Table I

substr	RM	conditions	product	yield	stereoselectivity[e]
7	CH_3Li	Et$_2$O, −10 °C, 10 min	*trans*-11a	87%, 99%[c]	1:>99
7	C_6H_5Li	Et$_2$O, −10 °C, 10 min	*trans*-11b	77%, 91%[c]	<5:>95[d]
7	$H_2C=CHCH_2Li$[a]	Et$_2$O, −10 °C, 10 min	*trans*-11c	81%, 63%[c]	4.9:95.1
7	$H_2C=CHLi$[b]	Et$_2$O, −10 °C, 10 min	*trans*-11d	86%, 88%[c]	1:>99
7	*t*-BuLi	Et$_2$O, −10 [c], 10 min	*trans*-11e	46%, 85%[c]	3.6:96.4
7	$(CH_3)_3SiC≡CLi$	THF, 0 °C, 30 min	*trans*-11f	67%, 65%[c]	1:>99
8	$(CH_3)_2CuLi$	Et$_2$O or THF, −78 °C, 20 min	*cis*-11a	99%	98.7:1.3
8	CH_3Li	THF, −78 °C, 10 min	*cis*-11a	33%	72.8:27.2
8	CH_3CeCl_2	THF, −78 °C, 25 min	*cis*-11a	95%	97.4:2.6
8	$(C_6H_5)_2CuLi$	THF, −78 °C, 20 min	*cis*-11b	91%	>95:5[d]
8	$(CH_2=CHCH_2)_2CuLi$[a]	THF, −78 °C, 20 min	*cis*-11c	91%	>99:1
8	$(CH_2=CH)_2CuLi$[b]	THF, −78 °C, 20 min	*cis*-11d	78%	>99:1
8	$(t$-$Bu)_2CuLi$	THF, −78 °C, 30 min	*cis*-11e	25%	96.1:3.9
8	$(CH_3)_3SiC≡CLi$	THF, −40 °C, 10 min	*cis*-11f	85%	>99:1

[a] Via transmetalation from tetraallyltin. [b] Via transmetalation from vinyltri-*n*-butyltin. [c] The first yield reported corresponds to the conjugate-addition reaction with **7**, the second yield represents the overall yield for the alkylation/elimination reaction. [d] *trans*-11b and *cis*-11b could not be separated by HPLC; the figures given represent a minimum ratio derived from 470-MHz ^{1}H NMR. [e] See ref 10 for HPLC conditions.

followed by immediate treatment with dimethylamine produces amino vinyl sulfone **7**[6] via a "Lawton" reaction[8] in 87% yield. Reaction of **7** with methyl trifluoromethanesulfonate followed by counterion exchange with sodium tetrafluoroborate produces quaternary ammonium salt **8**[6,9] as a stable crystalline material, mp 157–62 °C (92% yield) (Scheme II).

Treatment of amino vinyl sulfone **7** with methyl, phenyl, allyl, vinyl, *tert*-butyl, and (trimethylsilyl)ethynyllithium affords monoadducts **9a–f**[6] in excellent yield. Reaction of these amines with methyl trifluormethanesulfonate produces the corresponding trimethylammonium sulfonates **10a–f** which were not fully characterized but subsequently treated with DBU to afford the trans isomers **11a–f**[6] respectively (Scheme III). Alternatively, direct reaction of allylammonium salt **8** in THF at −78 °C with the corresponding homo cuprate reagents instantaneously affords the cis adducts **11a–f**[6] in excellent yield. Comparison of each of these reaction products by analytical HPLC[10] establishes the stereoselectivity *of all of these reactions to be in excess of 95%* (Table I).

The stereoselectivity observed in each of these reactions is worthy of comment. The trans additions to amino vinyl sulfone **7** are apparently occurring under steric control; it is interesting to note that coordination of the amine moiety to the lithium reagents is apparently not occurring since this could have afforded the cis adducts, although such a directed addition would have required a 6-endo-trig[11,12] transition state. The complete reversal of stereochemistry seen in the cuprate additions to allylammonium salt **8** is quite striking. Reaction of allylammonium salts with organocuprates has been previously observed in simple systems,[13] but this example provides the first opportunity to observe the stereochemistry of the process in a system biased toward the S$_N$2′ Lawton[8] reaction. Although it is tempting to invoke an "ammonium cuprate" ion pair as the control element for additions

to **8**, the observation that methylcerium dichloride[14] and dimethylamine[3] also proceed via a syn addition pathway suggests that further research will be required to elaborate the intimate details of these reactions.[15–17]

(14) Imamoto, T.; Sugiura, Y.; Takiyama, N. *Tetrahedron Lett.* **1984**, *25*, 4233.

(15) Reaction of **8** with more basic reagents is far less satisfactory. Methylmagnesium bromide does not provide any evidence for the generation of *cis*- or *trans*-11a; methyllithium affords a low yield of adducts with substantially diminished stereocontrol (see Table I).

(16) It should be noted that both enantiomers of **7** are available via enantioconvergent synthesis,[8] thereby also providing efficient access to chiral material.

(17) Studies relating to the scope and generality of this ammonium ion directed S$_N$2′ reaction are currently under active investigation.

Homogeneous Catalysis of Hydrogen Reduction of SO$_2$ to Sulfur and Water Using $[(\eta^5\text{-}Me_nCp)Mo(S)(SH)]_2$

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Industrial processes involving heterogeneously catalyzed reduction of SO$_2$ by CH$_4$ or H$_2$S are well established, and H$_2$ reduction on Ru/Al$_2$O$_3$ has been demonstrated under mild conditions.[1] Homogeneous studies of CO reduction by H$_2$ have provided a wealth of mechanistic information relevant to heterogeneous catalysis and have led to homogeneous systems that are catalytic. Similar studies of SO$_2$ reductions with H$_2$ and metal hydrides should produce information pertinent to the elementary steps and even to practical reduction chemistry. Reactions of SO$_2$ with hydride complexes generally terminate with the formation of metal sulfide or oxy sulfide complexes,[2] precluding standard hydrogenation methods. However, Rakowski DuBois has shown that an organometallic Mo–S complex catalyzes $^1/_8S_8$ + H$_2$ →

(8) For references to the Lawton reaction, see ref 14 in: Saddler, J. C.; Donaldson, R. E.; Fuchs, P. L. *J. Am. Chem. Soc.* **1981**, *103*, 2110. For recent references to Lawton reactions with acyclic beta′-halo vinyl sulfones, see: (a) Anzeveno, P. B.; Mathews, D. P.; Barney, C. L.; Barbuch, R. J. *J. Org. Chem.* **1984**, *49*, 3134. (b) Knochel, P.; Normant, J. F. *Tetrahedron Lett.* **1985**, *26*, 425.

(9) The ((*tert*-butyl*dimethyl*silyl)oxy)ammonium salt had been previously prepared[3] but was not routinely isolated. Although the tetrafluoroborate counterion was used throughout this entire study, we have found that the crude triflate precursor to **8** affords *cis*-11a in identical yield and stereoselectivity.

(10) For all HPLC analyses, a normal phase econosphere silica 5 μm, 15 cm × 4.6 mm column was used with 3.5% THF in hexane (v/v) as mobile phase. Flow rate was 2.5 mL/min with UV detection at 254 nm.

(11) Baldwin, J. E. *J. Chem. Soc., Chem. Comm.* **1976**, 734.

(12) Addition of a vinyllithium reagent to *cis*-4-(dimethylamino)-1-(silyloxy)-2-cyclopentenyl sulfone also occurs via the trans-addition mode;[3] again avoiding the 6-endo-trig[11] directed addition option.

(13) (a) Commercon-Bourgain, M.; Normant, J. P.; Villieras, J. *C. R. Seances Acad. Sci., Ser. C* **1977**, *285*, 211. (b) Decodts, G.; Dressiare, G.; Langlois, Y. *Synthesis* **1979**, 510. (c) Dressiare, G.; Langlois, Y. *Tetrahedron Lett.* **1980**, *21*, 67. (d) Langlois, Y.; VanBac, N.; Fall, Y. *Tetrahedron Lett.* **1985**, *26*, 1009.

(1) Moody, D. C.; Ryan, R. R.; Salazar, K. V. *J. Catal.* **1981**, *70*, 221.

(2) (a) Kubas, G. J.; Ryan, R. R. *Inorg. Chem.* **1984**, *23*, 3181. (b) Kubas, G. J.; Wasserman, H. J.; Ryan, R. R. *Organometallics* **1985**, *4*, 419. (c) Kubas, G. J.; Wasserman, H. J.; Ryan, R. R. *Organometallics*, in press.

**Table I.** Summary of Catalytic Reactions of SO_x (3–8 mmol) and H_2 (12–27 mmol) To Give Sulfur and H_2O^a

solvent	catalyst molarity	temp, °C	P_{H_2}, atm	reaction time, h	catalyst turnovers/h $(av)^b$
$CHCl_3$	0.0056	75	2.8	144	0.4
PhCl	0.0017	100	2.8	5.8	18.4
PhCl	0.0017	100	1.2	1.4	7.8
4:1 PhCl–BzOH	0.0017	100	1.2	1.0	34.0
4:1 PhCl–BzOH	0.0017	20	1.2	15.5	1.8
4:1 PhCl–BuOH	0.0020	75	2.8	1.4	110
1:1 PhCl–BuOH	0.0017	75	2.8	1.0	203
1:1 PhCl–BuOH	0.033	75	2.8	0.6	183
PhCl + Bu_3N^c	0.0017	75	2.8	1.2	121
1:1 PhCl–BuOH + Bu_3N^d	0.0016	75	2.8	0.6	355

^{a} Magnetically stirred in a closed 250-mL flask, using 0.04–0.1 mmol of $[Me_5CpMoS(SH)]_2$ in 25 mL of solvent. ^{b} On the basis of SO_2 consumption (see ref 17), assuming 2 mmol of catalyst converts 1.5 mmol SO_2 according to reaction scheme; reaction times represent 50–80% consumption of initial SO_2. ^{c} 0.1 mL (0.42 mmol). ^{d} 0.025 mL (0.105 mmol).

H_2S without catalyst poisoning.^{3} We now report its use to effect the first example of homogeneous catalytic hydrogenation of SO_2.

The catalyst, $[(Me_nCp)Mo(\mu$-$S)(\mu$-$SH)]_2$ (1), is effectively sulfur-saturated and contains reducing SH groups uniquely regenerable from sulfide groups by H_2.^{3,4} We find that conversion of SO_2 to S_8 and H_2O proceeds under mild conditions (20–100 °C, 1–3 atm H_2, H_2/SO_2 = ca. 4) similar to those for S_8–H_2 reaction^3 (Table I). In the absence of H_2, stoichiometric reaction of SO_2 with 1 (1:2) at 20 °C produces water and the known^5 (for n = 5, cluster, $(Me_nCp)_2Mo_2(\mu$-$S)_2(\mu$-$S_2)$ (2).^{6} This is consistent with SO_2 reduction and concomitant oxidation of the two μ-SH ligands of the catalyst to μ-S_2 ligand. Only small amounts of the two known isomers^{5,7} of 2, $(Me_nCp)_2Mo_2(\mu$-$S)_2(S)_2$ and $(Me_nCp)_2Mo_2(S)_2(\mu$-$S_2)$, form.^{8} A third product (22% yield) of the reaction analyzes^9 as "$[Me_nCpMoS_3]_x$" (3), an insoluble, presumably polymeric species containing the sulfur from the reduced SO_2 (S_8 is *not* formed in the stoichiometric reaction). Complex 3 is observed as a precipitate during the catalytic SO_2–H_2 reaction for n = 0 or 1, but for n = 5 the catalyst solution remains visibly homogeneous. Both 3^9 and 2^4 react with H_2 (1 atm) in $CHCl_3$ to quantitatively regenerate 1, the excess sulfur in 3 being released as H_2S. Thus, in the catalysis, the SO_2 is apparently initially reduced to H_2S, which is indeed present in small quantities. However, since a closed vessel rather than a flow system is used, the H_2S rapidly reacts with unconsumed SO_2 (Claus reaction) to yield the final observed products, S_8 and H_2O.^{10} On the basis

of the above independently observed reactions, the following catalytic scheme is proposed:

$$H_2S + 0.5SO_2 \xrightarrow{4} 1.5S + H_2O$$

$$\text{overall:} \quad 1.5 SO_2 + 3H_2 \longrightarrow 1.5S + 3H_2O$$
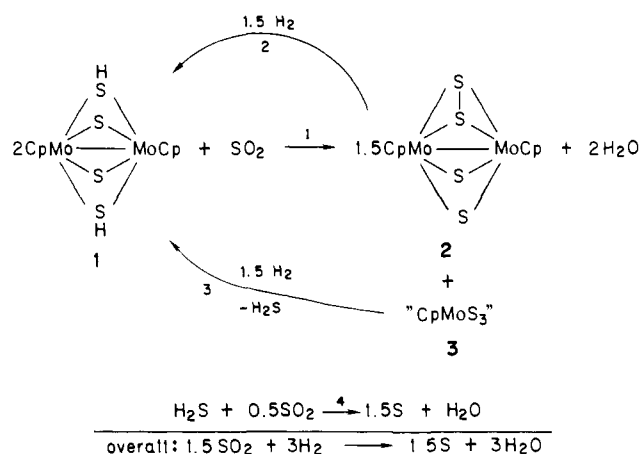
If the catalysis is terminated at or before complete SO_2 consumption, S_8 is the product. If the reaction is allowed to continue (assuming excess H_2 is present), S_8 is hydrogenated to H_2S as final product. Actually, a parallel cycle based on SO_2 reduction by H_2S from S_8–H_2 reaction undoubtedly occurs in addition to the cycle shown above. However, this cycle probably is not dominant since the rate of reduction as monitored by pressure drop was highest early on (no appreciable induction period), decreasing somewhat with time. Importantly, the catalyst solution is stable to oxygenation by SO_2 and is reusable, although the presence of atmospheric oxygen results in inactive $(Me_5Cp)_2Mo_2(O)S_3^5$ being formed.

Both reaction 1 (in the scheme) and the overall catalysis have been carefully studied in regard to variations in reaction conditions (Table I). In both instances, SO_2 reduction proceeds at a slow rate if $CHCl_3$ is used as solvent. However, the rate of catalysis increases several-hundred-fold (e.g., from 0.4 to 355 turnovers/h) if weakly basic solvents such as alcohols and/or catalytic amounts of Brønsted bases such as amines are present. For example, by use of 0.04 mmol of 1, 6.1 mmol of SO_2 is cleanly reduced in 34 min at 75 °C in 1:1 n-BuOH–PhCl containing 0.1 mmol of Bu_3N. Similar enhancements by weak bases occur for reaction 1 and the Claus reaction, (4).^{10} The rate-limiting step of the catalysis is undoubtedly regeneration of the μ-SH groups in 1 by H_2 since reaction 1 is found to occur instantly in the presence of weak bases and a large excess of SO_2. Even for a ratio of $SO_2/$ $[Me_5CpMoS(SH)]_2$ (0.016 M) as low as 4:1, ^{1}H NMR evidence shows that conversion to 2 and 3 is complete within 2 min in $CDCl_3$–CD_3OD or in $CDCl_3$ containing catalytic amounts of Et_3N (vs. 6 h in $CDCl_3$ and >2 h in acetone).^{11} Acids are found to inhibit this reaction. We also find that $^1/_8 S_8 + H_2 \xrightarrow{1 (n = 5)} H_2S$ occurs at a rate of 194 catalyst turnovers/h in 1:1 PhCl–n-BuOH (75 °C, 2.4 atm H_2), 17 times faster than that previously reported^3 in $CHCl_3$. This rate is very similar to the SO_2 rate (203 turnovers/h) and also indicative of base promotion. In this context, the reactivities of $(\mu$-$SH)_2Fe_2(CO)_6$ and $Cp_2Ti(SH)_2Mo(CO)_4$ are also promoted by bases such as amines.^{12}

In regard to the mechanism of the SO_2–H_2 catalysis, bases enhance three reactions, (1), (4), and S_8–H_2, but which is most important in enhancing the overall catalysis rate is presently unknown. The mechanism for base promotion of reaction 1 may be proton abstraction followed by electrophilic attack of SO_2 on –S^-. In this regard, the complex μ-$SH[W(CO)_5]_2^-$ was found^{13} to be much more reactive toward heterocumulenes (e.g., MeN=C=O) in its deprotonated form, and SO_2 is a type of

(3) Rakowski DuBois, M.; VanDerveer, M. C.; DuBois, D. L.; Haltiwanger, R. C.; Miller, W. K. *J. Am. Chem. Soc.* **1980**, *102*, 7456. An alternate synthesis has been reported: Curtis, M. D.; Williams, P. D. *Inorg. Chem.* **1983**, *22*, 2661.

(4) Brunner, H.; Kauermann, H.; Meier, W.; Wachter, J. *J. Organomet. Chem.* **1984**, *263*, 183. We find that 2 → 1 occurs in minutes at 75 °C, using only 1 atm of H_2.

(5) Brunner, H.; Meier, W.; Wachter, J.; Guggolz, E.; Zahn, T.; Ziegler, L. *Organometallics* **1982**, *1*, 1107.

(6) Yield of 2 (n = 5, 4:1 $CHCl_3$–MeOH, 18 h) 77%, corresponding to the stoichiometry in reaction 1. H_2O was analyzed by Karl–Fischer titration.

(7) Rakowski DuBois, M.; DuBois, D. L.; VanDerveer, M. C.; Haltiwanger, R. C. *Inorg. Chem.* **1981**, *20*, 3064 and references therein.

(8) The isomers of $(Me_5Cp)_2Mo_2S_4$ are photochemically interconvertible: Bruce, A. E.; Tyler, D. R. *Inorg. Chem.* **1984**, *23*, 3433. We find that 2 *thermally* converts to $[Me_5CpMoS(\mu$-$S)]_2$ in solution at 100 °C. Examination of catalyst solutions after quenching in midreaction reveals that the latter is the principle species present.

(9) Found for n = 5, C, 37.5; H, 4.8; S, 28.0; Mo, 27.9; S:Mo = 3.01. For n = 1, S:Mo = 3.3. Similar or identical polymers have been previously described which form 1 on reaction with H_2.^{7}

(10) H_2S and SO_2 react rapidly in donor or weakly basic organic solvents: Albertson, N. F.; McReynolds, J. P. *J. Am. Chem. Soc.* **1943**, *65*, 1690. If $CHCl_3$ is the solvent, the Claus reaction occurs inefficiently mainly along the upper flask walls (sulfur deposition is observed) where H_2O (from SO_2 reduction) condenses and promotes it. If ROH or amines are present in the catalyst solution, the H_2S–SO_2 reaction (4) occurs efficiently in the solution phase.

(11) 3 does not form if stoichiometric amounts of amine are present. This reaction is under investigation.

(12) (a) Seyferth, D.; Henderson, R. S. *J. Organomet. Chem.* **1981**, *218*, C34. (b) Seyferth, D.; Womack, G. B. *J. Am. Chem. Soc.* **1982**, *104*, 6839. (c) Seyferth, D.; Womack, G. B.; Song, L.-C.; Cowie, M.; Hames, B. W. *Organometallics* **1983**, *2*, 928. (d) Ruffing, C. J.; Rauchfuss, T. B. *Ibid.* **1985**, *4*, 524.

heterocumulene. Alternatively, SO_2 could initially coordinate to the sulfur atom of -SH, similar to $RS-SO_2$ in $L_nCuSR\cdot SO_2$.[14] In both cases, base-assisted proton transfer to an oxygen atom could result in formation of an $MSSO_2H$ group. Since the SO_2H unit is unstable in both RSO_2H[15] and novel MSO_2H complexes,[2c] the proposed $MSSO_2H$ group would likewise be expected to decompose to reduced sulfur species, such as **3**, and H_2O. The implications of this chemistry could extend to heterogeneous sulfide

catalysts such as hydrodesulfurization catalysts[16] and we plan to investigate these catalysts for SO_2 reduction.

(13) Angelici, R. J.; Gingerich, R. G. W. *Organometallics* **1983**, *2*, 89.
(14) Eller, P. G.; Kubas, G. J. *J. Am. Chem. Soc.* **1977**, *99*, 4346.
(15) (a) Oae, S. "Organic Chemistry of Sulfur"; Plenum: New York, 1977; Chapter 11. (b) Detoni, S.; Hadzi, D. *J. Chem. Soc.* **1955**, 3163.

(16) (a) Schuman, S. C.; Shalit, H. *Catal. Rev.* **1970**, *4*, 245. (b) Grange, P. *Catal. Rev.—Sci. Eng.* **1980**, *21*, 135.
(17) SO_2 amounts were measured on a vacuum line by using $P-V-T$ data. After the reaction mixture was quenched (−196 °C) and H_2 pumped off, unreacted SO_2 was isolated by pumping (25 °C) and passage through a −95 °C trap.

Computer Software Reviews *

MacDraw. By Mark Cutter. Apple Computer, Inc.: Cupertino, CA. List price $195.00.

MACDRAW is a graphic design program for use in creating pictorial layouts that involve relatively fixed, uniform objects. MACDRAW is a release of Apple Corporation and will operate only on the MacIntosh computer. The disk operating system is the standard MacIntosh Finder and the current release, 1.7, is non-copy protected. MACDRAW will operate on either a 128K or 512K MacIntosh although it was evaluated for this review on a machine with the larger memory capacity.

MACDRAW is an object oriented drawing program and as such differs from the more well known MACPAINT as the latter maniuplates and stores information in screen pictal point format. Thus, the basic underlying principle of these two programs is entirely different and each has its strengths and weaknesses. However, for use in creating scientific layouts such as chemical structures, MACDRAW is superior. MACDRAW has a standard set of drawing tools that allow the creation of such objects as lines, circles, ovals, squares, rectangles, and odd-shaped polygons with an unlimited number of corners. In addition, there is the capability of drawing arcs and random lines. When an object, such as a square, is created, certain defaults are automatically assigned to the object such as the line width and the fill. These defaults may be changed and there are four different line thicknesses as well as the opportunity to create an object with no border line. There are as well a whole series of fill patterns that can be used. All of the characteristics of an object can be modified.

As each object is created, it is not only placed on the diagram in an X–Y coordinate sense but also it is stacked in front of all previous objects. This has the result that objects with fill will cover those which were created first. This stacking order is not permanent and can be changed by selecting objects and either moving them to the front or moving them to the back of the stack. This is an extremely useful feature because it allows the creation of small shapes with the fill white but no lines. Placing such an object between two polygons whose lines cross creates the sense of three-dimensionality since the line of the back polygon will be broken. This has the interesting feature that simply by reordering the stacking position the objects can be switched from one mirror image sense to the other. Once objects are created they may be moved, duplicated, flipped along either the vertical or horizontal axis, and rotated by 90° increments. They may also be resized, and with the option of showing size active the dimensions of any object will be displayed on the screen. In addition, when the show size option is activated the dimensions of objects are displayed as they are created. Thus, the length of a line is dynamically displayed as it is formed and it is quite easy to obtain precise lengths. For squares, rectangles, circles, and ovoids, the two pertinent dimensions are displayed while for polygons the rise and run number from the last point is illustrated. This feature makes it quite simple to create regular patterns such as hexagons or the normal zigzag of an acyclic carbon chain based on simple trigonometric calculations. Not every line length and rise and run is available, however, as MACDRAW will allow no greater precision than the pictal display on the screen. One can operate either in an English or metric system and in both cases the actual size on the screen is quite close to the printed version. In the metric mode, one can access dimensions that vary by approximately 0.03 cm. This would appear to be more than sufficiently precise for routine structure drawing purposes.

There are three views which can be accessed of any document that is currently active: the normal view which, as indicated above, has nearly

the same scale as the printed version; an intermediate view; and a reduced to fit mode that displays the entire document. The document can be adjusted to print on anywhere from one 8.5 × 11 in. sheet to a maximum of 5 × 12 such sheets which can then be pasted together to make an extremely large layout.

The reviewer found it convenient to work with structures that had a uniform 2 cm bond length. A template was created with common structural subunits such as hexagons, pentagons, etc., and these were quite easy to create with nearly exact dimensions. Up to four documents can be kept active on the desktop at one time, and thus the template can be kept accessible. Objects can be copied from the template to the clipboard and then pasted into the drawing being created. After objects are pasted into the active document they may be moved with facility and the lines of two adjacent objects such as two hexagons can be made to merge.

A collection of objects such as that which would represent the steroid nucleus can then be grouped together in which case MACDRAW treats them as a single object. They can then be duplicated, placed in various positions around the diagram, and further manipulated by the addition of structural subunits that vary from one to another. A very useful feature of MACDRAW is that when an object is duplicated and then moved in the diagram a repeat of the duplication object will result in a second copy being placed at the same displacement from the first duplicate as the first duplicate was from the original. This permits very ready setup of repetitive layouts, for instance in synthetic schemes where the basic structure stays unchanged and functional manipulations are being carried out. Thus, for instance, a single steroid nucleus could be placed in the upper left hand corner of a document, duplicated, the duplicate placed on the same line but in the middle, duplicated again to create a third all of which are evenly spaced across the top of the document. These three then can be duplicated together and if that set of duplicates is moved to the middle of the sheet and duplicated again one will arrive at nine identical units placed uniformly on the document. MACDRAW has the feature of showing rulers along the left and top margin which indicate the position on the page. While this can be used to align objects, the reviewer found it easier simply to create temporary vertical and horizontal lines as an alignment grid. Once objects were appropriately positioned, these temporary lines were removed.

Text may be created in two modes, a caption and a paragraph display. The former is useful for short text entries such as structure numbers and information that would typically go about a transformation arrow while the latter contains the feature of work wraparound and is useful in creating fairly extensive amounts of text. Text, like other objects, can have fill and for creating structure diagrams the most useful fill is white where a single letter such as an "N" or an "O" will cover up structure lines that are on objects behind the letter. Text within the caption mode can also either be left, centered, or right justified and for the purpose of adding heteroatoms to structures the center mode is to be preferred since then the fill cover is then symmectrical about the letter.

Printing MACDRAW diagrams can be accomplished either with the Apple Imagewriter or with the Apple Laserwriter. The former has the option of printing either full scale or in a 50% reduce mode where the latter reduces both dimensions by half, resulting in a final printed area of $^1/_4$ of the original as it was operated on under MACDRAW. With 2-cm bonds the dimensions then are reduced to 1 cm, which are slightly too large for final printed versions. However, these may be reduced during the publication process to whatever is appropriate for a particular journal or the originals may be reduced by using photocopiers of the Xerox type