Electronic Supplementary Information (ESI)

R/X Exchange Reactions on Pd and Pt Complexes Containing Phosphine Ligands, *cis*-$[M(R)_2\{P(X)(NMeCH_2)_2\}_2]$ (M = Pd, Pt), *via* a Phosphenium Intermediate and Theoretical Approach

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General: All reactions were carried out under an atmosphere of dry nitrogen by using standard Schlenk tube techniques. Benzene and hexane were distilled from sodium metal and were stored under a nitrogen atmosphere. CH_3CN and CH_2Cl_2 were distilled from CaH_2 under dry nitrogen prior to use. $Pd(Me)_2(cod)$,[1] $Pt(R)_2(cod)$ (R = Me,[2] Et,[2] Ph,[2] *p*-tol,[3] *p*-CF_3Ph[4]), $Pt(I)_2(cod)$,[5] and $P(X)(NMeCH_2)_2$ (X = Cl: **1a**[6], Br: **1b**[7]) were synthesized according to the reported procedures. NMR spectra (^1H, ^{13}C, ^{19}F and ^{31}P) were measured on a JEOL JNM-AL400 spectrometer at 25 °C. ^1H and ^{13}C NMR data were referred to residual peaks of solvent as an internal standard. Peak positions of $^{19}F\{^1H\}$ and $^{31}P\{^1H\}$ NMR spectra were referenced to external $CFCl_3$ and 85% H_3PO_4, respectively.

Synthesis: Synthesis of *cis*-[Pd(Cl)$_2${P(Me)(NMeCH$_2$)$_2$}$_2$] (2). A hexane solution (10 mL) of a palladium complex $Pd(Me)_2(cod)$, which was prepared by a reaction of $Pd(I)_2(cod)$ (1.405 g, 3.0 mmol) with 2 equiv of MeMgBr *in situ*, was slowly added to a hexane solution (2 mL) of **1a** (1.091 g, 7.05 mmol) at room temperature. The mixture was stirred for 10 min at room temperature. Volatile materials were removed under reduced pressure, and the resulting residue was washed with hexane (2 mL × 3), collected by filtration, and dried in *vacuo* to give a yellow solid of **2** (382.6 mg, 0.866 mmol, 29%). Single-crystals of **2** were obtained by solvent diffusion over a few days from a CH_2Cl_2 layer containing **2** and an overlayer of hexane. ^1H NMR (400.0 MHz, $CDCl_3$, δ, ppm, r.t.); 1.87 (apparent t, $^{2+4}J_{PH}$ = 4.9 Hz, 6H, PMe), 2.74 (apparent t, $^{3+5}J_{PH}$ = 6.4 Hz, 12H), NMe), 3.11 (dt, $^3J_{PH}$ = 6.8 Hz, $^3J_{HH}$ = 6.8 Hz, 4H, NCH_2), 3.16-3.22 (m, 4H, NCH_2). $^{13}C\{^1H\}$ NMR (100.4 MHz, $CDCl_3$, δ, ppm, r.t.); 21.04 (apparent t, $^{1+3}J_{PC}$ = 14.1 Hz, PMe), 34.17 (apparent t, $^{2+4}J_{PC}$ = 5.0 Hz, NMe), 51.28 (s, NCH_2). $^{31}P\{^1H\}$ NMR (161.7 MHz, $CDCl_3$, δ, ppm, r.t.); 108.15 (s). Elemental Analysis. Calcd. for $C_{10}H_{26}Cl_2N_4P_2Pd$: C, 27.20; H, 5.93; N, 12.69; Found: C, 26.79; H, 5.81; N, 12.59%.

Synthesis of *cis*-[Pt(Me)$_2${P(Cl)(NMeCH$_2$)$_2$}$_2$] (3a). A mixture of **1a** (298.0 mg, 1.953 mmol) and $Pt(Me)_2(cod)$ (325.5 mg, 0.977 mmol) in hexane (5 mL) was stirred for 10 min at room temperature. Volatile materials were removed under reduced pressure, and the resulting residue was washed with hexane (2 mL × 3) at –40 ºC, collected by filtration, and dried in *vacuo* to give a gray solid of **3a** (440.9 mg, 0.835 mmol, 85%). Single-crystals of **3a** were obtained by solvent diffusion over a few days from a benzene layer containing $Pt(Me)_2(cod)$ and **1a** and an overlayer of hexane. ^1H NMR (400 MHz, C_6D_6, δ, ppm): 1.52 (apparent t, $^3J_{PH}$ = 10.8 Hz, J_{PtH} = 71.9 Hz, 6H, PtMe), 2.47 (d, $^3J_{PH}$ = 14.4 Hz, 12H, NMe), 2.60-2.62 (m, 2H, NCH_2), 2.64-2.65 (m, 2H, NCH_2), 2.69-2.70 (m, 4H,

NCH_2). $^{13}C\{^1H\}$ NMR (100.4 MHz, C_6D_6, δ, ppm): 8.42 (dd, $^2J_{PC}$ = 9.9, 142.5 Hz, J_{PtC} = 751.2 Hz, PtMe), 33.0 (apparent t, $^{2+4}J_{PC}$ = 5.0 Hz, NMe), 51.05 (apparent t, $^{2+4}J_{PC}$ = 3.3 Hz NCH_2). $^{31}P\{^1H\}$ NMR (161.9 MHz, C_6D_6, δ, ppm): 155.18 (s, J_{PtP} = 2373 Hz). Elemental Analysis. Calcd. For $C_{10}H_{26}Cl_2N_4P_2Pt$: C, 22.65; H, 4.94; N, 10.57; Found: C, 22.91; H, 5.02; N, 10.16%.

Synthesis of *cis*-[Pt(Et)$_2${P(Cl)(NMeCH$_2$)$_2$}$_2$] (3b). A hexane solution (7 mL) of $Pt(Et)_2$(cod) (398.6 mg, 1.103 mmol) was added to **1a** (340.5 mg, 2.206 mmol) at room temperature. The mixture was stirred for 30 min at room temperature. The solvent was removed by filtration, and the resulting residue was washed with hexane (2 mL × 3), collected by filtration, and dried in *vacuo* to give a yellow solid of **3b** (317.7 mg, 0.569 mmol, 51%). ^1H NMR (400 MHz, C_6D_6, δ, ppm): 1.68 (dt, $^4J_{PH}$ = 14.4 Hz, $^3J_{HH}$ = 7.2 Hz, J_{PtH} = 76.3 Hz, 6H, $PtCH_2CH_3$), 2.23 (m, J_{PtH} = 73.9 Hz, 4H, $PtCH_2CH_3$), 3.46 (d, $^3J_{PH}$ = 15.6 Hz, 12H, NMe), 2.64-2.70 (m, 4H, NCH_2), 2.71-2.74 (m, 4H, NCH_2). $^{13}C\{^1H\}$ NMR (100.4 MHz, C_6D_6, δ, ppm): 16.90 (d, $^3J_{PC}$ = 6.6 Hz, J_{PtC} = 29.9 Hz, $PtCH_2CH_3$), 22.61 (dd, $^2J_{PC}$ = 139.6, 9.0 Hz, J_{PtC} = 676.0 Hz, $PtCH_2CH_3$), 32.95 (d, $^2J_{PC}$ = 12.4 Hz, NMe), 51.05 (d, $^2J_{PC}$ = 8.3 Hz NCH_2). $^{31}P\{^1H\}$ NMR (161.9 MHz, C_6D_6, δ, ppm): 159.56 (s, J_{PtP} = 2039 Hz). Elemental Analysis. Calcd. For $C_{12}H_{30}Cl_2N_4P_2Pt$: C, 25.81; H, 5.42; N, 10.03; Found: C, 23.88; H, 5.30; N, 9.67%.

Synthesis of *cis*-[Pt(Ph)$_2${P(Cl)(NMeCH$_2$)$_2$}$_2$] (3c). A mixture of **1a** (270.3 mg, 1.772 mmol) and $Pt(Ph)_2$(cod) (404.8 mg, 0.885 mmol) in benzene (5 mL) was stirred for 30 min at room temperature. Volatile materials were removed under reduced pressure, and the resulting residue was washed with hexane (2 mL × 3), collected by filtration, and dried in *vacuo* to give a white powder of **4c** (492.9 mg, 0.753 mmol, 85%). ^1H NMR (400 MHz, C_6D_6, δ, ppm): 2.40-2.44 (m, 4H, NCH_2), 2.52-2.57 (d, $^3J_{PH}$ = 15.6 Hz, 16H, 12H of NMe and 4H of NCH_2), 6.89 (t, $^3J_{HH}$ = 7.6 Hz, 2H, *p*-Ph), 7.09 (t, $^3J_{HH}$ = 6.8 Hz, 4H, *m*-Ph), 7.48 (t, $^3J_{HH}$ = 7.2 Hz, J_{PtH} = 63.1 Hz, 4H, *o*-Ph). $^{13}C\{^1H\}$ NMR (100.4 MHz, C_6D_6, δ, ppm): 33.14 (t, $^{2+4}J_{PC}$ = 5.8 Hz, NMe), 50.84 (t, $^{2+4}J_{PC}$ = 3.31 Hz, J_{PtC} = 15.76 Hz, NCH_2), 123.29 (s, J_{PtC} = 5.7, *p*-Ph), 127.35 (t, $^3J_{PC}$ = 4.9 Hz, J_{PtC} = 68.9 Hz, *o*-Ph), 136.98 (t, $^4J_{PC}$ = 3.3 Hz, J_{PtC} = 36.6 Hz, *m*-Ph), 156.48 (dd, $^1J_{PC}$ = 169.2, $^3J_{PC}$ = 16.6 Hz, J_{PtC} = 864.2 Hz, *ipso*-Ph). $^{31}P\{^1H\}$ NMR (161.9 MHz, C_6D_6, δ, ppm): 145.65 (s, J_{PtP} = 2419 Hz). Elemental Analysis. Calcd. For $C_{20}H_{30}Cl_2N_4P_2Pt$: C, 36.71; H, 4.62; N, 8.56; Found: C, 36.93; H, 4.82; N, 8.19%.

Synthesis of *cis*-[Pt(*p*-tol)$_2${P(Cl)(NMeCH$_2$)$_2$}$_2$] (3d). A mixture of **1a** (546.1 mg, 3.579 mmol) and Pt(*p*-tol)$_2$(cod) (667.9 mg, 1.377 mmol) in benzene (5 mL) was stirred for 15 min at room temperature. Volatile materials were removed under reduced pressure, and the resulting residue was washed with hexane (2 mL × 3), collected by filtration, and dried in *vacuo* to give a gray solid of **3d** (677.5 mg, 0.993 mmol, yield 87%). ^{1}H NMR (400 MHz, C_6D_6, δ, ppm): 2.13 (s, 6H, Me in *p*-tol), 2.42 -2.51 (m, 4H, NCH_2), 2.57 (d, $^3J_{PH}$ = 15.6 Hz, 16H, 12H of NMe and 4H of NCH_2), 6.94 (d, $^3J_{HH}$ = 6.0 Hz, 4H, *m*-Ph), 7.39 (t, $^3J_{PH}$ = 8.0 Hz, J_{PtH} = 170.6 Hz, 4H, *o-Ph*). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6, δ, ppm): 21.58 (s, Me in *p*-tol), 33.60 (m, NMe), 51.22 (t, $^{2+4}J_{PC}$ = 3.32 Hz, NCH_2), 129.07 (s, *p*-Ph), 131.46 (s, J_{PtC} = 12.44 Hz, *m*-Ph), 136.70 (s, J_{PtC} = 38.98 Hz, *o*-Ph), 153.83 (dd, $^1J_{PC}$ = 153.4, $^3J_{PC}$ = 17.4 Hz, J_{PtC} = 870.8 Hz, *ipso*-Ph). ^{31}P{^{1}H} NMR(162 MHz, C_6D_6, δ, ppm): 146.32 (s, J_{PtP} = 2395 Hz). Elemental Analysis. Calcd. for $C_{22}H_{34}Cl_2N_4P_2Pt$: C, 38.72; H, 5.02; N, 8.21; Found: C, 37.33; H, 5.37; N, 7.99%.

Synthesis of *cis*-[Pt(*p*-CF$_3$Ph)$_2${P(Cl)(NMeCH$_2$)$_2$}$_2$] (3e). A mixture of **1a** (311.5 mg, 2.042 mmol) and Pt(*p*-CF_3Ph)$_2$(cod) (511.2 mg, 0.861 mmol) in benzene (4 mL) was stirred for 20 min at room temperature. Volatile materials were removed under reduced pressure, and the resulting residue was washed with hexane (2 mL × 3), collected by filtration, and dried in *vacuo* to give a yellow solid of **3e** (642.2 mg, 0.812 mmol, 94%). ^{1}H NMR (400 MHz, C_6D_6, δ, ppm): 2.23-2.32 (m, 4H, NCH_2), 2.37 (d, $^3J_{PH}$ = 15.1 Hz, 12H, NMe), 2.46 (m, 4H, NCH_2), 7.29 (d, $^3J_{HH}$ = 7.3 Hz, 4H, *m*-Ph), 7.34 (m, J_{PtH} = 61.5 Hz, 4H, *o*-Ph). ^{13}C{^{1}H} NMR (100.4 MHz, C_6D_6, δ, ppm): 31.80 (t, $^2J_{PC}$ = 10.8 Hz, NMe), 50.73 (s, NCH_2), 123.41 (s, J_{PtC} = 63.11 Hz, *o*-Ph), 125.28 (q, $^2J_{FC}$ = 30.7 Hz, *p*-Ph), 125.89 (q, $^1J_{FC}$ = 271.5 Hz, CF_3), 136.73 (s, J_{PtC} = 38.2 Hz, *m*-Ph), 162.49 (dd, $^1J_{PC}$ = 167.7, $^3J_{PC}$ = 17.4 Hz, J_{PtC} = 862.0 Hz, *ipso*-Ph). ^{31}P{^{1}H} NMR (161.7 MHz, C_6D_6, δ, ppm): 141.52 (s, J_{PtP} = 2533 Hz). ^{19}F{^{1}H} NMR (376 MHz, C_6D_6, δ, ppm): –61.53 (s). Elemental Analysis. Calcd. for $C_{22}H_{28}Cl_2F_6N_4P_2Pt$: C, 33.43; H, 3.57; N, 7.09%; Found: C, 33.15; H, 3.52; N, 7.10%.

Synthesis of *cis*-[Pt(Me)$_2${P(Br)(NMeCH$_2$)$_2$}$_2$] (3f). A hexane solution (9 mL) of Pt(Me)$_2$(cod) (355.7 mg, 1.07 mmol) was added to **1b** (420.7 mg, 2.14 mmol) at room temperature. The mixture was stirred for 5 min at room temperature. The solvent was removed by filtration, and the resulting residue was washed with hexane (2 mL × 3), collected by filtration, and dried in *vacuo* to give a yellow solid of **3f** (568.1 mg, 0.918 mmol, 86%). ^{1}H NMR (400 MHz, C_6D_6, δ, ppm): 1.63 (apparent t, $^3J_{PH}$ = 10.8 Hz, J_{PtH} = 73.1 Hz, 6H, PtMe), 2.35 (d, $^3J_{PH}$ = 16.8 Hz, 12H, NMe), 2.53-2.54 (m, 2H, NCH_2), 2.58 (m, 2H, NCH_2), 2.62 (m, 4H, NCH_2). ^{31}P{^{1}H} NMR (161.7 MHz, C_6D_6, δ, ppm): 166.77 (s, J_{PtP} = 2179 Hz). Elemental Analysis was not achieved due to instability.

Synthesis of *cis*-[Pt(I)$_2${P(Cl)(NMeCH$_2$)$_2$}$_2$] (3g). A CH_2Cl_2 solution (4 mL) of Pt(I)$_2$(cod) (314.3 mg, 0.565 mmol) was added to **1a** (172.4 mg, 1.130 mmol) at room temperature. The mixture was stirred for 3 days at room temperature. The solvent was removed by filtration and the residue was dried in *vacuo* to give dark red crystals of **3g** (266.0 mg, 0.353 mmol, 62%). ^{1}H NMR (400.0 MHz, $CDCl_3$, δ, ppm, r.t.); 2.86 (d, $^3J_{PH}$ = 15.6 Hz, 12H, NMe), 3.32-3.37 (m, 8H, CH_2). ^{13}C{^{1}H} NMR (100.4 MHz, $CDCl_3$, δ, ppm): 33.66 (t, $^2J_{PC}$ = 5.0 Hz, NMe), 50.73 (t, $^2J_{PC}$ = 13.5 Hz, NCH_2). ^{31}P{^{1}H} NMR (161.7 MHz, $CDCl_3$, δ, ppm, r.t.); 85.83 (s, J_{PtP} = 5254 Hz). Elemental Analysis. Calcd. for $C_8H_{20}Cl_2I_2N_4P_2Pt$: C, 12.74; H, 2.67; N, 7.43%; Found: C, 12.83; H, 2.61; N, 7.25%.

Synthesis of *cis*-[Pt(Me)$_2${P(Cl)(NMe$_2$)$_2$}$_2$] (3h). A hexane solution (7 mL) of Pt(Me)$_2$(cod) (319.0 mg, 0.927 mmol) was added to **1a** (286.6 mg, 0.927 mmol) at room temperature. The mixture was stirred for 15 min at room temperature. Volatile materials were removed under reduced pressure until the residual solution became ca. 2 mL, and the solvent was removed by filtration at –78 °C. The resulting residue was washed with cold hexane (1 mL × 3), collected by filtration at –78 °C, and dried in *vacuo* to give a gray solid of **3h** (350.6 mg, 0.656 mmol, 71%). ^{1}H NMR (400 MHz, C_6D_6, δ, ppm): 1.26 (apparent t, $^3J_{PH}$ = 8.3 Hz, J_{PtH} = 71.6 Hz, 6H, PtMe), 2.58 (d, $^3J_{PH}$ = 11.2 Hz, 24H, NMe). ^{31}P{^{1}H} NMR (161.7 MHz, C_6D_6, δ, ppm): 156.04 ppm (s, J_{PtP} = 2665 Hz). Sufficient data of the elemental analysis were not obtained due to its instability.

Synthesis of *cis*-[Pt(Cl)$_2${P(Me)(NMeCH$_2$)$_2$}$_2$] (4a). An acetonitrile solution (10 mL) of *cis*-[Pt(Me)$_2${P(Cl)(NMeCH$_2$)$_2$}$_2$] (**3a**) (393.0 mg, 0.741 mmol) was stirred for 3 h at room temperature. Volatile materials were removed under reduced pressure, and the resulting residue was washed with hexane (2 mL × 3), collected by filtration, and dried in *vacuo* to give a white solid of **4a** (390.4 mg, 0.736 mmol, 99%). Single-crystals of **4a** were obtained by solvent diffusion over a few days from a CH_2Cl_2 layer containing **4a** and an overlayer of hexane. ^{1}H NMR (400 MHz, $CDCl_3$, δ, ppm): 1.78 (d, $^2J_{PH}$ = 10.0 Hz, 6H, PMe), 2.69 (d, $^3J_{PH}$ = 12.39 Hz, 12H, NMe), 3.09-3.18 (m, 8H, NCH_2). ^{13}C{^{1}H} NMR (100.4 MHz, $CDCl_3$, δ, ppm): 18.66 (dd, $^1J_{PC}$ = 43.2, $^3J_{PC}$ = 2.5 Hz, J_{PtC} = 153.5 Hz, PMe), 33.88 (apparent t, $^{2+4}J_{PC}$ = 5.0 Hz, NMe), 51.15 (s, NCH_2). ^{31}P{^{1}H} NMR (161.7 MHz, $CDCl_3$, δ, ppm): 76.62 (s, J_{PtP} = 4406 Hz). Elemental Analysis. Calcd. for $C_{10}H_{26}Cl_2N_4P_2Pt$: C, 22.65; H, 4.94; N, 10.57; Found: C, 22,41; H, 4.95; N, 10.23%.

Synthesis of *cis*-[Pt(Cl)$_2${P(Et)(NMeCH$_2$)$_2$}$_2$] (4b). An acetonitrile solution (15 mL) of *cis*-

$[Pt(Et)_2\{P(Cl)(NMeCH_2)_2\}_2]$ (**3b**) (138.1 mg, 0.247 mmol) was stirred for 40 min at room temperature. Volatile materials were removed under reduced pressure, and the resulting residue was washed with hexane (2 mL × 3), collected by filtration, and dried in *vacuo* to give a white solid of **4b** (135.9 mg, 0.243 mmol, 99%). ^{1}H NMR (400 MHz, $CDCl_3$, δ, ppm): 0.94 (dt, $^3J_{PH}$ = 18.4 Hz, $^3J_{HH}$ = 7.6 Hz, 6H, PCH_2CH_3), 2.44 (m, 4H, PCH_2CH_3), 2.73 (d, $^3J_{PH}$ = 11.2 Hz, 12H, NMe), 3.16-3.26 (m, 8H, NCH_2). $^{13}C\{^1H\}$ NMR (100.4 MHz, $CDCl_3$, δ, ppm): 8.36 (apparent t, $^{2+4}J_{PC}$ = 3.3 Hz, PCH_2CH_3), 28.69 (dd, $^1J_{PC}$ = 43.1, $^3J_{PC}$ = 1.4 Hz, J_{PtC} = 157.6 Hz, PCH_2CH_3), 33.80 (apparent t, $^{2+4}J_{PC}$ = 4.1 Hz, NMe), 51.57 (s, NCH_2). $^{31}P\{^1H\}$ NMR (161.7 MHz, $CDCl_3$, δ, ppm): 82.61 (s, J_{PtP} = 4380 Hz). Elemental Analysis. Calcd. For $C_{12}H_{30}Cl_2N_4P_2Pt$: C, 25.81; H, 5.42; N, 10.03; Found: C, 25.84; H, 5.46; N, 9.86%.

Synthesis of *cis*-$[Pt(Cl)_2\{P(Ph)(NMeCH_2)_2\}_2]$ (4c). An acetonitrile solution (7 mL) of *cis*-$[Pt(Ph)_2\{P(Cl)(NMeCH_2)_2\}_2]$ (**3c**) (284.5 mg, 0.435 mmol) was stirred for 30 min at room temperature. Volatile materials were removed under reduced pressure, and the resulting residue was washed with hexane (2 mL × 3), collected by filtration, and dried in *vacuo* to give a white solid of **4c** (275.9 mg, 0.422 mmol, 97%). ^{1}H NMR (400 MHz, $CDCl_3$, δ, ppm): 2.59 (d, $^3J_{PH}$ = 11.6 Hz, 12H, NMe), 2.94-3.03 (m, 8H, NCH_2), 7.15 (s, 2H, *p*-Ph), 7.29 (t, $^3J_{HH}$ = 7.20 Hz, 4H, *m*-Ph), 7.30-7.53 (m, 4H, *o*-Ph). $^{31}P\{^1H\}$ NMR (161.7 MHz, $CDCl_3$, δ, ppm): 75.78 (s, J_{PtP} = 4409 Hz). Elemental Analysis. Calcd. For $C_{20}H_{30}Cl_2N_4P_2Pt$: C, 36.71; H, 4.62; N, 8.56; Found: C, 36.71; H, 4.62; N, 8.56%.

Synthesis of cis-$[Pt(Cl)_2\{P(p\text{-tol})(NMeCH_2)_2\}_2]$ (4d). In a procedure analogous to that outlined in the case of complex **4c**, $Pt(p\text{-tol})_2\{P(Cl)(NMeCH_2)_2\}_2$ (**3d**) (314.4 mg, 0.460 mmol) in acetonitrile (20 mL) gave a white powder of **4d** (307.9 mg, 0.451 mmol, 98%). Single-crystals of **4d** were obtained by solvent diffusion over a few days from a CH_2Cl_2 layer containing **4d** and an overlayer of hexane. ^{1}H NMR (400 MHz, $CDCl_3$, δ, ppm): 2.36 (s, 6H, Me in *p*-tol), 2.67 (d, $^3J_{PH}$ = 11.2 Hz, 12H, NMe), 3.02-3.13 (m, 8H, NCH_2), 7.19 (d, $^3J_{HH}$ = 6.4 Hz, 4H, *m*-Ph), 7.50 (dd, $^3J_{PH}$ = 11.2 Hz, $^3J_{HH}$ = 8.0 Hz, 4H, *o*-Ph). $^{13}C\{^1H\}$ NMR (100.4 MHz, $CDCl_3$, δ, ppm): 21.57(s, Me in *p*-tol), 35.28 (apparent t, $^{2+4}J_{PC}$ = 4.2 Hz, NMe), 51.25 (s, NCH_2), 128.34 (d, J_{PC} = 12.4 Hz, J_{PtC} = 10.7, Ph), 130.20 (d, J_{PC} = 12.4 Hz, J_{PtC} = 10.7, Ph), 133.70 (d, $^1J_{PC}$ = 71.3 Hz, J_{PtC} = 144.3 Hz, *ipso*-Ph), 140.68 (s, *C*Me). $^{31}P\{^1H\}$ NMR (161.7 MHz, $CDCl_3$, δ, ppm): 75.64 (s, J_{PtP} = 4417 Hz). Elemental Analysis. Calcd. for $C_{22}H_{34}Cl_2N_4P_2Pt$: C, 38.72; H, 5.02; N, 8.21; Found: C, 38.10; H, 4.97; N, 7.95%.

Synthesis of *cis*-[Pt(Cl)$_2${P(*p*-CF_3Ph)(NMeCH$_2$)$_2$}$_2$] (4e). An acetonitrile solution (15 mL) of *cis*-[Pt(*p*-CF_3Ph)$_2${P(Cl)(NMeCH$_2$)$_2$}$_2$] (**3e**) (1.280 g, 1.62 mmol) was stirred for 4 h at 55 ºC. Volatile materials were removed under reduced pressure, and the resulting residue was washed with hexane (2 mL × 3), collected by filtration, and dried in *vacuo* to give a white solid of **4e** (*cis* and *trans* isomers in the 7 : 1 ratio determined by ^{31}P NMR) (1.175 g, 1.49 mmol, 92%). ^{31}P{^{1}H} NMR (161.7 MHz, C_6D_6, δ, ppm): 72.17 (s, J_{PtP} = 4450 Hz for *cis* isomer), 98.03 (s, J_{PtP} = 3495 Hz for *trans* isomer). Signals in ^{1}H and ^{13}C{^{1}H} NMR spectra could not unambiguously be assigned due to severe overlapping of resonances.

Synthesis of *cis*-[Pt(Br)$_2${P(Me)(NMeCH$_2$)$_2$}$_2$] (4f). An acetonitrile solution (7 mL) of *cis*-[Pt(Me)$_2${P(Br)(NMeCH$_2$)$_2$}$_2$] (**3f**) (533.9 mg, 0.862 mmol) was stirred for 1 h at room temperature. Volatile materials were removed under reduced pressure, and the resulting residue was washed with hexane (2 mL × 3), collected by filtration, and dried in *vacuo* to give a yellow solid of **4f** (513.0 mg, 0.829 mmol, 96%). Single-crystals of **4f** were obtained by solvent diffusion over a few days from a CH_2Cl_2 layer containing **4f** and an overlayer of hexane. ^{1}H NMR (400 MHz, $CDCl_3$, δ, ppm): 1.93 (d, $^2J_{PH}$ = 8.3 Hz, J_{PtH} = 26.4 Hz, 6H, PMe), 2.71 (d, $^3J_{PH}$ = 12.2 Hz, J_{PtH} = 26.4 Hz, 12H, NMe), 3.10-3.20 (m, 8H, NCH_2). ^{13}C{^{1}H} NMR (100.7 MHz, $CDCl_3$, δ, ppm): 21.15 (d, $^1J_{PC}$ = 39.9 Hz, J_{PtC} = 163.6 Hz, PMe), 33.84 (d, $^2J_{PC}$ = 9.1 Hz, NMe), 50.93 (s, J_{PtC} = 29.1 Hz, NCH_2). ^{31}P{^{1}H} NMR (161.7 MHz, $CDCl_3$, δ, ppm): 76.23 (s, J_{PtP} = 4361 Hz). Elemental Analysis. Calcd. for $C_{10}H_{26}Br_2N_4P_2Pt$: C, 19.40; H, 4.23; N, 9.05; Found: C, 19.50; H, 4.23; N, 8.81%.

Synthesis of *cis*-[Pt(Cl)$_2${P(Me)(NMe$_2$)$_2$}$_2$] (4h). An acetonitrile solution (2 mL) of *cis*-[Pt(Me)$_2${P(Cl)(NMe$_2$)$_2$}$_2$] (**3h**) (81.1 mg, 0.152 mmol) was stirred for 10 min at room temperature. Volatile materials were removed under reduced pressure, and the resulting residue was washed with hexane (2 mL × 3), collected by filtration, and dried in *vacuo* to give a yellow solid of **4h** (78.7 mg, 0.147 mmol, 97%). ^{1}H NMR (400 MHz, C_6D_6, δ, ppm): 1.76 ppm (d, $^2J_{PH}$ = 8.4 Hz, J_{PtH} = 24.4 Hz, 6H, PMe), 2.76 ppm (d, $^3J_{PH}$ = 9.6 Hz, 24H, NMe). ^{13}C{^{1}H} NMR (100.4 MHz, $CDCl_3$, δ, ppm): 16.93 (dd, $^{1+3}J_{PC}$ = 68.8, 2.4 Hz, PMe), 39.09 (t, $^{2+4}J_{PC}$ = 2.5 Hz, NMe). ^{31}P{^{1}H} NMR (161.7 MHz, C_6D_6, δ, ppm): 66.07 ppm (s, J_{PtP} = 4314 Hz). Elemental Analysis. Calcd. for $C_{10}H_{30}Cl_2N_4P_2Pt$: C, 22.48; H, 5.66; N, 10.49; Found: C,22.40; H, 5.84; N, 9.15%.

X-ray crystallography measurements

Crystals (**2**, **3a**, **3g**, **4a**, **4d** and **4f**) suitable for X-ray diffraction studies were separately mounted in a glass capillary. All of data were collected at 200 K on Rigaku AFC-7/Mercury CCD area-detector diffractometer equipped with monochromated MoKα radiation. All of calculations were performed with the CrystalClear software package of Molecular Structure Corporation. A full-matrix least-squares refinement was used for the non-hydrogen atoms with anisotropic thermal parameters. Hydrogen atoms were located by assuming the ideal geometry and were included in the structure calculation without further refinement of the parameters. Those crystal data are listed in Tables S1 and S2. Crystallographic data for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre, CCDC No. 1040103 for **2**, 1041011 for **3a**, 1041007 for **3g**, 1041008 for **4a**, 1041009 for **4d**, and 1041010 for **4f**. Copies of this information may be obtained free of charge from the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (Fax: +44-1223-336-033; e-mail: deposit@ccdc.cam.ac.uk or http://www.ccdc.cam.ac.uk).

Table S1. Crystallographic data and details of structure refinement of complexes **2**, **3a** and **4a**.

	2	**3a**	**4a**
empirical formula	$C_{10}H_{26}Cl_2N_4P_2Pd$	$C_{10}H_{26}Cl_2N_4P_2Pt$	$C_{10}H_{26}Cl_2N_4P_2Pt$
formula weight	441.59	530.28	530.28
T (K)	200(2)	200(2)	200(2)
crystal system	Orthorhombic	Monoclinic	Orthorhombic
space group	$Pna2_1$	$C2/c$	$Pna2_1$
a (Å)	11.9253(19)	11.246(3)	12.007(2)
b (Å)	16.170(3)	9.1156(19)	16.096(3)
c (Å)	9.0441(12)	17.511(4)	9.0774(16)
β (°)		96.035(5)	
volume (Å^3)	1744.0(5)	1785.2(7)	1754.2(5)
Z	4	4	4
ρ_{calcd} (mg m^{-3})	1.682	1.973	2.008
μ (mm^{-1})	1.547	8.332	8.479
F(000)	896	1024	1024
crystal size (mm^3)	0.24 × 0.20 × 0.05	0.25 × 0.10 × 0.05	0.30 × 0.20 × 0.12
reflections collected	16484	8531	16812
independent reflections (R(int))	3737 (0.0395)	2044 (0.0379)	3898 (0.0416)
$R1$ ($I > 2\sigma(I)$)	0.0349	0.0283	0.0336
w$R2$	0.0675	0.0586	0.0555
Goodness of fit	1.138	1.169	1.187

Table S2. Crystallographic data and details of structure refinement of complexes **4d**, **4f** and **3g**.

	4d	**4f**	**3g**
empirical formula	$C_{22}H_{34}Cl_2N_4P_2Pt$	$C_{10}H_{26}Br_2N_4P_2Pt$	$C_8H_{20}Cl_2I_2N_4P_2Pt$
formula weight	682.46	619.20	754.01
T (K)	200(2)	200(2)	200(2)
crystal system	Monoclinic	Tetragonal	Orthorhombic
space group	$P2_1/c$	$P\text{-}42_1c$	$Pna2_1$
a (Å)	10.0497(4)	19.7900(17)	16.534(2)
b (Å)	32.6793(15)	19.7900(17)	12.1735(15)
c (Å)	16.1968(7)	9.3200(9)	9.4837(12)
β (°)	91.935(2)		
volume (Å^3)	5316.3(4)	3650.1(6)	1908.8(4)
Z	8	8	4
ρ_{calcd} (mg m^{-3})	1.705	2.254	2.624
μ (mm^{-1})	5.617	12.236	11.026
F(000)	2688	2336	1376
crystal size (mm^3)	0.38 × 0.07 × 0.06	0.10 × 0.08 × 0.02	0.12 × 0.08 × 0.07
reflections collected	40696	27014	18154
independent reflections (R(int))	11745 (0.0440)	4149 (0.0645)	4033 (0.0423)
$R1$ ($I > 2\sigma(I)$)	0.0484	0.0473	0.0320
w$R2$	0.0701	0.0737	0.0655
Goodness of fit	1.191	1.251	1.114

Calculation Section

<u>path A: *via* metallaphosphorane</u>

For metallasphophorane complexes **6a** and **7a**, geometry searches for local minima (LM) and transition states (TS) were performed using B3PW91/BS2. The results are shown in Figs. S1–S2. The energy minimum search for **6a** lead to a structure similar to the reactant complex **3a** (see Figure S1(c)), and TS search lead to a structure similar to TS (**10a** → **11a**) of path C (see Fig. S1(d)). For **7a**, the minimum and TS searches lead to a three-coordinated complex in which a Cl^- ion was situated far from the Pt (Fig. S2). The LM and TS structures of metallaphosphorane type were not found for both complexes. Therefore, the path A is unfavorable reaction pathway.

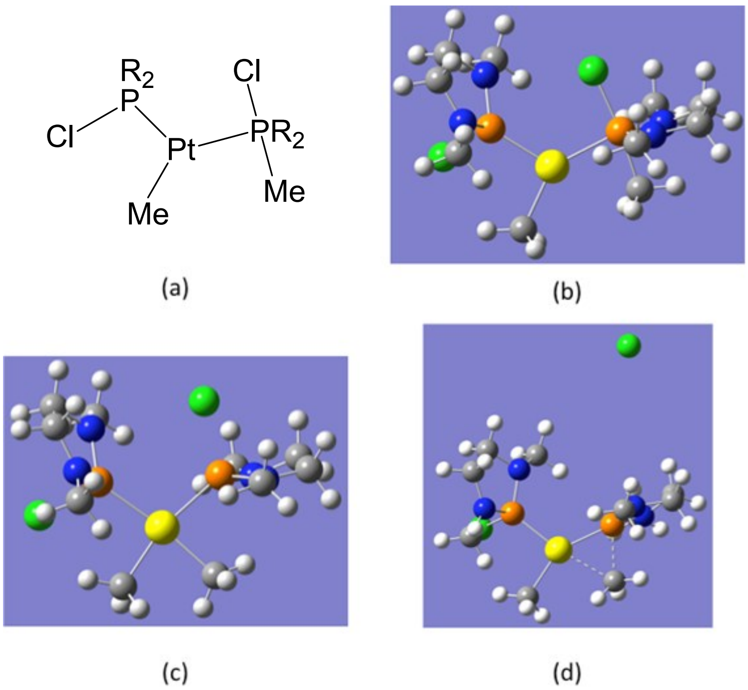


Fig. S1. (a) Chemical formula of **6a**, (b) an initial structure of **6a**, (c) the optimized structure (local minimum)**,** and (d) the obtained TS structure.

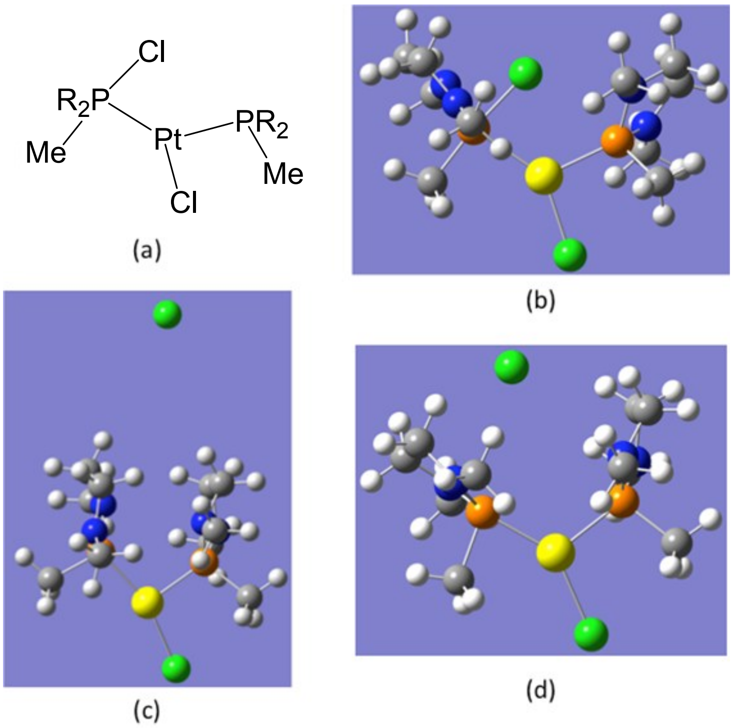


Fig. S2. (a) Chemical formula of **7a**, (b) an initial structure of **7a**, (c) the optimized structure (local minimum), and (d) the obtained TS structure.

path B: *via* oxidative addition

Path B is the reaction sequences involving oxidative addition of the P–Cl bond of **3a** (**5a**) to give a phosphide complex $Pt(Cl)(Me)_2(PR_2)(PClR_2)$ (**8a**) ($Pt(Cl)_2(Me)(PR_2)(PR_2Me)$ (**9a**)) followed by reductive elimination of the Me and PR_2 groups to give $Pt(Cl)(Me)(PR_2Cl)(PR_2Me)$ (**5a**) (($Pt(Cl)_2(PMeR_2)_2$ (**4a**)). As $Pt(Cl)(Me)_2(PR_2)(PClR_2)$ (**8a**) is supposed to be formed by the oxidative addition of one of P–Cl bonds in **3a**, it might be reasonable that the PR_2 and Cl ligands are situated *cis* to each other right after the oxidative addition. The same situaton is postulated for **9a**. Thus, five five-coordinated isomers are conceivable for **8a** and **9a** as well. The five initial structures are named as A_{init}, B_{init}, C_{init}, D_{init}, and E_{init} for **8a**, and A'_{init}, B'_{init}, C'_{init}, D'_{init}, and E'_{init} for **9a** (see Figs. S3 and S4). A_{init}, B_{init}, and E_{init} (A'_{init}, B'_{init}, and E'_{init}) have the phosphide ligand in a basal position. C_{init} and D_{init} (C'_{init} and D'_{init}) have the phosphide ligand at the top of the pyramidal structure. Next, geometries of these ten complexes (A_{init}–E_{init} and A'_{init}–E'_{init}) were optimized at the B3PW91/BS2 level. The results are shown on the right-hand side of Figs. S3 and S4 for **8a** and **9a**, respectively. For **8a**, A_{opt} and B_{opt} are quite similar four-coordinated complexes with a Cl atom far away from Pt. Therefore, A_{opt} and B_{opt} are not the products caused by oxidative addition. C_{opt} and D_{opt} have a phosphide ligand at the top of the pyramidal structure with two Me ligands at the *cis* and *trans* positions, respectively. As the phosphide phosphorus does not adopt a planar geometry, the phosphide serves as a 1e-donor ligand in both C_{opt} and D_{opt}. E_{opt} has almost the same geometry as that of C_{opt}. Thus, two types of optimized geometries C_{opt} and D_{opt} were obtained for five-coordinated complex **8a**. Comparing the energy of C_{opt} with that of D_{opt}, C_{opt} is more stable. D_{opt} is less stable than the reactant **3a**, by 10.23 kcal/mol. C_{opt} is less stable but comparable in energy to **3a**. The energy difference between them is only 2.14 kcal/mol. As for **9a**, quite similar results were obtained (see Fig. S4). The only difference between the structures in **8a** and **9a** is that B'_{opt} is quite similar to C'_{opt} for **9a**. These results suggest that the Me/Cl exchange may provide five-coordinated complexes such as C_{opt} and C'_{opt}. Then, scan calculations for the inverse reaction, i.e., the Cl transfer from Pt to phosphine (**8a** → **3a** and **9a** → **5a**) were performed starting from the obtained stable five-coordinated structures C_{opt} and C'_{opt}. The results are shown in Figs. S5 and S6. The potential energy rose with the transfer of Cl ion in both cases, and the saddle point P in Fig. S5 was found for **8a**. For the saddle point of **8a** (point P: $r_{Pt–Cl}$ = 3.44 Å, $r_{P–Cl}$ = 3.30 Å) and the local maximum of **9a** (point Q: $r_{Pt–Cl}$ = 3.73 Å, $r_{P–Cl}$ = 2.91 Å), TS search calculations were performed. However, the obtained structures were found to be not a TS but a stable five-coordinated complex (see Figs. S7 and S8). Another PES calculation was also calculated against Pt–Cl distance and the P(1)–Pt–P(2)–C(1) dihedral angle. In this PES calculation, because the corresponding phosphenium ligand had been eliminated from Pt with the decreasing of dihedral angle, Pt–P(2) distance was fixed. The saddle point R was found as shown in Fig. S9. For the point R (r(Pt–Cl) = 2.9 Å, d(P–Pt–P–C) = 146º), TS search calculation was performed. The obtained TS structure with one negative force constant was not for the Cl transfer from P to Pt, but corresponded to the Cl transfer from the eliminated phosphine to Pt or the P–Pt cleavage by Cl. The product by IRC calculation from the TS was the four-coordinated complex, $PtCl(Me)_2P(NMeCH)_2$, and the free phosphenium (See Figure S10). Additionally, the energy difference between the complex **3a** and the TS was too large (221.24 kcal/mol). These results suggested that this route was energetically unfavorable although the addition of the free phosphenium to $PtCl(Me)_2P(NMeCH)_2$ might lead to the C_{opt}. Therefore, path B is not a plausible pathway.

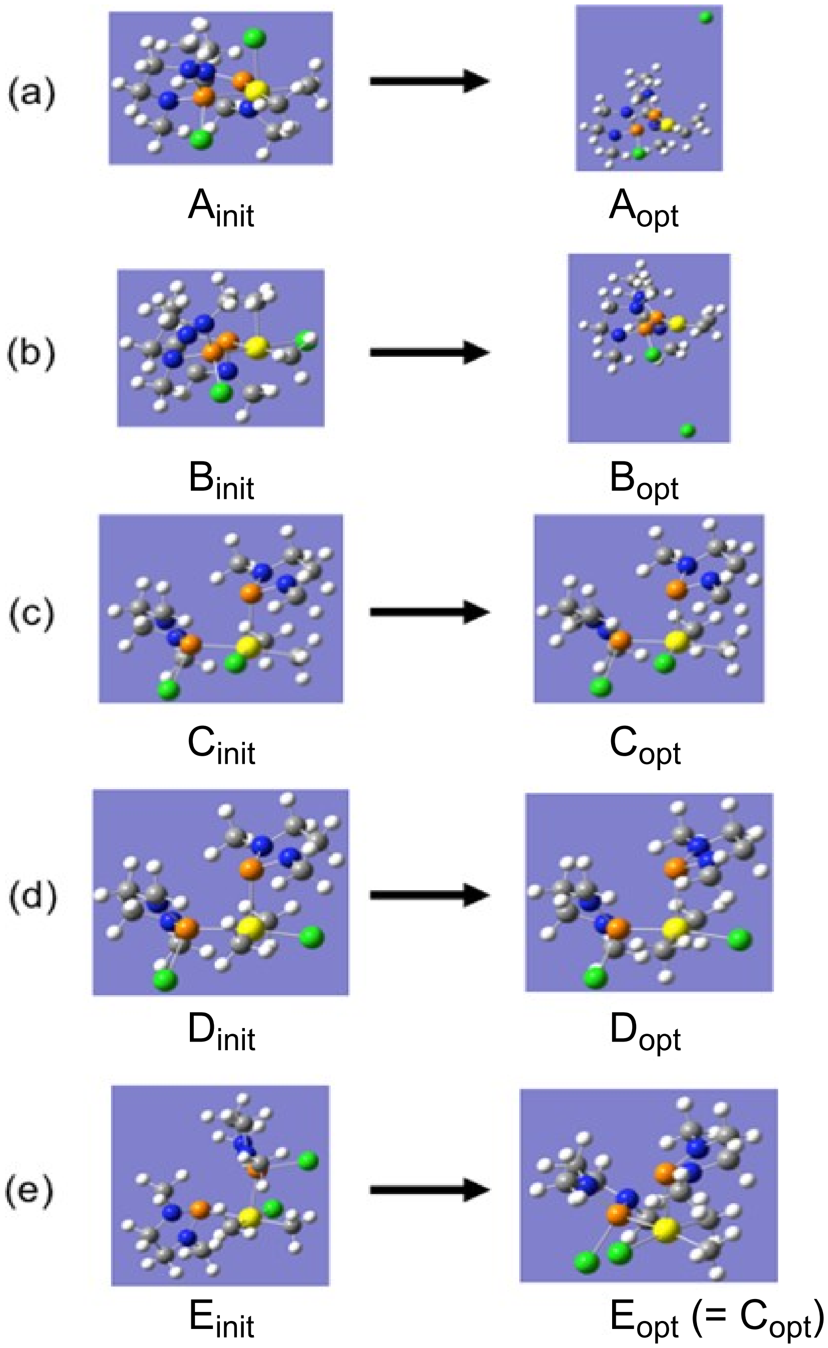


Fig. S3. Five initial structures (A_{init} – E_{init}) of **8a** and the obtained optimized structures (A_{opt} – E_{opt}); (a) Cl is located at the top of the pyramidal structure (A_{init}), (b) Me is at the pyramidal summit (B_{init}), (c) phosphide ligand is at the pyramidal summit and two Me ligands are in *cis*-position (C_{init}), (d) phosphide ligand is at the pyramidal summit and two Me ligands are in *trans*-position (D_{init}), and (e) phosphine ligand is at the pyramidal summit (E_{init}).

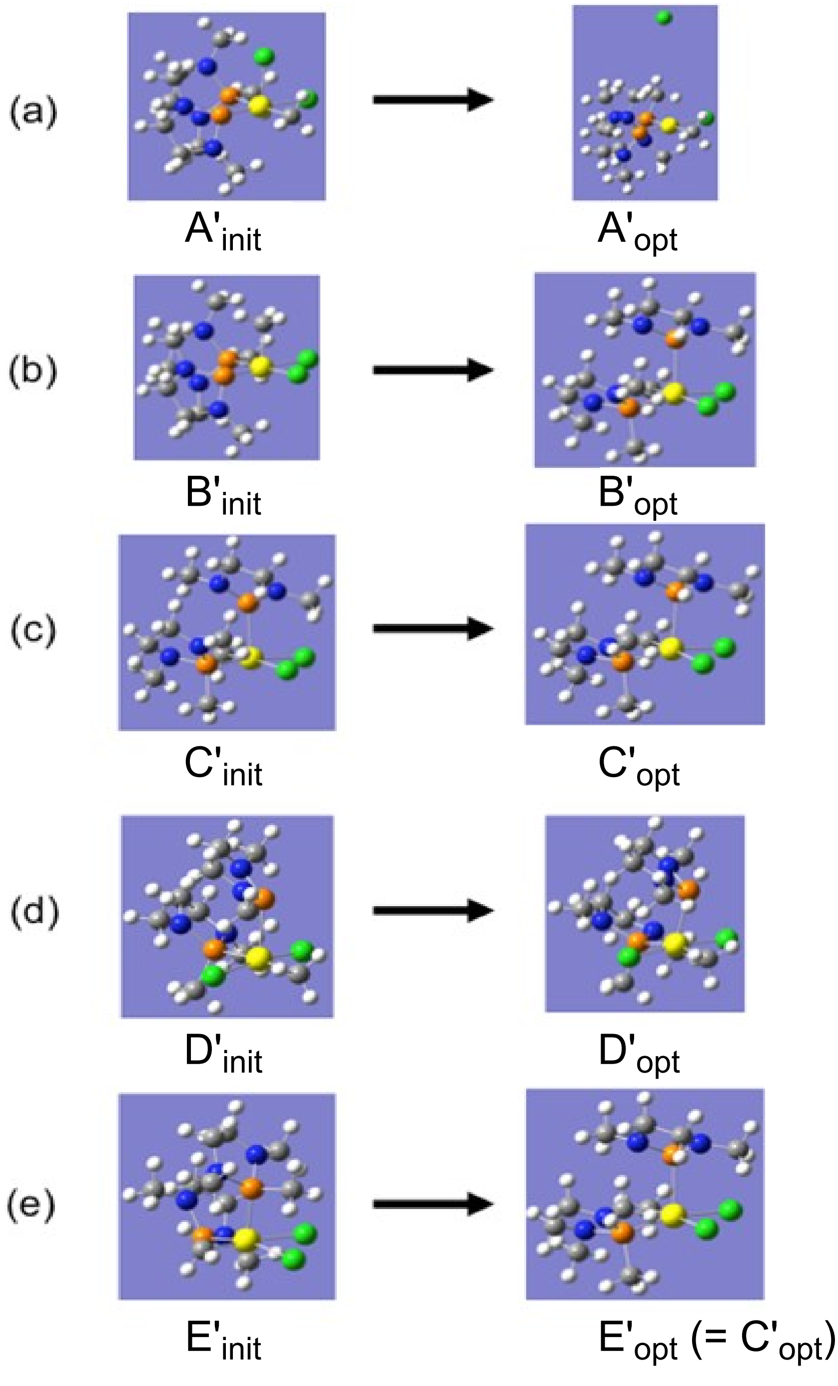


Fig. S4. Five initial structures (A’$_{init}$ – E’$_{init}$) of **9a** and the obtained optimized structures (A’$_{opt}$ – E’$_{opt}$); (a) complex A’, (b) complex B’, (c) complex C’, (d) complex D’, and (e) complex E’. See the figure caption in Fig. S3 in more details.

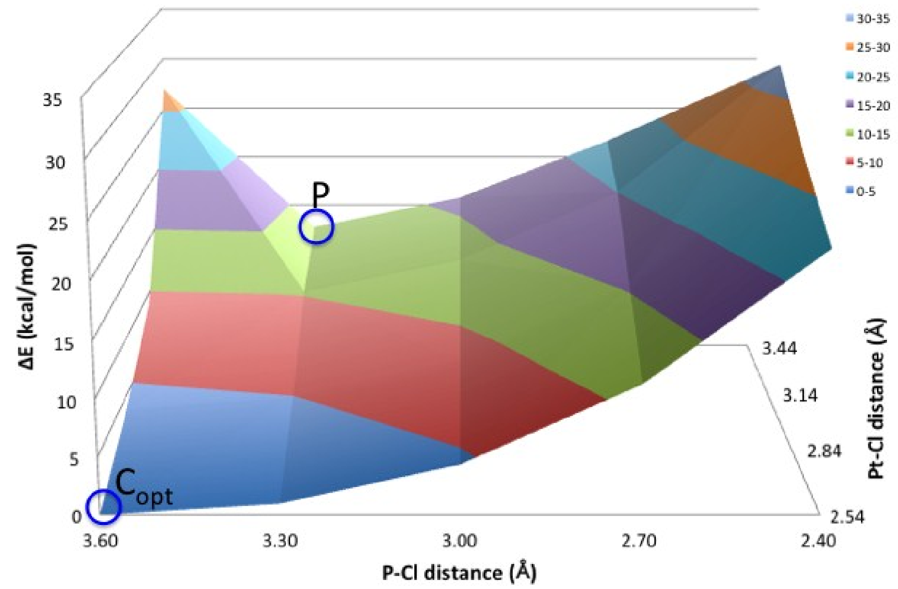


Fig. S5. Potential energy surface (PES) for the Pt–Cl and P–Cl distances of **8a**. Point P is a saddle point with the Pt–Cl bond length of 3.44 Å and the P–Cl bond length of 3.30Å.

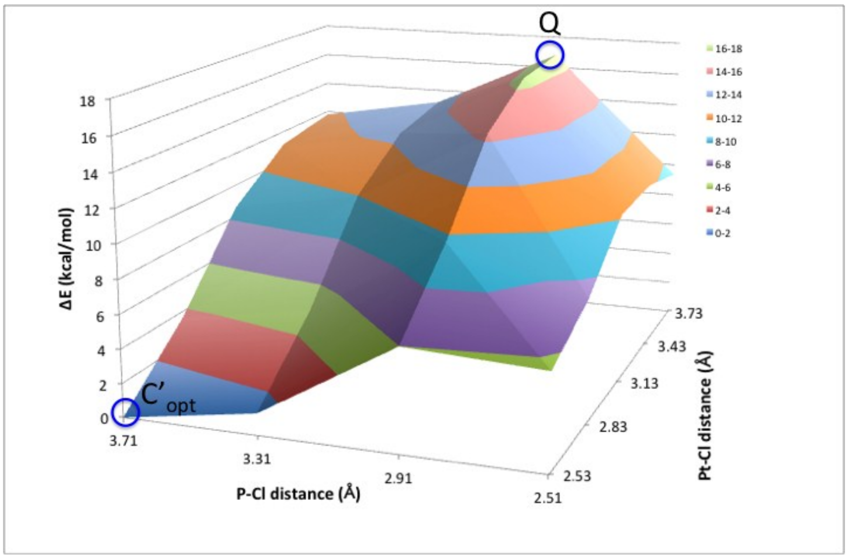


Fig. S6. Potential energy surface (PES) for the Pt–Cl and P–Cl distances of **9a**. Point Q is a local maximum with the P–Cl bond length of 3.73 Å and the P–Cl bond length of 2.91 Å.

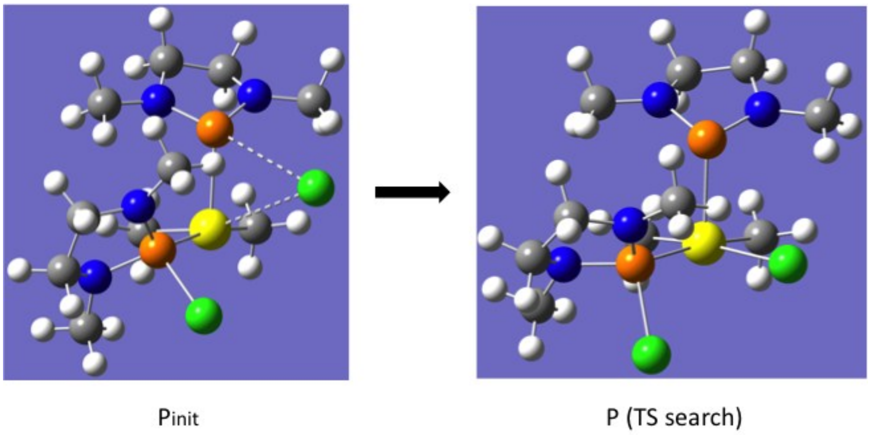


Fig. S7. Initial structure (P_{init}) from the saddle point on the PES shown in Figure S5 and the obtained structure (P(TS search)) by the TS search for Cl transfer in the first half of the reaction.

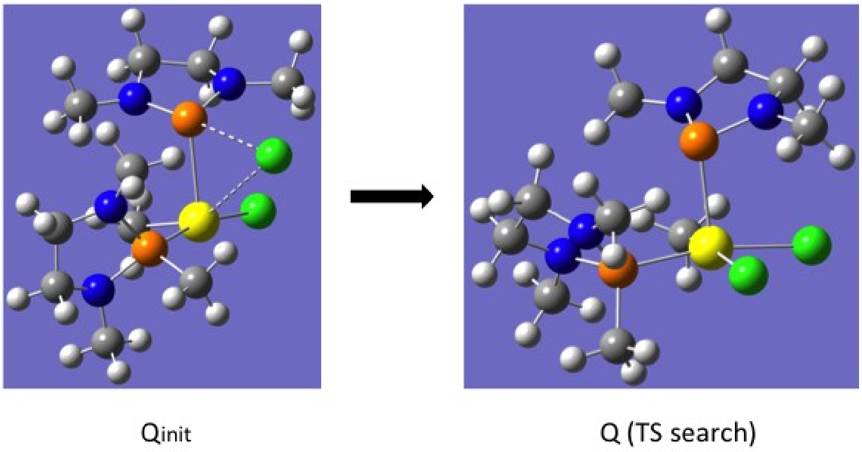
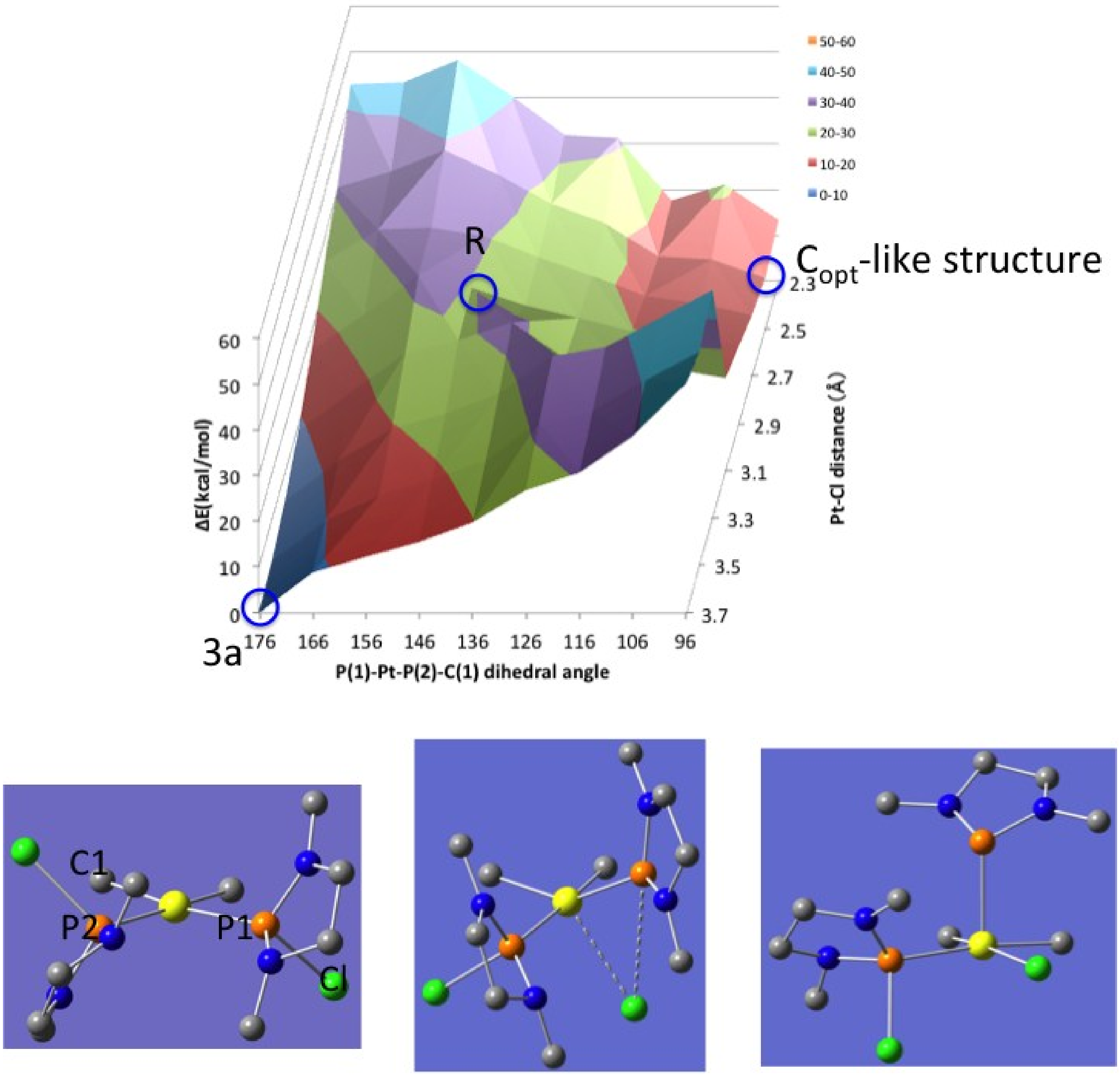


Fig. S8. Initial structure (Q_{init}) from the energy-maximum structure on the PES shown in Figure S6 and the obtained structure (Q(TS search)) by the TS search for Cl transfer in the second half of the reaction.



3a R C_{opt}-like structure

Fig. S9. Potential energy surface (PES) for the P(1)–Pt–P(2)–C(1) dihedral angle and Pt–Cl distances of **3a** and the structures denoted by blue circles. Point R is a saddle point with the P(1)–Pt–P(2)–C(1) dihedral angle of 176º and the Pt–Cl bond length of 2.9 Å.

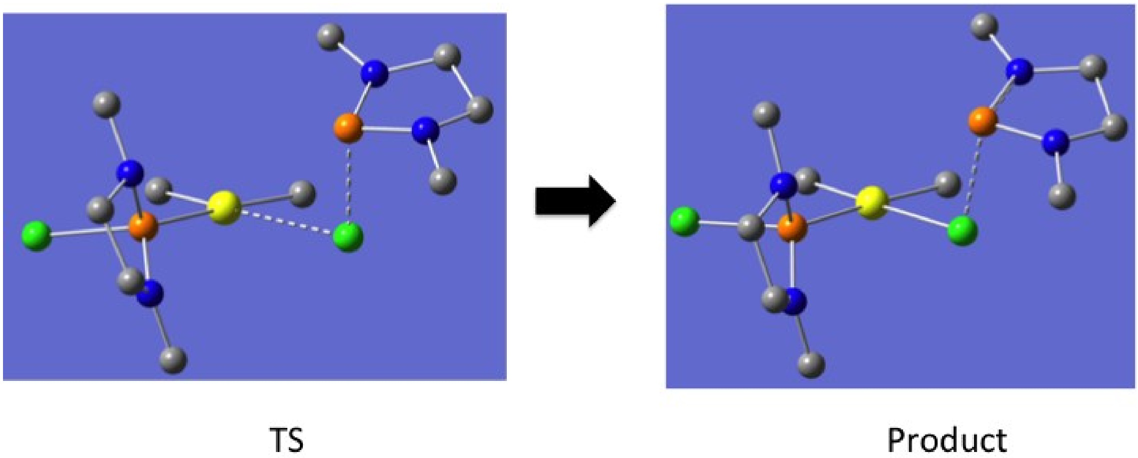


Fig. S10. TS structure from the point R and the product structure by IRC calculation from the TS.

path C: *via* phosphenium

Cl⁻ elimination from Pt complex

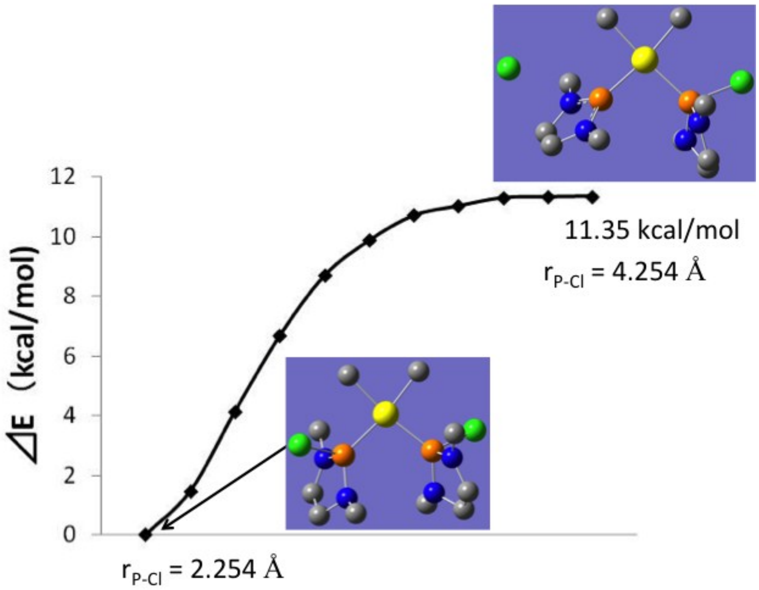


Fig. S11. Potential energy curve by scan calculations at the B3PW91/BS2 level for the P–Cl cleavage in the first half of path C. Hydrogen atoms are omitted for clarity.

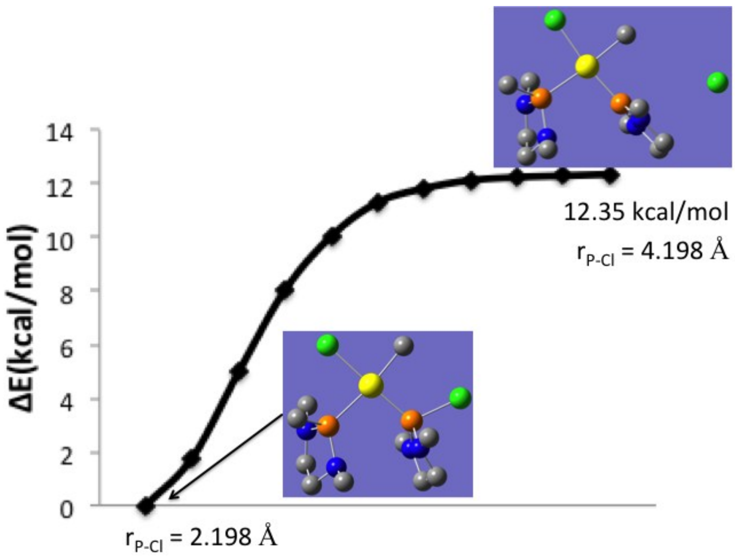


Fig. S12. Potential energy curve by scan calculations at the B3PW91/BS2 level for the P–Cl cleavage in the second half of path C. Hydrogen atoms are omitted for clarity.

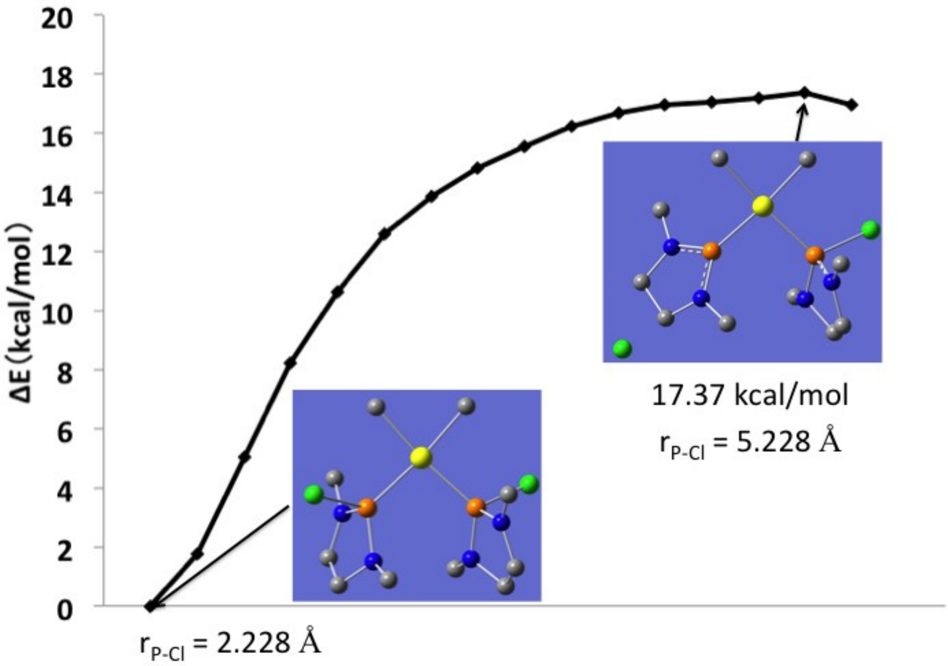


Fig. S13. Potential energy curve by scan calculations at the B3PW91-D3/BS2 level for the P–Cl cleavage in the first half of path C. Hydrogen atoms are omitted for clarity.

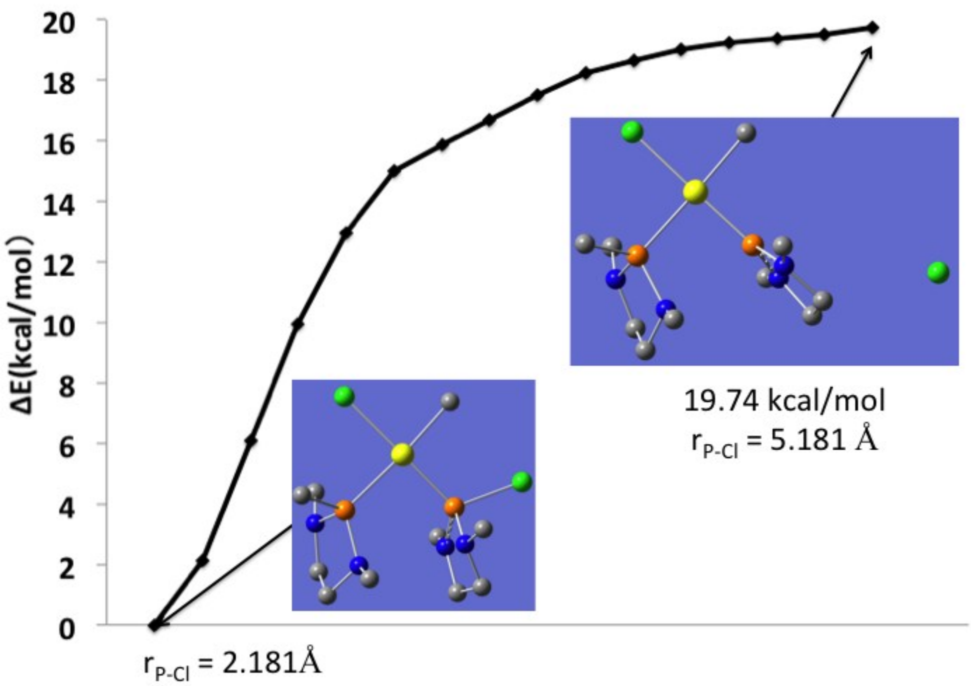
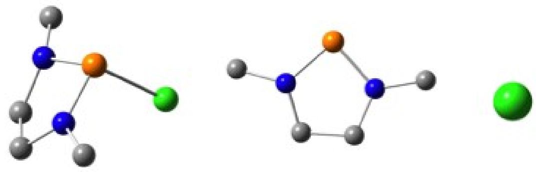


Fig. S14. Potential energy curve by scan calculations at the B3PW91-D3/BS2 level for the P–Cl cleavage in the second half of path C. Hydrogen atoms are omitted for clarity.

Table S3. The bond dissociation energy for radical splitting and ionic bond cleavage at B3PW91/BS2 with or without PCM (solvent: acetonitrile)



P-Cl P Cl

		ΔG (= (P + Cl) – P-Cl) (kcal/mol)
radical splitting	(gas)	71.32
radical splitting	(acetonitrile)	74.68
ionic bond cleavage	(gas)	113.22
ionic bond cleavage	(acetonitrile)	3.99

Molecular orbital change during the Me migration

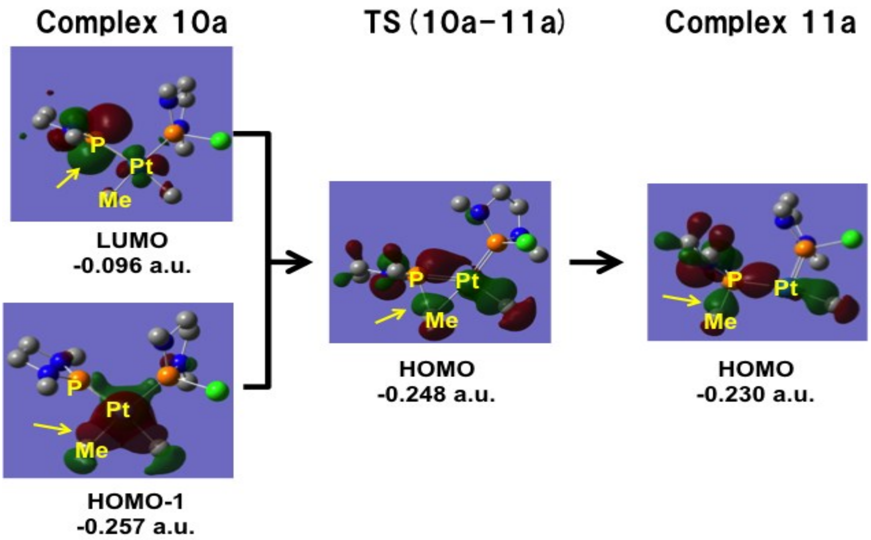


Fig. S15. Change of the molecular orbitals during the Me transfer reaction in the first half of path C.

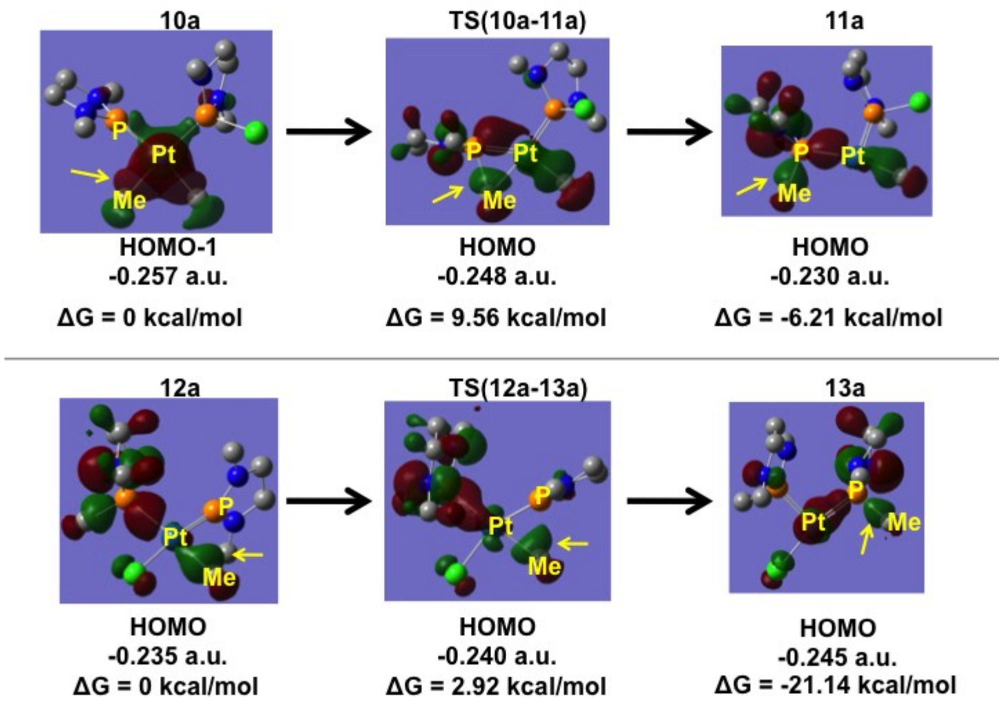


Fig. S16. Change of the frontier molecular orbitals with orbital energies related to the Me transfer reaction and Gibbs free energies. Me migration of the first half (upper) and the second half (lower).

Another possibility for path C

As another possibility for path C, the route via the complex **11a'** was investigated. Complex **11a'** is an isomer of the phosphenium complex **11a** in which the PR_2Me moves to the trans position of PR_2Cl. The calculation results are shown in Figs. S17 and S18. The route consists of 7 steps, and the route from **3a** to **11**a is the same as the Path C. Isomerization reaction in the third step (**11a**→**11a'**) is accompanied by the transfer of PR_2Me. Complex **11a'** is more stable than **11a** by 11.40 kcal/mol, and the activation energy (TS(**11a-11a'**) is low (10.05 kcal/mol). Therefore, **11a**/**11a'** isomerization is conceivable. The fourth step (**11a'** → **5a'**) is Cl^- coordination process to Pt. Complex **5a'** is more stable than **11a'**. The fifth step (**5a'** → **12a'**) is Cl^- elimination from the phosphine ligand, and the generated phosphenium complex (**12a'**) is less stable than complex **5a'** by 9.51 kcal/mol. This energy difference is large compared to the corresponding one (step **5a** → **12a**: 4.08 kcal/mol) of the original path C. The sixth step (**12a'** → **13a'**) is the generation of three-coordinated complex accompanied with the Me transfer from Pt to P. The activation energy, 15.79 kcal/mol, is also larger than the corresponding one (step **12a** → **13a'**: 2.92 kcal/mol) for the original path C. These results indicate that the route via **11a'** is possible but unfavorable compared with the original path C.

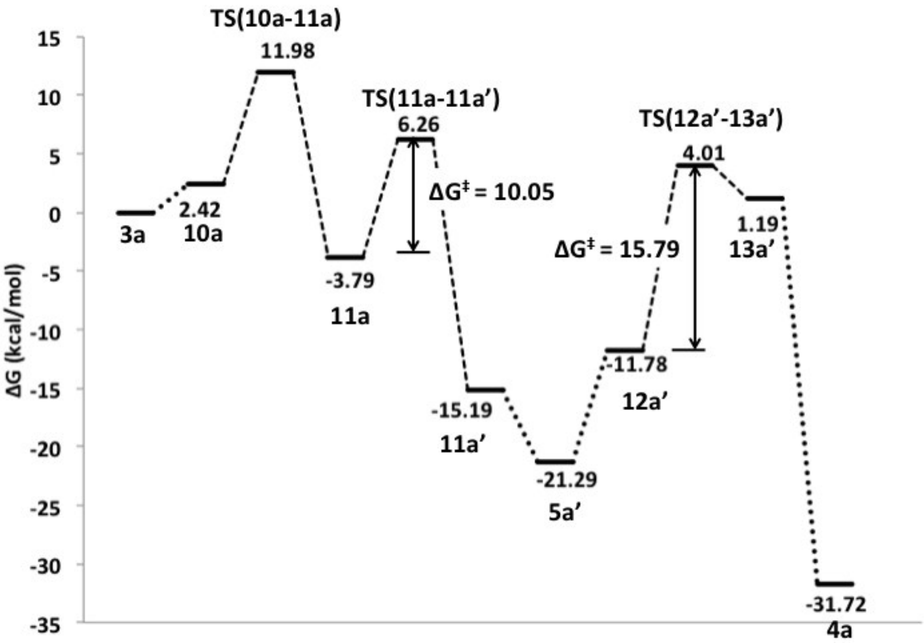
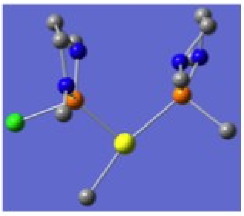
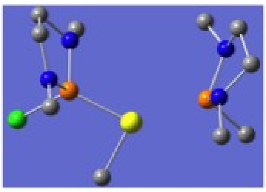


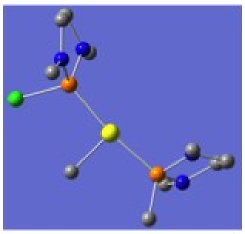
Fig. S17. Gibbs free energy profile for another path of path C based on the B3PW91/BS2 calculations.



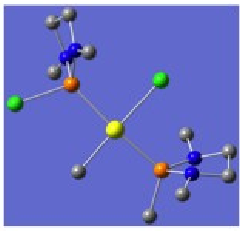
11a



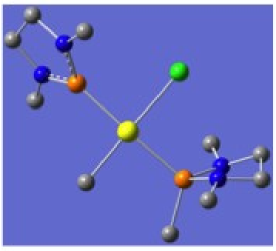
TS(11a-11a′)



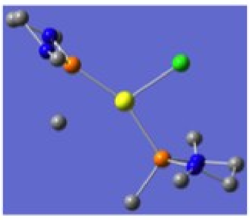
11a′



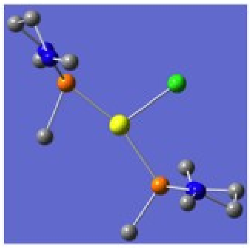
5a′



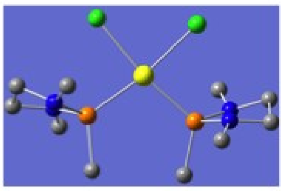
12a′



TS(12a′-13a′)



13a′



4a′

Fig. S18. Optimized strictures of LM and TS for energy profile of Fig. 17.

Coordinates of the optimized geometries at B3PW91/BS2 for route C in Å.

Complex **3a**

78	0.000000	1.189017	0.000000
6	1.346807	2.784233	-0.231842
1	1.175850	3.212970	-1.225183
1	2.402502	2.514382	-0.167141
1	1.134303	3.557531	0.511381
15	1.738291	-0.322901	-0.123130
7	2.699483	-0.517996	1.202521
6	3.270111	-1.857460	1.345636
1	2.865567	-2.317953	2.254530
1	4.358646	-1.808962	1.443658
6	2.860651	-2.627774	0.088671
1	3.655083	-2.594321	-0.669510
1	2.641622	-3.675328	0.306822
7	1.651436	-1.969247	-0.418149
6	3.012559	0.491853	2.191451
1	2.828099	0.094919	3.194728
1	2.373138	1.362892	2.046871
1	4.060373	0.803701	2.125565
6	1.129520	-2.479393	-1.673661
1	1.871390	-2.418407	-2.480345
1	0.242474	-1.917152	-1.966214
1	0.839124	-3.523705	-1.540468
17	3.154503	0.277841	-1.770853
6	-1.346809	2.784231	0.231846
1	-1.175852	3.212967	1.225188
1	-2.402504	2.514379	0.167145
1	-1.134306	3.557531	-0.511376
15	-1.738291	-0.322903	0.123130
7	-2.699491	-0.517986	-1.202516
6	-3.270120	-1.857449	-1.345639
1	-2.865583	-2.317936	-2.254540
1	-4.358656	-1.808951	-1.443653
6	-2.860652	-2.627773	-0.088683
1	-3.655079	-2.594327	0.669503
1	-2.641625	-3.675326	-0.306844
7	-1.651433	-1.969251	0.418135
6	-3.012573	0.491870	-2.191437
1	-2.828120	0.094943	-3.194718
1	-2.373148	1.362906	-2.046855
1	-4.060386	0.803720	-2.125541
6	-1.129510	-2.479407	1.673639
1	-1.871374	-2.418423	2.480329
1	-0.242459	-1.917173	1.966188
1	-0.839120	-3.523720	1.540437
17	-3.154491	0.277826	1.770867

Complex **10a**

78	-0.135639	-1.131266	-0.200459
15	1.660182	0.316227	0.189819
7	2.272711	1.220227	-1.043699
7	1.468099	1.638527	1.197497
6	2.697195	2.565812	-0.642569
1	2.089460	3.301609	-1.179896
1	3.746577	2.732200	-0.901833
6	2.484646	2.648831	0.871577
1	3.416063	2.437744	1.413543
1	2.126880	3.633329	1.179026
6	2.610484	0.729845	-2.364419
1	2.290952	1.454732	-3.118078
1	2.090890	-0.209802	-2.556533
1	3.688433	0.565959	-2.468245
6	1.164121	1.462875	2.609470
1	2.053794	1.190138	3.190712
1	0.411585	0.682451	2.734576
1	0.757858	2.396038	3.004589
15	-1.771789	0.368106	-0.017523
7	-3.034849	0.422084	1.003547
7	-2.309729	1.539190	-1.008479
6	-4.116278	1.322350	0.572376
1	-4.463375	1.908016	1.424479
1	-4.947715	0.714857	0.203268
6	-3.524535	2.216983	-0.524903
1	-4.219664	2.348116	-1.355107
1	-3.245391	3.203663	-0.143918
6	-3.239742	-0.456998	2.144211
1	-3.385245	0.138894	3.047312
1	-2.367963	-1.097287	2.277734
1	-4.119726	-1.083172	1.978138
6	-1.613869	2.063297	-2.173077
1	-2.277677	2.029433	-3.039119
1	-0.732524	1.458214	-2.381501
1	-1.306050	3.096191	-1.993598
6	1.132476	-2.759925	-0.504956
1	1.494011	-3.063732	0.482444
1	0.616407	-3.598070	-0.972794
1	1.995859	-2.481627	-1.113778
17	3.387777	-0.722836	1.069132
6	-1.629090	-2.571414	-0.617745
1	-2.664101	-2.241019	-0.503184
1	-1.490599	-2.908132	-1.647986
1	-1.463113	-3.416930	0.054024

Complex TS(**10a→11a**)

6	-3.375192	1.552437	1.581108
6	-2.923206	2.545575	0.513226
6	-3.264790	-0.937936	1.895404
6	-1.052880	2.749920	-1.113374
6	2.180087	-1.936954	0.034721
6	4.141755	1.468980	-0.445612
6	4.177297	1.082299	1.030735
6	2.777115	0.808534	-2.456684

6	2.459182	0.446027	2.760967
6	-1.001455	-2.715831	-0.307289
7	-2.862916	0.244947	1.160618
7	-1.678806	1.994507	-0.040778
7	3.049115	0.688202	-1.035306
7	2.789238	0.759108	1.380844
17	-2.910336	-0.070985	-1.896124
15	-1.794691	0.331386	-0.084440
15	1.961393	0.155827	0.084738
78	0.031556	-0.903122	-0.094335
1	-2.957729	1.798511	2.564023
1	-4.464707	1.526201	1.662513
1	-3.679876	2.653549	-0.275370
1	-2.723026	3.531780	0.935487
1	-3.075896	-0.792714	2.963468
1	-2.692422	-1.801780	1.562276
1	-4.329319	-1.143578	1.749145
1	-1.708865	2.848877	-1.986830
1	-0.126753	2.262330	-1.419433
1	-0.806327	3.746520	-0.742630
1	2.304754	-2.317230	-0.977603
1	1.657097	-2.654798	0.672755
1	3.166108	-1.821648	0.492132
1	3.940867	2.539282	-0.573889
1	5.083322	1.229238	-0.944843
1	4.827939	0.214758	1.202751
1	4.529475	1.905154	1.655233
1	2.597966	1.852611	-2.734696
1	1.894091	0.223884	-2.718758
1	3.624634	0.428914	-3.032350
1	2.997560	-0.439229	3.117881
1	1.386557	0.266928	2.850428
1	2.719126	1.296094	3.394812
1	-2.024794	-2.654951	-0.679523
1	-0.409730	-3.301397	-1.020139
1	-1.000140	-3.240948	0.654092

Complex **11a**

78	-0.343257	-1.323666	-0.007746
15	-1.399415	0.551314	-0.091750
7	-1.532625	1.464027	1.264647
7	-0.784794	1.776808	-1.035413
6	-1.227416	2.880472	1.043417
1	-0.262093	3.114906	1.503683
1	-1.996665	3.508411	1.499631
6	-1.189344	3.072125	-0.471634
1	-2.174603	3.364457	-0.858795
1	-0.464352	3.833861	-0.764478
6	-1.932523	1.004803	2.578947
1	-1.224421	1.363133	3.330895
1	-1.937802	-0.085295	2.607873
1	-2.932185	1.369237	2.835325
6	-0.770320	1.679217	-2.486336
1	-1.746299	1.927678	-2.921139
1	-0.499549	0.667279	-2.789423
1	-0.022819	2.369306	-2.882114
15	1.876160	-0.406077	0.096558
7	2.815519	0.238327	-1.151749
7	2.131708	0.929849	1.114294
6	2.855119	-1.825616	0.737964
1	2.885573	-2.608049	-0.025495
1	2.381979	-2.242587	1.631169
1	3.878151	-1.522386	0.971745
6	3.330152	1.566662	-0.828797
1	2.686336	2.351334	-1.250739
1	4.335713	1.690596	-1.242889
6	3.344573	1.634045	0.690932
1	4.250554	1.155780	1.093969
1	3.316326	2.664650	1.053558
6	2.646709	-0.104632	-2.549003
1	2.024370	0.623369	-3.084275
1	2.183870	-1.088154	-2.646055
1	3.622728	-0.147864	-3.041922
6	1.946734	0.771443	2.546805
1	2.779988	0.239719	3.027641
1	1.026491	0.217419	2.742643
1	1.854178	1.755440	3.012862
6	-2.026516	-2.510962	0.198628
1	-2.752723	-2.177667	0.942469
1	-2.540154	-2.645718	-0.757311
1	-1.595993	-3.470637	0.522174
17	-3.395610	0.292396	-0.828642

Complex **5a**

15	1.620922	0.200371	0.158938
7	2.119129	1.149218	-1.118061
7	1.538523	1.457072	1.217526
6	2.823226	2.329483	-0.607322
1	2.752933	3.137814	-1.338294
1	3.885675	2.100756	-0.447488
6	2.131524	2.694391	0.709401
1	2.848788	3.100979	1.428329
1	1.335890	3.430733	0.554334
6	2.614487	0.557730	-2.348395
1	2.555210	1.297168	-3.150080
1	1.990658	-0.295106	-2.622695
1	3.655185	0.221842	-2.256075
6	1.105211	1.372426	2.593579
1	1.953637	1.432530	3.284697
1	0.587429	0.426611	2.761211
1	0.410904	2.186698	2.820439
15	-1.726307	0.543797	-0.398121
7	-2.751493	0.907858	0.918692
7	-1.296743	2.187218	-0.637340
6	-2.867054	0.140957	-1.777520
1	-3.388263	-0.789589	-1.552057

1	-2.299249	-0.000912	-2.701075
1	-3.595076	0.943828	-1.913799
6	-2.749587	2.336845	1.227480
1	-2.037941	2.559674	2.036368
1	-3.744087	2.653797	1.558318
6	-2.337150	3.035732	-0.054503
1	-3.199390	3.147207	-0.731925
1	-1.933167	4.033575	0.138249
6	-2.886521	0.022589	2.061242
1	-2.077549	0.154815	2.793995
1	-2.896087	-1.018036	1.738371
1	-3.836420	0.228291	2.564158
6	-0.829564	2.613528	-1.946390
1	-1.635173	2.653211	-2.694623
1	-0.046825	1.943285	-2.301881
1	-0.396061	3.613808	-1.863253
6	1.146537	-2.858431	0.139495
1	1.976224	-2.835225	-0.572152
1	1.566093	-2.891747	1.149022
1	0.548896	-3.755064	-0.032501
17	3.501526	-0.780791	0.752756
78	-0.083324	-1.181173	-0.081546
17	-1.917689	-2.754093	-0.243895

Complex **12a**

78	0.064351	-1.062775	-0.073053
15	-1.686740	0.147127	-0.162878
7	-2.953440	0.224357	0.842160
7	-2.241109	1.201523	-1.257971
6	-4.064051	1.034895	0.313750
1	-4.457702	1.670208	1.107540
1	-4.855996	0.360135	-0.022994
6	-3.487953	1.867097	-0.841118
1	-4.174162	1.906554	-1.687386
1	-3.250219	2.888633	-0.531951
6	-3.142573	-0.574499	2.043784
1	-3.347455	0.082656	2.890690
1	-2.239063	-1.148236	2.248836
1	-3.979718	-1.262515	1.905028
6	-1.541224	1.650486	-2.451152
1	-2.185329	1.514389	-3.321743
1	-0.634209	1.062927	-2.587368
1	-1.276614	2.705817	-2.354442
15	1.648620	0.622196	0.515935
7	2.616386	1.257068	-0.724221
7	0.993761	2.143865	0.932075
6	2.803794	0.106061	1.831587
1	3.394971	-0.737783	1.471984
1	2.244891	-0.220307	2.712004
1	3.468988	0.930633	2.095739
6	2.381695	2.690339	-0.906950
1	1.632489	2.868640	-1.691482
1	3.311300	3.183644	-1.205720
6	1.885358	3.197357	0.435920
1	2.725685	3.375018	1.123847
1	1.325906	4.130946	0.336375
6	2.916381	0.493185	-1.923522
1	2.108379	0.546660	-2.665983
1	3.085504	-0.554260	-1.672847
1	3.830134	0.883943	-2.378962
6	0.458596	2.354024	2.269354
1	1.243530	2.455258	3.031364
1	-0.189436	1.522767	2.555110
1	-0.144194	3.265203	2.275225
17	1.818501	-2.681461	-0.019889
6	-1.183296	-2.695026	-0.642146
1	-0.719945	-3.108191	-1.540146
1	-1.113021	-3.413929	0.176690
1	-2.236362	-2.498539	-0.850342

Complex TS(**12a**→**13a**)

78	-0.038440	-0.906751	-0.036206
15	1.775066	0.170205	0.112044
7	2.888524	0.588570	-0.998243
7	2.485278	0.906590	1.373242
6	4.097553	1.168602	-0.392053
1	4.462779	1.982448	-1.019619
1	4.873135	0.398092	-0.330988
6	3.685484	1.669734	0.996718
1	4.474015	1.499065	1.731187
1	3.437588	2.735440	0.987949
6	2.937129	0.096816	-2.366731
1	3.160569	0.924522	-3.042020
1	1.971652	-0.328377	-2.641737
1	3.706544	-0.673304	-2.471584
6	1.910822	1.064096	2.699916
1	2.609465	0.692934	3.452342
1	0.983048	0.495845	2.769518
1	1.695280	2.117994	2.894138
15	-1.833658	0.484483	-0.422462
7	-2.805989	0.909508	0.899171
7	-1.438343	2.089274	-0.793145
6	-2.960577	-0.174876	-1.693305
1	-3.385479	-1.115526	-1.338628
1	-2.405112	-0.377738	-2.612079
1	-3.761438	0.540656	-1.889989
6	-2.687302	2.340028	1.192650
1	-1.879375	2.529110	1.914504
1	-3.624416	2.704852	1.621863
6	-2.381291	2.999438	-0.140385
1	-3.298292	3.133351	-0.733342
1	-1.912282	3.978190	-0.011150
6	-2.956782	0.030906	2.048131
1	-2.096983	0.084861	2.730098
1	-3.077550	-1.002755	1.723450
1	-3.855552	0.318795	2.599222

6	-0.978747	2.455608	-2.121489
1	-1.792814	2.502326	-2.857664
1	-0.235183	1.737164	-2.472034
1	-0.498848	3.436126	-2.076792
17	-1.439928	-2.854566	0.011905
6	1.807972	-2.151964	0.383050
1	1.451530	-2.619831	1.299957
1	1.739256	-2.808256	-0.483772
1	2.862592	-1.900055	0.528938

Complex **13a**

78	-0.764099	-0.987894	-0.086124
15	1.470294	-0.961393	0.170857
7	2.122733	0.085089	1.315767
7	2.569868	-0.538476	-1.010555
6	3.480157	0.480990	0.928714
1	4.221137	-0.245864	1.291743
1	3.714457	1.454623	1.366025
6	3.472724	0.531207	-0.594042
1	3.122689	1.503995	-0.959667
1	4.472118	0.350864	-0.999872
6	1.878630	-0.126667	2.732741
1	2.508900	-0.920451	3.155080
1	0.831278	-0.388726	2.894875
1	2.081290	0.798465	3.277303
6	2.480969	-0.895183	-2.411298
1	2.293862	-0.018016	-3.039343
1	1.667133	-1.604198	-2.572220
1	3.411904	-1.364360	-2.744633
15	-1.024755	1.192435	-0.336051
7	-1.214314	2.095124	1.057112
7	0.239368	2.110812	-0.932962
6	-2.491724	1.446222	-1.378389
1	-3.373385	1.073662	-0.857322
1	-2.388419	0.895672	-2.314542
1	-2.591767	2.515695	-1.575000
6	-0.066129	2.981992	1.266919
1	0.714772	2.483095	1.851564
1	-0.393027	3.873983	1.806487
6	0.425948	3.326476	-0.130375
1	-0.159467	4.152982	-0.556144
1	1.479701	3.613808	-0.129517
6	-1.927095	1.608761	2.226409
1	-1.269661	1.064214	2.914030
1	-2.737493	0.944661	1.924033
1	-2.362410	2.458164	2.757896
6	0.455913	2.238250	-2.366091
1	-0.201029	2.993905	-2.815181
1	0.279033	1.284479	-2.865048
1	1.491284	2.529239	-2.554081
17	-3.109225	-1.547527	-0.033650
6	1.827811	-2.701418	0.622460
1	1.201567	-3.024040	1.456979
1	1.630363	-3.353912	-0.231124
1	2.881775	-2.785539	0.897456

Complex **4a**

78	0.000000	-1.002577	-0.000001
15	1.669452	0.453160	0.488805
7	2.898475	0.628594	-0.670132
7	1.390936	2.113761	0.610658
6	2.492684	-0.030718	2.046248
1	2.950551	-1.012478	1.937707
1	1.758311	-0.077102	2.853870
1	3.256876	0.712934	2.284329
6	3.040066	2.026961	-1.082860
1	2.453867	2.225765	-1.991060
1	4.089182	2.241841	-1.305169
6	2.531173	2.857408	0.081592
1	3.316493	2.988574	0.842743
1	2.207093	3.850700	-0.241111
6	3.124514	-0.348775	-1.723390
1	2.397962	-0.250382	-2.542176
1	3.064690	-1.359953	-1.324561
1	4.127671	-0.199772	-2.131743
6	0.748321	2.672700	1.783190
1	1.447071	2.805004	2.621427
1	-0.065260	2.026036	2.113627
1	0.319848	3.646373	1.533844
15	-1.669447	0.453166	-0.488807
7	-2.898479	0.628580	0.670121
7	-1.390935	2.113770	-0.610635
6	-2.492668	-0.030688	-2.046264
1	-2.950537	-1.012448	-1.937740
1	-1.758289	-0.077061	-2.853881
1	-3.256857	0.712969	-2.284341
6	-3.040087	2.026944	1.082856
1	-2.453899	2.225747	1.991065
1	-4.089208	2.241814	1.305153
6	-2.531186	2.857404	-0.081582
1	-3.316498	2.988569	-0.842742
1	-2.207120	3.850696	0.241133
6	-3.124505	-0.348795	1.723375
1	-2.397949	-0.250402	2.542157
1	-3.064679	-1.359971	1.324539
1	-4.127660	-0.199799	2.131734
6	-0.748308	2.672725	-1.783151
1	-1.447047	2.805035	-2.621397
1	0.065280	2.026070	-2.113583
1	-0.319845	3.646399	-1.533789
17	-1.601724	-2.797437	-0.448591
17	1.601717	-2.797443	0.448588

Complex TS(**11a→11a'**)

78	-0.047531	-0.874037	-0.232688

15	-1.949902	0.143912	0.104002
7	-2.290632	0.675198	1.627738
7	-2.038848	1.650684	-0.598039
6	-2.541181	2.118054	1.683109
1	-1.652586	2.629388	2.073030
1	-3.383998	2.328797	2.345754
6	-2.841344	2.542295	0.248877
1	-3.909552	2.435225	0.017207
1	-2.548746	3.577441	0.063864
6	-1.995856	-0.040509	2.854284
1	-1.146480	0.414380	3.375057
1	-1.747147	-1.078458	2.633639
1	-2.866021	-0.027874	3.515683
6	-2.132155	1.825157	-2.038475
1	-3.151970	1.662913	-2.407774
1	-1.457956	1.127580	-2.537531
1	-1.821591	2.840326	-2.292180
15	2.377706	-0.129170	-0.314688
7	2.857189	1.396746	-0.897994
7	3.048141	0.132504	1.224642
6	3.409141	-1.328875	-1.233707
1	3.102236	-1.324260	-2.283038
1	3.248468	-2.335586	-0.838370
1	4.467954	-1.069289	-1.168403
6	3.496317	2.183850	0.161924
1	2.761954	2.826952	0.668281
1	4.272568	2.822105	-0.270100
6	4.074356	1.171421	1.137430
1	5.036020	0.776194	0.775964
1	4.237100	1.609420	2.125567
6	2.025472	2.138860	-1.830048
1	1.186888	2.646303	-1.333826
1	1.625617	1.472558	-2.595717
1	2.636676	2.892327	-2.333496
6	3.291317	-0.984578	2.119562
1	4.163985	-1.586971	1.831197
1	2.413312	-1.635296	2.143315
1	3.454956	-0.606254	3.131597
6	-1.048922	-2.638343	-0.427083
1	-1.717800	-2.862021	0.403954
1	-1.600374	-2.645171	-1.368020
1	-0.210465	-3.342972	-0.452512
17	-3.738619	-0.853172	-0.556640

Complex **11a’**

78	0.161801	-0.026784	0.327603
15	-2.150944	-0.028556	-0.033140
7	-2.994353	1.384851	-0.048283
7	-2.627822	-0.454317	-1.572954
6	-3.938962	1.505789	-1.163565
1	-3.604298	2.313718	-1.823599
1	-4.938889	1.752351	-0.796291
6	-3.930554	0.152030	-1.877203
1	-4.742697	-0.492714	-1.515718
1	-4.036020	0.262097	-2.958136
6	-2.931190	2.426148	0.956962
1	-2.787136	3.397697	0.475305
1	-2.086919	2.250029	1.624979
1	-3.849335	2.460451	1.552236
6	-2.366915	-1.778144	-2.115348
1	-3.099877	-2.517511	-1.769782
1	-1.368108	-2.106189	-1.822462
1	-2.404638	-1.729202	-3.205470
15	2.460522	0.061006	0.335767
7	3.348087	-1.118536	-0.503995
7	2.902967	1.306416	-0.717725
6	3.306116	0.234021	1.940386
1	3.272401	-0.713405	2.483374
1	2.818608	1.000259	2.546853
1	4.351219	0.500361	1.771490
6	3.830955	-0.583718	-1.780762
1	3.096589	-0.744798	-2.583265
1	4.760475	-1.087527	-2.058873
6	4.043766	0.901572	-1.540569
1	4.998282	1.085921	-1.026252
1	4.041703	1.468572	-2.474677
6	2.915050	-2.507245	-0.511132
1	2.058488	-2.677511	-1.177275
1	2.641877	-2.827423	0.495715
1	3.744989	-3.135537	-0.843043
6	2.808361	2.701277	-0.320896
1	3.646642	3.018597	0.313343
1	1.875517	2.868884	0.222108
1	2.793689	3.329834	-1.214305
6	0.031663	-0.916351	2.146159
1	-0.737193	-0.397076	2.722243
1	-0.272248	-1.953354	1.982507
1	0.974170	-0.887687	2.690226
17	-3.260196	-1.381036	1.281932

Complex **5a’**

15	-2.183530	0.100214	-0.095554
7	-2.927258	-0.957108	-1.114618
7	-2.884441	-0.545641	1.274228
6	-3.902495	-1.827470	-0.458444
1	-3.490681	-2.841815	-0.386266
1	-4.829722	-1.871381	-1.036665
6	-4.138489	-1.221113	0.923192
1	-4.968173	-0.501042	0.904662
1	-4.362991	-1.985432	1.670039
6	-2.550647	-1.209330	-2.488503
1	-2.191827	-2.236959	-2.604129
1	-1.745304	-0.535846	-2.784180
1	-3.401517	-1.049748	-3.158243
6	-2.837841	0.150863	2.548645
1	-3.595012	0.942668	2.613873

1	-1.850622	0.594046	2.689678
1	-3.008880	-0.566249	3.354317
15	2.412919	0.433252	0.221369
7	3.108419	-0.677629	1.302172
7	3.278888	-0.153984	-1.110922
6	3.152290	2.029994	0.716575
1	2.789751	2.314096	1.707001
1	2.893289	2.823678	0.014134
1	4.237070	1.914165	0.757177
6	3.914866	-1.667688	0.585582
1	3.309682	-2.543973	0.317129
1	4.743322	-1.996375	1.220671
6	4.414085	-0.957705	-0.663115
1	5.294160	-0.335229	-0.438162
1	4.692616	-1.667771	-1.446840
6	2.380533	-1.159851	2.463554
1	1.667448	-1.952453	2.205643
1	1.833052	-0.341225	2.934192
1	3.093895	-1.546788	3.196751
6	3.448336	0.648927	-2.306711
1	4.216691	1.427725	-2.197848
1	2.502181	1.128504	-2.568374
1	3.733941	0.001038	-3.139624
6	0.065139	2.428450	0.132687
1	0.649581	2.887600	-0.672125
1	-0.954080	2.807387	0.066689
1	0.490413	2.748671	1.088599
17	-3.351523	1.973981	-0.396891
78	0.123431	0.378898	-0.055764
17	0.262074	-2.098879	-0.369140

Complex **12a’**

15	2.278932	0.017909	-0.101170
7	3.325465	1.235020	-0.320830
7	3.352368	-1.044810	0.485974
6	4.673459	0.953591	0.204979
1	4.807283	1.520134	1.130721
1	5.418790	1.283948	-0.519201
6	4.744243	-0.561891	0.438266
1	5.262391	-1.080593	-0.373094
1	5.240345	-0.800960	1.379360
6	3.001838	2.569906	-0.801893
1	3.197960	3.302280	-0.015691
1	1.948922	2.618236	-1.075529
1	3.614014	2.800630	-1.675771
6	3.075726	-2.416262	0.886617
1	3.591952	-3.110331	0.219747
1	2.003233	-2.602528	0.841992
1	3.421123	-2.570950	1.910445
15	-2.241775	-0.493938	-0.168676
7	-2.922684	-0.470361	1.377846
7	-3.123982	0.834322	-0.712287
6	-2.889176	-2.015815	-0.934159
1	-2.490093	-2.889910	-0.415031
1	-2.613500	-2.083529	-1.987327
1	-3.976396	-2.011283	-0.837383
6	-3.726828	0.739810	1.573832
1	-3.118661	1.549505	1.996257
1	-4.547634	0.521633	2.263082
6	-4.241240	1.111641	0.192055
1	-5.130971	0.520621	-0.071238
1	-4.504097	2.170926	0.130938
6	-2.208662	-0.973498	2.539976
1	-1.481473	-0.248147	2.923795
1	-1.682818	-1.897313	2.292768
1	-2.931347	-1.203890	3.327008
6	-3.313588	1.098356	-2.126836
1	-4.083427	0.459714	-2.580798
1	-2.374582	0.949452	-2.664033
1	-3.609562	2.141719	-2.259561
6	0.187290	-1.720167	-1.669897
1	-0.415833	-1.463038	-2.544853
1	1.207587	-1.898281	-2.011260
1	-0.192401	-2.647698	-1.236051
78	0.060764	-0.168465	-0.293569
17	-0.123194	1.785713	1.244951

Complex TS(**12a’**→**13a’**)

15	2.256274	0.031671	-0.064030
7	3.313082	1.279264	0.122392
7	3.409359	-1.140474	-0.092458
6	4.693958	0.822153	0.321033
1	4.930603	0.812160	1.391243
1	5.382807	1.503187	-0.183004
6	4.754194	-0.580396	-0.278668
1	5.007388	-0.552149	-1.345606
1	5.483796	-1.207273	0.236359
6	2.938781	2.622388	0.531199
1	3.114067	2.772266	1.601334
1	1.881098	2.794196	0.326703
1	3.522440	3.353333	-0.032487
6	3.157166	-2.529179	-0.438546
1	3.357611	-2.720755	-1.498280
1	2.117563	-2.780580	-0.223627
1	3.798450	-3.174412	0.165051
15	-2.176150	0.084399	-0.638766
7	-3.227216	-1.202186	-0.301297
7	-3.117356	1.224629	0.178842
6	-2.326824	0.366289	-2.439212
1	-1.944128	-0.502709	-2.981008
1	-1.753347	1.246406	-2.740785
1	-3.376432	0.507646	-2.704183
6	-4.288894	-0.779658	0.617064
1	-3.998605	-0.962568	1.660900
1	-5.203179	-1.342464	0.407741
6	-4.474444	0.707983	0.366370

1	-5.103774	0.884142	-0.519053
1	-4.940062	1.206794	1.220249
6	-2.721790	-2.554321	-0.125385
1	-2.285021	-2.709959	0.869444
1	-1.962092	-2.776173	-0.876976
1	-3.542033	-3.263190	-0.264360
6	-2.967820	2.645220	-0.081008
1	-3.446193	2.961394	-1.018139
1	-1.907913	2.905289	-0.124472
1	-3.415189	3.209513	0.740792
6	1.363313	0.331761	-1.870321
1	1.483914	1.385213	-2.107040
1	2.070245	-0.292272	-2.421546
1	0.389912	-0.014991	-2.243253
78	0.073554	-0.066107	0.070607
17	-0.588935	-0.427577	2.278298

Complex **13a'**

15	2.284104	0.058633	-0.220974
7	3.351554	1.294604	0.102442
7	3.388207	-1.157046	0.008332
6	4.626655	0.774332	0.609661
1	4.619709	0.745691	1.706712
1	5.442262	1.423211	0.282441
6	4.756061	-0.626364	0.025322
1	5.175217	-0.598469	-0.989049
1	5.386597	-1.265398	0.646483
6	2.923170	2.611720	0.547264
1	2.824639	2.660822	1.637792
1	1.961040	2.866109	0.100366
1	3.653978	3.356023	0.223741
6	3.166682	-2.525908	-0.423922
1	3.466645	-2.681990	-1.467156
1	2.111202	-2.781814	-0.316800
1	3.744263	-3.200865	0.210776
15	-2.257658	0.008154	-0.593243
7	-3.258162	-1.243981	-0.041899
7	-3.147481	1.216897	0.184325
6	-2.553324	0.100783	-2.396007
1	-2.163015	-0.802126	-2.872756
1	-2.039344	0.965721	-2.822915
1	-3.623871	0.174609	-2.598034
6	-4.257760	-0.739310	0.903651
1	-3.892407	-0.817756	1.936997
1	-5.177537	-1.325047	0.816742
6	-4.480186	0.715659	0.523766
1	-5.176968	0.801057	-0.323654
1	-4.886069	1.293459	1.358122
6	-2.729923	-2.571855	0.224438
1	-2.250867	-2.640173	1.209519
1	-1.997922	-2.849267	-0.535993
1	-3.545571	-3.298340	0.180267
6	-3.032484	2.608049	-0.215247
1	-3.587163	2.836858	-1.135689
1	-1.981930	2.864870	-0.368736
1	-3.417062	3.244938	0.585058
6	1.616003	0.215650	-1.971766
1	1.880702	1.187439	-2.384297
1	1.971724	-0.615547	-2.580152
1	0.492079	0.160937	-2.090910
78	0.060771	-0.026486	-0.054168
17	-0.392669	-0.281807	2.193774

Complex **4a'**

15	-1.786311	0.850648	-0.085072
7	-2.990034	0.445181	-1.205284
7	-2.816253	0.712785	1.245122
6	-4.210836	-0.001311	-0.533088
1	-4.208544	-1.090864	-0.405579
1	-5.081647	0.281278	-1.132666
6	-4.213400	0.703638	0.816085
1	-4.614525	1.724908	0.726305
1	-4.818966	0.165184	1.550472
6	-2.689524	-0.162261	-2.488496
1	-2.582064	-1.251230	-2.415258
1	-1.764679	0.249881	-2.896612
1	-3.495525	0.068555	-3.191015
6	-2.502851	1.340460	2.513905
1	-2.749287	2.411491	2.533413
1	-1.439285	1.223774	2.734138
1	-3.063217	0.845692	3.311564
15	1.786304	0.850615	0.085126
7	2.990289	0.445093	1.204997
7	2.816008	0.713227	-1.245196
6	1.554992	2.633691	0.405884
1	1.009886	2.789395	1.338699
1	1.031466	3.130615	-0.408841
1	2.551493	3.067778	0.505985
6	4.211051	-0.001054	0.532560
1	4.209023	-1.090605	0.405002
1	5.081903	0.281717	1.131997
6	4.213240	0.704002	-0.816587
1	4.614448	1.725251	-0.726885
1	4.818580	0.165569	-1.551183
6	2.690308	-0.162311	2.488334
1	2.583152	-1.251318	2.415202
1	1.765455	0.249575	2.896682
1	3.496434	0.068791	3.190618
6	2.502076	1.340149	-2.514178
1	2.748856	2.411080	-2.534484
1	1.438346	1.223657	-2.733714
1	3.061754	0.844697	-3.311909
6	-1.555210	2.633842	-0.405221
1	-1.010074	2.789937	-1.337952
1	-2.551725	3.067933	-0.505195
1	-1.031730	3.130469	0.409684

78	-0.000028	-0.555122	0.000059
17	1.650780	-2.348054	-0.081862
17	-1.650567	-2.348398	0.082064

Coordinates of the optimized geometries at B3PW91/BS1 for complexes **8a** and **9a** of route B in Å.

Complex **8a** of Fig. S3(c)

78	0.290922	-0.771780	-0.595428
15	-1.813324	0.116620	0.129217
7	-2.040342	0.800817	1.613884
7	-2.600971	1.362046	-0.671717
6	-2.971388	1.931149	1.629055
1	-2.420359	2.842515	1.886877
1	-3.749258	1.777510	2.382706
6	-3.570299	2.004629	0.226331
1	-4.530386	1.472814	0.179633
1	-3.735543	3.035351	-0.094460
6	-1.547358	0.281902	2.873687
1	-1.068317	1.083002	3.444557
1	-0.814286	-0.503767	2.691770
1	-2.367125	-0.133383	3.470485
6	-3.052451	1.200627	-2.046281
1	-4.008519	0.664282	-2.095285
1	-2.314628	0.649172	-2.627037
1	-3.179321	2.186379	-2.499386
15	1.567387	0.754197	0.829247
7	1.946703	2.148131	-0.017086
7	3.184934	0.345545	0.956300
6	1.950066	-1.688063	-1.425780
1	2.708428	-0.995044	-1.795132
1	2.396404	-2.367966	-0.698214
1	1.582816	-2.275031	-2.276120
6	3.371362	2.415367	-0.190554
1	3.690580	3.183321	0.527303
1	3.571571	2.791580	-1.198419
6	4.074600	1.087898	0.066006
1	4.232813	0.526318	-0.864372
1	5.047229	1.228891	0.544167
6	1.017202	3.233571	-0.241613
1	1.229541	4.081015	0.422024
1	-0.004877	2.900182	-0.056918
1	1.077772	3.580824	-1.277473
6	3.674317	-0.877711	1.557091
1	4.044686	-1.574485	0.797347
1	2.871969	-1.368762	2.108088
1	4.490863	-0.651996	2.249892
6	0.373840	0.437414	-2.270010
1	-0.095686	-0.107666	-3.096690
1	-0.151826	1.382620	-2.126010
1	1.407160	0.654795	-2.541831
17	-3.317769	-1.530302	-0.000020
17	0.243287	-2.568660	1.198351

Complex **8a** of Figure S3(d)

78	0.166192	-0.829951	-0.288999
15	-1.807197	0.084978	0.154675
7	-2.035813	1.184212	1.361388
7	-2.662825	0.976362	-0.975319
6	-2.992593	2.242036	1.026709
1	-2.456091	3.192881	0.931592
1	-3.738271	2.345497	1.819737
6	-3.643802	1.824059	-0.288854
1	-4.571293	1.262685	-0.109020
1	-3.882071	2.684968	-0.916940
6	-1.514032	1.124993	2.710419
1	-1.087327	2.094227	2.984081
1	-0.726120	0.377344	2.777548
1	-2.303904	0.871649	3.426034
6	-3.124996	0.364821	-2.211922
1	-4.044442	-0.214078	-2.056974
1	-2.357878	-0.294735	-2.614312
1	-3.323129	1.149965	-2.944796
15	1.403588	1.119044	0.674728
7	2.088428	2.053145	-0.524914
7	2.906673	0.607833	1.193550
6	3.547055	2.029062	-0.601751
1	3.946321	2.968017	-0.195624
1	3.874801	1.943718	-1.642216
6	3.982307	0.825310	0.226336
1	4.097198	-0.073433	-0.392552
1	4.922517	1.009179	0.752096
6	1.378521	3.068494	-1.271509
1	1.723355	4.070150	-0.987986
1	0.308420	3.004808	-1.071578
1	1.534356	2.936356	-2.346020
6	3.120938	-0.382160	2.227327
1	3.290725	-1.374442	1.795453
1	2.254442	-0.430677	2.886925
1	3.992404	-0.100133	2.825046
6	0.275406	0.021075	-2.254874
1	-0.110199	-0.729717	-2.956290
1	-0.280372	0.947991	-2.411725
1	1.324413	0.198211	-2.501967
17	-3.200591	-1.556234	0.575471
6	0.082048	-2.077977	1.466237
1	-0.363816	-3.017927	1.117907
1	1.092558	-2.297564	1.816617
1	-0.514285	-1.735996	2.316547
17	2.126972	-2.096840	-0.913845

Complex **8a** of Figure S3(e)

78	0.290482	-0.771385	-0.595463

15	-1.813877	0.116805	0.129828
7	-2.041769	0.799035	1.615195
7	-2.601225	1.363145	-0.670064
6	-2.970445	1.931205	1.630964
1	-2.417406	2.841573	1.888137
1	-3.748073	1.779259	2.385204
6	-3.570050	2.005515	0.228676
1	-4.530271	1.473897	0.182212
1	-3.735228	3.036434	-0.091527
6	-1.545167	0.281978	2.874308
1	-1.062485	1.083340	3.441786
1	-0.814318	-0.505545	2.691485
1	-2.363643	-0.130416	3.474837
6	-3.053225	1.202896	-2.044604
1	-4.009410	0.666766	-2.093698
1	-2.315726	0.651780	-2.626094
1	-3.180072	2.189053	-2.496844
15	1.567640	0.754301	0.828312
7	1.949013	2.147193	-0.019055
7	3.184665	0.344078	0.956813
6	3.374159	2.413226	-0.190459
1	3.693115	3.180724	0.528025
1	3.576126	2.789439	-1.197972
6	4.075789	1.085106	0.066884
1	4.233972	0.523117	-0.863253
1	5.048251	1.225154	0.545665
6	1.021005	3.233905	-0.243772
1	1.233673	4.080697	0.420612
1	-0.001671	2.901637	-0.060348
1	1.083056	3.581713	-1.279357
6	3.672351	-0.879194	1.558926
1	4.041592	-1.577434	0.799971
1	2.869362	-1.368397	2.110632
1	4.489317	-0.653823	2.251343
6	0.372704	0.437926	-2.270017
1	-0.097496	-0.107016	-3.096410
1	-0.152629	1.383256	-2.125614
1	1.405912	0.655094	-2.542440
17	-3.318185	-1.530235	-0.002396
6	1.949298	-1.687655	-1.426477
1	1.581761	-2.274398	-2.276847
1	2.707529	-0.994523	-1.795878
1	2.395771	-2.367742	-0.699160
17	0.242397	-2.568932	1.197265

Complex **9a** of Fig. S4(b)

78	0.394089	-0.987910	-0.141334
15	1.475383	1.080420	-1.047920
7	0.395707	2.373487	-1.075146
7	2.418762	1.820915	0.113344
6	0.819785	3.526994	-0.277012
1	-0.043681	4.007459	0.196367
1	1.302044	4.266683	-0.933617
6	1.806194	2.984231	0.751637
1	2.577567	3.719618	1.001760
1	1.309708	2.682231	1.684605
6	-0.417303	2.653408	-2.249216
1	-1.366345	3.109981	-1.951597
1	-0.637651	1.727929	-2.785364
1	0.098126	3.342337	-2.933532
6	3.574506	1.217709	0.749360
1	4.382579	1.955914	0.805901
1	3.916564	0.361785	0.163788
1	3.326743	0.870442	1.759664
15	-1.715592	-0.413643	0.470252
7	-2.135554	0.977024	1.323799
7	-2.853773	-0.122302	-0.761180
6	-2.295169	-1.811287	1.505325
1	-1.692133	-1.842561	2.417450
1	-3.349846	-1.667549	1.759813
1	-2.161456	-2.758178	0.972661
6	-3.000543	1.861898	0.551589
1	-2.419447	2.603281	-0.015182
1	-3.666299	2.402832	1.233249
6	-3.785775	0.938565	-0.366068
1	-4.652893	0.517757	0.168183
1	-4.151986	1.458316	-1.258000
6	-1.435279	1.542042	2.458999
1	-0.794026	2.385254	2.167211
1	-0.809728	0.785737	2.935054
1	-2.168439	1.907519	3.188349
6	-3.483218	-1.242054	-1.452143
1	-4.306990	-1.677683	-0.866077
1	-2.754175	-2.025568	-1.664155
1	-3.888296	-0.891930	-2.407528
17	1.113188	-0.912178	2.256366
6	-0.185367	-1.350589	-2.096831
1	0.703971	-1.289705	-2.729178
1	-0.576427	-2.374714	-2.147414
1	-0.947401	-0.653951	-2.454788
17	2.490996	-2.213543	-0.684490

Complex **9a** of Fig. S4(c)

78	0.364404	-0.990306	-0.111768
15	1.502670	1.018001	-1.111731
7	0.476297	2.348551	-1.054655
7	2.526594	1.686855	0.019726
6	0.978949	3.453073	-0.235139
1	0.156310	3.962747	0.273880
1	1.483569	4.185745	-0.880232
6	1.958225	2.822581	0.742813
1	2.751509	3.516118	1.031279
1	1.461840	2.466540	1.654278
6	-0.357572	2.699596	-2.192027
1	-1.255668	3.220959	-1.854718
1	-0.668028	1.800629	-2.725144

1	0.176860	3.354139	-2.892072
6	3.681598	1.021561	0.589413
1	4.507611	1.734582	0.663776
1	3.987554	0.193095	-0.048479
1	3.452001	0.625676	1.583565
15	-1.736091	-0.351258	0.465569
7	-2.134156	1.106393	1.194606
7	-2.885002	-0.161141	-0.770658
6	-2.310469	-1.657872	1.609804
1	-1.710147	-1.613226	2.520036
1	-3.363811	-1.500530	1.852378
1	-2.173599	-2.643665	1.159690
6	-3.081369	1.895914	0.417151
1	-2.568291	2.639956	-0.204232
1	-3.751148	2.431525	1.096471
6	-3.846521	0.888824	-0.423298
1	-4.687141	0.471063	0.151025
1	-4.248201	1.335641	-1.336767
6	-1.456641	1.753099	2.297249
1	-0.882902	2.625448	1.964501
1	-0.773301	1.061668	2.787378
1	-2.195311	2.092295	3.031269
6	-3.483433	-1.333797	-1.393498
1	-4.282097	-1.766488	-0.775218
1	-2.732982	-2.101103	-1.576167
1	-3.911838	-1.050127	-2.358174
17	1.080835	-0.754008	2.277864
6	-0.206262	-1.415057	-2.055694
1	0.682846	-1.373147	-2.685250
1	-0.595311	-2.438081	-2.079587
1	-0.964581	-0.732519	-2.440527
17	2.450750	-2.239428	-0.593535

Complex **9a** of Fig. S4(d)

78	0.329588	-1.070710	0.082016
15	1.895661	0.496862	-1.107425
7	1.049613	1.922811	-1.338066
7	2.971238	1.245507	-0.073019
6	1.670247	3.104132	-0.739072
1	0.907094	3.794780	-0.370663
1	2.263615	3.630255	-1.499290
6	2.555635	2.572711	0.378979
1	3.433814	3.203395	0.536222
1	2.015878	2.493092	1.331027
6	0.139275	2.114368	-2.451311
1	-0.706730	2.732609	-2.142420
1	-0.245506	1.149105	-2.782669
1	0.640273	2.605055	-3.294752
6	3.999990	0.554519	0.677165
1	4.900074	1.174097	0.715569
1	4.255050	-0.384141	0.184418
1	3.669987	0.336979	1.698463
15	-1.795351	0.036093	0.549774
7	-2.028555	1.593988	1.207850
7	-2.940040	0.307179	-0.699477
6	-2.605660	-1.069352	1.775413
1	-2.022641	-1.050210	2.699142
1	-3.624703	-0.736987	1.986071
1	-2.620061	-2.098663	1.406511
6	-2.922666	2.409445	0.394852
1	-2.359387	3.030057	-0.318367
1	-3.503775	3.080433	1.036177
6	-3.814738	1.421523	-0.329999
1	-4.634861	1.088501	0.326535
1	-4.259628	1.853414	-1.231078
6	-1.029343	2.308772	1.973487
1	-0.378283	2.924006	1.338473
1	-0.406271	1.613263	2.534610
1	-1.526930	2.972677	2.687900
6	-3.641916	-0.829127	-1.278158
1	-4.418349	-1.229066	-0.608869
1	-2.937073	-1.623507	-1.519782
1	-4.125589	-0.515499	-2.207545
17	0.998727	-0.708017	2.326924
6	1.899409	-2.443704	-0.064606
1	1.478215	-3.402877	0.257965
1	2.725418	-2.187180	0.601218
1	2.257310	-2.541115	-1.091033
17	-0.343235	-1.805955	-2.092092

Complex **9a** of Fig. S4(e)

78	0.346745	-1.000312	-0.109554
15	1.527035	0.993710	-1.104960
7	0.522851	2.339718	-1.065985
7	2.556189	1.656913	0.023214
6	1.048155	3.452179	-0.272045
1	0.235638	3.987372	0.226592
1	1.563860	4.161656	-0.934056
6	2.018062	2.825118	0.717728
1	2.829141	3.507553	0.982362
1	1.519198	2.507776	1.642012
6	-0.329682	2.677049	-2.192904
1	-1.216580	3.211379	-1.846636
1	-0.657263	1.771098	-2.703275
1	0.196001	3.314428	-2.914968
6	3.697104	0.977650	0.603984
1	4.552124	1.659434	0.627603
1	3.956057	0.105758	0.004127
1	3.472065	0.640956	1.620592
15	-1.736684	-0.315280	0.470128
7	-2.092607	1.177546	1.141070
7	-2.903605	-0.153135	-0.754509
6	-2.321924	-1.572187	1.664821
1	-1.705606	-1.514035	2.563355
1	-3.367273	-1.382928	1.919762
1	-2.216205	-2.574310	1.243173

6	-3.098623	1.926654	0.398308
1	-2.633811	2.677293	-0.252616
1	-3.755269	2.452319	1.098369
6	-3.871319	0.888531	-0.397281
1	-4.687374	0.469311	0.210742
1	-4.308991	1.309455	-1.306458
6	-1.394133	1.851227	2.213351
1	-0.937152	2.783354	1.863246
1	-0.608419	1.214052	2.616388
1	-2.092400	2.098383	3.020993
6	-3.505118	-1.342220	-1.342595
1	-4.281149	-1.775771	-0.696565
1	-2.750500	-2.102933	-1.535386
1	-3.963679	-1.077314	-2.298668
17	1.075911	-0.761672	2.275922
6	-0.233881	-1.420013	-2.051486
1	0.651835	-1.377325	-2.685822
1	-0.622822	-2.443047	-2.074522
1	-0.994687	-0.737484	-2.431165
17	2.411752	-2.283610	-0.590586

TS of Figure S10

78	0.936059	-1.299817	-0.290850
6	2.478105	-2.426066	0.379008
1	2.670261	-2.175241	1.426333
1	3.366063	-2.188202	-0.212774
1	2.250631	-3.489888	0.292003
15	1.913266	0.759252	0.122235
7	1.901262	1.922086	-1.051160
6	1.679288	3.282675	-0.565566
1	0.701596	3.634143	-0.916775
1	2.444869	3.963157	-0.950320
6	1.731981	3.194796	0.959945
1	2.742925	3.409254	1.333489
1	1.037821	3.893380	1.432305
7	1.351292	1.818891	1.295243
6	2.073549	1.685910	-2.467913
1	1.228814	2.102315	-3.026395
1	2.111620	0.612242	-2.660591
1	2.998267	2.142767	-2.836585
6	1.390454	1.461617	2.702461
1	2.389959	1.600242	3.134753
1	1.096149	0.418199	2.827904
1	0.681885	2.085440	3.251931
17	4.105670	0.612415	0.687326
6	-0.045891	-3.049760	-0.748868
1	0.491912	-3.614471	-1.519757
1	-1.041945	-2.798517	-1.134289
1	-0.163867	-3.701228	0.124363
15	-2.920627	0.927554	0.511918
7	-3.332503	-0.517813	1.199508
6	-4.707174	-0.963951	0.959736
1	-5.288335	-0.843868	1.882211
1	-4.724678	-2.020330	0.678297
6	-5.232361	-0.073477	-0.160162
1	-5.061932	-0.529700	-1.144756
1	-6.300084	0.131067	-0.056004
7	-4.470901	1.175616	-0.053911
6	-2.503156	-1.270000	2.119619
1	-2.978427	-1.327715	3.104780
1	-1.531605	-0.787173	2.231853
1	-2.337971	-2.285413	1.748422
6	-4.777740	2.225500	-1.009200
1	-4.616893	1.893471	-2.042009
1	-4.149368	3.097457	-0.821008
1	-5.821411	2.527195	-0.894585
17	-1.797718	0.278180	-1.559143

product of Figure S10

78	0.657495	-1.271632	-0.304174
6	2.026170	-2.603200	0.418600
1	2.245374	-2.380941	1.468357
1	2.962271	-2.515038	-0.143302
1	1.668777	-3.633511	0.344413
15	1.883883	0.620052	0.147868
7	2.241548	1.691434	-1.057490
6	2.194881	3.097686	-0.665600
1	1.349563	3.583816	-1.168616
1	3.111446	3.616754	-0.962486
6	2.023109	3.101672	0.854105
1	2.995872	3.169624	1.360921
1	1.403581	3.935980	1.191227
7	1.367043	1.834099	1.184636
6	2.542246	1.338401	-2.426806
1	1.862683	1.857397	-3.111312
1	2.409822	0.264149	-2.567408
1	3.572626	1.602334	-2.689425
6	1.141261	1.564074	2.592628
1	2.077435	1.550208	3.166228
1	0.644571	0.598840	2.707314
1	0.487844	2.335292	3.007201
17	3.938586	0.182526	1.039834
6	-0.486819	-2.925516	-0.795977
1	0.065968	-3.584298	-1.476643
1	-1.417979	-2.622926	-1.285415
1	-0.734151	-3.512220	0.096767
15	-2.688787	0.979958	0.675185
7	-3.442060	-0.417381	1.105539
6	-4.798003	-0.592295	0.572460
1	-5.519631	-0.430252	1.381375
1	-4.927822	-1.608741	0.193688
6	-4.941109	0.447288	-0.535055
1	-4.687512	0.027814	-1.516689
1	-5.952108	0.856180	-0.585432
7	-3.988030	1.512691	-0.201102
6	-2.937413	-1.370135	2.076626

1	-3.579072	-1.389174	2.963169
1	-1.926980	-1.094199	2.379614
1	-2.903506	-2.371876	1.641448
6	-3.936050	2.678530	-1.066423
1	-3.701333	2.395940	-2.098549
1	-3.174184	3.373793	-0.711848
1	-4.901459	3.188927	-1.049710
17	-1.165781	0.241494	-1.305926

Coordinates of the optimized geometries at B3PW91−D3/BS2 for route C in Å.

Complex **3a**

78	-0.000021	1.236583	0.000009
6	1.369326	2.821851	-0.216219
1	1.238849	3.238427	-1.221669
1	2.421071	2.543213	-0.111746
1	1.143827	3.611020	0.507596
15	1.673666	-0.305904	-0.141057
7	2.582793	-0.611183	1.196810
6	3.026619	-1.998357	1.319608
1	2.553515	-2.442559	2.203315
1	4.111534	-2.052317	1.448224
6	2.583873	-2.699611	0.030303
1	3.398380	-2.722174	-0.707442
1	2.262720	-3.726787	0.216640
7	1.456194	-1.920065	-0.480054
6	2.928791	0.355901	2.214175
1	2.667847	-0.036616	3.202229
1	2.364173	1.275307	2.053105
1	3.998901	0.587580	2.197831
6	0.851071	-2.350133	-1.723318
1	1.588148	-2.419694	-2.533879
1	0.071431	-1.646208	-2.018832
1	0.384562	-3.326675	-1.576473
17	3.138825	0.260160	-1.721223
6	-1.369455	2.821756	0.216159
1	-1.239488	3.237882	1.221867
1	-2.421142	2.543129	0.111022
1	-1.143604	3.611249	-0.507192
15	-1.673700	-0.305922	0.141056
7	-2.582908	-0.611204	-1.196746
6	-3.026562	-1.998425	-1.319613
1	-2.553332	-2.442546	-2.203294
1	-4.111462	-2.052514	-1.448309
6	-2.583814	-2.699652	-0.030296
1	-3.398316	-2.722208	0.707456
1	-2.262644	-3.726827	-0.216605
7	-1.456142	-1.920074	0.480017
6	-2.928752	0.355862	-2.214166
1	-2.667585	-0.036612	-3.202181
1	-2.364185	1.275278	-2.052921
1	-3.998870	0.587510	-2.198027
6	-0.850850	-2.350156	1.723187
1	-1.587807	-2.419730	2.533855
1	-0.071161	-1.646240	2.018592
1	-0.384366	-3.326696	1.576251
17	-3.138819	0.260029	1.721268

Complex **10a**

78	-0.169135	-1.202064	-0.171827
15	1.568810	0.262214	0.240394
7	2.311390	0.954621	-1.053555
7	1.250759	1.733707	0.965910
6	2.762729	2.327338	-0.810829
1	2.308522	2.981490	-1.562063
1	3.849641	2.400836	-0.907881
6	2.311682	2.687293	0.613137
1	3.145234	2.603871	1.322610
1	1.915602	3.702833	0.671261
6	2.778340	0.236083	-2.220617
1	2.611298	0.846593	-3.111710
1	2.211530	-0.689505	-2.332345
1	3.844792	-0.002845	-2.148917
6	0.754254	1.789658	2.330847
1	1.556104	1.646424	3.066026
1	0.000512	1.014600	2.484924
1	0.286536	2.761255	2.499739
15	-1.711641	0.380192	-0.147102
7	-3.140037	0.420506	0.618614
7	-1.838153	1.845191	-0.830449
6	-3.961193	1.592254	0.273508
1	-4.425580	1.988994	1.176951
1	-4.749144	1.275201	-0.416219
6	-3.007425	2.610129	-0.366740
1	-3.469291	3.118394	-1.213649
1	-2.666034	3.362192	0.351238
6	-3.701956	-0.658002	1.415309
1	-3.988867	-0.273298	2.395640
1	-2.958419	-1.444090	1.545093
1	-4.580698	-1.073465	0.916171
6	-0.807680	2.499334	-1.618501
1	-1.247413	2.889041	-2.538216
1	-0.027646	1.782562	-1.872090
1	-0.366116	3.318276	-1.046124
6	1.137014	-2.837704	-0.162268
1	1.402360	-3.016286	0.885180
1	0.679444	-3.737983	-0.574010
1	2.060804	-2.623946	-0.707633
17	3.146239	-0.588718	1.462114

6	-1.612254	-2.665039	-0.676498
1	-2.629600	-2.295625	-0.827311
1	-1.291973	-3.155761	-1.599479
1	-1.631423	-3.412862	0.122256

Complex TS(**10a**→**11a**)

6	-3.292405	1.573772	1.620583
6	-2.859022	2.552608	0.529174
6	-3.155700	-0.918996	1.963010
6	-1.007767	2.708233	-1.135646
6	2.186195	-1.930097	-0.023101
6	4.092615	1.508019	-0.391866
6	4.118417	1.071095	1.072870
6	2.730293	0.887227	-2.429346
6	2.388730	0.318237	2.750307
6	-1.012347	-2.719209	-0.353801
7	-2.807448	0.258419	1.195743
7	-1.625558	1.988791	-0.035034
7	3.009498	0.739244	-1.013197
7	2.727709	0.735960	1.400833
17	-2.942030	-0.046222	-1.849633
15	-1.775296	0.330712	-0.074471
15	1.926246	0.165991	0.079647
78	0.032243	-0.910412	-0.123370
1	-2.840744	1.823186	2.587512
1	-4.379088	1.560985	1.734531
1	-3.629361	2.647604	-0.248427
1	-2.651122	3.544783	0.932643
1	-2.898191	-0.766287	3.015674
1	-2.600960	-1.781489	1.597348
1	-4.226130	-1.129277	1.884923
1	-1.675717	2.790797	-2.002006
1	-0.093818	2.196684	-1.441456
1	-0.741005	3.710226	-0.795605
1	2.383448	-2.245569	-1.046459
1	1.659025	-2.705995	0.539420
1	3.136127	-1.800874	0.501693
1	3.884084	2.580220	-0.486732
1	5.038893	1.290176	-0.891600
1	4.764948	0.195188	1.218356
1	4.468014	1.870463	1.728122
1	2.517433	1.931849	-2.680016
1	1.864346	0.280220	-2.700142
1	3.587137	0.546763	-3.014879
1	2.945678	-0.577577	3.048196
1	1.319642	0.103977	2.805635
1	2.617389	1.126150	3.447531
1	-2.051421	-2.646732	-0.680832
1	-0.452629	-3.286608	-1.106825
1	-0.974176	-3.273722	0.590864

Complex **11a**

78	-0.470683	-1.354002	0.070457
15	-1.231415	0.649070	-0.062285
7	-1.061226	1.629374	1.235559
7	-0.504380	1.683442	-1.141502
6	-0.544372	2.954271	0.893641
1	0.485922	3.034707	1.251047
1	-1.149769	3.731940	1.365610
6	-0.614088	3.056767	-0.631373
1	-1.562746	3.505775	-0.955785
1	0.205959	3.654829	-1.032927
6	-1.471765	1.307306	2.584815
1	-0.728021	1.676853	3.293680
1	-1.542525	0.223747	2.699552
1	-2.441725	1.754746	2.824843
6	-0.708430	1.499607	-2.568453
1	-1.683033	1.884728	-2.893444
1	-0.651548	0.438061	-2.814192
1	0.077864	2.024745	-3.113364
15	1.767310	-0.574257	0.160607
7	2.572684	-0.061356	-1.230524
7	2.053199	0.875122	0.991417
6	2.826038	-1.876993	0.886189
1	2.826279	-2.742550	0.218634
1	2.424380	-2.188656	1.853708
1	3.849280	-1.514002	1.005069
6	2.976191	1.338563	-1.136233
1	2.202986	1.994169	-1.560215
1	3.908811	1.500876	-1.684628
6	3.148104	1.604495	0.351571
1	4.130944	1.252705	0.702417
1	3.065100	2.669259	0.585809
6	2.253129	-0.588902	-2.541746
1	1.606337	0.089304	-3.108648
1	1.737688	-1.547233	-2.449017
1	3.168750	-0.750499	-3.118439
6	2.035772	0.856312	2.441083
1	2.953487	0.431653	2.871931
1	1.185944	0.267969	2.792570
1	1.920121	1.874503	2.820921
6	-2.342959	-2.275585	0.067762
1	-3.018355	-1.906121	0.843819
1	-2.841030	-2.185163	-0.901566
1	-2.113762	-3.333792	0.263982
17	-3.300598	0.735663	-0.576471

Complex **5a**

15	1.548823	-0.040784	0.130484
7	2.101418	0.892503	-1.123898
7	1.576064	1.185011	1.227013
6	2.887083	2.011492	-0.603200
1	2.855587	2.837393	-1.316879
1	3.935848	1.712546	-0.466083
6	2.237004	2.391862	0.731875
1	2.987677	2.739949	1.446693

1	1.482676	3.172819	0.596800
6	2.510516	0.287683	-2.375331
1	2.480034	1.040923	-3.165856
1	1.814409	-0.512926	-2.635364
1	3.525088	-0.127819	-2.321389
6	1.309870	1.007341	2.634700
1	2.235876	0.889459	3.209897
1	0.693267	0.117733	2.778525
1	0.761245	1.867487	3.025655
15	-1.556914	0.795298	-0.373381
7	-2.303358	1.422903	1.020623
7	-0.770137	2.263609	-0.741135
6	-2.901666	0.626187	-1.598219
1	-3.600128	-0.137210	-1.254840
1	-2.484576	0.304066	-2.555689
1	-3.422281	1.578772	-1.719366
6	-1.866390	2.792032	1.286304
1	-1.012775	2.805134	1.978831
1	-2.679238	3.367506	1.739885
6	-1.460830	3.358675	-0.063339
1	-2.345924	3.695382	-0.627649
1	-0.786080	4.213308	0.041100
6	-2.515455	0.575174	2.179621
1	-1.613993	0.475344	2.799425
1	-2.825113	-0.421238	1.862717
1	-3.311992	0.999498	2.797542
6	-0.383906	2.521949	-2.115666
1	-1.234321	2.828551	-2.742725
1	0.066815	1.630160	-2.550324
1	0.366248	3.316717	-2.138580
6	0.679179	-3.033120	0.125113
1	1.499620	-3.130267	-0.593249
1	1.104412	-3.120423	1.130516
1	-0.033767	-3.845500	-0.033135
17	3.303780	-1.219771	0.667919
78	-0.300074	-1.191125	-0.098167
17	-2.370357	-2.444416	-0.189999

Complex **12a**

78	0.092619	-1.093781	-0.103537
15	-1.635202	0.128230	-0.229021
7	-3.041965	0.017939	0.555257
7	-1.974337	1.461416	-1.071868
6	-4.031215	1.012426	0.108030
1	-4.528555	1.441152	0.978371
1	-4.776945	0.506540	-0.511343
6	-3.252468	2.079247	-0.680320
1	-3.791870	2.390193	-1.575008
1	-3.035856	2.962534	-0.072713
6	-3.425129	-1.053017	1.460937
1	-3.745148	-0.625682	2.412653
1	-2.571358	-1.708258	1.632509
1	-4.242270	-1.632776	1.026093
6	-1.047778	2.170645	-1.935668
1	-1.535141	2.387140	-2.887545
1	-0.174803	1.546188	-2.120532
1	-0.731527	3.099584	-1.457618
15	1.543055	0.631560	0.583122
7	2.618805	1.251274	-0.563162
7	0.781727	2.129825	0.851939
6	2.528978	0.192746	2.045219
1	3.161504	-0.659476	1.790036
1	1.861026	-0.104987	2.856963
1	3.149518	1.035363	2.356430
6	2.424588	2.690568	-0.760053
1	1.813253	2.878496	-1.653179
1	3.390588	3.182419	-0.904285
6	1.717630	3.197507	0.489093
1	2.436258	3.399766	1.297633
1	1.163612	4.118902	0.293790
6	2.967508	0.478502	-1.744785
1	2.185318	0.521020	-2.515850
1	3.129640	-0.565660	-1.477470
1	3.895039	0.870523	-2.168883
6	0.010465	2.336586	2.066846
1	0.643005	2.506994	2.948554
1	-0.619134	1.465854	2.268180
1	-0.643967	3.201163	1.935221
17	1.886407	-2.660668	0.023149
6	-1.098561	-2.752268	-0.719985
1	-0.581526	-3.185404	-1.579096
1	-1.077080	-3.460298	0.112492
1	-2.138312	-2.562702	-0.995615

Complex TS(**12a→13a**)

78	-0.112988	-0.948654	-0.013215
15	1.704729	0.093768	0.124571
7	2.826323	0.448959	-0.990374
7	2.397305	0.876250	1.359140
6	4.035030	1.039894	-0.395286
1	4.423461	1.815777	-1.055643
1	4.795261	0.260189	-0.281833
6	3.605532	1.615793	0.961758
1	4.382230	1.481977	1.715701
1	3.358353	2.679632	0.892955
6	2.866883	-0.132893	-2.322112
1	3.106285	0.643574	-3.050188
1	1.890388	-0.554833	-2.565239
1	3.618241	-0.925723	-2.372129
6	1.771633	1.112025	2.649520
1	2.446645	0.801862	3.448971
1	0.850313	0.532548	2.717906
1	1.531841	2.172284	2.763295
15	-1.757765	0.567807	-0.445015
7	-2.629911	1.151992	0.880940
7	-1.156126	2.087306	-0.879633

6	-2.976306	0.001116	-1.663855
1	-3.489204	-0.873981	-1.260039
1	-2.461937	-0.294898	-2.580913
1	-3.695043	0.795904	-1.872045
6	-2.316583	2.565753	1.110333
1	-1.461621	2.671409	1.794719
1	-3.180515	3.066441	1.555012
6	-1.972818	3.130261	-0.259150
1	-2.882949	3.343324	-0.839875
1	-1.390528	4.051723	-0.183197
6	-2.769960	0.322048	2.067661
1	-1.855271	0.311329	2.676495
1	-3.005420	-0.704471	1.783668
1	-3.592017	0.704501	2.677083
6	-0.657466	2.317785	-2.222686
1	-1.459295	2.410257	-2.967835
1	-0.001822	1.495548	-2.519868
1	-0.066081	3.236013	-2.233214
17	-1.621540	-2.806970	0.063231
6	1.679046	-2.248678	0.460748
1	1.320925	-2.681328	1.394943
1	1.601887	-2.936601	-0.381546
1	2.737526	-2.002763	0.593216

Complex **13a**

78	-0.907227	-0.903179	-0.095046
15	1.305790	-1.083094	0.160291
7	1.992026	-0.111907	1.346984
7	2.410032	-0.655007	-0.997577
6	3.396149	0.148308	1.020847
1	4.042716	-0.655553	1.402022
1	3.709596	1.085510	1.487161
6	3.465467	0.223056	-0.504296
1	3.307742	1.246372	-0.860580
1	4.439504	-0.118085	-0.866208
6	1.674133	-0.368015	2.740816
1	2.217893	-1.231722	3.146240
1	0.602147	-0.549215	2.845211
1	1.926892	0.509957	3.339712
6	2.387041	-1.092490	-2.375387
1	2.614281	-0.256794	-3.042140
1	1.392187	-1.462308	-2.635099
1	3.115406	-1.890185	-2.558852
15	-0.818163	1.278351	-0.370312
7	-0.924134	2.192820	1.023982
7	0.608694	1.960608	-0.895092
6	-2.163548	1.764553	-1.482036
1	-3.116983	1.545295	-1.002160
1	-2.102779	1.195215	-2.410283
1	-2.068712	2.834114	-1.679489
6	0.359403	2.846791	1.301691
1	1.003449	2.197609	1.902529
1	0.180488	3.775448	1.847935
6	0.977311	3.109889	-0.063785
1	0.581864	4.036722	-0.502055
1	2.064718	3.191278	-0.002568
6	-1.702483	1.732303	2.162671
1	-1.149337	1.005954	2.769629
1	-2.625403	1.262278	1.820952
1	-1.962949	2.590036	2.786072
6	0.914851	2.028047	-2.312086
1	0.422352	2.879040	-2.799350
1	0.598889	1.109549	-2.807452
1	1.992572	2.129500	-2.449906
17	-3.316334	-1.074769	-0.045305
6	1.558545	-2.848272	0.566429
1	0.912631	-3.146395	1.395004
1	1.314544	-3.459840	-0.305100
1	2.605713	-3.004237	0.83563

Complex **4a**

78	-0.000183	1.006584	-0.000026
15	-1.636047	-0.455458	0.500642
7	-2.869995	-0.629602	-0.649605
7	-1.324998	-2.103662	0.596253
6	-2.437376	-0.003424	2.072715
1	-2.922470	0.966428	1.979085
1	-1.680650	0.056506	2.858106
1	-3.172811	-0.772175	2.320545
6	-2.993891	-2.028594	-1.070994
1	-2.413960	-2.211104	-1.986384
1	-4.041393	-2.257869	-1.284276
6	-2.456867	-2.863048	0.080070
1	-3.228290	-3.016869	0.851356
1	-2.118930	-3.846482	-0.258070
6	-3.048025	0.349528	-1.711773
1	-2.248388	0.293647	-2.464137
1	-3.065430	1.357240	-1.300588
1	-4.005678	0.161802	-2.203364
6	-0.615507	-2.656091	1.728647
1	-1.279728	-2.856629	2.580838
1	0.161604	-1.964344	2.054437
1	-0.128474	-3.588737	1.434434
15	1.636330	-0.454803	-0.500658
7	2.870351	-0.628583	0.649603
7	1.325847	-2.103111	-0.596283
6	2.437466	-0.002639	-2.072802
1	2.922418	0.967279	-1.979202
1	1.680683	0.057174	-2.858147
1	3.173005	-0.771275	-2.320686
6	2.994602	-2.027518	1.071060
1	2.414658	-2.210158	1.986417
1	4.042152	-2.256494	1.284419
6	2.457902	-2.862151	-0.080010
1	3.229417	-3.015772	-0.851241
1	2.120219	-3.845670	0.258136

6	3.048236	0.350588	1.711766
1	2.248613	0.294607	2.464138
1	3.065512	1.358296	1.300588
1	4.005916	0.162998	2.203358
6	0.616594	-2.655825	-1.728692
1	1.280942	-2.856191	-2.580823
1	-0.160732	-1.964372	-2.054588
1	0.129856	-3.588617	-1.434458
17	1.604538	2.798687	-0.473595
17	-1.606024	2.797599	0.473750

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