The coordinating atoms in polydentate chelates are primarily heteroatoms. We present the first examples of polydentate chelates with all binding atoms of the chelating agent being carbon atoms, denoted as CCCCC chelates. Having up to five metal-carbon bonds in the equatorial plane has not been previously observed in transition metal chemistry. Density functional theory calculations showed that the planar metallacycle has extended Craig-Möbius aromaticity arising from 12-center–12-electron $d_xp_y \pi$-conjugation. These planar chelates have broad absorption in the ultraviolet-visible–near-infrared region and, thus, notable photothermal performance upon irradiation by an 808-nm laser, indicating that these chelates have potential applications in photothermal therapy. The combination of facile synthesis, high stability, and broad absorption of these complexes could make the polydentate carbon chain a novel building block in coordination chemistry.

**RESULTS AND DISCUSSION**

**Synthesis and structural characterization**

In the presence of AgBF$_4$ treatment of complex 1 (9) with phenylacetylene (PhC≡CH) at room temperature for 2 hours led to the formation of 2a (Fig. 1A). Complex 2a exhibits excellent thermal stability both in solution and in the solid state. For instance, the solid sample of 2a was stable even when exposed to air at room temperature for 1 year or when heated at 150°C in air for 3 hours. The molecular structure of 2a was confirmed by X-ray diffraction (Fig. 1B), with the osmium center adopting a slightly distorted pentagonal bipyramidal geometry. All five coordination sites in the equatorial plane are occupied by carbon atoms, and the axial positions are occupied by two phosphorus atoms. Note that this system contains five metal-carbon bonds in the equatorial plane, which has not been previously observed in coordination chemistry. The maximum carbon coordination number for a transition metal in a planar geometry is previously four (10). Therefore, complex 2a represents the highest carbon coordination number in planar metallacycles known to date.

The metallacyclic unit in 2a is almost coplanar, as reflected by the small mean deviation from the least-squares plane (0.0523 Å). Structurally, complex 2a is constituted by a 12-atom carbon chain (C1–C12) as a polydentate ligand chelating to a central transition-metal atom (Os). The sum of the angles in the fused five-membered rings (5MRs) and the 6MR are 540.1°, 540.0°, and 719.7°, which are close to the ideal values of 540° and 720°. The bond distances of Os1–C1 (2.088 Å), Os1–C4 (2.107 Å), Os1–C7 (2.090 Å), and Os1–C11 (2.025 Å) are within the range of those of osmapentalene (1.926 to 2.139 Å) reported previously (7), indicating the delocalized metal-carbon bonds. The Os1–C12 (2.253 Å) bond distance is similar to that of the Os–C(sp$^3$) bond in complex 1 (2.272 Å) (9).
The molecular structure of 2a was further confirmed by nuclear magnetic resonance (NMR) spectroscopy, high-resolution mass spectrometry (HRMS), and elemental analysis. A doublet signal at 13.22 parts per million (ppm) in the 1H NMR spectrum is assigned to the H1 proton, which is shifted slightly downfield compared to those in the spectra of osmapentalene (11.94 to 12.46 ppm) (7). The signal of the proton on the fused 5MRs and 6MRs are observed in the aromatic region (8.71 to 7.55 ppm). In the 31PNMR spectrum, the CPPh3 signal appears at 9.24 ppm, and two OsPPh3 signals appear at −8.45 and −19.22 ppm. The 13C NMR spectrum of 2a displays metal-bonded carbon atoms in the typical downfield regions for C1 (208.0 ppm), C4 (200.8 ppm), C7 (232.0 ppm), and C11 (218.7 ppm) and an upfield signal for C12 (14.9 ppm), as expected for sp3 hybridization.

A plausible mechanism for this ring expansion reaction is proposed in fig. S1. To explore the scope of this protocol, we treated a variety of alkynes with complex 1 (Fig. 1A). The reactions of 1 with 3-ethynylthiophene, ethynylcyclohexane, or ethynylcyclopropane afforded the expected products 2b, 2c, and 2d, respectively. All of these complexes were characterized by multidimensional NMR spectra, HRMS, and elemental analysis. The structural features of 2c are essentially identical to those observed for 2a, as confirmed by single-crystal x-ray diffraction (Fig. 1C).

Notably, this reaction is not limited to alkynes; allene is also an effective reagent to form the ring-expanded product 2e. For the synthesis of 2e, complex 1 was reacted with allenylboronic acid pinacol ester in the presence of AgBF4 at room temperature for 12 hours (Fig. 1A). The molecular structure of 2e was confirmed by NMR spectroscopy, HRMS, and elemental analysis, as well as by single-crystal x-ray diffraction (Fig. 1D). The most notable structural feature of 2e is the planarity of the metallacycle, as reflected by the small mean deviation from the least-squares plane (0.0345 Å) and by the sum of the angles in the fused 5MRs (539.9°) and the 6MR (719.9°). The pentagonal bipyramidal geometry, Os–C bond distances, and proton chemical shift for 2e are similar to those for 2a. Therefore, through the reactions of 1 with alkynes or allene, a series of previously undescribed pentadentate chelates were constructed with a 12-atom carbon chain (C1–C12) and an osmium center (with axial PPh3 ligands).

These structures prompted us to reexamine the scope of the pincer complexes. Traditionally, the term “pincer” has been used to describe planar tridentate ligands (I) (24, 25). The analogous planar tetratadentate (II) and pentadentate (III) chelates, such as metalloporphyrin and complex 2, can be included in the family of pincer or pincer-type complexes.

**DFT calculations**

To elucidate the bonding and electronic structure of these unique pentadentate carbon chain chelates, we performed DFT calculations on simplified unsubstituted models of 2′ by replacing the PPh3 ligands with PH3 groups. The DFT-optimized structural parameters of 2′, especially the bond distances in the metallacycle, agree well with those observed for the crystal structure of 2a. The calculated Wiberg bond indices for the Os–C bonds in 2′ are 0.88, 0.72, 0.87, 0.73, and 0.62 for Os1–C1, Os1–C4, Os1–C7, Os1–C11, and Os1–C12, respectively, indicating strongly covalent Os–C bonding between the osmium center and these carbons, as depicted in the resonance structures (fig. S2). The pentadentate CCCCC chelate formed by the 12-atom carbon chain with the osmium center exhibits aromatic character.

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Fig. 1. Syntheses and x-ray molecular structures of pentadentate carbon chain chelates. (A) Ring expansion reactions of complex 1 with alkynes or allene, leading to the formation of 2a to 2e. (B to D) X-ray molecular structures of the cations of 2a (B), 2c (C), and 2e (D) drawn with 50% probability (the protons in PPh3 are omitted for clarity). RT, room temperature.
which was confirmed by experimental observations (for example, high stability, perfect planarity, and downfield proton chemical shift) and DFT calculations.

The isomerization stabilization energy (ISE) (26) was computed to evaluate the $\pi$-aromaticity of complex 2. The ISE values for the fused 5MRs and the 6MR are $-8.9$, $-16.2$, and $-6.3$ kcal mol$^{-1}$ (fig. S3). The sum of these values ($-31.4$ kcal mol$^{-1}$) is close to the global ISE value ($-29.0$ kcal mol$^{-1}$) of 2', indicating that such carbon chain chelates benefit from extra stability arising from quite strong 12c-12e $d_{\pi}-p_{\pi}$ $\pi$-conjugation. Note that the global ISE value of 2' is comparable to that computed for the osmapentalene ($-31.4$ kcal mol$^{-1}$) (7), which has planar Craig-type Möbius aromaticity pertaining to its 4ne (8c-8e) $d_{\pi}-p_{\pi}$ $\pi$-conjugation.

To probe the nature of the aromaticity in complex 2', we first analyzed its electronic structure. The seven-coordinated Os center has three electrons in its two unhybridized $d_{\pi}$ atomic orbitals (AOs), and the 11-center carbon chain ligand contributes 11 electrons. These $\pi$-AOs constitute seven occupied $\pi$-MOs of 2', as shown in fig. S4. Among them, six key occupied $\pi$-MOs selected in fig. 2 reflect the $\pi$-delocalization along the perimeter of the tricyclic system, which are jointly responsible for the planar 4ne (12c-12e) $d_{\pi}-p_{\pi}$ $\pi$-conjugation of Craig-type Möbius aromaticity (16, 27).

The aromaticity in the model complex 2' was further confirmed by the anisotropy of the current-induced density (ACID) calculations (28). The ACID method is a versatile, intuitive, and generally applicable approach to investigating and visualizing electron delocalization. The clockwise ring current in the $\pi$-system is displayed along the periphery of the fused 5MRs and the 6MR, indicating the $\pi$-aromaticity (Fig. 3A and fig. S5). The current-density vectors plotted on the ACID isosurface of the $\sigma$-system indicate a diatropic ring current only in the 3MR, suggesting the $\sigma$-aromaticity in the 3MR of 2' (Fig. 3B and fig. S6).

The $\sigma$-aromaticity in the 3MR of 2’ was further examined by canonical MO (CMO) nucleus-independent chemical shift (NICS) calculations (fig. S4) (29, 30). The results reveal that the total contribution of the NICS($1)_zz$ value ($-38.3$ ppm) for the 3MR from all the $\sigma$ orbitals is more negative than that ($-23.5$ ppm) from all the $\sigma$ and $\pi$ orbitals, showing $\sigma$-aromaticity in the 3MR, as previously observed in the reactant, complex 1 (9). The NICS($1)_zz$ values for the fused 5MRs and the 6MR from all occupied MOs are $-27.9$, $-16.7$, and $-6.8$ ppm, indicating aromaticity in these rings. Thus, the nature of the aromaticity in complex 2' could be considered as a combination of Craig-type Möbius aromaticity with $\sigma$-aromaticity. Overall, the ISE values, in conjunction with the ACID analysis and NICS calculations, unambiguously confirm the aromaticity, which is critical in stabilizing these planar pentadentate CCCCCC chelating structure.

**UV-vis–NIR absorption spectra**

All complexes, 2a to 2e, exhibit a broad absorption band in the UV-vis–NIR region (Fig. 4). The absorption maxima of 2a and 2b in low-energy absorption bands are 810 nm (log $\varepsilon = 2.53$, $\varepsilon$ is the molar absorption coefficient in M$^{-1}$ cm$^{-1}$) and 805 nm (log $\varepsilon = 2.48$), respectively. The absorption maxima of 2c to 2e in the low-energy absorption regions are blue-shifted to 740 nm. These results indicate that the photophysical properties of these novel pentadentate carbon chain chelates can be effectively modulated by structural modifications.

To understand the NIR absorption spectra, we carried out time-dependent DFT (TD-DFT) calculations on the cations of 2a and 2c. The lowest unoccupied MO (LUMO) level of 2a delocalized over its aryl substituent is 0.21 eV lower than that of 2c, and the highest occupied MO (HOMO) levels of 2a and 2c are similar (fig. S7). These results suggest that the aryl substituents on the metallacycle lower the LUMO levels substantially but have a small effect on the HOMO levels. The theoretical spectra are consistent with the trends of the experimental spectra. Specifically, the observed absorption bands (around 810 nm for complex 2a and around 740 nm for 2c) can be ascribed to their HOMO→LUMO transitions.

**PTT in vitro and in vivo**

PTT usually uses NIR light-absorbing agents to generate heat from energy, leading to the thermal ablation of cancer cells (31). Because of the broad absorbance spectra in the NIR region, the photothermal effect of these pentadentate carbon chain chelates was first examined by measuring the temperature increase of various concentrations of 2a under NIR laser (808 nm, 1 W cm$^{-2}$) radiation. As shown in Fig. 5A, the temperature of the water-ethanol solution (95% v/v) containing

![Fig. 3. ACID isosurfaces of the model complex 2' separated into the $\pi$- and $\sigma$-contribution. Current-density vectors are plotted onto the ACID isosurface of 0.035. (A) and (B)]. The diatropic ring current displayed in the periphery of the 6MR and the fused 5MRs indicates the $\pi$-aromaticity (A), whereas the diatropic ring current only exists in the 3MR, indicating the $\sigma$-aromaticity (B). The magnetic field vector is orthogonal with respect to the ring plane and points upward (clockwise currents are diatropic).
complex 2a (0.1 mg ml$^{-1}$) significantly increased from 28°C to 52°C within 5 min, whereas the solvent (without complex 2a) exhibited a negligible temperature change (less than 3°C) under similar conditions. Because of the strong d$_n$-p$_{π}$ π-conjugation between the osmium center and the 12-atom carbon chain, 2a exhibited good photothermal stability under the laser irradiation conditions (fig. S8). The photothermal effect of 2b was similar to that of 2a, which is more preferable than that of reported organometallics (10). These results suggest that these chelates have potential applications in PTT.

PTT often requires preferential tumor accumulation of these photo-absorbing agents to reach sufficient hyperthermia. Generally, amphiphilic polymers serve as useful nanocarriers with high clinical translational potential for loading and delivering hydrophilic compounds, and polyethylene glycol (PEG) has widely emerged as a powerful coating for nanoparticles to achieve a long circulation time and high accumulation in the tumor via the enhanced permeability and retention effects (32–34). Here, the amphiphilic polymer alkyl–polyethylenimine (PEI)$_{2k}$–PEG$_{2k}$ (35, 36) was prepared and used for the solubilization of complex 2a. Transmission electron microscopy (TEM) image and dynamic light scattering (DLS) data showed that the complex 2a–loaded micelles (2a@NPs) were well dispersed in water, with an average diameter of approximately 70 nm (fig. S9). Formulation of 2a with a large loading capacity (61.2 weight percent), high water solubility, good photothermal activity, and biocompatibility was achieved by generating 2a@NPs for cancer PTT applications (figs. S10 and S11). As expected, SCC7 cells (a squamous cell carcinoma cell line) with 2a@NPs clearly exhibited lower cell viability under...
laser irradiation as compared to control experiments without laser irradiation (Fig. 5B).

Because 2a@NPs exhibited excellent tumor accumulation (fig. S12) and photothermal performance in vivo after intravenous injection (fig. S13), we investigated the feasibility of using 2a@NPs as a PTT reagent for tumor ablation in vivo. SCC7 tumor–bearing mice were randomly divided into four groups (five mice per group): a group with saline injection and NIR laser irradiation, a group with only saline injection, a group treated with 2a@NPs plus NIR laser irradiation, and a group treated with only 2a@NPs. As shown in Fig. 5C, the tumor volumes of the control experiment increased exponentially and were up to 12 times larger at day 14 than those at day 1; however, the group of mice that received both intravenous injection and irradiation of 2a@NPs showed tumor ablation 2 days after treatment and exhibited thorough regression of the tumor in 14 days (Fig. 5, C and D). To the best of our knowledge, this work represents the first example of organometallics used for PTT; this treatment showed comparable efficacy and show broad absorption spectra in the UV-vis region for tumor ablation in vivo. SCC7 tumor cells (fig. S11), suggest that 2a@NPs have good biocompatibility. For photothermal injury, the SCC7 cells were incubated with 2a@NPs for 24 hours at room temperature. We observed that the solvent was vaporized to dryness under vacuum, and the resulting residue was washed with diethyl ether and then dried under vacuum. 1H NMR plus 1H-13C HSQC (500.1 MHz, CD2Cl2): δ = 13.22 (dd, J,P-H = 21.1 Hz, 1H, H1), 8.71 (s, 1H, H3), 8.12 (s, 1H, H8), 7.76 (s, 1H, H10), 7.63 (s, 1H, H5), 7.55 (s, 1H, H6), 6.73 (dd, J,P-H = 13.8, 2.5 Hz, 1H, H12), 8.10–5.78 ppm (m, 55H, other aromatic protons). 31P NMR (202.5 MHz, CD2Cl2): δ = 9.24 (t, J,P-P = 25.7 Hz, CPLL), –8.45 (dd, J,P-P = 254.7 Hz, J,P-P = 6.7 Hz, OsPPh3), –19.22 (dd, J,P-P = 254.7 Hz, J,P-P = 6.7 Hz, OsPPh3). 13C NMR plus DEPT-135, 1H-13C HMBC, and 1H-13C HSQC (125.8 MHz, CD2Cl2): δ = 232.0 (s, C7), 218.7 (s, C11), 208.0 (br, C1), 200.8 (d, J,P-C = 25.7 Hz, C4), 163.4 (s, C6), 159.2 (s, C5), 159.1 (s, C9), 136.6 (s, C1), 128.6 (s, C8), 120.7 (d, J,P-C = 87.1 Hz, C2), 114.4 (s, C10), 14.9 (s, C12), 148.4 (s, Ph), 142.7 (s, Ph), 134.4–124.6 ppm (m, other aromatic carbons). HRMS (ESI): mass/charge ratio (m/z) calcd for [C72H62O8P3]+, 1283.3681; found, 1283.3680. Anal. calc (%) for C72H62O8P3: C 68.42, H 4.56; found: C 68.62, H 4.77.

Preparation of 2a@NPs. The 2a@NPs were prepared according to the method described in a previous report, Liu et al. (35), with some modifications. Briefly, PEG2k was activated with N,N′-carbonyldimidazole in tetrahydrofuran and reacted with alkyl-PEI2k for 24 hours at room temperature. The product (alkyl-PEI2k-PEG2k) was obtained after precipitation in cold ether and dialysis against water to remove the residue PEG. Then, 2a was mixed with alkyl-PEI2k-PEG2k in chloroform. The mixed solutions were added to distilled water dropwise under sonication, and the resulting solution was shaken overnight. Subsequently, the residual chloroform was removed by rotary evaporation to obtain the 2a@NPs.

In vitro cytotoxicity

The cells were maintained in Dulbecco’s modified Eagle’s medium containing 10% fetal bovine serum and 1% streptomycin/ampicillin at 37°C with 5% CO2. To confirm the cytotoxicity of the 2a@NPs, 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) assays were conducted on SCC7, SCC7G9011, and 4T1 cell lines following incubation with 2a@NPs (2a concentration: 0.10, 0.20, 0.40, 0.80, and 0.10 mg ml−1) for 5 hours (39, 40). We observed that 2a@NPs exhibited low cell cytotoxicity on SCC7, SCC7G9011, and 4T1 cancer cells (fig. S11), suggesting that 2a@NPs have good biocompatibility. For photothermal injury, the SCC7 cells were incubated with 2a@NPs for 5 hours, and the medium was replaced with fresh medium, irradiated...
with an 808-nm NIR laser (1 W cm\(^{-2}\)) for 10 min, and then incubated overnight before being subjected to the standard MTT assay.

**In vivo efficacy**

Female BALB/c nude mice (18 to 20 g) were used under protocols approved by the Xiamen University Laboratory Animal Center. For the SCC7 carcinoma model, about 5 \(\times\) 10\(^6\) SCC7 cells in 50 \(\mu\)l of phosphate-buffered saline were injected subcutaneously into the hind flank of mice. The mice were used when the tumor volumes reached 50 to 60 mm\(^3\). To demonstrate the tumor biodistribution behavior of 2a@NPs, dynamic IR thermal images were obtained (fig. S12A).

2a@NPs (2a: 10 mg kg\(^{-1}\)) were intravenously injected into the tumor-bearing mice, the tumors were irradiated with an 808-nm NIR laser (1 W cm\(^{-2}\)) for 10 min, and the temperature curves were recorded at 1, 3, 5, 7, and 10 hours after injection. The biodistribution of 2a@NPs at various tissues was carried out using inductively coupled plasma MS (ICP-MS). The organs (including heart, liver, spleen, lung, and kidney) and tumors were extracted at 5 hours after injection. Each tissue was further treated with 2.0 ml of aqua regia for 48 hours until all the tissues were digested in the solutions. The distribution of Os was calculated according to the concentration of Os from 2a@NPs measured by ICP-MS (fig. S12B).

For PTT, SCC7 tumor-bearing mice were intravenously injected with 2a@NPs (2a: 10 mg kg\(^{-1}\)), and the tumors were photoirradiated for 10 min (1 W cm\(^{-2}\)) at 5 hours after injection. To monitor the PTT efficiency, the tumor volumes were measured every other day for 2 weeks (39, 40). The following equation was used to monitor the volume change of tumors: tumor volume = length \(\times\) width\(^2\)/2. In the equation, length is the largest diameter, and width is the smallest diameter. The body weights of the mice in all groups showed no obvious decrease, suggesting low toxicity of all treatments (fig. S14).

**Experimental results are means ± SD. Statistical analysis was performed using Student’s t test. \(* P < 0.05\) was considered statistically significant.**

**X-ray crystallographic analysis**

All single crystals suitable for x-ray diffraction were grown from a dichloromethane solution layered with hexane. Single-crystal x-ray diffraction data were collected at 173 K on a Rigaku R-AXIS SPIDER IP CCD (charge-coupled device) area detector using graphite-monochromated Mo K\(\alpha\) radiation (\(\lambda = 0.71073\) Å). Semiempirical or multiscan absorption corrections (SADABS) were applied (41). All structures were solved by the Patterson function, completed by subsequent difference Fourier map calculations, and refined by full-matrix least squares on \(F^2\) using the SHELXTL program package (42). All nonhydrogen atoms were refined isotropically unless otherwise stated. Hydrogen atoms were placed at idealized positions and assumed the riding model. Crystal data and structure refinement for 2a, 2c, and 2e are given in table S1. All of the x-ray molecular structures, selected bond distances, and angles (in degrees) can be found in figs. S15 to S17.

**Computational details**

All structures were optimized at the B3LYP level of DFT (43–45). In addition, frequency calculations were performed to confirm the characteristics of the calculated structures as minima. In the B3LYP calculations, the effective core potentials of Hay and Wadt with a double-\(\zeta\) valence basis set (LanL2DZ) were used to describe the Os and P atoms, whereas the standard 6-311++G(d,p) basis set was used for the C and H atoms (46). Polarization functions were added for Os \([\zeta(\mu) = 0.886], \text{CI} \ [\zeta(\zeta) = 0.514], \text{and P} \ [\zeta(\zeta) = 0.34] (47)\) in all calculations. NICS values were calculated at the B3LYP-GIAO/6-311++G(d,p) level. All of the optimizations were performed with the Gaussian 09 software package (48). To understand the absorption spectra, we performed TD-DFT calculations on 2a and 2c at the BLYP/6-31G (d) level (49). In TD-DFT calculations, the structures were extracted from x-ray diffraction data, and the polarizable continuum model was used, with dichloromethane as the solvent (50). The CMO-NICS calculations were carried out with the NBO 5.0 program (30), and the ACID calculations were carried out with the ACID program (28). See data file S1 for the Cartesian coordinates.

**SUPPLEMENTARY MATERIALS**

Supplementary material for this article is available at http://advances.sciencemag.org/cgi/content/full/2/6/ea610031/DC1

**Supplementary Materials and Methods**

fig. S1. A plausible mechanism for the formation of complex 2a from osmapentalene 1.

fig. S2. The major resonance structures for the cation of 2.

fig. S3. The aromaticity of model 2e evaluated by the ISE method.

fig. S4. NICS(1)zz (in ppm) contributions of the MOs of model 2e.

fig. S5. ACID isosurfaces of the model complex 2e separated into the \(\sigma\)-contribution.

fig. S6. ACID isosurfaces of the model complex 2e separated into the \(\pi\)-contribution.

fig. S7. Frontier MOs of 2a and 2c and their eigenvalues predicted at the BLYP/6-31G(d) level of theory.


fig. S9. The average diameter of 2a@NPs confirmed by DLS and TEM.

fig. S10. Photothermal effect of 2a, 2a@NPs, alkyl-PEI-PEG, and water under laser irradiation.

fig. S11. The cytotoxicity of 2a@NPs was measured in vitro without laser irradiation.

fig. S12. Pharmacological evaluation of 2a@NPs.

fig. S13. Photothermal performance in vivo of 2a@NPs.

fig. S14. The body weights of the mice in all groups.

figs. S15 to S17. Molecular structure, selected bond distance, and angles of 2a, 2c, and 2e.

figs. S18 to S22. HRMS spectra of 2a to 2e.

figs. S23 to S52. All NMR spectra of 2a, 2c, and 2e.

figs. S24 to S30. All X-ray crystallographic data.

fig. S31. Crystal data and structure refinement for 2a, 2c, and 2e.

**REFERENCES AND NOTES**


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CCCCC pentadentate chelates with planar Möbius aromaticity and unique properties
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