

SUPPORTING INFORMATION

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EXPERIMENTAL:

General Considerations.

All air- and moisture-sensitive manipulations were carried out using standard vacuum line Schlenk techniques or in an MBraun inert atmosphere dry-box containing an atmosphere of purified argon. THF-*d*₈, CD₂Cl₂ and C₆D₆ were purchased from Cambridge Isotope Laboratories. CD₂Cl₂ was dried over CaH₂ and distilled, THF-*d*₈ and C₆D₆ were distilled over potassium. All glassware was stored in a 120°C oven for several hours and was degassed prior to use. Solvents were degassed prior to the filtration over alumina in the PureSolv-purification system by “inert”, the water content was determined by Karl Fischer titration. Solvents were additionally tested using a ketyl test to guarantee oxygen and moisture free conditions. Phosphorus halides were used as purchased. The Na(OCP) and the azadiphospholide Na[1]¹, [Mo(Mes)(CO)₃]² have been synthesized using literature procedures.

¹H NMR spectra were recorded on Bruker spectrometers operating at 300, 400 and 500 MHz, ¹³C NMR at 75.46 MHz 100.61 MHz. ³¹P NMR at 101.28, 121.494 and 161.97 MHz. All ¹H and ¹³C NMR chemical shifts are reported relative to SiMe₄ using the ¹H (residual) and ¹³C chemical shifts of the solvent as a secondary standard. Peak widths at half heights (in Hz) are given for broad signals. Infrared spectra were collected on a Bruker-alpha FT-IR-spectrometer. UV/Vis spectra were recorded on UV/VIS/NIR lambda-19-spectrometer in a cell with a 1 or 2 mm path length. Elemental analyses were performed at the Mikrolabor of ETH Zürich.

Single crystals suitable for X-ray diffraction were coated with polyisobutylene oil in a glovebox, transferred to a nylon loop and then transferred to the goniometer of a Bruker X8 APEX2 or D8-Venture diffractometer or on an Oxford Excalibur equipped with a molybdenum X-ray tube ($\lambda = 0.71073 \text{ \AA}$). Preliminary data was collected to determine the crystal system. The space group was identified and the data were processed using the Bruker SAINT+ program and corrected for absorption using SADABS. The structures were solved using direct methods (SHELXS) on OLEX2 completed by Fourier synthesis and refined by full-matrix least-squares procedures.

Preparation of compound 2: Na[1] (1.7 g, 4.6 mmol) was dissolved in 20 mL of THF and was added dropwise to a solution of PhSiCl₃ (322 mg, 1.5 mmol) in THF cooled to -78°C. The reaction mixture was warmed up to room temperature and was stirred for additional 2 hours. The reaction mixture was filtered through Celite and the volatiles were removed under reduced pressure. The product was washed with a minimal amount of a THF/diethylether (1:1) mixture. To yield 632 mg (70 %) of a yellow solid. MF: C₂₄H₁₇N₃O₃P₆Si, MW: 609.35 g/mol, MP: 178 °C, EA[calc]: C, 47.31; H, 2.81; N, 6.90, EA[found]: C, 46.71; H, 2.75; N, 6.97, Absorption max [$\lambda \text{ nm}$]: 395.2, 341.4, 326.8. ³¹P{¹H}-NMR (CD₂Cl₂, 121.5 MHz): δ (ppm) = 123.07 (d, ¹J_{P,P} = 442.58 Hz), 118.84 (d, ¹J_{P,P} = 442.64 Hz). ¹H-NMR (CD₂Cl₂, 121.5 MHz): δ (ppm) = 8.58 (d, *J* = 7.08 Hz, 3H, CH), 8.10 (d, *J* = 6.84 Hz, 2H, CH), 7.84-7.96 (m, 3H, CH), 7.65 (t, *J* = 7.52 Hz, 1H CH), 7.52 (t, *J* = 7.40 Hz, 2H, CH), 6.89 (m, 6H, CH). IR[cm⁻¹]: 1504.63, 1448.88, 1430.30, 1336.24, 1309.93, 1246.68, 1211.41, 1119.90, 1067.00, 1023.36, 981.55, 882.00, 853.53, 730.31, 689.58

Preparation of compound Na[3]: Na[1] (1 g, 2.52 mmol) was dissolved in 20 mL of THF and was added dropwise to a solution of PhBCl₂ (100 mg, 0.63 mmol) in THF cooled to -78°C. The reaction mixture was warmed up to room temperature and was stirred for additional 2 hours. The reaction mixture was filtered through Celite the solution was concentrated to 5 mL of THF layered with hexanes and placed in the freezer to yield 438 mg (69

%) of a yellow crystalline solid. MF: $C_{44}H_{59}BN_3NaO_9P_6$, MW: 993.61 g/mol for $Na[3](THF)_4(DME)_1$. MP: 168 °C dec.), Absorption max [λ nm]: 417.6, 353.3; $^{31}P\{^1H\}$ -NMR (121 MHz, THF-d8): δ (ppm) = 115.11 (d, $^1J_{P,P}$ = 414.6 Hz), 107.11 (d, $^1J_{P,P}$ = 414.6 Hz). 1H -NMR (300 MHz, THF): δ (ppm) = 8.93 (d, J = 7.3 Hz, 3H), 7.81 (d, J = 6.4 Hz, 2H), 7.54 (dd, J = 5.3, 8.5 Hz, 3H), 6.85 – 7 (m, CH, 3H), 6.62 (t, J = 6.6 Hz, 3H), 6.48 (dd, J = 7.0, 7.8 Hz, 2H). ^{13}C -NMR (75 MHz, THF-d8): δ (ppm) = 175.93 (dd, $^1J_{P,C}$ = 3.3, 85.9 Hz), 158.71 (dd, $^1J_{P,C}$ = 4.6, 64.4 Hz), 131.75 (s), 126.57 (d, $^1J_{P,C}$ = 21.7 Hz), 126.1 (s), 123.9 (s), 112.52 (d, $^1J_{P,C}$ = 19.3 Hz), 110.36 (d, $^1J_{P,C}$ = 2.5 Hz).

Synthesis of 4: $POCl_3$ (580 mg, 3.78 mmol) was dissolved in 20 mL THF and was added dropwise at $-78^\circ C$ to a solution of the sodium salt of the azadiphospholide $Na[1]$ (4.2 g, 11.35 mmol, 3 eq) in THF (15 mL). The solution was stirred at $-78^\circ C$ for 1 hour. After that time the reaction mixture was warmed up to room temperature whereupon the colour changed from red to yellow and a precipitate was formed. The solvent was removed under reduced pressure and the remaining solid was dissolved in 40 mL of DCM, filtered through Celite and was dried under reduced pressure to give 1.15 g of a yellow powder (55 % yield). The solid was extracted twice with THF (20 mL) to yield another 609 mg of product. Combined 1.759 g (84 % yield) of product were isolated. The compound is soluble in THF and DCM and only barely soluble in diethyl ether and toluene and insoluble in hexane. MF: $C_{18}H_{12}N_3O_4P_7$, MW: 551.13 g/mol, MP: 140 °C (decomposition), EA[calc]: C, 39.23; H, 2.19; N, 7.62, EA[found]: C, 38.99; H, 2.43; N, 7.36, Absorption max [λ nm] : 395.2, 341.4, 326.8. ^{31}P -NMR{ 1H } (CD_2Cl_2 , 121.5 MHz): δ (ppm) = 140.24 (d, $^1J_{P,P}$ =446.5 Hz), 129.41 (d, $^1J_{P,P}$ =446.5 Hz), - 20.78 (s, PO). 1H -NMR (CD_2Cl_2 , 300 MHz): δ (ppm) = 8.18 – 8.32 (m, 1H, CH_{arom}), 7.81 – 7.94 (m, 1H, CH_{arom}), 6.75 – 6.92 (m, 2H, CH_{arom}). $^{13}C\{^1H\}$ -NMR (CD_2Cl_2 , 300 MHz): δ (ppm) = 162.84 (d, $J_{P,C}$ = 72.88 Hz), 158.82 (d, $J_{P,C}$ = 86.85 Hz), 128.42 (d, $J_{P,C}$ = 23.27 Hz), 117.96 (d, $J_{P,C}$ = 18.72 Hz), 115.40 (d, $J_{P,C}$ = 2.68 Hz). IR[cm^{-1}] : 2963, 1261 (P=O), 1091, 1021, 799

Preparation of complex 5: Compound **2** (100 mg, 0.11 mmol) and $[MesMo(CO)_3]$ (45 mg, 0.15 mmol) were placed in a scintillation vial in the glovebox and were suspended in 4 mL of THF. The reaction mixture was left unstirred overnight. The colour of the reaction mixture changed from yellow to red and was filtered then over a glass filter and was layered with hexane before it was placed in the freezer at $-35^\circ C$ for crystallization. After 72 hours a dark yellow crystalline material was formed which was filtered off and washed with hexane to yield 64 mg (74 %) of product. Once crystallized the product was nearly insoluble in the common deuterated organic solvents. MF: $C_{27}H_{17}MoN_3O_6P_6Si$, MW: 789.34 g/mol, MP: no < 400 °C, EA[calc]: C, 41.08; H, 2.17; N, 5.32, EA[found]: C, 40.98; H, 2.08; N, 5.27, Absorption max [λ nm] : 426.7, 333.7, 270.9. $^{31}P\{^1H\}$ -NMR (CD_2Cl_2): 141.77 (m), 98.27 (m). IR[cm^{-1}] : 1959.58, 1896.16, 1870.90, 1609.73, 1355.60, 1308.51, 1253.60, 1221.42, 1123.46, 875.45, 724.85

Preparation of compound Na[6]: $Na[3]$ (200 mg, 0.2 mmol) and $[MesMo(CO)_3]$ (80 mg, 0.26 mmol) were placed in a scintillation vial in the glovebox and 4 mL of THF and 18C6 (52 mg, 0.2 mmol) was added. The reaction was stirred overnight to form a yellow microcrystalline solid. The colour of the reaction mixture changed from yellow to red. The reaction mixture was filtered to isolate 230 mg (95 %) of a yellow solid of composition $Na(18C6)_1(THF)_2[Mo(CO)_3(3)]$. The mother liquor was placed in the freezer to obtain single crystals suitable for X-ray diffraction. MF: $C_{47}H_{57}BMoN_3NaO_{14}P_6$, MW: 1203.6 g/mol, MP: 198 °C (dec.), EA[calc]: C, 46.90; H, 4.77; N, 3.49, EA[found]: C, 45.46; H 4.40; N 3.53; Absorption max [λ nm] : 445.1; 1H NMR (500 MHz, CD_2Cl_2):

= δ 8.29 (d, $J = 7.2$ Hz, 3H, CH_{arom}), 7.97 (d, $J = 7.4$ Hz, 2H, CH_{arom}), 7.69 (t, $J = 7.3$, 3H, CH_{arom}), 7.41 (m, 2H, CH_{arom}), 7.36 (m, 1H, CH_{arom}), 6.64 (dd, $J = 7.1, 8.0$ Hz, 3H, CH_{arom}), 6.56 (dt, $J = 1.3, 6.6$ Hz, 3H, CH_{arom}). ³¹P{¹H}-NMR (121 MHz, CD₂Cl₂): δ (ppm) = 125.6 (m), 89.3 (m) with $^1J_{A,X} = 450.1$ Hz, $J_{A,A'} = 38.03$ Hz, $J_{A,X'} = 2.2$ Hz, $^1J_{X,X'} = 9.43$ Hz. ¹³C-NMR (125.8 MHz, THF-d₈): δ (ppm) = 220.0 (m, broad, CO), 173.7 (broad, CP), 160.73 (d, $J_{P,C} = 67.95$ Hz, CP), 131.5 (s), 127.97 (d, $J_{P,C} = 26.23$ Hz), 127.7 (s), 126.8 (s), 126.4, 125.4 (s), 116.13 (1C, d, $J_{P,C} = 20.27$ Hz), 116.14 (s).

Preparation of compound 7: CpTiCl₃ (48 mg, 0.22 mmol) and Na[1] (210 mg, 0.65 mmol) were placed in a scintillation vial in the glovebox and the solids were covered with 1 mL of hexane. 3 mL of toluene were slowly added. The reaction was let unstirred overnight and the product crystallized over 3 days as purple blocks. The solid was collected on a glass frit. To remove the remaining NaCl, the product was dissolved in THF and was filtered through Celite. The volatiles were removed and 40 mg of a dark purple solid was isolated. The purple reaction solution was layered with hexane and put in the freezer for 14 days to crystallize another 16 mg of the product. A total amount of 56 mg (41 % yield) was isolated.

Alternative route for the synthesis of compound 7: CpTiCl₃ (48 mg, 0.22 mmol) was dissolved in 10 mL of THF and was cooled to -78°C. The Na[1] (210 mg, 0.65 mmol) was dissolved in 10 mL of THF and was added slowly under vigorous stirring. It is not recommended to use an excess of the sodium salt of the phospholide Na[1]. The sodium salt replaced the cyclopentadienyl group to form the product Na₂[8_{Ti}]. The reaction mixture was stirred for 1 hour at this temperature before it was warmed up to room temperature. The reaction mixture was left unstirred for 2 hours to settle the precipitate. The mixture was then filtered through Celite. The filtrate was concentrated to roughly 4 mL and was layered with 4 mL of hexane. The layered solution was placed in the freezer at -35 °C for one week. Dark purple crystals formed, which were collected on a glass frit and were dried under reduced pressure to obtain 62 mg (46 %) of a purple solid. MF: C₂₃H₁₇N₃O₃P₆Ti, MW: 617.12 g/mol, MP: 228 °C, EA[calc]: C, 44.77; H, 2.78; N, 6.81, EA[found]: C, 44.12; H, 2.79; N, 6.43, Absorption max [λ nm]: 393, 498. ¹H/³¹P{¹H} NMR were measured in CD₂Cl₂ but the product slowly decomposes. Therefore the ¹³C NMR spectrum was measured in THF. ³¹P{¹H}-NMR (CD₂Cl₂, 121.5 MHz): δ (ppm) = 129.7 (d, $^1J_{P,P} = 444.3$ Hz), 120.6 (d, $^1J_{P,P} = 444.3$ Hz). ¹H-NMR (CD₂Cl₂, 300 MHz): δ (ppm) = 8.42 (d, $^3J_{H,H} = 6.81$ Hz, 3H, CH), 7.86 (dd, $^3J_{H,H} = 7.51$ Hz, $^3J_{H,H} = 5.93$ Hz, 3H, CH), 6.9 – 6.75 (m, 3H, CH), 6.79 (s, 5H, CH), 5.24 (m, 3H, CH). ¹³C{¹H}-NMR (THF, 121.5 MHz): δ (ppm) = 182.60 (d, $J_{P,C} = 69.97$ Hz), 159.43 (d, $J_{P,C} = 68.86$ Hz), 127.43 (d, $J_{P,C} = 22.28$ Hz, CH), 123.6 (s, CH), 120.53 (s, CH, Cp), 115.74 (d, $J_{P,C} = 18.36$ Hz, CH), 113.38 (d, $J_{P,C} = 2.60$ Hz, CH). IR[cm⁻¹]: 1318.85, 1281.72, 1212.15, 1111.04, 1013.50, 780.15, 735.00, 687.54

Preparation of complex Na₂[8_{Ti}](DME)₆: Titanium tetrachloride di tetrahydrofuran, [TiCl₄(THF)₂], (400 mg 1.2 mmol) was dissolved in 10 mL of THF and then added to a solution of Na[1] (2.7 g 7.2 mmol) in THF. The reaction mixture turned dark green to black immediately. The solution was stirred for 1 h at room temperature. The volatiles were removed under vacuum and the remaining product was dissolved in 20 mL of DCM. The mixture was filtered to remove NaCl. All volatiles were removed under reduced pressure. To the solid, DME (2 mL) and hexanes (8 mL) were added. The suspension was filtered and the product was collected on the glass frit. 1.932 g (98 %) of a dark green solid was isolated. The product was recrystallized from a saturated DCM solution at -30°C for single crystals suitable for X-ray structure analysis. MF: C₆₀H₈₄N₆Na₂O₁₈P₁₂Ti, MW: 1642.87 g/mol, MP: 137 °C, Absorption max [λ nm]: 520 nm. ³¹P{¹H}-NMR (CD₂Cl₂, 121.5 MHz, 298 K): δ = 111.7 (d, $^1J_{P,P} = 434.5$ Hz),

110.3 (d, $^1J_{P,P} = 434.5$ Hz). $^1\text{H-NMR}$ (CD_2Cl_2 , 300 MHz): δ (ppm) = 8.58 (m, CH, 6H), 7.57 (m, CH, 6H), 6.46 (m, CH, 6H), 6.23 (m, CH, 6H). $^{13}\text{C}\{^1\text{H}\}$ -NMR (CD_2Cl_2 , 100.5 MHz): δ (ppm) = 186.2 (dd, $J_{P,C} = 16.99, 57.74$ Hz), 160.1 (dd, $J_{P,C} = 7.93, 52.65$ Hz), 128.4 (d, $J_{P,C} = 17.63$ Hz), 126.9 (s), 116.02 (d, $J = 16.4$ Hz), 112.6 (s). IR[cm^{-1}]: 1341, 1289, 1079, 1063

Preparation of complex $\text{Na}_2[\mathbf{8}_{\text{Zr}}](\text{DME})_6$: Zirconium tetrachloride THF adduct, $[\text{ZrCl}_4(\text{THF})_2]$, (97 mg 0.26 mmol) was suspended in 4 mL of THF. To this suspension, Na[1] (592 mg 1.6 mmol) in 4 mL of THF was added dropwise while stirring. The solution was stirred for 2 h at room temperature and the volatiles were removed under reduced pressure. The yellow solid was dissolved in DCM and filtered over Celite. The volatiles were removed under reduced pressure and the product was washed with a minimal amount of cold DME (2 mL) and hexanes (3×4 mL) to give 396 mg (90 %) of a yellow crystalline material. $^1\text{H-NMR}$ analysis revealed the co-crystallization of two DME molecules per sodium ion. MF: $\text{C}_{60}\text{H}_{84}\text{N}_6\text{Na}_2\text{O}_{18}\text{P}_{12}\text{Zr}$, MW: 1686.22 g/mol $(\text{DME})_6$, MP: 141 $^\circ\text{C}$, Absorption max [λ nm]: 422.5, 356.7, 345.8. $^{31}\text{P}\{^1\text{H}\}$ -NMR (CD_2Cl_2 , 121.5 MHz): δ (ppm) = 105.1 (d, $^1J_{PP} = 426.2$ Hz), 99.4 (d, $^1J_{PP} = 426.2$ Hz). $^1\text{H-NMR}$ (CD_2Cl_2 , 300 MHz): δ (ppm) = 8.64 (m, 6H, CH), 7.57 (m, 6H, CH), 6.46 (m, 6H, CH), 6.24 (m, 6H, CH). $^{13}\text{C}\{^1\text{H}\}$ -NMR (CD_2Cl_2 , 75 MHz): δ (ppm) = 184.1 (dd, $J_{P,C} = 5.7, 64.7$ Hz), 161.7 (d, $J_{P,C} = 60.4$ Hz), 129.2 (d, $J_{P,C} = 20.7$ Hz), 126.4 (s), 116.3 (d, $J_{P,C} = 18.4$ Hz), 113.6 (d, $J_{P,C} = 2.0$ Hz), IR[cm^{-1}]: 3095, 2989, 2912, 2823, 1348, 1293, 1070, 1063

Preparation of complex $\text{Na}_2[\mathbf{8}_{\text{Hf}}](\text{DME})_6$: Hafnium tetrachloride (32 mg 0.1 mmol) and Na[1] (223 mg 0.6 mmol) were suspended in 4 mL of DME. The solution was stirred for 16 h at room temperature. The yellow product precipitated out of the solution and was filtered off. The solid was extracted with DCM and filtered again to remove the NaCl. The volatiles were removed under reduced pressure to yield 138 mg (78 %) of a yellow solid. Single crystals suitable for X-ray analysis were grown from a DCM solution at -35 $^\circ\text{C}$. MF: $\text{C}_{60}\text{H}_{84}\text{N}_6\text{Na}_2\text{O}_{18}\text{P}_{12}\text{Hf}$, MW: 1773.49 g/mol $(\text{DME})_6$, MP: 143.3 $^\circ\text{C}$, Absorption max [λ nm]: 409.0. $^{31}\text{P}\{^1\text{H}\}$ -NMR (CD_2Cl_2 , 121.5 MHz): δ (ppm) = 104.9 (d, $^1J_{P,P} = 426.3$ Hz), 98.8 (d, $^1J_{P,P} = 426.3$ Hz). $^1\text{H-NMR}$ (CD_2Cl_2 , 300 MHz): δ (ppm) = 8.50 (m, 6H, CH), 7.50 (m, 6H, CH), 6.39 (m, 6H, CH), 6.15 (m, 6H, CH). $^{13}\text{C}\{^1\text{H}\}$ -NMR (CD_2Cl_2 , 75 MHz): δ (ppm) = 171.3 (dd, $J_{P,C} = 66.1$ Hz, $J_{P,C} = 4.3$ Hz), 160.5 (d, $J_{P,C} = 61.3$ Hz), 127.9 (d, $J_{P,C} = 21.0$ Hz), 125.0 (s), 115.0 (d, $J_{P,C} = 18.8$ Hz), 112.2 (s). IR[cm^{-1}]: 3095, 2989, 2910, 2823, 1399, 1351, 1259, 1113, 1080, 1013

Preparation of complex **9:** **7** (31 mg, 0.05 mmol) was dissolved in 6 mL of THF. $[\text{MoMes}(\text{CO})_3]$ (15 mg, 0.05 mmol) was added to the solution and the reaction mixture was stirred for 15 minutes. The reaction was filtered over a glass filter paper and left unstirred over the weekend, upon dark red crystals grow directly from the reaction mixture. 32 mg (80 %) of product was isolated. The product was nearly insoluble in common deuterated organic solvents. MF: $\text{C}_{26}\text{H}_{17}\text{MoN}_3\text{O}_6\text{P}_6\text{Ti}$, MW: 797.11 g/mol, MP: no < 400 $^\circ\text{C}$, EA[calc]: C, 39.18; H, 2.15; Mo, 12.04; N, 5.27, EA[found]: C, 39.36; H, 2.42; N, 4.89, Absorption max [λ nm]: 423.2. $^1\text{H-NMR}$ (THF-d_8 , 300 MHz): δ (ppm) = 8.47 - 8.39 (m, br, 3H), 7.74-7.64 (m, br, 3H), 7.41 (s, 5H, Cp), 7.05-6.92 (m, br, 3H), 6.79-6.69 (m, br, 3H). IR[cm^{-1}]: 1943.31 (CO), 1862.74 (CO), 1319.60, 1290.62, 1253.59, 732.10

Attempts for the preparation of complex $\text{Na}_2[\mathbf{10}_{\text{Ti}}]$: $\text{Na}_2[\mathbf{8}_{\text{Ti}}]$ (190 mg, 0.116 mmol), 18-crown-6 (54 mg, 0.2 mmol) and $[\text{MoMes}(\text{CO})_3]$ (60 mg, 0.202 mmol) were dissolved in 12 mL of THF. The solution was left unstirred overnight upon a dark green micro crystalline solid precipitated from the reaction mixture. The solid was filtered off and dried under reduced pressure. 220 mg (96 %) were isolated. The product is insoluble in common organic solvents. MF: $\text{C}_{66}\text{H}_{72}\text{TiMo}_2\text{N}_6\text{Na}_2\text{O}_{24}\text{P}_{12}$, MW: 1990.71 g/mol, IR[cm^{-1}]: 1925 (CO), 1829 (CO)

Preparation of complex Na₂[10_{Hf}]: Na₂[8_{Hf}] (180 mg, 0.101 mmol), 18-crown-6 (54 mg, 0.2 mmol) and [MoMes(CO)₃] (60 mg, 0.202 mmol) were dissolved in 12 mL of DCM. The solution was left unstirred for 16 hours upon dark red crystals grow directly from the reaction mixture. The solid was filtered off and dried under reduced pressure to isolate 132 mg (61 %). The product is only badly soluble in THF and nearly insoluble in other common deuterated organic solvents. Single crystals for X-ray analysis were picked from the first crop of isolated product. MF: C₆₆H₇₂HfMo₂N₆Na₂O₂₄P₁₂, MW: 2121.39 g/mol, MP: 224 °C, Absorption max [λ nm]: 428.6, 443.2 (shoulder). ¹H-NMR (DMF-d₇, 300 MHz): δ (ppm) = 7.90 (m, 1H, CH), 7.62 (m, 1H, CH), 6.44 (m, 1H, CH), 5.96 (m, 1H, CH). ³¹P{¹H}-NMR (DMF-d₇, 121.5 MHz): δ (ppm) = 111.8 (m), 84.5 (m). ¹³C{¹H}-NMR (DMF-d₇, 75.5 MHz): δ (ppm) = 214.54 (m, carbonyl), 176.31 (s-broad), 154.70 (d, *J*_{P,C} = 67.35 Hz), 122.68 (d, *J*_{P,C} = 25.67 Hz), 118.1 (s), 110.75 (d, *J*_{P,C} = 18.71 Hz), 107.9 (s). IR[cm⁻¹] : 2870.07, 1929.57 (CO), 1817.34 (CO), 1605.99, 1500.46, 1450.60, 1394.73, 1348.95, 1293.22, 1245.96, 1088.34, 1015.54, 945.82, 775.56, 732.02, 689.30

Preparation of compound 11: Na[1] (740 mg, 2 mmol) was suspended in toluene and (Pr₂N)₂PCl (532 mg, 2 mmol) dissolved in 5 mL of toluene was added dropwise to the stirred suspension. The colour of the mixture changed from orange to dark yellow. The mixture was stirred for 16 hours at room temperature before it was filtered through Celite. The volatiles were removed to isolate 655 mg of a yellow solid (82 %). Single crystals were obtained from a saturated toluene solution at -35 °C. In solution two isomers were observed, only isomer A was fully characterized by NMR spectroscopy. MF: C₁₈H₃₂N₃OP₃, MW: 399.4 g/mol, MP: 148°C, EA[calc]: C, 54.13; H, 8.08; N, 10.52, EA[found]: C, 54.00; H, 7.96; N, 10.58, Absorption max [λ nm]: 398 , 331 **Isomer A:** ³¹P{¹H}-NMR (C₆D₆, 121.5 MHz): δ (ppm) = 134.3 (dd, ¹*J*_{P,P} = 121.8 Hz, ²*J*_{P,P} = 18.7 Hz), 121.8 (dd, ¹*J*_{P,P} = 425.5 Hz, ²*J*_{P,P} = 20.0 Hz), 109.0 (dd, ¹*J*_{P,P} = 425.5 Hz, ¹*J*_{P,P} = 120.7 Hz). ¹H-NMR (C₆D₆, 300 MHz): δ (ppm) = 8.38 (d, ³*J*_{H,H} = 7.03 Hz, 1H, CH), 7.64 (dd, ³*J*_{H,H} = 8.84 Hz, ³*J*_{H,H} = 9.11 Hz, 1H, CH), 6.28 (pseudo-t, ³*J*_{H,H} = 6.6 Hz, 1H, CH), 6.15 (dd, ³*J*_{H,H} = 7.03 Hz, ³*J*_{H,H} = 9.11 Hz, 1H, CH), 3.52 (*sept*, ³*J*_{H,H} = 6.55 Hz, 4H, CH), 1.12 (d, ³*J*_{H,H} = 6.55 Hz, 24H, CH₃). ¹³C{¹H}-NMR (C₆D₆, 125.8 MHz): δ (ppm) = 173.98 (dd, *J*_{P,C} = 22.12, 85.97 Hz), 162.67 (dd, *J*_{P,C} = 6.53, 71.56 Hz), 130.03 (d, *J*_{P,C} = 22.32 Hz), 123.9 (s), 115.85 (d, *J*_{P,C} = 20.05 Hz), 114.30 (d, *J*_{P,C} = 2.87 Hz), 45.91 (d, *J*_{P,C} = 12.59 Hz), 24.50 (d, *J*_{P,C} = 9.14 Hz), 24.07 (d, *J*_{P,C} = 5.53 Hz). IR[cm⁻¹] : 2970.63, 2926.97, 2865.76, 1453.98, 1390.86, 1362.40, 1318.36, 1302.31, 1249.03, 1197.08, 1175.71, 1152.72, 1113.87, 1024.44, 955.86, 871.51, 782.40, 741.15, 692.17 **Isomer B:** ³¹P{¹H}-NMR (DME, 121.5 MHz): δ (ppm) = 136.1 (s), 116.45 (d, ¹*J*_{P,P} = 442.2 Hz), 96.76 (d, ¹*J*_{P,P} = 442.2 Hz).

Synthesis of 12: [Mo(Mes)(CO)₃] (30 mg, 0.1 mmol) and **11** (40 mg, 0.1 mmol) were placed in a 10 mL Schlenk tube. DCM (2 mL) was added and the solution was left unstirred at room temperature. Overnight orange crystals of composition [{Mo(CO)₃(**11**) }₄] were formed. The solid was filtered off and dried under reduced pressure to isolate 48 mg (83 %) of an orange crystalline material. The crystals formed were of suitable quality to get single crystal X-ray analysis of the solid. The product was insoluble in common deuterated organic solvents. MF: C₂₁H₃₂MoN₃O₄P₃, MW: 579.39 g/mol, MP: 198 °C (dec.), EA[calc]: C, 43.53; H, 5.57; N, 7.25; EA[found]: C, 43.76; H, 5.71; N, 6.99. IR[cm⁻¹] : 2965.09, 1964.90, 1949.96, 1897.80, 1848.94, 1355.65, 1312.23, 1250.88, 1176.22, 1114.99, 966.47, 859.61

	9	Na ₂ [8 Ti]	Na[8 Hf]	Na ₂ [10 Hf]
CCDC	CCDC 1494722	CCDC 1494723	CCDC 1494718	CCDC 1494720
Empirical formula	C ₃₀ H ₂₅ MoN ₃ O ₇ P ₆ Ti	C ₆₂ H ₈₈ Cl ₄ N ₆ Na ₂ O ₁₈ P ₁₂ Ti	C ₆₀ H ₈₄ HfN ₆ Na ₂ O ₁₈ P ₁₂	C ₆₈ H ₈₈ Cl _{3.92} HfMo ₂ N ₆ Na ₂ O ₂₄ P ₁₂
Formula weight	869.19	1812.70	1773.44	2300.25
Temperature/K	100	99.55	293(2)	104(2)
Crystal system	monoclinic	monoclinic	monoclinic	triclinic
Space group	P2 ₁ /c	P2 ₁ /n	P2 ₁ /n	P-1
a/Å	11.0367(3)	12.9086(7)	15.9451(3)	13.1135(3)
b/Å	19.6039(7)	24.9553(13)	13.2815(2)	13.1212(4)
c/Å	15.6787(6)	13.7959(7)	18.8611(5)	16.9409(4)
α/°	90	90	90.00	83.345(2)
β/°	93.440(3)	108.1170(10)	90.052(3)	68.758(2)

X-RAY TABLES

Table S1: Crystal data and structure refinement.

	5	Na[3]	Na[6]	7	7
CCDC	CCDC 1494719	CCDC 1494721	CCDC 1494716	CCDC 1494717	CCDC 1494802
Empirical formula	C ₃₉ H ₄₁ MoN ₃ O ₉ P ₆ Si	C _{36.46} H _{44.9} BN ₃ N aO _{7.4} P ₆	C ₅₅ H ₇₃ BMoN ₃ N aO ₁₆ P ₆	C ₃₀ H ₂₅ N ₃ O ₃ P ₆ Ti	C ₂₄ H ₁₉ Cl ₂ N ₃ O ₃ P ₆ Ti
Formula weight	1005.60	863.20	1347.72	709.25	702.04
Temperature/K	106.48(14)	106(9)	107(6)	104.7(10)	104.6(2)
Crystal system	orthorhombic	orthorhombic	monoclinic	orthorhombic	monoclinic
Space group	Pbca	Pna2 ₁	P2 ₁ /n	P2 ₁ 2 ₁ 2 ₁	P2 ₁ /n
a/Å	28.4804(10)	33.7644(14)	12.9566(4)	13.1587(2)	7.4263(3)
b/Å	18.1858(6)	12.0728(6)	29.5914(8)	20.1174(3)	15.2635(8)
c/Å	16.8840(4)	11.6209(5)	16.6475(5)	24.1036(4)	26.3095(15)
α/°	90	90	90	90	90
β/°	90	90	90.824(3)	90	92.364(4)
γ/°	90	90	90	90	90
Volume/Å ³	8744.9(5)	4737.1(4)	6382.1(3)	6380.68(17)	2979.7(3)
Z	8	4	4	8	4
ρ _{calc} /cm ³	1.528	1.210	1.403	1.477	1.565
μ/mm ⁻¹	0.603	0.281	0.429	0.606	0.822
F(000)	4112.0	1799.0	2800.0	2896.0	1416.0
Reflections collected	47716	34644	43016	30300	26042
Independent reflections	6938	9513	14875	15821	12040
R _{int}	0.1278	0.1077	0.0653	0.0300	0.0526
R _{sigma}	0.0823	0.0965	0.0988	0.0599	0.0806
Data/restraints/parameters	6938/0/532	9513/61/436	14875/0/748	15821/0/777	12040/0/352
GOF	1.335	1.059	1.060	1.048	1.068
R ₁ [I > 2σ (I)]	0.0972	0.1122	0.0740	0.0521	0.0671
wR ₂ [I > 2σ (I)]	0.1556	0.2802	0.1282	0.1083	0.1633
Largest diff. peak/hole / e Å ⁻³	0.92/-0.74	0.73/-0.65	0.68/-0.50	1.50/-0.40	1.33/-1.58

$\gamma/^\circ$	90	90	90.00	60.501(3)
Volume/ \AA^3	3386.17(19)	4223.9(4)	3994.33(14)	2357.64(12)
Z	4	2	2	1
$\rho_{\text{calc}}/\text{g/cm}^3$	1.705	1.425	1.475	1.620
μ/mm^{-1}	0.941	0.530	1.622	1.754
F(000)	1744.0	1876.0	1808.0	1154.0
Reflections collected	25661	50291	13164	38086
Independent reflections	10325	8349	7328	13365
R_{int}	0.0676	0.0748	0.0365	0.0236
R_{sigma}	0.1100	0.0781	0.0629	0.0285
Data/restraints/parameters	10325/102/449	8349/0/481	7328/0/454	13365/534/564
GOF	0.976	0.906	1.032	1.032
$R_1 [I > 2\sigma(I)]$	0.0563,	0.0374	0.0415	0.0230
$wR_2 [I > 2\sigma(I)]$	0.0825	0.0642	0.0723	0.0529
Largest diff. peak/hole / $e \text{\AA}^{-3}$	1.47/-0.76	0.54/-0.37	0.61/-0.51	0.66/-0.55

	4	11	12
CCDC	CCDC 1495123	CCDC 1495143	CCDC 1495146
Empirical formula	C ₅₀ H ₅₀ N ₂ O ₄ P ₇	C ₁₈ H ₃₂ N ₃ OP ₃	C _{22.5} H _{34.4} Cl _{2.71} Mo N ₃ O ₄ P ₃
Formula weight	959.71	399.37	695.90
Temperature/K	105(1)	104.79(12)	106.05(13)
Crystal system	triclinic	orthorhombic	orthorhombic
Space group	P-1	Pbca	Fdd2
a/Å	8.6804(3)	12.9301(4)	59.1004(11)
b/Å	11.7969(5)	11.3677(4)	34.6994(6)
c/Å	12.7633(5)	29.4791(17)	12.38327(19)
α/°	112.956(4)	90	90
β/°	104.532(3)	90	90
γ/°	93.858(3)	90	90
Volume/Å ³	1144.80(9)	4333.0(3)	25394.9(8)
Z	1	8	32
ρ _{calc} /cm ³	1.392	1.224	1.456
μ/mm ⁻¹	0.318	0.286	0.824
F(000)	501.0	1712.0	11376.0
Reflections collected	12458	14270	32415
Independent reflections	4678	5923	12027
R _{int}	0.0325	0.0210	0.0374
R _{sigma}	0.0458	0.0312	0.0436
Data/restraints/para meters	4678/0/329	5923/0/234	12027/1/671
GOF	1.180	1.113	1.093
R ₁ [I>2σ (I)]	0.0589	0.0396	0.0487
R ₁ [I>2σ (I)]	0.1087	0.0844	0.1120
Largest diff. peak/hole / e Å ⁻³	0.47/-0.65	0.44/-0.30	0.91/-0.80

CALCULATION DETAILS HOMO LUMO REPRESENTATIONS

[Ti(1)₆]²⁻

-2 1

C	-3.17872705	-3.27975595	-3.07012544
N	-1.98736405	-2.81607730	-2.48659605
C	-0.77150802	-3.43472743	-2.74498833
C	-0.69697342	-4.49855392	-3.58935297
C	-1.87583348	-4.99654223	-4.21681066
C	-3.07659677	-4.39027869	-3.94797299
C	-2.06626796	-1.71285505	-1.62458961
O	-0.94397979	-1.29683356	-1.12640616
Ti	-0.00002069	-0.00006187	-0.00001213
O	-0.65606525	1.46490913	-1.12480306
C	-0.45700619	2.64375346	-1.62614937
N	-1.45499065	3.12486424	-2.48576115
C	-1.26318188	4.38715683	-3.07279223
C	-2.27895798	4.85157182	-3.94848793
C	-3.40518675	4.11396913	-4.21158306
C	-3.56111486	2.84566503	-3.58029031
C	-2.59951402	2.38042926	-2.73819384
P	0.20639447	5.25860549	-2.66625870
P	0.92311372	3.71131775	-1.35504465
P	-4.66653192	-2.44322627	-2.65661500
P	-3.67969147	-1.05121481	-1.34686219
O	0.94389758	1.29675647	1.12633147
C	2.06614963	1.71284268	1.62452715
N	1.98714737	2.81609354	2.48647925
C	0.77126748	3.43478903	2.74464659
C	0.69662812	4.49862172	3.58899262
C	1.87539706	4.99656267	4.21666010
C	3.07618675	4.39025740	3.94803232
C	3.17842798	3.27972986	3.07020315
P	4.66628480	2.44320481	2.65686578
P	3.67956580	1.05102436	1.34719948
O	1.59200811	-0.16551849	-1.13094238
C	2.51250472	-0.92830695	-1.63269650
N	3.42756171	-0.30629477	-2.49401534
C	3.35582302	1.05681274	-2.74802378
C	4.23874356	1.65525962	-3.59212065
C	5.25790197	0.88462865	-4.22367034
C	5.33295820	-0.45925166	-3.95900361
C	4.42333039	-1.10504281	-3.08156913
P	4.44252209	-2.81299313	-2.67311452
P	2.74590907	-2.65724542	-1.36003055
O	0.65601854	-1.46505239	1.12476809
C	0.45690761	-2.64387825	1.62614279
N	1.45501719	-3.12510372	2.48553114
C	1.26324563	-4.38742713	3.07250691
C	2.27916451	-4.85195909	3.94797493
C	3.40549200	-4.11444241	4.21089490
C	3.56138843	-2.84611930	3.57962945
C	2.59965073	-2.38076924	2.73775305
P	-0.20640264	-5.25881290	2.66609628
P	-0.92333727	-3.71133524	1.35522188
O	-1.59202083	0.16546260	1.13096168
C	-2.51241214	0.92836074	1.63274122
N	-3.42750290	0.30651560	2.49414707
C	-3.35599207	-1.05660474	2.74815331
C	-4.23894222	-1.65488830	3.59233647
C	-5.25789220	-0.88406753	4.22398959
C	-5.33271303	0.45982986	3.95934635
C	-4.42305204	1.10545326	3.08182140
P	-4.44194710	2.81341667	2.67341436
P	-2.74538500	2.65739313	1.36029779

H	2.56709881	1.57970046	-2.22604180
H	-0.27290103	4.95353972	3.76228938
H	4.44071625	-2.23354181	3.74842795
H	2.12713378	-5.82662358	4.40369743
H	5.96582222	1.35873895	-4.89826773
H	3.99803923	4.74509744	4.40085228
H	-0.07748492	3.01286205	2.22544396
H	6.10006968	-1.07934530	-4.41484793
H	1.82057307	5.84661161	4.89151836
H	2.65648217	-1.43594477	2.21612338
H	4.14824518	2.72287847	-3.76231797
H	4.17145053	-4.49027930	4.88400104
H	-2.56741476	-1.57963643	2.22609381
H	0.27254573	-4.95342320	-3.76283697
H	-4.44036178	2.23301432	-3.74924183
H	-2.12688693	5.82620627	-4.40426225
H	-5.96583773	-1.35804770	4.89865230
H	-3.99851042	-4.74513059	-4.40065903
H	0.07732261	-3.01275235	-2.22595818
H	-6.09965702	1.08006688	4.41527717
H	-1.82109223	-5.84657107	-4.89170101
H	-2.65637579	1.43562676	-2.21653432
H	-4.14863061	-2.72252487	3.76252079
H	-4.17103091	4.48971120	-4.88487213

Excitation energies and oscillator strengths:

Excited State	1:	Singlet-A	2.0369 eV	608.70 nm	f=0.0003
<S**2>=0.000					
	266 -> 269	0.37478			
	266 -> 270	-0.28409			
	267 -> 269	0.39501			
	267 -> 270	0.32958			
Excited State	2:	Singlet-A	2.0385 eV	608.21 nm	f=0.0052
<S**2>=0.000					
	266 -> 268	0.35938			
	266 -> 269	-0.29106			
	266 -> 270	0.30477			
	267 -> 268	0.23344			
	267 -> 269	0.26457			
	267 -> 270	0.24482			
Excited State	3:	Singlet-A	2.0387 eV	608.15 nm	f=0.0052
<S**2>=0.000					
	266 -> 268	-0.23391			
	266 -> 269	0.23492			
	266 -> 270	0.31001			
	267 -> 268	0.35483			
	267 -> 269	0.21632			
	267 -> 270	-0.33539			
Excited State	4:	Singlet-A	2.0929 eV	592.39 nm	f=0.0155
<S**2>=0.000					
	263 -> 268	-0.27257			
	266 -> 269	0.32898			
	266 -> 270	0.31999			
	267 -> 269	-0.31805			
	267 -> 270	0.32846			
Excited State	5:	Singlet-A	2.1001 eV	590.37 nm	f=0.0000
<S**2>=0.000					
	264 -> 269	0.47221			
	264 -> 270	-0.14875			
	265 -> 269	-0.14988			
	265 -> 270	-0.46978			
Excited State	6:	Singlet-A	2.1104 eV	587.50 nm	f=0.0826
<S**2>=0.000					

263 -> 269	0.28719				
266 -> 268	-0.23750				
266 -> 269	-0.17030				
266 -> 270	-0.21764				
267 -> 268	0.44184				
267 -> 269	-0.21653				
267 -> 270	0.17013				
Excited State 7:	Singlet-A	2.1106 eV	587.45 nm	f=0.0826	
<S**2>=0.000					
263 -> 270	-0.28690				
266 -> 268	0.44217				
266 -> 269	0.21710				
266 -> 270	-0.17248				
267 -> 268	0.23711				
267 -> 269	-0.16878				
267 -> 270	-0.21673				
Excited State 8:	Singlet-A	2.1133 eV	586.70 nm	f=0.0000	
<S**2>=0.000					
264 -> 269	-0.23896				
264 -> 270	-0.11747				
265 -> 268	0.57964				
265 -> 269	0.11804				
265 -> 270	-0.24529				
Excited State 9:	Singlet-A	2.1135 eV	586.64 nm	f=0.0000	
<S**2>=0.000					
264 -> 268	0.57862				
264 -> 269	-0.11622				
264 -> 270	0.24145				
265 -> 269	-0.24520				
265 -> 270	-0.11973				
Excited State 10:	Singlet-A	2.1826 eV	568.07 nm	f=0.0000	
<S**2>=0.000					
262 -> 269	0.24324				
264 -> 268	0.14503				
264 -> 269	0.39991				
265 -> 268	0.29644				
265 -> 270	0.39736				
Excited State 11:	Singlet-A	2.1828 eV	568.00 nm	f=0.0000	
<S**2>=0.000					
262 -> 270	0.24330				
264 -> 268	0.29830				
264 -> 270	-0.39454				
265 -> 268	-0.14492				
265 -> 269	0.40149				
Excited State 12:	Singlet-A	2.2083 eV	561.46 nm	f=0.0000	
<S**2>=0.000					
262 -> 268	0.38753				
264 -> 269	0.13847				
264 -> 270	0.39183				
265 -> 269	0.38211				
265 -> 270	-0.14045				
Excited State 13:	Singlet-A	2.2663 eV	547.07 nm	f=0.1377	
<S**2>=0.000					
263 -> 269	0.61856				
263 -> 270	-0.13232				
266 -> 269	0.10249				
267 -> 268	-0.21596				
267 -> 270	-0.10799				
Excited State 14:	Singlet-A	2.2669 eV	546.92 nm	f=0.1381	
<S**2>=0.000					
263 -> 269	0.13264				

263 -> 270	0.61883
266 -> 268	0.21590
266 -> 270	-0.10351
267 -> 269	-0.10673

Excited State 15: Singlet-A 2.2781 eV 544.25 nm f=0.2288
<S**2>=0.000

263 -> 268	0.64582
266 -> 269	0.11115
266 -> 270	0.16711
267 -> 269	-0.16051
267 -> 270	0.10772

[CpTi(1)₃]

0 1

Ti	4.39180000	9.17680000	3.35350000
P	5.30970000	13.37790000	7.27900000
P	8.79650000	5.67710000	1.78100000
P	8.26670000	7.48810000	2.74200000
P	-1.05640000	7.78990000	2.23510000
P	0.93870000	7.09720000	2.05840000
P	3.85560000	12.28890000	6.19050000
O	4.66340000	9.97960000	4.98820000
N	6.27930000	11.14400000	6.13340000
C	1.03160000	9.84140000	4.97880000
H	1.91990000	9.86560000	5.25700000
O	5.63850000	7.83230000	3.39160000
C	7.91760000	12.35210000	7.39020000
H	8.15440000	13.07230000	7.92770000
N	6.16350000	5.87210000	2.31760000
C	-0.67770000	8.91400000	3.51190000
C	7.16360000	5.06150000	1.76250000
C	1.53300000	8.15160000	3.28770000
C	4.46610000	4.29710000	1.78130000
H	3.56860000	4.05370000	1.76200000
N	0.64740000	8.98380000	3.93880000
C	4.82920000	5.49000000	2.31640000
H	4.18320000	6.05130000	2.68270000
C	6.59250000	7.08130000	2.82980000
C	7.24910000	10.19750000	5.80660000
H	7.02670000	9.47130000	5.27150000
C	5.46350000	10.79300000	2.08500000
H	6.29250000	11.11490000	2.35730000
C	-1.61190000	9.75490000	4.16750000
H	-2.50540000	9.72880000	3.90960000
C	6.58720000	12.25550000	6.91870000
C	6.75440000	3.80820000	1.24860000
H	7.39390000	3.22880000	0.90150000
C	0.12240000	10.63000000	5.57520000
H	0.38420000	11.20140000	6.25970000
C	5.22800000	9.69060000	1.24370000
H	5.87540000	9.15340000	0.84840000
C	5.44240000	3.42600000	1.25340000
H	5.19370000	2.59920000	0.91110000
C	3.86600000	9.55580000	1.11360000
H	3.43180000	8.90190000	0.61460000
C	4.97400000	11.05450000	5.71210000
C	-1.23820000	10.59580000	5.16300000
H	-1.86590000	11.14710000	5.57030000
C	8.50320000	10.33230000	6.26450000
H	9.14530000	9.69860000	6.04040000
C	8.85580000	11.42670000	7.08160000
H	9.72430000	11.51120000	7.40460000
C	4.21870000	11.31400000	2.43690000
H	4.07520000	12.05230000	2.98160000
C	3.24760000	10.55760000	1.84630000
H	2.33040000	10.69240000	1.92110000
O	2.81730000	8.26540000	3.64660000

Excited State 1: Singlet-A 2.4515 eV 505.75 nm f=0.0087 <S**2>=0.000
 155 ->158 -0.37319
 155 ->159 0.20247
 156 ->157 -0.24423
 156 ->158 0.46892

Excited State 2: Singlet-A 2.4581 eV 504.40 nm f=0.0146
 <S**2>=0.000
 155 ->157 0.57822
 155 ->158 0.11448
 155 ->159 -0.19432
 156 ->158 0.29899

Excited State	3:	Singlet-A	2.4817 eV	499.60 nm	f=0.0543
<S**2>=0.000					
	154 ->158	-0.13189			
	155 ->159	0.21272			
	156 ->157	0.56866			
	156 ->158	0.16968			
	156 ->159	0.22782			
Excited State	4:	Singlet-A	2.5305 eV	489.97 nm	f=0.0434
<S**2>=0.000					
	154 ->158	0.30640			
	155 ->157	-0.18019			
	155 ->158	0.36221			
	156 ->157	-0.15463			
	156 ->159	0.44590			
Excited State	5:	Singlet-A	2.5476 eV	486.66 nm	f=0.0609
<S**2>=0.000					
	154 ->157	0.12482			
	154 ->158	-0.17512			
	154 ->159	-0.21085			
	155 ->157	0.24611			
	155 ->159	0.43657			
	156 ->157	-0.13653			
	156 ->158	-0.25091			
	156 ->159	0.23646			
Excited State	6:	Singlet-A	2.6093 eV	475.17 nm	f=0.0293
<S**2>=0.000					
	154 ->157	0.41988			
	155 ->158	-0.34074			
	155 ->159	-0.29028			
	156 ->157	0.11304			
	156 ->158	-0.10100			
	156 ->159	0.28622			
Excited State	7:	Singlet-A	2.6720 eV	464.02 nm	f=0.1742
<S**2>=0.000					
	154 ->158	0.57395			
	155 ->157	0.13331			
	155 ->158	-0.13796			
	155 ->159	0.17734			
	156 ->157	0.20198			
	156 ->158	-0.12002			
	156 ->159	-0.16667			
Excited State	8:	Singlet-A	2.7105 eV	457.42 nm	f=0.1220
<S**2>=0.000					
	154 ->159	0.63496			
	155 ->157	0.16193			
	155 ->159	0.10364			
	156 ->158	-0.14717			

NOTES AND REFERENCES

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