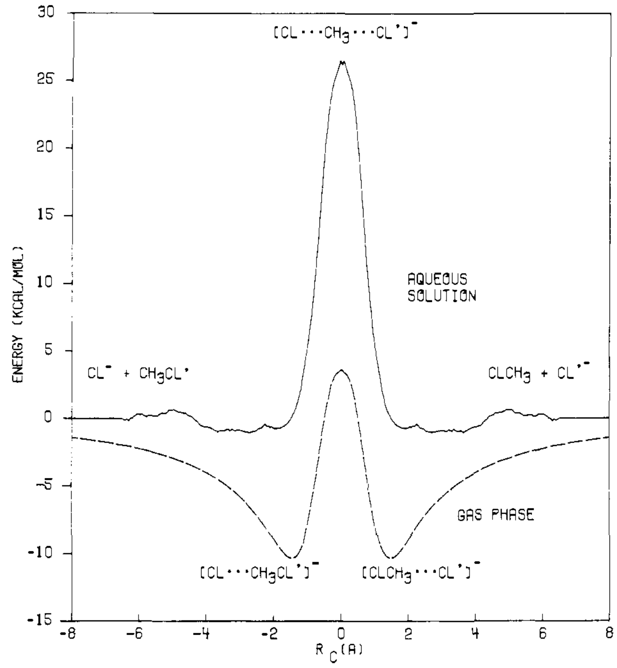

Figure 1. Calculated internal energies in the gas phase (dashed curve) and the potential of mean force in aqueous solution (solid curve) for the system $[ClCH_3Cl]^-$ as a function of the reaction coordinate, r_c (in angstroms).

The principal goal of the solution simulations was to obtain the potential of mean force, $w(r_c)$, which represents the relative free energy of the system as a function of r_c. The function is given by $-kT \ln g(r_c)$, where $g(r_c)$ is the probability of occurrence of each value of r_c. Precise computation of $g(r_c)$ requires the use of importance sampling methods.[13] Thus, simulations were carried out for six overlapping regions covering the entire reaction. The solute was constrained within limited ranges of r_c by imposing a harmonic force. Furthermore, an additional biasing function, $\exp(-25r_c^2)$, was included to enable sufficient sampling near the high-energy transition state. All calculated properties were normalized to remove the effects of this non-Boltzmann sampling.[13] The $g(r_c)$ from the different "windows" were spliced together at points of maximum overlap to form a single distribution from which $w(r_c)$ was obtained.

Monte Carlo simulations were executed for the solute cluster and 250 water molecules in the NPT ensemble at 25 °C and 1 atm. As in previous work, periodic boundary conditions and a preferential sampling algorithm to enhance solute-solvent statistics were employed.[14] Equilibration for 1000-2000K configurations was followed by averaging over 2600K configurations for each window. In all, this required ca. 50 h on a Cyber 205 computer.

The calculated potential of mean force (Figure 1, solid curve) is distinctly different from the gas-phase profile. Part of the difference is because the former is a free energy curve while the latter indicates the change in internal energy (for the hypothetical vibrationless system at 0 K). The minima in the gas phase would be less deep on the free energy scale because of the large negative entropy accompanying their formation from the separated species.[15] However, the entropy change from **1** to **2** is expected to be much smaller leaving the intrinsic barrier essentially unchanged.[16] Clearly, solvation leads to a flattening of the ion-dipole minima and to a large increase in the free energy of activation. Although putative minima exist, they are very shallow and would have negiligible influence on the reaction kinetics. Thus, the calculations firmly support the conventional view of a unimodal energy surface in aqueous solution. The calculated free energy of activation (26.3 ± 0.5 kcal/mol)[17] is in quantitative agreement with the experimental value (26.6 kcal/mol).[18] This along with the reasonable computed heat of solution for the reactants (88 ± 6 kcal/mol)[19] supports the viability of the computational model, though consideration of vibrational effects and the full multidimensional nature of the surface are desirable.

The sharp onset of the barrier at the position of the ion-dipole complex in solution is also interesting. It reveals that the desolvation of the ion up to this stage is compensated by the ion-dipole attraction. The enhanced barrier in solution then results primarily from less solute-solvent attraction for the charge delocalized transition state than for the separated reactants. Further structural and thermodynamic analyses of this system will be reported shortly.[20]

Registry No. CH_3Cl, 74-87-3; Cl^-, 16887-00-6.

Supplementary Material Available: Details of the intermolecular potential functions used in the simulations (4 pages). Ordering information is given on any current masthead page.

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(15) At 298 K, ΔH for the formation of the ion-dipole complex is -8.6 kcal/mol, while ΔG for the process is only -4.1 kcal/mol.[10]

(16) For the intrinsic barrier, ΔH and ΔG are implicitly assumed to be similar in ref 3b and 11.

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(20) Gratitude is expressed to the National Science Foundation for support.

Reactions of Coordinated Molecules. 40. Addition of a Pt-H Bond across Metal Acetylide C-C Triple Bonds: A Direct Route to Dinuclear μ-Vinylidene Complexes

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Recent theoretical calculations have supported the general opinion that the orbitals of the carbon-carbon triple bonds of metal acetylide ligands do not interact greatly with the valence orbitals of the metal atoms to which they are bonded.[2] Because M-H bonds are known to add to the carbon-carbon triple bonds of alkynes, a similar addition to metal acetylides might provide an interesting and general route to the preparation of homo- and heterodinuclear complexes. The first example of this type of reaction is reported below.

When the platinum phenylacetylide complex, *trans*-$Pt(PEt_3)_2(C{\equiv}CPh)_2$[3] (**1**), is treated with 1 equiv of $[$*trans*-$Pt(PEt_3)_2(H)(acetone)]BF_4$[4] (**2**), in acetone solution at 25 °C for 20 min,

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(1) (a) Department of Chemistry. (b) Department of Physics and Astronomy.

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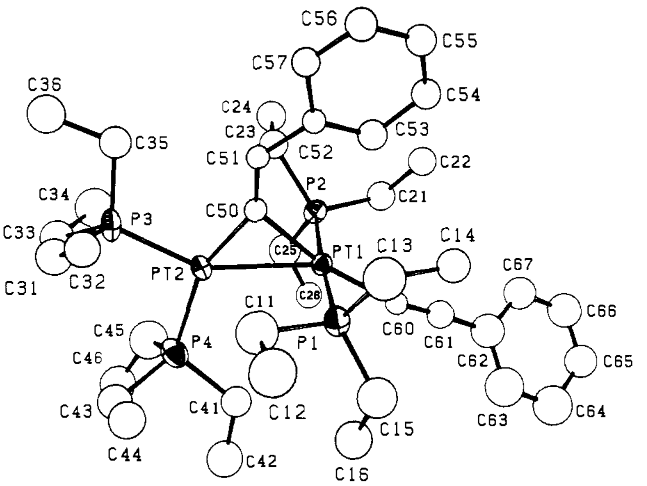
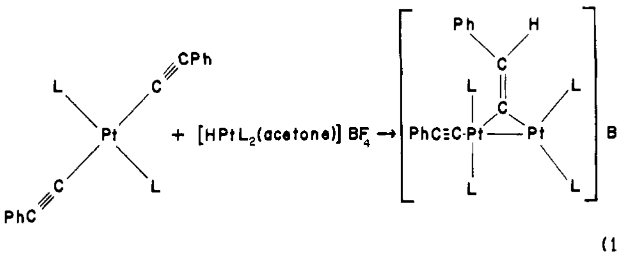


Figure 1. ORTEP view (thermal ellipsoids at 15% probability) of the cation of **3**. Some selected interatomic distances (Å) and angles (deg): Pt(1)–Pt(2), 2.750 (2); Pt(1)–P(1), 2.325 (5); Pt(1)–P(2), 2.329 (5); Pt(2)–P(3), 2.228 (8); Pt(2)–P(4), 2.351 (8); Pt(1)–C(60), 2.17 (2); C(60)–C(61), 1.14[15]; Pt(1)–C(50), 2.10 (2); Pt(2)–C(50), 1.93 (2); C(50)–C(51), 1.33 (3); P(1)–Pt(1)–P(2), 176.1 (3); C(50)–Pt(1)–C(60), 169.1 (7); P(1)–Pt(1)–C(60), 86.2 (4); P(2)–Pt(1)–C(60), 91.1 (4); P(3)–Pt(2)–P(4), 100.2 (3); Pt(1)–C(50)–Pt(2), 86.2 (7); C(50)–C(51)–C(52), 132 (2); Pt(1)–C(60)–C(61), 163[15]; C(60)–C(61)–C(62), 172[15]. Hydrogen atoms are omitted for clarity.

the diplatinum complex, $[Pt_2(\mu\text{-C}{=}CHPh)(C{\equiv}CPh)(PEt_3)_4]BF_4$[5] (**3**) is isolated as a red solid, as shown in eq 1.



(1)

1, L = PEt$_3$ **2**, L = PEt$_3$ **3**, L = PEt$_3$

Complex **3** contains a μ-vinylidene ligand formed by the 1,2-addition of the Pt-H bond of **2** across the C-C triple bond of one of the phenylacetylide ligands of **1**. This reaction represents a new method of preparing vinylidene ligands and one of the few direct and easily rationalized routes to μ-vinylidene complexes.[6-14]

The molecular structure of **3**, as determined by X-ray diffraction, confirms the structure as shown.[15] An ORTEP view of the cationic portion of **3** is shown in Figure 1. The Pt(1)-Pt(2) distance of 2.750 (2) Å represents a bona fide Pt-Pt single-bond length. The principal coordination geometry about Pt(1), excluding Pt(2), is nearly square [the atoms Pt(1), P(1), P(2), C(50), and C(60) are nearly coplanar having a maximum atomic deviation from coplanarity of 0.11 Å for Pt(1)], while the principal coordination geometry about Pt(2), excluding Pt(1), is described best as distorted "Y" or "T" shaped.[11a] The angle between the planes defined by [Pt(1), Pt(2), P(1), P(2)] and [Pt(1), Pt(2), P(3), P(4), C(50), C(60)] is 86.9°. A terminal phenylacetylide ligand is coordinated to Pt(1). The presence of a μ-phenylvinylidene ligand is also evident. The C(50)-C(51) distance of 1.33 (3) Å is as expected for a C-C double bond, and the overall structure of this ligand is consistent with that reported for $(\eta\text{-}C_5H_5)_2Mn_2(CO)_4(\mu\text{-C}{=}CHPh)$.[7g] Positive electron density amounting to 0.29e$^-$/Å^3 was located on electron density maps at the calculated position for the vinylidene proton bonded to C(51).

A proposed mechanism for the formation of **3** from **1** and **2** can be devised by analogy to the extensive mechanistic work reported by Clark for the reactions of **2** (and related complexes) with alkynes.[4,16] For the reaction shown in eq 1, a probable mechanism is the following: (1) loss of acetone from **2** upon formation of an η^2-alkyne complex with one of the phenyl acetylide ligands of **1**, (2) isomerization of this trans "alkyne" complex to the cis isomer, and (3) cis-1,2-addition of the Pt-H bond across the C-C triple bond with concomitant formation of the Pt-Pt bond giving **3**. The metal-metal bond formation presumably results from having the Pt atom of the phenyl acetylide complex act as an intramolecular Lewis base that donates an electron pair to the 3-coordinate cationic platinum atom produced after the 1,2-addition.

Two important consequences of this mechanism that are evident from the structure of **3** are (1) the Pt-H bond adds to the C-C triple bond to give a cis-addition product and (2) the formation of the Pt-Pt bond locks in the cis phosphine coordination geometry at the Pt atom which added to the C-C triple bond (this isomer is the one expected for the kinetic product after addition[16c]). Furthermore, addition of the hydrogen atom of **2** to the phenyl-substituted acetylide carbon atom would result if the Pt-H bond polarity is $^{\delta-}$Pt-H$^{\delta+}$ (as appears to be the general observation[16a]), because electrophiles prefer to attack at C$_\beta$ of acetylide ligands.[7c,8]

The formation of **3** represents a direct, rational route for preparing dinuclear clusters. This synthetic method corresponds

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(4) Complex **2** is prepared by a procedure analogous to that used in preparing the PF$_6^-$ salt; see: Clark, H. C.; Fiess, P. L.; Wong,, C. S. *Can. J. Chem.* **1977**, *55*, 177–188.

(5) Complex **3** is isolated in 43% yield by crystallization from a THF/hexane solution at −15 °C. Detailed characterization data: mp 134–137 °C dec; IR (CH$_2$Cl$_2$) ν (C≡C) 2100 (w) cm^{-1}; ^{1}H NMR (CD$_2$Cl$_2$) δ 1.00, 1.08, 1.16, 1.24, 1.33 ("quintet", 36, CH$_3$, J_{obsd} = 7.5 Hz), 1.98 (m, 24, CH$_2$), 7.28, 7.88 (complex m, 11, 2Ph + CH?); ^{13}C NMR (CD$_2$Cl$_2$) δ 8.3 (q, CH$_3$, J = 124 Hz), 16.9, 17.8 18.2, 18.9, 19.2 ("t", CH$_2$, $J \sim$ 132 Hz), 124.9, 126.1, 127.0, 128.9, 130.7 ("d", CH, $J \sim$ 161 Hz), 140.3 (s, C, Ph), 142.0 (s, C, Ph). The μ-vinylidene quarternary donor carbon and the two acetylide quarternary carbons were not observed in the ^{13}C NMR spectrum of **3** for an ~0.2 M solution after 28 000 pulses. Anal. Calcd for $C_{40}H_{71}BF_4P_4Pt_2$: C, 41.66; H, 6.15; F, 6.67; P, 10.74. Found: C, 39.98; H, 6.23; F, 6.63; P, 10.76.

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(15) Crystallographic data are summarized below: Space group $P2_1/c$, with a = 13.130 (3) Å, b = 15.792 (4) Å, c = 24.958 (5) Å, β = 113.07 (2)° (λ = .70926 Å), and Z = 4. Data were collected on an orange-red crystal measuring *ca.* 0.35 mm × 0.26 mm × 0.22 mm on a four-circle automated Picker diffractometer using Mo Kα radiation. Data were acquired by 2θ step scans out to 50° 2θ. Of the total 8436 observed unique reflections, only 4444 with intensity $>2\sigma(F^2)$ were used in the refinement. An absorption correction was applied to the data. The structure was solved by the Patterson method, and final full-matrix least-squares refinement gave R = 6.9% and R_w = 7.7%. All non-hydrogen atoms were included in the refinements, although some atomic positions [C(43)–C(46) and C(61)–C(67)] were fixed in the final refinement due to a slight disorder. Details of these procedures are included in the supplementary material.

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to a new type of bridge-assisted, addition reaction for cluster synthesis.[17] Because of the possible variation of metal acetylide[2b] (and hydride) reagents, this approach might also afford heterodinuclear clusters. In addition, complex **2** (and related hydrides) might add to other types of unsaturated bonds to give di- and polynuclear clusters or to other types of unsaturated bonds to give di- and polynuclear clusters having different types of bridging groups. The investigations of these possibilities as well as the reaction chemistry of complex **3** are being pursued.[18]

Acknowledgment. C.M.L. thanks the National Science Foundation (Grant CHE-8106140), the donors of the Petroleum Research Fund, administered by the American Chemical Society, and the University Research Council of Vanderbilt University for support of this research. P.G.L. acknowledges support from NIH BRSG (Grant RR 07089-13). D.A. thanks Dr. Thomas M. Harris for assistance in acquiring NMR spectra.

Supplementary Material Available: A complete listing of final positional and thermal parameters, final observed and calculated structure factors, selected interatomic distances and angles, and selected least-squares planes data, and a brief description of the details of the solution and refinement (33 pages). Ordering information is given on any current masthead page.

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(18) In separate but analogous reactions, complex 2 reacts with acetylide complexes of Ni(II), Pd(II), Ir(I), and (η-C_5H_5)(OC)$_2$Fe(C≡CPh) to give distinctive color changes like that observed for eq 1. Preliminary spectroscopic data are consistent with the formation of heterodinuclear complexes that are analogous to 3.

Structural Rearrangements in the Two-Electron Oxidations of Dimetal Cyclooctatetraene Compounds. Structure of the 34-Electron "Triple-Decker" Dication†

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A study of the two-electron oxidation[2] of the pseudo-triple-decker dicobalt compound (CpCo)$_2$(cot) (Cp = η^5-C_5H_5; cot = η^8-cyclooctatetraene) (**1**) suggested that the dication might have a flattened cyclooctatetraene ring since this would give a delocalized 34-electron[3] triple-decker structure. **1**$^{2+}$ was too unstable to be structurally characterized, but we now report the isolation of analogous dications in which the central C_8H_8 ring has two planar four-carbon fragments connected by a minor twist and the metal atoms are slipped to the sides of the C_8 ligand. Voltammetry experiments suggest that electron-transfer-induced movement of the two metal atoms over the C_8 ligand is much more facile for cobalt than for rhodium.

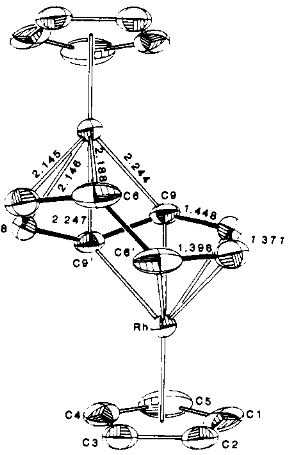
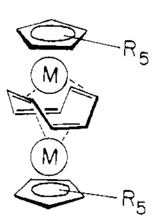


Figure 1. Thermal ellipsoid (40% probability) diagram and label scheme for [CpRh(cot)RhCp](PF$_6$)$_2$. A crystallographic 2-fold axis is perpendicular to the drawing and passes through the midpoints of the C6–C6' and C9–C9' bonds. Important bond distances not given on the figure are C6–C6' 1.501, C9–C9' 1.500, Rh–centroid (Cp) 1.823 Å. Estimated standard deviations on Rh–C bonds, 0.006; on C–C bonds, 0.01.

Cyclic voltammetric (CV) and controlled potential coulometric experiments on **2**[4] and the dirhodium complex[5] **3** show that both



2, M = Co; R = CH_3
3, M = Rh; R = H

undergo chemically reversible two-electron oxidations in which the electron transfer is either quasi-reversible (for **2**) or irreversible (for **3**). The (η^5-C_5Me_5)Co$_2$ complex **2** undergoes oxidation at a $E°$ potential (−0.24 V vs. SCE) 140 mV lower than **1**. Unlike **1**, for which a nearly Nernstian CV peak separation (ΔE_p) as low as 32 mV was obtained,[2] the smallest peak separation found for **2** in dichloromethane was 61 mV (v = 16 mV/s). Moreover, the peak potentials are scan-rate and temperature dependent, giving a ΔE_p of ca. 380 mV (v = 160 mV/s) at −40 °C.

Even larger CV peak separations are observed for the dirhodium complex **3** (E_{pa} = +0.47, E_{pc} = −0.17 V at v = 200 mV/s in 1:1 acetone/dichloromethane and E_{pa} = +0.55, E_{pc} = −0.14 V in dichloromethane). Bulk electrolysis of **3** in dichloromethane at +0.9 V caused the precipitation of the dicationic complex. **3**$^{2+}$ was also obtained by chemical oxidation of **3** with 2 mol equiv of AgPF$_6$ in CH$_2$Cl$_2$. The product precipitated as dark red crystals and was separated from silver by dissolution in nitromethane, filtration, and crystallization by addition of benzene. The structure **3**$^{2+}$(PF$_6$)$_2$ was determined by single-crystal X-ray diffraction studies. The key feature of the structure (Figure 1) is that the metal atoms are slipped to the side of the C_8 ring, which has two nearly planar C_4 fragments twisted by 34.8°. Each Rh is formally bonded to five carbons, requiring two carbons (C9 and C9') to be bridging between the metals to give a 34-electron structure. The ^{1}H NMR spectrum of **3**$^{2+}$ at reduced temperatures suggests that it retains this structure in solution (four sets of resonances from the C_8 ring).[7]

[†] Structural Consequences of Electron-Transfer Reactions 9. Part 8: *J. Am. Chem. Soc.* **1983**, *105*, 1772.

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(6) [(CpRh)$_2$(cot)](PF$_6$)$_2$ crystallizes in the orthorhombic, noncentrosymmetric group $P2_12_12$: a = 14.073 (3) Å, b = 11.353 (2) Å, c = 6.748 (1) Å, V = 1078.1 (4) Å^3, d(calcd) = 2.25 g cm^{-3}, Z = 2 (asymmetric unit consists of one Cp ring, one Rh atom, and one half of a cot ring). Refinement converged at R_F = 0.0299, R_{wF} = 0.0346, and GOF = 1.305.

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