Reversible Modulation of the Electronic and Spatial Environment around Ni(0) Centers Bearing Multifunctional Carbene Ligands with Triarylamuminum

Yasuhiro Yamauchi,[a] Yutaka Mondori,[a] Yuta Uetake,*[a,b] Yasuo Takeichi,[c] Takahiro Kawakita,[a] Hidehiro Sakurai,[a,b] Sensuke Ogoshi,*[a] and Yoichi Hoshimoto*[a,d]

[a] Department of Applied Chemistry, Faculty of Engineering, Osaka University, Suita, Osaka 565-0871, Japan
[b] Innovative Catalysis Science Division, Institute for Open and Transdisciplinary Research Initiatives (ICS-OTRI), Osaka University, Suita, Osaka 565-0871, Japan
[c] Department of Applied Physics, Graduate School of Engineering, Osaka University, Suita, Osaka 565-0871, Japan
[d] Center for Future Innovation (CFi), Division of Applied Chemistry, Faculty of Engineering, Osaka University, Suita, Osaka 565-0871, Japan

*Please address correspondence to: hoshimoto@chem.eng.osaka-u.ac.jp; uetake@chem.eng.osaka-u.ac.jp

Abstract

Designing and modulating the electronic and spatial environment surrounding metal centers is a crucial issue in a wide range of chemistry fields that use organometallic compounds. Herein, we demonstrate a Lewis-acid-mediated reversible expansion, contraction, and transformation of the spatial environment surrounding nickel(0) centers that bear N-phosphine oxide-substituted N-heterocyclic carbenes (henceforth referred to as (S)PoxIm). Reaction between trigonal-planar (syn-κ-C,O-(S)PoxIm)Ni(CO)₂ and Al(C₆F₅)₃ smoothly afforded heterobimetallic Ni/Al species such as tetrahedral {κ-C-Ni(CO)₂}{μ-anti-(S)PoxIm}{κ-O-Al(C₆F₅)₃} via a complexation-induced rotation of the N-phosphine oxide moieties, while the addition of 4-dimethylaminopyridine resulted in the quantitative regeneration of the former Ni complex. The shape and size of the space around the Ni(0) center was drastically changed through this Lewis-acid-mediated interconversion. Moreover, the multinuclear NMR, IR, and XAS analyses clarified the details of the changes in the electronic states on the Ni centers. The results presented in this work thus provide a strategy for reversibly modulating the electronic and spatial environment of organometallic complexes, in addition to the well-accepted Lewis-base-mediated ligand-substitution methods.

Key words: Lewis acids, N-heterocyclic carbenes, multifunctional ligands, Nickel, X-ray absorption spectroscopy
**Introduction**

Designing the spatial environment around a metal center is a critical issue in terms of the electronic and/or steric properties and hence the reactivity of organometallic complexes. Chemists have thus focused on the design of the structural, electronic, and dynamic properties of supported ligands, as demonstrated in the field of, e.g., homogenous catalysis, supramolecular chemistry, and materials science. One well-known strategy for reversibly modulating the electronic/spatial environment around metal centers is based on a ligand-substitution process on metal centers bearing multifunctional ligands including a hemi-labile coordination moiety (L’) in the presence of an external Lewis base (LB) (Figure 1A, left). However, these processes often yield an equilibrium mixture that is difficult to separate. In this context, we have reported the reversible, recyclable, and pressure-responsive room-temperature-chemisorption of carbon monoxide (CO) on a zero-valent nickel complexes that bear multifunctional multipurpose carbene ligands, namely N-phosphine oxide-substituted imidazolylidenes (SPoxIms) and the corresponding imidazolylidenes (PoxIms) (Figure 1B, left). (S)PoxIm ligands in tetrahedral (S)PoxImNi(CO), complexes selectively adopt either a κ-C- (n = 3) or κ-C,O- (n = 2) coordination mode, which can be interconverted through the addition/exclusion of CO.

A strategy based on the use of Lewis acids (LAs) is another potential option for reversibly modulating the electronic/spatial environment around metal centers that bear multifunctional ligands (Figure 1A, right). The LA-mediated process can cause a substantial change in both the electronic state and spatial environment of the metal center due to the change in the number of ligands. This feature clearly distinguishes LA-mediated processes from LB-mediated ones, as the latter commonly proceeds without changing the number of ligands. However, examples of such LA-mediated reactions have been severely limited, because LAs often trigger the irreversible decomposition of the organometallic complex via the abstraction of ligands to form an LA–LB adduct. A judicious combination of multifunctional ligands and LAs is thus essential for constructing an LA-mediated system that can reversibly regulate the electronic/spatial environment around the metal centers. It should be noted that Fan et al. have reported an example that relies predominantly on an electrostatic interactions involving the reversible complexation of Na⁺ and a crown-ether moiety included in a Rh complex that bears Aza-CrownPhos; the reactivity of the Rh complex can be regulated through the Na⁺-mediated interconversion. The authors evaluated the change in the spatial environment around the Rh center using multinuclear NMR spectroscopy and ESI mass spectrometry, even though a quantitative evaluation of how much the field expanded/diminished via the reaction was not discussed.

Herein, we present a novel strategy to reversibly transform the spatial environment around a nickel center by combining (S)PoxIms 1a–d (Figure 1C) as multifunctional ligands and
tris(pentafluorophenyl)aluminum as an LA, where the geometry of the Ni center is interconverted between tetrahedral and trigonal planar (Figure 1B, right). We quantitatively evaluated the variation of the spatial environment, i.e., the volume and shape of the space, and the electronic state around the nickel center based on single-crystal X-ray diffraction (SC-XRD) and X-ray absorption spectroscopy (XAS) analyses.

**Figure 1.** (A) A simplified scheme of the reversible modulation of the spatial environment around a metal center in an organometallic complex, mediated by Lewis bases (LBs, left) or Lewis acids (LAs, right). (B) Reversible transformation of Ni/(S)PoxIm complexes using Lewis-basic CO (our previous work, left) and Lewis-acidic aluminum species (this work, right). (C) The (S)PoxIm used in this work (Dipp = 2,6-diisopropylphenyl, Mes = 2,4,6-trimethylphenyl).

### Results and Discussion

Previously, we have reported that (S)PoxIm include *syn*- and *anti*-conformers with respect to the N–P bonds, which can interconvert easily at room temperature via rotation of the
$N$-phosphinoyl groups ($\Delta E \sim 12$ kcal mol$^{-1}$ for previously reported PoxIms), even though the \textit{anti}-conformers are thermodynamically favorable (Figure 2).\textsuperscript{15,16} Importantly, the volume and shape of the space can be drastically varied via rotation of the $N$-phosphinoyl groups, and a relatively limited space is present around the carbene carbon atoms in the \textit{anti-}(S)PoxIms. Due to this limited spatial environment, only group-11 metals such as Cu\textsuperscript{20} and Au\textsuperscript{21} have been confirmed to form complexes that bear \textit{anti-}(S)PoxIms in a $\kappa$-C fashion, given that these metals tend to adopt two-coordinated linear complexation geometries (Figure 2). We have also reported the synthesis of heterobimetallic complexes of the type ($\kappa$-C-Cu)($\mu$-\textit{anti-}(S)PoxIm)($\kappa$-O-Al) through complexation between \textit{anti-}(\kappa-O-(S)PoxIm)Al(C$_6$F$_5$)$_3$ and CuO'Bu followed by an irreversible intramolecular Cu–O'Bu/Al–C$_6$F$_5$ transmetalation triggered by the rotation of the $N$-phosphinoyl moiety.\textsuperscript{20} However, reversible spatial modifications around the metal center between isolable species remain challenging.

![Figure 2](image_url)

\textbf{Figure 2.} Interconversion between \textit{syn-} and \textit{anti-}conformers of (S)PoxIms, as well as complexation between (S)PoxIms and transition metals that prefer different coordination geometries.

In this work, we envisioned an Al(C$_6$F$_5$)$_3$-mediated reversible interconversion between complexes bearing \textit{syn-} and \textit{anti-}(S)PoxIms based on the use of Ni(0), i.e., an interconversion between tetrahedral ($\kappa$-C,O-(S)PoxIm)Ni(CO)$_2$ and trigonal-planar \{($\kappa$-C-Ni(CO)$_2$)$_2$($\mu$-\textit{anti-}(S)PoxIm)\}$\{($\kappa$-O-Al(C$_6$F$_5$)$_3$)$_2$\} (Figure 1B, right). The preparation of trigonal-planar Ni(0) di-carbonyl complexes that bear bulky $N$-heterocyclic carbenes (NHCs) such as (I'Bu)Ni(CO)$_2$ and (IAd)Ni(CO)$_2$\textsuperscript{22,23} (I'Bu = 1,3-di-tert-butylimidazol-2-ylidene; IAd = 1,3-di-adamantylimidazol-
2-ylidene) has already been reported which inspired us to explore the preparation of a Ni(0) complexes bearing bulky anti-(S)PoxIm ligands (Figure 2).

We started our study with the reaction between \((\text{syn-} \kappa\text{-}C,\text{O-1a})\text{Ni(CO)}_2\) (2a) and an equimolar amount of \(\text{Al(C}_6\text{F}_3)_3(\text{tol})_{0.5}\), which resulted in the selective formation of heterobimetallic Ni/Al complex 3a in 90% yield (Figure 3A). We also confirmed that the \(\text{Al(C}_6\text{F}_3)_3\)-mediated rotation of \(N\)-phosphinoyl moieties in 2b–d afforded the corresponding heterobimetallic Ni/Al complexes (3b–d) in good-to-high yield. The molecular structures of 3a–d were fully characterized using NMR and ATR-infrared (IR) absorption spectroscopy as well as SC-XRD analysis \((\text{vide infra})\). Subsequently, we treated 3a with slightly excess amounts of 4-dimethylaminopyridine (DMAP) and confirmed the quantitative regeneration of 2a with the concomitant formation of the adduct DMAP–\(\text{Al(C}_6\text{F}_3)_3\) (Figure 3B). These results demonstrated that the interconversion between 2a and 3a can be successfully mediated by the addition/removal of \(\text{Al(C}_6\text{F}_3)_3\).

Next, we compared the electronic and geometric parameters of 2a and 3a. In the \(^{31}\text{P}\) NMR spectrum of 3a, the resonance corresponding to the \(N\)-phosphinoyl moiety is observed at \(\delta = 82.0\) in toluene-\(d_8\), which represents a significant downfield shift compared to that of 2a (\(\delta = 68.0\) in THF-\(d_8\))\(^{14}\) while it is almost identical to that of \((\kappa\text{-}O\text{-1a})\text{Al(C}_6\text{F}_3)_3\) (\(\delta = 79.8\) in CD\(_2\)Cl\(_2\)).\(^{20}\) These results indicate that the 1a moiety in 3a should adopt predominantly the anti-conformation. The geometric parameters of 3a obtained from the SC-XRD analyses are shown in Figure 3C. As previously reported, the Ni center in 2a, which bear the \(\kappa\text{-}C,\text{O-syn-1a}\) ligand (C–N–P–O torsion angle: 8.5(1)°), adopts a tetrahedral geometry.\(^{14}\) In stark contrast, 3a features a trigonal-planar Ni center (sum of bond angles around Ni: 358.9°) bearing anti-1a (C1–N2–P–O1 torsion angle: 159.7(2)°)\(^{21}\), as shown in Figure 3C. The Ni(CO)\(_2\) unit is located slightly out of ideal alignment with the carbene lone pair (Z1–C1–Ni angle: 169.9°; Z1 = centroid of the imidazolinylidene ring), most likely due to the high steric demand of the ‘Bu groups.

Interestingly, a non-covalent interaction between the Ni and H1 atoms was confirmed in the gas-phase-optimized structure of 3a (level: PBE0/def2-TZVPD//M06L/def2-SVPD for O, F, and Ni; def2-SVP for all other atoms) via a topological analysis of the electron density, which was calculated using the quantum-theory-of-atoms-in-molecule (AIM) method (Figure 3D).\(^{24,25}\) It should also be noted here that the geometric parameters of the solid state structure of 3a confirmed by SC-XRD analysis were closely reproduced in the theoretically calculated gas-phase-optimized structure, e.g., the interatomic distances between the Ni and C5 atoms was 3.18 Å in the gas-phase and 3.240(4) Å in the crystalline state. In fact, the Ni···H1 distance (2.13 Å)\(^{26}\) and the relatively high electron density (\(\rho = 0.026\) e \(\text{Å}^{-3}\)) as well as the positive value of the Laplacian of the electron density (\(\nabla^2\rho = +0.061\) e \(\text{Å}^{-3}\)) at the bond-critical point (BCP) between these atoms, suggests the participation of an agostic Ni···H interaction.\(^{24,25}\)
Dissociation of the \(N\)-phosphinoyl moiety from the tetrahedral \(2a\) to afford trigonal planar \(3a\) also caused obvious changes in the wavenumbers of the stretching vibration of the CO ligands. In fact, the signal corresponding to the stretching vibration of the CO ligands in \(3a\) was observed at 2019 cm\(^{-1}\), i.e., at higher wavenumber than that of \(2a\) (1967 cm\(^{-1}\)). The AIM analysis clarifies the increase in the delocalization indices \(\delta(Ni, C_{CO})\) and \(\delta(Ni, O_{CO})\) in \(3a\) compared to those in \(2a\), which represent a number of electron pairs delocalized between the Ni and carbonyl carbon atoms (\(C_{CO}\)) and the Ni and carbonyl oxygen atoms (\(O_{CO}\), respectively. (Figures S7–S8)\(^{25}\) The mean values of \(\delta(Ni, C_{CO})\) and \(\delta(Ni, O_{CO})\) increase from 0.51 (\(2a\)) to 1.20 (\(3a\)) and from 0.063 (\(2a\)) to 0.23 (\(3a\)), respectively, indicating that electrons become effectively delocalized through the Ni, \(C_{CO}\), and \(O_{CO}\) atoms in \(3a\). On the other hand, the values of \(\delta(C_{CO}, O_{CO})\) are nearly identical between \(2a\) (1.70–1.71) and \(3a\) (1.60–1.62). Thus, we attribute the aforementioned blue-shift to the increased polarization of the \(\pi\) CO bonding orbitals due to an increased cationic nature on the Ni in \(3a\) (AIM atomic net charge = 0.50 e) compared to \(2a\) (AIM atomic net charge = −0.1 e).\(^{27}\)

Based on the aforementioned geometric parameters of \(2a\) and \(3a\) in the crystalline state, the impact of the \(N\)-phosphinoyl rotation on the spatial environment surrounding the Ni center was quantitatively evaluated on the basis of percent buried volume (%\(V_{bur}\)) (Figure 3E).\(^{2,28}\) Topographic steric maps that visualize the %\(V_{bur}\) values in the north-western (NW), north-eastern (NE), south western (SW), and south-eastern (SE) quadrants, as well as their average (Av), are also depicted; these maps were produced using the program SambVca 2.1.\(^2\) The Av(%\(V_{bur}\)) values in \(2a\) and \(3a\) were calculated to be 43.9 and 51.2, respectively, clearly demonstrating that the space around the Ni center is significantly altered via rotation of the \(N\)-phosphinoyl moiety. Importantly, the drastic expansion/contraction of the space can be precisely and reversibly triggered by the addition/removal of \(Al(C_{6}F_{5})_3\). In addition, this rotational transformation alters the shape of the space around the Ni center, as clearly confirmed by the comparison of both the %\(V_{bur}\)(NE) and %\(V_{bur}\)(SE) values of \(2a\) and \(3a\).
Figure 3. (A) Synthesis of heterobimetallic Ni/Al complexes 3 via the reaction between \((\text{syn-}_\kappa\text{-C,O-1})\text{Ni(CO)}_2\) (2) and an equimolar amount of Al(C\(_6\)F\(_5\))\(_3\)(tol)\(_{0.5}\). (B) Reaction of 3a with DMAP. (C) Molecular structure of 3a with thermal ellipsoid at 30% probability; H atoms (except those bound to C3 and C4) are omitted for clarity. Selected bond lengths (Å) and angles (°): Ni–C1 1.945(3), Ni–C2 1.759(3), Ni–C5 3.240(4), C2–O2 1.140(4), P–O1 1.524(2), O1–Al 1.799(2), Z1–C1–Ni 169.9 C1–N2–P–O1 159.7(2). (D) The quantum theory of AIM bond paths (black lines) and bond-critical points (green dots), overlaid with the contour plots of \(\nabla^2 \rho\) through the plane defined by the C1, Ni, and C5 atoms. Selected atoms and values of electron density \((e \cdot r_{\text{bohr}}^{-3})\) are shown. The values of \(\nabla^2 \rho\) \((e \cdot r_{\text{bohr}}^{-5})\) are shown in square brackets. (E) Topographic
stereic maps and \%\Vbar values of 2a/3a calculated using the program Samb\Vca (r = 3.5 Å; \(d = 2.0\) Å; bond radii scaled by 1.17; mesh spacing 0.05; H atoms are omitted) based on the structural parameters obtained from the SC-XRD analysis.

We then carried out solution-phase XAS measurements to determine whether the results obtained from the SC-XRD analysis could be extended to the solvated states of 2a and 3a. A magnified view of the pre-edge and edge region of the Ni K-edge X-ray absorption near edge structure (XANES) is shown in Figure 4A. In the case of 2a, a pre-edge peak corresponding to the electric dipole transition from the Ni 1s orbital to the Ni 4p(-3d) orbitals was observed at 8326 eV and no characteristic peak was detected at the absorption edge, which is typical for nickel complexes with tetrahedral geometry.\(^{14}\) Meanwhile, a remarkable peak appeared in the edge region (8331 eV) for 3a, along with the greater pre-edge peak intensity compared to 2a. We attribute the characteristic edge peak to the Ni 1s→4p transition in 3a, given the presence of the non-bonding 4p\_\(z\) orbital (\(a''\) symmetry) (Figure 4C). Considering that such non-bonding 4p\_\(z\) orbitals are commonly found in trigonal-planar 16-electron complexes, the results of the solution-phase XAS experiments clearly rationalize the adoption of a trigonal-planar geometry by 3a, even in toluene, as observed in the crystal structure.

To gain further insight, the Ni K-edge XAS spectra of 2a and 3a were simulated using the time-dependent DFT (TDDFT) calculation at the B3LYP level with the zeroth-order regular approximation (ZORA)\(^{29–31}\) to take the relativistic effect into consideration.\(^{32}\) The CP(PPP) basis set was used for Ni, while the ZORA-def2-TZVP(-f) basis set was used for all other elements. The intensities of the pre-edge and edge peaks of the simulated XAS spectra show good agreement with those of the experimental spectra (Figures 4A and 4B). To identify the predominant contribution to the pre-edge peaks, we then analyzed the molecular orbitals (MOs) in 2a and 3a. In the case of 2a, the transition from the Ni 1s orbital to the LUMO+2 significantly contributes to the pre-edge peak, where the LUMO+2 mainly consists of the Ni 3d (6.7%), Ni 4p (7.8%), and CO 2p (30.7%) orbitals (Figure 4D). On the other hand, in the case of 3a, the increased intensity of the corresponding pre-edge peak can be rationalized predominantly by the transition from the Ni 1s orbital to the LUMO. The LUMO of 3a features increased contribution from the Ni 4p orbitals (17.1%) and CO ligands (52.3%) compared to their contributions to the LUMO+2 in 2a (Figure 4E), while the Ni 3d orbitals exhibit a nearly identical degree of contribution to the respective MOs in 2a and 3a. We therefore attributed the increase in the pre-edge peak intensity of 3a induced by the Al(C\(_6\)F\(_3\))\(_3\)-mediated geometric change to the increased efficiency of the Ni 3d-4p mixing and contribution of CO ligands (\(e'\) symmetry) in the trigonal planar geometry.

Finally, we further explored the electronic structures of the Ni 3d orbitals in the solid state for 2a and 3a based on Ni L\(_{2,3}\)-edge XAS experiments using the partial fluorescence yield
(PFY) method. In the cases of 2a and Ni(cod)$_2$, the absorption maxima on the Ni L$_3$-edge appear at 856.0 and 856.2 eV, respectively, with a shoulder peak in their lower-energy regions (Figure 4F). These Ni L$_{2,3}$-edge XAS spectra represent spectroscopic features characteristic of tetrahedral nickel complexes with a d$^{10}$ electron configuration (formally Ni(0)). In contrast, for 3a, the peak maximum shifts toward the lower-energy region to 852.9 eV, clearly indicating that the 3d orbitals are stabilized through the formation of the 16-electron complex with a vacant 4p$_z$ orbital. In fact, the energy levels of the unoccupied frontier MOs of 3a are substantially lower than those of 2a, showing good agreement with the experimental Ni L$_{2,3}$-edge XAS data (Table S4). Furthermore, a broad signal is observed in the higher energy region at 854–858 eV. Based on the results of the Cu L$_{2,3}$-edge XAS experiments previously reported by Lancaster et al., we attribute this signal to the transitions from the Ni 2p$_{3/2}$ orbital to the ligand and Ni 3d orbitals, given the occupied d$^{10}$ electron configuration in 3a.
Figure 4. (A) Ni K-edge XANES spectra of 2a/3a in toluene. (B) The simulated Ni K-edge XAS spectra of 2a and 3a using the TDDFT method at the ZORA-B3LYP/CP(PPP) (for Ni), ZORA-def2-TZVP-f (for C, H, O, N, F, P, and Al) level. (C) Qualitative MO diagram of the trigonal-planar complex. The purple bars denote electric dipole allowed, and the gray bars forbidden transition orbitals in the Ni K-edge XAS. (D) Kohn–Sham LUMO+2 for 2a. (E) Kohn–Sham LUMO for 3a. (F) Ni L\textsubscript{2,3}-edge XAS spectra of Ni(cod)\textsubscript{2}, 2a, and 3a in PFY method.
In summary, we have reported a strategy that reversibly modulate the electronic state and spatial environment around metal centers that bear multifunctional ligands based on the use of Lewis acids. To this end, a series of N-phosphine oxide-substituted N-heterocyclic carbenes, referred to as (S)PoxIms, was employed, as (S)PoxIms can afford heterobimetallic species in a κ-C-M1 and κ-O-M2 fashions without the formation of quenched NHC–Lewis acid-adducts. In fact, the reaction between trigonal-planar (syn–κ-C,C,O-(S)PoxIm)Ni(CO)2 and Al(C6F5)3 smoothly afforded heterobimetallic Ni/Al species such as tetrahedral {κ-C-Ni(CO)2} (μ-anti-(S)PoxIm) {κ-O-Al(C6F5)3} through the complexation-induced rotation of the N-phosphine oxide moiety, while the addition of DMAP quantitatively triggered the formation of the former complex. We experimentally and theoretically confirmed that the shape and size of the space around the Ni(0) center drastically expanded/contracted through this Lewis-acid-mediated procedure. Furthermore, a detailed discussion based on multinuclear NMR, IR absorption, and X-ray absorption spectroscopy shed light on the changes in the electronic states of the Ni centers. Thus, this work manifests a conceptually novel and effective approach to design and modulate the electronic and spatial environment surrounding metal centers in organometallic compounds using a combination of multifunctional ligands and Lewis acids.

Acknowledgements

We thank T. Honma (Japan Synchrotron Radiation Research Institute), S. Yamashita (High Energy Accelerator Research Organization), and H. Iwayama (Institute for Molecular Science) for their support of the XAS experiments. Ni K-edge XAS measurements were performed at the BL14B2 beamline of SPring-8 with the approval of the Japan Synchrotron Radiation Research Institute (under proposal no. 2020A1871, 2021A1630, 2022A1767, and 2022A1784). Ni L2,3-edge XAS measurements were performed at the BL-19B beamline of KEK under the approval of the Photon Factory Program Advisory Committee (under proposal no. 2022P013), and at the BL4B beamline of the UV Sor Synchrotron Facility with the approval of Institute for Molecular Science (under proposals no. 21-697). This project was supported by Grants-in-Aid for Scientific Research (C) (JSPS KAKENHI grants 21K05070 to Y.H. and 22K05095 to Y.U.), and Grants-in-Aid for Transformative Research Area (A) Digitalization-driven Transformative Organic Synthesis (JSPS KAKENHI grant 22H05363 to Y.H.). Part of this work was supported by JST SPRING (grant JPMJSP2138 to Y.Y.). Part of the computation was performed using resources from the Research Center for Computational Science, Okazaki, Japan (Project: 22-IMS-C107).
Competing interests
The authors declare the absence of any competing interests.

Author contributions
Y.H. conceived and directed this project. Y.Y., Y.M. T.K. and Y.H. synthesized and characterized the nickel complexes. Y.U. and Y.H. performed the theoretical calculations. Y.Y., Y.M., Y.U., and Y.T. conducted the XAS experiments and analysis. Y.Y., Y.U., and Y.H. prepared the manuscript with feedback from all authors.

Supporting Information.
Full details pertaining to the experimental methods, identification of the compounds, and DFT calculations. CCDC 2263787-2263791 contain the supplementary crystallographic data for this paper.

References


