6.61917107	2.24692224	0.79816388
C	-7.04654790	5.39631955	-0.41072293
H	-5.56716416	6.51412092	-1.48821700

H	-8.31442124	4.02424470	0.68934259
C	-5.10562224	-3.33669205	0.27366714
C	-4.83248398	-4.56332708	0.92121459
C	-6.38248443	-3.18069273	-0.29813713
C	-5.78164393	-5.57275296	0.99002875
H	-3.85796832	-4.71013151	1.37830129
C	-7.34371337	-4.19034800	-0.23553974
H	-6.61847775	-2.24737714	-0.80013048
C	-7.04676957	-5.39581683	0.41093814
H	-5.56827570	-6.51265971	1.49064655
H	-8.31373860	-4.02469862	-0.69136292
C	3.07702089	-9.25237844	-1.31042008
H	3.87412576	-9.82435703	-0.82410438
H	2.12257970	-9.71230930	-1.02118707
H	3.18128706	-9.37856457	-2.39346382
C	8.26381930	-1.62065033	2.01872448
H	8.73799069	-2.32746522	2.71286526
H	8.95829290	-1.46788757	1.18594019
H	8.15735466	-0.66870132	2.55029884
C	8.26400880	1.61962002	-2.01839949
H	8.73820633	2.32619647	-2.71276311
H	8.95849002	1.46705145	-1.18558748
H	8.15746505	0.66752011	-2.54969037
C	3.07829188	9.25234294	1.30968327
H	3.87820855	9.82326666	0.82673079
H	2.12571809	9.71352133	1.01629725
H	3.17809569	9.37844577	2.39314236
O	-7.91148886	-6.45208166	0.53183421
O	-7.91119633	6.45264995	-0.53151796
C	-9.20418019	-6.31950556	-0.02859912
H	-9.16271603	-6.16478610	-1.11574786
H	-9.72206156	-7.25813138	0.18064209
H	-9.76213362	-5.48991106	0.42729305
C	-9.20437709	6.31955192	0.02766625
H	-9.16386127	6.16394269	1.11472563
H	-9.72211157	7.25832797	-0.18125797
H	-9.76188654	5.49030439	-0.42939612

Complex 1d:

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-0.44359420	3.47959181	0.22676314
C	-1.73231553	2.90806571	0.18045977
C	-1.80270680	1.50398290	0.08616789
C	-0.63999372	0.74027720	0.05158275
C	0.66809090	2.65872089	0.18306478
C	-0.64009197	-0.74020410	-0.05152550
C	-1.80290762	-1.50375433	-0.08613700
C	-1.73270183	-2.90784264	-0.18045260
C	-0.44405689	-3.47954037	-0.22674156
C	0.66773871	-2.65882070	-0.18301192
H	-0.31149843	4.55131915	0.30537828
H	1.67723758	3.05577896	0.22379809
H	-0.31210559	-4.55128430	-0.30537371
H	1.67683337	-3.05601148	-0.22373796
N	0.58980230	-1.31822105	-0.09930198
N	0.58997762	1.31813021	0.09936992
Pt	2.24946392	-0.00015565	0.00003121
H	-2.77044385	-1.02446081	-0.02731579
H	-2.77030685	1.02482055	0.02732808
C	3.62485874	1.38047596	0.11606398
C	3.62467523	-1.38096635	-0.11602909
N	-2.88251563	3.69166670	0.22141042
N	-2.88299931	-3.69130912	-0.22143658
C	-2.84688258	-5.07281225	0.16016823
C	-2.32597646	-5.45789366	1.40255796
C	-3.36412275	-6.05219983	-0.69573115
C	-2.30833900	-6.80269133	1.76663725
H	-1.93721975	-4.70334260	2.07997670
C	-3.35566823	-7.39180552	-0.31155112
H	-3.77647256	-5.75986258	-1.65661451
C	-2.82140616	-7.79525375	0.91969071
H	-1.89969513	-7.08338457	2.73451444
H	-3.76429248	-8.13895120	-0.98782820
C	-4.13618402	-3.15147972	-0.65533228
C	-5.28536587	-3.32834876	0.12460652
C	-4.23948329	-2.46855700	-1.87517246
C	-6.51168565	-2.83077404	-0.31239852
H	-5.21329913	-3.85742520	1.06990597
C	-5.46854764	-1.96145444	-2.29141922
H	-3.35633976	-2.33632714	-2.49318115

C	-6.62896694	-2.13726023	-1.52428165
H	-7.39340295	-2.97736236	0.30717839
H	-5.52814136	-1.43150974	-3.23927799
C	-2.84624170	5.07318084	-0.16013799
C	-3.36344793	6.05258544	0.69575999
C	-2.32522001	5.45825758	-1.40248202
C	-3.35484954	7.39220362	0.31162335
H	-3.77589126	5.76025591	1.65660555
C	-2.30743933	6.80306461	-1.76651617
H	-1.93649147	4.70369293	-2.07990170
C	-2.82047446	7.79564508	-0.91957047
H	-3.76344893	8.13936295	0.98790016
H	-1.89870629	7.08375356	-2.73435718
C	-4.13577969	3.15193577	0.65521719
C	-5.28484802	3.32874722	-0.12482612
C	-4.23921903	2.46918788	1.87518772
C	-6.51126215	2.83127648	0.31216281
H	-5.21269733	3.85771786	-1.07017819
C	-5.46830692	1.96222844	2.29140386
H	-3.35612709	2.33705297	2.49329197
C	-6.62867610	2.13794985	1.52408821
H	-7.39292267	2.97784600	-0.30748890
H	-5.52801367	1.43246806	3.23936509
C	4.43303468	-2.29877684	-0.19465702
C	4.43334041	2.29818192	0.19465012
C	5.40241012	-3.34191378	-0.26657687
C	5.15301848	-4.53547678	-0.97443588
C	6.65624677	-3.21257236	0.36929566
C	6.10917597	-5.54603120	-1.03885791
H	4.20070629	-4.65525194	-1.48372851
C	7.60296095	-4.22928570	0.29934986
H	6.87317922	-2.29869877	0.91408708
C	7.35042312	-5.41778510	-0.40196710
H	5.88835507	-6.45342921	-1.59819748
H	8.56173636	-4.09765198	0.79776926
C	5.40280155	3.34124378	0.26652598
C	5.15380872	4.53447558	0.97518217
C	6.65625746	3.21220903	-0.37004758
C	6.10998143	5.54494613	1.03964251
H	4.20179158	4.65393993	1.48510083
C	7.60305631	4.22890789	-0.30005304
H	6.87293691	2.29859694	-0.91537666
C	7.35091473	5.41701721	0.40195726
H	5.88949269	6.45202282	1.59964602

H	8.56158337	4.09751430	-0.79899876
C	-2.77594304	9.25363079	-1.31247924
H	-3.57457697	9.82454711	-0.82742924
H	-1.82253958	9.71422032	-1.02087226
H	-2.87803531	9.38044854	-2.39563429
C	-7.96465450	1.62095350	2.00399633
H	-8.43842493	2.32646028	2.69971268
H	-8.65877619	1.47105149	1.17042486
H	-7.85945671	0.66754406	2.53322344
C	-7.96502074	-1.62045086	-2.00417567
H	-8.44294442	-2.33030668	-2.69260484
H	-8.65616401	-1.46196716	-1.16968776
H	-7.85887461	-0.67165465	-2.54137632
C	-2.77703314	-9.25323068	1.31264775
H	-3.57584684	-9.82404217	0.82776922
H	-1.82375714	-9.71397928	1.02087473
H	-2.87893930	-9.37999144	2.39582642
C	8.37510972	6.52734998	0.44805933
H	9.39434702	6.13153900	0.52795612
H	8.34165752	7.14610292	-0.45974283
H	8.20575215	7.19370548	1.30106698
C	8.37492541	-6.52782566	-0.44832175
H	9.39314314	-6.13213163	-0.54134517
H	8.35066105	-7.13870687	0.46506296
H	8.19790313	-7.20146549	-1.29398588

Complex 2a:

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	0.39899076	3.43102750	0.42998691
C	-0.91964043	2.95563412	0.25805423
C	-1.07279509	1.56476699	0.08246370
C	0.03927288	0.72933003	0.07044275
C	1.45691603	2.54298312	0.38569230
C	-0.05317196	-0.74158642	-0.10505549
C	-1.26040756	-1.43293610	-0.10944944
C	-1.28077459	-2.83364256	-0.27297083
C	-0.03195527	-3.46980677	-0.44584988
C	1.12753449	-2.71883776	-0.41201930
H	0.59602592	4.48351865	0.58845157
H	2.48514192	2.87144315	0.49772381
H	0.03245945	-4.53993912	-0.59537365

H	2.10726066	-3.17160233	-0.52487210
N	1.13662745	-1.38486319	-0.23605109
N	1.30043192	1.21902886	0.20085993
Pt	2.87641372	-0.18691632	-0.02033871
H	-2.18940749	-0.90159109	0.04363662
H	-2.06036666	1.15257003	-0.07113218
C	4.33077361	1.09034035	0.23945691
C	4.16199285	-1.63283494	-0.28245726
N	-2.01057422	3.81399111	0.25546178
N	-2.46924211	-3.55024675	-0.25700367
C	-2.48277932	-4.96728810	-0.02717753
C	-1.89199890	-5.51861236	1.11285446
C	-3.12874263	-5.81843340	-0.93709465
C	-1.92066553	-6.89649207	1.34062917
H	-1.39580396	-4.86938417	1.82828405
C	-3.17919327	-7.18608692	-0.70872406
H	-3.59522920	-5.39802668	-1.82280716
C	-2.57031517	-7.73911413	0.42968530
H	-1.44586413	-7.29341904	2.23031832
H	-3.67622786	-7.85296492	-1.40595193
C	-3.74004252	-2.89661589	-0.38298846
C	-4.69495270	-3.01980025	0.62856747
C	-4.06153337	-2.15987913	-1.53449283
C	-5.95399225	-2.43031871	0.50365718
H	-4.45623669	-3.59202384	1.51985281
C	-5.30642207	-1.55696441	-1.66042152
H	-3.33020212	-2.06625968	-2.33207016
C	-6.26712062	-1.69390893	-0.64563293
H	-6.67238339	-2.54743303	1.30628262
H	-5.56600796	-0.99009429	-2.54883544
C	-1.84588023	5.22414846	0.04159725
C	-2.35778265	6.13926748	0.97437099
C	-1.20921393	5.70887243	-1.10383213
C	-2.22997424	7.50477661	0.76424287
H	-2.85919545	5.77070383	1.86409143
C	-1.05923167	7.08165077	-1.31424164
H	-0.81741499	5.00942659	-1.83651221
C	-1.57325294	7.98897580	-0.37901254
H	-2.62040135	8.22139416	1.47971164
H	-0.55381856	7.42603594	-2.20897697
C	-3.35211842	3.32412388	0.38739405
C	-4.30002001	3.60149631	-0.60000926
C	-3.74695025	2.59723864	1.52247325
C	-5.62183685	3.17276997	-0.46787220

H	-4.00477598	4.16841077	-1.47761226
C	-5.05600713	2.15263211	1.65429997
H	-3.02135297	2.38562046	2.30243436
C	-6.00721420	2.44288054	0.66338241
H	-6.33244987	3.40677254	-1.25181727
H	-5.37110685	1.59343931	2.52952713
C	4.91024241	-2.58712538	-0.45975033
C	5.18470501	1.95178292	0.41301244
C	5.81278644	-3.67500242	-0.64662184
C	5.45815693	-4.79858200	-1.42406278
C	7.09526798	-3.65824094	-0.05574183
C	6.34636295	-5.85704021	-1.60088797
H	4.47781233	-4.82322272	-1.89186205
C	7.97833066	-4.72009305	-0.23503823
H	7.38181487	-2.79812446	0.54167500
C	7.61100990	-5.82583717	-1.00728497
H	6.05087381	-6.71061618	-2.20676396
H	8.96086756	-4.68403685	0.22961149
H	8.30307092	-6.65238123	-1.14667351
C	6.18179523	2.95202265	0.61534652
C	6.79033959	3.12795243	1.87681421
C	6.58788897	3.79789827	-0.43929151
C	7.76006510	4.10887187	2.07189523
H	6.49076759	2.48029438	2.69546905
C	7.55843021	4.77662704	-0.23761360
H	6.13276383	3.66830206	-1.41691743
C	8.15003873	4.93971855	1.01797185
H	8.21603465	4.22436021	3.05247768
H	7.85723475	5.41447938	-1.06633091
H	8.90818135	5.70319621	1.17257535
O	-7.46829201	-1.09012419	-0.87445887
O	-2.66820159	-9.09126212	0.55524612
O	-7.27128900	1.98645948	0.89677612
O	-1.49086720	9.34379381	-0.48433557
C	-8.27711313	2.29438474	-0.05871371
H	-8.06890956	1.81547363	-1.02341868
H	-9.20783849	1.89671235	0.34946163
H	-8.38031471	3.37815661	-0.19761234
C	-0.81743977	9.89372127	-1.60694905
H	-1.31371902	9.62141920	-2.54775928
H	-0.85805849	10.97660757	-1.47843630
H	0.23129723	9.57151619	-1.64451329
C	-2.06200759	-9.71007353	1.68033670
H	-2.25554989	-10.77871290	1.57372204

H	-0.97804075	-9.53752878	1.69924422
H	-2.50149780	-9.35392978	2.62137153
C	-8.48763625	-1.24400776	0.10401229
H	-8.20717897	-0.76296548	1.04907950
H	-9.37057558	-0.75031125	-0.30558749
H	-8.71775972	-2.30251944	0.28026679

Complex 2b:

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	0.81429843	-3.46344188	0.29011861
C	2.10968287	-2.91731876	0.15061953
C	2.19396703	-1.51349475	0.03437998
C	1.04262512	-0.73441454	0.04600617
C	-0.28523540	-2.62717163	0.27362334
C	1.06391737	0.74528586	-0.06924619
C	2.23645421	1.49209350	-0.04787688
C	2.19171827	2.89811266	-0.15931800
C	0.91293193	3.48048399	-0.30420182
C	-0.20923011	2.67460048	-0.29851703
H	0.66802103	-4.52996513	0.40229665
H	-1.29546823	-3.01225546	0.36344418
H	0.79741255	4.55127414	-0.41178405
H	-1.20867071	3.08586287	-0.39298799
N	-0.15572819	1.33575673	-0.17540021
N	-0.19398890	-1.29026456	0.14524979
Pt	-1.83386599	0.04564311	-0.02353260
H	3.18945425	0.99892230	0.08318774
H	3.16100608	-1.04705365	-0.09164369
C	-3.22943099	-1.30663223	0.15994996
C	-3.19312507	1.43308714	-0.21843032
N	3.24039546	-3.71816215	0.12259912
N	3.34394935	3.66735618	-0.12100768
C	3.28912698	5.07886134	0.14031409
C	2.69476256	5.57245181	1.30438815
C	3.87027875	5.98161044	-0.76333467
C	2.65593205	6.94463551	1.56298865
H	2.24975183	4.88162542	2.01458981
C	3.85277524	7.34472293	-0.50549262
H	4.33959176	5.60526265	-1.66718955
C	3.24021818	7.83989239	0.65765236
H	2.18135725	7.29702729	2.47136523

H	4.29868621	8.05224762	-1.19713958
C	4.64498341	3.07934362	-0.26630503
C	5.59909974	3.23231560	0.74180775
C	4.99476410	2.37993762	-1.43273150
C	6.88445149	2.70712354	0.59969409
H	5.33882439	3.77706828	1.64417535
C	6.26634897	1.83999885	-1.57552386
H	4.26459378	2.26526111	-2.22861517
C	7.22552083	2.00565642	-0.56354852
H	7.60150460	2.84591931	1.40007286
H	6.54751307	1.30162306	-2.47499151
C	3.14749972	-5.12903474	-0.13165559
C	3.69483756	-6.04308184	0.78166067
C	2.54822862	-5.61157399	-1.29780356
C	3.63850397	-7.40658772	0.53165831
H	4.16783971	-5.67538520	1.68715612
C	2.47051612	-6.98349146	-1.54880784
H	2.12959693	-4.91189372	-2.01533841
C	3.02015511	-7.89025774	-0.63327686
H	4.05725342	-8.12298550	1.23109479
H	1.99294521	-7.32723902	-2.45891108
C	4.55656776	-3.16581784	0.27149659
C	5.51196621	-3.35344652	-0.72952914
C	4.91919406	-2.46779994	1.43484868
C	6.81080044	-2.86367161	-0.58350139
H	5.24174957	-3.89756105	-1.62935476
C	6.20467923	-1.96296365	1.58138967
H	4.18788036	-2.32648124	2.22537237
C	7.16466392	-2.16321755	0.57651386
H	7.52836125	-3.02864086	-1.37850115
H	6.49560549	-1.42580396	2.47847816
C	-4.00140312	2.34644637	-0.34091992
C	-4.04984989	-2.20914760	0.27994429
C	-4.97825744	3.37319391	-0.46296036
C	-4.63525166	4.66909213	-0.90748826
C	-6.33137432	3.12314793	-0.14080378
C	-5.59499195	5.66819759	-1.01771718
H	-3.60287970	4.87824862	-1.17119776
C	-7.29007993	4.12273707	-0.25129672
H	-6.61281957	2.13025003	0.19471979
C	-6.92858334	5.40193275	-0.68970198
H	-5.31338218	6.65653432	-1.36738777
H	-8.32562175	3.91023271	-0.00464924
C	-5.00401968	-3.25700254	0.41336321

C	-5.42905710	-3.69890024	1.68537888
C	-5.54869413	-3.89383371	-0.72416936
C	-6.35323400	-4.72960781	1.81384063
H	-5.02128432	-3.21901558	2.56950628
C	-6.47113046	-4.92463995	-0.59388520
H	-5.23361668	-3.56432876	-1.70922646
C	-6.87756404	-5.35121931	0.67583279
H	-6.66477668	-5.05976078	2.79965279
H	-6.87427541	-5.40736846	-1.47893349
O	8.45223328	1.46383678	-0.80899035
O	3.26946712	9.19153285	0.81128015
O	8.40471640	-1.65420384	0.82541753
O	3.00919756	-9.24307895	-0.77819918
C	9.42261979	-1.87716418	-0.14146893
H	9.19170272	-1.36904232	-1.08577203
H	10.33470144	-1.45478656	0.28345844
H	9.57440979	-2.94861565	-0.32379931
C	2.38230018	-9.79496753	-1.92704278
H	2.87547607	-9.46670899	-2.85138403
H	2.48161709	-10.87725836	-1.83008837
H	1.31785496	-9.53041156	-1.97042911
C	2.65665647	9.75466735	1.96225974
H	2.79290132	10.83375713	1.87494860
H	1.58366384	9.52604563	1.99930600
H	3.13445831	9.40208644	2.88569202
C	9.47073174	1.65308685	0.16449875
H	9.22119440	1.14556211	1.10434482
H	10.37325079	1.20879233	-0.25851246
H	9.65042695	2.71890344	0.35434490
C	-7.91240031	-6.42863684	0.80559693
C	-7.95164166	6.49657272	-0.74591700
F	-7.83634791	-7.07083989	1.99502625
F	-7.79179235	-7.36652890	-0.16529089
F	-9.17496262	-5.94185923	0.70990700
F	-8.04966937	7.16467688	0.43205048
F	-7.65505882	7.42490302	-1.68677131
F	-9.18982625	6.02496948	-1.02204370

Complex 2c:

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	0.39543878	-3.46457863	0.37061722

C	1.68183446	-2.90451245	0.20930173
C	1.74864744	-1.50351429	0.06622057
C	0.58670997	-0.73813404	0.07358542
C	-0.71528231	-2.64275379	0.34766887
C	0.58673144	0.73815211	-0.07355789
C	1.74869217	1.50349715	-0.06620623
C	1.68192035	2.90449684	-0.20928971
C	0.39554034	3.46460197	-0.37059566
C	-0.71520528	2.64281064	-0.34763570
H	0.26445889	-4.53089239	0.50315538
H	-1.72173895	-3.03520913	0.45123813
H	0.26459170	4.53091929	-0.50313570
H	-1.72165112	3.03529563	-0.45119785
N	-0.64130755	1.30787690	-0.19441735
N	-0.64134549	-1.30782178	0.19445338
Pt	-2.30241303	0.00005209	0.00002088
H	2.70869206	1.02779714	0.07863774
H	2.70866001	-1.02784309	-0.07863328
C	-3.67671421	-1.36624630	0.23925440
C	-3.67667866	1.36638696	-0.23920624
N	2.82406528	-3.69399420	0.18555404
N	2.82417709	3.69394118	-0.18555885
C	2.74756869	5.10517003	0.06541596
C	2.13409360	5.59944493	1.21951723
C	3.32364698	6.01037223	-0.83924010
C	2.07087311	6.97294316	1.46613581
H	1.69176849	4.90777545	1.93047030
C	3.28256669	7.37519925	-0.59264822
H	3.80697715	5.63421298	-1.73576931
C	2.64994956	7.87000162	0.55957846
H	1.58057479	7.32477745	2.36630131
H	3.72402877	8.08390645	-1.28600407
C	4.13256211	3.12468748	-0.32980327
C	5.09271482	3.31297341	0.66675875
C	4.48451739	2.40665691	-1.48445415
C	6.38522446	2.80533481	0.52454976
H	4.83054472	3.87161244	1.56002609
C	5.76329995	1.88392465	-1.62686105
H	3.74939547	2.26342971	-2.27101548
C	6.72766066	2.08502144	-0.62649495
H	7.10629233	2.97132928	1.31613394
H	6.04539651	1.33124370	-2.51734888
C	2.74740518	-5.10521919	-0.06542569
C	3.32346552	-6.01044504	0.83921807

C	2.13389503	-5.59946805	-1.21951951
C	3.28233384	-7.37526963	0.59262131
H	3.80682229	-5.63430638	1.73574157
C	2.07062264	-6.97296305	-1.46614248
H	1.69158292	-4.90778021	-1.93046283
C	2.64968169	-7.87004539	-0.55959758
H	3.72378165	-8.08399503	1.28596770
H	1.58029789	-7.32477655	-2.36630170
C	4.13247198	-3.12478735	0.32978802
C	5.09260697	-3.31310103	-0.66678589
C	4.48446715	-2.40678037	1.48444144
C	6.38513720	-2.80551203	-0.52458676
H	4.83040633	-3.87172343	-1.56005465
C	5.76327079	-1.88409701	1.62683866
H	3.74935971	-2.26353341	2.27101268
C	6.72761299	-2.08522126	0.62646026
H	7.10619041	-2.97152740	-1.31617991
H	6.04539805	-1.33143485	2.51732843
C	-4.48362741	2.27466427	-0.40095785
C	-4.48367988	-2.27450694	0.40101405
C	-5.45037760	3.30935833	-0.56833642
C	-5.18006578	4.45793222	-1.34718627
C	-6.71787776	3.22708907	0.03867058
C	-6.12275413	5.46331583	-1.50633866
H	-4.21303073	4.54584995	-1.83428267
C	-7.67257147	4.23345671	-0.11426671
H	-6.95186851	2.35441116	0.64073282
C	-7.37840157	5.36070053	-0.89002676
H	-5.91150133	6.34261950	-2.10786731
H	-8.63549689	4.12604917	0.37304713
C	-5.45042401	-3.30920920	0.56838015
C	-5.18021479	-4.45764372	1.34747082
C	-6.71781342	-3.22708743	-0.03887791
C	-6.12289574	-5.46303584	1.50661303
H	-4.21326854	-4.54544244	1.83476488
C	-7.67249823	-4.23346605	0.11404623
H	-6.95172452	-2.35451718	-0.64112710
C	-7.37843094	-5.36057008	0.89004785
H	-5.91172359	-6.34223103	2.10832855
H	-8.63533671	-4.12617457	-0.37346477
O	7.96127258	1.55636822	-0.87061994
O	2.65485322	9.22415864	0.70197863
O	7.96124798	-1.55661786	0.87057679
O	2.65453566	-9.22420198	-0.70200310

C	8.97999731	1.77085928	0.09661695
H	8.73809960	1.27524405	1.04487982
H	9.88615758	1.32948589	-0.32188733
H	9.14962280	2.84117728	0.27036636
C	2.01250130	9.78557093	1.83698934
H	2.12565177	10.86659168	1.73982151
H	0.94445664	9.53296542	1.86096670
H	2.48367906	9.45435730	2.77181521
C	8.97995397	-1.77113972	-0.09667302
H	8.73806599	-1.27550589	-1.04492863
H	9.88613604	-1.32980605	0.32182585
H	9.14953549	-2.84146275	-0.27043436
C	2.01214477	-9.78558739	-1.83700504
H	2.48331863	-9.45438731	-2.77183769
H	2.12525838	-10.86661253	-1.73984294
H	0.94410871	-9.53294372	-1.86096358
O	-8.23746008	6.40664989	-1.10742663
O	-8.23748929	-6.40651807	1.10745602
C	-9.52139739	-6.34473758	0.51596455
H	-9.46327801	-6.30568441	-0.58075821
H	-10.03667734	-7.26014040	0.81535390
H	-10.09233186	-5.47611149	0.87230813
C	-9.52146735	6.34473764	-0.51616416
H	-9.46353250	6.30549237	0.58056101
H	-10.03671586	7.26018205	-0.81548033
H	-10.09232419	5.47616282	-0.87275748

Complex 2d:

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-0.10278810	-3.46360229	-0.38162347
C	-1.38913050	-2.90388914	-0.21884483
C	-1.45573576	-1.50309515	-0.07153867
C	-0.29380400	-0.73803299	-0.07605271
C	1.00801935	-2.64192969	-0.35635667
C	-0.29379184	0.73804322	0.07612628
C	-1.45571101	1.50312435	0.07159876
C	-1.38908077	2.90392088	0.21887771
C	-0.10272916	3.46361414	0.38165639
C	1.00806275	2.64192101	0.35641431
H	0.02815242	-4.52950779	-0.51731936
H	2.01424868	-3.03444085	-0.46178991
H	0.02822799	4.52952007	0.51733315

H	2.01429842	3.03441303	0.46185750
N	0.93412260	1.30752468	0.19887654
N	0.93410195	-1.30753484	-0.19880317
Pt	2.59520769	-0.00001564	0.00002182
H	-2.41575093	1.02786028	-0.07429223
H	-2.41576558	-1.02781566	0.07436809
C	3.96891713	-1.36560044	-0.24401724
C	3.96894416	1.36555044	0.24401031
N	-2.53128013	-3.69293496	-0.19769269
N	-2.53121699	3.69298022	0.19767858
C	-2.45473125	5.10550056	-0.04675081
C	-1.84319027	5.60484201	-1.19966753
C	-3.02919045	6.00652723	0.86303769
C	-1.78039688	6.97941669	-1.44026066
H	-1.40218932	4.91632804	-1.91450539
C	-2.98840266	7.37244833	0.62255234
H	-3.51112068	5.62632687	1.75861650
C	-2.35785362	7.87239430	-0.52861860
H	-1.29175220	7.33529458	-2.33973055
H	-3.42869869	8.07805311	1.31979651
C	-3.83973168	3.12303761	0.33925116
C	-4.79904355	3.31405962	-0.65756979
C	-4.19248530	2.40193050	1.49171040
C	-6.09163745	2.80601752	-0.51772635
H	-4.53619977	3.87518101	-1.54908257
C	-5.47138530	1.87884869	1.63175342
H	-3.45799061	2.25666328	2.27849326
C	-6.43498691	2.08267733	0.63118618
H	-6.81212688	2.97416961	-1.30937399
H	-5.75420467	1.32385618	2.52056764
C	-2.45481704	-5.10544727	0.04678918
C	-3.02923838	-6.00649436	-0.86300358
C	-1.84333954	-5.60476369	1.19974988
C	-2.98847617	-7.37240938	-0.62248011
H	-3.51111678	-5.62631337	-1.75861856
C	-1.78057267	-6.97933244	1.44038361
H	-1.40236447	-4.91623643	1.91459112
C	-2.35799115	-7.87233059	0.52873678
H	-3.42874246	-8.07802686	-1.31973024
H	-1.29197759	-7.33518911	2.33988859
C	-3.83978520	-3.12297605	-0.33928799
C	-4.79914212	-3.31403344	0.65748499
C	-4.19248473	-2.40181579	-1.49172918
C	-6.09172370	-2.80597058	0.51761033

H	-4.53634359	-3.87519682	1.54898413
C	-5.47137377	-1.87871213	-1.63180052
H	-3.45796155	-2.25652612	-2.27848087
C	-6.43501691	-2.08257480	-0.63128332
H	-6.81224727	-2.97414894	1.30922186
H	-5.75414804	-1.32367742	-2.52060278
C	4.77478313	2.27409989	0.40939578
C	4.77472772	-2.27416960	-0.40943019
C	5.73863045	3.31050922	0.58130472
C	5.49208815	4.41690990	1.42025292
C	6.97953517	3.26791258	-0.09044049
C	6.43963690	5.42520131	1.57739938
H	4.54533461	4.47322095	1.95042942
C	7.91794318	4.28188664	0.07307704
H	7.19019566	2.42701645	-0.74433612
C	7.67139918	5.37940980	0.91107472
H	6.21866153	6.26648068	2.23203963
H	8.86420677	4.22137311	-0.46169228
C	5.73853779	-3.31061011	-0.58136516
C	5.49210534	-4.41678930	-1.42063393
C	6.97929588	-3.26826508	0.09067207
C	6.43961589	-5.42511690	-1.57780132
H	4.54547288	-4.47289837	-1.95104763
C	7.91766271	-4.28227004	-0.07286920
H	7.18987291	-2.42753601	0.74480966
C	7.67122434	-5.37958062	-0.91118121
H	6.21873000	-6.26622091	-2.23269648
H	8.86381026	-4.22195181	0.46212837
C	8.71046760	6.45899669	1.10833429
H	9.45058945	6.17293924	1.86885909
H	9.26331887	6.65956413	0.18313784
H	8.25465596	7.39920549	1.43831285
C	8.71025413	-6.45920656	-1.10843160
H	8.25451584	-7.39911526	-1.43935960
H	9.45096469	-6.17275932	-1.86823488
H	9.26242127	-6.66049156	-0.18297943
O	-7.66872604	1.55353106	0.87300701
O	-2.36301657	9.22708658	-0.66492828
O	-7.66874065	-1.55339901	-0.87312523
O	-2.36317283	-9.22701932	0.66508322
C	-8.68707596	1.77119764	-0.09401211
H	-8.44504997	1.27812848	-1.04355328
H	-9.59354208	1.32903880	0.32296753
H	-8.85615137	2.84207187	-0.26474319

C	-1.72399946	9.79364316	-1.79933189
H	-1.83741875	10.87417246	-1.69724578
H	-0.65590870	9.54165239	-1.82726969
H	-2.19759031	9.46614568	-2.73422597
C	-8.68713597	-1.77113983	0.09382801
H	-8.44516332	-1.27812957	1.04341483
H	-9.59358579	-1.32896411	-0.32316839
H	-8.85620635	-2.84202603	0.26448518
C	-1.72418796	-9.79355521	1.79951550
H	-2.19781869	-9.46605778	2.73438960
H	-1.83758521	-10.87408742	1.69743559
H	-0.65610269	-9.54154523	1.82749025

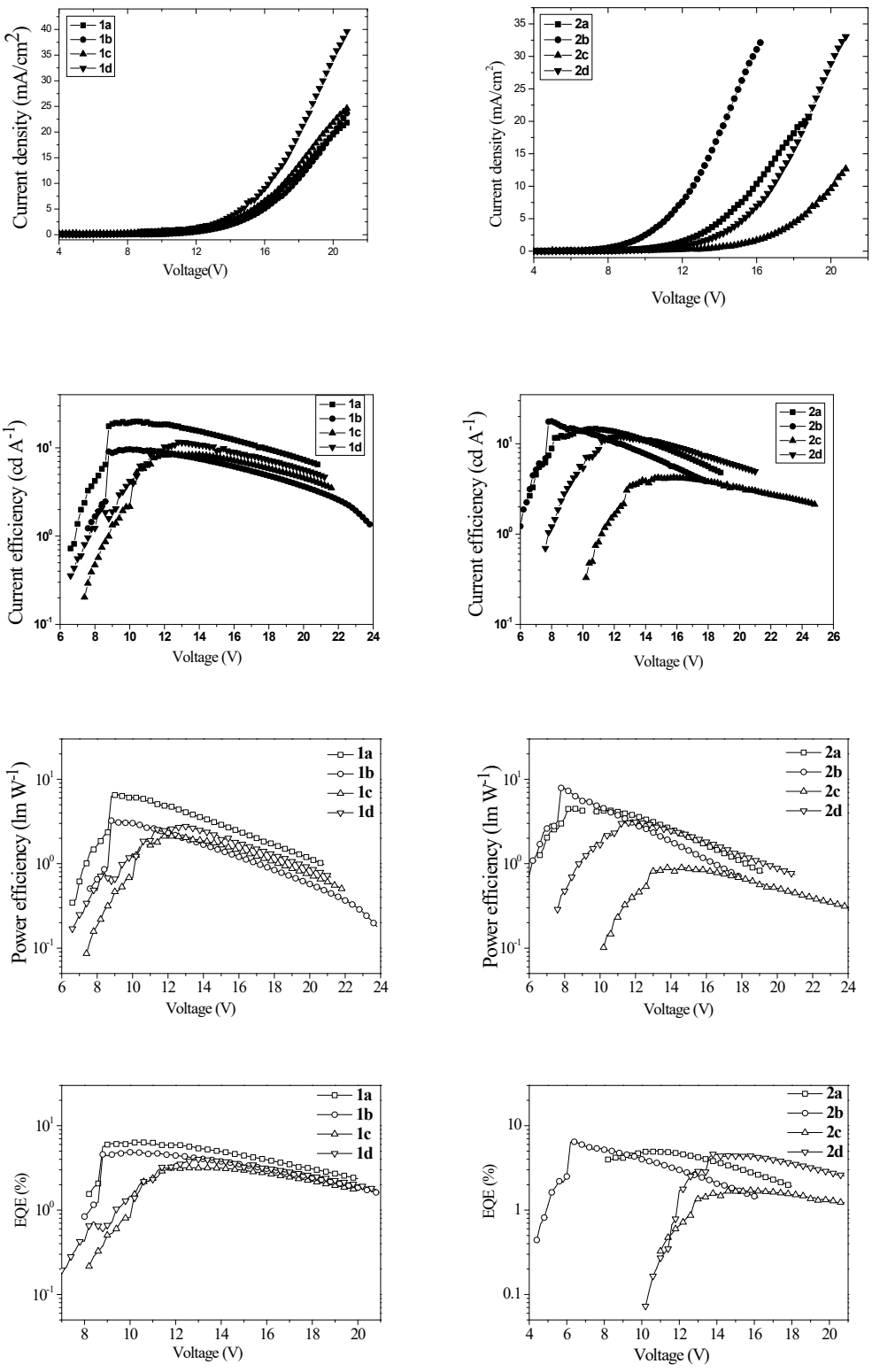
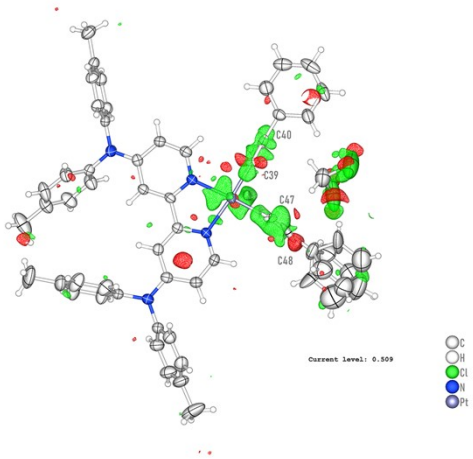
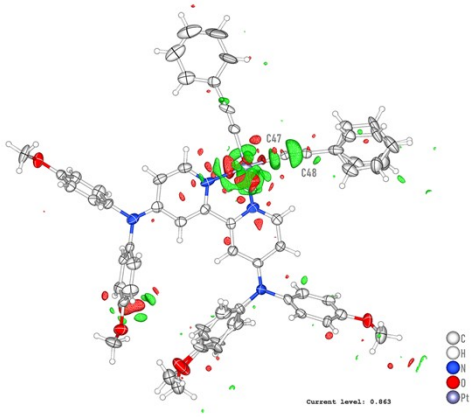


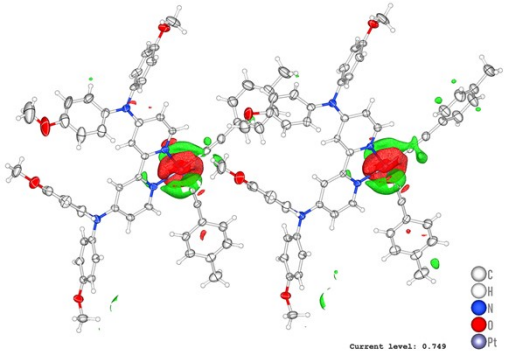
Fig. S9 Comparison of OLED performance data for series **1** and **2** complexes

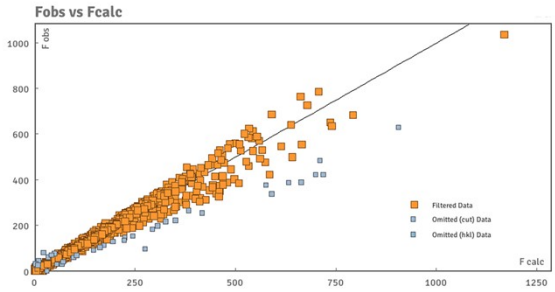


1a



2a





2d

Fig. S10 Electron density maps of **1a**, **2a** and **2d**. For **2d**, the Fobs vs. Fcalc plot with a deviation from linearity to indicate the unsatisfactory data quality is also shown.

Table S1 X-ray crystallographic data for **Pt-1**·CH_2Cl_2, **1a**·CH_2Cl_2, **2a**, **2b** and **2d**

Compound	**Pt-1**·CH_2Cl_2	**1a**·CH_2Cl_2	**2a**	**2b**	**2d**
CCDC	2362301	2362297	2362298	2362299	2362300
chemical formula	$C_{38}H_{34}Cl_2N_4Pt.CH_2Cl_2$	$C_{54}H_{44}N_4Pt.CH_2Cl_2$	$C_{54}H_{44}N_4O_4Pt$	$C_{56}H_{42}F_6N_4O_4Pt$	$C_{56}H_{48}N_4O_4Pt$
formula weight	897.61	1028.94	1008.01	1144.02	1036.07
wavelength	0.71073	0.71073	0.71073	0.71073	1.54178
crystal system	Monoclinic	Monoclinic	Monoclinic	Triclinic	Monoclinic
space group	$P2_1/n$	$P2_1/c$	$P2_1/c$	P-1	$P2_1/c$
a [Å]	15.44(1)	14.5715(9)	13.549(2)	11.270(3)	27.028(1)
b [Å]	9.409(7)	10.8846(7)	9.877(1)	13.603(3)	9.9741(5)
c [Å]	25.814(2)	29.960(2)	33.703(4)	18.951(5)	34.505(2)
α [°]	90.0	90.0	90.0	101.556(4)	90.0
β [°]	102.0(1)	96.820(1)	99.076(2)	105.572(5)	97.533(2)
γ [°]	90.0	90.0	90.0	104.303(4)	90.0
V [Å^3]	3666.8(5)	4718.2(5)	4453.9(9)	2599(1)	9221.7(8)
Z	4	4	4	2	8
ρ_{calc} [g·cm^{-3}]	1.626	1.449	1.503	1.462	1.492
μ [mm^{-1}]	4.152	3.128	3.202	2.769	6.105
F (000)	1776	2064	2024	1140	4164
θ range [°]	2.55–28.28	2.63–25.03	2.563–25.027	2.700–24.995	2.88–68.12
reflections collected	21912	22949	20743	11998	84428
independent reflections	8803	8238	7788	8527	15476
R_{int}	0.0410	0.0378	0.0703	0.0492	0.0259
no. of parameters	433	590	606	676	1183
$R1$, $wR2$ [I >2.0 (I)] [a]	0.0352, 0.0864	0.0424, 0.0993	0.0605, 0.1168	0.0656, 0.1512	0.0588, 0.1613
$R1$, $wR2$ (all data)	0.0466, 0.0925	0.0598, 0.1080	0.0968, 0.1279	0.0901, 0.1675	0.0625, 0.1695
GoF on F^2 [b]	1.103	1.103	1.143	0.980	1.007

[a] $R1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$. $wR2 = \{\Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]\}^{1/2}$.

[b] $GoF = [(\Sigma w|F_o| - |F_c|)^2 / (N_{obs} - N_{param})]^{1/2}$.

Table S2 Selected bond lengths [Å] and angles [°] in **Pt-1**·CH_2Cl_2, **1a**·CH_2Cl_2, **2a**, **2b** and **2d** with estimated standard deviations (esds) given in parentheses.

Pt-1·CH_2Cl_2		**1a**·CH_2Cl_2		**2a**		**2b**		**2d**	
Pt1–N1	2.012(3)	Pt1–N1	2.059(5)	Pt1–N1	2.053(8)	Pt1–N1	2.053(8)	Pt1–N1	2.057(4)
								Pt2–N5	2.065(5)
Pt1–N3	2.001(3)	Pt1–N3	2.053(5)	Pt1–N3	2.061(7)	Pt1–N3	2.077(7)	Pt1–N3	2.051(4)
								Pt2–N7	2.042(4)
Pt1–Cl1	2.30(1)	Pt1–C39	1.991(6)	Pt1–C39	1.991(8)	Pt1–C39	2.000(9)	Pt1–C39	1.977(7)
								Pt2–C95	1.991(7)
Pt1–Cl2	2.30(9)	Pt1–C47	2.100(6)	Pt1–C47	2.053(7)	Pt1–C48	1.94(1)	Pt1–C48	1.974(6)
								Pt2–C104	1.966(6)
		C39–C40	1.072(8)	C39–C40	1.080(6)	C39–C40	1.17(1)	C39–C40	1.19(1)
								C95–C96	1.17(1)
		C47–C48	1.100(4)	C47–C48	1.080(6)	C48–C49	1.21(1)	C48–C49	1.184(8)
								C104–C105	1.188(8)
N1–Pt1–N3	80.5(1)	N1–Pt1–N3	78.8(1)	N1–Pt1–N3	78.6(3)	N1–Pt1–N3	78.3(3)	N1–Pt1–N3	78.4(2)
								N5–Pt2–N7	78.3(2)
N3–Pt1–Cl1	176.02(8)	N1–Pt1–C39	96.7(2)	N1–Pt1–C39	94.7(3)	N1–Pt1–C39	95.4(4)	N1–Pt1–C39	94.9(2)
								N5–Pt2–C95	95.2(2)
N1–Pt1–Cl2	174.42(8)	N3–Pt1–C47	98.1(2)	N3–Pt1–C47	96.4(3)	N3–Pt1–C48	96.4(4)	N3–Pt1–C48	95.6(2)
								N7–Pt2–C104	95.2(2)
Cl1–Pt1–Cl2	89.49(3)	C39–Pt1–C47	86.4(2)	C39–Pt1–C47	90.4(3)	C39–Pt1–C48	89.9(4)	C39–Pt1–C48	91.2(2)
								C95–Pt2–C104	91.5(2)
		Pt1–C39–C40	176.6(6)	Pt1–C39–C40	177(1)	Pt1–C39–C40	172(1)	Pt1–C39–C40	169.9(5)
								Pt2–C95–C96	169.3(5)
		Pt1–C47–C48	164.4(6)	Pt1–C47–C48	166.9(8)	Pt1–C48–C49	175.7(9)	Pt1–C48–C49	173.5(5)
								Pt2–C104–C105	171.9(5)

The structure of **2d** was not solved very accurately due to poor diffraction data obtained but there is no doubt that the molecular skeleton of **2d** should be similar to other related structures such as **2a** and **2b**. So, the structural parameters for **2d** should not be treated so accurate here.