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### Molybdenum and nickel atrane complexes with a rigid tripodal tetraphosphine ligand incorporating imidazole rings

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Dedicated to Professor Ionel Haiduc on the occasion of his 80<sup>th</sup> birthday

#### Abstract

tetraphosphine ligand tris(1H-2-diisopropylphosphinoimidazol-1-Tripodal, tetradentate yl)phosphine (1) was synthesized in three straightforward steps from widely available starting materials. The ligand crystallized in a  $C_3$ -like conformation suitable for metal coordination. Nickel(II) complex 2 was prepared from 1 and Ni(dme) $Br_2$  and adopted a classical atrane structure with trigonal pyramidal geometry at the metal, a bromine covalently bonded in the axial position, and a bromide ion in the outer coordination sphere. Molybdenum(III) complex 3 was prepared from 1 and MoCl<sub>3</sub>(thf)<sub>3</sub> and could be structurally characterized using a co-crystal with Cp<sub>2</sub>Co and [Cp<sub>2</sub>Co]Cl. It displayed a face-capped octahedral geometry at the seven-coordinated metal. Complexes 2 and 3 proved to be prone to decomposition under reductive and oxidative conditions, hindering the investigation of their chemistry. Crystallization attempts from acetonitrile led to the isolation of dinuclear hydrolysis product 4, with the Mo(III) centres bridged by two chlorides and two 2-(diisopropylphosphino)imidazole moieties in a paddlewheel arrangement.

#### **1. Introduction**

Tripodal phosphine ligands have received substantial attention for their ability to stabilize highly reactive species with unique electronic properties. Most notable is their success in dinitrogen activation and subsequent reduction via homogeneous catalysis and the most prominent examples in this regard are atrane architectures **I** and **II** bearing boron and silicon central elements (Chart 1).<sup>1,2,3,4</sup> Known for more than five decades, the neutral analogs with group 15 donors at the transannular site have been the focus of renewed interest in recent times for the ability of their metal complexes to catalyze hydrogenation and dehydrogenation reactions.<sup>5,6,7,8,9</sup> Ligands **III** (R = Me,<sup>10</sup> Ph<sup>11</sup>) pioneered by Venanzi,<sup>12</sup> represent the earliest

prototypes of tetraphosphine ligands. Significant effort has been directed to the preparation of complexes bearing flexible alkyl linkages such as **IV** ( $\mathbf{R} = \mathbf{Me}$ ,<sup>13</sup> Et,<sup>14</sup> *i*Pr,<sup>15</sup> Cy,<sup>16</sup> Ph<sup>17</sup>) and **V** ( $\mathbf{R} = \mathbf{Me}$ ,<sup>18</sup> Et,<sup>18</sup> *i*Pr,<sup>19</sup> Ph<sup>20</sup>), in part due to the synthetic accessibility of such constructs. More recently, ligand **VI** ( $\mathbf{R} = \mathbf{Ph}$ ) has been shown to undergo reversible ortho-metallation on Ir(I), leading to a distorted octahedral coordination environment at the metal.<sup>21</sup> Rh(I) and Ir(I) complexes with the extremely sterically demanding tetradentate ligand **VII** ( $\mathbf{R} = 2,4,6-tBu_3C_6H_2$ ) featured the expected trigonal bipyramidal geometry.<sup>22</sup>



Chart 1. C<sub>3</sub>-symmetric tetradentate atrane ligands bearing equatorial phosphine donors.

All-phosphine ligands have emerged as attractive frameworks for metal-centred reactivity as it pertains to the functionalization of N<sub>2</sub>. Mézailles reported the enforcement of a  $C_3$  geometry for a Mo<sup>II</sup> centre by using strongly donating equatorial cyclohexyl phosphine substituents.<sup>23</sup> In this configuration, important intermediates involved in the reduction of N<sub>2</sub>, including one incorporating an M=NTMS fragment generated at a metal centre by the reduction of N<sub>2</sub>, could be isolated (Chart 2).



**Chart 2.** N<sub>2</sub> reduction products **XI** and **XII** and their precursor **X**, featuring a neutral allphosphine donor ligand of type **IV**.

The groups of van der Vlugt and Pérez-Prieto have demonstrated that substituting flexible alkyl linkers with their indolyl fragments in linkage isomers **VIII** (R = iPr, Ph) and **IX** (R = Ph) removes conformational freedom and enforces tetradenticity.<sup>24,25,26</sup> Rh(I), Rh(II), Pd(II), and Cu(I) complexes incorporating ligands **VIII** and **IX** have been characterized. Notwithstanding

their facile synthesis and rigid coordination geometry, the applications of these ligands have not yet been pursued past the initial reports and no information regarding their coordination chemistry with earlier transition metals is available.

As an extension to our investigations on pincer ligands,<sup>27,28</sup> we report herein the synthesis and coordination chemistry of C<sub>3</sub>-symmetric tripodal tetraphosphine **1**, incorporating imidazole moieties.<sup>29</sup> These provide the advantage of a straightforward, modular synthesis, a rigid framework, and excellent crystallization properties. The coordination chemistry of nickel(II) and molybdenum(III) with ligand **1** is also described. The low oxidation state complexes these metals can form with tetrapodal ligands<sup>30,23</sup> are of interest to us for small molecule activation.

#### 2. Experimental

#### 2.1. General considerations

Synthesis and handling of compounds was performed under an atmosphere of dry, oxygen-free argon employing vacuum lines and glove boxes, unless specified otherwise. Benzene and pentane solvents were dried and purified using the Grubbs/Dow purification system and stored in evacuated 500 mL glass vessels over potassium/benzophenone. Hexamethyldisiloxane (HMDSO) and tetrahydrofuran (THF) were distilled over potassium/benzophenone while acetonitrile was distilled off CaH<sub>2</sub>. Solvents were vacuum transfered directly into the reaction vessels from their storage ampoules.  ${}^{1}H{}^{31}P{}$ ,  ${}^{13}C{}^{1}H{}$  and  ${}^{31}P{}^{1}H{}$  NMR spectra were acquired on Bruker Advance 400 and 600 MHz spectrometers. <sup>1</sup>H and <sup>13</sup>C NMR were internally referenced relative to THF-d<sub>7</sub> (1.76 ppm, <sup>1</sup>H), THF-d<sub>8</sub> (25.31 ppm, <sup>13</sup>C), CHDCl<sub>2</sub> (5.32 ppm, <sup>1</sup>H) and CD<sub>2</sub>Cl<sub>2</sub> (54.24 ppm, <sup>13</sup>C). NMR samples were prepared in the glove box, capped with a septum and sealed with parafilm. <sup>1</sup>H-<sup>13</sup>C HSQC experiments were carried out using conventional pulse sequences to aid in the assignment of peaks in the  ${}^{13}C{}^{1}H$  NMR spectroscopy. Coupling constants (J) are reported as absolute values. All glassware was dried overnight at 150 °C and evacuated for 1 h prior to use. Combustion analyses were performed in-house employing a Perkin Elmer 2400 Series II CHNS Analyzer. THF-d<sub>8</sub> was purchased from Sigma Aldrich and was dried over potassium, distilled, degassed and stored under argon in a glove box. X-ray crystallographic analyses were performed on suitable single crystals coated in Paratone oil and mounted on a glass fibre. Data were collected on a Bruker APEX II CCD diffractometer. Full

details can be found in the independently deposited crystallography information file (cif) under the CCDC deposition numbers 1559365 (1), 1559366 ( $2 \cdot CH_2Cl_2$ ), 1559367 { $3_2 \cdot (Cp_2Co)_2 \cdot [Cp_2Co]Cl \cdot THF$ }, and 1559368 ( $4 \cdot 2CH_3CN$ ). Ni(dme)Br<sub>2</sub> was prepared via Soxhlet extraction of NiBr<sub>2</sub> with 1,2-dimethoxyethane (DME), and MoCl<sub>3</sub>(thf)<sub>3</sub> was prepared according to previously reported procedures.<sup>31</sup>

#### 2.2 Synthesis of the ligand and its complexes

#### 2.2.1. Synthesis of 2-(diisopropylphosphino)imidazole

A solution of n-BuLi (18.4 mL, 29.4 mmol, 1.6 M in heptane) was added dropwise in small portions with stirring at -78 °C to a solution of 1-(diethoxymethyl)imidazole<sup>32</sup> (5g, 29.4 mmol) in dry THF (50 mL). The cooling bath was warmed to -40 °C and chlorodi-*iso*-propylphosphine (4.6 g, 29.4 mmol) was added dropwise. The reaction was allowed to warm up to room temperature overnight with continuous stirring and the solvent was subsequently removed in vacuo. The residue was extracted into pentane (50 mL), and methanol (10 mL) and excess chlorotrimethylsilane (0.25 mL) were added to the pentane extract. After 1 h, the volatiles were removed in vacuo and the oily residue was triturated multiple times with pentane, followed each time by removal of the volatiles in vacuo, in order to remove residual methanol. The residue was then washed with pentane and filtered, leaving behind the product as a white solid (3.8 g, 71%). The NMR spectra matched the values reported in the literature.<sup>33</sup>

#### 2.2.2. Synthesis of ligand 1.

To a suspension of 2-(diisopropylphosphino)imidazole (1.85 g, 10 mmol) in benzene (50 mL) phosphorus trichloride (6.5 mL, 3.25 mmol, 0.5 M solution in C<sub>6</sub>H<sub>6</sub>) and excess triethylamine (2.5 mL) were added, and the mixture was heated to the boiling point of the solvent in a sealed, thick-walled glass vessel. The reaction mixture was then transferred to a swivel frit and the precipitate was removed by filtration and washed three times with benzene. The filtrates were united and the volatiles were removed in vacuo; the residue was triturated with pentane (50 mL) followed by HMDSO (10 mL). The resulting thick oil that solidified on standing was washed with HMDSO (10 mL) yielding the product a white solid (1.1 g, 57 %). <sup>1</sup>H NMR (400 MHz, THF-d<sub>8</sub>):  $\delta$  0.93 (dd, 18H, <sup>3</sup>J<sub>PH</sub> = 13.0 Hz, <sup>3</sup>J<sub>HH</sub> = 7.0 Hz, CH(CH<sub>3</sub>)<sub>2</sub>), 1.06 (dd, 18H, <sup>3</sup>J<sub>PH</sub> = 17.2 Hz, <sup>3</sup>J<sub>HH</sub> = 7.0 Hz, CH(CH<sub>3</sub>)<sub>2</sub>), 2.30 (sep, 6H, <sup>3</sup>J<sub>HH</sub> = 7.1 Hz, CH(CH<sub>3</sub>)<sub>2</sub>), 6.56 (s, 3H, NCH), 7.24 (s, 3H, NCH). <sup>13</sup>P{<sup>1</sup>H} NMR (162 MHz, THF-d<sub>8</sub>):  $\delta$  -16.2 (d, 3P, <sup>3</sup>J<sub>PP</sub> = 152.2 Hz, *P*<sub>eq</sub>), 51.1 (q, <sup>3</sup>J<sub>PH</sub> = 151.0 Hz, *P*<sub>ax</sub>). <sup>13</sup>C{<sup>1</sup>H} NMR (101 MHz, THF-d<sub>8</sub>):  $\delta$  20.0 (d, <sup>2</sup>J<sub>PC</sub> = 9.1 Hz, CH(CH<sub>3</sub>)<sub>2</sub>), 20.5 (d, <sup>2</sup>J<sub>PC</sub> = 18.8 Hz, CH(CH<sub>3</sub>)<sub>2</sub>), 25.3 (m, CH(CH<sub>3</sub>)<sub>2</sub>), 122.8 (d, J<sub>PC</sub> = 4.1 Hz, NCH), 134.1 (d, J<sub>CP</sub> = 2.3 Hz, NCH), 152.7 (dd, J<sub>CP</sub> = 19.6 Hz, 16.8 Hz, NCP).

#### 2.2.3. Synthesis of nickel complex 2.

Ni(dme)Br<sub>2</sub> (212 mg, 0.69 mmol) was added to a solution of ligand **1** (400 mg, 0.69 mmol) in THF (25 mL). The solution was stirred for 4 h at which point the blue precipitate was collected by filtration and washed with THF (25 mL) followed by pentane (25 mL) and dried in vacuo. The complex was isolated as a dark blue solid (480 mg, 87 %). <sup>1</sup>H{<sup>31</sup>P} NMR (400 MHz, CD<sub>2</sub>Cl<sub>2</sub>):  $\delta$  1.17 (s, br, 18H, CH(CH<sub>3</sub>)<sub>2</sub>), 1.44 (s, br, 18H, CH(CH<sub>3</sub>)<sub>2</sub>), 3.02 (s, br, 6H, CH(CH<sub>3</sub>)<sub>2</sub>), 7.68 (s, 3H, NCH), 9.64 (s, 3H, NCH). <sup>31</sup>P{<sup>1</sup>H} NMR (162 MHz, CD<sub>2</sub>Cl<sub>2</sub>):  $\delta$  18.1 (d, <sup>3</sup>J<sub>PP</sub> = 55.7 Hz, *P*<sub>eq</sub>), 101.4 (q, <sup>3</sup>J<sub>PP</sub> = 53.3 Hz, *P*<sub>ax</sub>). <sup>13</sup>C{<sup>1</sup>H} NMR (101 MHz, CD<sub>2</sub>Cl<sub>2</sub>):  $\delta$  18.7 (s, CH(CH<sub>3</sub>)<sub>2</sub>), 19.2 (s, CH(CH<sub>3</sub>)<sub>2</sub>), 29.8 (m, br, CH(CH<sub>3</sub>)<sub>2</sub>), 124.9 (s, NCH), 142.0 (d, *J*<sub>CP</sub> = 8.50 Hz, NCH), 149.9 (m, NCP). Elemental analysis (%): Calcd for C<sub>27</sub>H<sub>48</sub>Br<sub>2</sub>N<sub>6</sub>NiP<sub>4</sub>: C 40.58, H 6.05, N 10.52; Found: C 40.64, H 5.86, N 10.52.

#### 2.2.4. Synthesis of molybdenum complexes 3 and 4.

MoCl<sub>3</sub>(thf)<sub>3</sub> (72 mg, 017 mmol) was added to a solution of **1** (100 mg, 0.17 mmol) in THF (10 mL). The solution was stirred overnight at 60 °C and the red precipitate that formed was recovered by filtration and washed with THF (5 mL) followed by pentane (10 mL), and dried in vacuo, yielding 45 mg product (34 %). The characterization of this complex was hindered by its facile decomposition. Attempts to crystallize **3** from acetonitrile led reproducibly to the formation of single crystals of **4**. A solution of cobaltecene (33 mg, 174 µmol) in THF (0.5 mL) was added to a suspension of **3** (45 mg, 57 µmol) in THF (0.5 mL). The solution was heated to 60 °C overnight and subsequently cooled to room temperature, leading to the precipitation of crystalline {**3**<sub>2</sub>·(Cp<sub>2</sub>Co)<sub>2</sub>·[Cp<sub>2</sub>Co]Cl·THF}.

#### 3. Results and discussion

3.1 Ligand synthesis.



Scheme 1. Synthesis of ligand 1

reaction Ligand was obtained from the of the 1 already reported 2-(diisopropylphosphino)imidazole<sup>32</sup> with PCl<sub>3</sub> and excess triethylamine (Scheme 1). The isolation of clean 1 was complicated by the affinity of the ligand for benzene, which was used as a solvent, and required multiple trituration steps with pentane followed by solvent removal and washing with hexamethyldisiloxane (HMDSO). Following this procedure, the ligand was reproducibly obtained in low yields and high purity as a white solid with good solubility in organic solvents, including *n*-pentane. In the  ${}^{31}$ P NMR spectrum the ligand exhibits a doublet resonance at -16.2 ppm corresponding to the three equivalent phosphine donors and a quartet at 51.1 ppm for the central phosphine, in a 3 : 1 intensity ratio. As reflected by the <sup>1</sup>H and <sup>13</sup>C

NMR, the methyl groups on the isopropyl substituents are diastereotopic in the free ligand **1** and its complexes. Single crystals of the ligand were obtained from a pentane solution at -40 °C and the X-ray diffraction study confirmed the proposed structure (Figure 1). The metric parameters in the solid-state structure fall in the expected ranges and will not be further discussed. The ligand crystalizes in a  $C_3$ -like conformation suitable for metal coordination in a typical atrane geometry.



**Fig. 1.** Solid-state structure of **1** with thermal ellipsoids drawn at 50% probability level. All hydrogen atoms have been omitted for clarity.

3.2 Nickel coordination chemistry.



Scheme 2. Synthesis of Ni complex 2.

That Complex 2 was obtained in high purity as a dark blue, microcrystalline solid upon mixing of 1 with Ni(dme)Br<sub>2</sub> in THF (Scheme 2). The diamagnetic Ni(II) complex was characterized by 1D and 2D NMR methods. It exhibited a doublet resonance at 18.1 ppm corresponding to the three equatorial phosphine donors and a quartet resonance at 101.4 ppm marking the axial donor phosphine in the <sup>31</sup>P NMR spectrum. Single crystals of this complex were obtained by layering a dichloromethane solution of the complex with pentane at -40 °C. The crystal structure revealed a trigonal bipyramidal metal with one covalently bound bromide in the axial position a bromide ion in the outer coordination sphere. The non-coordinated bromide ion is situated on the P1-Ni1-Br1 axis, at a distance of 4.884(1) Å from P1. The cationic complex

shows classic atrane geometry with a transannular Ni1-P1 bond distance of 2.063(1) Å. This is noticeably shorter than in all other known nickel P<sub>4</sub>-atrane complexes (2.142(3) - 2.181(2) Å),<sup>34,35</sup> all of which incorporate the lest rigid ligand **IV**. With 2.266(1) - 2.337(1) Å, the Ni-P bonds involving the equatorial phosphines are longer than the axial Ni-P bond and comparable with the equatorial Ni-P measured in other nickel P<sub>4</sub>-atrane complexes (*av.* 2.28 Å).



**Fig. 2.** Solid-state structure of the cation in **2** with thermal ellipsoids drawn at 50% probability level. All hydrogen atoms, the bromide counterion, and one molecule of co-crystallized dichloromethane have been omitted for clarity. Selected bond distances (Å) and angles (°): Ni1-Br1 2.3380(8), Ni1-P1 2.063(1), Ni1-P2 2.266(1), Ni1-P3 2.333(1), Ni1-P4 2.337(1); P(1)-Ni1-P 84.77(5)-86.35(4), P1-Ni1-Br1 175.81(5).

Attempts to reduce complex 2 with either KC<sub>8</sub> and 1% Na amalgam, or to produce a Ni(0) complex by combining an appropriate nickel source such as Ni(COD)<sub>2</sub> and Ni(PPh<sub>3</sub>)<sub>4</sub> with 1 invariably led to intractable mixtures of products resulting from ligand decomposition. This is likely initiated by metal insertion into the labile N-P bonds in the ligand skeleton.

3.3 Molybdenum complexes



Scheme 3. Synthesis of products 3 and 4.

The synthesis, isolation and characterization of coordination complexes of molybdenum with ligand 1 was hindered by the facile decomposition via cleavage of P-N bonds. Complex 3 was isolated in low yields as a paramagnetic orange-red solid by heating a mixture of  $MoCl_3(thf)_3$  and 1 in THF. Attempts to purify this complex by crystallization from an acetonitrile solution at -40 °C yielded X-ray quality crystals of an edge-sharing, dinuclear, pseudo-octahedral Mo(III) complex with a Mo-Mo interaction (Figure 3). Bonding parameters indicate a standard Mo-Mo single bond as compared with the literature value for Mo<sub>2</sub>Cl<sub>6</sub>(dmpm)<sub>2</sub> (Mo-Mo 2.7394(5), dmpm = bis(dimethylphosphino)methane)<sup>36</sup> and Mo<sub>2</sub>Cl<sub>6</sub>(dppm)<sub>2</sub> (Mo-Mo 2.789(1), bis(diphenylphosphino)methane).<sup>37</sup> dppm = The regeneration of the 2-(diisopropylphosphino)imidazole ligand is in all likelihood a result of hydrolysis due to the presence of adventitious moisture in the acetonitrile solvent.



**Fig. 3.** Solid-state structure of **4** with thermal ellipsoids drawn at 50% probability level. Hydrogen atoms on the phosphine substituents and co-crystallized acetonitrile molecule have been omitted for clarity. The hydrogen atom on N2 was located from the Fourier difference map. Selected bond distances (Å) and angles (°): Mo1-Mo1 2.7443(3), Mo1-Cl1 2.3789(5), Mo1-Cl2 2.4196(6), Mo1-Cl3 2.4194(6), Mo1-N1 2.195(2), Mo1-P1 2.5615(6).

Direct reduction of **3** with KC<sub>8</sub> or 1% Na/Hg gave complex mixtures of products. Crystals of the complex in  $3 \cdot \text{Cp}_2\text{Co}\cdot[\text{Cp}_2\text{Co}]\text{Cl}\cdot\text{THF}$  were isolated from the reaction of **3** with Cp<sub>2</sub>Co. An equivalent of cobaltocene and a highly disordered cobaltocenium chloride pair, as well as a molecule of co-crystalized THF were present in the unit cell, along with the coordination complex **3**. Co-crystallized cobaltocenium suggests successful electron transfer to molybdenum, however, a reduced species was not observed in our studies.



**Fig. 4.** Solid-state structure of **3** in  $3 \cdot \text{Cp}_2\text{Co}\cdot[\text{Cp}_2\text{Co}]\text{Cl}\cdot\text{THF}$  with thermal ellipsoids drawn at 50% probability level. Hydrogen atoms on the phosphine substituents and one unit of each cobaltocene, cobaltocenium chloride, and co-crystallized tetrahydrofuran have been omitted for clarity. Selected bond distances (Å) and angles (°): Mo1-Cl1 2.572(2), Mo1-Cl2 2.545(2), Mo1-Cl3 2.555(2), Mo1-P1 2.251(2), Mo1 - P2 2.507(1), Mo1 - P3 2.539(1), Mo1 - P4 2.557(2); P1-Mo1-Cl1 129.15(7), P1-Mo1-Cl2 133.69(8), P1-Mo1-Cl3 130.02(7), P1-Mo1-P2 75.53(7), P1-Mo1-P3 75.15(7), P1-Mo1-P4 74.43(7).

In the mononuclear complex **3**, molybdenum is bound by three chloride and four phosphine donors in a 7-coordinate mono-capped octahedron enforced by the rigid ligand architecture. The

complex is best described as having a pseudooctahedral *fac*-(PR<sub>3</sub>)<sub>3</sub>MoCl<sub>3</sub> core with the (P<sub>eq</sub>)<sub>3</sub> face capped by the axial phosphorus atom. This structural motif has been described in (PR<sub>3</sub>)<sub>3</sub>MoCl<sub>4</sub> derivatives,<sup>38,39</sup> where one chloride takes the position of the capping P<sub>ax</sub> in **3**. Seven-coordinated metal complexes incorporating tetrapodal, *C*<sub>3</sub>-symmetric E<sub>4</sub> (E = N, P, As) ligands are rare, with the only known examples containing either hydride/dihydrogen,<sup>40,41</sup> or enynyl ligands.<sup>42,43</sup> The axial Mo1-P1 bond in **3** is, with 2.2508(19) Å, much shorter than in complexes **XI** and **XII** reported by Mézailles (2.420(1) - 2.4911(7) Å),<sup>23</sup> which are the only P<sub>4</sub>-atrane complexes of molybdenum that are available for comparison. In turn, the equatorial Mo1-P bonds (2.507(1) - 2.557(2) Å) are longer than in the compounds available for reference (2.414(2) – 2.444(1) Å).<sup>23</sup>

#### 4. Conclusions

The new, rigid,  $C_3$ -symmetric tetrapodal phosphine ligand 1 and its Ni(II) (2) and Mo(III) (3) complexes were isolated and characterized. The structures of the atrane complexes revealed very short bonds between the metal and the axial phosphorus atom, the shortest ever reported for this type of compound. This indicates strong electron donation from phosphorus to the metal, which is expected to translate into increased ability to activate molecules such as dinitrogen, that would coordinate in the axial position. At the same time, the ligand backbone was less robust than expected, and all attempts to reduce the metal led to complex reaction mixtures. We postulate that the P-N bonds in the ligand framework are susceptible to not only hydrolysis but also oxidative addition in the presence of a highly electron rich metal. The susceptibility to hydrolysis led to the isolation of dinuclear Mo(III) complex 4, featuring a single Mo-Mo bond, which was also structurally characterized.

#### **Supplementary Material**

CCDC 1559365-1559368 contains the crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data\_request/cif. All NMR spectra, as well as crystallographic parameters for compounds 1 - 4 are available in the supporting information.

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- A  $C_3$ -symmetric tetraphosphine ligand incorporating imidazole moieties is reported
- Its Ni(II) complex has a trigonal pyramidal geometry with an outer sphere bromide
- The Mo(III) analog features an uncommon face-capped pseudoctahedral structure

Acceleration

