roughly 17 kcal/mol would have to be supplied to the planar triplet in order for it to cross to the singlet at the orthogonal geometry. However, there may be a lower energy pathway for intersystem crossing from the triplet to the singlet (for instance, rotating two methylene groups) than twisting to the orthogonal geometry.

(23) It is almost certain that methylene rotation *coupled* with bond length changes would provide the lowest energy pathway from a planar to an orthogonal minimum. It should also be noted that an orthogonal minimum is not a global one, since rotation of a second methylene group leads to methylenecyclopropane.

(24) Because of relief of steric compression on methylene twisting in substituted derivatives of trimethylenemethane, the stabilization energy on twisting will be greater in these molecules than in the unsubstituted parent. Therefore, the numbers in parentheses in Figure 5 most certainly represent algebraic upper limits.

(25) J. A. Berson, L. R. Corwin, and J. H. Davis, *J. Am. Chem. Soc.*, **96**, 6177 (1974), have shown that in an isomer of **9**, in which the two methyl groups are both attached to the unique carbon, the singlet is trapped by diylophiles to give, preferentially, fused rather than bridged adducts. They have interpreted this finding as evidence for the orthogonal geometry, expected in such a derivative of **8**. It is conceivable that **9** or **10** would preferentially give, instead, bridged adducts; since, electronically, if planar, the lowest singlet might be expected to react most readily at the ring carbon atoms. Thus, an alteration in regioselectivity would be indicative of a planar singlet in these molecules. However, steric effects would tend to favor attack at the least substituted, exocyclic carbon, and so fused adducts might again be obtained, even if the lowest singlet preferred a planar geometry. A better probe for a planar singlet in **9** and **10** would be a stereochemical one, in which preservation of geometrical integrity about the double bond in these molecules was examined by substituting deuterium for one of the hydrogens in the methylene group and labeling the ring with a stereochemical point of reference.

(26) The relative energy of the orthogonal geometry of **11** is probably represented adequately by the number in parentheses for the appropriate form of **5** in Figure 5, since the energy gain on methylene rotation in **11** should be comparable to that in unsubstituted trimethylenemethane.

(27) These conclusions are in good agreement with the known experimental facts about trimethylenemethane and its derivatives.[2]

Internal Rotation in the Ground Electronic State of Allene[1]

Clifford E. Dykstra

Contribution from the Department of Chemistry and Materials and Molecular Research Division, Lawrence Berkeley Laboratory, University of California, Berkeley, California 94720. *Received September 10, 1976*

Abstract: The internal rotation potential of allene has been studied with ab initio self-consistent field (SCF) methods using a double-ζ basis set of 38 contracted Gaussian functions and an extended set of 65 functions including polarization functions, and with the method self-consistent electron pairs (SCEP) using the double-ζ set. The ground state of allene is a closed shell $^1A_1$ state in D_{2d} symmetry. In the D_2 symmetry of the twisted form, this closed shell state mixes with a $2b_3 \rightarrow 3b_3$ open shell $^1A_1$ state which correlates with a ^1A_u state in the D_{2h} symmetry of the planar form of the molecule. The planar closed shell state, ^1A_g, is higher in energy than the ^1A_u state. Examination of pair correlation energies indicates that correlation effects will not reverse this order. The internal rotation barrier is predicted to be about 49 kcal, after geometry optimization, and there is little effect on relative energies from including polarization functions.

Allene is the simplest molecule containing two carbon-carbon double bonds and like ethylene, the effects of internal rotation on electronic structure have been of theoretical interest. The lowest energy structure of the ground state of allene is with the two CH_2 groups in perpendicular planes. A detailed molecular orbital comparison of the planar ground state (D_{2h}) structure of ethylene and the out-of-plane (D_{2d}) structure of allene has been given by Buenker.[2a] Experimental studies of allene include the UV spectrum taken by Sutcliffe and Walsh[2b] who identified several Rydberg series at short wavelengths. Maki and Toth[3] used high-resolution infrared spectra to determine the structure of allene: $R_{C=C}$ = 1.308 Å, R_{C-H} = 1.087 Å, and ∠HCH = 118.2°.

There have been several ab initio theoretical studies of allene. The largest basis set allene calculation appears to be that of Hariharan and Pople[4] who showed that polarization functions were important in comparing energetics of C_3H_4 isomers. FSGO calculations include those of Talaty, Schwartz, and Simons[5] who found a C=C length 0.03 Å longer than experiment and a rather large H-C-H angle of 126° in the nonplanar structure. Weimann and Christoffersen[6] used FSGO to predict a barrier to rotation (to the planar ^1A_g state) of 75.1 kcal. Earlier calculations on a large number of molecules by Preuss and Janoschek[7] gave a 65 kcal difference between planar and nonplanar closed shell states. A partial geometry optimization determined the C=C bond length to be 1.310 Å in the D_{2d} form, quite close to experiment, and 1.323 in the planar form. A geometry optimization of the D_{2d} form by Radom, Lathan, Hehre, and Pople[8] used a minimum STO-3G basis and gave the C=C length as 1.288 Å and the bond angle as 116.2°. In another STO-3G study, by Radom and Pople,[9] a separation of 92 kcal for the closed shell states was given from calculations performed without optimization of the geometry.

Schaad, Burnelle, and Dressler[10] studied the excited states of allene in the D_{2d} and D_{2h} structures and confirmed Buenker's[2a] result that the lowest planar allene electronic state is a ^3A_u state ($1b_{2g} \rightarrow 2b_{2u}$) and that the lowest singlet is a ^1A_u state arising from the same occupancy. (The convention for distinguishing b_2 and b_3 symmetry species of the D_{2h} point group used by Buenker and Schaad et al. is opposite that used here.) Buenker[2a] determined that the open shell singlet was about 6 kcal lower than the closed shell singlet and estimated that the real difference could be five times that. The separation between the ^3A_u and ^1A_u states was estimated to be less than 0.1 eV (2.3 kcal). Furthermore, it was suggested that the singlet might have a relative minimum in the planar form. The SCF calculations of Schaad and co-workers[10] yield a smaller value for the energy difference of the closed shell states, 3.15 eV (73 kcal), a ^3A_u-^1A_u separation of 0.09 eV and a very small separation for the ^1A_u and ^1A_g states of 0.03 eV (0.7 kcal). The open shell energies were calculated using the virtual orbitals from a closed shell calculation. Correlated wave functions were not used in any of the studies.

The closeness of the two lowest planar singlet states of allene determined in these two SCF calculations suggests that even small correlation effects or the inclusion of polarization functions could reverse the relative ordering of these states and

Table I. Allene Closed Shell State Optimized Structures and Energies[a]

	$R_{C=C}$	$R_{C\text{-}H}$	∠HCH, deg	Energy
90°	1.310	1.074	117.6	−115.8303
	(1.308)	(1.087)	(118.2)	
75°	1.310	1.075	117.6	−115.8267
55°	1.314	1.075	117.3	−115.8110
35°	1.319	1.076	117.0	−115.7836
15°	1.327	1.076	117.1	−115.7465
0°, planar	1.330	1.074	119.6	−115.7195

[a] Bond lengths are in ångströms and energies are in atomic units. The basis set used in these calculations was the DZ set. Experimental results[3] are in parentheses.

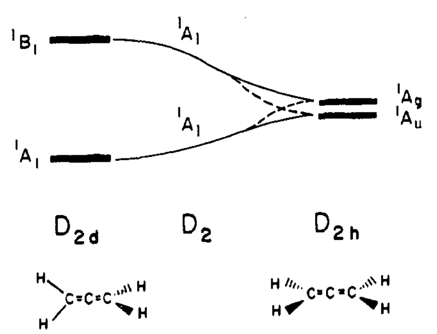


Figure 1. Qualitative potential curves for the D_2 symmetry $^1A_1$ states which could correlate with the nonplanar D_{2d} $^1A_1$ ground state. The avoided crossing is indicated by the broken lines.

change the nature of the correspondence of the electronic states upon internal rotation (see Figure 1). Another potentially important effect not taken into account is geometry optimization of the various states. This is especially important since the likely planar ground state is an open shell state. In recent SCF calculations on small carbonyl systems, including glyoxal,[11] ketene,[12] and acrolein,[13] we have found large energy changes upon geometry optimization of certain low-lying open shell states and thus this effect should not be overlooked in studying allene.

Theoretical Approach

A double-ζ (DZ) basis set of Dunning-contracted functions,[14,15] carbon (9s 5p/4s 2p) and hydrogen (4s/2s), was used in the (SCF) geometry optimization calculations and the SCEP calculations. In addition, SCF calculations were performed at the optimized geometries with a double-ζ plus polarization (DZ+P) basis of 115 primitives contracted to 65 functions. In this set, hydrogen p functions with an exponent of 1.0 and carbon d functions with an exponent of 0.75 were added as in a previous study of ketene.[12] The ground state occupancy was confirmed to be $1a_1{}^2\,1b_2{}^2\,2a_1{}^2\,3a_1{}^2\,2b_2{}^2\,4a_1{}^2\,3b_2{}^2\,1e^4\,2e^4$ in D_{2d} symmetry. In the D_{2h} planar form, the lowest closed shell occupancy is $1a_g{}^2\,1b_{1u}{}^2\,2a_g{}^2\,3a_g{}^2\,2b_{1u}{}^2\,4a_g{}^2\,3b_{1u}{}^2\,1b_{3u}{}^2\,1b_{2g}{}^2\,1b_{2u}{}^2\,1b_{3g}{}^2$ and in the intermediate D_2 structure is $1a_1{}^2\,2b_1{}^2\,2a_1{}^2\,3a_1{}^2\,2b_1{}^2\,4a_1{}^2\,3b_1{}^2\,1b_3{}^2\,1b_2{}^2\,2b_2{}^2\,2b_3{}^2$.

A complete geometry optimization was performed for the closed shell SCF wave functions at several internal rotation angles and for the two open shell planar states. The three structural parameters were optimized cyclically with simple parabolic fits used to determine the minimum for a given parameter and a few cycles through the three parameters were used.

Some consideration of correlation effects has been achieved using the recently introduced method of self-consistent electron pairs (SCEP)[16,17] due to Meyer. SCEP is an efficient method for obtaining correlated wave functions which include singly and doubly substituted configurations from a closed shell reference determinant. The calculations reported here are all variational fixed ψ_0 calculations[17] where the singly substituted configurations are included explicitly in the wave function after convergence of the iterative treatment of the doubly substituted configurations. This neglects the very small effect of the singles on the doubles which is typically less than 0.1% of the correlation energy.[17] Conveniently obtained from an SCEP calculation are variationally additive pair correlation energies for each pair of electrons in the closed shell reference determinant. For each such pair, there is a doubly substituted function given directly in terms of basis functions which implicitly includes all double substitutions of the pair by virtual or external orbitals. Explicit manipulation of a configuration list and an explicit integral transformation are avoided.

Results and Discussion

The results of the geometry optimization of the closed shell states are given in Table I and it is seen that the calculated structure of the lowest energy D_{2d} form is quite close to the experimental structure.[3] Most of the changes in structure upon internal rotation are minor, though the carbon-carbon distance increases by 0.02 Å. The structures and energies for the D_2 intermediate forms may be somewhat different than those determined since a proper description of the wave function in this region should include at least two configurations. The energy difference between the closed shell $^1A_1$ (D_{2d}) and ^1A_g (D_{2h}) is about 70 kcal with the DZ basis which is close to the 73 kcal value obtained by Schaad et al.[10] Orbital energies obtained from the closed shell calculations at the optimized

Table II. Allene SCF Orbital Energies (in au) at Optimum Geometries

	D_{2d} symmetry		D_2 symmetry					D_{2h} symmetry	
		90°		75°	55°	35°	15°		0°, planar
Improved virtuals (IVO's)	$5a_1$	0.2946	$5a_1$	0.2945	0.2940	0.2932	0.2919	$5a_g$	0.2854
	$4b_2$	0.2619	$4b_1$	0.2618	0.2618	0.2619	0.2627	$4b_{1u}$	0.2665
	3e	0.1596	$3b_2$	0.1758	0.1931	0.2036	0.2036	$2b_{2u}$	0.1842
			$3b_3$	0.1413	0.1145	0.0861	0.0569	$2b_{3u}$	0.0327
Occupied	2e	−0.3776	$2b_3$	−0.3588	−0.3328	−0.3063	−0.2797	$1b_{3g}$	−0.2567
			$2b_2$	−0.3955	−0.4178	−0.4384	−0.4603	$1b_{2u}$	−0.4979
	1e	−0.6141	$1b_2$	−0.6085	−0.6002	−0.5917	−0.5841	$1b_{2g}$	−0.5795
			$1b_3$	−0.6189	−0.6237	−0.6265	−0.6274	$1b_{3u}$	−0.6301
	$3b_2$	−0.6317	$3b_1$	−0.6319	−0.6326	−0.6338	−0.6352	$3b_{1u}$	−0.6353
	$4a_1$	−0.7193	$4a_1$	−0.7195	−0.7203	−0.7214	−0.7218	$4a_g$	−0.7161
	$2b_2$	−0.9667	$2b_1$	−0.9697	−0.9675	−0.9669	−0.9667	$2b_{1u}$	−0.9804
	$3a_1$	−1.0821	$3a_1$	−1.0872	−1.0832	−1.0822	−1.0821	$3a_g$	−1.1058

Table III. Correlation and Basis Set Effects in Allene Closed Shell States

Calcn	$^1A_1$ energy, au 90°	^1A_g energy, au Planar	Diff, kcal
SCF-DZ	−115.8303	−115.7195	69.5
SCF-DZ+P	−115.8834	−115.7750	68.0
SCEP-DZ; 9 frozen orbitals[a]	−115.8884	−115.7651	77.4
Pair energies[b] $2e_x^2$	−0.0243	$1b_{3g}^2$ −0.0223	
$2e_y^2$	−0.0243	$1b_{2u}^2$ −0.0133	
Sum of pair energies	−0.0573	−0.0450	7.7
SCEP-DZ; 7 frozen orbitals	−115.9394	−115.8165	77.1
SCEP-DZ; 6 frozen orbitals	−115.9739	−115.8524	76.2

[a] Orbitals were frozen with respect to substitution in the SCEP wave function on the basis of orbital energies. In the D_{2d} structure, the degenerate e orbitals have been counted as two orbitals for comparison with the D_{2h} wave function where no orbital is occupied by more than two electrons. [b] The pair energies given are for pairs with both electrons in the same orbital. However, with nine frozen orbitals there are a total of four electron pairs (see ref 17).

Table IV. Allene Planar Open Shell States[a]

	^3A_u ($1b_{3g}$ → $2b_{3u}$)	^1A_u ($1b_{3g}$ → $2b_{3u}$)
Energy at ^1A_g optimum geometry: DZ	−115.7539	−115.7518
DZ+P	−115.8057	−115.8026
Optimized structures:		
$R_{C=C}$	1.360	1.361
R_{C-H}	1.078	1.077
∠HCH, deg	116.6	116.6
Energy (DZ)	−115.7566	−115.7545

[a] Results from SCF calculations with energies in atomic units and bond lengths in ångströms. The DZ basis was used for the optimization.

geometries are given in Table II. As Buenker[2a] has explained, the removal of the 2e and 3e orbital degeneracy upon rotation produces a very low-lying virtual orbital, $2b_{3u}$, and an occupied orbital, $1b_{3g}$, higher in energy than in the out-of-plane form. Promotion of an electron from this highest filled occupied orbital to the low-lying virtual yields the ^1A_u and ^3A_u states.

As shown in Table III, the addition of polarization functions (DZ+P) changed the relative closed shell state energies very slightly. As seen in Table IV, the DZ and DZ+P sets yielded about the same relative energies for the planar open-shell states as well. Some understanding of correlation effects can be obtained from the SCEP results in Table III. Including only single and double substitutions from the 2e orbital (D_{2d}) and the two D_{2h} orbitals which correlate with the 2e (see Table II) raises the energy of the ^1A_g relative to the $^1A_1$ by about 8 kcal. Comparison of pair correlation energies suggests that the two electrons in the planar $1b_{2u}$ orbital show less correlation than electrons in the D_{2d} 2e orbital. The diagonal pair energies (i.e., pair energies with both electrons of the pair in the same internal orbital) for planar allene with nine frozen orbitals are −0.0223 for $1b_{3g}^2$ and − 0.0133 for $1b_{2u}^2$. A calculation with 10 frozen orbitals gave essentially the same pair energy for the $1b_{3g}$ electrons. The diagonal pair energies for orbitals which correlate with the D_{2d} 1e orbital, however, do not show as much difference. With seven frozen orbitals, the additional correlation energy from these electrons is 0.0510 in D_{2d} and 0.0514 in D_{2h}. The effect of unfreezing additional orbitals on the relative energies of the closed shell states is likely to be small since contributions to the total energy from lower lying electrons will tend to be same for both structures. For example, with six frozen orbitals, the D_{2d} $3b_2^2$ diagonal pair energy is −0.0045 while the D_{2h} $3b_{1u}^2$ diagonal pair energy is −0.0048 and the overall effect on relative energies is only 0.0014 au. It seems clear that correlation effects will raise the separation between the ^1A_g and $^1A_1$ by about 10% relative to the SCF determined difference and this results primarily from the unexpectedly small correlation contribution of the $1b_{2u}$ electrons.

The geometries of the open shell ^1A_u and ^3A_u states were optimized and the results are given in Table IV. Geometry optimization had only a small effect, less than 2 kcal, on the energy relative to the ^1A_g state; however, the bond length of the carbon–carbon bond was determined to be 0.03 Å longer than for the ^1A_g state. The energy difference between the D_{2d} ground state and the planar ^1A_u state is 0.0785 au or 49.3 kcal. Interestingly, the ^3A_u and ^1A_u are very close in energy, 0.0021 au with DZ basis and 0.0031 au with DZ+P basis. The fact that these energies are so close suggests little correlation energy for the $1b_{3g}$ $2b_{3u}$ pair. Thus, we can take as an estimate of the upper limit on the lowering of the ^1A_g–^1A_u separation from correlation effects to be the $1b_{3g}^2$ electrons' pair energy, −0.0223 au. But this energy is still less than the SCF determined separation energy of 0.0350 au (DZ) or 0.0276 au (DZ+P). Thus, it is clear that the planar open shell singlet, and not the closed shell state, correlates with the D_{2d} $^1A_1$ ground state. The SCF predicted internal rotation barrier (^1A_u–$^1A_1$ energy difference) is 49.3 kcal which is substantially lower than previous reported values. The maximum effect of correlation energy should be the change in the closed shell state energies from correlation plus the $1b_{3g}^2$ pair energy, which is used as the maximum ^1A_u–^1A_g correlation energy difference. From this analysis, we conclude that (1) the value for the barrier is about 49 kcal, though possibly as much as 70 kcal due to correlation, (2) the ^1A_u–^3A_u separation is, in fact, small, about 2 kcal, and (3) the ^1A_g is higher than both open shell states.

Acknowledgments. I thank Professor H. F. Schaefer for his many useful comments and suggestions in the course of this work and for a careful reading of the manuscript. This work was supported in part by Professor Schaefer's National Science Foundation Grants GP-39317 and GP-41509X.

References and Notes

(1) Work performed under the auspices of the U.S. Energy Research and Development Administration.
(2) (a) R. J. Buenker, *J. Chem. Phys.*, **48,** 1368 (1968); (b) L. H. Sutcliffe and A. D. Walsh, *J. Chem. Soc.*, 899 (1952).
(3) A. G. Maki and R. A. Toth, *J. Mol. Spectrosc.*, **17,** 136 (1965).
(4) P. C. Hariharan and J. A. Pople, *Chem. Phys. Lett.*, **16,** 217 (1972).
(5) E. R. Talaty, A. K. Schwartz, and G. Simons, *J. Am. Chem. Soc.*, **97,** 972 (1975).
(6) L. J. Weimann and R. E. Christoffersen, *J. Am. Chem. Soc.*, **95,** 2074 (1973).
(7) H. Preuss and R. Janoschek, *J. Mol. Struct.*, **3,** 423 (1969).
(8) L. Radom, W. A. Lathan, W. J. Hehre, and J. A. Pople, *J. Am. Chem. Soc.*, **93,** 5339 (1971).
(9) L. Radom and J. A. Pople, *J. Am. Chem. Soc.*, **92,** 4786 (1970).

(10) L. J. Schaad, L. A. Burnelle, and K. P. Dressler, *Theor. Chim. Acta*, **15**, 91 (1969).
(11) C. E. Dykstra and H. F. Schaefer, *J. Am. Chem. Soc.*, **98**, 401 (1976).
(12) C. E. Dykstra and H. F. Schaefer, *J. Am. Chem. Soc.*, **98**, 2689 (1976).
(13) C. E. Dykstra, *J. Am. Chem. Soc.*, **98**, 7182 (1976).
(14) T. H. Dunning, *J. Chem. Phys.*, **53**, 2823 (1970).
(15) T. H. Dunning and P. J. Hay, "Modern Theoretical Chemistry", H. F. Schaefer, Ed., Plenum Press, New York, N.Y., 1976.
(16) W. Meyer, *J. Chem. Phys.*, **64**, 2901 (1976).
(17) C. E. Dykstra, H. F. Schaefer, and W. Meyer, *J. Chem. Phys.*, **65**, 2740 (1976).

Generalized Stereoisomerization Modes

James G. Nourse*

Contribution from the Department of Chemistry, Princeton University, Princeton, New Jersey 08540. *Received June 28, 1976*

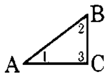
Abstract: A stereoisomerization mode can be defined as a set of symmetry equivalent degenerate rearrangements of a molecular skeleton. The key mathematical constructions in this definition are the double cosets of the skeletal point group in some larger permutation group of identically substituted skeletal sites. This concept is generalized to include the more practical case in which the sites are not identically substituted and in which rearrangements can therefore be degenerate or nondegenerate. A symmetry group, $S_{n\mathrm{L}} \times S_{n\mathrm{S}}$, is defined which includes all permutations which act on ligand and site labels separately. The generalized stereoisomerization modes are found to be collections of double cosets in this group. It is then shown that the schemes used in some previously solved problems can be viewed as restrictions of this scheme. The methods are also applicable to the site exchange problems often encountered in problems in dynamic stereochemistry.

Recently there has been a considerable amount of work making use of permutation group theory to define key symmetry-based concepts in dynamic stereochemistry.[1] Although definitions and terminology vary somewhat the most important concept is probably the stereoisomerization *mode* which is defined by various double coset decompositions of a permutation group by a skeletal site point group.[1b-f] Generally, the existing treatments only consider isomerizations which can be expressed by permutations of nuclei of identical chemical composition. The purpose of this article is to generalize the mode concept by including isomerizations which can be expressed by permutations of nuclei of different chemical composition. This will be done by using a formalism which takes the ligand symmetry (i.e., the number of ligands of identical chemical composition) and site symmetry (e.g., skeletal point group) of the dynamic problem into account simultaneously. The experimental question addressed is this: By changing the number and kind of substituents on a molecule undergoing a skeletally degenerate rearrangement, how many more potentially observable processes are there? Such rearrangements are encountered, for example, in the study of various molecular propellers,[2] pentacoordinate system,[3] and hydrocarbons.[4] In all cases treated here the assumption will be made that the different substituents do not seriously deform the skeleton but may significantly alter the favored rearrangement mechanism. The present treatment does not deal with the case of a skeletally nondegenerate rearrangement.

Ligand-Site Permutation Group

The formulation requires a permutation group which acts on the molecular skeletal site labels and ligand labels separately. The construction of and need for such a group will be shown.

A number of existing treatments make use of the idea of an ordered molecule which is a $2 \times n$ matrix indicating the mapping of a set of n ligands to a set of n molecular sites.[1,5] Each $2 \times n$ matrix corresponds to one of the possible isomers obtained by placing the n ligands on the n sites. For example, consider the simple case of three ligands and three sites. The triangular structures used throughout are simply abstract models of molecules.



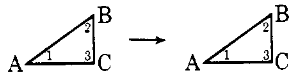
$$\begin{vmatrix} A & B & C \\ 1 & 2 & 3 \end{vmatrix}$$

1

Structure **1** is described by the $2 \times n$ matrix indicated. Isomerization can now be represented by permutations which act on either the ligand labels or the site labels. However, the same overall change can be effected by either a ligand permutation or site permutation (e.g., the ligand permutation (ABC) and site permutation (132) have the same effect on structure **1**) and these permutations are generally identified.[1e] (The conventions for defining and multiplying permutations are given in the section Notations and Conventions at the end of this paper.) Thus for certain problems it suffices to make use of only one type of permutation; site permutations are usually chosen.[1,6]

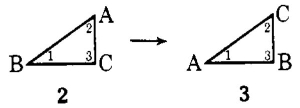
In the present formulations the $2 \times n$ matrix represents an *isomerization* rather than an isomer. Consider the examples:

$$\begin{vmatrix} A & B & C \\ 1 & 2 & 3 \end{vmatrix}$$



1 **1**

$$\begin{vmatrix} B & A & C \\ 3 & 1 & 2 \end{vmatrix}$$



2 **3**

The top row of the matrix gives the position of each ligand on the starting isomer (site labels increase from left to right in the matrix). Thus in the second example above, ligand B starts in site 1, ligand A starts in site 2, and ligand C starts in site 3. The bottom row of the $2 \times n$ matrix gives the site permutation effected by the isomerization. Again in the second example above the permutation is: the ligand in site 1 goes to site 3, the ligand in site 3 goes to site 2, and the ligand in site 2 goes to site 1. The first example above gives the $2 \times n$ matrix for the trivial isomerization of isomer **1** to itself. There will be six such trivial isomerizations since there are six possible isomers. Since each

---

* Address correspondence to the Department of Computer Science, Stanford University, Stanford, Calif. 94305.