Electronic Supplementary Information

First examples of tri- and tetraphosphametacyclophanes: synthesis and isolation of an unusual hexapalladium complex containing pincer units with Pd—P covalent bonds

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Supporting Information contains

(S1) Experimental Section

General procedures

All experimental manipulations were performed under inert atmosphere of dry nitrogen or argon, using standard Schlenk line techniques. All the solvents were purified by conventional procedures[1] and distilled prior to use. The metal precursor AgOTf was purchased from Aldrich chemicals and used as received. Metal reagent [$AuCl(SMe_2)$] and $PhPH_2$ were prepared according to published procedures.[2] The ^1H and $^{31}P\{^1H\}$ NMR (δ in ppm) spectra were obtained from either Bruker Avance-400 MHz or Bruker Avance- 500 MHz spectrometer. The samples for NMR recording were washed with Et_2O or CH_2Cl_2 and dried under vacuum at room temperature, whereas for elemental analyses, the samples were dried using modified Abderhalden apparatus circulating boiling pentanes. The spectra were recorded in $CDCl_3$ solution with $CDCl_3$ (or DMSO-d_6) as an internal lock; TMS and 85%

H_3PO_4 were used as internal and external standards for ^1H and $^{31}P\{^1H\}$ NMR, respectively. Positive values indicate downfield shifts. The UV-Vis and Fluorescence spectra were recorded at 298 K on Perkin-Elmer UV-Vis and fluorescence spectrometers, respectively, using a quartz cell (1 cm width). Mass spectra were recorded on BRUKER mass spectrometer using Electro-spray ionization mass spectrometry (ESI-MS) method. Microanalyses were carried out on a Carlo Erba (model 1106) elemental analyzer. Melting points of all compounds were determined on a Veego melting point apparatus and are uncorrected.

Synthesis of tri- and tetraphosphametacylophanes (*m*-{-C(O)-C_5H_3N(C(O)PPh)}$_3$ (1), (*m*-{-C(O)-C_5H_3N(C(O)PPh)}$_4$) (2)

To a solution of phenylphosphine ($PhPH_2$) (1.08 g, 9.8 mmol) in diethyl ether (50 mL) was added dropwise a solution of 2,6-pyridinedicarbonyl dichloride (2 g, 9.8 mmol) in the same solvent (30 mL) over 10-15 minutes at -78 ^oC in presence of Et_3N (1.98 g, 2.73 mL, 19.6 mmol) during which time the color of the solution turned to bright yellow. The reaction mixture was warmed to room temperature and stirred for further 16 h. The reaction mixture was passed through celite and the solvent was removed under reduced pressure to give yellow solid in 90% (2.12 g) yield. The yellow solid was dissolved in dichloromethane (15 mL) and saturated with 5 ml of petroleum ether and stored overnight at room temperature to give 1.48 g (*ca*. 70%) of *m*-{-C(O)-C_5H_3N(C(O)PPh)}$_3$ (**1**) as yellow crystals. The mother liquor was again dried under reduced pressure and added 5 mL of dichloromethane and layered with 3 mL of diethyl ether and stored at room temperature for 24 h to give 0.64 g (*ca*. 30%) of *m*-{-C(O)-C_5H_3N(C(O)PPh)}$_4$ (**2**) as thin yellow needles.

Compound **1**: Mp: 170-173 °C (dec). Anal. Calcd. for $C_{39}H_{24}N_3O_6P_3 \cdot CH_2Cl_2$: C, 59.42; H, 3.24; N, 5.19. Found: C, 59.70; H, 3.39; N, 4.97. MS (ESI): *m/z* Calc for $C_{39}H_{24}N_3O_6P_3$ (M+H): 724.0951, Found: 724.0981 (err 4.1 ppm). FT-IR (KBr disc) cm^{-1}: υ_{CH}: 2972, 2937,

2737, 2676, 2490 s, $\upsilon_{C=O}$: 1735 s, $\upsilon_{C=C}$: 1651 m. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.40 (d, J = 8 Hz, 6H, Py-H), 7.81-7.76 (m, 9H, Ph-H), 7.57 (t, J = 8 Hz, 3H, Py-H), 7.48 (td, J = 8 Hz, 6H, Ph-H), 3.09 (q, J = 7.2 Hz, 4H, Et_2O), 1.39 (t, J = 7.2 Hz, 6H, Et_2O) ppm. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 211.9 (d, J_{CP} = 37.3 Hz, C=O), 153.0 (d, J_{CP} = 32.4 Hz, *ipso*-C-Ph), 139.0 (C-Ar), 136.68-136.9 (m, C-Ar), 130.6 (C-Ar), 128.8 (C-Ar), 124.1 (C-Ar), 45.9 (CH_2-O, Et_2O), 8.7 (CH_3, Et_2O) ppm. $^{31}P\{^{1}H\}$ NMR (202.45 MHz, $CDCl_3$): δ 23.3 (s) ppm.

Compound **2**: Mp: 180-185 °C (dec). Anal. Calcd. for $C_{52}H_{32}N_4O_8P_4{\cdot}Et_2O$: C, 64.74; H, 4.07; N, 5.39. Found: C, 64.70; H, 3.69; N, 5.21. MS (ESI): *m*/*z* Calc for $C_{52}H_{32}N_4O_8P_4$ (M+K): 1003.0802, Found: 1003.0772 (err -3.0 ppm). FT-IR (KBr disc) cm^{-1}: υ_{CH}: 2932, 2675, 2489 m, $\upsilon_{C=O}$: 1735 s, $\upsilon_{C=C}$: 1654 s. δ 8.40 (d, J = 8 Hz, 8H, Py-H), 7.81-7.76 (m, 12H, Ph-H), 7.57 (t, J = 8 Hz, 4H, Py-H), 7.48 (td, J = 8 Hz, 8H, Ph-H) ppm. $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 211.9 (d, J_{CP} = 36.2 Hz, C=O), 153.0 (d, J_{CP} = 33.7 Hz, *ipso*-C-Ph), 139.0 (C-Ar), 136.73-136.9 (m, C-Ar), 130.6 (C-Ar), 128.8 (C-Ar), 124.1 (C-Ar), 45.9 (CH_2-O, Et_2O), 8.7 (CH_3, Et_2O) ppm. $^{31}P\{^{1}H\}$ NMR (202.45 MHz, $CDCl_3$): δ 23.3 (s) ppm.

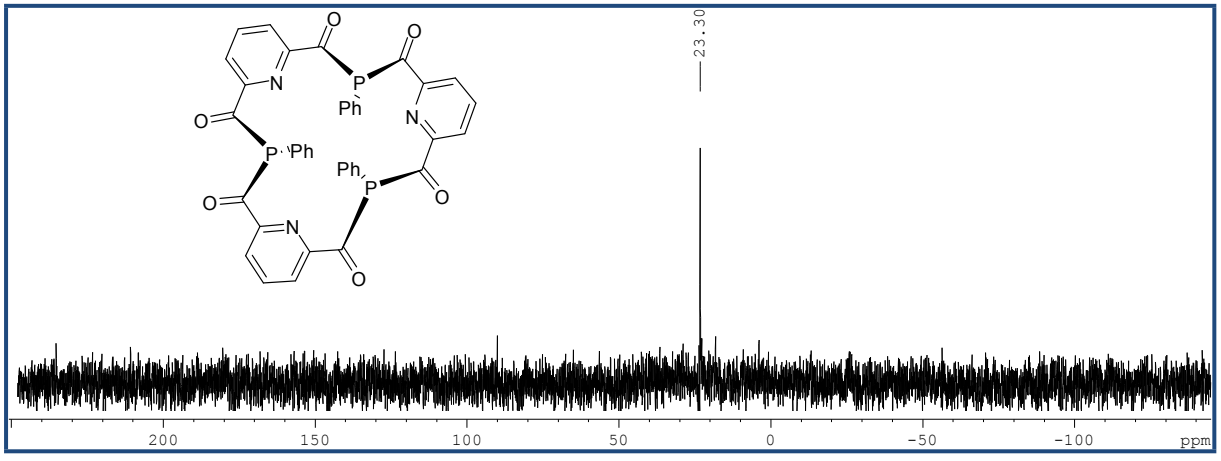


Fig. S1-a. $^{31}P\{^{1}H\}$ NMR spectrum of **1** in $CDCl_3$

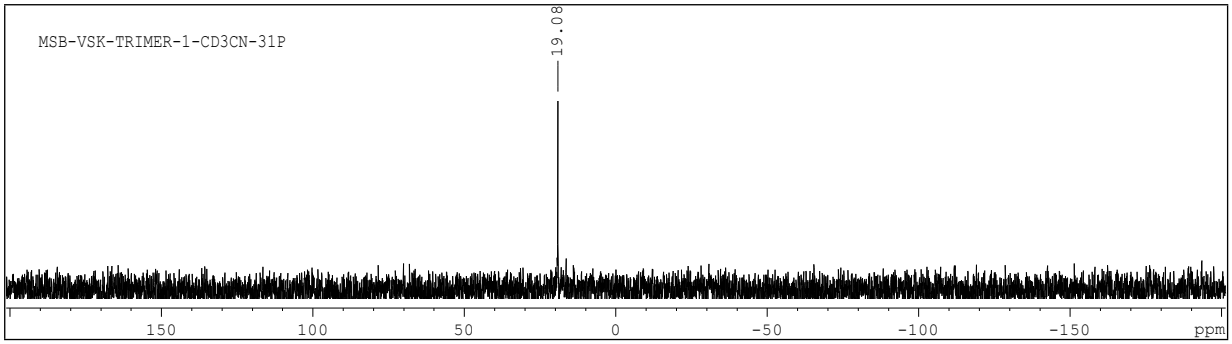


Fig. S1-a'. $^{31}P\{^{1}H\}$ NMR spectrum of **1** in CD_3CN

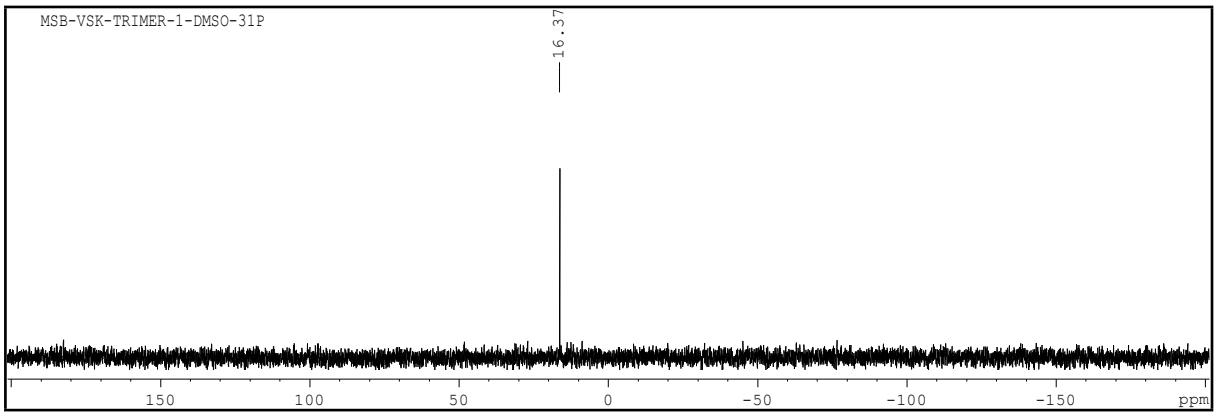


Fig. S1-a". $^{31}P\{^{1}H\}$ NMR spectrum of **1** in DMSO(d_6)

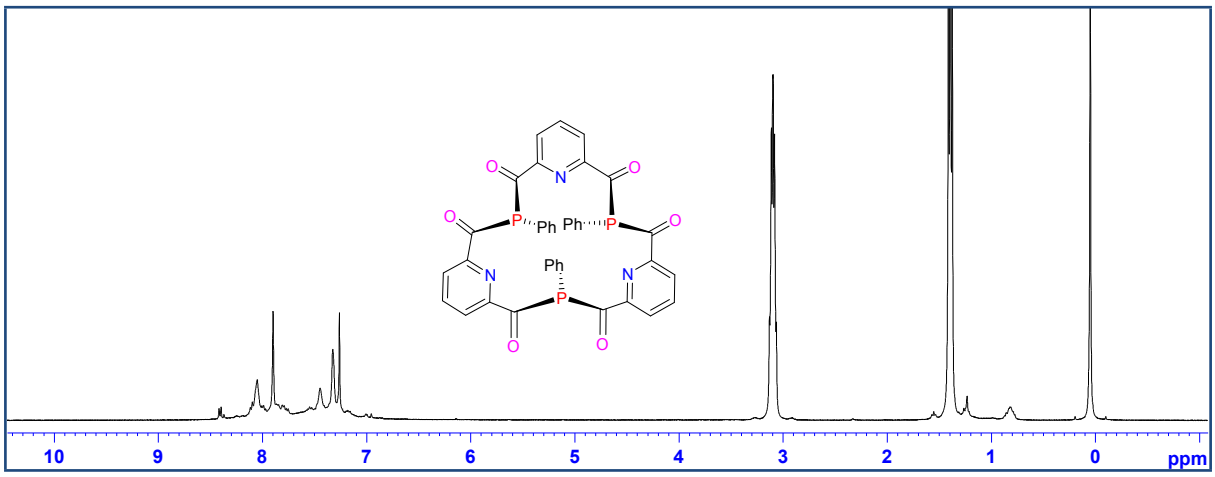


Fig. S1-b. ^{1}H NMR spectrum of **1**

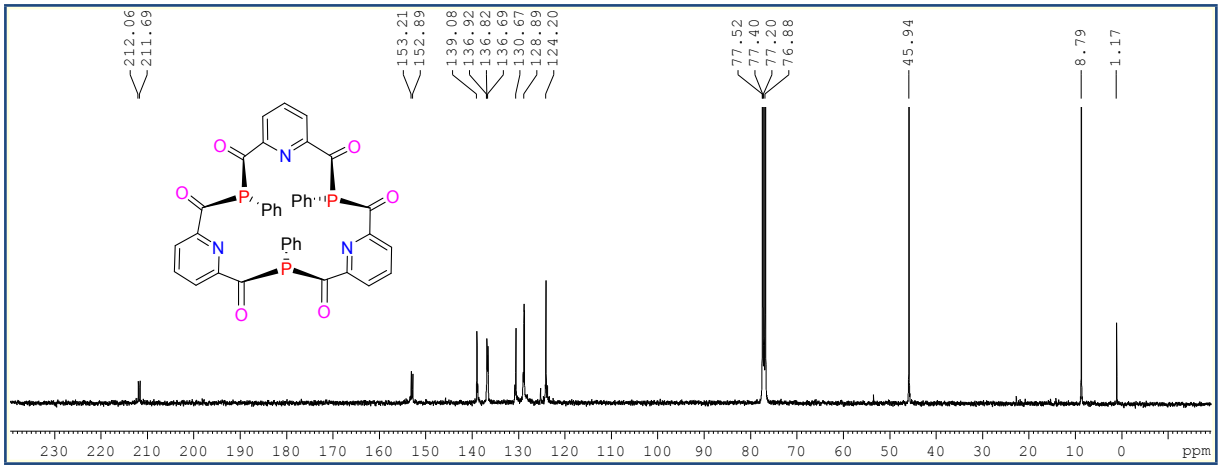


Fig. S1-c. $^{13}C\{^{1}H\}$ NMR spectrum of **1**

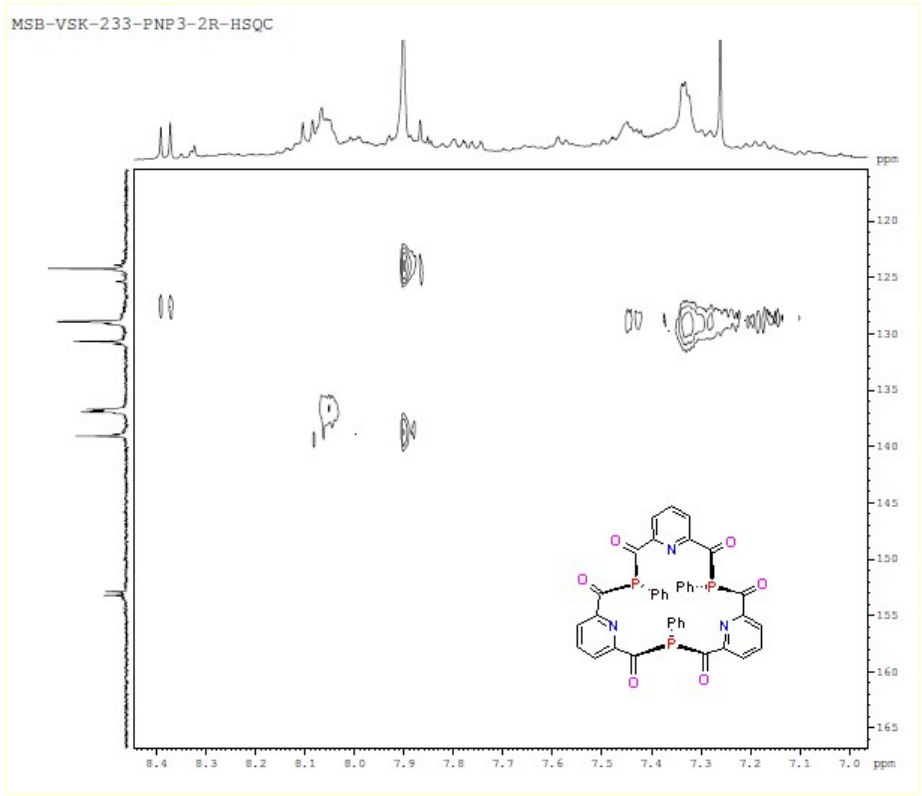


Fig. S1-d. 2D-HSQC NMR spectrum of **1**

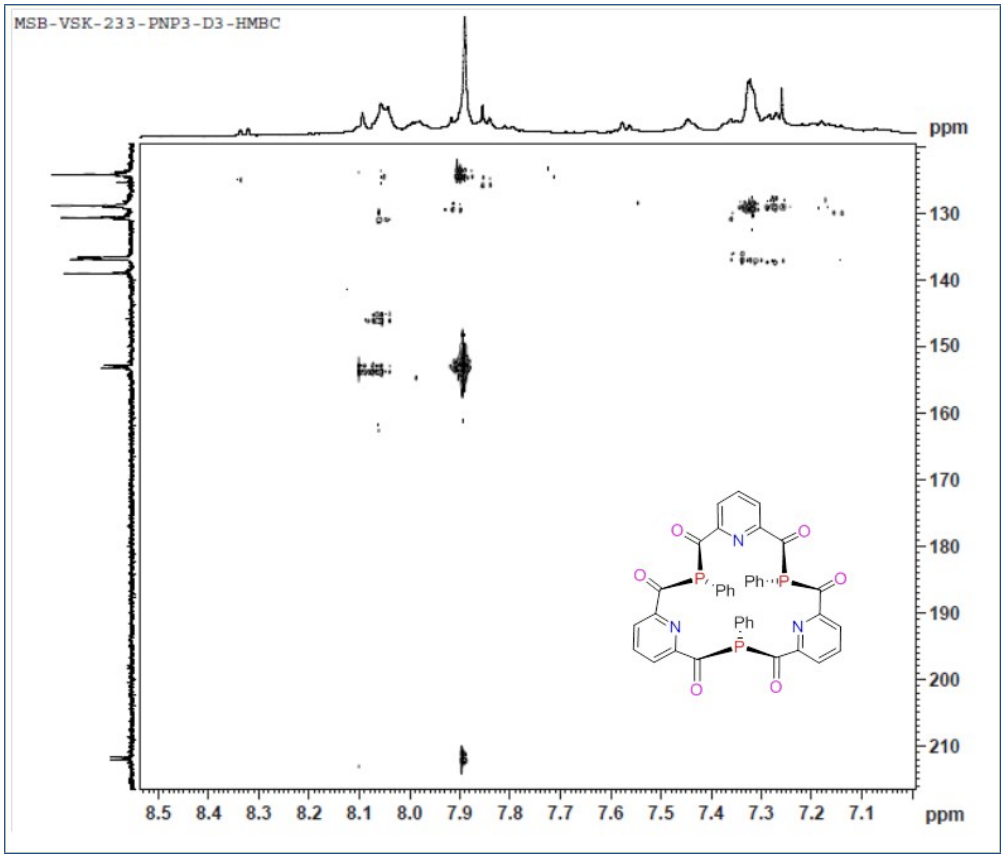


Fig. S1-e. 2D-HMBC NMR spectrum of **1**

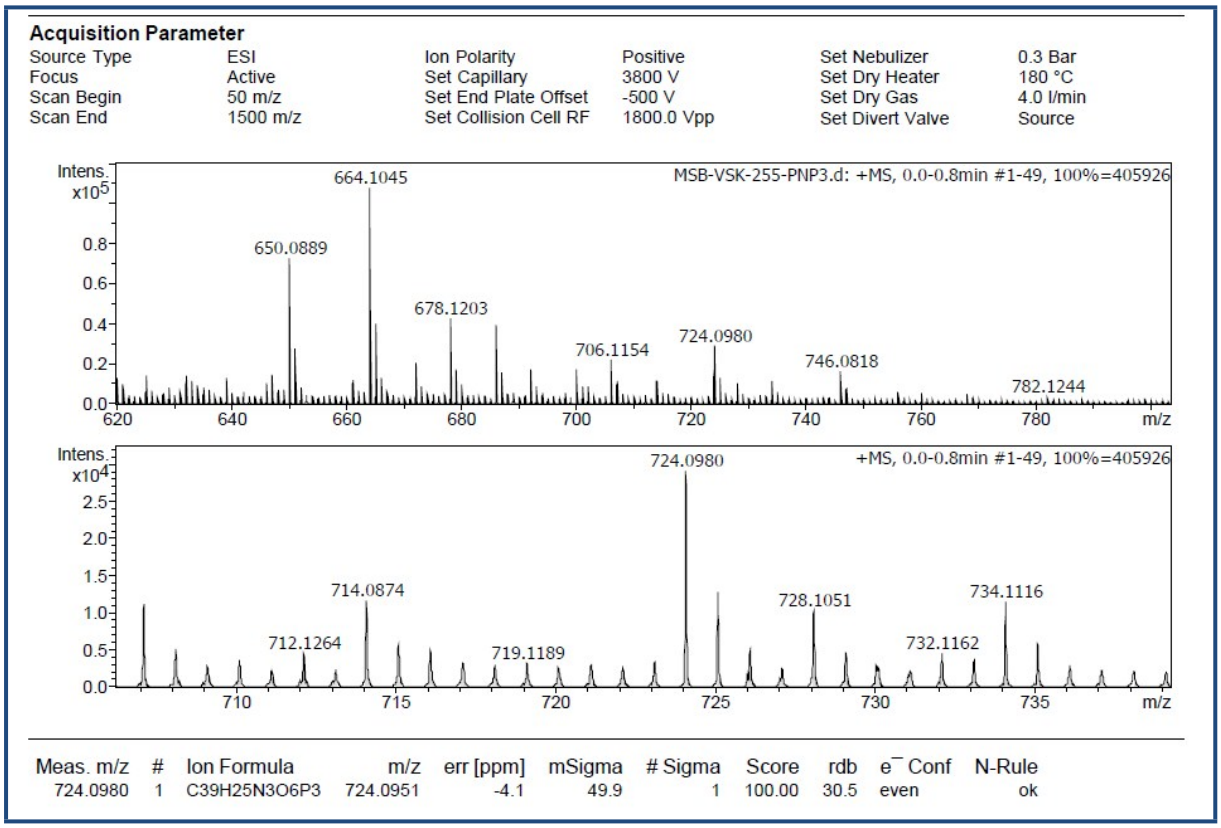


Fig. S1-f. MS (ESI) of **1**

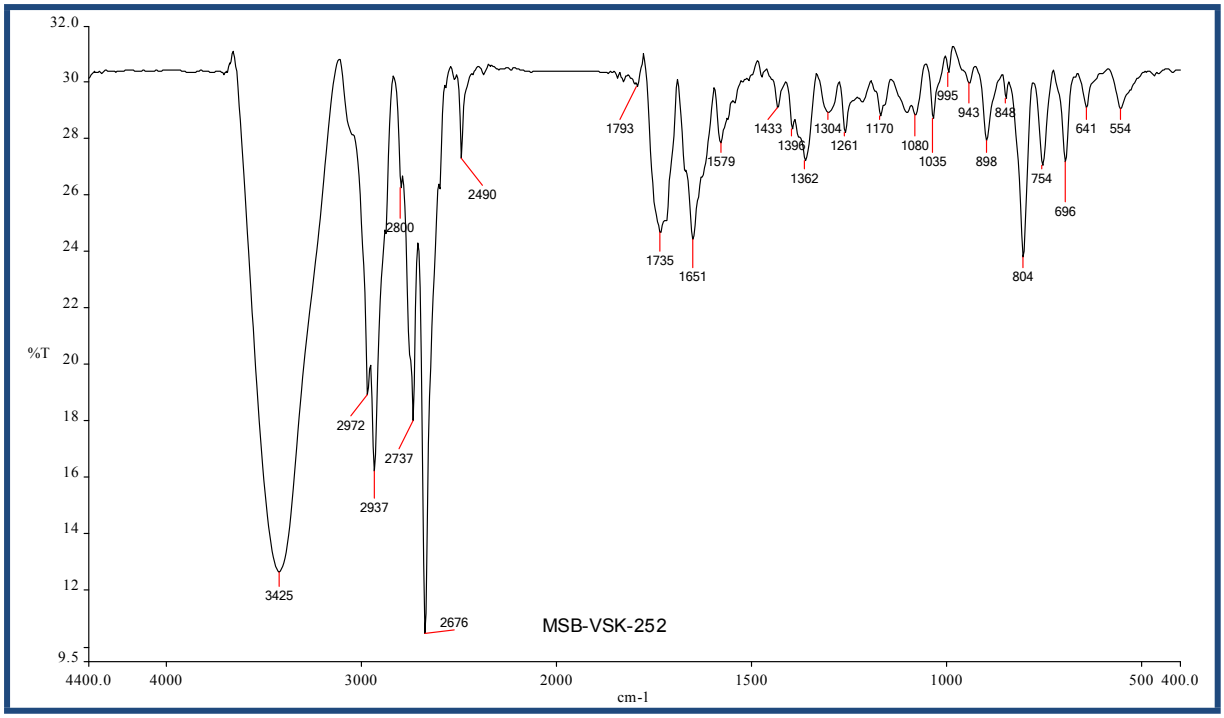


Fig. S1-g. FT-IR spectrum of **1**.

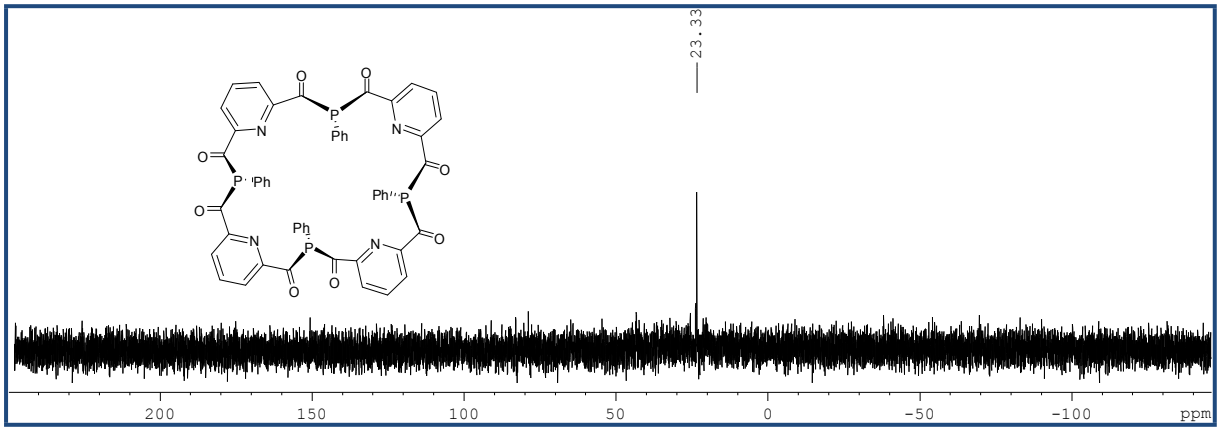


Fig. S2-a. $^{31}P\{^{1}H\}$ NMR spectrum of **2** in $CDCl_3$

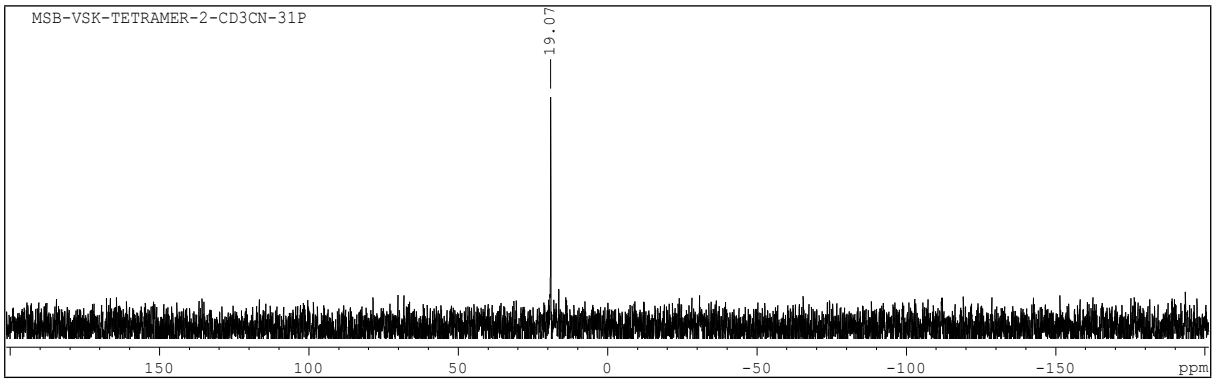


Fig. S2-a'. $^{31}P\{^{1}H\}$ NMR spectrum of **2** in CD_3CN

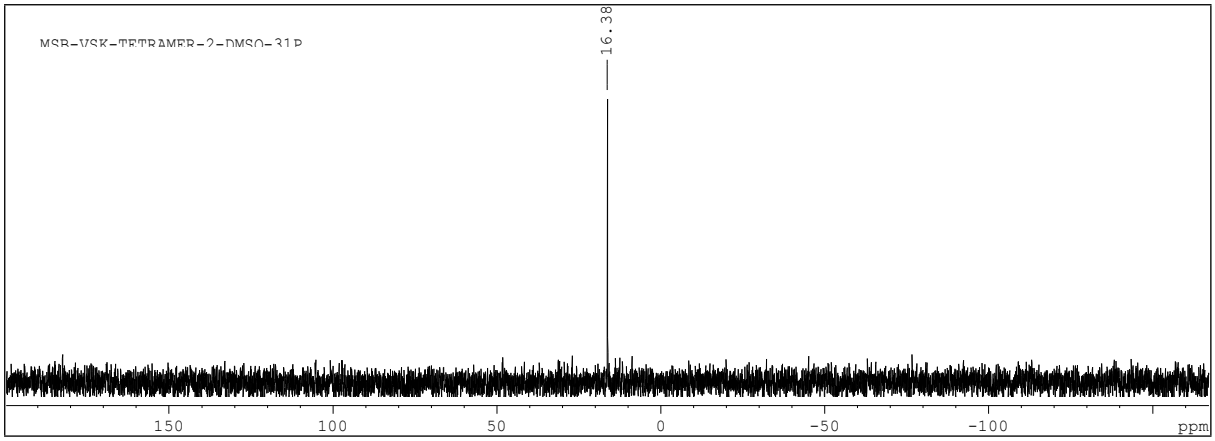


Fig. S2-a". $^{31}P\{^{1}H\}$ NMR spectrum of **2** in DMSO(d_6)

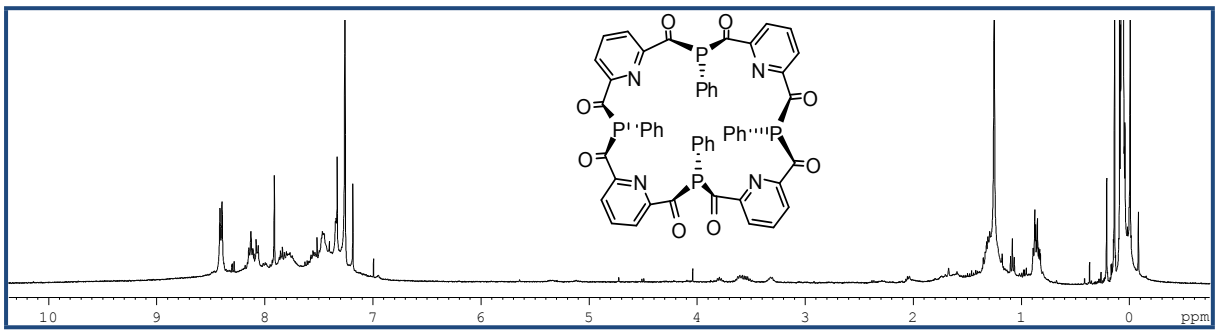


Fig. S2-b. ^{1}H NMR spectrum of **2**

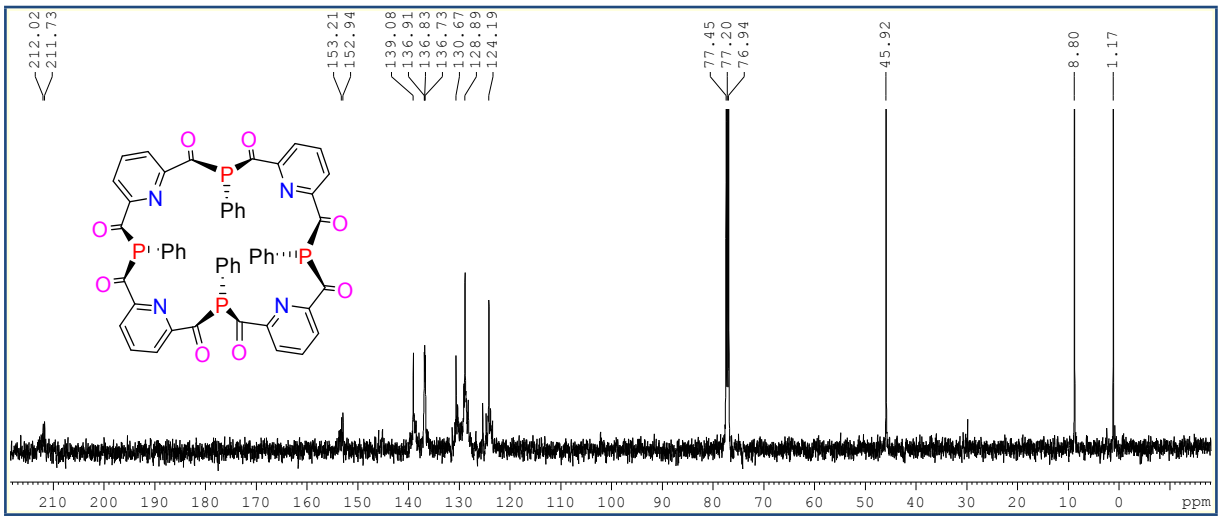


Fig. S2-c. $^{13}C\{^{1}H\}$ NMR spectrum of **2**

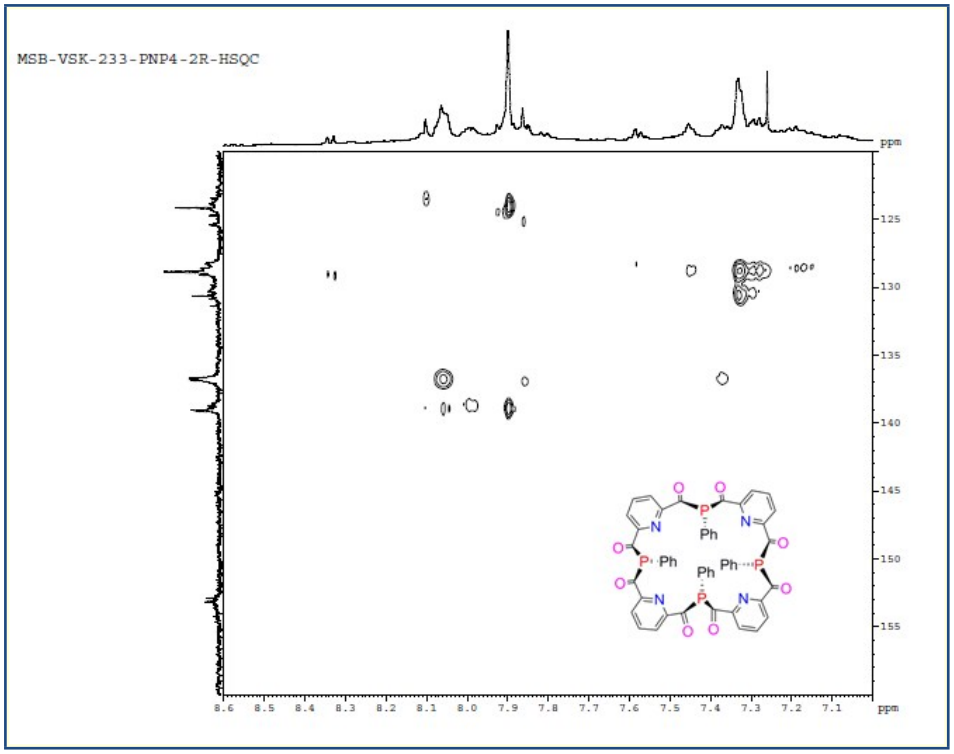


Fig. S2-d. 2D-HSQC NMR spectrum of **2**

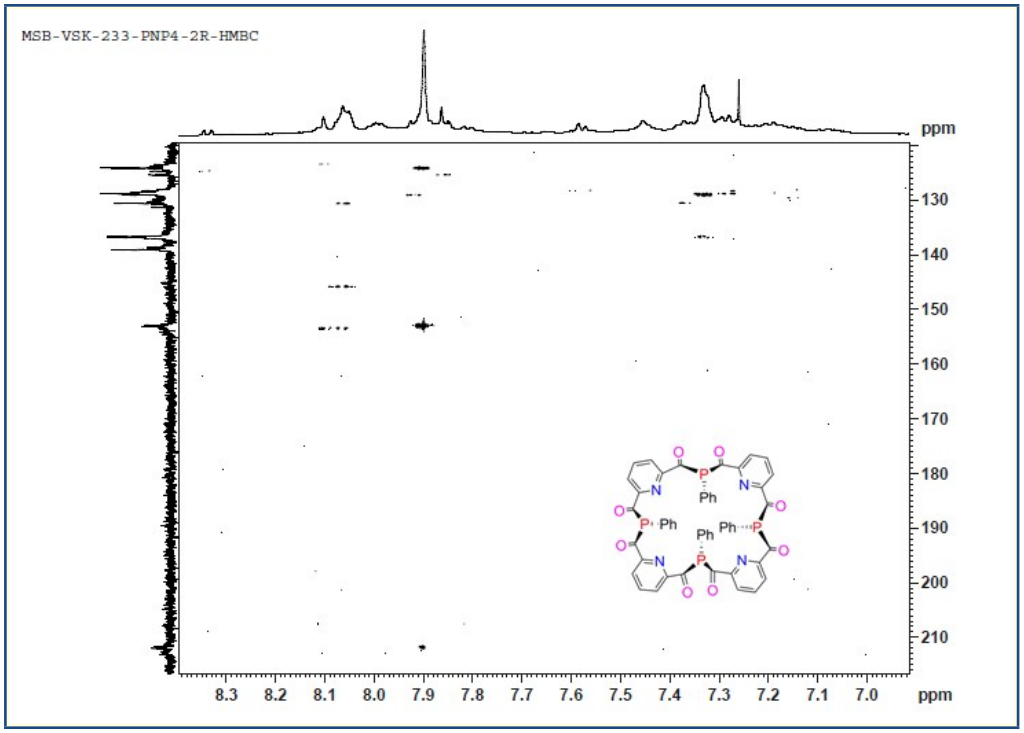


Fig. S2-e. 2D-HMBC NMR spectrum of **2**

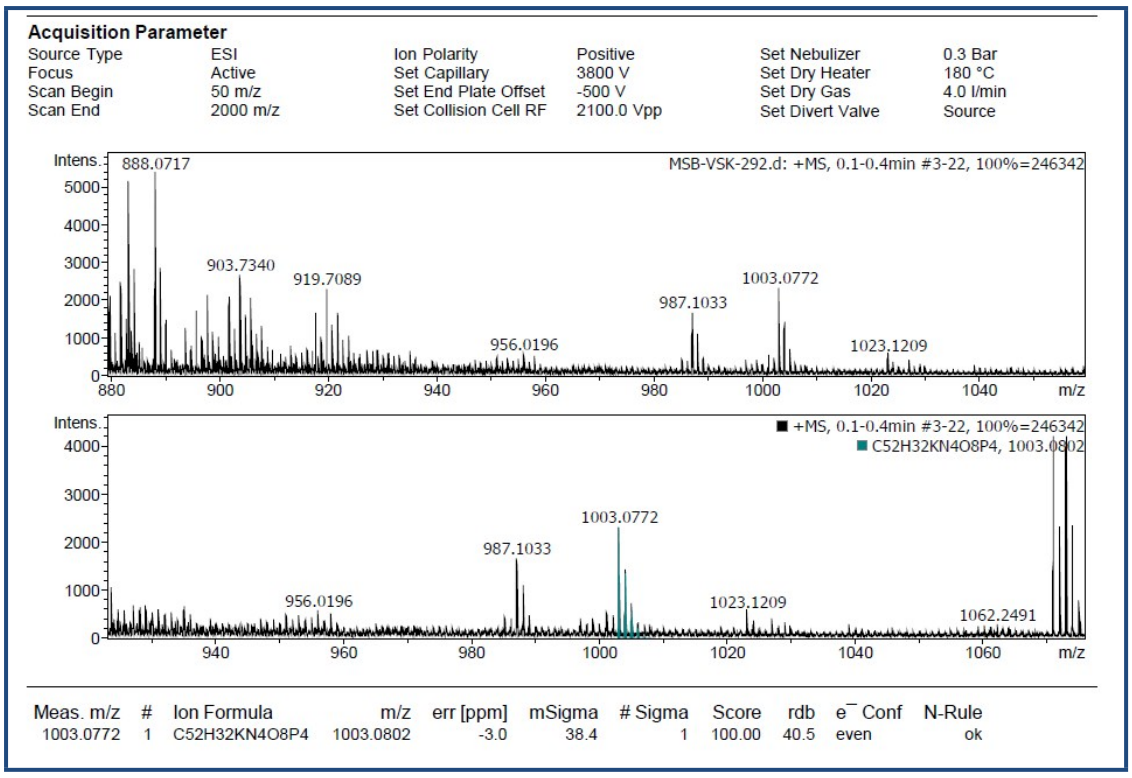


Fig. S2-f. MS (ESI) of **2**

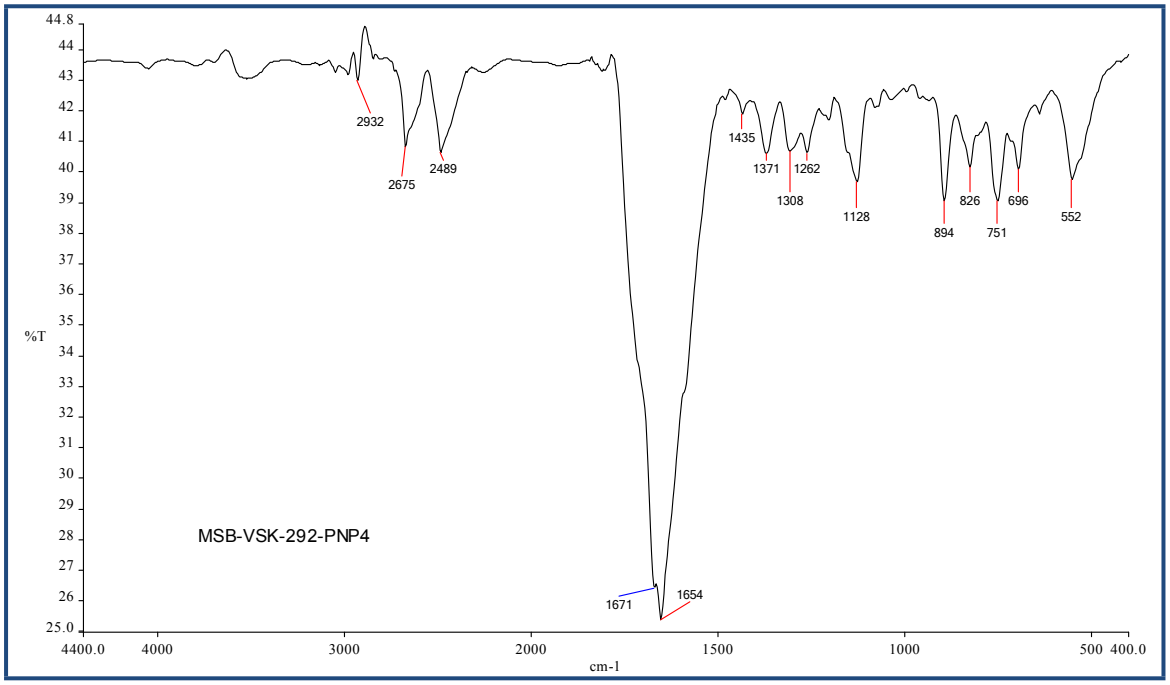


Fig. S2-g. FT-IR spectrum of **2**.

Synthesis of $[Pd_4(\mu\text{-}Cl)_4(\eta^3\text{-}C_3H_5)_2\{PdClP(Ph)C(O)C_5H_3N(C(O)PPh\text{-}\kappa\text{-}P,P,N\}_2]$ (3)

To a solution of **1** (0.010 g, 0.014 mmol) in dichloromethane (5 mL) was added a solution of $[Pd(\eta^3C_3H_5)Cl]_2$ (0.0075 g, 0.020 mmol) in the same solvent (5 mL) at room temperature and

the reaction mixture was stirred for 6 h. The reaction mixture was concentrated to a small bulk, 1 mL of petroleum ether was added and stored at room temperature to obtain X-ray quality crystals of **3** as brick red needles. Yield: 35% (0.004 g). Mp: 186-188 °C (dec). Anal. Calcd. for $C_{44}H_{36}Cl_6N_2O_4P_4Pd_6$: C, 32.38; H, 2.22; N, 1.72. Found: C, 32.45; H, 2.19; N, 1.65. MS (ESI): *m/z* Calc for $C_{44}H_{36}N_2O_4P_4Pd_6Cl_6$ (M-Cl): 1596.4294, Found: 1596.6993. FT- IR (KBr disc) cm^{-1}: $\upsilon_{C=O}$: 1653 s, $\upsilon_{C=C}$: 1460 m. ^1H NMR (500 MHz, DMSO-d_6): δ 8.31-7.39 (br, m, 26H, Ar), 5.75 (quintet, J = 9.75 Hz, 2H, $CH{=}CH_2$), 3.06 (d, J = 9.75 Hz, 8H) ppm. $^{31}P\{^1H\}$ NMR (202 MHz, DMSO-d_6): δ 12.6 (s) ppm.

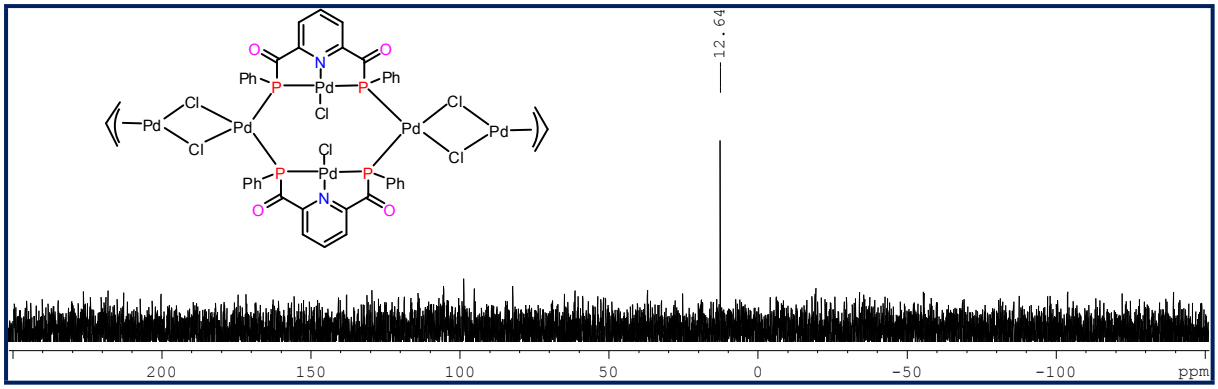


Fig. S3-a. $^{31}P\{^1H\}$ NMR spectrum of **3**

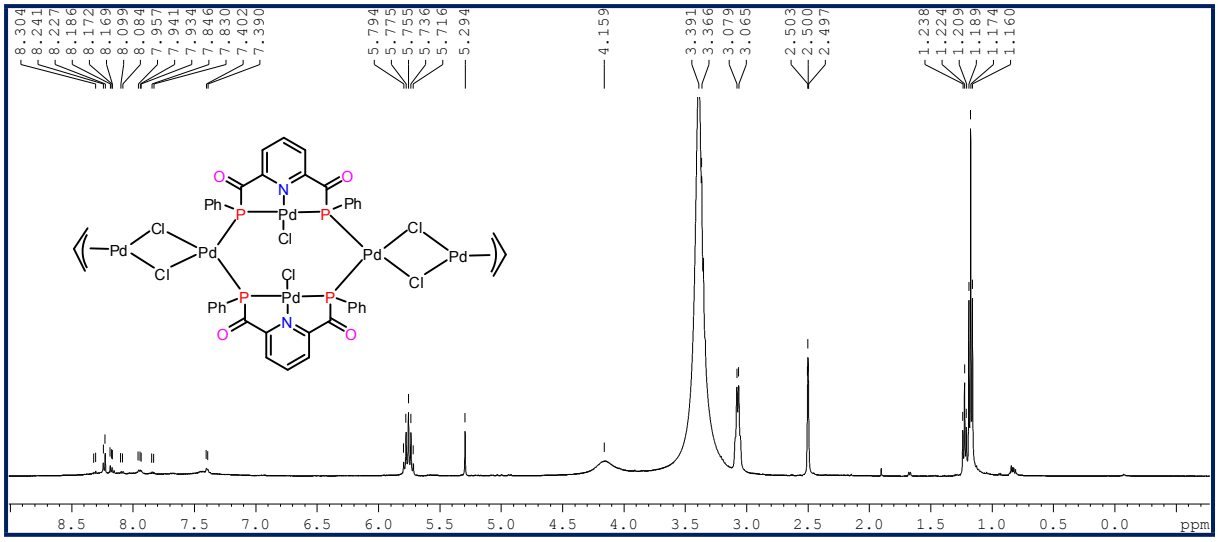


Fig. S3-b. ^1H NMR spectrum of **3**

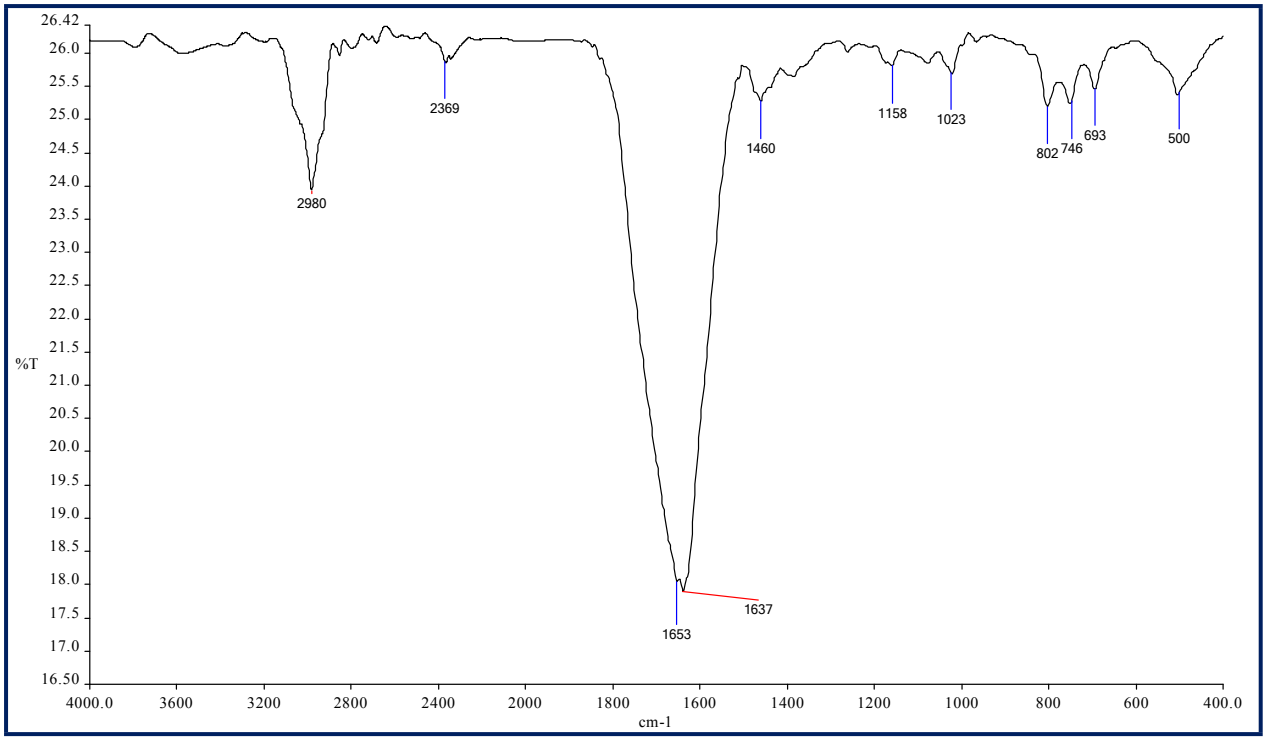


Fig. S3-c. FT-IR spectrum of **3**

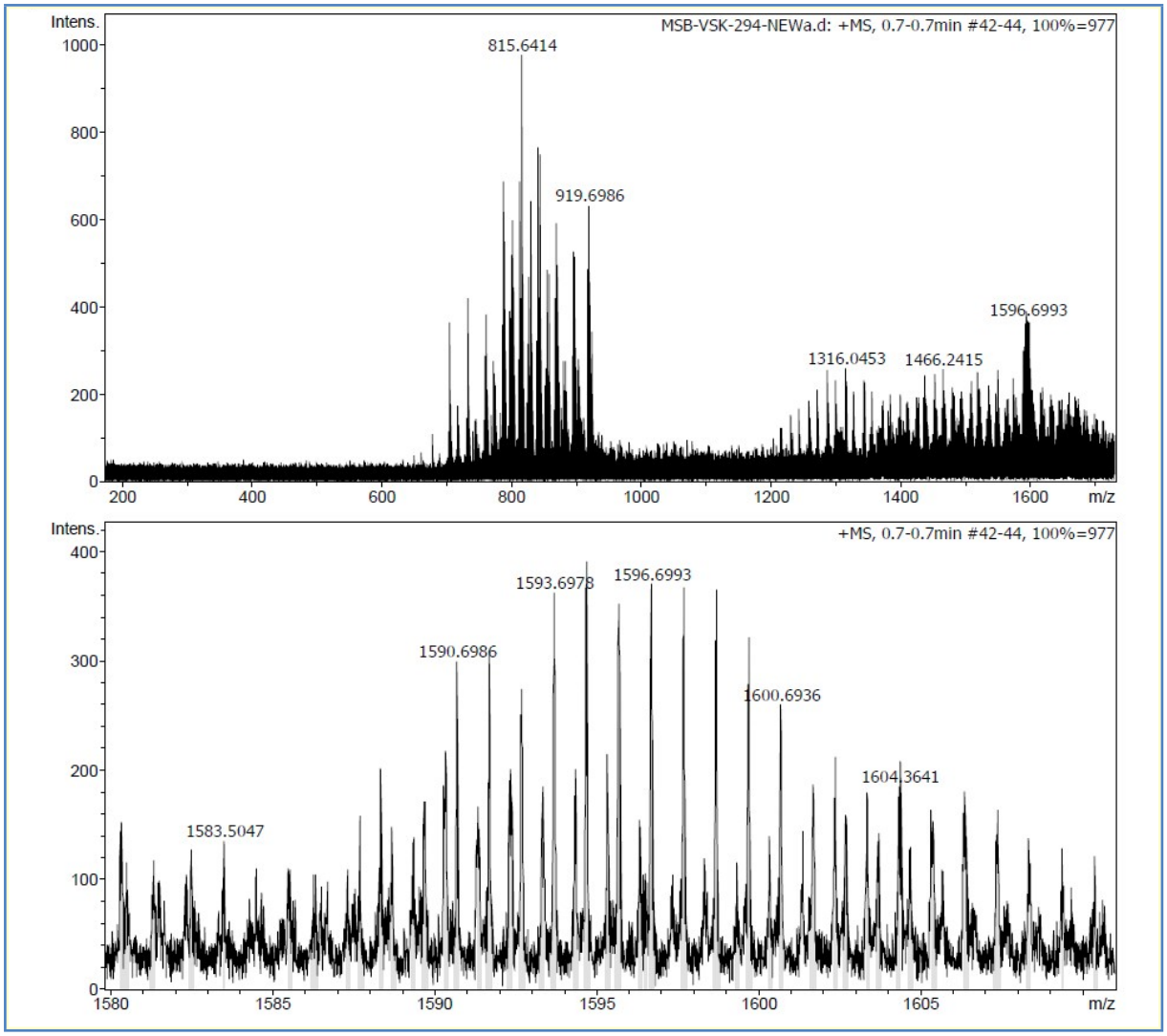


Fig. S3-d. MS (ESI) of **3**

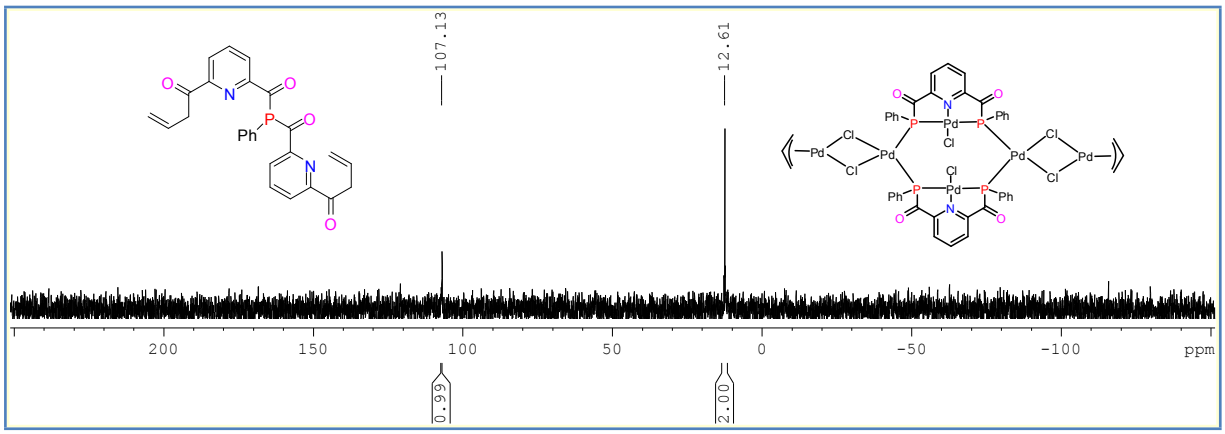


Fig. S4-a. $^{31}P\{^{1}H\}$ NMR spectrum of **3** and **4** (NMR tube reaction showed formation of **3** and **4**)

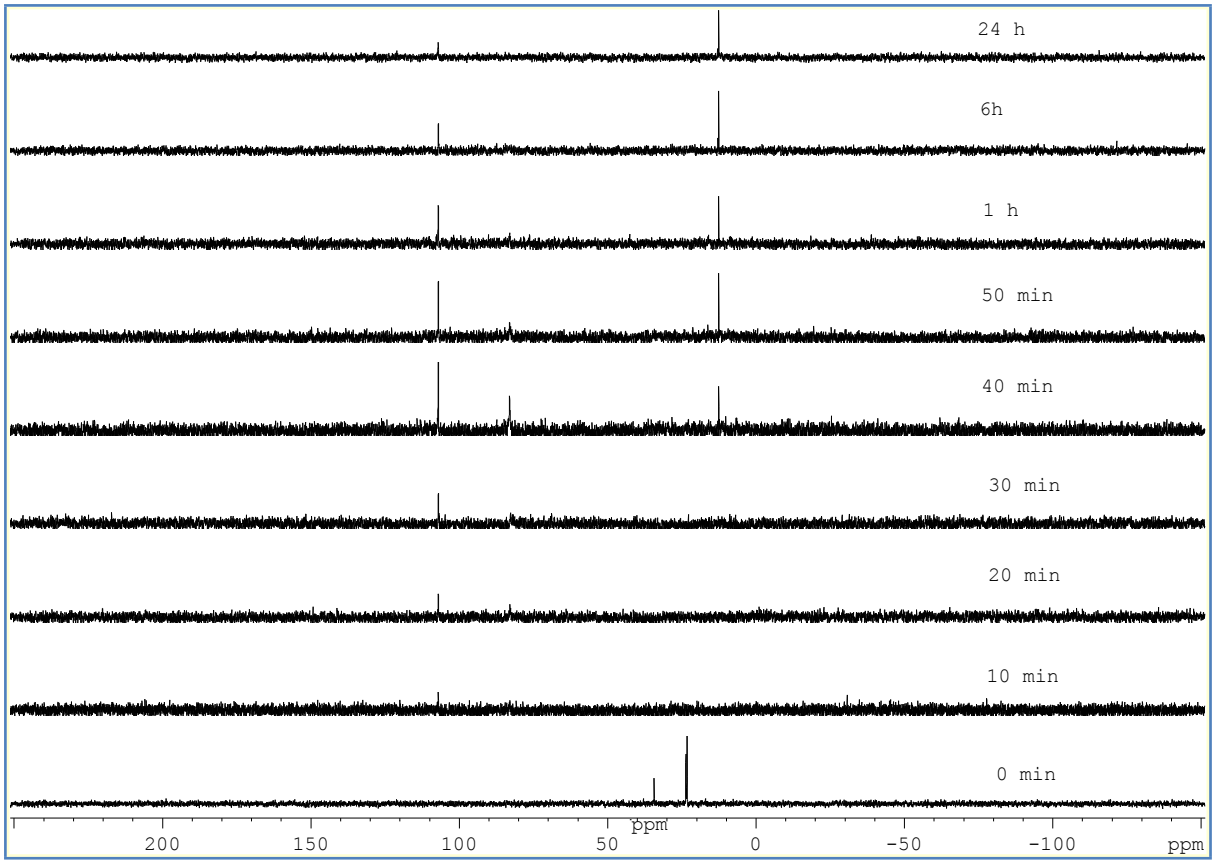


Fig. S4-b. Time-dependent $^{31}P\{^{1}H\}$ spectrum of reaction mixture containing **3** and **4** (NMR tube reaction showed formation of **3** and **4**)

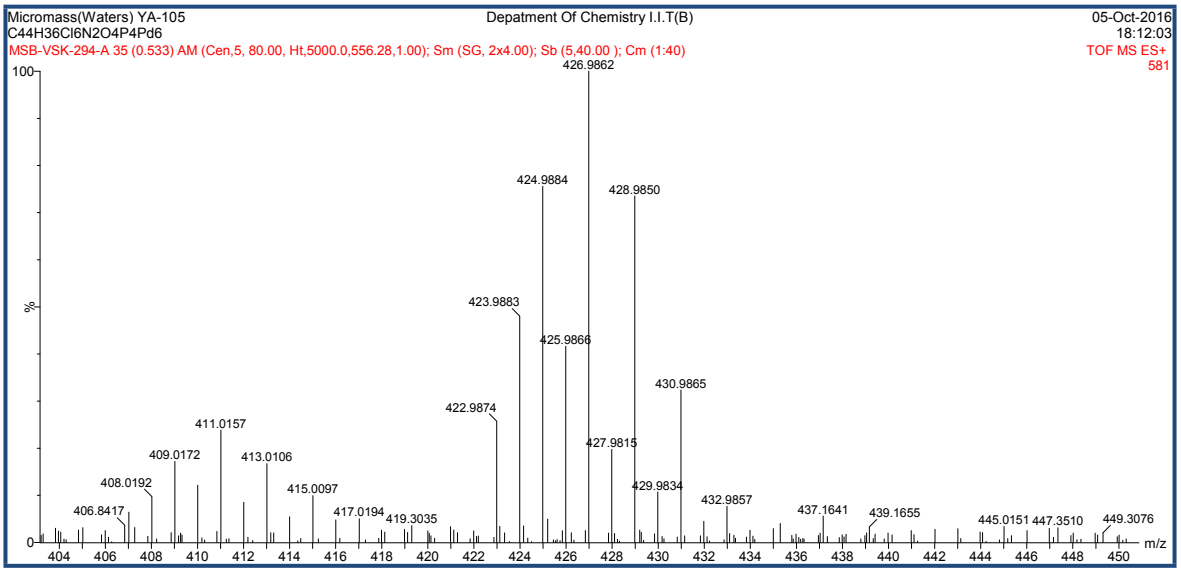


Fig. S4-c. MS (ESI) for fragmented compound **4** observed in the spectrum of reaction mixture, *m*/*z* Calc. for $C_{26}H_{21}N_2O_4P$ (M-CH_2CH): 429.1004, Found: 428.9850.

(S2) X-ray Crystallography

The structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre for compounds **1**, **2** and **3**. A crystal of each of the compound in the present work suitable for single-crystal X-ray diffraction study was mounted in a cryoloop with a drop of paratone oil and placed in the cold nitrogen stream of the kryoflex attachment of the Rigaku Saturn 724+ (4×4 bin mode) CCD diffractometer for compound **1**, **2** and **3**. Data were collected at 100 K using graphite-monochromated Mo Kα radiation (λα = 0.71073 Å) with the ω-scan technique. The data were reduced by using Crystal Clear-SMExpert 2.1 b24 software. Crystal data and summary of data collection for compounds **1**, **2** and **3** are given in Table S1. The structures were solved by direct methods and refined by least-squares against F2 utilizing the software packages SHELXL-97/2013[3], SIR-92[4] and WINGX[5]. All non-hydrogen atoms were refined anisotropically.

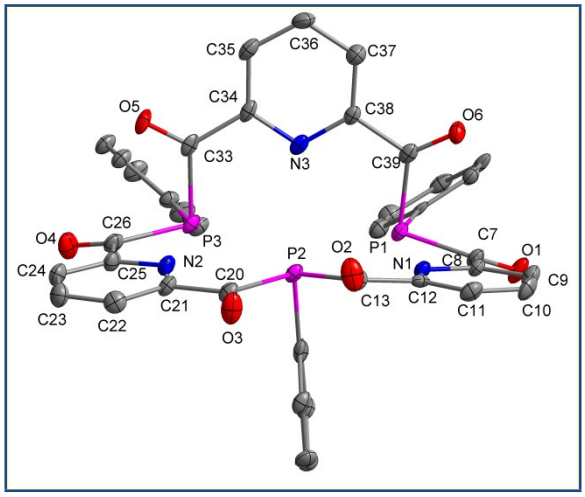


Fig. S5. Crystal structure of compound **1**. All hydrogen atoms and solvent molecule have been omitted for clarity. Thermal ellipsoids are drawn at the 50% probability level. Selected bond distances (Å) and bond angles (deg): P1–C19 = 1.879(3), P1–C46 = 1.888(3), C19–P1–C46 = 92.64(11).

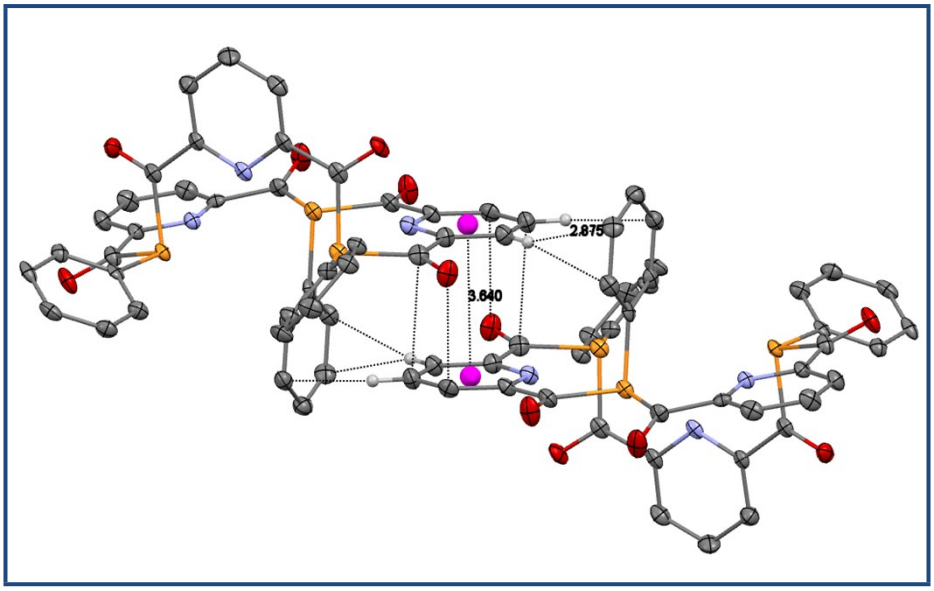


Fig. S6. Crystal structure of compound **1** showing π–π interactions in dimeric structure between two pyridine rings (N2C21C22C23C24C25) and CH–π interactions between pyridine and phenyl rings.

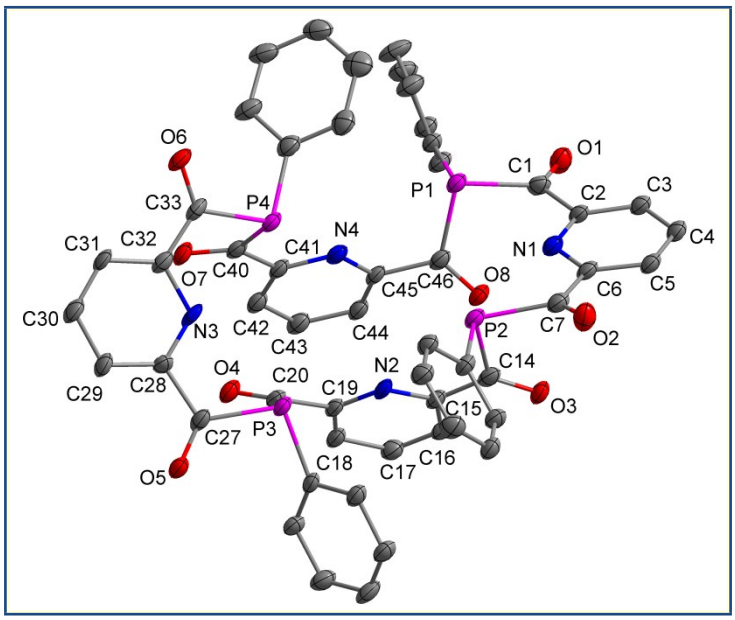


Fig. S7. Crystal structure of **2**. All hydrogen atoms and solvent molecule have been omitted for clarity. Thermal ellipsoids are drawn at the 50% probability level. Selected bond distances (Å) and bond angles (deg): P3 -C27= 1.888(6), P4-C33 = 1.912(6), O6-C33 = 1.233(7), C32-C33-P4 = 116.4(4), N3-C32-C33= 116.9(5), O6-C33-C32 = 122.3(5), O6-C33-P4 = 121.1(5).

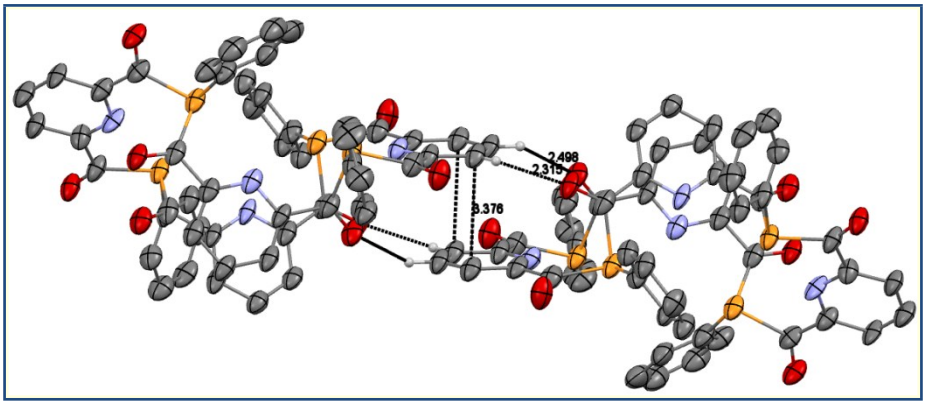


Fig. S8. Crystal structure of **2** showing one dimensional expansion due to partial π–π interactions between two pyridine rings and also showing hydrogen bonding between O–H of pyridine rings.

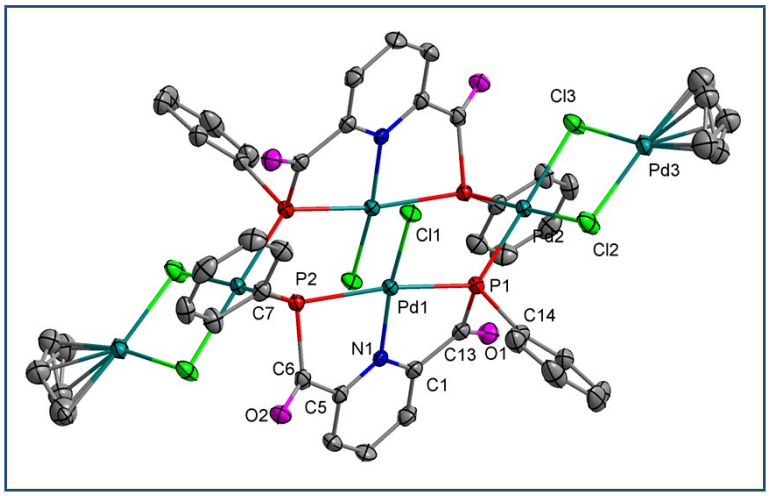


Fig. S9. Crystal structure of complex **3**. All hydrogen atoms and solvent molecule have been omitted for clarity. Thermal ellipsoids are drawn at the 50% probability level. Selected bond distances (Å) and bond angles (deg): Pd1-N1 = 2.056(3), Pd1-P1 = 2.2835(9), Pd1-Cl1 = 2.2930(9), Pd1-P2 = 2.3451(9), Pd2-P1 = 2.2448(9), Pd2-P2 = 2.2881(9), N1-Pd1-P1 = 84.63(8), N1-Pd1-Cl1 = 172.49(8), P1-Pd1-Cl1 = 91.36(3), N1-Pd1-P2 = 82.94(8), P1-Pd1-P2 = 166.74(3), Cl1-Pd1-P2 = 101.49(3).

Table S1. Crystallographic data for compounds **1**, **2** and **3**.

Compound	**1**	**2**	**3**
Emp. formula	$C_{39}H_{24}N_3O_6P_3{\cdot}CH_2Cl_2$	$C_{52}H_{32}N_4O_8P_4{\cdot}(CH_3CH_2)_2O$	$C_{44}H_{36}Cl_6N_2O_4P_4Pd_6$
fw	808.45	1038.81	1631.73
Crystal system	Triclinic	Monoclinic	Triclinic
space group	P -1	P 21/c	P -1
a, Å	8.8960(5)	12.9200(3)	10.0974(2)
b, Å	13.1019(6)	19.0391(8)	10.1677(3)
c, Å	16.2731(7)	20.9881(6)	13.9117(3)
α, deg	93.834(4)	90	102.789(2)
β, deg	96.273(4)	97.725(2)	95.8839(19)
γ, deg	106.767(5)	90	113.851(2)
V, Å^3	1795.52(16)	5115.9(3)	1244.01(6)
Z	2	4	1
$D_{calc,}$ g cm^{-3}	1.495	1.349	2.178
μ (MoKα), mm^{-1}	0.369	1.877	2.618
F (000)	828.0	2152.0	784.0
T (K)	100	100	150
2θ range, deg	1.959 - 24.999	3.1250 - 72.6190	4.576-49.996
Total no. reflns	6317	9815	4353
No.of indep reflns	5463	6159	4043
S	1.029	1.099	1.061
R_1[a]	0.0480	0.0819	0.0252
wR_2[b]	0.1273	0.2652	0.0646

([a]$R = \Sigma||F_o|-|Fc||/\Sigma|F_o|$. [b]$wR_2 = \{[\Sigma w(F_o^2-F_c^2)/\Sigma w(F_o^2)^2]\}^{1/2}$; $w = 1/[\sigma^2(F_o^2)+(xP)^2]$ where $P = (F_o^2+2F_c^2)/3$).

Table S2. Bond lengths (Å) and bond angles (deg) for **1**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl2	C40	1.748(3)	C23	H23	0.9500
Cl1	C40	1.774(3)	C23	C22	1.399(3)
P3	C26	1.879(2)	C23	C24	1.373(3)
P3	C27	1.830(2)	C15	H15	0.9500
P3	C33	1.888(2)	C15	C14	1.387(3)
P2	C14	1.840(2)	C15	C16	1.392(3)
P2	C13	1.890(2)	C38	C37	1.397(3)
P2	C20	1.876(2)	C29	H29	0.9500
P1	C39	1.894(2)	C29	C28	1.377(3)
P1	C1	1.830(2)	C29	C30	1.400(3)
P1	C7	1.890(3)	C37	H37	0.9500
O1	C7	1.212(3)	C37	C36	1.381(3)
O5	C33	1.217(3)	C14	C19	1.404(3)
O6	C39	1.213(3)	C3	H3	0.9500
O4	C26	1.213(3)	C3	C2	1.380(3)
O2	C13	1.208(3)	C3	C4	1.389(3)
O3	C20	1.206(3)	C21	C20	1.510(3)
N2	C25	1.344(3)	C21	C22	1.387(3)
N2	C21	1.334(3)	C27	C28	1.396(3)
N3	C34	1.345(3)	C27	C32	1.399(3)
N3	C38	1.346(3)	C10	H10	0.9500
N1	C12	1.338(3)	C10	C11	1.386(3)
N1	C8	1.342(3)	C10	C9	1.391(3)
C39	C38	1.496(3)	C28	H28	0.9500
C25	C26	1.491(3)	C19	H19	0.9500
C25	C24	1.397(3)	C19	C18	1.388(3)
C1	C6	1.401(3)	C13	C12	1.510(3)
C1	C2	1.403(3)	C11	H11	0.9500
C31	H31	0.9500	C11	C12	1.391(3)
C31	C32	1.378(3)	C9	H9	0.9500
C31	C30	1.381(3)	C9	C8	1.389(3)
C34	C35	1.390(3)	C7	C8	1.496(3)
C34	C33	1.496(3)	C5	H5	0.9500
C4	H4	0.9500	C35	H35	0.9500
C16	H16	0.9500	C35	C36	1.376(3)
C16	C17	1.389(3)	C6	H6	0.9500
C40	H40a	0.9900	C18	H18	0.9500
C40	H40b	0.9900	C18	C17	1.374(4)
C17	H17	0.9500	C2	H2	0.9500
C24	H24	0.9500	C22	H22	0.9500
C5	C6	1.385(3)	C36	H36	0.9500
C5	C4	1.387(3)	C30	H30	0.9500
C32	H32	0.9500			

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C27	P3	C26	101.21(10)	C16	C15	C14	120.5(2)
C33	P3	C26	92.64(10)	C39	C38	N3	116.7(2)
C33	P3	C27	96.46(10)	C37	C38	N3	123.2(2)
C13	P2	C14	97.33(10)	C37	C38	C39	120.0(2)
C20	P2	C14	100.49(10)	C30	C29	C28	120.4(2)
C20	P2	C13	99.32(11)	C36	C37	C38	118.8(2)
C1	P1	C39	96.30(10)	C15	C14	P2	119.66(18)
C7	P1	C39	92.17(10)	C19	C14	P2	121.13(18)
C7	P1	C1	98.27(10)	C19	C14	C15	119.2(2)
C21	N2	C25	118.19(19)	C4	C3	C2	120.4(2)
C38	N3	C34	116.59(19)	C20	C21	N2	115.57(19)
C8	N1	C12	117.1(2)	C22	C21	N2	123.5(2)
O6	C39	P1	122.39(18)	C22	C21	C20	120.8(2)
C38	C39	P1	117.69(16)	C28	C27	P3	125.89(18)
C38	C39	O6	119.9(2)	C32	C27	P3	115.71(17)
C26	C25	N2	115.22(19)	C32	C27	C28	118.4(2)
C24	C25	N2	122.1(2)	C9	C10	C11	118.8(2)
C24	C25	C26	122.7(2)	C27	C28	C29	120.6(2)
C6	C1	P1	117.31(17)	C18	C19	C14	119.9(2)
C2	C1	P1	123.77(17)	O2	C13	P2	126.35(18)
C2	C1	C6	118.7(2)	C12	C13	P2	113.84(17)
C30	C31	C32	120.7(2)	C12	C13	O2	119.8(2)
O4	C26	P3	124.29(18)	C12	C11	C10	118.9(2)
C25	C26	P3	113.86(16)	C13	C12	N1	116.8(2)
C25	C26	O4	121.6(2)	C11	C12	N1	123.2(2)
C35	C34	N3	123.5(2)	C11	C12	C13	120.0(2)
C33	C34	N3	116.4(2)	C8	C9	C10	118.1(2)
C33	C34	C35	120.1(2)	O1	C7	P1	123.92(19)
C24	C23	C22	119.3(2)	C8	C7	P1	114.29(16)
C3	C2	C1	120.4(2)	C8	C7	O1	121.5(2)
O5	C33	P3	122.60(17)	C4	C5	C6	120.4(2)
C34	C33	P3	117.04(17)	C27	C32	C31	120.8(2)
C34	C33	O5	120.4(2)	C9	C8	N1	123.9(2)
C21	C22	C23	117.8(2)	C7	C8	N1	115.7(2)
C35	C36	C37	118.8(2)	C7	C8	C9	120.4(2)
C29	C30	C31	119.0(2)	C36	C35	C34	119.0(2)
C5	C4	C3	119.7(2)	C5	C6	C1	120.3(2)
C17	C16	C15	119.6(2)	O3	C20	P2	124.81(18)
Cl1	C40	Cl2	111.71(15)	C21	C20	P2	114.39(16)
C16	C17	C18	120.5(2)	C21	C20	O3	120.2(2)
C23	C24	C25	119.0(2)	C17	C18	C19	120.3(2)

Table S3. Bond lengths (Å) and bond angles (deg) for **2**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P4	C13	1.886(5)	N4	C8	1.337(5)
P4	C20	1.894(5)	N3	C21	1.335(5)
P4	C14	1.816(4)	N3	C25	1.335(6)
P2	C39	1.889(4)	N2	C34	1.332(5)
P2	C46	1.875(5)	N2	C38	1.344(5)
P2	C40	1.834(4)	O9	C54	1.416(6)
P3	C27	1.843(4)	O9	C55	1.431(7)
P3	C26	1.874(5)	C47	C46	1.497(5)
P3	C33	1.886(4)	C47	C48	1.399(7)
P1	C52	1.876(5)	C39	C38	1.492(6)
P1	C7	1.885(4)	C11	C12	1.391(6)
P1	C1	1.832(4)	C11	C10	1.377(6)
O7	C20	1.214(5)	C22	C23	1.377(7)
O3	C46	1.222(5)	C22	C21	1.380(6)
O2	C52	1.215(4)	C52	C51	1.491(6)
O6	C26	1.199(5)	C13	C12	1.496(6)
O4	C39	1.219(5)	C9	C8	1.401(6)
O5	C33	1.203(5)	C9	C10	1.379(6)
O1	C7	1.207(5)	C34	C35	1.380(5)
O8	C13	1.216(5)	C34	C33	1.510(5)
N1	C47	1.332(5)	C7	C8	1.497(6)
N1	C51	1.337(5)	C23	C24	1.390(5)
N4	C12	1.335(5)	C32	C27	1.380(6)
C32	C31	1.396(6)	C2	C3	1.376(6)
C1	C2	1.399(7)	C37	C36	1.375(6)
C1	C6	1.366(6)	C50	C49	1.383(6)
C21	C20	1.488(6)	C17	C18	1.391(6)
C25	C24	1.396(7)	C17	C16	1.386(6)
C25	C26	1.512(5)	C41	C42	1.383(7)
C38	C37	1.389(6)	C48	C49	1.393(6)
C28	C27	1.382(7)	C15	C16	1.377(6)
C28	C29	1.391(5)	C30	C31	1.361(7)
C35	C36	1.379(6)	C3	C4	1.380(6)
C29	C30	1.384(7)	C43	C42	1.366(8)
C14	C19	1.395(5)	C43	C44	1.378(8)
C14	C15	1.391(6)	C4	C5	1.365(8)
C19	C18	1.383(6)	C6	C5	1.390(7)
C40	C41	1.405(6)	C44	C45	1.399(7)
C40	C45	1.374(7)	C54	C53	1.483(9)
C51	C50	1.381(7)	C56	C55	1.491(8)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C13	P4	C20	92.6(2)	O4	C39	P2	122.6(3)
C14	P4	C13	96.8(2)	O4	C39	C38	120.6(4)
C14	P4	C20	100.53(19)	C38	C39	P2	116.5(3)
C46	P2	C39	93.98(19)	C10	C11	C12	118.3(4)
C40	P2	C39	99.35(18)	C23	C22	C21	118.4(4)
C40	P2	C46	99.4(2)	O2	C52	P1	123.2(3)
C27	P3	C26	95.03(19)	O2	C52	C51	120.9(4)
C27	P3	C33	100.88(18)	C51	C52	P1	115.8(3)
C26	P3	C33	94.7(2)	O8	C13	P4	123.3(3)
C52	P1	C7	95.65(18)	O8	C13	C12	120.2(4)
C1	P1	C52	98.3(2)	C12	C13	P4	116.4(3)
C1	P1	C7	97.24(19)	C10	C9	C8	118.4(4)
C47	N1	C51	117.5(4)	N2	C34	C35	123.3(3)
C12	N4	C8	116.6(4)	N2	C34	C33	115.2(3)
C25	N3	C21	116.5(4)	C35	C34	C33	121.5(4)
C34	N2	C38	117.4(3)	O1	C7	P1	123.1(3)
C54	O9	C55	113.8(4)	O1	C7	C8	120.1(4)
N1	C47	C46	117.5(4)	C8	C7	P1	116.4(3)
N1	C47	C48	123.3(4)	C22	C23	C24	118.9(4)
C48	C47	C46	119.2(4)	N4	C12	C11	124.1(4)
N4	C12	C13	116.0(4)	O6	C26	C25	121.5(4)
C11	C12	C13	119.9(4)	C25	C26	P3	112.8(3)
C27	C32	C31	120.0(5)	C11	C10	C9	119.1(4)
C2	C1	P1	124.3(3)	C41	C40	P2	122.4(4)
C6	C1	P1	117.3(4)	C45	C40	P2	118.4(3)
C6	C1	C2	118.2(4)	C45	C40	C41	119.2(4)
N3	C21	C22	124.4(4)	N1	C51	C52	118.2(4)
N3	C21	C20	115.5(4)	N1	C51	C50	123.3(4)
C22	C21	C20	120.1(4)	C50	C51	C52	118.5(4)
N4	C8	C9	123.5(4)	C3	C2	C1	121.3(4)
N4	C8	C7	117.3(4)	C36	C37	C38	118.7(4)
C9	C8	C7	119.3(4)	C51	C50	C49	119.2(4)
N3	C25	C24	123.7(4)	C16	C17	C18	118.8(4)
N3	C25	C26	116.3(4)	C42	C41	C40	119.7(5)
C24	C25	C26	119.8(4)	C49	C48	C47	118.2(4)
N2	C38	C39	115.4(3)	C37	C36	C35	118.9(4)
N2	C38	C37	122.8(4)	C16	C15	C14	120.9(4)
C37	C38	C39	121.8(3)	C19	C18	C17	120.1(4)
O7	C20	P4	122.2(4)	C31	C30	C29	120.2(4)
O7	C20	C21	121.5(4)	O5	C33	P3	124.5(3)
C21	C20	P4	116.2(3)	O5	C33	C34	122.0(4)
C27	C28	C29	120.4(4)	C34	C33	P3	113.3(3)
C32	C27	P3	116.1(4)	C50	C49	C48	118.3(5)
C32	C27	C28	119.4(4)	C2	C3	C4	119.3(5)

C28	C27	P3	124.4(3)	C15	C16	C17	121.0(4)
C36	C35	C34	118.9(4)	C42	C43	C44	120.2(5)
C30	C29	C28	119.6(5)	C43	C42	C41	120.8(5)
O3	C46	P2	122.7(3)	C30	C31	C32	120.4(5)
O3	C46	C47	120.6(4)	C5	C4	C3	120.2(4)
C47	C46	P2	116.6(3)	C1	C6	C5	120.8(5)
C23	C24	C25	118.0(4)	C43	C44	C45	119.8(5)
C19	C14	P4	124.8(3)	O9	C54	C53	110.1(5)
C15	C14	P4	117.1(3)	C40	C45	C44	120.3(5)
C15	C14	C19	117.9(4)	O9	C55	C56	113.4(5)
C18	C19	C14	121.2(4)	C4	C5	C6	120.2(4)
O6	C26	P3	125.7(3)				

Table S4. Bond lengths (Å) and bond angles (deg) for complex **3**

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Pd2	P1	2.2448(9)	N1	C1	1.350(5)
Pd2	P2[1]	2.2881(9)	C5	C4	1.376(5)
Pd2	Cl2	2.4108(10)	C5	C6	1.508(5)
Pd2	Cl3	2.4154(9)	C4	C3	1.381(6)
Pd1	N1	2.056(3)	C7	C12	1.388(5)
Pd1	P1	2.2835(9)	C7	C8	1.395(5)
Pd1	Cl1	2.2930(9)	C8	C9	1.384(5)
Pd1	P2	2.3451(9)	C2	C1	1.374(5)
Pd3	C20	2.055(15)	C2	C3	1.386(6)
Pd3	C22	2.095(10)	C9	C10	1.364(6)
Pd3	C21A	2.113(9)	C19	C14	1.385(6)
Pd3	C22A	2.137(11)	C19	C18	1.394(6)
Pd3	C20A	2.139(9)	C10	C11	1.381(6)
Pd3	C21	2.139(9)	C16	C17	1.355(7)
Pd3	Cl2	2.3849(10)	C16	C15	1.393(6)
Pd3	Cl3	2.3983(10)	C11	C12	1.390(6)
P2	C7	1.815(4)	C1	C13	1.501(5)
P2	C6	1.866(4)	C15	C14	1.393(5)
P2	Pd2[1]	2.2881(9)	C20	C21	1.260(17)
P1	C14	1.832(4)	C18	C17	1.371(7)
P1	C13	1.873(4)	C22	C21	1.030(13)
O1	C13	1.207(4)	C22A	C21A	1.299(14)
O2	C6	1.209(4)	C21A	C20A	1.469(13)
N1	C5	1.348(5)			

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
P1	Pd2	P2[1]	88.55(3)	C5	N1	C1	118.3(3)
P1	Pd2	Cl2	92.89(3)	C5	N1	Pd1	120.4(2)

P2[1]	Pd2	Cl2	178.56(3)	C1	N1	Pd1	121.3(2)
P1	Pd2	Cl3	175.69(3)	N1	C5	C4	122.4(3)
P2[1]	Pd2	Cl3	94.27(3)	N1	C5	C6	116.3(3)
Cl2	Pd2	Cl3	84.29(3)	C4	C5	C6	121.3(3)
N1	Pd1	P1	84.63(8)	C5	C4	C3	119.2(3)
N1	Pd1	Cl1	172.49(8)	C12	C7	C8	119.7(3)
P1	Pd1	Cl1	91.36(3)	C12	C7	P2	119.9(3)
N1	Pd1	P2	82.94(8)	C8	C7	P2	120.4(3)
P1	Pd1	P2	166.74(3)	C9	C8	C7	119.8(4)
Cl1	Pd1	P2	101.49(3)	C1	C2	C3	119.6(3)
C20	Pd3	C22	61.0(5)	C10	C9	C8	120.2(4)
C21A	Pd3	C22A	35.6(4)	C14	C19	C18	119.1(4)
C21A	Pd3	C20A	40.4(3)	C9	C10	C11	120.8(4)
C22A	Pd3	C20A	74.2(4)	C4	C3	C2	118.6(3)
C20	Pd3	C21	34.9(5)	C17	C16	C15	119.3(4)
C22	Pd3	C21	28.1(4)	C10	C11	C12	119.8(4)
C20	Pd3	Cl2	167.3(4)	C7	C12	C11	119.7(4)
C22	Pd3	Cl2	107.2(3)	N1	C1	C2	121.9(3)
C21A	Pd3	Cl2	136.5(2)	N1	C1	C13	117.0(3)
C22A	Pd3	Cl2	102.4(3)	C2	C1	C13	121.0(3)
C20A	Pd3	Cl2	176.4(3)	O1	C13	C1	122.1(3)
C21	Pd3	Cl2	134.4(2)	O1	C13	P1	124.4(3)
C20	Pd3	Cl3	106.9(4)	C1	C13	P1	113.3(2)
C22	Pd3	Cl3	167.0(3)	C16	C15	C14	119.8(4)
C21A	Pd3	Cl3	133.7(3)	O2	C6	C5	121.7(3)
C22A	Pd3	Cl3	166.6(3)	O2	C6	P2	127.2(3)
C20A	Pd3	Cl3	98.4(3)	C5	C6	P2	111.1(2)
C21	Pd3	Cl3	138.9(2)	C21	C20	Pd3	76.2(8)
Cl2	Pd3	Cl3	85.23(3)	C17	C18	C19	119.9(4)
Pd3	Cl3	Pd2	94.61(3)	C19	C14	C15	120.0(4)
C7	P2	C6	105.50(16)	C19	C14	P1	119.8(3)
C7	P2	Pd2[1]	110.48(12)	C15	C14	P1	119.9(3)
C6	P2	Pd2[1]	98.99(11)	C16	C17	C18	121.7(4)
C7	P2	Pd1	127.50(13)	C21	C22	Pd3	78.3(8)
C6	P2	Pd1	93.55(12)	C22	C21	C20	133.7(13)
Pd2[1]	P2	Pd1	114.15(4)	C22	C21	Pd3	73.5(7)
C14	P1	C13	96.57(16)	C20	C21	Pd3	68.9(8)
C14	P1	Pd2	108.93(12)	C21A	C22A	Pd3	71.2(6)
C13	P1	Pd2	115.97(12)	C22A	C21A	C20A	137.3(9)
C14	P1	Pd1	109.38(12)	C22A	C21A	Pd3	73.2(6)
C13	P1	Pd1	97.20(12)	C20A	C21A	Pd3	70.7(5)
Pd2	P1	Pd1	124.88(4)	C21A	C20A	Pd3	68.8(5)
Pd3	Cl2	Pd2	95.08(3)				

(S3) Computational Details

Density functional theory calculations were performed using the Gaussian 09 suite of quantum chemical programs.[6] Crystal structure geometries (coordinates) are considered as the starting point for the optimization and calculated all optimized geometries with frequency calculations using freq=noraman as keyword. The optimized molecular structures and determination of energies were calculated by using M062X/6-31G** level of theory. Molecular orbital analysis have been done to find the HOMO-LUMO energy gap using the iop(6/7=3) at M062X/6-31G** level of theory.[7] Graphical representations of the optimized geometries of compounds **I(a, b, c)−III(a, b, c), 1** and **2** were created by using CYLView.[8]

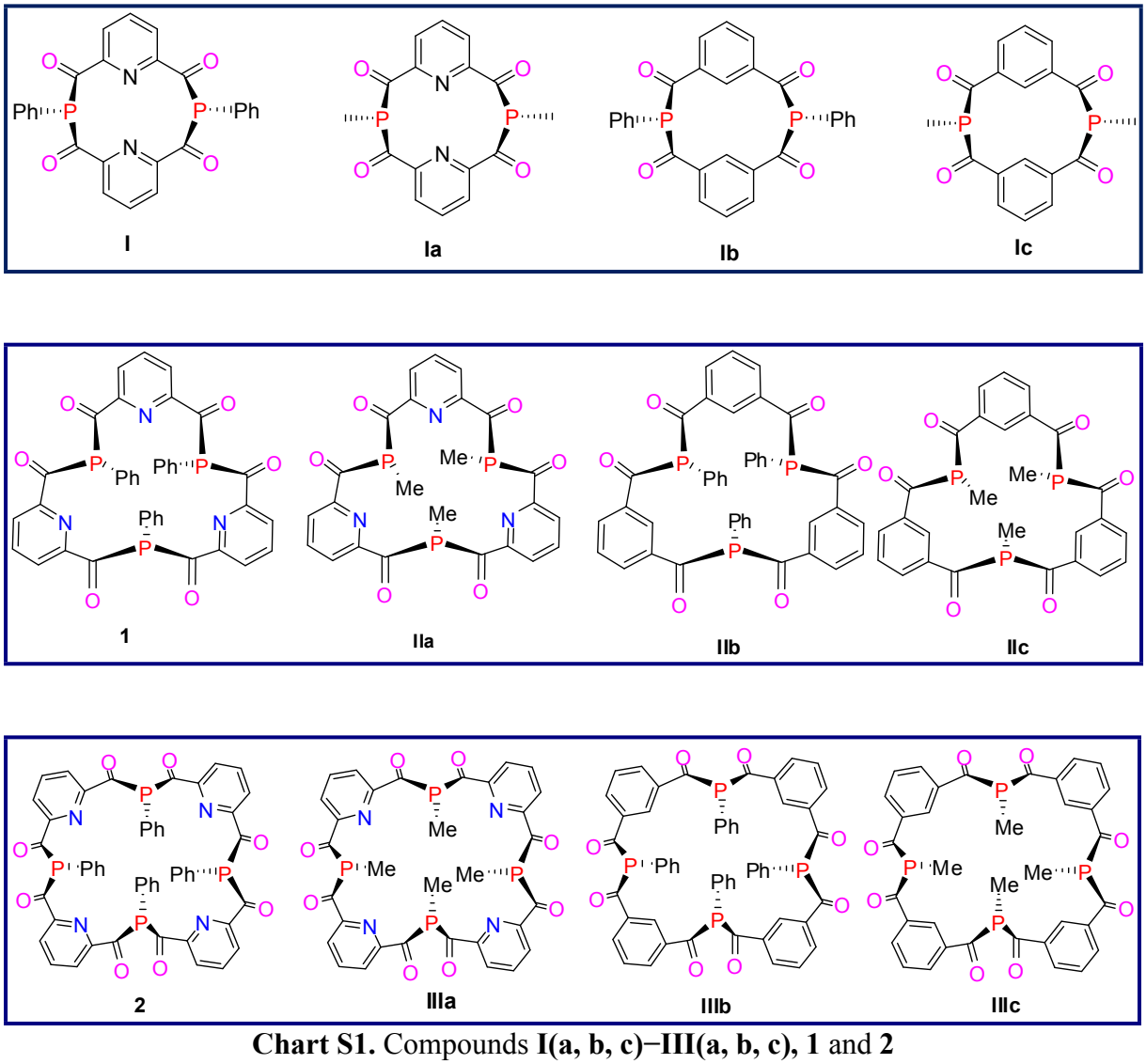
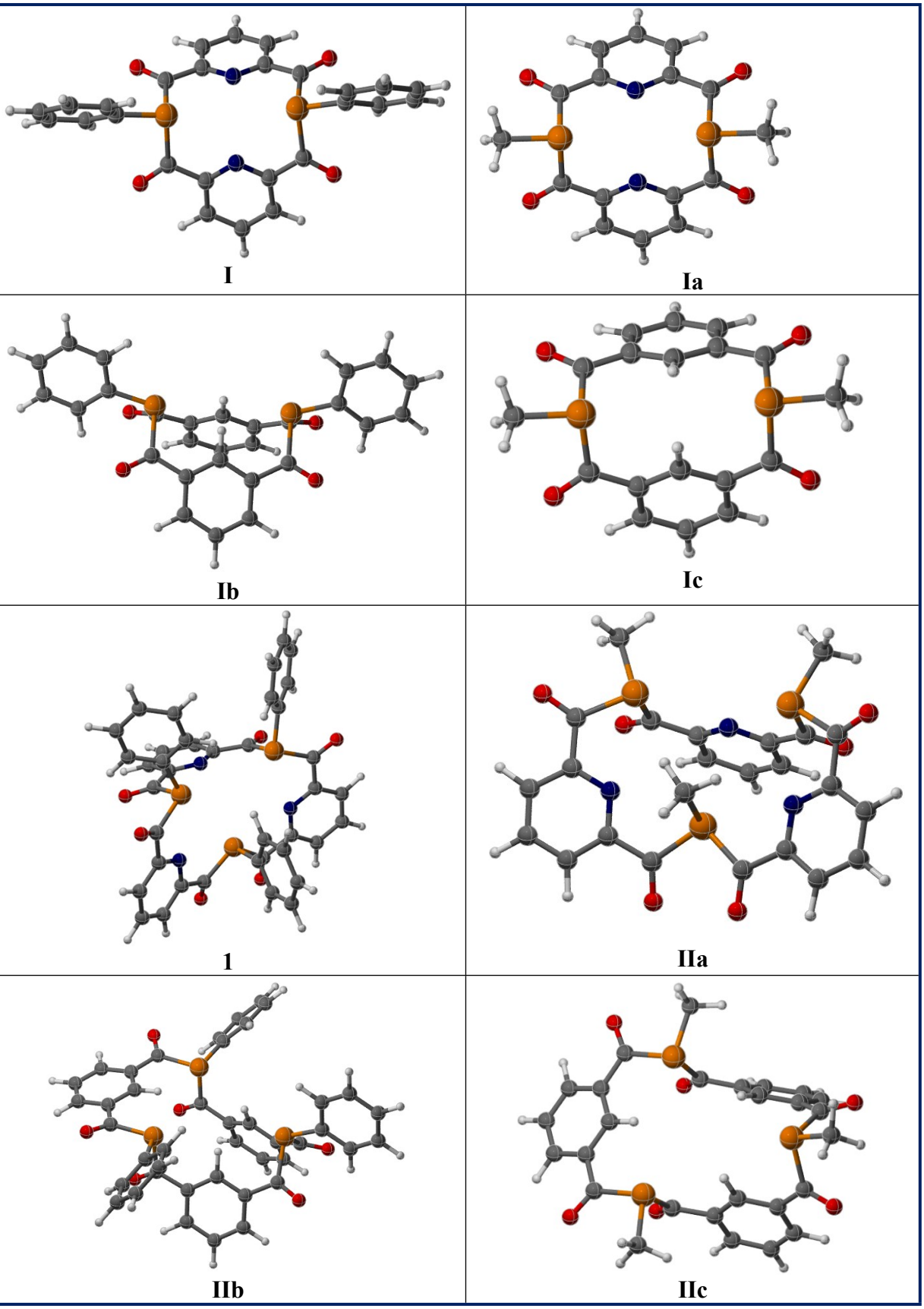


Chart S1. Compounds **I(a, b, c)−III(a, b, c), 1** and **2**


I
Ia
Ib
Ic
1
IIa
IIb
IIc

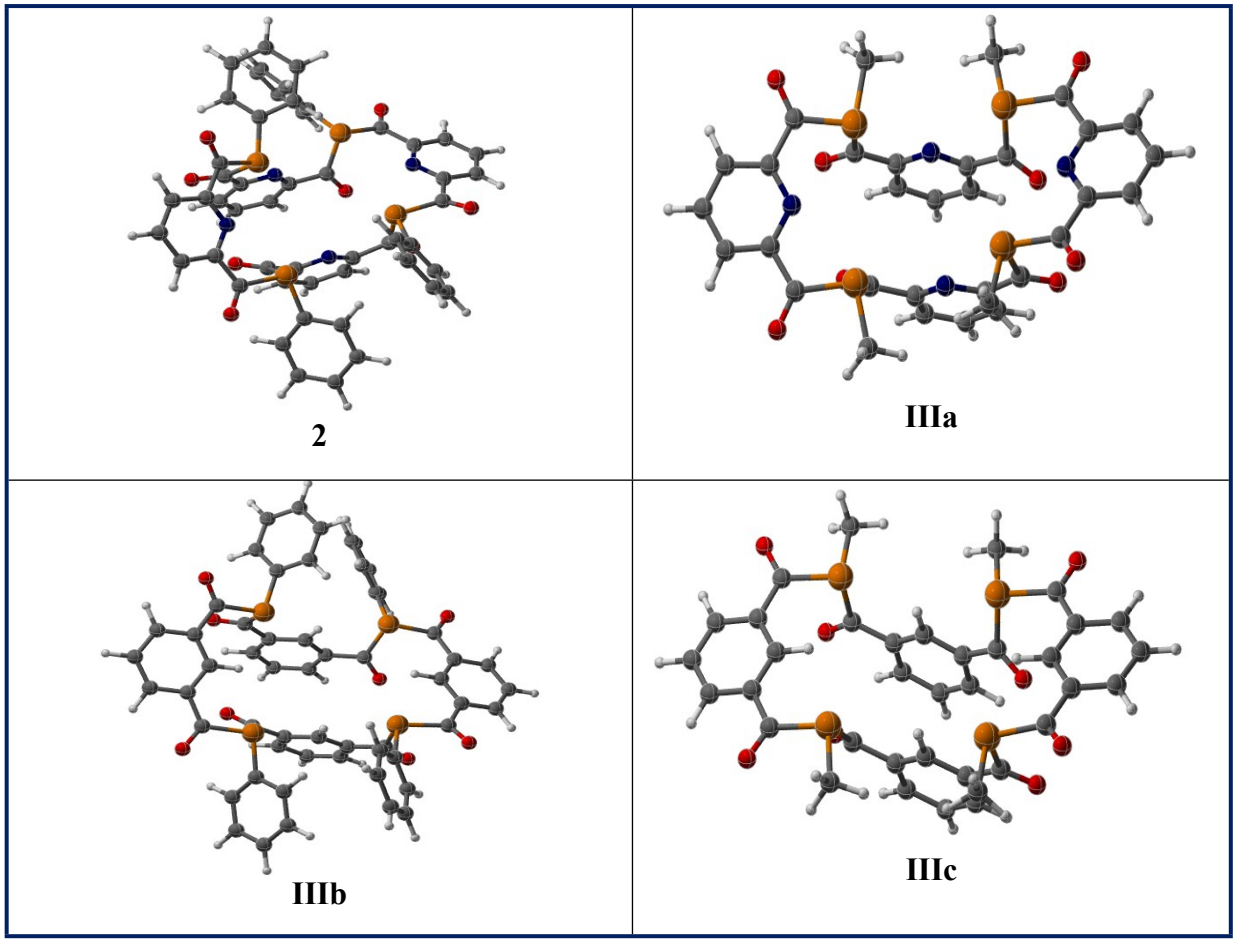
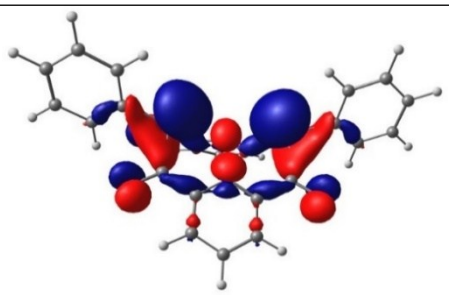
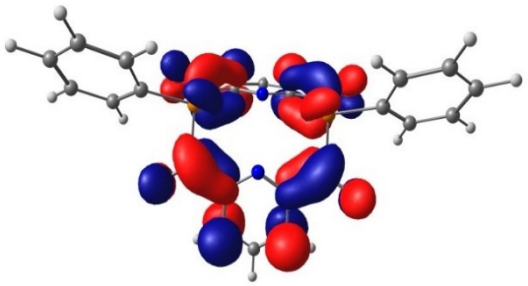
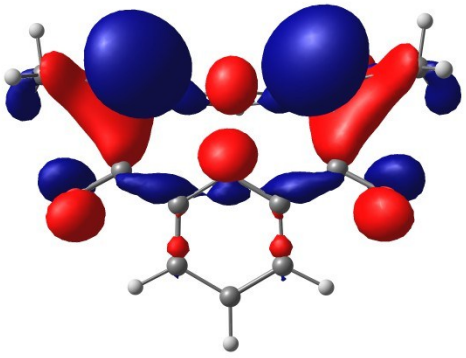
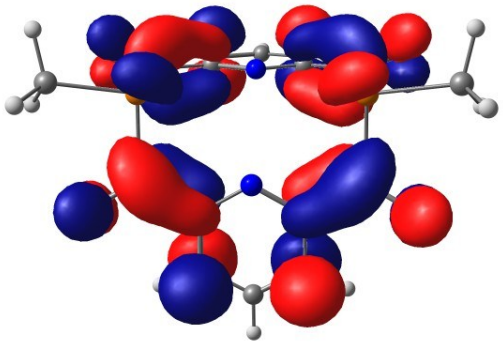
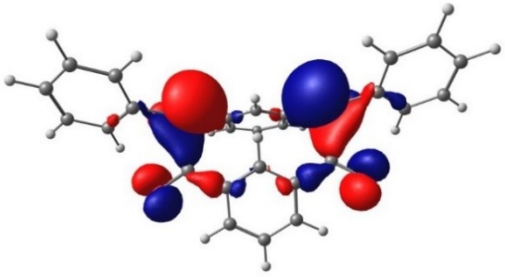
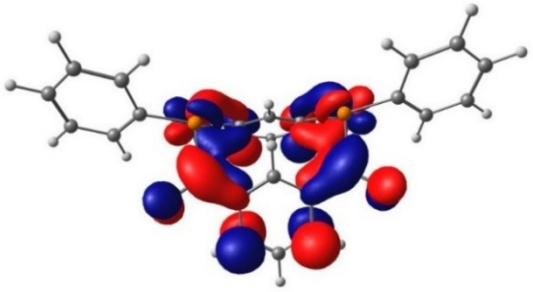
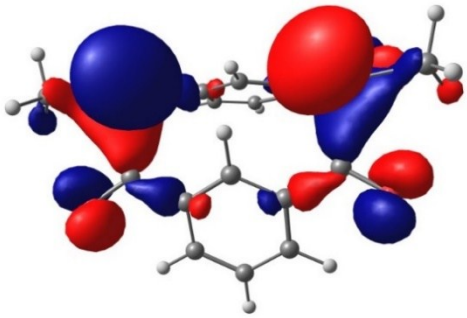
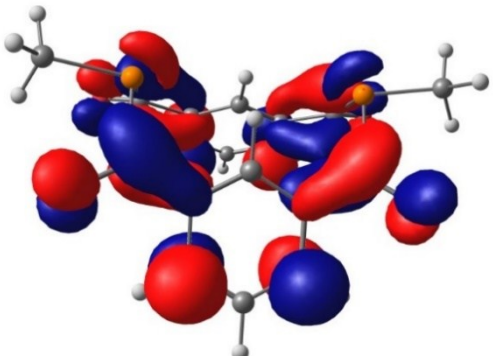
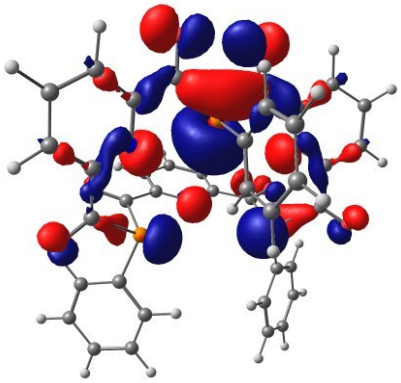
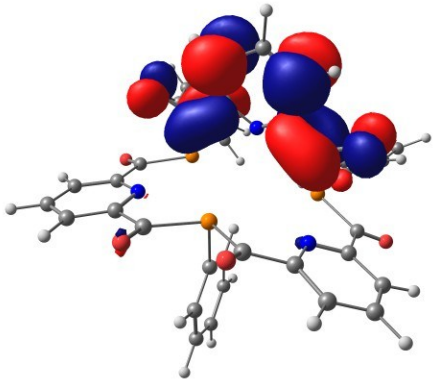
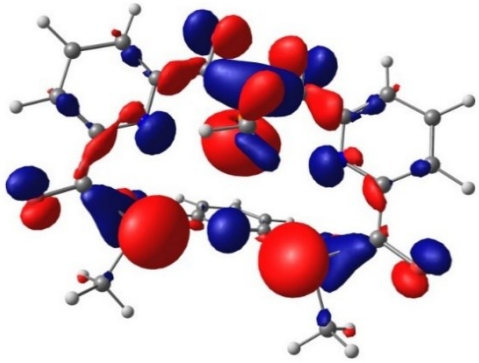
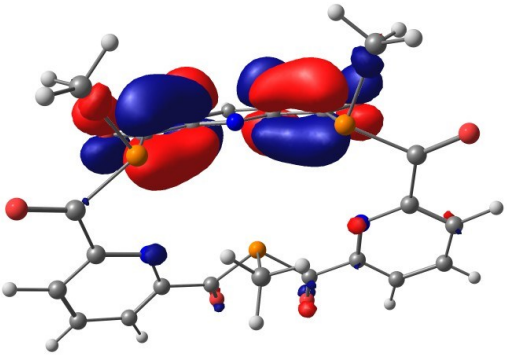
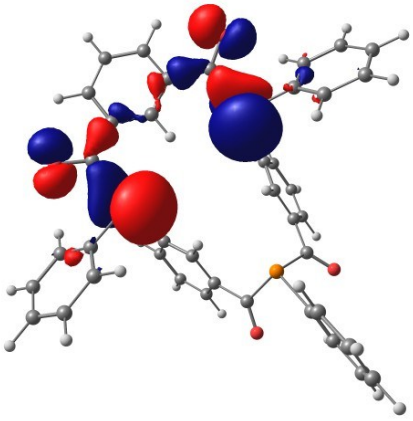
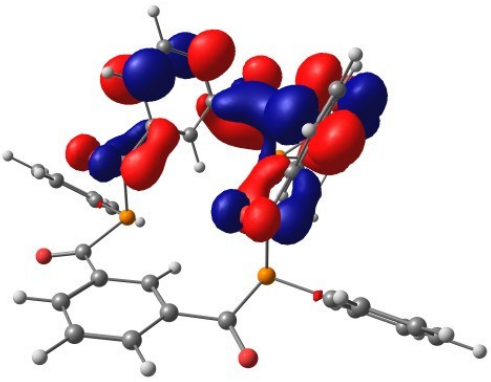
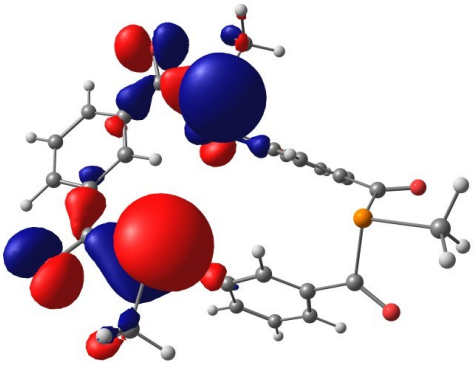
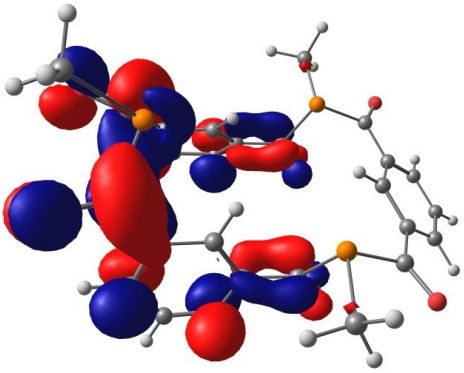


Fig. S10. Optimized structures of **I(a, b, c)−III(a, b, c), 1** and **2** at M062X/6-31G** level of theory.

	HOMO	LUMO
I		
Ia		
Ib		
Ic		

1		
IIa		
IIb		
IIc		

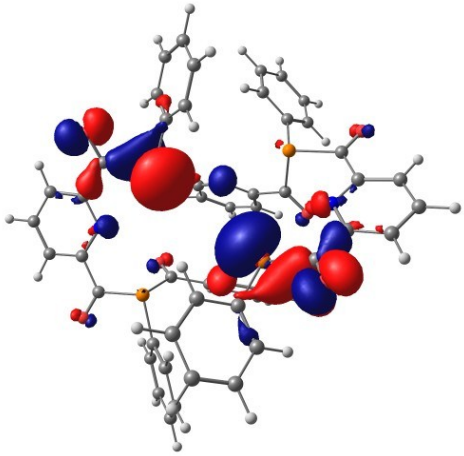
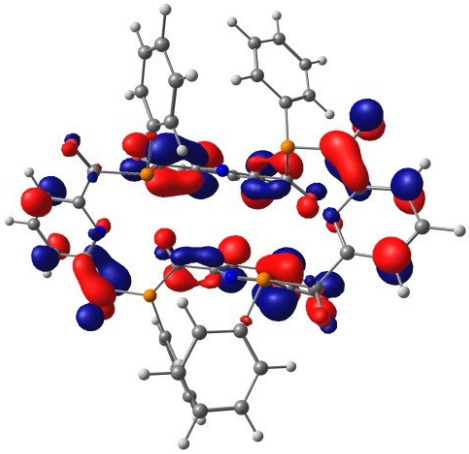
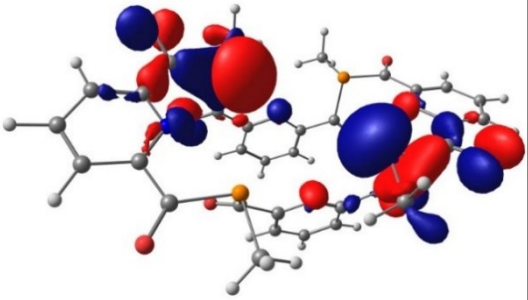
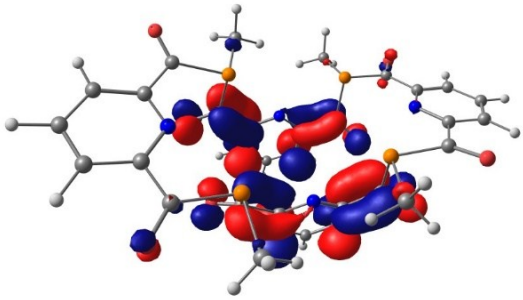
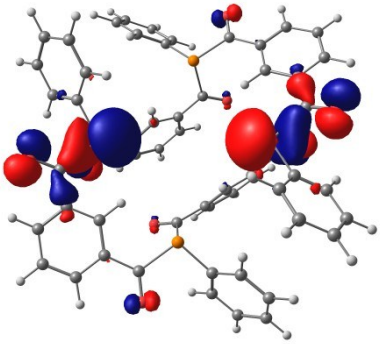
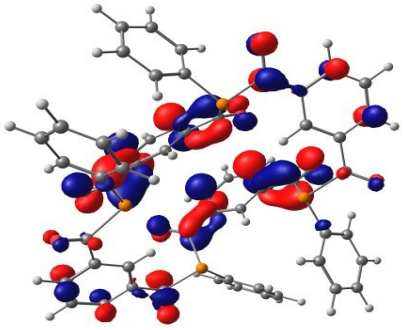
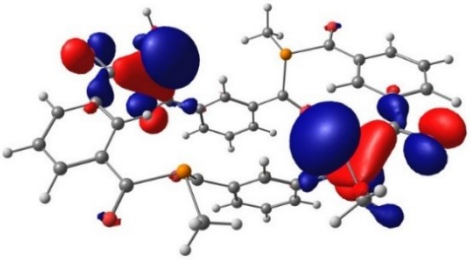
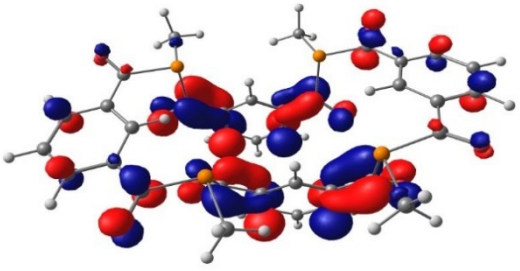
2		
IIIa		
IIIb		
IIIc		

Fig. S11. Representative molecular orbitals surfaces of HOMO and LUMO for **I(a, b, c)−III(a, b, c), 1** and **2**

Table S5. ΔG (kcal/mol) energy values of compound **I(a, b, c)−III(a, b, c), 1** and **2** at M062X/6-31G** level of theory.

Compound	**ΔG**	**Compound**	**ΔG**	**Compound**	**ΔG**	**Compound**	**ΔG**
I	0.0	Ia	0.0	Ib	0.0	Ic	0.0
1	-6.7	IIa	1.7	IIb	0.9	IIc	4.4
2	-12.8	IIIa	-2.7	IIIb	-5.3	IIIc	5.5

Table S6. Energies (eV) of Selected Molecular Orbitals of **I(a, b, c)−III(a, b, c), 1** and **2**

	I	Ia	Ib	Ic	1	IIa	IIb	IIc	2	IIIa	IIIb	IIIc
HOMO	-7.68	-7.71	-7.99	-8.04	-7.59	-7.54	-7.87	-7.90	-7.46	-7.47	-7.79	-7.89
LUMO	-1.70	-1.67	-1.55	-1.55	-1.44	-1.45	-1.47	-1.64	-1.31	-1.54	-1.35	-1.49

Table S7. Selected Experimental and DFT Calculated Bond Lengths (Å) and Bond Angles (deg) of compound **1**

Bond lengths (Å)	X-ray	DFT	Bond angles (deg)	X-ray	DFT
C-O	1.2115	1.2079	C_{CO}-P-C_{CO}	94.71	94.636
C_{CO}-P	1.8861	1.8912	C_{CO}-P-C_{Ph}	98.34	97.983
C_{Ph}-P	1.833	1.8394			

Table S8. Selected Experimental and DFT Calculated Bond Lengths (Å) and Bond Angles (deg) of compound **2**

Bond lengths (Å)	X-ray	DFT	Bond angles (deg)	X-ray	DFT
C-O	1.2118	1.2088	C_{CO}-P-C_{CO}	94.232	93.83
C_{CO}-P	1.8831	1.8919	C_{CO}-P-C_{Ph}	98.441	98.37
C_{Ph}-P	1.8312	1.8548			

Total electronic energies and Gibbs free energies (in a.u) and Cartesian coordinates of optimized geometries of I(a, b, c)−III(a, b, c), 1 and 2 at the M062X/6-31G level of theory**

I			
Zero-point correction=	0.364246		
Thermal correction to Energy=	0.392332		
Thermal correction to Enthalpy=	0.393277		
Thermal correction to Gibbs Free Energy=	0.302353		
Sum of electronic and zero-point Energies=	-2092.500567		
Sum of electronic and thermal Energies=	-2092.472480		
Sum of electronic and thermal Enthalpies=	-2092.471536		
Sum of electronic and thermal Free Energies=	-2092.562459		
6	0.727665000	0.709497000	2.842207000
6	2.037388000	0.003958000	3.080068000
6	4.303674000	0.125632000	3.255987000
6	4.412416000	-1.238228000	3.538072000
1	5.394262000	-1.661400000	3.718297000
6	3.248298000	-1.996482000	3.585016000
1	3.288355000	-3.058867000	3.802106000
6	2.031164000	-1.365383000	3.356469000
1	1.083159000	-1.890475000	3.391003000
6	5.553145000	0.968249000	3.228644000
6	5.714228000	2.294533000	0.775698000
6	4.529438000	1.847187000	-0.039974000
6	2.268865000	1.670614000	-0.243144000
6	2.370897000	1.084298000	-1.507221000
1	1.464274000	0.814844000	-2.037124000
6	3.639000000	0.879714000	-2.038415000
1	3.762458000	0.427939000	-3.017221000
6	4.745635000	1.273054000	-1.295095000
1	5.762346000	1.157317000	-1.653391000
6	0.901315000	1.926195000	0.336359000

8	-0.309969000	0.162887000	3.126904000
8	6.590113000	0.515803000	3.649309000
8	6.799785000	2.390711000	0.256909000
8	-0.075205000	1.824962000	-0.365662000
15	0.804582000	2.490405000	2.159465000
15	5.395393000	2.765383000	2.597942000
7	3.145187000	0.737661000	3.030511000
7	3.321150000	2.044418000	0.478580000
6	-0.973433000	2.914057000	2.241894000
6	-2.029079000	2.110941000	1.790879000
6	-1.263056000	4.156967000	2.816470000
6	-3.341650000	2.550836000	1.915257000
1	-1.823180000	1.146166000	1.346371000
6	-2.578708000	4.595568000	2.940576000
1	-0.449315000	4.785488000	3.169327000
6	-3.618722000	3.790500000	2.488739000
1	-4.153920000	1.922457000	1.564038000
1	-2.787317000	5.561639000	3.388797000
1	-4.646576000	4.127174000	2.583039000
6	7.063401000	3.375842000	3.036075000
6	8.272802000	2.727058000	2.754270000
6	7.091411000	4.604022000	3.706638000
6	9.478194000	3.301437000	3.139632000
1	8.267868000	1.778039000	2.234326000
6	8.300085000	5.178098000	4.091299000
1	6.157368000	5.114071000	3.928241000
6	9.494451000	4.524949000	3.807019000
1	10.410672000	2.792380000	2.917597000
1	8.306760000	6.130694000	4.611091000
1	10.439973000	4.967699000	4.105081000

Ia

Zero-point correction=	0.256534
Thermal correction to Energy=	0.278366

Thermal correction to Enthalpy= 0.279310

Thermal correction to Gibbs Free Energy= 0.204931

Sum of electronic and zero-point Energies= -1709.292628

Sum of electronic and thermal Energies= -1709.270796

Sum of electronic and thermal Enthalpies= -1709.269852

Sum of electronic and thermal Free Energies= -1709.344231

6	0.711398000	0.903287000	2.902066000
6	2.009955000	0.191159000	3.165854000
6	4.274530000	0.299640000	3.365050000
6	4.370929000	-1.060814000	3.667109000
1	5.348094000	-1.487981000	3.863027000
6	3.201241000	-1.810718000	3.710907000
1	3.231521000	-2.870430000	3.942182000
6	1.991252000	-1.174362000	3.459735000
1	1.039191000	-1.692457000	3.489030000
6	5.526238000	1.134532000	3.333064000
6	5.704440000	2.422055000	0.856492000
6	4.518852000	2.000646000	0.031962000
6	2.256714000	1.864619000	-0.180973000
6	2.353237000	1.281455000	-1.446827000
1	1.443855000	1.029591000	-1.980773000
6	3.619604000	1.055302000	-1.973368000
1	3.739184000	0.603942000	-2.952846000
6	4.729958000	1.426030000	-1.223783000
1	5.746168000	1.291831000	-1.577230000
6	0.895688000	2.138736000	0.399121000
6	-1.062506000	2.917960000	2.203925000
1	-1.285464000	3.825485000	1.639141000
1	-1.400196000	3.049235000	3.233945000
1	-1.581609000	2.071795000	1.754988000
6	7.187822000	3.333192000	3.014206000
1	7.310280000	3.454034000	4.092464000

1	7.417791000	4.280504000	2.522333000
1	7.866502000	2.560987000	2.653422000
8	-0.339387000	0.369870000	3.169962000
8	6.561493000	0.692982000	3.773721000
8	6.801104000	2.492586000	0.353452000
8	-0.086864000	2.071652000	-0.301522000
15	0.765925000	2.677871000	2.219276000
15	5.424210000	2.916190000	2.671704000
7	3.123085000	0.917214000	3.117977000
7	3.312165000	2.217278000	0.547209000

Ib

Zero-point correction= 0.388920

Thermal correction to Energy= 0.417089

Thermal correction to Enthalpy= 0.418033

Thermal correction to Gibbs Free Energy= 0.328447

Sum of electronic and zero-point Energies= -2060.405320

Sum of electronic and thermal Energies= -2060.377152

Sum of electronic and thermal Enthalpies= -2060.376208

Sum of electronic and thermal Free Energies= -2060.465794

6	0.612660000	0.813793000	2.879497000
6	1.963385000	0.188766000	3.045260000
6	3.119331000	0.952356000	3.197472000
1	3.047795000	2.031619000	3.290772000
6	4.364634000	0.329947000	3.257941000
6	4.446386000	-1.065296000	3.221637000
1	5.426330000	-1.527984000	3.283454000
6	3.290985000	-1.830494000	3.103416000
1	3.357367000	-2.912805000	3.073100000
6	2.051489000	-1.206049000	3.010425000
1	1.136067000	-1.779539000	2.903643000
6	5.642140000	1.107661000	3.330904000
6	5.806408000	2.405094000	0.841657000

6	4.574485000	1.939693000	0.128111000
6	3.294022000	2.301157000	0.543550000
1	3.167166000	3.013289000	1.352912000
6	2.175478000	1.772360000	-0.098322000
6	2.341924000	0.921194000	-1.194849000
1	1.455986000	0.529835000	-1.684882000
6	3.619033000	0.585892000	-1.632046000
1	3.745315000	-0.077094000	-2.481360000
6	4.733868000	1.089067000	-0.969819000
1	5.740779000	0.831010000	-1.282286000
6	0.780544000	2.055560000	0.368279000
8	-0.396601000	0.213531000	3.159104000
8	6.650297000	0.618041000	3.778944000
8	6.875159000	2.454224000	0.282709000
8	-0.164910000	1.941235000	-0.373214000
15	0.556644000	2.594445000	2.189140000
15	5.617442000	2.904646000	2.675996000
6	7.309277000	3.439646000	3.073646000
6	8.460257000	2.706590000	2.758339000
6	7.434367000	4.663191000	3.740631000
6	9.711864000	3.197595000	3.109979000
1	8.372052000	1.759532000	2.241516000
6	8.689723000	5.151373000	4.091304000
1	6.543496000	5.234749000	3.986817000
6	9.828066000	4.416760000	3.775435000
1	10.601115000	2.626617000	2.863597000
1	8.777035000	6.101321000	4.608395000
1	10.809108000	4.793540000	4.047747000
6	-1.227782000	2.939628000	2.238791000
6	-2.214228000	2.068195000	1.760556000
6	-1.605881000	4.163516000	2.801805000
6	-3.554736000	2.424143000	1.849920000
1	-1.930848000	1.118807000	1.324759000

6	-2.949300000	4.516418000	2.888925000
1	-0.843433000	4.842282000	3.174571000
6	-3.923232000	3.644762000	2.412615000
1	-4.315735000	1.745569000	1.478516000
1	-3.232789000	5.467576000	3.327593000
1	-4.972453000	3.915540000	2.478950000

Ic

Zero-point correction= 0.280657

Thermal correction to Energy= 0.302763

Thermal correction to Enthalpy= 0.303707

Thermal correction to Gibbs Free Energy= 0.229230

Sum of electronic and zero-point Energies= -1677.197426

Sum of electronic and thermal Energies= -1677.175320

Sum of electronic and thermal Enthalpies= -1677.174376

Sum of electronic and thermal Free Energies= -1677.248853

6	0.604622000	0.960339000	2.922636000
6	1.943228000	0.324164000	3.121442000
6	3.104507000	1.081000000	3.264560000
1	3.041632000	2.162917000	3.332439000
6	4.343283000	0.449469000	3.354105000
6	4.413034000	-0.946820000	3.355253000
1	5.388512000	-1.415780000	3.437393000
6	3.251683000	-1.704559000	3.245509000
1	3.308392000	-2.787811000	3.244035000
6	2.018943000	-1.071849000	3.122639000
1	1.099220000	-1.639082000	3.019264000
6	5.622486000	1.221669000	3.409905000
6	5.800196000	2.483813000	0.901547000
6	4.567336000	2.053786000	0.171840000
6	3.292180000	2.426709000	0.593052000
1	3.175305000	3.126966000	1.414553000
6	2.166461000	1.929391000	-0.060879000

6	2.320507000	1.098238000	-1.174241000
1	1.428816000	0.731254000	-1.672765000
6	3.593006000	0.751155000	-1.616248000
1	3.709719000	0.103649000	-2.478790000
6	4.714873000	1.222011000	-0.942037000
1	5.718078000	0.952454000	-1.256712000
6	0.780408000	2.224786000	0.417556000
6	-1.297932000	2.889808000	2.181973000
1	-1.556063000	3.766265000	1.585227000
1	-1.667809000	3.023645000	3.199905000
1	-1.747260000	1.999792000	1.742002000
6	7.429410000	3.332799000	3.022063000
1	7.588566000	3.464821000	4.093574000
1	7.704819000	4.249938000	2.498763000
1	8.038842000	2.505397000	2.659102000
8	-0.420322000	0.373028000	3.178569000
8	6.633305000	0.741564000	3.866899000
8	6.881848000	2.503077000	0.362383000
8	-0.175411000	2.141748000	-0.317667000
15	0.530934000	2.736034000	2.235528000
15	5.647543000	3.001114000	2.728221000

1

Zero-point correction= 0.546961

Thermal correction to Energy= 0.590075

Thermal correction to Enthalpy= 0.591019

Thermal correction to Gibbs Free Energy= 0.466146

Sum of electronic and zero-point Energies= -3138.773507

Sum of electronic and thermal Energies= -3138.730393

Sum of electronic and thermal Enthalpies= -3138.729448

Sum of electronic and thermal Free Energies= -3138.854321

15	-1.552891000	10.216004000	2.509793000
15	-4.907288000	8.234824000	4.606494000

15	-1.061944000	6.010921000	4.610261000
8	-0.749440000	4.133098000	6.589330000
8	-3.365875000	10.244705000	0.463891000
8	-2.666948000	4.048079000	3.586784000
8	-1.763715000	12.931233000	2.148205000
8	-7.056811000	7.042726000	5.886785000
8	-7.347995000	9.550207000	4.627463000
7	-4.306544000	10.872879000	3.453040000
7	-2.619025000	7.332442000	2.305334000
7	-3.728430000	5.906097000	5.964229000
6	-2.364858000	5.214950000	3.475676000
6	-3.760715000	12.005889000	3.013999000
6	0.408239000	5.102638000	3.984705000
6	2.144976000	10.175324000	0.785322000
1	3.120696000	9.789359000	1.062669000
6	-2.347316000	11.930484000	2.486430000
6	-3.279624000	8.101374000	1.441780000
6	-5.731172000	13.268609000	3.502522000
1	-6.286666000	14.200633000	3.520261000
6	-2.519767000	9.099455000	5.790685000
1	-2.053160000	8.689602000	4.901065000
6	-3.049649000	6.081351000	2.456562000
6	0.716316000	11.336170000	-0.773374000
1	0.581816000	11.855338000	-1.716975000
6	-4.137172000	5.545664000	1.762856000
1	-4.422027000	4.517681000	1.956043000
6	-3.905159000	9.025626000	5.937040000
6	1.610484000	3.106500000	3.344030000
1	1.645337000	2.027456000	3.232437000
6	-5.553940000	10.920119000	3.920389000
6	-0.200060000	10.502154000	1.300929000
6	-4.692701000	4.298873000	8.028770000
1	-5.068545000	3.671295000	8.830337000

6	-0.366062000	11.172260000	0.083056000
1	-1.342516000	11.558872000	-0.190268000
6	-4.510768000	9.551308000	7.082947000
1	-5.591412000	9.494542000	7.200856000
6	-5.862025000	7.056057000	5.720430000
6	-5.517095000	5.236897000	7.417975000
1	-6.554249000	5.380801000	7.699507000
6	-4.984459000	6.022187000	6.395954000
6	-3.378834000	4.177367000	7.592191000
1	-2.678349000	3.470220000	8.021774000
6	-1.531331000	4.873941000	6.044741000
6	2.673784000	5.262088000	3.140451000
1	3.533526000	5.867164000	2.871152000
6	1.061801000	10.009551000	1.644681000
1	1.193607000	9.497033000	2.593686000
6	-2.948285000	5.000607000	6.551868000
6	-4.378036000	7.665649000	0.697036000
1	-4.858627000	8.363501000	0.020840000
6	1.522967000	5.870297000	3.635788000
1	1.487116000	6.949646000	3.754701000
6	-6.161409000	9.626375000	4.423672000
6	-3.733375000	10.147048000	8.072751000
1	-4.207243000	10.554290000	8.960290000
6	0.460436000	3.711366000	3.837479000
1	-0.401140000	3.109302000	4.106420000
6	-2.856254000	9.536335000	1.302990000
6	-6.311778000	12.090520000	3.958367000
1	-7.326208000	12.043403000	4.338241000
6	-4.815165000	6.358202000	0.863860000
1	-5.670523000	5.983534000	0.311160000
6	1.971203000	10.838784000	-0.424561000
1	2.812643000	10.971416000	-1.097478000
6	2.716924000	3.879747000	2.994599000

1	3.612821000	3.402363000	2.610008000
6	-1.745464000	9.695825000	6.781518000
1	-0.668163000	9.749445000	6.658723000
6	-2.350564000	10.219598000	7.921622000
1	-1.745374000	10.684731000	8.693538000
6	-4.426986000	13.230912000	3.023045000
1	-3.908866000	14.109749000	2.656023000

IIa

Zero-point correction= 0.385497

Thermal correction to Energy= 0.419135

Thermal correction to Enthalpy= 0.420079

Thermal correction to Gibbs Free Energy= 0.320133

Sum of electronic and zero-point Energies= -2563.948226

Sum of electronic and thermal Energies= -2563.914588

Sum of electronic and thermal Enthalpies= -2563.913644

Sum of electronic and thermal Free Energies= -2564.013590

15	-1.520795000	10.224513000	2.506862000
15	-4.968842000	8.067081000	4.535781000
15	-1.145421000	5.972659000	4.654868000
8	-0.835305000	3.997889000	6.523743000
8	-3.175248000	10.191802000	0.340217000
8	-2.670274000	4.020786000	3.510234000
8	-1.801878000	12.926711000	2.232122000
8	-6.985798000	7.293205000	6.273010000
8	-7.375411000	9.344533000	4.407389000
7	-4.341125000	10.778350000	3.377841000
7	-2.641497000	7.332002000	2.316504000
7	-3.793086000	5.828906000	6.021387000
6	-2.410674000	5.201681000	3.460123000
6	-3.817475000	11.934349000	2.970973000
6	-2.381866000	11.903828000	2.510608000
6	-3.281220000	8.114912000	1.449430000

6	-5.834607000	13.132791000	3.426388000
1	-6.418016000	14.047616000	3.440832000
6	-3.096430000	6.088022000	2.460029000
6	-4.187486000	5.573434000	1.756677000
1	-4.486042000	4.547003000	1.937393000
6	-5.597035000	10.785059000	3.825331000
6	-4.737691000	4.248353000	8.107905000
1	-5.109367000	3.626284000	8.915714000
6	-5.846466000	7.129175000	5.914414000
6	-5.534370000	5.250346000	7.563819000
1	-6.539452000	5.457986000	7.913579000
6	-5.014125000	6.016491000	6.520670000
6	-3.452846000	4.064543000	7.608804000
1	-2.769562000	3.318939000	7.999616000
6	-1.623433000	4.768051000	6.027734000
6	-3.026809000	4.886647000	6.566242000
6	-4.390462000	7.704782000	0.705443000
1	-4.851886000	8.411284000	0.024752000
6	-6.178227000	9.472279000	4.304160000
6	-2.778465000	9.517989000	1.263238000
6	-6.389242000	11.933492000	3.858374000
1	-7.409562000	11.852734000	4.216326000
6	-4.853064000	6.405309000	0.866494000
1	-5.715350000	6.050605000	0.311492000
6	-4.518327000	13.139601000	2.978831000
1	-4.015621000	14.038611000	2.640227000
6	-0.234958000	10.715536000	1.264466000
1	0.329606000	11.547285000	1.690095000
1	0.440482000	9.879030000	1.079276000
1	-0.700540000	11.046000000	0.333870000
6	0.311682000	4.978372000	4.079530000
1	1.045134000	4.966336000	4.887843000
1	0.020158000	3.950542000	3.855363000

1	0.756108000	5.450486000	3.201676000
6	-3.566189000	8.855481000	5.477966000
1	-2.724833000	8.979802000	4.794006000
1	-3.850555000	9.825508000	5.888363000
1	-3.260843000	8.192715000	6.286499000

IIb

Zero-point correction= 0.583473

Thermal correction to Energy= 0.627098

Thermal correction to Enthalpy= 0.628043

Thermal correction to Gibbs Free Energy= 0.501957

Sum of electronic and zero-point Energies= -3090.615717

Sum of electronic and thermal Energies= -3090.572092

Sum of electronic and thermal Enthalpies= -3090.571148

Sum of electronic and thermal Free Energies= -3090.697233

15	-0.544601000	10.210805000	2.165535000
15	-3.128607000	8.881564000	6.847872000
15	-1.346238000	5.065935000	4.308535000
8	-1.858378000	2.643840000	5.452092000
8	-0.487365000	9.308581000	-0.431598000
8	-4.066297000	5.063439000	3.959540000
8	-2.298867000	12.161362000	1.351786000
8	-4.300548000	8.193689000	9.214978000
8	-5.387507000	7.673842000	5.888207000
6	-3.021581000	5.495293000	3.527622000
6	-3.413004000	10.491774000	2.594373000
6	-0.788366000	3.927349000	2.986753000
6	2.695080000	12.622367000	1.702952000
1	3.581795000	12.845332000	2.287240000
6	-2.209835000	11.133086000	1.976972000
6	-1.962478000	8.032297000	0.907167000
6	-5.773806000	10.004562000	2.421812000
1	-6.714631000	10.088123000	1.888174000

6	-2.943181000	11.602029000	7.376367000
1	-1.903440000	11.473916000	7.087773000
6	-2.976436000	6.340398000	2.292338000
6	1.346297000	12.959518000	-0.269155000
1	1.185567000	13.447500000	-1.224980000
6	-3.981525000	6.164948000	1.337128000
1	-4.769798000	5.447200000	1.540934000
6	-3.801715000	10.499903000	7.377181000
6	-1.149253000	2.073976000	1.478830000
1	-1.784310000	1.276416000	1.107107000
6	-4.501220000	9.195103000	4.310461000
6	0.611523000	11.413232000	1.435048000
6	-4.111138000	4.019149000	8.724803000
1	-4.572236000	3.336112000	9.430348000
6	0.409787000	12.047032000	0.202372000
1	-0.474170000	11.825879000	-0.380810000
6	-5.140169000	10.667218000	7.751229000
1	-5.808610000	9.811336000	7.758287000
6	-3.803899000	7.744665000	8.209841000
6	-4.232541000	5.392899000	8.906200000
1	-4.782911000	5.808801000	9.744059000
6	-3.641988000	6.273991000	7.997003000
6	-3.401194000	3.519710000	7.638045000
1	-3.293989000	2.452451000	7.473050000
6	-2.055336000	3.830099000	5.566274000
6	0.934158000	3.291024000	1.411803000
1	1.921321000	3.444624000	0.988282000
6	1.760166000	11.707417000	2.178641000
1	1.921097000	11.217768000	3.135543000
6	-2.806945000	4.396666000	6.726647000
6	-2.931414000	7.808568000	-0.074124000
1	-2.881747000	8.380671000	-0.995469000
6	0.481757000	4.118199000	2.437312000

1	1.117324000	4.915263000	2.813242000
6	-4.507749000	8.457883000	5.612925000
6	-5.607252000	11.922904000	8.120105000
1	-6.645053000	12.047980000	8.411619000
6	-1.604153000	2.899872000	2.499255000
1	-2.589769000	2.745804000	2.928690000
6	-0.957232000	9.113585000	0.662507000
6	-5.707409000	9.285591000	3.609303000
1	-6.580712000	8.791023000	4.022293000
6	-3.949066000	6.886583000	0.149043000
1	-4.715780000	6.731752000	-0.602584000
6	2.486361000	13.248436000	0.477911000
1	3.212898000	13.962566000	0.102858000
6	0.119535000	2.269415000	0.934803000
1	0.471766000	1.623268000	0.136965000
6	-3.414650000	12.859759000	7.744335000
1	-2.743129000	13.712012000	7.741310000
6	-4.745703000	13.018918000	8.116010000
1	-5.114422000	13.998346000	8.403932000
6	-4.632060000	10.622530000	1.923296000
1	-4.659189000	11.202822000	1.006240000
6	-3.346843000	9.783884000	3.793839000
1	-2.398254000	9.692446000	4.318488000
6	-1.973151000	7.286704000	2.085354000
1	-1.207414000	7.449384000	2.840629000
6	-2.928017000	5.770637000	6.913465000
1	-2.446171000	6.454728000	6.220159000

IIc

Zero-point correction=	0.420372
Thermal correction to Energy=	0.454439
Thermal correction to Enthalpy=	0.455384
Thermal correction to Gibbs Free Energy=	0.350963
Sum of electronic and zero-point Energies=	-2515.796817

Sum of electronic and thermal Energies= -2515.762750

Sum of electronic and thermal Enthalpies= -2515.761806

Sum of electronic and thermal Free Energies= -2515.866226

15	-1.460026917	10.470334651	2.245180077
15	-5.164558898	8.178000511	4.618468319
15	-0.909932297	5.665933932	4.699025623
8	-0.888422422	3.748734426	6.606887017
8	-3.092596157	10.109186155	0.100648466
8	-2.369579377	3.855892417	3.289405495
8	-1.975644095	13.098913096	1.862478138
8	-7.169549809	7.122276923	6.160856056
8	-7.463193122	9.648232024	4.860402950
6	-2.163621459	5.043562341	3.390319781
6	-3.856911311	12.067538912	2.852244835
6	-2.481167438	12.076189478	2.261521790
6	-3.143800348	8.166523926	1.437649520
6	-5.848245125	13.280743267	3.479955459
1	-6.411929969	14.206915586	3.516429832
6	-2.895273840	6.025405518	2.526592527
6	-4.033915571	5.560714762	1.859119143
1	-4.344439675	4.534624470	2.028028324
6	-5.673176992	10.919717898	3.968191698
6	-4.809159246	4.194523835	8.056549887
1	-5.199067378	3.577240701	8.858973788
6	-5.996314846	7.064801924	5.889360662
6	-5.603186422	5.196013543	7.503490075
1	-6.613879036	5.378146388	7.855271764
6	-5.108163008	5.993484806	6.469342579
6	-3.516295870	3.986747547	7.587092090
1	-2.872808996	3.221767329	8.009539103
6	-1.611032678	4.560933840	6.078902798
6	-3.016240103	4.776853784	6.548258782

6	-4.281665230	7.690637790	0.776743342
1	-4.788590126	8.355641450	0.084910987
6	-6.297547143	9.678456988	4.553401822
6	-2.684260062	9.550799962	1.092829994
6	-6.393699443	12.115167087	4.012081352
1	-7.379662228	12.105640838	4.466286044
6	-4.738595635	6.398580203	1.004040766
1	-5.630863027	6.039960856	0.502203095
6	-4.581556280	13.261996952	2.906131488
1	-4.130040994	14.159242695	2.495406466
6	-0.285609713	11.028402544	0.933147727
1	0.214233835	11.927166656	1.297438240
1	0.455889762	10.250665132	0.744312116
1	-0.831999930	11.271470853	0.020158500
6	0.473188830	4.526492312	4.251365700
1	1.112431327	4.419665724	5.129032695
1	0.077923724	3.546426562	3.978220173
1	1.051305592	4.952536451	3.429900207
6	-3.738252573	8.862226059	5.633263745
1	-2.792034889	8.699694188	5.106336696
1	-3.861818208	9.932895358	5.801020342
1	-3.682844149	8.368972589	6.604656906
6	-2.466158749	7.343285103	2.342029367
1	-1.591640681	7.714837330	2.873029065
6	-4.411498598	10.904402397	3.374905112
1	-3.850593046	9.975573397	3.322917946
6	-3.818324161	5.766414055	5.991136000
1	-3.429805945	6.369830744	5.175943581

2

Zero-point correction= 0.730945

Thermal correction to Energy= 0.788332

Thermal correction to Enthalpy= 0.789277

Thermal correction to Gibbs Free Energy= 0.637515

Sum of electronic and zero-point Energies= -4185.051861

Sum of electronic and thermal Energies= -4184.994473

Sum of electronic and thermal Enthalpies= -4184.993529

Sum of electronic and thermal Free Energies= -4185.145290

15	1.095081000	8.830998000	4.619576000
15	5.326839000	10.438504000	6.827186000
15	1.652025000	11.175616000	8.897757000
15	4.161432000	10.387796000	2.059201000
8	-0.725474000	10.295604000	3.177173000
8	6.093679000	13.014229000	7.387182000
8	1.816971000	11.856389000	2.052891000
8	3.001475000	13.454528000	8.093521000
8	7.568232000	10.030931000	8.400740000
8	1.723059000	12.270493000	11.428244000
8	3.835117000	10.256977000	-0.676879000
8	-0.501000000	6.838270000	3.550536000
7	4.169732000	12.099775000	4.592820000
7	1.723847000	8.844784000	1.743786000
7	1.093205000	11.554548000	5.908100000
7	4.486472000	11.243459000	9.527088000
6	4.671511000	12.931177000	5.502411000
6	6.443731000	10.467561000	8.361726000
6	-0.008934000	7.470541000	0.818712000
1	-0.842619000	6.807682000	1.021175000
6	-0.175552000	12.815821000	4.299297000
1	-0.786669000	12.777186000	3.405199000
6	2.899406000	11.691396000	2.568418000
6	0.268232000	7.735946000	3.307532000
6	1.498426000	8.633023000	-0.634889000
1	1.883595000	8.911305000	-1.609486000
6	3.874884000	11.740216000	10.599096000
6	3.359983000	9.977470000	0.398608000

6	0.131140000	13.999232000	4.955990000
1	-0.252507000	14.948253000	4.594987000
6	0.682929000	8.032715000	1.892235000
6	-1.076836000	10.931684000	8.495446000
1	-0.798574000	9.973752000	8.069384000
6	5.424403000	11.632451000	1.554146000
6	0.347852000	11.624750000	4.808075000
6	2.127316000	9.125327000	0.507039000
6	1.394826000	12.700799000	6.517954000
6	5.798477000	11.044637000	9.591951000
6	0.078842000	10.336814000	4.079909000
6	-0.452689000	13.012098000	9.548663000
1	0.305037000	13.671666000	9.959808000
6	-0.089739000	11.762996000	9.029979000
6	4.542923000	12.083686000	11.772916000
1	3.974548000	12.486791000	12.603747000
6	-1.785904000	13.407291000	9.547429000
1	-2.061223000	14.374383000	9.956616000
6	5.454880000	12.318737000	6.630877000
6	0.952127000	13.947604000	6.078729000
1	1.248206000	14.836197000	6.626027000
6	0.090863000	8.309187000	6.067708000
6	-1.304499000	8.196332000	6.032864000
1	-1.844728000	8.458943000	5.128014000
6	2.185444000	12.611061000	7.798332000
6	0.404345000	7.789626000	-0.469195000
1	-0.112495000	7.381250000	-1.331628000
6	6.584456000	9.920939000	5.591496000
6	3.411943000	12.628495000	3.631508000
6	5.237620000	12.584856000	0.544273000
1	4.333158000	12.571652000	-0.055134000
6	6.562351000	11.338342000	10.722276000
1	7.627481000	11.137461000	10.702609000

6	3.143408000	13.991875000	3.523386000
1	2.507141000	14.342415000	2.717731000
6	-1.303750000	7.370504000	8.301912000
1	-1.846287000	7.005070000	9.168175000
6	7.863132000	10.486409000	5.507662000
1	8.140784000	11.294845000	6.177763000
6	4.493924000	14.316292000	5.469847000
1	4.953585000	14.919132000	6.244340000
6	5.918227000	11.878937000	11.828779000
1	6.477199000	12.130244000	12.724225000
6	0.777053000	7.961667000	7.235054000
1	1.857477000	8.069000000	7.274064000
6	-1.996792000	7.727486000	7.145101000
1	-3.077837000	7.634739000	7.108055000
6	-2.766802000	12.567916000	9.020675000
1	-3.806159000	12.881758000	9.021265000
6	2.381178000	11.866502000	10.498892000
6	3.717532000	14.853867000	4.453239000
1	3.550907000	15.924608000	4.390536000
6	6.216068000	13.543797000	0.302502000
1	6.067791000	14.276982000	-0.484146000
6	0.081938000	7.492587000	8.348553000
1	0.624697000	7.230037000	9.250791000
6	8.432181000	8.954484000	3.729734000
1	9.150570000	8.579675000	3.007567000
6	8.782125000	10.002491000	4.581245000
1	9.773600000	10.441118000	4.524210000
6	-2.410755000	11.332415000	8.490220000
1	-3.163882000	10.672505000	8.070415000
6	7.379994000	13.570948000	1.070053000
1	8.137418000	14.325236000	0.880169000
6	6.591937000	11.668475000	2.320469000
1	6.729622000	10.947778000	3.118555000

6	7.159698000	8.395635000	3.799705000
1	6.878272000	7.588886000	3.130708000
6	6.238074000	8.877990000	4.727958000
1	5.239354000	8.452429000	4.774867000
6	7.565580000	12.634576000	2.081888000
1	8.464442000	12.648358000	2.690786000

IIIa

Zero-point correction= 0.514171

Thermal correction to Energy= 0.559778

Thermal correction to Enthalpy= 0.560722

Thermal correction to Gibbs Free Energy= 0.434975

Sum of electronic and zero-point Energies= -3418.613614

Sum of electronic and thermal Energies= -3418.568008

Sum of electronic and thermal Enthalpies= -3418.567064

Sum of electronic and thermal Free Energies= -3418.692811

15	-0.270100000	-2.793831000	-1.076659000
15	0.267957000	2.795586000	-1.074198000
15	3.362394000	-0.040930000	-0.310982000
15	-3.363632000	0.041730000	-0.306302000
8	-1.188412000	-4.068199000	1.187936000
8	1.189625000	4.067174000	1.190584000
8	-2.812722000	-1.542481000	1.884172000
8	2.814621000	1.541040000	1.881852000
8	0.956200000	5.236449000	-2.128679000
8	5.932525000	0.850720000	0.000685000
8	-5.933343000	-0.850260000	0.007342000
8	-0.959653000	-5.233531000	-2.133013000
7	-1.079306000	1.387924000	1.165370000
7	-3.178217000	-2.831145000	-0.877798000
7	1.079949000	-1.388482000	1.162503000
7	3.176369000	2.832559000	-0.879078000
6	-0.272461000	2.292212000	1.714805000

6	1.365285000	4.243722000	-1.572887000
6	-3.741739000	-5.094023000	-1.432537000
1	-3.383650000	-6.057709000	-1.776996000
6	0.107951000	-2.443995000	3.090545000
1	-0.564473000	-3.213504000	3.452407000
6	-2.608483000	-0.482117000	1.335723000
6	-1.368012000	-4.241529000	-1.575397000
6	-5.451239000	-3.576565000	-0.712806000
1	-6.475891000	-3.314400000	-0.473641000
6	4.458743000	2.601971000	-0.615384000
6	-4.798327000	-1.189205000	-0.234005000
6	0.805526000	-1.587324000	3.931329000
1	0.710316000	-1.671232000	5.009591000
6	-2.830293000	-4.049284000	-1.282142000
6	0.274113000	-2.293544000	1.712136000
6	-4.460260000	-2.600864000	-0.612215000
6	1.716520000	-0.547276000	1.978076000
6	2.827948000	4.051115000	-1.281755000
6	-0.487565000	-3.179529000	0.763048000
6	5.449614000	3.577760000	-0.716238000
1	6.474563000	3.315352000	-0.478618000
6	0.487650000	3.179426000	0.765624000
6	1.610729000	-0.600961000	3.367320000
1	2.154380000	0.122523000	3.965341000
6	2.609475000	0.481281000	1.332574000
6	-5.077208000	-4.849925000	-1.130760000
1	-5.817378000	-5.637514000	-1.227301000
6	-1.714485000	0.545690000	1.980965000
6	3.739235000	5.095964000	-1.432320000
1	3.380749000	6.059991000	-1.775411000
6	-1.606285000	0.597563000	3.370098000
1	-2.148950000	-0.126653000	3.968127000
6	-0.103782000	2.440769000	3.093114000

1	0.569464000	3.209643000	3.454789000
6	5.075084000	4.851531000	-1.132478000
1	5.815155000	5.639191000	-1.229198000
6	4.797271000	1.189871000	-0.239218000
6	-0.799965000	1.583071000	3.933992000
1	-0.702819000	1.665519000	5.012194000
6	4.315651000	-1.502504000	0.337189000
1	4.877092000	-1.936399000	-0.492666000
1	5.022554000	-1.217420000	1.118241000
1	3.616090000	-2.252935000	0.710865000
6	-1.359125000	3.657771000	-1.311726000
1	-2.155189000	2.984218000	-0.988906000
1	-1.417093000	4.610511000	-0.782140000
1	-1.473849000	3.852000000	-2.380035000
6	-4.316082000	1.502514000	0.344891000
1	-4.879317000	1.936874000	-0.483497000
1	-5.021339000	1.216605000	1.127123000
1	-3.616007000	2.252863000	0.717769000
6	1.356629000	-3.655946000	-1.316889000
1	1.415458000	-4.608774000	-0.787550000
1	1.469590000	-3.850063000	-2.385409000
1	2.153222000	-2.982456000	-0.995261000

IIIb

Zero-point correction= 0.778218

Thermal correction to Energy= 0.836619

Thermal correction to Enthalpy= 0.837563

Thermal correction to Gibbs Free Energy= 0.681297

Sum of electronic and zero-point Energies= -4120.843102

Sum of electronic and thermal Energies= -4120.784700

Sum of electronic and thermal Enthalpies= -4120.783756

Sum of electronic and thermal Free Energies= -4120.940022

15	-0.277306000	-3.118665000	-1.430532000

15	0.277087000	3.116829000	-1.434395000
15	3.849948000	-0.066430000	-0.313901000
15	-3.850081000	0.065611000	-0.313849000
8	-1.058940000	-4.255073000	0.922744000
8	1.059233000	4.255718000	0.917488000
8	-2.847486000	-1.602995000	1.640578000
8	2.847466000	1.604815000	1.638367000
8	1.167671000	5.569876000	-2.255080000
8	6.275591000	1.116746000	0.006003000
8	-6.275565000	-1.117364000	0.008229000
8	-1.167597000	-5.572942000	-2.247960000
6	-0.344797000	2.402951000	1.331883000
6	1.516535000	4.516178000	-1.782166000
6	-3.882601000	-5.255688000	-1.494460000
1	-3.547675000	-6.243177000	-1.795334000
6	0.139720000	-2.482345000	2.716952000
1	-0.542330000	-3.238804000	3.090363000
6	-2.772991000	-0.502301000	1.141535000
6	-1.516567000	-4.518621000	-1.776521000
6	-5.600865000	-3.736903000	-0.750573000
1	-6.626126000	-3.522544000	-0.466512000
6	4.668701000	2.695363000	-0.714089000
6	-5.121101000	-1.340315000	-0.275413000
6	0.783238000	-1.594311000	3.568187000
1	0.620459000	-1.653379000	4.639586000
6	-2.945627000	-4.220691000	-1.450388000
6	4.566537000	-2.709399000	0.139319000
1	3.976402000	-2.913189000	-0.750293000
6	-4.727403000	1.397638000	0.589788000
6	0.344891000	-2.401645000	1.334861000
6	-4.668697000	-2.696794000	-0.710090000
6	1.842845000	-0.541765000	1.670071000
6	2.945632000	4.218459000	-1.455998000

6	-0.391511000	-3.359030000	0.457219000
6	5.477280000	-1.153121000	1.748554000
1	5.605038000	-0.136616000	2.107186000
6	4.727266000	-1.397277000	0.591505000
6	5.601005000	3.735286000	-0.756276000
1	6.626322000	3.521164000	-0.472240000
6	6.067384000	-2.210081000	2.431080000
1	6.650999000	-2.013619000	3.324795000
6	0.391655000	3.359214000	0.453071000
6	1.619540000	-0.610586000	3.045289000
1	2.111672000	0.112286000	3.689206000
6	1.298415000	-4.001300000	-1.735909000
6	1.652433000	-5.162891000	-1.041281000
1	0.978284000	-5.569368000	-0.292773000
6	2.772943000	0.503467000	1.140773000
6	-5.207589000	-5.011039000	-1.147927000
1	-5.933523000	-5.816606000	-1.180628000
6	-1.298486000	3.999500000	-1.740369000
6	-1.842862000	0.543605000	1.669443000
6	-5.476748000	1.155171000	1.747617000
1	-5.604008000	0.139232000	2.108026000
6	3.882739000	5.253262000	-1.501777000
1	3.547842000	6.240371000	-1.803926000
6	-1.619677000	0.614246000	3.044589000
1	-2.111882000	-0.107777000	3.689406000
6	3.706152000	-5.297535000	-2.303002000
1	4.642423000	-5.801846000	-2.521066000
6	-1.652272000	5.161636000	-1.046559000
1	-0.978037000	5.568523000	-0.298348000
6	-0.139741000	2.485476000	2.713882000
1	0.542386000	3.242347000	3.086321000
6	5.207793000	5.008925000	-1.155274000
1	5.933833000	5.814338000	-1.189318000

6	2.157598000	-3.496597000	-2.717822000
1	1.887339000	-2.593322000	-3.258073000
6	2.855141000	-5.802783000	-1.320431000
1	3.124867000	-6.703142000	-0.777299000
6	5.907746000	-3.517147000	1.972519000
1	6.369784000	-4.339601000	2.509650000
6	5.121102000	1.339410000	-0.277775000
6	-0.783395000	1.598636000	3.566259000
1	-0.620697000	1.659127000	4.637592000
6	-6.066873000	2.213078000	2.428661000
1	-6.649975000	2.017922000	3.323001000
6	3.355874000	-4.147498000	-3.005521000
1	4.017042000	-3.752060000	-3.769628000
6	-3.706049000	5.295701000	-2.308235000
1	-4.642254000	5.800007000	-2.526596000
6	-2.854885000	5.801520000	-1.326087000
1	-3.124442000	6.702289000	-0.783551000
6	5.155521000	-3.766411000	0.829759000
1	5.020125000	-4.780293000	0.466724000
6	-5.907928000	3.519429000	1.967831000
1	-6.369970000	4.342611000	2.503840000
6	-4.567353000	2.709067000	0.135323000
1	-3.977756000	2.911562000	-0.754951000
6	-3.356010000	4.145097000	-3.009938000
1	-4.017294000	3.749218000	-3.773719000
6	-2.157816000	3.494209000	-2.721847000
1	-1.887756000	2.590475000	-3.261431000
6	-5.156380000	3.767039000	0.824275000
1	-5.021532000	4.780351000	0.459464000
6	-3.346943000	-2.943607000	-1.069186000
1	-2.624511000	-2.132775000	-1.060668000
6	1.209689000	-1.443244000	0.813998000
1	1.379055000	-1.377083000	-0.258688000

6	-1.209581000	1.443896000	0.812210000
1	-1.378835000	1.376284000	-0.260407000
6	3.346872000	2.941850000	-1.073129000
1	2.624342000	2.131122000	-1.063223000

IIIc

Zero-point correction= 0.562181

Thermal correction to Energy= 0.608329

Thermal correction to Enthalpy= 0.609274

Thermal correction to Gibbs Free Energy= 0.480949

Sum of electronic and zero-point Energies= -3354.407606

Sum of electronic and thermal Energies= -3354.361457

Sum of electronic and thermal Enthalpies= -3354.360513

Sum of electronic and thermal Free Energies= -3354.488838

15	0.137288000	-4.285705000	-0.517215000
15	-0.137567000	4.286350000	-0.519799000
15	2.693497000	0.159706000	-0.944389000
15	-2.693916000	-0.159992000	-0.946928000
8	-1.130219000	-4.443204000	1.896988000
8	1.128739000	4.444374000	1.894917000
8	-2.554124000	-1.588966000	1.367933000
8	2.554636000	1.588967000	1.370391000
8	1.248735000	6.578263000	-0.894021000
8	5.313553000	0.732668000	-1.312767000
8	-5.313737000	-0.733598000	-1.315789000
8	-1.248181000	-6.578317000	-0.890563000
6	-0.341875000	2.593159000	1.853406000
6	1.378819000	5.380689000	-0.783612000
6	-3.859395000	-5.508433000	-0.950250000
1	-3.741811000	-6.586557000	-0.909474000
6	0.358397000	-2.469121000	3.250244000
1	-0.155607000	-3.222575000	3.838684000
6	-2.312103000	-0.511654000	0.866633000

6	-1.378594000	-5.380675000	-0.781320000
6	-5.225213000	-3.529777000	-1.091820000
1	-6.191729000	-3.041976000	-1.166995000
6	4.079640000	2.730385000	-1.038727000
6	-4.240556000	-1.249051000	-1.097831000
6	1.028542000	-1.409162000	3.847409000
1	1.051241000	-1.319895000	4.928795000
6	-2.710104000	-4.714297000	-0.899680000
6	0.341428000	-2.592752000	1.855994000
6	-4.079643000	-2.731002000	-1.040264000
6	1.637234000	-0.562658000	1.666692000
6	2.710294000	4.713965000	-0.900449000
6	-0.354100000	-3.774105000	1.256809000
6	5.225342000	3.528967000	-1.090367000
1	6.191821000	3.040967000	-1.164754000
6	0.353168000	3.774896000	1.254451000
6	1.662232000	-0.452328000	3.058223000
1	2.175080000	0.396457000	3.499802000
6	2.312131000	0.511719000	0.869216000
6	-5.113500000	-4.915741000	-1.045381000
1	-6.004851000	-5.532945000	-1.079747000
6	-1.637285000	0.562849000	1.664003000
6	3.859713000	5.507905000	-0.951104000
1	3.742233000	6.586077000	-0.911359000
6	-1.661668000	0.452061000	3.055512000
1	-2.174096000	-0.397016000	3.497009000
6	-0.358215000	2.469063000	3.247624000
1	0.155914000	3.222429000	3.836062000
6	5.113794000	4.914976000	-1.045069000
1	6.005240000	5.532039000	-1.079490000
6	4.240373000	1.248379000	-1.095416000
6	-1.027874000	1.408779000	3.844738000
1	-1.050031000	1.319112000	4.926103000

6	1.296898000	-5.631640000	0.005322000
1	2.208885000	-5.184533000	0.407769000
1	0.826373000	-6.278364000	0.747679000
1	1.551186000	-6.226221000	-0.873305000
6	3.531790000	-1.491850000	-0.864238000
1	4.427694000	-1.416673000	-1.484121000
1	3.834746000	-1.758920000	0.149729000
1	2.871815000	-2.263277000	-1.265095000
6	-3.532577000	1.491383000	-0.866904000
1	-4.428677000	1.415801000	-1.486458000
1	-3.835235000	1.758635000	0.147104000
1	-2.872960000	2.262883000	-1.268203000
6	-1.296732000	5.632927000	0.002074000
1	-2.209268000	5.186358000	0.403866000
1	-0.826320000	6.279297000	0.744811000
1	-1.550026000	6.227728000	-0.876690000
6	2.825149000	3.328216000	-0.947722000
1	1.934134000	2.706164000	-0.920810000
6	-0.979465000	1.639368000	1.064171000
1	-0.933613000	1.724807000	-0.018958000
6	0.978923000	-1.638854000	1.066829000
1	0.932586000	-1.723938000	-0.016314000
6	-2.825118000	-3.328611000	-0.948242000
1	-1.934187000	-2.706454000	-0.921399000

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