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Non-Empirical LCAO-MO-SCF Calculations with Gaussian Type Functions on the Electrocyclic Transformation of Cyclopropyl to Allyl

II. Anion Transformation

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Non-empirical molecular quantum chemical calculations have been performed on the electrocyclic transformation of planar and non planar cyclopropyl anions, to allyl anions in the LCAO-MO-SCF framework using gaussian type functions as atomic orbitals. Employing a total of 37 GTF 3 disrotatory and 2 conrotatory modes of transformation have been considered. A total of 34 calculations have been carried out. In the transformation of planar and non planar cyclopropyl anions to allyl anions, both the disrotatory and conrotatory modes possess activations barriers, those for the conrotatory modes being the lower by substantial margins. A detailed analysis of the energy terms involved show that is little theoretical justification for the postulate that the mode of ring opening depends only on the symmetries of the highest occupied orbitals.

Nichtempirische SCF-MO-Rechnungen mit Gaußfunktionen (GF) für den Übergang des planaren und des unplanaren Cyclopropylanions zum Allyanion wurden vorgenommen. Mit einem Basissatz von 37 GF wurden 34 Rechnungen für 3 disrotatorische und 2 conrotatorische Übergänge durchgeführt. Sowohl die disrotatorischen als auch die conrotatorischen Übergänge besitzen Aktivierungsbarrieren, von denen diejenigen für die conrotatorischen Übergänge stets kleiner sind. Die Analyse der Energieterme gibt wenig Anlaß zu der Annahme, daß die Art der Ringöffnung nur von der Symmetrie des obersten besetzten Orbitals abhängt.

Des calculs *ab-initio* en orbitales gaussiennes ont été effetués sur la transformation de cations cyclopropyliques en cations allyliques. Les barrières d'activation sont toujours plus basses pour la mode conrotatoire que pour la mode disrotatoire. Il est peu evident que l'ouverture du cycle dépende que de la symmetrie de la plus haute orbitale occupée.

1. Introduction

In Part I [1] we presented the results of an *ab initio* treatment of the transformations of cyclopropyl to allyl cation. In this paper we present similar results for the anion transformations.

In a previous communication [2] the ground state and lower excited singlet and triplet state energy differences between various modes of transformation of cyclopropyl to allyl anion have been investigated by a semi empirical all valence

SCF MO method. The motivation for this investigation was to clarify the original predictions of Woodward and Hoffmann [10] and Longuet-Higgins and Abrahamsom [8] particularly for transformations involving excited states. However, although the semi empirical all valence SCF MO treatment is on a surer theoretical basis for charged species, than EHT used in the original work, the method is unsatisfactory [2, 3] for calculating energy changes between species in which the bond lengths are different. On the other hand an *ab initio* treatment has the principal disadvantages of requiring relatively powerful computing facilities but has the major advantage that all the terms of the total energy are effectively calculated and that one can then distinguish the contribution of each of them to a global energetic effect. This allows a detailed comparison of energy differences between various modes of transformation to test the validity of the Woodward Hoffmann approach.

As in the previous work [1] the transformations of both planar and non planar cyclopropyl species have been investigated, the definition of the various modes being as described previously. However the emphasis of the work is slightly changed from that of the cationic species since calculations show that a free cyclopropyl anion is non planar anyway so that the Dis(1), Dis(2) and Con(1) modes of transformations [1, 3] are prototypes for both the *concerted* and *non concerted* transformation of cyclopropyl to allyl anion. The Dis(0) and Con(0) [1, 3] modes then represent hypothetical transformations of a planar cyclopropyl anion to allyl anion. However this also has considerable interest since one of the most unsual findings in the cationic case [1] was that in the disrotatory transformation of *planar* cyclopropyl cation after $\sim 30°$ angle of rotation on the reaction co-ordinate the *non planar* species corresponding to the Dis(2) mode became the more favoured. It is of interest therefore to see if this behaviour is mirrored in the case of a non planar cyclopropyl anion where perhaps the planar species might become the favoured one as the transformation proceeds.

2. Method of Calculation

The calculations performed in this work were carried out using the Polyatom system [4, 5] tailored to make use of the extensive disc handling facilities of the NUMAC IBM 360/67. The five modes of transformation were studied at 15° intervals in the rotation of the H2–C2–H3 (H4–C3–H5) planes with respect to the plane of the ring. The numbering system co-ordinate axes, bond angles and bond lengths used in the calculations were as previously given [1, 3]. The integrals generated for each point on the reaction co-ordinate, for the cationic species were stored on disc (IBM 2314) and were then utilized in the SCF procedure for both the cation and anion. In particular cases however difficulty was experienced with convergence of the SCF procedure, and despite using several devices which we have previously found to be useful in such cases, convergent solutions were not obtained for the points corresponding to Dis(1) and Con(1) 45°. However for a 50° angle of rotation the solutions were convergent. A total of 34 calculations have been carried out, a basis set of 37 GTF being used as previously described.

3. Results and Discussion

3.1. Energies for Bent and Planar Cyclopropyl and Allyl anions

Table 1 shows the energies and symmetries of the occupied and two lowest energy virtual orbitals for bent and planar cyclopropyl and allyl anions. The energy of each orbital is considerably higher than the corresponding orbital of the cation [1], in particular the effect of the extra two electrons on the carbon 1*s* orbitals should be noted. For the planar cyclopropyl anion the highest occuped and lowest energy virtual orbitals are of "pseudo" π-symmetry, consisting of the carbon p_x orbitals and anti symmetric combinations of the hydrogen 1*s* orbitals. The occupied orbital is concentrated about C1 whereas the virtual orbital is spread over C2, C3 and the hydrogen atoms. In allyl anion the corresponding orbitals are of π-symmetry the highest occupied orbital consisting of an anti symmetric combination of C2 and C3 p_x orbitals, whilst the lowest virtual orbital is concentrated largely on C1. Applying Koopman's theorem the ionisation potential of the anions, equal to the negative of the electron affinity of the corresponding radicals are calulated to be 0.971 eV, 0.283 eV and 0.629 eV for planar, non planar cyclopropyl and allyl respectively. These values would appear to be reasonable (cf. CH_3 1.08 eV [9]).

Table 1. *Energies and symmetries of the occupied and two lowest energy virtual orbitals for bent and planar cyclopropyl and allyl anions (energies in a. u.)*

	Cyclopropyl anion		Allyl anion
	Bent	*Planar*	
Virtual orbitals	+0.6003 A'' $14\sigma^*$	+0.6002 $B2$ $14\sigma^*$	+0.5507 $A1$ $14\sigma^*$
	+0.5272 A' $13\sigma^*$	+0.5584 $B1$ $13\sigma^*$	+0.4694 $B1$ $13\pi^*$
Occupied orbitals	+0.0104 A' 12σ	+0.0357 $B1$ 12σ	+0.0231 $A2$ 12π
	−0.1439 A'' 11σ	−0.1351 $B2$ 11σ	−0.1698 $B1$ 11π
	−0.1879 A' 10σ	−0.1933 $A1$ 10σ	−0.2486 $B2$ 10σ
	−0.2781 A'' 9σ	−0.2684 $A2$ 9σ	−0.2538 $A1$ 9σ
	−0.3360 A' 8σ	−0.3589 $A1$ 8σ	−0.3140 $B2$ 8σ
	−0.4157 A' 7σ	−0.4008 $B1$ 7σ	−0.3768 $A1$ 7σ
	−0.5067 A' 6σ	−0.4879 $A1$ 6σ	−0.4966 $A1$ 6σ
	−0.5727 A'' 5σ	−0.5650 $B2$ 5σ	−0.6218 $B2$ 5σ
	−0.8656 A' 4σ	−0.8494 $A1$ 4σ	−0.7672 $A1$ 4σ
	−10.5179 A' 3σ	−10.5131 $A1$ 3σ	−10.5471 $A1$ 3σ
	−10.6360 A'' 2σ	−10.6354 $B2$ 2σ	−10.5472 $B2$ 2σ
	−10.6358 A' 1σ	−10.6362 $A1$ 1σ	−10.6289 $A1$ 1σ
Electronic energy	−180.26367	−179.86996	−176.18932
Nuclear energy	68.42081	68.02974	64.24261
Total energy	−111.84286	−111.84022	−111.94671

The calculations indicate that a free cyclopropyl anion will adopt a "bent" configuration about C1, the difference in energy between the bent and planar configurations being 1.66 kals/mole. The nuclear energy favours the planar form by a considerable margin but this is just offset by the lower electronic energy of the non planar form.

For the transformation of non planar cyclopropyl to allyl anion the calculated energy change is 0.1039 a. u. (65.2 kals/mole). This is almost indentical to the value obtained for the cation transformation with the same size basis set [1].

3.2. Analysis of Energy Terms for the Disrotatory and Conrotatory Modes of Transformation for a Bent Cyclopropyl Anion, Analogue for a Concerted and Non Concerted Reaction Process

As we have already indicated the situation involving the anion is somewhat different from that of the cation where the free cyclopropyl species adopted a planar configuration about C1 [1]. For the anion the non planar configuration of cyclopropyl is energetically preferred so that the Dis(1), Dis(2) and Con(1) modes serve as models for both the concerted and non concerted processes.

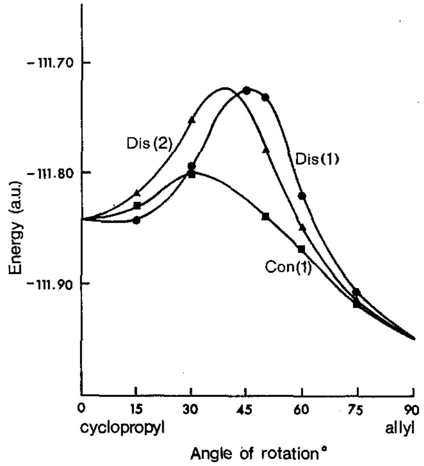

Fig. 1. Energy (a. u.) versus angle of rotation ° for Dis(1), Dis(2) and Con(1) transformation of cyclopropyl to allyl anion

Fig. 1 shows a plot of energy versus reaction co-ordinate for the three modes. An interesting feature here is that in contrast to the cation case where the favoured Dis(0) mode showed no activation barrier, all three modes of transformation possess activation barriers of 73.95 kals/mole, 73.95 kals/mole and 26.92 kals/mole for the Dis(1), Dis(2) and Con(1) modes respectively. For the non concerted reaction therefore in which an initially formed cyclopropyl carbanion is produced which then rearranges, one would expect the anion to have a substantial lifetime, this is in contrast to the cation which has a great propensity ro rearrange since the Dis(0) modes requires no activation barrier. The conrotatory mode is clearly favoured as predicted by EHT in the original work [10] and confirmed by the all valence electron SCF MO calculations [2]. Since the effect of the leaving group is not specifically taken into account for the concerted reaction we cannot say anything about the activation barriers for this type of process, however the *energy differences* between the modes should be mirrored in the non concerted transformation of the non planar cyclopropyl anion so that again the conrotatory process should be clearly favoured. There appears to be no experimental evidence as yet for the ring opening of cyclopropyl anion itself, however a derivative of the isoelectronic aziridine ring system has been studied. Huisgen and co-workers [6] have studied the thermolysis of both cis and trans dimethyl 1 (4 methoxy phenyl) aziridine 2,3 dicarboxylate and by trapping the intermediate ring opened azomethine ylids with dimethyl acetylene dicarboxylate have shown that ring opening occurs stereospecifically in a conrotatory fashion.

Fig. 2 shows a plot of the orbital energies for both the occupied and two lowest energy virtual orbitals for the Dis(1), Dis(2) and Con(1) modes of transformation. For the disrotatory modes the highest occupied orbital of bent cyclopropyl anion correlates with the lowest virtual orbital of allyl anion. As in the cation case [1] there are significant changes in the inner shell carbon 1*s* orbital energies.

The various energy terms contributing to the total energy may be written as follows Eq. (1).

$$E_{\mathrm{Total}} = E_1 + E_2 + E_3 \tag{1}$$

where E_1 = sum of orbital energies,

E_2 = sum of electron repulsion terms,

E_3 = nuclear repulsion term.

Table 2 gives an analysis of these energy terms for the Dis(1), Dis(2) and Con(1) modes and also the energy differences between the modes. Also included are the contributions to the orbital energy term arising from the highest occupied orbitals, since according to Woodward and Hofmann [10] it is the energy differences arising in these orbitals that largely determines the energy difference between disrotatory and conrotatory modes. Considering first the energy terms for the Dis(1) and Con(1) modes, the major energy differences between these modes occurs in the region corresponding to 30°–60° angle of rotation along the reaction co-ordinate.

In each of the cases corresponding to 30°, 50°, and 60° angles of rotation the lower energy of the Con(1) mode results largely from the lower electronic energy, the nuclear energy terms being much smaller and favouring the Con(1) mode. For a 30° angle of rotation the lower electronic energy of the Con(1) mode is attributed to the lower electron repulsion energy term, the orbital energy term actually favouring the disrotatory mode even though the contribution to the latter term arising from the highest occupied orbital is opposite in sign. At 50° and 60° the lower energy of the Con(1) mode is largely due to the lower orbital energy term the electron repulsion terms in each case strongly favouring the Dis(1) mode. However the contribution to ΔE_1 arising from the highest occupied orbital is by no means predominant. In fact there is very little correlation between ΔE_1 and the particular term in this summation arising from the highest occupied orbital as suggested by Woodward and Hoffmann [10]. The largest energy differences between the Dis(2) and Con(1) modes also occur in the region 30°–60°, in this case however the nuclear energy terms are substantially larger and in each case favour the Con(1) mode. At 30° the lower energy of the Con(1)

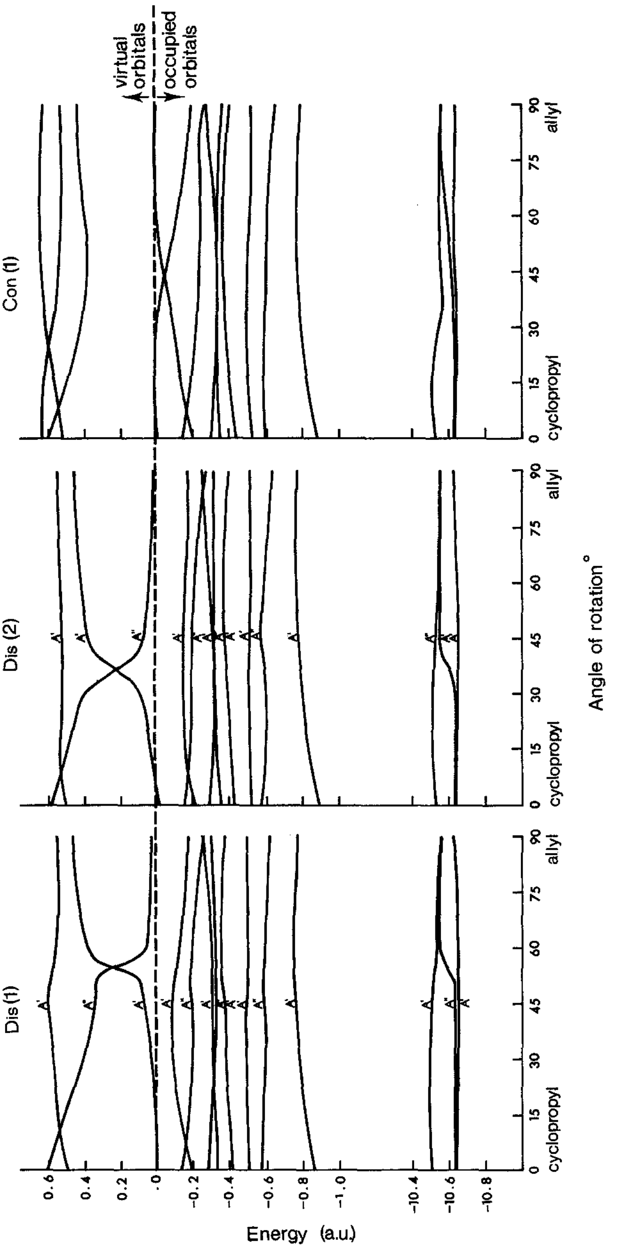

Fig. 2. Orbital correlations for Dis(1), Dis(2) and Con(1) modes of transformation of cyclopropyl to allyl *anion*

mode arises mainly from ΔE_1 the orbital energy term, however for 50° and 60° angles of rotation the orbital energy and electron repulsion terms are of comparable magnitude, the preference for the Con(1) mode arising from a combination of nuclear and electronic energies. For a 75° angle of rotation however the electronic energy term actually favours the Dis(2) mode and the small preference for the Con(1) mode then arises from the nuclear energy term. It is clear however that

Table 2. *Detailed comparison of energy terms for the* Dis(1), Dis(2) *and* Con(1) *modes (all energies in a. u.)*

Angle of rotation		Electronic energy			Nuclear energy	Energy differences relative to Con(1) mode					
and mode		E_1	E_2	E_1+E_2	E_3	ΔE_1	ΔE_2	$\Delta(E_1+E_2)$	$\Delta\varepsilon^*_{\mathrm{HOC}}$	ΔE_3	$\Delta E_{\mathrm{Total}}$
0°	Dis(1)	−70.1774	−110.0863	−180.2637	68.4208	0	0	0	0	0	0
	Dis(2)										
	Con(1)										
15°	Dis(1)	−70.0732	−108.4799	−178.5531	66.7125	−0.0584	0.0512	−0.0072	−0.0115	−0.0033	−0.0105
	Dis(2)	−70.1006	−108.4450	−178.5456	66.7269	−0.0858	0.0861	+0.0003	0.0201	0.0112	0.0113
	Con(1)	−70.0148	−108.5311	−178.5459	66.7158	0	0	0	0	0	0
30°	Dis(1)	−69.9306	−107.4478	−177.3784	65.5835	−0.0632	0.0674	0.0042	0.0144	0.0002	0.0044
	Dis(2)	−69.8390	−107.5169	−177.3559	65.6030	0.0284	−0.0017	0.0267	0.0694	0.0197	0.0464
	Con(1)	−69.8674	−107.5151	−177.3826	65.5835	0	0	0	0	0	0
50°	Dis(1)	−69.5294	−106.9357	−176.4651	64.7339	0.2041	−0.1011	0.1030	0.1646	0.0033	0.1063
	Dis(2)	−69.5976	−106.9317	−176.5293	64.7494	0.1359	−0.0971	0.0388	0.1634	0.0188	0.0576
	Con(1)	−69.7335	−106.8346	−176.5681	64.7306	0	0	0	0	0	0
60°	Dis(1)	−69.6494	−106.4296	−176.0790	64.2598	0.0914	−0.0484	0.0430	0.0343	0.0035	0.0465
	Dis(2)	−69.6866	−106.4311	−176.1177	64.2697	0.0542	−0.0499	0.0043	0.0383	0.0134	0.0177
	Con(1)	−69.7408	−106.3812	−176.1220	64.2563	0	0	0	0	0	0
75°	Dis(1)	−69.8540	−106.2563	−176.1103	64.2049	−0.0648	0.0733	0.0086	0.0034	0.0012	0.0098
	Dis(2)	−69.8466	−106.2744	−176.1210	64.2078	−0.0574	0.0552	−0.0022	0.0043	0.0041	0.0019
	Con(1)	−69.7892	−106.3296	−176.1189	64.2037	0	0	0	0	0	0
90°	Dis(1)	−69.8974	−106.2919	−176.1893	64.2426	0	0	0	0	0	0
	Dis(2)										
	Con(1)										

as for the Dis(1) mode there is little correlation between the ΔE_1 terms and the individual terms arising from the highest occupied orbitals, indicating the gross oversimplification of Woodward and Hoffmann's arguments [10] for the cyclopropyl-allyl anion transformation.

3.3. Disrotatory and Conrotatory Transformation of an Initially Planar Cyclopropyl Anion

As we have indicated a free cyclopropyl anion adopts a non planar configuration so that the transformation involving a planar species are to some extent academic. However there are two points of interest. Firstly do the energy curves for the preferred conrotatory modes, Con(1) and Con(0), involving the non planar and planar species respectively, cross over as the corresponding disrotatory modes do for the cation? Secondly for the planar species the two disrotatory modes Dis(1) and Dis(2) become identical, Dis(0) and it is of interest to compare the energy difference between a conrotatory and disrotatory process as we have done for the cationic species.

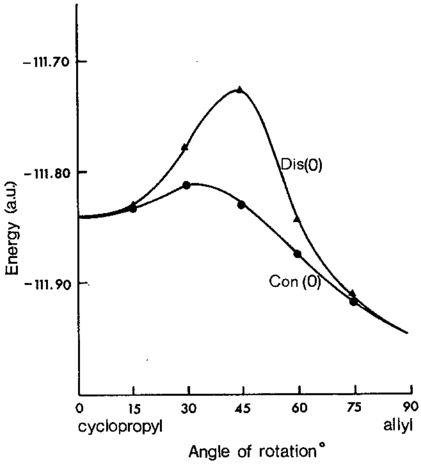

Fig. 3. Energy (a. u.) versus angle of rotation ° for Dis(0) and Con(0) transformation of planar cyclopropyl to allyl anion

Fig. 3 shows a plot of the energy of transformation against the reaction coordinates for the two modes of transformation. Both modes show activation barriers of 18.82 kals/mole and 70.90 kals/mole respectively for the Con(0) and Dis(0) modes. The activation energy difference 52.08 kals/mole may be compared with 46.2 kals/mole obtained [1] for the transformation involving the planar cations, the Con(0) mode being favoured for the anion and Dis(0) mode for the cation.

Table 3 shows an analysis of the energy terms for the Con(1) and Con(0) modes. The surprising feature here is that the planar species is actually the more stable for angles of rotation greater than 15° and this results from a lower nuclear energy, the electronic energy terms favouring the non planar species. Hence the transformation of a free cyclopropyl anion to allyl anion involves an initially

Table 3. *Detailed comparison of energy terms for the* Con(1) *and* Con(0) *modes (all energies in a. u.)*

Angle of rotation		Electronic energy			Nuclear energy	Energy differences Con(1)–Con(0)				
and mode		E_1	E_2	E_1+E_2	E_3	ΔE_1	ΔE_2	$\Delta(E_1+E_2)$	ΔE_3	ΔE_{Total}
0°	Con(1)	−70.1774	−110.0863	−180.2637	68.4208	−0.0647	−0.3290	−0.3937	0.3911	−0.0026
	Con(0)	−70.1127	−109.7573	−179.8700	68.0297					
15°	Con(1)	−70.0148	−108.5311	−178.5459	66.7158	−0.0018	−0.2558	−0.2576	0.2608	0.0032
	Con(0)	−70.0130	−108.2753	−178.2883	66.4550					
30°	Con(1)	−69.8674	−107.5152	−177.3826	65.5833	−0.0546	−0.0935	−0.1481	0.1592	0.0111
	Con(0)	−69.8128	−107.4217	−177.2345	65.4241					
60°	Con(1)	−69.7408	−106.3817	−176.1220	64.2563	0.0564	−0.0946	−0.0282	0.0355	0.0073
	Con(0)	−69.8072	−106.2886	−176.0938	64.2208					
75°	Con(1)	−69.7892	−106.3296	−176.1188	64.2037	0.1368	−0.1429	−0.0061	0.0083	0.0022
	Con(0)	−69.9260	−106.1867	−176.1867	64.1954					
90°	Con(1) Con(0)	−69.8974	−106.2919	−176.1893	64.2426	0	0	0	0	0

non planar species which rapidly assumes a planar configuration about C1 as the reaction proceeds in a conrotatory fashion. This is exactly the opposite behaviour to that exhibited by the cation [1].

3.4. Electronic Distributions

The gross atomic and bond overlap populations of the cyclopropyl and allyl anions are presented in Table 4. For all three anions the negative charge is spread over all the atoms. As might be expected there is a close similarity in electron distribution between the two cyclopropyl anions, except for the occupancy of the C1 p_x and H1 orbitals. The charge distribution in allyl anion is somewhat similar to that of the cyclopropyl anions and this is in marked contrast to the cation case [1]. The explanation for this equalization of charge is evident from the form of the highest occupied orbitals which produce a localisation of electrons in the C1 p_x orbitals and in the C2, C3 p_x orbitals for the cyclopropyl and allyl anions respectively (i. e. on those atoms in the corresponding cation which were positively charged).

Table 4. *Electron densities and bond populations of bent and planar cyclopropyl and allyl anions*

Electron densities		Planar cyclopropyl anion	Bent cyclopropyl anion	Allyl anion
C1	S	2.538	2.620	2.642
	P_x	1.827	1.569	0.904 (π)
	P_y	0.944	0.904	1.319
	P_z	1.106	1.088	1.208
Total		6.415	6.181	6.073
C2, C3	S	2.602	2.618	2.576
	P_x	1.126	1.137	1.548 (π)
	P_y	1.073	1.095	1.071
	P_z	1.324	1.360	1.074
Total		6.125	6.210	6.269
H1		1.099	1.211	1.026
H2, H4		1.059	1.034	1.106
H3, H5		1.059	1.062	1.075
Bond populations				
C1–C2		0.700	0.693	0.839
C2–C3		0.475	0.504	−0.053
C1–H1		0.717	0.661	0.747
C2–H2		0.719	0.751	0.753
C2–H3		0.719	0.706	0.743

The difference between allyl and cyclopropyl anions however is manifest in the C2–C3 bond overlap populations, the latter being strongly bonding for the cyclopropyl anions and slightly antibonding for the allyl anion. The changes in C2–C3 bond overlap populations for the Dis(0), Con(0) and Dis(1), Dis(2) and Con(1) modes are illustrated in Figs. 4 and 5 respectively. Considering firstly the Dis(0) and Con(0) modes, for angles of rotation $> 50°$ the bond overlap populations are both negative, that for the Dis(0) mode being the larger, whilst

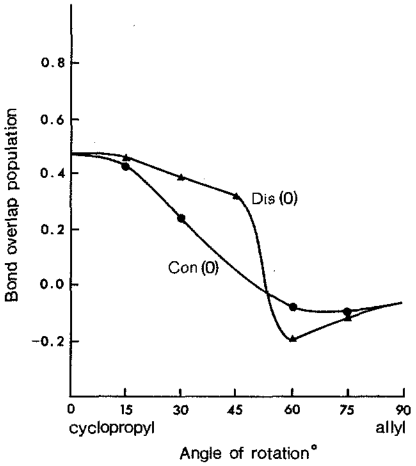

Fig. 4. Bond overlap populations between atoms C 2–C 3 for Dis (0) and Con (0) modes of transformation of planar cyclopropyl to allyl anion

for angles of rotation < 50° the bond overlap populations are positive, again that for the Dis(0) mode being the larger. Comparing this with the energy plot Fig. 3 shows quite clearly that for a 45° angle of rotation where the energy gap between the Dis(0) and Con(0) modes is the largest the Dis(0) mode in fact has the larger C2–C3 bond overlap population, again pointing to the inadequacy of the simple Woodward-Hoffmann pictorial treatment [10]. In the case of the Dis(1), Dis(2) and Con(1) modes however, the situation is somewhat better. Comparison of the energy curves Fig. 1 and Fig. 5 the C2–C3 bond overlap populations for the three modes shows some correlation between the two. Thus the antibonding situation develops more rapidly for the Dis(2) mode

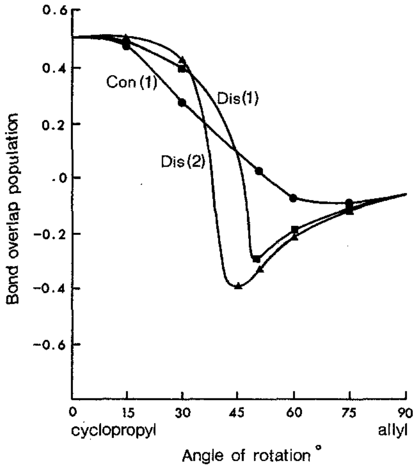

Fig. 5. Bond overlap populations between atoms C2–C3 for Dis(1), Dis(2) and Con(1) modes of transformation of cyclopropyl to allyl anion

with respect to the Dis(1) mode and the major energy difference between the corresponding modes and the Con(1) mode also develops in the same way.

In the case of the cation a simple pictorial explanation has been advanced [7] for the lower energy of the Dis(2) mode with respect to the Dis(1) mode, a concerted reaction in terms of a favourable bonding interaction between orbitals on C2 and C3 and the vacant orbital of the developing carbonium ion at C1. Our calculations [1] gave some support to this hypothesis, and indicated that for angles of rotation <45° where the energy difference between the two disrotatory modes was largest, there was a significant difference in the C1–C2 (C3) bond overlap populations as required by the simple model. In the case of the anion however one might expect this argument to be set in reverse i. e. the interaction between orbitals located at C2 and C3 with the doubly occupied orbital of the developing carbanion at C1 should be unfavourable and again show up as a difference in C1–C2 (C3) bond overlap populations. For angles of rotation less than ~40° (see Fig. 1) the Dis(1) mode is of considerably lower energy than the Dis(2) mode. Fig. 6 shows the C1–C2 (C3) bond overlap populations and again there is some evidence for the pictorial explanation since the major difference in C1–C2 (C3) bond overlap population between the Dis(1) and Dis(2) modes occurs in the same region.

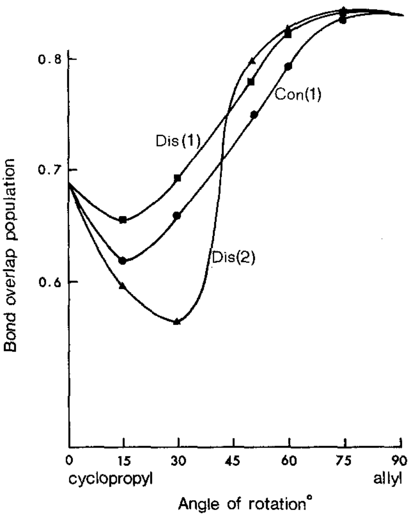

Fig. 6. Bond overlap populations between atoms C1–C2 (C3) for Dis(1), Dis(2) and Con(1) modes of transformation of cyclopropyl to allyl anion

3.5. Bond Length Variation in Allyl Anion

The molecular geometries used are those previously described for the cation transformation [1, 3]. However as a check we have carried out calculations on allyl anion varying the C–C bond length with the C–H bond length fixed at 1.08 Å. This shows a calculated minimum at 1.38 Å, and this is almost identical to that obtained for the cation (1.37 Å). This would indicate that the assumed initial and final geometries are reasonable.

By fitting a parabola to the potential energy curve a force constant for the symmetric stretching vibration of the C–C bonds of 13.47 mdyne $Å^{-1}$ was obtained.

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