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## Structures and Stabilities of $C_3H_3^-$ Anions: an *ab initio* Molecular Orbital Study

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The various minima and some of the saddle points on the  $C_3H_3^-$  potential energy surface have been studied with *ab initio* molecular orbital calculations. The structures of these species have been determined by full geometry optimizations at the Hartree-Fock level with the diffuse-function augmented basis sets 3-21+G and 6-31+G\*. In addition, improved energy comparisons have been obtained at the MP3/6-31++G\*\* level, and vibrational frequency analysis of the various species have been carried out in order to characterize the stationary points as well as to determine zero-point vibrational energies of these species.

Eight stable species have been found on the potential energy surface of  $C_3H_3^-$ . In descending order of stability, they are: 1-propynyl (1), allenide (3), cyclopropen-1-ide (5), prop-2-en-1-yliden-1-ide (6), three isomers (EZ, EE, ZZ) of prop-1-en-3-yliden-1-ide (7, 8, 9) and cyclopropen-3-ide (10) ions. The transition structures found are those for the methyl migration of 1, the inversion at the anionic center of 3, and the pseudorotation of 10.

In addition, for all the equilibrium structures found, the electron affinities of the corresponding free radicals have been calculated. From these results, it is deduced that, among the eight anionic equilibrium structures, only 10 is unstable toward spontaneous electron loss.

### INTRODUCTION

The study of carbocations, either using gas-phase experimental methods<sup>1</sup> or employing theoretical calculations,<sup>2</sup> has been making steady progress in recent years. In fact, the aforementioned two methods often complement each other. Yet, until quite recently, the same statement cannot be made for the carbanions, even though these ions do play a very important role in organic reactions.

In the past few years, some significant advances have been made in the study of carbanions. As far as theoretical investigations are concerned, it has been found that quantitatively useful chemical information can be obtained for anions from calculations with sufficiently large basis sets (such as diffuse-function augmented sets) and with adequate incorporation of electron correlation.<sup>3</sup> At such high levels of theory, properties such as ion structures and energies of reactions involving closed-shell species may be

determined with an accuracy comparable to that achievable for neutral molecules or cations. On the experimental side, new and useful techniques have also been developed for the study of carbanions. For instance, ions may be generated by inducing charge inversion collisionally, a method pioneered some years ago by Bursley *et al.*<sup>4</sup> Indeed, applying this method, Burgers and his co-workers have been able to investigate the collisionally induced fragmentations of a variety of  $C_3H_3^+$  and  $C_3H_3^-$  ions.<sup>5</sup>

The cations investigated by Burgers *et al.*,  $C_3H_3^+$  had been previously<sup>6,7</sup> studied theoretically by Pople and co-workers using *ab initio* molecular orbital calculations. Hence, it appears desirable to carry out a similar study for the  $C_3H_3^-$ . In this work, most of the structures studied are minima on the  $C_3H_3^-$  surface while some saddle points are also included. It should be pointed out that, while some of the minima on the  $C_3H_3^-$  potential energy surface have already been reported in the literature, a comprehensive study of this system using suitable basis functions and including correlation effects and vibrational analysis should be useful in determining the various structures and their relative energies.

#### METHOD OF CALCULATION AND RESULTS

The *ab initio* molecular orbital calculations have been carried out by using the Gaussian 82 system of programs.<sup>8</sup> Geometries of the stationary points on the  $C_3H_3^-$  potential energy surface have been determined at the Hartree-Fock (HF) level by employing gradient optimization technique with basis sets 3-21+G<sup>9</sup> and 6-31+G\*.<sup>9,10</sup> These diffuse-function augmented basis sets have been shown to yield satisfactory results for anionic systems.<sup>11</sup> It has been demonstrated that the inclusion of diffuse functions to split valence basis sets improves anion energy calculations significantly.

In order to characterize the stationary points found as minima (equilibrium structures) or saddle points (transition structures) and to include the effects of zero-point vibrational energies (ZPVEs) in estimating the relative energies of various structures, harmonic vibrational frequencies have been calculated at the HF level with the 3-21+G basis using geometries optimized with this basis set. As this sort of calculation is known to overestimate vibrational frequencies by about 10%, the ZPVE contributions have been scaled by a factor of 0.9. In addition, the effects of valence-electron correlation on relative energies have been determined from third-order Møller-Plesset perturbation theory<sup>12,13</sup> (MP3) calculations with the 6-31++G\*\* basis set. In other words, our best relative energies are the MP3/6-31++G\*\*//HF/6-31+G\* values.

Optimized geometries (HF/6-31+G\*) of the various species are displayed within the text. In these drawings, structural parameters determined with the 3-21+G basis set are enclosed in parentheses. Bond lengths are given in ångströms and bond angles in degrees. Calculated total energies, ZPVE and relative energies are summarized in Tables I and II, and calculated frequencies for equilibrium and transition structures are listed in Table III. Unless otherwise noted, relative energies quoted in the text correspond to MP3/6-31++G\*\* values, together with ZPVE contributions.

TABLE I  
 Calculated Total Energies (Hartrees) and Zero-point Vibrational Energies (ZPVE,  $\text{kJmol}^{-1}$ ) of  $C_3H_3^-$  Anions<sup>a</sup>

Anion	Symmetry	HF/3-21+G <sup>b</sup>	HF/6-31+G <sup>*</sup>	HF/6-31+G <sup>*</sup>	MP2/6-31+G <sup>*</sup>	MP3/6-31+G <sup>**</sup>	ZPVE <sup>c</sup>
1-Propynyl (1)	$C_{3v}$	-114.61569	-115.24621	-115.25097	-115.65671	-115.67273	111
TS for methyl migration of 1 (2)	$C_s$	-114.53116	-115.17139	-115.17631	-115.58417	-115.60298	102
Allene (3)	$C_s$	-114.59902	-115.23241	-115.23890	-115.64856	-115.66479	102
TS for inversion of 3 (4)	$C_{2v}$	-114.59530	-115.22337	-115.23041	-115.64012	-115.65402	100
Cyclopropen-1-ide (5)	$C_s$	-114.54239	-115.19336	-115.19919	-115.61570	-115.63242	105
Prop-2-en-1-yliden-1-ide (6)	$C_s$	-114.53069	-115.16406	-115.17069	-115.56047	-115.58527	101
E,Z-Prop-1-en-3-yliden-1-ide (7)	$C_s$	-114.51806	-115.15649	-115.16244	-115.54927	-115.57478	101
E,E-Prop-1-en-3-yliden-1-ide (8)	$C_{2v}$	-114.51740	-115.15614	-115.16216	-115.54955	-115.57464	101
Z,Z-Prop-1-en-3-yliden-1-ide (9)	$C_{2v}$	-114.50937	-115.14949	-115.15563	-115.54179	-115.56814	99
Cyclopropen-3-ide (10)	$C_s$	-114.47806	-115.12757	-115.13395	-115.55459	-115.57028	100
TS for pseudorotation of 10 (11)	$C_2$	-114.45819	-115.11336	-115.11960	-115.55148	-115.56230	97

<sup>a</sup> Geometries optimized using 6-31+G\* basis set unless otherwise noted.

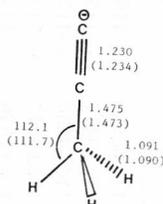
<sup>b</sup> Geometry optimized with the 3-21+G basis set.

<sup>c</sup> Calculated at the 3-21+G//3-21+G level; values have been scaled by 0.9 (see text).

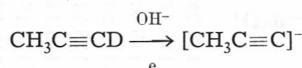
## DISCUSSION

*Geometries and Relative Energies: 1-Propynyl Anion (1)*

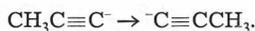
The most stable  $C_3H_3^-$  species is the 1-propynyl anion, which has been observed in mass spectrometric studies.<sup>5</sup> The 6-31+G\* structure is not



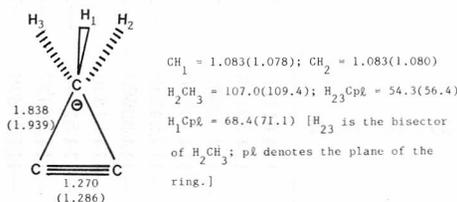
very different from that using the 4-31G basis set.<sup>14</sup> As expected, this ion is generated in the mass spectrometer by the proton abstraction of propyne:<sup>5</sup>



An interesting rearrangement of 1 is its methyl migration:



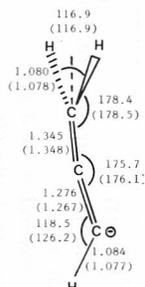
By symmetry consideration, and confirmed by vibrational frequency analysis,



the transition structure of this reaction is 2. The barrier of the rearrangement is calculated to be 174 kJ mol<sup>-1</sup>.

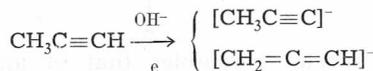
*Allenide Anion (3)*

This anion is less stable than 1 by only 12 kJ mol<sup>-1</sup>. The optimized

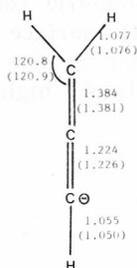


structure is quite similar to those obtained using the 4-31G<sup>14</sup> of the double-zeta<sup>15</sup> basis sets. Gas-phase experiments suggest<sup>16</sup> that 3 is less stable than

1, but that the difference in stabilities could be less than the calculated (MP2/6—31G\*\*//HF/4—31G) value of 22 kJmol<sup>-1</sup>.<sup>14</sup> The present result is in agreement with this conclusion. Also, it is noted that both 1 and 3 can be generated by the proton abstraction of propyne:



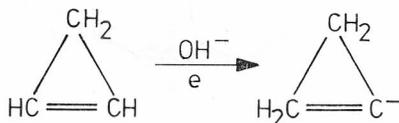
The inversion at the anionic center of 3 is also of interest. It is found that the transition structure for this process is 4. This structure is similar



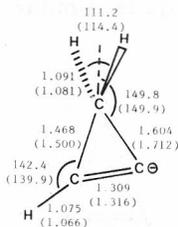
of that obtained by Wilmshurst and Dykstra<sup>15</sup>, except that their double bond between the central carbon and the anionic center is 1.237 Å. Their calculated barrier (double zeta basis, with correlation but without ZPVE correction) is 30 kJmol<sup>-1</sup>, as compared to 26 kJmol<sup>-1</sup> of the present work.

### Cyclopropen-1-ide (5)

This ion has also been observed by mass spectrometry; it is generated by the proton abstraction of cyclopropene:

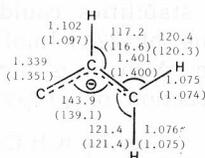


The structure of 5 features a long C—C bond (1.604 Å) and a short »double bond« (1.309 Å). In terms of stability, 5 is of much higher energy (by 100 kJmol<sup>-1</sup>) than 1.



### Prop-2-en-1-yliden-1-ide (6)

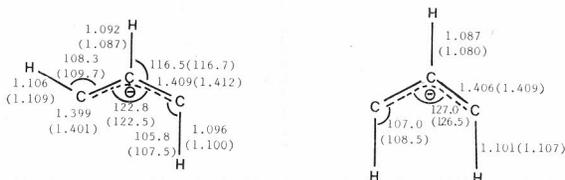
This ion is about 120 kJmol<sup>-1</sup> less stable than 5 and has not yet been observed experimentally.



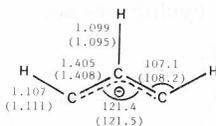
The structure of this species resembles that of an »unsaturated carbene.«

### Prop-1-en-3-yliden-1-ides (7, 8, 9)

There are three possible geometric isomers for this ion; all of them are found to be minima on the  $C_3H_3^-$  surface. The most stable is the EZ-isomer (7). The EE-isomer (8) is less stable by less than  $1 \text{ kJmol}^{-1}$ . The least stable is the ZZ-isomer (9); it lies  $16 \text{ kJmol}^{-1}$  higher in energy than 8.

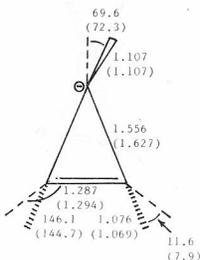


Such an energy ordering is in excellent agreement with that of a recent theoretical (MP2/6-31+G\*\*/HF/4-31+G) study.<sup>17</sup> As pointed out by these authors, all three isomers have the electronic structure with only  $2\pi$  electrons and two lone pairs on the terminal carbenes. As the two lone pairs are best oriented away from each other, the *cis-trans* (7) and *trans-trans* (8) geometries are energetically more favorable than the *cis-cis* (9) form.



### Cyclopropen-3-ide (10)

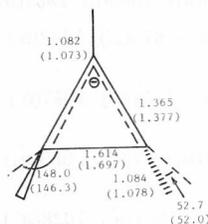
The »cyclopropenyl« anion is the subject of two recent studies: at MP2/6-31+G\*\*/HF/6-31+G<sup>17</sup> and MP2/6-31+G\*\*/HF/4-31+G<sup>18</sup> levels. As expected, their optimized structures are quite similar to the one included here. As



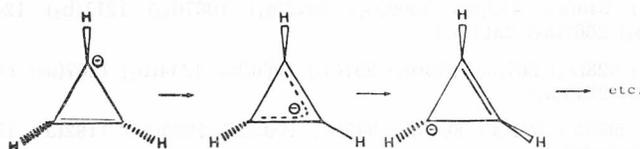
mentioned by these authors,<sup>18</sup> the anion is »doing all that is possible to avoid cyclic conjugation of the four  $\pi$  electrons.« This nonplanar structure for the

cyclopropenyl anion is the result of the Jahn-Teller effect for the equilateral triangular structure.<sup>19</sup>

Another intriguing structure of the »cyclopropenyl« anion is that of 11. This structure has also been included in the work<sup>17</sup> mentioned above. Ap-



parently, these authors have taken 11 as a minimum on the  $C_3H_3^-$  surface, while our vibrational frequency analysis shows that, having one imaginary frequency, it is a transition structure. Indeed, upon examining the vibrational mode with the imaginary frequency, it may be concluded that 11 is the transition structure for the pseudorotation of 10:



The barrier for this process is calculated to be 18 kJmol<sup>-1</sup>. Also, a similar pseudorotation process has been proposed for the cyclopropenyl radical.<sup>20</sup>

Finally, it is perhaps worth pointing out that, judging by the relative energies shown in Table II, *in general*, MP2 overestimates correlation effects

TABLE II  
Relative Energies (kJ mol<sup>-1</sup>) of  $C_3H_3^-$  Anions<sup>a</sup>

Anion	HF/3-21+G	HF/6-31+G*	HF/6-31++G**	MP2/6-31++G**	MP3/6-31++G**	MP3/6-31++G** <sup>b</sup>
1 ( $C_{3v}$ )	0	0	0	0	0	0
2 ( $C_s$ )	222	196	196	190	183	174
3 ( $C_s$ )	44	36	32	21	21	12
4 ( $C_{2v}$ )	54	60	54	44	49	38
5 ( $C_s$ )	192	139	136	108	106	100
6 ( $C_s$ )	223	216	211	253	230	220
7 ( $C_s$ )	256	236	232	282	257	247
8 ( $C_{2v}$ )	258	236	233	281	257	247
9 ( $C_{2v}$ )	279	254	250	302	275	263
10 ( $C_s$ )	362	311	307	268	269	258
11 ( $C_2$ )	413	349	345	276	290	276

<sup>a</sup> Calculated from total energies in Table I.

<sup>b</sup> Including zero-point vibrational contribution.

TABLE III  
*Calculated Vibrational Frequencies (cm<sup>-1</sup>) of C<sub>3</sub>H<sub>3</sub><sup>-</sup> Anions<sup>a</sup>*

1 (C <sub>3v</sub> )	344(e)	847(a <sub>1</sub> )	1064(e)	1396(a <sub>1</sub> )	1500(e)	1987(a <sub>1</sub> )	2812(a <sub>1</sub> )	2829(e)				
2 (C <sub>s</sub> )	441i(a'')	72(a'')	590(a')	857(a'')	873(a')	1242(a')	1476(a'')	1484(a')	1663(a')	2897(a')	2959(a'')	2974(a')
3 (C <sub>s</sub> )	383(a'')	443(a')	612(a')	659(a')	833(a'')	1047(a')	1059(a'')	1438(a')	1794(a')	2921(a')	2970(a'')	2974(a')
4 (C <sub>2v</sub> )	150i(b <sub>1</sub> )	364(b <sub>1</sub> )	417(b <sub>2</sub> )	577(b <sub>1</sub> )	742(b <sub>2</sub> )	999(a <sub>1</sub> )	1050(b <sub>2</sub> )	1414(a <sub>1</sub> )	1914(a <sub>1</sub> )	2942(a <sub>1</sub> )	3002(b <sub>2</sub> )	3285(a <sub>1</sub> )
5 (C <sub>s</sub> )	472(a')	680(a'')	828(a')	844(a'')	911(a')	1028(a'')	1073(a')	1427(a')	1506(a')	2859(a')	2900(a'')	3031(a')
6 (C <sub>s</sub> )	375(a')	406(a'')	537(a'')	822(a'')	949(a')	993(a')	1140(a')	1387(a')	1442(a')	2796(a')	2957(a')	3025(a')
7 (C <sub>s</sub> )	423(a'')	518(a')	796(a'')	991(a'')	1003(a')	1097(a')	1210(a')	1255(a')	1391(a')	2608(a')	2722(a')	2848(a')
8 (C <sub>2v</sub> )	458(b <sub>1</sub> )	540(a <sub>1</sub> )	752(a <sub>2</sub> )	1009(b <sub>1</sub> )	1042(a <sub>1</sub> )	1087(b <sub>2</sub> )	1211(b <sub>2</sub> )	1245(a <sub>1</sub> )	1373(b <sub>2</sub> )	2619(b <sub>2</sub> )	2661(a <sub>1</sub> )	2911(a <sub>1</sub> )
9 (C <sub>2v</sub> )	397(b <sub>1</sub> )	528(a <sub>1</sub> )	867(a <sub>2</sub> )	970(b <sub>1</sub> )	991(a <sub>1</sub> )	1066(b <sub>2</sub> )	1244(b <sub>2</sub> )	1267(a <sub>1</sub> )	1413(b <sub>2</sub> )	2577(b <sub>2</sub> )	2578(a <sub>1</sub> )	2740(a <sub>1</sub> )
10 (C <sub>s</sub> )	297(a'')	560(a')	691(a')	884(a'')	949(a')	1005(a')	1035(a'')	1192(a')	1555(a')	2539(a')	3000(a'')	3049(a')
11 (C <sub>2</sub> )	880i(b)	497(a)	505(b)	886(b)	892(a)	971(a)	1079(b)	1238(b)	1327(a)	2898(b)	2900(a)	2945(a)

<sup>a</sup> Values listed have been scaled by 0.9 (see text).

while MP3 slightly underestimates them. Consequently, the MP3 results are closer to the HF ones than the MP2. Such a general trend, sometimes used as a rough guideline, has also been discussed elsewhere.<sup>21</sup>

### *Stabilities of the C<sub>3</sub>H<sub>3</sub><sup>-</sup> Ions with Respect to Electron Loss*

Finally, we attempt to answer the question of whether the various C<sub>3</sub>H<sub>3</sub><sup>-</sup> anions discussed above are stable toward spontaneous loss of an electron. The electron affinities (EAs) of a radical is the energy difference between the radical and its anion. However, the EAs obtained with this method are not always very accurate, especially for species leading to localized anions. Hence, in the results reported below, we have also included the approach of Schleyer and co-workers<sup>17</sup> by calculating the enthalpy change for the isogyric<sup>22</sup> reaction



The enthalpy change gives the EA of X<sup>-</sup> relative to that of CH<sub>3</sub><sup>-</sup>. Assuming the experimental value<sup>23</sup> (8 ± 2 kJmol<sup>-1</sup>) for the EA of CH<sub>3</sub><sup>-</sup> allows the EA of X<sup>-</sup> to be determined. Evaluation of EAs in this manner should be most effective when X<sup>-</sup> is similar to CH<sub>3</sub><sup>-</sup>. Thus, it is not certain whether, for C<sub>3</sub>H<sub>3</sub><sup>-</sup> radicals, EAs obtained *via* reaction (1) are likely to be more or less accurate than the directly calculated values.

TABLE IV

Calculated Total Energies<sup>a</sup> (Hartree) of  $CH_3^-$ ,  $CH_3^*$  and  $C_3H_3^*$  Radicals and Electron Affinities, (EA, in  $kJmol^{-1}$ ) of  $C_3H_3^*$  Radicals<sup>b</sup>

Radical	HF/6-31++G**	MP2/6-31++G**	MP3/6-31++G**	EA <sup>c</sup>	EA <sup>d</sup>
Methyl	-39.56679	-39.69650	-39.71392	—	—
1-Propynyl	-115.20461	-115.54995	-115.57485	257	324
Allenide	-115.26186	-115.61644	-115.64092	63	130
Cyclopropen-1-ide	-115.18514	-115.55756	-115.57996	138	205
Pro-2-en-1-yliden-1-ide	-115.20435	-115.53231	-115.56536	52	119
E,Z-Pro-1-en-3-yliden-1-ide	-115.14873	-115.48135	-115.51396	160	227
E,E-Prop-1-en-3-yliden-1-ide	-115.08758	-115.50626	-115.51673	152	219
Z,Z-Prop-1-en-3-yliden-1-ide	-115.09108	-115.47748	-115.49691	187	254
Cyclopropen-3-ide	-115.20345	-115.58036	-115.60151	-103	-36
Methyl Anion	-39.50758	-39.67844	-39.69148	—	—

<sup>a</sup> Based on the HF/6-31G\* optimized structures. <sup>b</sup> Evaluated at the MP3/6-31++G\*\* level. <sup>c</sup> Calculated by direct subtraction. <sup>d</sup> Evaluated *via* reaction (1).

Table IV summarizes the total energies as well as the EAs evaluated by direct subtraction and those calculated *via* reaction (1). These results indicate that, among the various radicals studied, only the cyclopropen-3-ide radical has a negative EA. In other words, the cyclopropen-3-ide anion is not stable toward spontaneous loss of an electron and, hence, should not be observable. A similar conclusion was reached in previous work.<sup>17</sup>

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### SAŽETAK

#### Strukture i stabilnosti $C_3H_3^-$

Wai-Kee Li

Različiti minimumi i neke točke sedla na površini potencijalne energije  $C_3H_3^-$  proučeni su *ab initio* MO računima. Strukture tih specija određene su potpunom geometrijskom optimizacijom na Hartree-Fock-ovoj razini s proširenim temeljnim skupovima difuzijske funkcije 3-21+G i 6-31+G.

Na površini potencijalne energije  $C_3H_3^-$  pronađeno je osam stabilnih specija. Poredane po silaznom redu stabilnosti, to su: 1-propinil (1), alenid (3), ciklopropen-1-id (5), prop-2-en-1-iliden-1-id (6), tri izomera (EZ, EE, ZZ) od prop-1-en-3-iliden-1-ida (7, 8, 9) i ciklopropen-3-id (10) ioni. Nađene su prijelazne strukture za metil-migraciju na 1, za inverziju anionskog centra na 3 i za pseudorotaciju na 10.

Nadalje, za sve nađene ravnotežne strukture izračunan je elektronski afinitet odgovarajućih slobodnih radikala. Iz tih rezultata zaključeno je da između osam anionskih ravnotežnih struktura samo 10 je nestabilna prema reakciji spontanog gubitka elektrona.