of Cp*(PMe$_3$)Ir(SH)H (**8**), Cp*(PMe$_3$)Ir(SMe)H (**9**), and Cp*(PMe$_3$)Ir(S-tBu)H (**10**), respectively. All three complexes can be isolated in pure form and fully characterized and show characteristic hydride doublets at high field in the ^{1}H NMR spectrum and iridium hydride stretches in the infrared spectrum.[13] The thiol hydride **8** also shows a doublet of doublets at δ −2.18 ppm (J_{P-H} = 4.6 Hz, J_{H-H} = 1.8 Hz) for the thiol proton in the ^{1}H NMR spectrum and a weak S–H stretch at 2524 cm^{-1} in the infrared spectrum.

Preliminary reactivity studies on some of these complexes have established that reactions with small molecules may take place at either the S–H bond or the metal center, depending on the structure of the complex and reagent. For example, metalla dithiol **4** reacts with solvent acetone in the presence of catalytic acid (HCl or aniline hydrochloride) to give a single new complex that exhibits inequivalent methyl groups at δ 2.02 and 1.81 ppm in the ^{1}H NMR spectrum. This, in addition to other spectroscopic and analytical data, led us to assign the structure of this product as Cp*(PMe$_3$)Ir(SCMe$_2$S) (**11**), to our knowledge the first 2,4-dithiametallacyclobutane complex.[14] An X-ray diffraction study confirms this assignment; once again, an ORTEP diagram is included in Scheme I. Treatment of **11** with H$_2$S at 80 °C for 24 h quantitatively regenerates the dithiol **4** and gives 2,2-propanedithiol[15] in 25% yield (^{1}H NMR).

In reactivity studies on thiol hydride complex **8**, insertion of carbon disulfide (CS$_2$) has been found to take place into the metal–hydrogen bond, rather than the metal–heteroatom bond as occurs in the PPh$_3$-substituted analogue of the ethoxy hydride **7**.[11] Thus, **8** reacts with 1 equiv of CS$_2$ in benzene to give the dithioformate complex **12** as the only product (^{1}H NMR).[16] In addition to the resonances attributable to the Cp* and PMe$_3$ ligands, a new thiol doublet (δ −2.01, J_{P-H} = 4.8 Hz) and a singlet integrating as one proton (δ 11.97) are seen in the ^{1}H NMR spectrum. Complex **12** is unstable and slowly decomposes to an as yet uncharacterized species.

In summary, mononuclear iridium complexes containing M–S bonds (some of which also possess other potentially reactive σ-bound ligands, such as hydrides) can be prepared in a straightforward way. These complexes are very robust, although they exhibit at least some reactivity toward small organic molecules; reaction may take place at either the metal or sulfur atom, depending on the structure of the molecule involved. Further investigations are under way aimed at understanding the physical principles that guide this choice.

Acknowledgment. We are grateful to the National Science Foundation for financial support of this work through Grant No. CHE-8722801 and to Dr. F. J. Hollander, director of the Berkeley X-ray diffraction facility (CHEXRAY), for carrying out the crystal structure determinations reported here. We also thank the Johnson-Matthey Co. for a generous loan of iridium trichloride.

Supplementary Material Available: Spectroscopic and analytical data for complexes **2–12** and details of the structure determinations for complexes **4**, **10**, and **11**, including experimental description, ORTEP drawings showing full atomic numbering, crystal and data collection parameters, general temperature factor expressions (*B*'s), root-mean-square amplitudes, positional parameters and their estimated standard deviations, and intramolecular distances and angles (37 pages); tables of observed and calculated structure factors for **4** and **10** (31 pages). Ordering information is given on any current masthead page.

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(13) Complex **8**: ^{1}H NMR (C$_6$D$_6$) δ_{Ir-H} −16.01 (dd, *J* = 36.7, 1.8 Hz, 1 H); IR (KBr pellet) ν_{Ir-H} 2093 cm^{-1}. Complex **9**: ^{1}H NMR (C$_6$D$_6$) δ_{Ir-H} −16.58 (d, *J* = 36.4 Hz, 1 H); IR (KBr pellet) ν_{Ir-H} 2114 cm^{-1}. Complex **10**: ^{1}H NMR (C$_6$D$_6$) δ_{Ir-H} −16.47 (d, *J* = 35.1 Hz, 1 H); IR (KBr pellet) ν_{Ir-H} 2096 cm^{-1}.

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Rhodium(II) Complex with a Highly Reactive Rhodium–Rhodium Bond: Insertion of Dioxygen and Nitrosobenzene

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We report the synthesis and some preliminary reaction chemistry of [Cp*Rh(μ-Cl)]$_2$ (**1**) (Cp* = C$_5$Me$_5$), a Rh(II) dimer with a reactive Rh–Rh bond.[1] While many Rh(II) complexes containing Rh–Rh bonds have been reported in the literature,[2] including several analogues of **1**,[3] the high reactivity of the Rh–Rh bond in **1** is remarkable and has allowed us to prepare several unusual products. The observed chemistry is outlined in Scheme I.

Complex **1** is produced by the reduction of [Cp*Rh(μ-Cl)Cl]$_2$[4] in CH$_2$Cl$_2$ with excess Na/Hg (0.4%).[5] Blue-black crystals of **1** are isolated in yields ranging from 65 to 75% by the addition of hexane to the filtered and reduced solutions and by cooling to −40 °C. An ORTEP diagram[6] of **1** is included in Scheme I. Complex **1** is soluble in aromatic solvents and slightly soluble in saturated hydrocarbons and Et$_2$O. Solubility is high in CH$_2$Cl$_2$; however, there is a slow reaction at ambient temperatures, and after solutions stand for 12 h, the starting complex, [Cp*Rh(μ-Cl)Cl]$_2$, is cleanly produced. A more rapid reaction occurs in CHCl$_3$, again producing mostly [Cp*Rh(μ-Cl)Cl]$_2$. Solutions are highly air sensitive, and the reaction of **1** with dry O$_2$ was investigated.

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(1) Presented at the 196th National Meeting of the American Chemical Society, Los Angeles, CA, Sept 1988; Inorganic Abstract 159.

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(5) ^{1}H NMR (C$_6$D$_6$, 90 MHz, 25 °C): 1.59 ppm.

(6) Crystal data for **1**, C$_{20}$H$_{30}$Cl$_2$Rh$_2$ (FW = 547.18): monoclinic (*C*2/*c*), a = 33.068 (8) Å, b = 13.173 (3) Å, c = 16.810 (4) Å, β = 117.77 (2)°, V = 6479.4 Å^3, Z = 12. Data (Mo Kα) were collected on a CAD4 diffractometer. The structure was solved by direct methods (MULTAN) and refined by full-matrix least-squares refinement (SDP) to R = 0.040 and R_w = 0.047 for 2326 absorption-corrected observations with $F_o^2 > 2\sigma(F_o^2)$ and 325 variables. Two independent molecules are present, one on a 2-fold site and the other on a general position (molecule shown in Scheme I). Selected bond distances and angles (2-fold site molecule in parentheses): Rh–Rh, 2.617 (1) (2.628 (1)); Rh–Cl, 2.411 (4) and 2.408 (3) (2.392 (3) and 2.393 (5)); Rh–Cl–Rh, 65.74 (8) and 65.92 (9) (66.6 (1)). Details will be provided in a forthcoming full paper.

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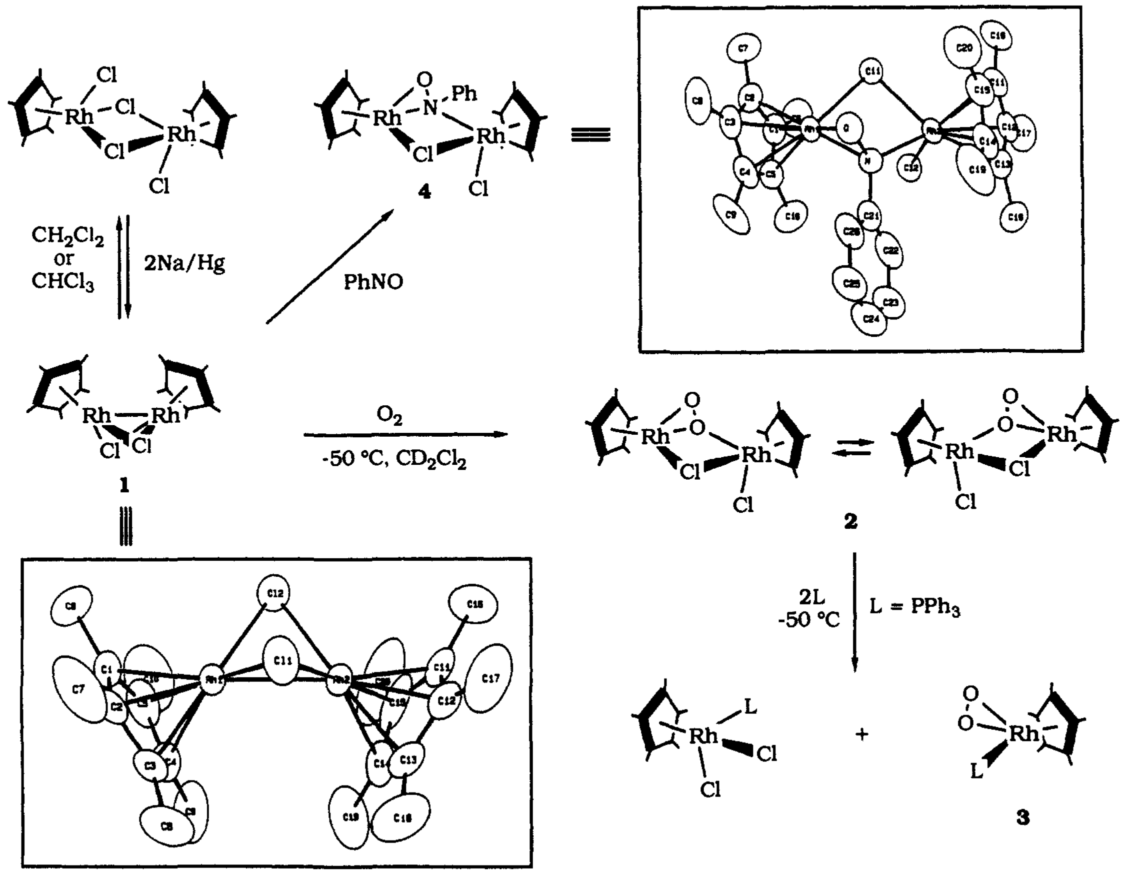
Scheme I



The injection of 1 equiv or more of O_2 into a deep blue CH_2Cl_2 solution of **1** at ca. −50 °C rapidly produces a red solution. Variable-temperature ^{1}H NMR spectroscopy shows the presence of a single new fluxional product formulated as $(Cp^*RhCl)_2O_2$ (**2**).[7] At −80 °C, two closely spaced Cp* resonances are observed.[8] As the temperature is increased, the two resonances collapse and coalesce and grow into a single resonance at a chemical shift midway between the two low-temperature peaks ($\Delta G^* \sim 50$ kJ/mol, $T_c \sim -45$ °C). The process is reversible provided that the temperature is kept below ca. −15 °C. Above this temperature, slow decomposition of the complex is evident by a darkening of the solution and the growth of several new Cp* peaks in the ^{1}H NMR spectra. Solid samples are much more stable and are obtained by solvent removal in vacuo at low temperature. IR spectroscopy (mineral oil mull) shows the presence of the O_2 ligand as the only new band at 812 cm^{-1}. The expected isotopic shift to 768 cm^{-1} is observed with $^{18}O_2$ substitution. A likely structure for **2**, consistent with the spectroscopic data, the reactivity (see below), and related structures, is shown in Scheme I. The $\mu,\eta^1:\eta^2$ bonding mode of the O_2 ligand has been observed only one other time in the closely related complex $[RhCl(PPh_3)_2(\mu,\eta^1:\eta^2\text{-}O_2)]_2$ (ν_{O-O} = 845 cm^{-1}).[9,10]

Support for the proposed structure of **2** is found from its reaction with PPh_3. A green solution initially forms but rapidly reverts to red. ^{1}H and ^{31}P NMR indicate the formation of two products. One of these is readily identified as the known complex $Cp^*RhCl_2(PPh_3)$.[4] The other product, unstable above ca. 0 °C, has very similar spectroscopic properties and can only be $Cp^*Rh(O_2)(PPh_3)$ (**3**).[11] This cleavage by PPh_3 is similar to that observed for $[Cp^*Rh(\mu\text{-}Cl)Cl]_2$, which is structurally and electronically[12] related to **2** (see Scheme I).

Nitrosobenzene, like dioxygen, gives a red product, $(Cp^*RhCl)_2(PhNO)$ (**4**), when added to solutions of **1**. However, unlike **2**, **4** is stable in solution at ambient temperatures. Crystals were obtained, and an ORTEP diagram[13] of **4** is shown in Scheme I. Complex **4**, proposed to have the same structure as **2**, is not fluxional[14] at ambient temperatures and gives a pair of Cp* peaks.[15] A related complex, $[CpCo(\mu,\eta^1:\eta^2\text{-}PhNO)]_2$, has been structurally characterized.[16]

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(7) Rh(II) and Ir(II) porphyrin dimers also insert O_2. See: Wayland, B. B.; Newman, A. R. *Inorg. Chem.* **1981**, *20*, 3093–3097. Collman, J. P.; Kim, K. *J. Am. Chem. Soc.* **1986**, *108*, 7847–7849.

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(10) $[(PPh_3)_2ClRh(\mu,\eta^1:\eta^2\text{-}O_2)]_2$ is actually isoelectronic with **2** if $(PPh_3)_2Cl$ is replaced with Cp* and if one O_2, considered as a peroxide, is replaced with one terminal and one bridging chloride.

(11) ^{1}H NMR (CD_2Cl_2, 90 MHz, −40 °C, TMS ref): 1.56 (d, J_{HP} = 2.4 Hz, Cp*) ppm, also phenyl peaks. ^{31}P NMR (CD_2Cl_2, 36 MHz, −40 °C, external H_3PO_4 ref): 31.0 (d, J_{PRh} = 184 Hz) ppm.

(12) In fact, they may be considered isoelectronic by replacement of a terminal and one bridging chloride with the $\mu,\eta^1:\eta^2\text{-}O_2$ (peroxide).

(13) Crystal data for **4**, $C_{26}H_{35}Cl_2NORh_2$ (FW = 654.29): triclinic ($P\bar{1}$), a = 9.290 (3) Å, b = 17.830 (3) Å, c = 8.941 (3) Å, α = 92.60 (2)°, β = 110.87 (3)°, γ = 104.36 (2)°, V = 1325.9 Å^3, Z = 2. Data (Mo Kα) were collected on a CAD4 diffractometer. The structure was solved by Patterson methods (SHELXS-86, Sheldrick, G. M. In *Crystallographic Computing 3*; Sheldrick, G. M., Kruger, C., Godard, R., Eds.; Oxford University Press: London, 1985; pp 175–189) and refined by full-matrix least-squares refinement (SDP) to R = 0.045 and R_w = 0.057 for 3570 absorption-corrected observations with $F_o^2 > 2\sigma(F_o^2)$ and 316 variables. The structure is disordered and was modeled with two orientations of the molecule. The major orientation (65%, shown in Scheme I) has O bonded to Rh1 and Cl2 bonded to Rh2. This is reversed in the minor orientation (35%, supplementary material). Selected bond distances and angles (minor orientation in parentheses): Rh1–Cl1, 2.456 (1); Rh2–Cl1, 2.457 (1); Rh2(1)–Cl2; 2.449 (2) (2.494 (4)); Rh1–N, 2.016 (4) (2.10 (1)); Rh2–N, 2.083 (6) (2.01 (1)); Rh1(2)–O, 2.020 (5) (2.01 (1)); N–O, 1.429 (9) (1.37 (2)); Rh1–Cl1–Rh2, 86.49 (5); Rh1–N–Rh2, 110.3 (3) (108.1 (6)); Rh1(2)–N–O; 69.4 (3) (68.4 (6)); Rh1(2)–O–N, 69.1 (3) (72.2 (7)). Details will be provided in a forthcoming full paper.

(14) The fluxional process observed for **2** probably involves a $\mu,\eta^1:\eta^1\text{-}O_2$. A similar process for **4** would not exchange the Cp* ligands if the nitrogen is the preferred bridging atom of the PhNO ligand.

(15) Anal. Calcd (found) for $C_{26}H_{35}Cl_2NORh_2$: C, 47.73 (48.15); H, 5.39 (5.53); N, 2.14 (2.08). ^{1}H NMR (C_6D_6, 90 MHz, 25 °C, TMS ref): 8.58, 7.50, 7.23, and 6.88 (m, Ph); 1.38 and 1.34 (s, Cp*1 and Cp*2) ppm.

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These preliminary results suggest that the reaction chemistry of **1** can be viewed as the disproprotionation of two Rh(II) centers into the Rh(III) fragment Cp*$RhCl_2$ and the Rh(I) fragment Cp*Rh. This latter species looks particularly interesting in view of the highly reactive nature of the Cp*ML (M = Rh and Ir, L = PMe_3 or CO) fragments.[17] Further chemistry with these complexes and the utilization of **1** as a source of Cp*Rh are under investigation and will be the subjects of a forthcoming full paper.

Acknowledgment. The support of this work by the Division of Chemical Sciences, Office of Basic Energy Sciences, Office of Energy Research, U.S. Department of Energy (DE-FG02-88ER13880), ARCO Chemical, and Johnson Matthey (a loan of $RhCl_3$) is gratefully acknowledged. The National Science Foundation provided a portion of the funds for the purchase of the X-ray (CHE-7820347) and NMR (PCM-8115599) equipment.

Supplementary Material Available: ORTEP diagrams of the second molecule of **1** (twofold site) and the minor orientation of **4** and tables of positional and thermal parameters for **1** and **4** (4 pages). Ordering information is given on any current masthead page.

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$^2B_2$: The Ground State of the Hexamethyl(Dewar benzene) Radical Cation. Time-Resolved Fluorescence Detected Magnetic Resonance[†]

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The hexamethyl(Dewar benzene) radical cation ($HMDB^{\bullet+}$) has attracted considerable interest as an assumed intermediate in the photosensitized conversion of HMDB to hexamethylbenzene (HMB).[1,2] Recently, the electronic structure of $HMDB^{\bullet+}$ has been studied extensively, but the assignment of its ground state is still in doubt. The two highest molecular orbitals of HMDB are the b_2 and a_1 orbitals.[2,3] In the $^2B_2$ state of $HMDB^{\bullet+}$, spin density is confined in the bonds between the two pairs of olefinic carbons, while in the $^2A_1$ state of $HMDB^{\bullet+}$, spin density is localized in the bond between the two transannular carbons. Ab initio calculations by Roth et al.[2] predict that $^2B_2$ is the ground state and is 8 kcal/mol more stable than the $^2A_1$ state. But a MINDO/3 calculation by Bews and Glidewell[4] predicts that $^2A_1$ has the minimum-energy geometry. In a CIDNP study of photoreactions of HMDB with excited (triplet) electron acceptors, Roth et al.[2] presented indirect evidence for the formation of both $^2B_2$ and $^2A_1$ states generated by competing pathways, and the ground state was not assigned experimentally. More recently, Rhodes[5] reported EPR studies of $HMDB^{\bullet+}$ in freon matrices. He observed $HMDB^{\bullet+}$ in the $^2B_2$ state in $CFCl_3$ and in the $^2A_1$ state in $CF_2ClCFCl_2$ and suggested that the ground state of $HMDB^{\bullet+}$ is $^2A_1$. We have studied $HMDB^{\bullet+}$ in freon matrices but failed to confirm the $^2A_1$ $HMDB^{\bullet+}$ in $CF_2ClCFCl_2$.[6] Recently, other workers have also reexamined this system.[7] In view of the strong interactions of solid freon matrices that can change the electronic state of the solute radical cations,[5,8] it is useful to examine $HMDB^{\bullet+}$ in nonpolar solvents. Here, we report our study of $HMDB^{\bullet+}$ in liquid alkanes by time-resolved fluorescence detected magnetic resonance (FDMR).[9] We conclude that the ground state of $HMDB^{\bullet+}$ is $^2B_2$ rather than $^2A_1$.

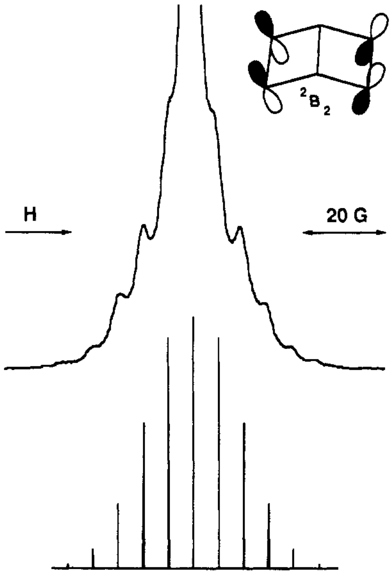

Figure 1. FDMR spectrum observed at 205 K in cyclopentane containing 10^{-2} M hexamethyl(Dewar benzene) and 10^{-4} M perdeuterated anthracene.

$HMDB^{\bullet+}$ was produced in a solution of 10^{-2} M HMDB and 10^{-4} M perdeuterated anthracene (A) in cyclopentane by using pulsed electron beam irradiation. Our observations were carried out at temperatures between 205 and 245 K. Electron beam pulses with a width of 12 ns were generated by a 3-MeV electron Van de Graaff accelerator at a repetition rate of 720 pulses/s. The ionizing radiation creates singlet-phased radical ion pairs in cyclopentane (RH) consisting of a cyclopentane radical cation and an electron (eq 1). Most of the ion pairs recombine geminately in a few picoseconds (eq 2). A few percent of the cyclopentane (gas-phase ionization potential (IP) = 10.5 eV)[10] cations are scavenged by transferring positive charge to HMDB (IP = 7.8 eV)[3] solute to form $HMDB^{\bullet+}$ (eq 3), while some of the electrons are converted to the scintillator radical anion ($A^{\bullet-}$) (eq 4). The resulting radical ion pairs consisting of $HMDB^{\bullet+}$ and $A^{\bullet-}$ are still spin-correlated. Upon recombination, an excited singlet state ($^1A^*$) is generated (eq 5), resulting in fluorescence (A*) which is detected.

$$RH \xrightarrow{e^-} RH^{\bullet+} + e^- \qquad (1)$$

$$RH^{\bullet+} + e^- \rightarrow RH^* \qquad (2)$$

$$RH^{\bullet+} + HMDB \rightarrow RH + HMDB^{\bullet+} \qquad (3)$$

$$e^- + A \rightarrow A^{\bullet-} \qquad (4)$$

$$HMDB^{\bullet+} + A^{\bullet-} \rightarrow HMDB + {}^1A^* \qquad (5)$$

[†] Work performed under the auspices of the Office of Basic Energy Science, Division of Chemical Science, US-DOE, under contract number W-31-109-ENG-38.

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