

apparently lower initial rate may be attributable to the time necessary for the system to reach an equilibrium in which CO is partitioned between ligand, solution, and atmospheric CO.

The above observations in conjunction with our studies of the photochemical system suggest a mechanism of the type shown in Scheme I.

Scheme I is undoubtedly a highly simplified representation of a very complex system. For example, the dimerization of RhL_2Cl or its addition to olefin may be expected²⁰ (followed in either case by a reaction with CO to regenerate **1**). Addition of RhL_2Cl to olefin can be invoked as one possible explanation for the observation of saturation in norbornene concentration above ca. 0.3 M. We also note that the H_2/CO substitution reactions may proceed via an indirect route. The observed inhibition by added

(20) Our photochemical studies indicate that reaction of RhL_2Cl with CO is not competitive with its reaction with cyclooctane under $P_{\text{CO}} < \text{ca. } 50 \text{ Torr}$. The first-order rate dependence on P_{H_2} of reaction 3 indicates that the addition of H_2 to RhL_2Cl is also not competitive with the reaction with alkane. This is an unsurprising conclusion given that (a) the concentration of H_2 is ca. 1/1000 that of C-H bonds even under 1500 psi of H_2 and (b) on the basis of Ford's flash photolysis studies^{9,15} we would expect the reaction of RhL_2Cl with H_2 to be much slower than its reaction with olefin. For a detailed description of the chemistry of $\text{Rh}(\text{PPh}_3)_2\text{Cl}$, which is very relevant to this work, see refs 15 and 16.

PMe_3 is consistent with our photokinetic studies, which indicate that H_2 elimination from $\text{RhL}_2\text{Cl}(\text{CO})\text{H}_2$ proceeds via phosphine loss;²¹ by the principle of microscopic reversibility, H_2 addition to **1** should also involve prior loss of phosphine. This is well preceded by studies of H_2 addition to $\text{Rh}(\text{PPh}_3)_3\text{Cl}$.¹⁶

In summary, an efficient catalytic system for alkane dehydrogenation is reported which requires an added hydrogen atmosphere. Our explanation for this almost paradoxical observation is that the thermodynamic barrier to CO loss from **1** is overcome by its being coupled with alkene hydrogenation. This affords the reactive fragment RhL_2Cl , which thermally dehydrogenates alkanes in accord with studies of its photocatalytic behavior. Further studies of mechanism and selectivity are in progress as are attempts to develop more effective routes to the fragment RhL_2Cl .

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(21) Maguire, J. A.; Goldman, A. S., to be submitted for publication.

Additions and Corrections

Tethered Oligonucleotide Probes. A Strategy for the Recognition of Structured RNA [*J. Am. Chem. Soc.* 1991, 113, 5109-5111].

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Pages 5110 and 5111: The sequence of one of the oligonucleotides used in this study was reported incorrectly. The sequence written as AAAUUUUGGA in the caption to Figure 2 and on lines 36-37 of page 5111 should read UCGGGCU-UUGGG.

Computer Software Reviews

ESR, ESR II, ESR^a and ESR^a II. Calleo Scientific Software Publishers: 1300 Miramont Drive, Fort Collins, CO 80524. List prices: \$175.00, \$245.00, \$225.00, and \$295.00.

ESR and ESR II are first-order isotropic electron spin resonance spectral simulation programs designed for the Apple MacIntosh family of computers. ESR II is a variant of ESR which takes advantage of the math coprocessor in the MacIntosh II computers (with considerable timesavings). With these programs, users can simulate spectra for systems with one unpaired electron containing up to 24 nuclear spin sets, and for $\sum I$ up to 90 for each set. In addition to varying hyperfine coupling constants, nuclear spin, and the number of equivalent nuclei, the user can define nuclear abundances, g value, spectrometer frequency, line width, spectrum width, plot resolution, and plot dimensions. All naturally occurring nuclei for the first 103 elements are included.

ESR^a and ESR^a II are companion programs similar to those described above except that they can additionally simulate first-order anisotropic spectra with anisotropic g or A tensors or both, as well as spectra with Gaussian or Lorentzian line shapes. Spectra generated by all four programs can be displayed and plotted in derivative and absorption modes, and with inverted phase and sweep. The software is not copy protected.

Those familiar with the standard Mac user-interface will find ESR and ESR^a easy to learn and use. In this regard, the programs seem ideal

for instructional purposes. They may be somewhat less ideal, however, for users who want to use the programs for fitting experimental spectra. The plotting routine, for example, only allows one to specify the plot dimensions in inches. Additionally, there is no option to save a spectrum as a data-array. This would be useful for a variety of purposes, such as transferring the spectral data to other machines for comparison with experimental spectra and for simulating superposition spectra.

Most unfortunately, pasting spectra generated by ESR and ESR^a into word processing and graphics programs (e.g. Microsoft Word, ChemDraw, ChemIntosh, Pagemaker, and Cricket Draw) presents serious difficulties. Spectra copied onto the Clipboard are invariably clipped due to the programming means by which the ESR creates high-resolution spectra. To get around this problem, one must first create a plotfile using ESR and then use a program capable of handling large drawing sizes (e.g. MacDraw) to read the plotfile and resize it. Only after this resizing operation can a spectrum be cut and pasted into other programs. Users who lack such a program will likely find this a serious inconvenience.

In summary, for the simulation of standard electron spin resonance spectra, ESR and ESR^a are convenient programs to both learn and use. For more demanding users, these programs lack a number of features that might otherwise make them much more attractive.

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