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# Ground States of Molecules. 60.[1] A MNDO Study of Conformations of Crotyl Anion and a Diaza Analogue, of Their BeH Derivatives, and of the Interconversion of Cyclopropyl Anion and Allyl Anion

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The cis and trans isomers of crotyl anion and of the anion obtained by C deprotonation of acetaldehyde hydrazone, the derivatives formed by these ions with BeH$^+$, and the electrocyclic interconversion of cyclopropyl and allyl anions have been studied by using the MNDO method.

The stereochemistry of methyl derivatives of conjugated carbanions has aroused much interest in recent years.[3] In particular, discrepant results have been reported for that of the crotyl anion (1). Various experiments[4] have indicated that in the case of its alkali metal salts in solution, the cis isomer (2, Chart I) is more stable than the trans (3). On the other hand, studies[5] by ion cyclotron resonance (ICR) spectroscopy have shown that the reverse is true in the gas phase. Several attempts have been made to explain this discrepancy by theoretical calculations,[6,7] but so far without success. The most recent and detailed of these, by Schleyer, Dill, Pople, and Hehre,[7] predicted the cis isomer (2) to be the more stable in the gas phase, in disagreement with experiment.

We recently reported[8] a detailed study of a vinylogous system, pentadienate anion (4), and its methyl derivatives using the MNDO method.[9] The results agreed well with experiment and clarified some analogous anomalies in the experimental data. We therefore decided to use MNDO to study 2 and 3 and appropriate metal derivatives. Since MNDO parameters were not available for metals other than beryllium[10] and aluminum,[11] we used the group BeH as a model for an alkali metal atom, a procedure which had given reasonable results in the case of 4.[8] Calculations were carried out for the beryllium hydride derivatives (5 and 6) of 2 and 3 and also for the analogous series of ions and beryllium hydride derivatives 7-10 derived from acetaldehyde hydrazone (11) by deprotonation. We also studied the electrocyclic conversion of cyclopropyl anion (12) to allyl anion (13) for reasons indicated below.

**Chart I**

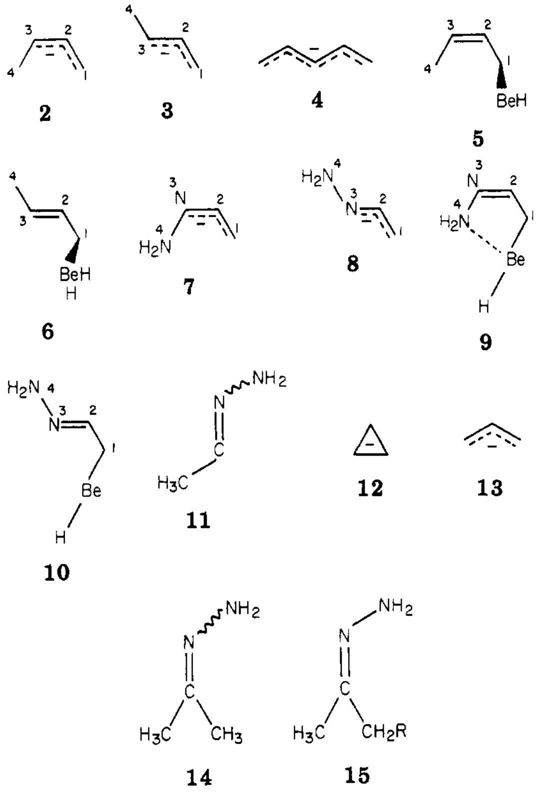

Table I. Heats of Formation ($\Delta H_f$) and Interconversion ($\Delta H$) (kcal/mol) of the Cis and Trans Isomers of Crotyl Anion and Acetaldehyde Hydrazone Anion and of the Corresponding HBe Complexes

| system | type | $\Delta H_f$ cis | $\Delta H_f$ trans | $\Delta H$, cis-trans |
|---|---|---|---|---|
| crotyl | anion | 9.63 | 9.27 | 0.36 |
| | HBe complex | −11.96 | −12.76 | 0.80 |
| hydrazone | anion | 27.73 | 27.82 | −0.09 |
| | HBe complex | −5.82 | 5.66 | −11.48 |

## Procedure

The calculations were carried out by using the standard MNDO method and parameters.[9,10] Geometries were calculated by minimizing the total energy by using the

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[2] Robert A. Welch Postdoctoral Fellow. Present address: Chemistry Dept., Purdue University, West Lafayette, Indiana 47907.

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[6] (a) Grunwell, J. R.; Sebastian, J. F.; Grunwell, J. R. *Tetrahedron* **1971**, *27*, 4387. (b) Sebastian, J. F.; Grunwell, J. R.; Hsu, B. *J. Organomet. Chem.* **1974**, *78*, C1.

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[11] Davis, L. P.; Guidry, R. M.; Williams, J. R.; Dewar, M. J. S.; Rzepa, H. S. *J. Am. Chem. Soc.*, in press.

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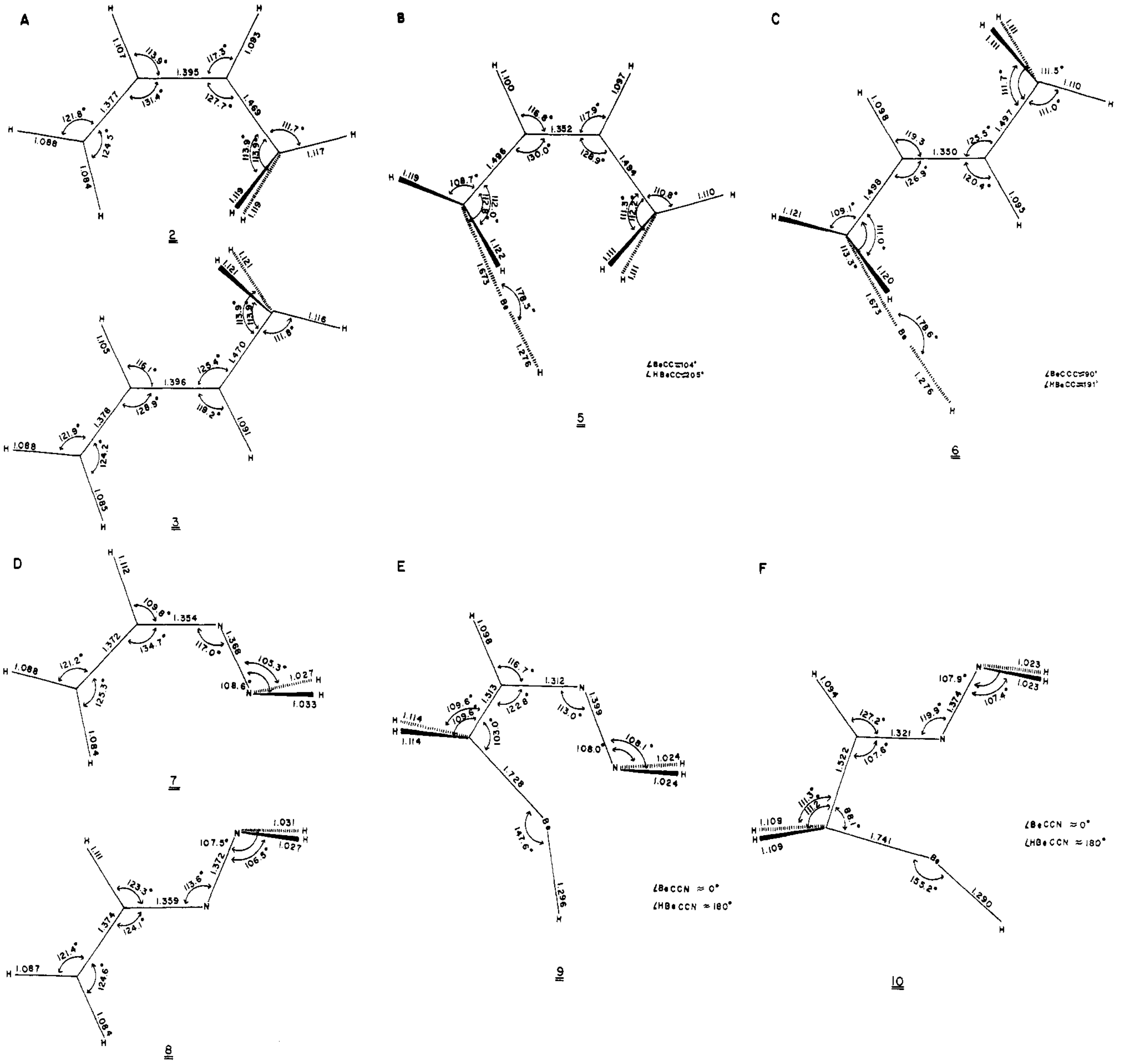

**Figure 1.** Geometries calculated for the allyl anion, the anion from acetaldehyde hydrazone, and for the corresponding HBe complexes.

Table II. Calculated Distributions of Formal Charge

| | formal charge (in units of e) at atom | | | | |
|---|---|---|---|---|---|
| compd | $C_1$ | $C_2$ | $C_3$ | $C_4$ | Be |
| 2 | −0.420 | 0.079 | −0.525 | 0.205 | |
| 3 | −0.418 | 0.077 | −0.200 | | |
| 5 | −0.234 | −0.046 | −0.140 | 0.076 | 0.485 |
| 6 | −0.234 | −0.043 | −0.146 | 0.073 | 0.484 |
| 7 | −0.463 | 0.153 | −0.549 | −0.122 | |
| 8 | −0.445 | 0.147 | −0.532 | −0.149 | |
| 9 | −0.267 | 0.124 | −0.242 | −0.082 | 0.276 |
| 10 | −0.272 | 0.205 | −0.242 | −0.154 | 0.343 |
| 12 | 0.048 | −0.783 | 0.048 | | |
| 13 | −0.494 | 0.107 | −0.494 | | |
| 14 | −0.137 | −0.446 | −0.137 | | |

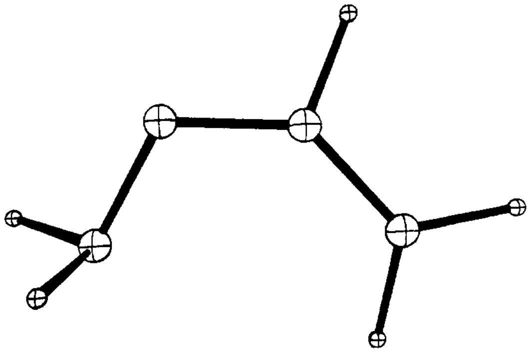

**Figure 2.** ORTEP plot for ion 7.

Davidon–Fletcher–Powell[12] procedure, standard in MNDO,[9] without making any assumptions. The transition state for 12 → 13 was found by taking the length of the breaking bond as the reaction coordinate and refined by minimizing the scalar gradient of the energy.[13] All stationary points were checked[13] by calculating and diagonalizing the Hessian (force constant) matrix using Cartesian coordinates. Convergence was confirmed by the presence of six near-zero eigenvalues, all the other eigenvalues being positive for minima while a transition state

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Table III. Some Bond Orders in Species Calculated by Using MNDO

| compd | bond order | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | $C_1,C_2$ | $C_1,C_3$ | $C_2,C_3$ | $C_3,C_4$ | $C_1,C_4$ | $C_1,H_4$ | $C_1,Be$ | $Be,C_4$ | $Be,H_4$ |
| 2 | 1.41 | 0.156 | 1.77 | 1.32 | 0.057 | 0.038 | | | |
| 3 | 1.41 | 0.141 | 1.92 | 1.20 | 0.102 | 0.036 | | | |
| 5 | 1.14 | 0.206 | 1.95 | 1.28 | 0.046 | 0.013 | 1.637 | 0.027 | 0.023 |
| 6 | 1.12 | 0.204 | 1.94 | 1.12 | 0.089 | 0.010 | 1.395 | 0.018 | 0.013 |
| 7 | 1.47 | 0.358 | 1.74 | 1.43 | 0.125 | 0.010 | | | |
| 8 | 1.45 | 0.325 | 1.66 | 1.23 | 0.134 | 0.002 | | | |
| 9 | 1.08 | 0.212 | 1.86 | 1.41 | 0.184 | 0.028 | 1.254 | 0.951 | 0.055 |
| 10 | 1.12 | 0.194 | 1.65 | 1.14 | 0.163 | 0.022 | 1.204 | 0.067 | 0.010 |
| 12 | 1.46 | 1.246 | 1.46 | | | | | | |
| 13 | 1.60 | 0.340 | 1.60 | | | | | | |
| 14 | 1.65 | 0.978 | 1.65 | | | | | | |

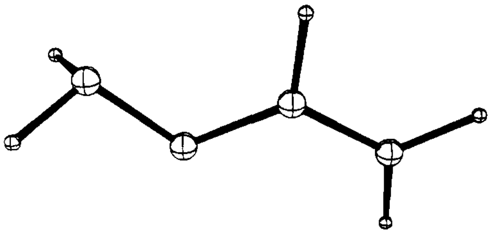

**Figure 3.** ORTEP plot for ion 8.

has one negative eigenvalues.[13]

## Results

The heats of formation calculated for **2**, **3**, and **5–10** are shown in Table I, together with the differences in energy between pairs of cis–trans isomers. Figure 1 shows geometries for **2**, **3**, and **5–10**. Table II lists calculated formal charges and Table III some relevant bond orders. ORTEP plots for ions **7** and **8** are depicted in Figures 2 and 3. Figure 4 shows the geometries and energies calculated for **12**, **13**, and the transition state **14** for their interconversion, the last being illustrated by the ORTEP plot in Figure 5.

## Discussion

As Table I shows, MNDO predicts the trans isomer (**3**) of **1** to be the more stable, in agreement with experiment[5] but in contrast to previous calculations.[6,7]

Clearly no strong conclusions can be drawn from these calculations because the calculated differences in energy between **2** and **3**, both ab initio[7] and MNDO, are so small. Furthermore, the ab initio calculations referred to molecules with the nuclei fixed at their equilibrium positions, no allowance being made for zero-point energy or thermal energy.

In MNDO these are taken into account via the parametrization, so errors in their tacit estimation are included in the overall errors in calculated heats of formation. The correction for vibronic energy seems to be rather effective, given the apparent success[7] of MNDO in predicting small differences in energy between conformational isomers such as that considered here. A further problem, however, is that equilibria are determined by free energies of reaction and so depend on differences in entropy which have not so far been considered and which, of course, have almost always been disregarded in ab initio calculations because of the lack, until recently, of techniques for calculating them and because of the cost of the calculations.

We therefore decided to calculate the relevant thermodynamic properties of **2** and **3**, partly as a check on the contributions of the vibronic terms to the enthalpy and partly to estimate the contributions of entropy to the equilibrium. Problems arise in calculating entropies of molecules which have free, or almost free, internal rotation, and while techniques for treating such cases have been developed, they have not yet been implemented in MNDO. However, the only relevant rotation in **2** or **3** is that about the C–$CH_3$ bonds, and the contribution to the total entropy is unlikely to differ significantly in the two cases. The entropies were therefore calculated by omitting the contribution of this particular normal mode. The results are shown in Table IV.

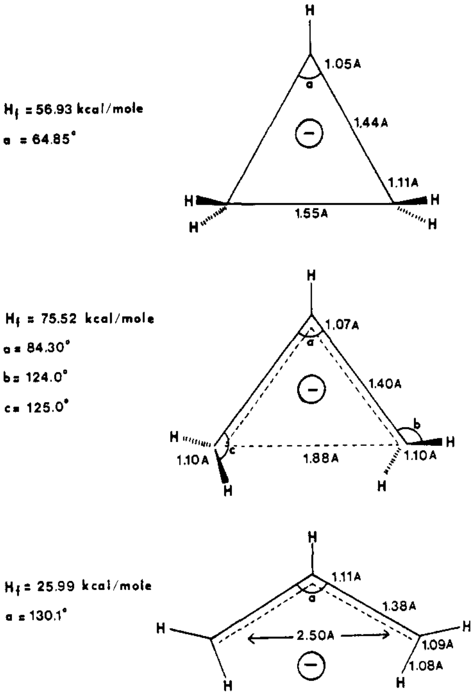

**Figure 4.** Bond lengths (Å) and heats of formation (kcal/mol) in (a) cyclopropyl anion (**12**); (b) allyl anion (**13**); (c) the transition state (**14**) for their interconversion.

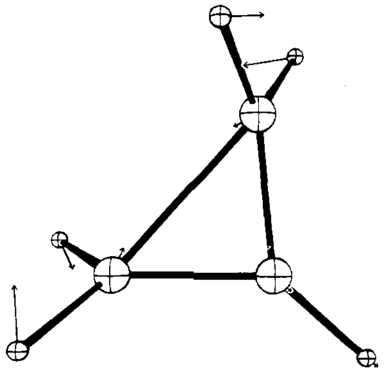

**Figure 5.** ORTEP plot of the transition state (**14**) for conversion of cyclopropyl anion (**12**) to allyl anion (**13**). The arrows indicate the transition coordinate.

It will be seen that the vibronic contributions to the enthalpies of **2** and **3** are almost identical and that the

Table IV. Vibronic Energies and Entropies of *cis*- and *trans*-1-Methylallyl Anions

| | cis (2) | trans (3) |
|---|---|---|
| zero point energy[a] | 62.36 | 62.19 |
| vibrational energy[a,b] | 1.53 | 1.67 |
| rotational energy[a,b] | 0.89 | 0.89 |
| total vibronic energy[a] | 64.78 | 64.75 |
| vibrational entropy[c,d] | 5.22 | 5.76 |
| rotational entropy[c] | 24.18 | 23.87 |
| translational entropy[c] | 37.92 | 37.92 |
| total entropy[c,d] | 67.32 | 67.55 |

[a] In kilocalories per mole at 25 °C. [b] Thermal contribution. [c] In calories per mole per degree. [d] Neglecting the contribution of internal rotation about the $C-CH_3$ bond.

difference between the calculated entropies is small. Furthermore, the difference in entropy further favors the trans isomer (**3**), the calculated difference in free energy between **2** and **3** at 25 °C being 0.43 kcal/mol.

It is clear that the preference for the cis isomer (**2**) in solution must arise from an interaction with the gegenion. We tried to model this using $BeH^+$ as an analogue for an alkali metal cation; unfortunately, no MNDO parameters for alkali metals are as yet available, due to the lack of gas-phase thermochemical data for their compounds. However, as Table I shows, the trans BeH derivative (**6**) is also predicted to be the more stable. In the case of the pentadienate anion (**4**), MNDO predicted the $HBe^+$ derivative to be most stable in the all-cis ("U") conformation, this being stabilized by interactions between the beryllium atom and the negatively charged carbon atoms of both terminal methylene groups. While the methylene groups rotate out of planarity to allow these interactions to take place,[8] the $\pi$ system of the anion retains much of its integrity, the bonding interactions between beryllium and carbon being less than in a typical C–Be covalent bond.

In **5** and **6**, however, the beryllium atom is covalently bound to the adjacent carbon atom which has a normal tetrahedral geometry, as indicated in **5**, **6**, and Table II. The $\pi$-allyl system is completely destroyed. The C–Be bond is almost coplanar with the axis of the adjacent carbon 2p $\pi$ AO. This geometry favors hyperconjugation between the CBe $\sigma$ bond and the CC $\pi$ bond. Indeed, **5** and **6** are derived from *cis*- and *trans*-2-butene by replacing one hydrogen atom by a BeH group. This conclusion is further supported by the calculated formal charges in **2**, **3**, **5**, and **6** (Table III). In **2** and **3**, there are large negative charges on the terminal allylic carbon atoms ($C_1$ and $C_3$), significant negative charges on the methyl hydrogen atoms, and quite a large positive charge on the methyl carbon, the last being a nice example of the charge-alternation effect.[14] In **5** and **6**, the atoms of the methyl group are almost neutral, and the charges on $C_1$ and $C_3$ are much smaller than those in **2** or **3**. The charge on beryllium is less than half a unit (of electronic charge), and the $C_1$–Be bond order (Table III) is very large.

It seems very likely that the preferred cis orientation in solution is due to the presence of dissociated species consisting of ion pairs of **2** and **3** with a metal cation, the cis isomer being favored because of electrostatic interactions between the cation and the negatively charged hydrogen atoms of the methyl group. Beryllium is, of course, less electropositive than any alkali metal, even lithium, so it would not be surprising if $BeH^+$ formed a covalent molecule with **1** under conditions where the alkali metal derivatives were ionic. However, it may well be, in the case of the lithium derivative at least, that these compounds are covalent in isolation, i.e., in the gas phase, but ionic in solution, due to solvation of the lithium cations. Even a relatively nonpolar solvent can stabilize cations quite effectively. Equally, the beryllium derivative might also be ionic in solution, as a result of similar solvation of $HBe^+$. Such solvation effects cannot, unfortunately, be reliably modeled by currently available procedures.

A stabilizing bifunctional interaction by the metal should be much stronger in the case of analogues of **5** or **6**, derived from an anion analogous to **1** but with the methyl carbon group replaced by a heteroatom, because here a lone pair of the (negatively charged) heteroatom can interact with the metal. Indeed, Jung and Shaw[15] have reported that deprotonation of acetone dimethylhydrazone (**14**) with lithium dimethylamide took place at the methyl group cis to the dimethylamino group and that reaction of the resulting anion with alkyl halide gave derivatives of **14** substituted at that methyl (i.e., **15**). We therefore carried out MNDO calculations for the simplest anion of this type, derived by deprotonation of acetaldehyde hydrazone (**11**) and capable of existing in syn (**7**) and anti (**8**) forms analogous to **2** and **3**. We also carried out calculations for the corresponding BeH derivatives, **9** and **10**.

As Table I shows, **7** and **8** are calculated to have almost identical energies, though this time it is the cis isomer that is marginally more stable. In the case of the BeH derivatives, however, the isomers differ dramatically in energy, the cis isomer now being very much more stable than the trans (**10**). Also, the beryllium atom in **5** or **6** lies out of the plane of the carbon atoms, the carbon–beryllium bond being almost coplanar with the 2p AO of the adjacent doubley bound carbon atom. This orientation should lead to maximum stabilization by hyperconjugation of the CBe bond with the $\pi$ electrons of the adjacent CC double bond.[16] On the other hand, the beryllium in **9** lies in the same plane as the other atoms, being simultaneously bonded to both terminal atoms (as indicated in **9**). The trans derivative (**10**) also has the beryllium atom in the same plane as carbon and nitrogen, the driving force here being presumably an interaction between it and the lone pair of the imine nitrogen. The bond order of the $C_4$–Be bond in **9** is also large (Table IV). Note also that the positive charges on beryllium in **9** and **10** are much less than those in **5** or **6** (Table II), although the heteroatoms in **16** should make it a less effective electron donor than **1**. Clearly this is compensated by the interactions with nitrogen lone pairs. Furthermore, the positive charge on beryllium is much less in the cis isomer **9** than in the trans isomer **10**, as would be expected, because steric repulsions should make the lone pair interaction smaller in the latter. A strong interaction between beryllium and the lone pair electrons of the imine nitrogen leads to a stronger stabilization than hyperconjugation between the CBe $\sigma$ bond and the CC $\pi$ bond. The existence of such an interaction is indeed indicated by the quite large value of the corresponding (NBe) bond order (Table IV).

The problems we have been discussing are related to the stability of the allyl anion with respect to processes which destroy the three-orbital $\pi$ system. We thought it would be a good idea to study another well-known process of this kind, namely, the electrocyclic conversion of allyl anion (**13**) to cyclopropyl anion (**12**), both as a test of the ability

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[14] See: Dewar, M. J. S. "The Molecular Orbital Theory of Organic Chemistry"; McGraw-hill: New York, 1969; Section 5.11.

[15] Jung, M. E.; Shaw, T. J. *Tetrahedron Lett.* **1977**, 3305.

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of MNDO in this connection and because this reaction is of interest as one of the simplest pericyclic processes. While a number of calculations have been reported[17] for it, none of these has used MNDO.

Figure 4 indicates the geometries and heats of formation calculated here for **12**, **13**, and the transition state for their interconversion. No experimental values are available for comparison.

Figure 5 is an ORTEP plot of the transition state showing the transition coordinate, i.e., the eigenvector corresponding to the normal mode with a negative force constant.

The reaction takes place conrotatorily, as expected[18] and as predicted by all previous calculations.[17] Our values lead to a heat of reaction (–30 kcal/mol) which agrees very well with that (–31 kcal/mol) given by an ab initio calculation,[17] but our estimate of the activation energy (–18.6 kcal/mol) is considerably less than the ab initio value (27 kcal/mol). The ab initio value is, however, likely to be too high because the procedure used to locate the transition state was inadequate.[13]

Judging by these results, there seems no reason to believe that MNDO encounters any special problems in systems of this kind. Calculations[19] for a number of anions have indeed indicated that difficulties arise only for very small anions where most of the formal negative charge is concentrated on a single atom.

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**Registry No.** **2**, 54078-18-1; **3**, 54078-26-1; **5**, 81389-28-8; **6**, 81389-29-9; **7**, 81389-30-2; **8**, 81389-31-3; **9**, 81389-32-4; **10**, 81389-33-5; **12**, 1724-45-4; **13**, 1724-46-5; **14**, 5281-20-9.

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[17] (a) Clark, D. T.; Armstrong, D. R. *Theor. Chim. Acta* **1969**, *14*, 370. (b) Clark, D. T.; Smale, G. *Tetrahedron Lett.* **1968**, 3673.

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[19] Dewar, M. J. S.; Rzepa, H. S. *J. Am. Chem. Soc.* **1978**, *100*, 784.

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# [(4-Nitrophenyl)thio](2,4,6-tri-*tert*-butylphenyl)aminyl: Its Preparation, Isolation, and Molecular Structure[1]

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[(4-Nitrophenyl)thio](2,4,6-tri-*tert*-butylphenyl)aminyl (**2a**) and related radicals have been generated and studied by ESR spectroscopy. Radical **2a**, produced by oxidation of *N*-[(4-nitrophenyl)thio]-2,4,6-tri-*tert*-butylaniline (**1a**) with lead dioxide, was isolated as pure dark brown needles in 45% yield and was stable for one month while exposed to air. The molecular structure has been determined by X-ray diffraction analysis. The radical crystallizes in the monoclinic space group $P2_1/c$ with $a = 9.352$ (2) Å, $b = 14.315$ (5) Å, $c = 18.426$ (3) Å, $\beta = 93.23$ (2)°, and $Z = 4$. The structure shows that the nitrogen and sulfur atoms, the *S*-phenyl ring, and the nitro group are almost in the same plane, while the *N*-phenyl ring is 90.7° twisted from the coplane. The S–N bond distance found for **2a** is 1.605 (8) Å, which lies between the typical S–N single and double bond distances. This intermediate bond distance is interpreted in terms of the formation of a three-electron bond between the nitrogen and sulfur atoms.

Free radicals are important intermediates in organic and photochemical reactions and are generally very reactive species. However, electronic stabilizations and steric protections often make them persistent. For instance, 2,2-diphenyl-1-1-picrylhydrazyl,[2] verdazyls,[3] and nitroxide radicals[4] can be isolated as pure crystals or oils. However, such extremely persistent free radicals are rather rare, and most of the free radicals generated so far are transient or have relatively short limited lifetimes under the usual conditions.[5,6] Therefore, it is of considerable interest to prepare a new class of isolable free radicals.

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[1] Part 17 in the series "ESR Studies of Nitrogen-Centered Free Radicals". For part 16, see: Miura, Y.; Nakamura, Y.; Kinoshita, M. *Bull. Chem. Soc. Jpn.* **1981**, *54*, 3217.

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