Chinese Chemical Letters 37 (2026) 111672

Contents lists available at ScienceDirect

Chinese Chemical Letters

journal homepage: www.elsevier.com/locate/cclet

Synthesis, characterization and hydride reduction of PNP-pincer molybdenum and tungsten carbyne complexes

Xiwen Yu[a,b], Haiqi Xu[a,b], Tao Xu[a,b], Tongling Liang[c], Yunhui Yang[a,b,*], Congyang Wang[a,b,*]

[a] Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Molecular Recognition and Function, Center for Carbon Neutral Chemistry, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China
[b] University of Chinese Academy of Sciences, Beijing 100049, China
[c] Center for Physicochemical Analysis and Measurement, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China

ARTICLE INFO

Article history:
Received 3 March 2025
Revised 19 July 2025
Accepted 4 August 2025
Available online 6 August 2025

Keywords:
PNP-pincer ligands
Molybdenum carbynes
Tungsten carbynes
Hydride reagents
η^6-Arene metal complexes

ABSTRACT

The first synthesis, characterization, and hydride reduction reactions of a series of PNP-pincer ligand supported molybdenum and tungsten carbyne complexes [(PNP)M(≡CAr)X(CO)] [M = Mo, W; PNP = $Ph_2P(CH_2)_2N^{(CH3)}(CH_2)_2PPh_2$, $R_2P(CH_2)_2N^{(H)}(CH_2)_2PR_2$, R = Ph, Cy] are reported. Treatment of [(PNP)M(≡CAr)X(CO)] with $LiAlH_4$ led to full reduction of the carbyne carbon, giving PP-bidentate η^6-arene molybdenum and tungsten complexes. Alternatively, when $NaBH_4$ was used as a reductant, the carbyne ligand completely dissociated from the molybdenum center to yield toluene and dimolybdenum biscarbonyl complex $[(PNP)Mo(CO)]_2$. These PNP-pincer molybdenum and tungsten carbyne complexes showed unique reactivity with hydride reagents preferably at the carbyne carbons, in contrast to the metal centers of non-pincer molybdenum and tungsten carbyne complexes in previous reports.

© 2026 Published by Elsevier B.V. on behalf of Chinese Chemical Society and Institute of Materia Medica, Chinese Academy of Medical Sciences.

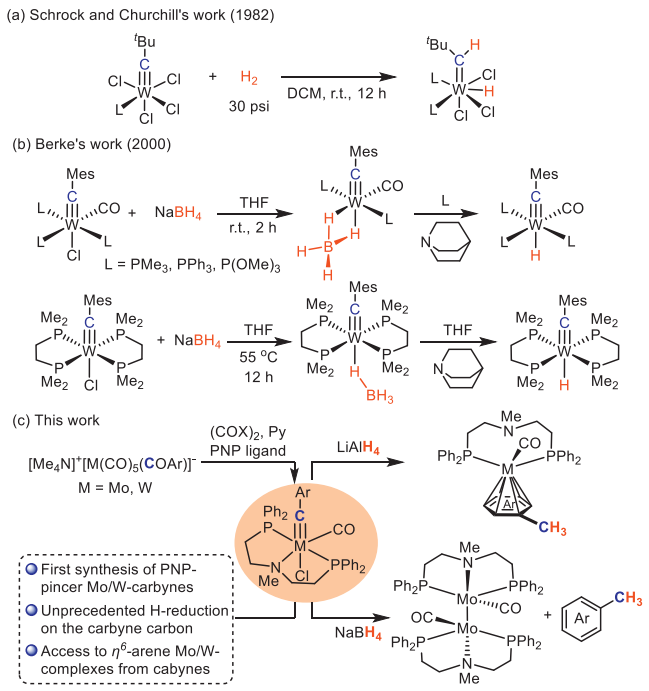
Since the synthesis of transition metal carbyne/alkylidyne complexes [$L_nM(\equiv CR)$] were reported by Fischer and Schrock [1,2], these species have been broadly applied in the fields of organic synthesis and material chemistry [3–8]. For instances, metal carbyne species had great potentials in catalytic hydrocarbon reforming reactions [9–12]. Also, high-valence metal carbyne complexes showed catalytic reactivity in alkyne metathesis reactions, thereby attracting extensive attentions [13–16]. Molybdenum and tungsten carbynes were widely studied in oxidative decarbonylation reactions [17–19] and construction of varied metal-carbon-bond containing compounds upon treatments with either nucleophiles or electrophiles [20–23].

It is noteworthy that metal carbyne species were identified as putative intermediates in Fischer–Tropsch process. Thus, reactions of metal carbyne complexes with dihydrogen or hydride reagents might give clues to the underlying mechanism of CO reduction [24,25]. However, explorations on the reduction reactions of metal carbynes were rather limited. Agapie *et al.* reported that a molybdenum carbyne carbonyl intermediate was gradually reduced by strongly reducing agent of KC_8 to give a coupling product of alkyne [26]. Only few reductive reactions of metal carbynes with milder hydrogen-based reducing agents were reported. Schrock, Churchill and coworkers showed that tungsten carbynes [W(≡C-^{t}Bu)Cl_3L_2 (L = PMe_3)] reacted with molecular hydrogen to yield the tungsten alkylidene hydride complexes [W(=CH-^{t}Bu)(H)Cl_3L_2] (Scheme 1a) [27]. When sodium borohydride ($NaBH_4$) was used as a reducing reagent to react with monodentate phosphine and/or CO supported tungsten carbynes, the corresponding dihydride-bridged W(≡CMes)(η^2-H_2BH_2)$(CO)_nL_{3-n}$ compounds were separated by Berke's group, which was further transformed with quinuclidine to tungsten carbyne hydride species (Scheme 1b) [28]. Bidentate-phosphine-coordinated tungsten carbyne complex, *trans*-W(≡CMes)Cl$(dmpe)_2$, reacted with $NaBH_4$ to form a monohydride-bridged complex, [*trans*-W(≡CMes)(η^1-BH_4)$(dmpe)_2$], and further removal of BH_3 with quinuclidine yielded the tungsten carbyne hydride complex *trans*-W(≡CMes)H$(dmpe)_2$ [29]. Of note, the formation of metal-hydride bonds was favoured towards electrophilic addition of the hydride to the carbyne carbon in the above-mentioned reactions. So far, dissociation of the carbyne moiety from the metal center has been rare due to the high bonding energy of metal carbynes [3,30–32], and complete reduction of the carbyne carbon by hydrides remains elusive.

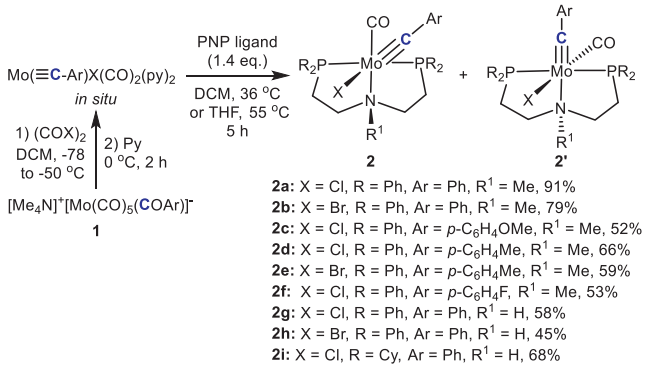
In order to achieve the reactivity on the carbyne carbon of metal carbynes with hydride reagents, we speculated that tridentate PNP-pincer ligands instead of previously-reported mono- and bidentate ones might tune the reactive sites of metal car-

* Corresponding authors at: University of Chinese Academy of Sciences, Beijing 100049, China.
E-mail addresses: yangyh@iccas.ac.cn (Y. Yang), wangcy@iccas.ac.cn (C. Wang).

https://doi.org/10.1016/j.cclet.2025.111672
1001-8417/© 2026 Published by Elsevier B.V. on behalf of Chinese Chemical Society and Institute of Materia Medica, Chinese Academy of Medical Sciences.



Scheme 1. Reaction modes of metal carbynes and hydride reagents.



Scheme 2. Synthesis of PNP-pincer molybdenum carbyne complexes.

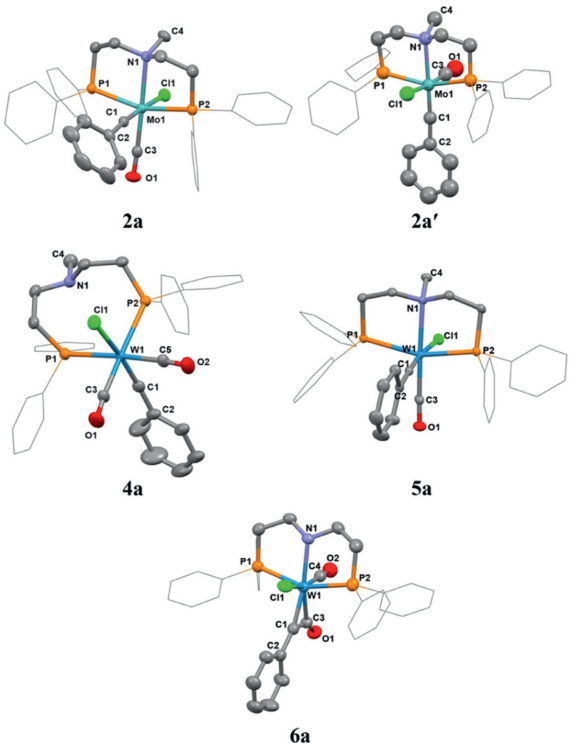


Fig. 1. Thermal ellipsoid drawing of the molecular structures of **2a**, **2a′**, **4a**, **5a**, **6a** at 50% probability. H atoms, some of the phenyl substituents, disordered parts, and solvent molecules are omitted for clarity.

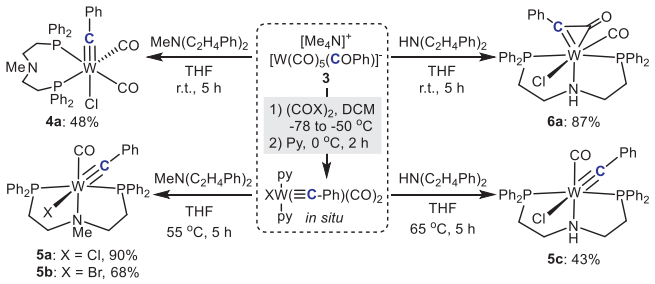
bynes with hydrides from the metal center to the carbyne carbon. Herein, we reported the first synthesis of a series of molybdenum and tungsten carbyne complexes bearing PNP-pincer ligands (Scheme 1c). Contrary to previous reactivity on the metal centers of mono- and bidentate tungsten carbynes with $NaBH_4$, tridentate PNP-pincer molybdenum and tungsten carbyne complexes underwent complete reduction of the carbyne carbon by hydride reagents. Specifically, PP-bidentate η^6-arene molybdenum and tungsten complexes [(η^6-arene)(PP)M(CO)] (M = Mo, W) were selectively accessed when $LiAlH_4$ was used as the reductant. On the other hand, treatment with $NaBH_4$ eventually gave toluene product and the dimerized dimolybdenum carbonyl complex $[(PNP)Mo(CO)]_2$, which showcased the diverse reactivity of PNP-pincer molybdenum and tungsten carbynes with hydride reagents.

According to Mayr's method [33], treatment of $[NMe_4]^+[Mo(CO)_5(CO)Ar]^-$ **1** (Ar = Ph, 4-fluorphenyl, 4-tolyl, 4-methoxyphenyl) with a slight excess of oxalyl halide $(COX)_2$ led to formation of *trans*-halotetracarbonylmetal carbyne complexes $[Mo(\equiv CAr)X(CO)_4]$, which was converted to carbyne complexes $[Mo(\equiv CAr)X(CO)_2(py)_2]$ (X = Cl, Br) upon addition of pyridine. Subsequent addition of a PNP-pincer ligand $[Ph_2P(CH_2)_2N^{(CH3)}(CH_2)_2PPh_2$; $R_2P(CH_2)_2N^{(H)}(CH_2)_2PR_2$, R = Ph, Cy] smoothly produced the corresponding PNP-pincer coordinated molybdenum carbyne complexes [(PNP)Mo(≡CAr)X(CO)], which contained two interconvertible stereoisomers **2** and **2′** (Scheme 2). The reaction yields (45%–91%) of these complexes were robust across various aromatic substituents (Ar) with electron-withdrawing or electron-donating groups. For **2a**, the characteristic carbon signals (Mo≡*C* and *C*O groups) in the ^{13}C NMR spectrum appeared at 271.68 ppm and 243.06 ppm, respectively (Fig. S7 in Supporting information). The two phosphorus atoms of the PNP-pincer ligand in the molybdenum carbyne product had the same chemical environment, exhibiting only one peak at 38.60 ppm in ^{31}P NMR. Meanwhile, the single crystal X-ray diffraction analysis confirmed the product structure and revealed its eight-coordinate, distorted octahedral geometry (Fig. 1). Specifically, the Mo-C1 bond length of **2a** was determined to be 1.808(4) Å (Table 1), which was in agreement with the Mo≡C bond length [3,34]. The bond angle of C1-Mo1-Cl1 was 173.14(11)°, indicating the chlorine atom was in a *trans* configuration to the carbyne ligand. This configuration predominated in the products presumably due to its more favorable electronic structure. Single crystal X-ray diffraction analysis of isomeric complex **2a′** showed that the bond angle of C1-Mo-Cl1 was 101.20(8)°, and the carbyne ligand was nearly perpendicular to the Mo-Cl bond (Fig. 1 and Table 1). In the ^{13}C NMR spectrum of **2a′**, the 'Mo≡*C*' and '*C*O' group showed signals at 288.97 ppm and 237.80 ppm, respectively (Fig. S26 in Supporting information), and the phosphorus signal of the PNP-pincer ligand was shown at 45.60 ppm in ^{31}P NMR.

Interestingly, when the congener tungsten precursor $[W(\equiv CAr)X(CO)_2(py)_2]$ was treated with the pincer ligand of $Ph_2P(CH_2)_2N^{(CH3)}(CH_2)_2PPh_2$ at room temperature, a bright-yellow tungsten carbyne complex **4a** was obtained in 48% isolated yield, in which the pincer ligand acted only as a bidentate PP-ligand

Table 1
Selected core bond lengths (Å) and bond angles (deg) of molybdenum and tungsten carbyne complexes.

Complex	M1-C1 (Å)	M1-C3 (Å)	M1-Cl (Å)	M1-N1 (Å)	C1-C2 (Å)	C1-M1-X1 (deg)	C1-M1-C3 (deg)
2a	1.808(4)	1.978(4)	2.5698(9)	2.355(3)	1.432(6)	173.14(11)	85.19(18)
2a′	1.796(3)	1.964(3)	2.5269(7)	2.464(2)	1.443(3)	101.20(8)	85.02(11)
4a	1.821(3)	2.023(3)	2.5504(7)	-	1.433(4)	169.33(9)	85.37(13)
5a	1.817(3)	1.963(3)	2.5445(7)	2.346(2)	1.443(4)	172.55(9)	85.27(12)
6a	2.007(3)	2.138(3)	2.5482(8)	2.313(3)	1.455(5)	90.29(10)	38.48(13)



Scheme 3. Synthesis of PP- and PNP-pincer tungsten carbyne complexes.

replacing two pyridine ligands of the precursor (Scheme 3). The single crystal X-ray diffraction analysis of **4a** indicated that the chlorine atom adopted a *trans* configuration relative to the carbyne ligand and two W-P bonds were perpendicular to each other, different from the linear configuration of PNP-pincer mode (Fig. 1). The bond length of the tungsten-carbon bond was 1.821(3) Å (Table 1), confirming its carbyne structure [35]. The ^{13}C NMR spectrum of **4a** revealed a triplet signal for the 'Mo≡C' group at 266.24 ppm, accompanied by two signals for the carbonyl carbons (*C*O) at 210.37 ppm and 210.02 ppm (Fig. S40 in Supporting information). The ^{31}P NMR spectrum of **4a** showed that the phosphine signal was at 8.58 ppm. When the reaction temperature was raised to 55 °C, the tridentate PNP-pincer tungsten carbyne complexes **5a** and **5b** were isolated in high yields. Characterization *via* ^{13}C NMR of **5a** displayed significant shifts of characteristic carbon signals (W≡*C* and *C*O), observed at 259.92 ppm and 241.79 ppm, respectively in comparison with those of **4a** (Fig. S43 in Supporting information). Surprisingly, similar PP-bidentate biscarbonyl tungsten carbyne species as **4a** could not be afforded when $Ph_2P(CH_2)_2N^{(H)}(CH_2)_2PPh_2$ was used in the reaction at room temperature. Instead, a PNP-pincer η^2-ketenyl complex **6a** was obtained as purple microcrystals. The single-crystal structure of **6a** revealed that the ketene group (C=C=O) lied in the equatorial coordination plane of tungsten (Fig. 1), with W-C1 bond elongated to 2.007 Å and the bond angle of Cl1-W1-C1 almost vertical [90.29(2)°] (Table 1). It was further found that complex **6a** slowly extruded CO to provide PNP-pincer tungsten carbyne complex **5c** when warmed up to 65 °C, which was in agreement with previous results reported by Hill and coworkers [36,37]. When the reaction temperature was directly raised to 65 °C, complex **5c** was obtained *via* a one-pot procedure in 43 % isolated yield.

To get more insights of the bonding nature and the reactivity properties of the carbyne carbon, computational studies of **2a** was carried out using Gaussian16 program (version RevC.01) [38]. The analysis of computation result was realized by Multifwn (Ver. 3.8) [39]. The optimized structures were in good agreement with the single-crystal XRD results, with small mean deviations for the bond lengths in the core coordination geometry, Mo1-C1 for 1.800 Å. The orbital diagram and corresponding energy level are shown in Fig. 2. HOMO orbital was stabilized due to the overlap of the d_{xz} orbital of Mo with the antibonding orbital of the CO fragment (Fig. 2a), and HOMO-1 and HOMO-2 orbitals participated in the π bond of the Mo≡C bond (Figs. 2c and d). LOL [40] was also used to

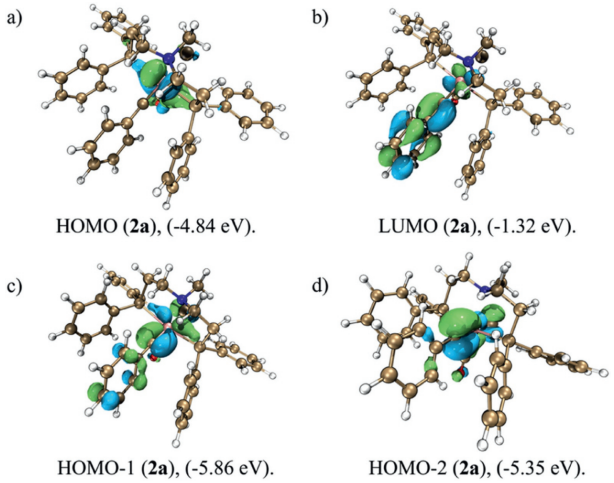


Fig. 2. Key molecular orbitals for the components of **2a.**

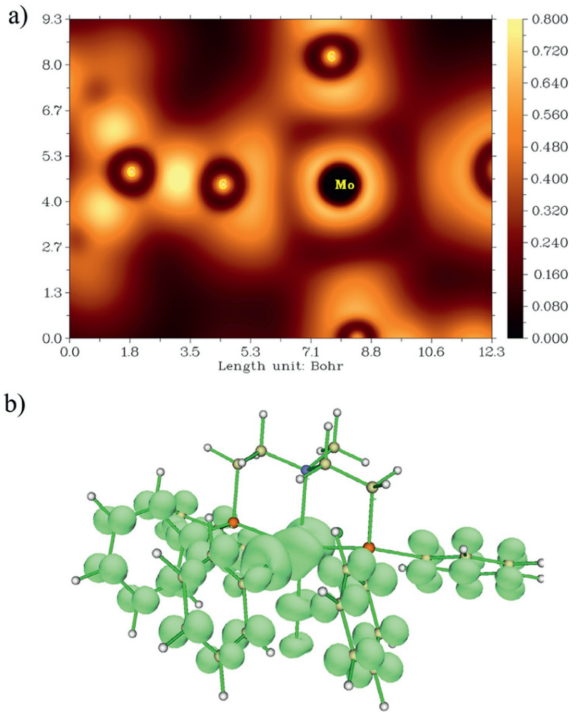
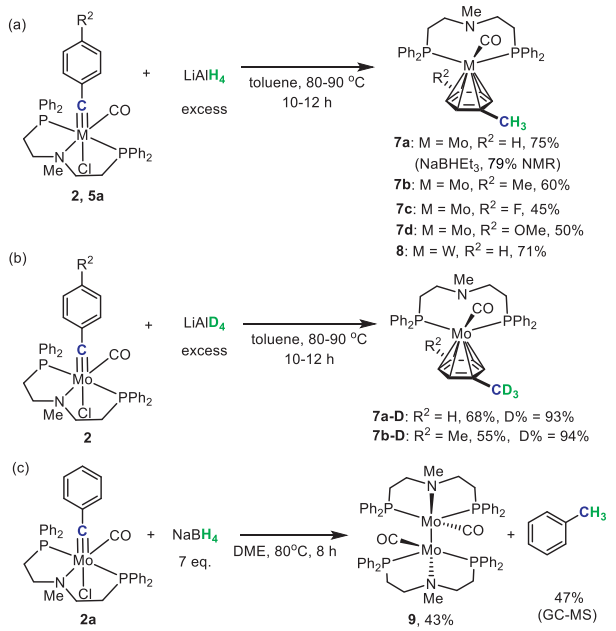


Fig. 3. (a) LOL color-filled diagram of **2a**. (b) f_w^+ isosurface map of **2a.**

determine the bonding characterization (Fig. 3a), and it is worth noting that the orbital localization component between Mo and C was polarized toward C atom of carbyne, and calculated Fuzzy bond order was 2.247, which showed a typical Mo≡C strength [41]. Electrophilic strength analysis using Fukui function (Fig. 3b) [42] showed that the f_w^+ was mainly located on Mo and C of carbyne, indicating that these two atoms were electrophilic sites.



Scheme 4. (a) Reaction of PNP-pincer Mo/W-carbyne complexes with $LiAlH_4$. (b) D-Labelling experiments with $LiAlD_4$. (c) Reaction of PNP-pincer Mo-carbyne complex with $NaBH_4$.

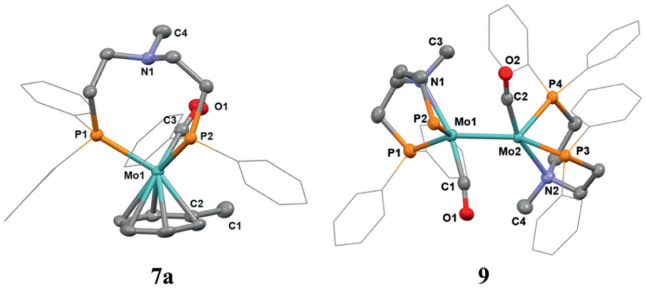


Fig. 4. Thermal ellipsoid drawing of the molecular structures of **7a**, **9** at 50% probability. H atoms, some of the phenyl substituents, disordered parts, and solvent molecules are omitted for clarity. Selected bond lengths (Å) and angles (deg): **7a**, Mo-C2 2.301(2) Å, Mo-C3 1.950(2) Å, C1-C2 1.510(3) Å, Mo1-C2-C1 129.17(17)°, C2-Mo1-C3 88.60(9)°. **9**, Mo1-Mo2 2.5795(3), Mo1-C1 1.922(3), Mo1-C2 1.910(3), P1-Mo1-P2, 94.81(2)°, P3- Mo1-P4, 122.42(2)°.

With the successful synthesis of PNP-pincer molybdenum and tungsten carbynes in hand, we commenced to investigate their reduction reactions with hydride reagents. It turned out that treatment of these metal carbyne complexes with excess amounts of $LiAlH_4$ in toluene at 80–90 °C yielded a series of unexpected PP-bidentate η^6-arene molybdenum and tungsten complexes **7a-d**, **8** (Scheme 4a). It is noteworthy that the substituents on the carbyne ligands were observed to appear on the η^6-arene moiety of the products, suggesting that the η^6-arene moiety was derived from the carbyne ligand and did not exchange with the toluene solvent in the reactions. Meanwhile, complex **7a** was also obtained in 79% NMR yield by treatment of **2a** with $NaBHEt_3$ in a THF solution (Fig. S55 in Supporting information). The ^1H NMR spectrum of **7a** in C_6D_6 showed that the benzene ring originated from the carbyne ligand changed to 4.08 ppm (2H), 3.86 ppm (1H), and 3.54 ppm (2H), while the signal of hydrogenated carbyne carbon was at 1.98 ppm (3H) (Fig. S52 in Supporting information). The single-crystal structure of complex **7a** revealed that the Mo-N distance was elongated, and the π-bond of η^6-benzene molybdenum complex was nearly equal to six benzene carbons (Fig. 4). The Mo-C(O) and Mo-P bond lengths remained unchanged and slight elongation of C1-C2 [1.510(3) Å] was observed. The deuterium-labelling experiments further confirmed that the carbyne carbons in complexes **2** were completely reduced by hydrides (Scheme 4b). Specifically, after treatment of **2a** with $LiAlD_4$, the ^1H NMR spectrum of product **7a-D** showed that the hydrogenated methyl peak of complex **7a** at 1.98 ppm almost disappeared. The integration ratio of this peak to the methyl group on the $PN^{(CH3)}P$ ligand was 0.07/1 indicating a 93% deuterium ratio, which was consistent with the 95% deuterium ratio of $LiAlD_4$ (Fig. S70 in Supporting information). Similar deuterium-labelling result was obtained for **7b**. The η^6-arene ring of complex **7b** corresponded to the signals at 3.71 ppm (4H) and 1.75 ppm (6H) for the two methyl groups in ^1H NMR (Fig. S56 in Supporting information). After the deuterium-labelling experiments, the integration of the two methyl signals at 1.75 ppm changed from 6 H to 3 H in **7b-D** (Fig. S72 in Supporting information).

To our surprise, when $NaBH_4$ was used as the reductant instead of $LiAlH_4$ to react with PNP-pincer molybdenum carbyne complex **2a**, a reduction pathway distinct from the previously observed reactions occurred and a dimolybdenum biscarbonyl complex $[(PNP)Mo(CO)]_2$ **9** was isolated after recrystallization in 43% yield (Scheme 4c). The single crystal X-ray diffraction analysis on the structure of **9** revealed complete detachment of the original carbyne ligand in **2a** (Fig. 4). Further analysis of the reaction mixture using GC–MS detected the formation of toluene with a yield of 47%, in a good agreement with the fact that the carbyne carbon was fully reduced with hydrides.

In summary, a series of PNP-pincer molybdenum and tungsten carbyne complexes were successfully synthesized and fully characterized for the first time. Furthermore, it was showed that PP-bidentate η^6-arene molybdenum and tungsten complexes were easily accessed from the reduction reactions of these PNP-pincer molybdenum and tungsten carbyne complexes with $LiAlH_4$. Meanwhile, toluene and dimolybdenum biscarbonyl complex $[(PNP)Mo(CO)]_2$ with the carbyne ligand fully reduced and detached, were generated when employing $NaBH_4$ as the hydride reductant. Such reactivity on the carbyne carbons of PNP-pincer molybdenum and tungsten carbyne complexes with hydride reagents are in sharp contrast to previous reactivity on the metal centers of monodentate and bidentate molybdenum and tungsten carbyne complexes with hydrides. Further investigations on new reactions and catalytic reactivity of these metal carbyne complexes are underway in our lab.

Declaration of competing interest

We herein declare that all the authors have no conflict of interest.

CRediT authorship contribution statement

Xiwen Yu: Writing – original draft, Validation, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Haiqi Xu:** Validation, Investigation. **Tao Xu:** Investigation, Data curation. **Tongling Liang:** Resources, Data curation. **Yunhui Yang:** Writing – review & editing, Supervision, Investigation. **Congyang Wang:** Writing – review & editing, Writing – original draft, Validation, Supervision, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis.

Acknowledgments

Financial supports from the National Key R&D Program of China (No. 2023YFA1507902), the National Natural Science Foundation of China (Nos. 22025109, 22371283), CAS Project for Young Scientists in Basic Research (No. YSBR-050), and the State Key Laboratory of

Fine Chemicals, Dalian University of Technology (No. KF2102) are gratefully acknowledged.

Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.cclet.2025.111672.

References

[1] E.O. Fischer, G. Kreis, C.G. Kreiter, et al., Angew. Chem. Int. Ed. 12 (1973) 564–565.
[2] S.J. McLain, C.J. Wood, L.W. Messerle, et al., J. Am. Chem. Soc. 100 (1978) 5962–5964.
[3] A. Mayr, H. Hoffmeister, Recent advances in the chemistry of metal-carbon triple bonds, in: F.G.A. Stone, R. West (Eds.), Advances in Organometallic Chemistry, Academic Press, 1991, pp. 227–324.
[4] R.R. Schrock, Chem. Rev. 102 (2002) 145–180.
[5] M. Cui, G. Jia, J. Am. Chem. Soc. 144 (2022) 12546–12566.
[6] A. Reinholdt, J. Bendix, Chem. Rev. 122 (2022) 830–902.
[7] Y. Yang, C. Wang, Chin. J. Chem. 39 (2021) 3481–3484.
[8] X. Wang, W.Y. Tong, B. Huang, et al., J. Am. Chem. Soc. 144 (2022) 4952–4965.
[9] K. Weiss, Angew. Chem. Int. Ed. 25 (1986) 359–360.
[10] C. Sergey, C.M. Alvaro, M. Logesh, K.V. Bukhryakov, Organometallics 39 (2020) 3453–3457.
[11] F. Blanc, J. Thivolle-Cazat, J.M. Basset, C. Copéret, Chem. Eur. J. 14 (2008) 9030–9037.
[12] T.J. Katz, T.H. Ho, N.Y. Shih, Y. Ying, V.I.W. Stuart, J. Am. Chem. Soc. 106 (1984) 2659–2668.
[13] A. Mortreux, M. Blanchard, J. Chem. Soc., Chem. Commun. (1974) 786–787.
[14] J.H. Wengrovius, J. Sancho, R.R. Schrock, J. Am. Chem. Soc. 103 (1981) 3932.
[15] R.R. Schrock, C. Czekelius, Adv. Synth. Catal. 349 (2007) 55–77.
[16] A. Fürstner, Angew. Chem. Int. Ed. 52 (2013) 2794–2819.
[17] A. Mayr, A.M. Dorries, G.A. McDermott, J. Am. Chem. Soc. 107 (1985) 7775–7776.
[18] A.C. Filippou, P. Portius, C. Jankowski, J. Organomet. Chem. 617-618 (2001) 656–670.
[19] J. Heppekausen, R. Stade, A. Kondoh, et al., Chem. Eur. J. 18 (2012) 10281–10299.
[20] M. Green, A.G. Orpen, I.D. Williams, J. Chem. Soc., Chem. Commun. (1982) 493–495.
[21] I.J. Hart, J.C. Jeffery, R.M. Lowry, F.G.A. Stone, Angew. Chem. Int. Ed. 27 (1988) 1703–1705.
[22] A.P. James, F.G.A. Stone, J. Organomet. Chem. 310 (1986) 47–54.
[23] N.H.T. Huy, J. Fischer, F. Mathey, Organometallics 7 (1988) 240–242.
[24] O.R. Inderwildi, S.J. Jenkins, D.A. King, J. Phys. Chem. C 112 (2008) 1305–1307.
[25] R.A. van Santen, A.J. Markvoort, I.A.W. Filot, M.M. Ghouri, E.J.M. Hensen, Phys. Chem. Chem. Phys. 15 (2013) 17038–17063.
[26] J. Buss, T. Agapie, Nature 529 (2016) 72–75.
[27] J.H. Wengrovius, R.R. Schrock, M.R. Churchill, H.J. Wasserman, J. Am. Chem. Soc. 104 (1982) 1739–1740.
[28] E. Bannwart, H. Jacobsen, F. Furno, H. Berke, Organometallics 19 (2000) 3605–3619.
[29] F. Furno, T. Fox, H.W. Schmalle, H. Berke, Organometallics 19 (2000) 3620–3630.
[30] N. Aristov, P.B. Armentrout, J. Am. Chem. Soc. 108 (1986) 1806–1819.
[31] R.L. Hettich, B.S. Freiser, J. Am. Chem. Soc. 108 (1986) 2537–2540.
[32] R.L. Hettich, B.S. Freiser, J. Am. Chem. Soc. 109 (1987) 3543–3548.
[33] G.A. McDermott, A.M. Dorries, A. Mayr, Organometallics 6 (1987) 925–931.
[34] H. Huang, R.P. Hughes, A.L. Rheingold, Dalton Trans. 40 (2011) 47–55.
[35] M.V. Baker, D.H. Brown, Tungsten compounds with CO or isocyanide, in: D.M.P. Mingos, R.H. Crabtree (Eds.), Comprehensive Organometallic Chemistry III, Comprehensive Organometallic Chemistry III, 5, Elsevier, Oxford, 2007, pp. 597–722.
[36] A.F. Hill, J.M. Malget, A.J.P. White, D.J. Williams, Chem. Commun. (1996) 721–722.
[37] A.F. Hill, J.M. Malget, Chem. Commun. (1996) 1177–1178.
[38] M.J. Frisch, G.W. Trucks, H.B. Schlegel, et al., Gaussian 16, Revision C.01, Wallingford CT, 2019.
[39] T. Lu, F. Chen, J. Comput. Chem. 33 (2012) 580–592.
[40] H.L. Schmider, A.D. Becke, J. Mol. Struct. 527 (2000) 51–61 (Theo).
[41] I. Mayer, P. Salvador, Chem. Phys. Lett. 383 (2004) 368–375.
[42] R. Pino-Rios, D. Inostroza, G. Cárdenas-Jirón, W. Tiznado, J. Phys. Chem. A 123 (2019) 10556–10562.