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CC Agostic Interactions

An Unsymmetrical bis C–C Agostic Heterobimetallic Lithium Yttrium Complex**

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Despite their relative scarcity, agostic complexes in which a C–C,[1] rather than a C–H, bond apparently interacts with a main-group or transition metal have been attracting much attention recently. This stems mainly from their involvement in metallacyclobutanes, which are intermediates in alkene metathesis reactions,[2] and also in their ability to model C–C σ-complexes and C–C bond cleavage.[3] We have characterized a series of α-C–C agostic cyclopropyl complexes [$\mathrm{Tp^{Me2}NbX}(c\text{-}\mathrm{C_3H_5})(\mathrm{MeCCMe})$] (X = Cl, Me, etc.) by different methods including X-ray diffraction, solution NMR and DFT modeling.[4] The poor overlap between the C orbitals within the strained C3 ring was suggested to be responsible for the preference of an α-CC over more classical α- or β-CH agostic distortions.[4b,c,5] The elongation of the α-CC agostic bond was accompanied by a lowering of the associated J_{CC} NMR spectroscopy coupling constant.[1j,2,4a] We also successfully calculated these J_{CC} values, realizing that computation is a reliable alternative to the inherently difficult problem of measuring J_{CC} values.[4a] We report herein an unprecedented example of a heterobimetallic complex [$\mathrm{Cp^*_2Y}(\mu\text{-}c\text{-}\mathrm{C_3H_5})_2\mathrm{Li(thf)}$] (**1**; Cp* = $\mathrm{C_5Me_5}$) that exhibits two different α-CC agostic distortions. We also discuss the nature of these distortions, showing that the α-CC agostic interaction with yttrium has a covalent nature whereas that with lithium has an electrostatic character.

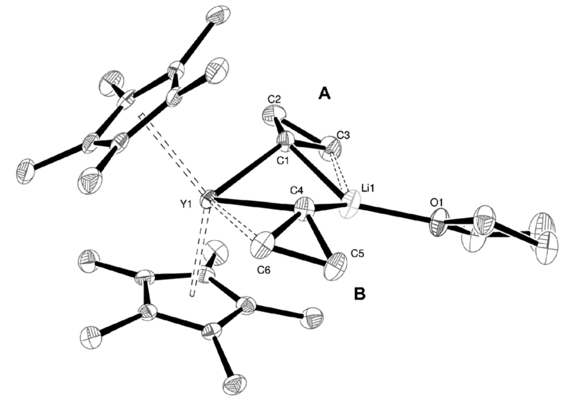
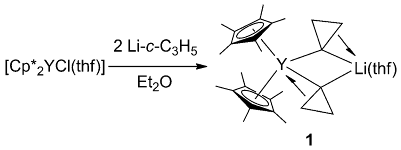


Figure 1. View of the molecular structure of complex **1** with hydrogen atoms omitted for clarity. Selected bond lengths [Å] and angles [°]: Y1–C1 2.477(5), Y1–C4 2.432(5), Li1–C1 2.131(11), Li1–C4 2.127(11), Li1–C3 2.473(11), Li1–O1 1.913(10), C1–C2 1.515(7), C1–C3 1.546(8), C2–C3 1.474(8), C4–C5 1.514(7), C4–C6 1.539(7), C5–C6 1.486(7); C1-Li1-C4 97.0(4), C1-Y1-C4 80.98(17), Y1-C1-Li1 80.8(3), Y1-C4-Li1 81.9(3), Y1-C1-C2 127.4(4), Y1-C1-C3 144.0(4), Y1-C4-C5 134.1(4), Y1-C4-C6 91.4(3), Li1-C1-C3 82.9(4), Li1-C4-C5 110.3(5), O1-Li1-C1 138.9(6), O1-Li1-C4 115.7(5).

The complex [$\mathrm{Cp^*_2Y}(\mu\text{-}c\text{-}\mathrm{C_3H_5})_2\mathrm{Li(thf)}$] (**1**) is obtained as white crystals in 75% yield by treatment of [$\mathrm{Cp^*_2YCl(thf)}$] with two equivalents of Li-c-$\mathrm{C_3H_5}$ in diethyl ether (Scheme 1). Its formulation comes from analytical, spectroscopic, and X-ray diffraction data. X-Ray diffraction on a single crystal reveals an unexpected unsymmetrical structure (Figure 1).[6] The yttrium is in a typical bent metallocene environment while the lithium is formally three coordinate. The yttrium and the lithium are bridged by two cyclopropyl groups by C1 (group A) and C4 (group B) with a puckered Y1-C1-Li1-C4 ring (48° between Y1-C1-C4 and Li1-C1-C4 planes). The bond lengths between these Cα and yttrium are unexceptional even if Y1–C1 is slightly longer than Y1–C4 [Y1-C1 2.477(5), Y1-C4 2.432(5) Å]. Typical Y–C bond lengths are 2.44(2) and 2.4071(18) Å in methyl [$\mathrm{Cp^*_2YCH_3(thf)}$][7a] and alkynyl [$\mathrm{Cp^*_2Y(CCPh)(thf)}$][7b] complexes, respectively, and 2.38(2) Å in the related μ-alkynyl bimetallic complex [$\mathrm{Cp^*_2Y}(\mu\text{-CC}t\mathrm{Bu})_2\mathrm{Li(thf)}$].[8] The bond lengths between these bridging secondary Cα and lithium are short [Li1-C1 2.131(11), Li1-C4 2.127(11) Å] most probably because of the low coordination number of the lithium as also observed in [$\mathrm{Cp^*_2Y}(\mu\text{-CC}t\mathrm{Bu})_2\mathrm{Li(thf)}$] [Li-C 2.09(3) Å].[8] There are no indications of CH agostic distortions of any kind.[9]



Scheme 1. Synthesis of complex **1**.

Several structures of secondary alkyl lithium compounds have been reported but not that of Li-c-$\mathrm{C_3H_5}$. In the clusters [$\{\mathrm{LiCH(CH_3)_2}\}_6$] and [$\{\mathrm{Li}\text{-}c\text{-}\mathrm{C_6H_{11}}\}_6$] Li–C bond lengths are in the range 2.160(3)–2.316(3) and 2.184(3)–2.300(4) Å, respectively.[10] The longer Li–C bond [Li-C 2.440(14) Å] in the dimer of 2,2-diphenyl-1-(phenylsulfonyl)cyclopropyllithium dimethoxyethane stems from the presence of four additional Li–O bonds with sulfonyl and ether moieties.[11] The two

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angles Y1-Cα-Li1 are very similar [Y1-C1-Li1 80.8(3), Y1-C4-Li1 81.9(3)°]. Despite the apparent symmetry, complex **1** shows strong distortions in the cyclopropyl rings themselves. The angles Y-Cα-Cβ as well as Li-Cα-Cβ are significantly different for the two cyclopropyl groups. The Y1-C1-C2 angle is 127.4(4)° whereas Y1-C4-C5 is 134.1(4)°. Similarly the Li1-C1-C3 angle is 82.9(4)° while Li1-C4-C5 is 110.3(5)°. The M⋯Cβ distances are consequently different, and most prominently, shorter M⋯Cβ distances and more acute M-Cα-Cβ are associated with longer Cα–Cβ bonds within the cyclopropyl rings. The cyclopropyl group A is tilted towards Li in such a way that Li1⋯C3 [2.473(11) Å] is shorter than Li1⋯C5 (3.01 Å) with C1–C3 [1.546(8) Å] not significantly longer than C1–C2 [1.515(7) Å]. The cyclopropyl group B, on the other hand, is tilted towards Y. C4–C6 [1.539(7) Å] directed towards Y and C4–C5 [1.514(7) Å] are statistically equal, and Y1⋯C6 [2.910(5) Å] is shorter than Y1⋯C2 [3.61 Å]. The interaction between Y and the cyclopropyl group B is similar to that observed in the α-CC agostic [$\mathrm{Tp^{Me2}NbCl}(c\text{-}\mathrm{C_3H_5})$(MeCCMe)] complex,[4b,c] with an even more pronounced distortion. The distortion of the cyclopropyl group A is reminiscent of that described in the "lithium-bonded" cyclopropyl edge in [{LiOC($\mathrm{CH_3}$)(c-$\mathrm{C_3H_5}$)$_2$}$_6$] (**2**) [Li⋯C 2.615(3), 2.644(3) Å] even though there is no Li–C bond in **2**.[1k] To our knowledge, **1** is the very first example in which two different CC agostic distortions, one with an alkaline metal, and one with a transition metal, are observed within the same complex.

Beyond solid-state structural data, solution ^{1}H and ^{13}C NMR spectra (Supporting Information) indicate a symmetrical structure at all temperatures (183–273 K). In the ^{1}H NMR spectrum, the CαH protons resonate as a triplet of triplets ($\delta = -1.50$, J_{HH} 9, 10 Hz), and CβH protons appear as two doublets of doublets at $\delta = 0.74$ (J_{HH} 10, 1 Hz) and 0.34 (J_{HH} 9, 1 Hz). Couplings with ^{89}Y and ^{6}Li are only apparent in the ^{13}C NMR spectrum where *C*αH signal appears as a broad multiplet at $\delta = 10.2$ (ddq, J_{CH} 111, J_{YC} 44, J_{LiC} 16 Hz). A single Cβ resonance is observed at $\delta = 5.4$ (t, J_{CH} 157 Hz). The inherently challenging measurement of J_{CC} was not attempted because of the fluxional behavior and the resulting overall symmetry in solution even at 183 K.

We have carried out DFT calculations on **1** with the goal of 1) firmly establishing the presence of α-CC agostic interactions, and 2) providing a description of the bonding situation.[12] Optimization of **1** yielded two minima: a symmetrical structure and an unsymmetrical distorted one. The symmetrical structure lies only 4 kJ mol^{-1} lower in energy, indicating a very low barrier for interconversion of agostic and non-agostic C–C structures as also observed by solution NMR spectroscopy. The calculated bond lengths and angles of the distorted structure match remarkably well the experimental parameters of the solid-state structure of **1** (Supporting Information). The core of the unsymmetrical optimized structure is depicted in Figure 2 together with relevant computed metrical parameters and J_{CC}. In this case the average calculated values for the $J_{\mathrm{C\alpha H}}$ and $J_{\mathrm{C\beta H}}$ of 106 and 145 Hz, respectively, serve as internal probes (experimental values of 111 and 157 Hz, respectively; see above). Also, at the same level of theory, the J_{CC} value computed for cyclopropane is 10.4 Hz, close to the experimental value of 12.4 Hz.[13] Overall the calculated J_{CC} values compare well with those recorded and computed for agostic cyclopropyl [$\mathrm{Tp^{Me2}NbX}(c\text{-}\mathrm{C_3H_5})$(MeCCMe)] niobium systems.[4a] Thus trends in coupling constants are fully reliable and furthermore there are only reasonably small shifts in absolute values. Most significantly, there is a clear relationship between distortion, C–C bond elongation and lowering of the corresponding J_{CC} value, with this parameter being a very sensitive probe of the distortion. Interactions between Y1 and the cyclopropyl group B on the one hand, and between Li1 and the cyclopropyl group A on the other hand, are characterized by a lengthening of the C–C bonds and by a considerable lowering of the J_{CC} value for the Cα–Cβ bonds facing the two metals, C4–C6 (1.53 Å, −4.1 Hz) for Y and C1–C3 (1.55 Å, −7.0 Hz) for Li. The other less elongated Cα–Cβ bonds, C1–C2 and C4–C5, also experience a lowering of the J_{CC} value (in part a result of the electropositive nature of Li and Y) albeit to a lesser extent. Computations on **2** and its "edge-coordinated" $\mathrm{Li^+}$-c-$\mathrm{C_3H_6}$ model have been reported but the corresponding J_{CC} values were neither recorded nor calculated.[1k] Therefore we have repeated the calculations on $\mathrm{Li^+}$-c-$\mathrm{C_3H_6}$ at the same level of theory used for **1** to provide direct comparisons. The results are very similar to those reported previously.[1k] The C–C bond "edge-coordinated" to $\mathrm{Li^+}$ has a bond length of 1.554 Å and a J_{CC} value of −0.27 Hz. These values differ from those obtained for the non-metal bridged C–C bonds (1.497 Å, 12.1 Hz). In both cases, the interactions of lithium with cyclopropyl, for **1**, or cyclopropane, for $\mathrm{Li^+}$-c-$\mathrm{C_3H_6}$, result in a distinctive lowering of J_{CC}.

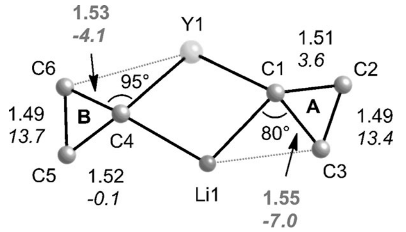

Figure 2. Core of the unsymmetrical optimized structure of **1** with relevant calculated parameters: Top value: CC bond length [Å]; Bottom value (italics): J_{CC} [Hz].

Having linked the structural distortions to a decrease in J_{CC} value, we sought to address the problem of the nature of the distortions, that is, the interactions themselves. Depending on metals, coordination spheres, and types of C–H bonds (particularly α- or β-CH in metal alkyl complexes), the interpretation of CH agostic distortions is still a matter of debate and embraces different situations. The agostic bonding can be described either as a direct CH–metal interaction, or as a relocation of M–C bonding electrons in the available low-lying orbitals located on the metal, on the alkyl ligand or on ancillary ligands.[14] We have carried out an NPA and NBO analysis[15] on complex **1** and on $\mathrm{Li^+}$-c-$\mathrm{C_3H_6}$, computing the natural charges (NC) and the bond delocalization. All the possible interactions between "filled" (donor) Lewis-type NBOs and "empty" (acceptor) non-Lewis NBOs have been considered and quantified according to their energetic contribution computed at the 2nd-order perturbation analysis. For Li^+-*c*-C_3H_6, the electrostatic nature of the interaction is confirmed with natural charges on Li and the edge carbons of 0.986 and −0.627 au, respectively. In addition, no significant second-order interaction between the σ-CC NBO and a vacant NBO on Li^+ is seen. In this case the second order interactions which allow internal benchmarking are those within the cyclopropyl group between the σ and σ*-CC NBOs which have an associated stabilization energy in the order of $30\,kJ\,mol^{-1}$. For complex **1**, strong donations ($55\,kJ\,mol^{-1}$) from the occupied Y1−C1 (NC −0.910 au) and Y1−C4 (NC −0.932 au) NBOs to a vacant Li^+ orbital (NC 0.911 au) point to an overall "ate" description $[Cp^*_2Y(c\text{-}C_3H_5)_2][Li(thf)]$. Most prominently, for the cyclopropyl group B, the NBO analysis further reveals a strong interaction ($67\,kJ\,mol^{-1}$) between the C4−C6 NBO and a Y-based d orbital, indicating the presence of an α-CC agostic interaction of marked covalent character. The natural charges for the two Cβ, C5 and C6, are identical at −0.476 au. On the contrary, no significant NBO second-order perturbation interaction is seen between C1−C3 and Li. The natural charge of C3 (−0.537 au) is significantly more negative than that of C5, C6, or C2 (−0.463 au), a very good indication that the α-CC agostic interaction of cyclopropyl group A with Li has a marked electrostatic character. Calculations on the symmetrical structure show that the "ate" formulation is preserved with C3 and C5 now exhibiting similar natural charges (−0.516 and −0.504 au, respectively). All other interactions linked to the distortions vanish.

A closer inspection of the NBO results reveals an additional relevant interaction. Indeed for cyclopropyl group B, a β-CH agostic interaction with Y appears to complement the α-CC agostic distortion just described. Although the two CH bonds on C6 have virtually the same length (C6-H6A, 1.091; C6-H6B, 1.087 Å; dihedral angles, Y-C4-C6-H: 35, −111°, respectively), the C6H6A bond closer to the Y-Cα-Cβ plane has a NBO that interacts quite strongly ($56\,kJ\,mol^{-1}$) with an empty d orbital on Y, indeed the same orbital involved in the interaction with the C4C6 NBO. The J_{C6H6A} (141 Hz) is marginally lower than J_{C6H6B} (149 Hz) and in addition the Cα−Cβ bond is elongated and not shortened as would be expected for a β-CH agostic interaction. This result suggests that the β-CH interaction may complement the more important α-CC agostic distortion. Actually there is no need to separate the two effects disclosed by the NBO analysis as only one unique interaction exists. Depending on the needs of the metal and the nature of the alkyl group, this situation would be a manifestation of the existence of a continuum between idealized "β-CH only" and "α-CC only" agostic structures as suggested previously[4b] but, to our knowledge, never observed before.

Experimental Section

In an argon-filled glove box, $[Cp^*_2YCl(thf)]$ (500 mg, 1.07 mmol) was dissolved in diethyloxyde (15 mL). Solid Li-*c*-C_3H_5 (320 mg, 2.20 mmol) was added slowly at room temperature to the stirred solution. A white precipitate appeared immediately. The slurry was stirred for 30 min and the volatiles were removed under reduced pressure. The residue was extracted with toluene (3 × 10 mL). A yellow residue was obtained after filtration and evaporation of the filtrate to dryness under vacuum. A minimum of pentane was added to give a solution which was cooled to −40 °C overnight to yield white crystals of **1** (420 mg, 0.80 mmol, 75 %). ^1H NMR ([D_8]toluene, 273 K, 500.3 MHz): $\delta = 3.27$ (m, 4H, OCH_2), 2.05 (s, 30H,C_5Me_5), 1.20 (m, 4H, $OCH_2\mathit{CH}_2$), 0.74 (dt, 4H, $J_{HH} = 10$, ≈1 Hz, $CH_{\beta'}$), 0.34 (dd, 4H, $J_{HH} = 9$, ≈1 Hz, CH_{β}), −1.50 ppm (tt, 2H, $J_{HH} = 10$, 9 Hz, YCH_{α}). ^{13}C NMR ([D_8]toluene, 273 K, 125.8 MHz): $\delta = 114.7$ (s, C_5Me_5), 68.2 (t, $J_{CH} = 146$ Hz, $O\mathit{C}H_2$), 25.2 (t, $J_{CH} = 132$ Hz, $OCH_2\mathit{C}H_2$), 11.4 (q, $J_{CH} = 124$ Hz, $C_5\mathit{Me}_5$), 10.2 (ddq, $J_{CH} = 111$, $J_{YC} = 44$, $J_{LiC} = 16$ Hz, $Y\mathit{C}HLi$), 5.4 ppm (t, $J_{CH} = 157$ Hz, $\mathit{C}H_2$). Elemental analysis (%) calcd for $C_{30}H_{48}LiOY$: C 69.2, H, 9.3; found: C 69.7, H 9.8 %.

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