distance between the nearest naphthyl groups which are attached to the neighboring turns is 5.5 Å for the 3_{10}-helix and 5.8 Å for the δ helix. These interchromophore distances are too far to form an excimer. The face-to-face longitudinal distance between the same pair of naphthyl groups is about 3 Å for the 3_{10}-helix and 4 Å for the δ helix, but the overlapping area of the two aromatic rings is very small.

Note Added in Proof: Ueno et al. informed us that they claimed a right-handed helix for a random copolymer of L-1-NapAla and γ-benzyl L-glutamate (67/33).[30a]

Registry No. Poly(L-1-NapAla) tetrablock copolymer, 84117-45-3; Poly(DL-1-NapAla) diblock copolymer, 84109-04-6; *N*-acetyl-L-1-naphthyl ethyl ester, 84109-03-5.

Communications to the Editor

Structures and Energies of $C_6H_6^{2+}$ Isomers. Fragmentation into $C_5H_3^+$ and CH_3^+[1]

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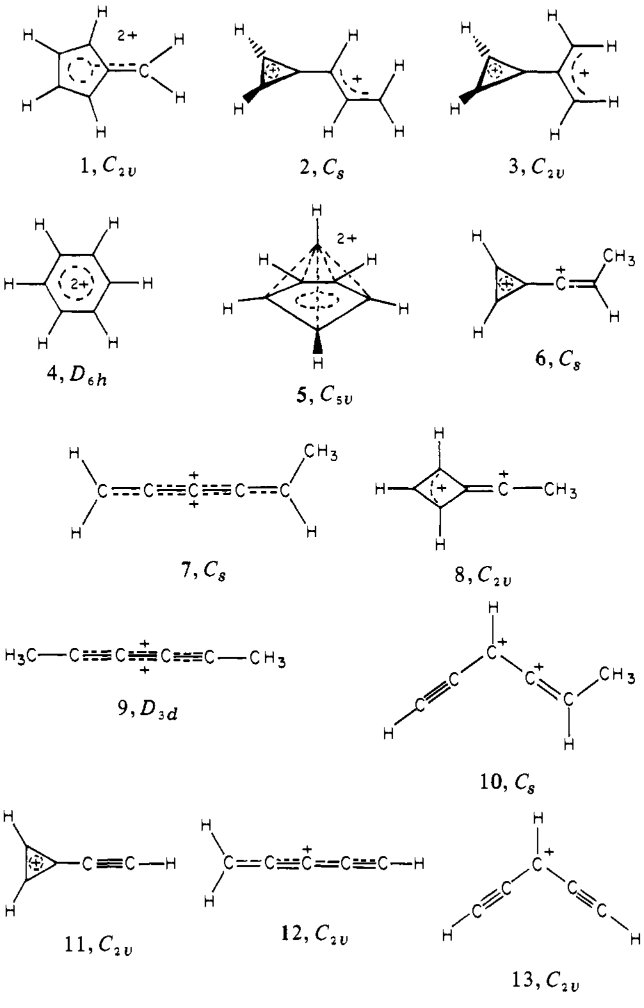
$C_6H_6^{2+}$, produced in high intensity by various ionization and mass spectrometric methods from numerous aromatic and aliphatic compounds, is a commonly observed gas-phase carbodication.[2-4] Structural reorganization may lead to the same $C_6H_6^{2+}$ species from various precursors. Although two $C_3H_3^+$ cyclopropenium ions would be the thermodynamically most stable cleavage products, the predominant fragmentation takes a curious course to give $C_5H_3^+$ (also of unknown structure) and CH_3^+.[2-4] This releases considerable kinetic energy (2.6 eV); the peak shape indicates a rather specific process involved.[2,3] A simple model has been used to interpret this result. If most of the energy release is attributed to Coulombic repulsion of the separating ions, the e^2/r relationship provides an estimate of r (5.5 Å), taken to be the initial intercharge distance (assuming idealized point charges). Since the diameter of the benzene ring (2.9 Å) is much smaller, acyclic $C_6H_6^{2+}$ structures, $CH_3C_4CH_3^{2+}$ in particular, have been postulated.[2,3] However, such idealized point-charge models are quite unrealistic for $C_6H_6^{2+}$ structural candidates; charge would be delocalized not only in the carbon π framework but to the hydrogens as well.[5,6] Charge delocalization also is expected in the fragmentation transition state.

Chart I



We present here the results of the first ab initio calculations on a set of $C_6H_6^{2+}$ isomers that should include the global energy

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Table I. Ab Initio Total Energies (in au), MNDO and MINDO/3 Heats of Formation, and Relative Energies (in kcal/mol) of $C_6H_6^{2+}$ and $C_5H_3^+$ Isomers and Reference Compounds

	STO-3G//STO-3G		3-21G//3-21G		MNDO		MINDO/3	
species	E	ΔE	E	ΔE	ΔH_f	$\delta\Delta H_f$	ΔH_f	$\delta\Delta H_f$
1	−227.15611	0.0	−228.58552	0.0	568.0	0.0	564.5	0.0
2	−227.14970	4.0	−228.57740	4.9	577.9	9.9	533.3	−31.2
3	−227.14817	5.0	−228.57558	6.0			548.8	−15.7
4, triplet opt, D_{6h}	−227.16117	−3.2 (16.8)[a]	−228.58956	−2.5 (17.5)[a]	571.0	3.0	563.9	−0.6
triplet, C_6H_6 geometry[b]			−228.58226	2.0 (22.0)[a]	576.9	8.9	571.4	6.9
singlet, opt, D_{2h}			−228.55573	18.7	578.2[c]	10.2	551.9[c]	−12.6
singlet, C_6H_6 geometry[b]			−228.52431	38.4	593.8	25.8	586.3	21.8
5	−227.14112[d]	9.4	−228.53928[d]	28.8	649.2	81.1	552.5	12.0
6	−227.10077	34.7	−228.52544	37.5	610.0	42.0	528.6	−35.9
7	−227.10118	34.5	−228.55575	18.4	581.9	13.9	528.5	−35.8
8	−227.08147	46.9	−228.50313	51.5	605.8	37.7	556.0	−8.5
9, triplet	−227.06832	55.1 (75.1)[a]	−228.51326	45.1 (65.1)[a]	614.7	46.7	535.6	−28.9
10	−227.05028	66.4	−228.50706	49.2	604.7	36.7	540.8	−23.7
11			−189.59121	0.0	311.5	11.8	269.4	0.0
12			−189.58597	3.3	299.7	0.0	273.6	4.2
13			−189.58122	6.3	301.5	1.8	279.1	9.7
C_6H_6, benzene	−227.89136[e]		−229.41945[e]		21.2[f]		28.8[g]	
CH_3^+	−38.77948[e]		−39.00913[e]		243.9[f]		260.3[g]	

[a] Corrected by 20 kcal/mol for triplet–singlet Hartree–Fock errors (see text). [b] Benzene geometry imposed. [c] Slightly nonplanar chairlike C_{2h} symmetry; ref 4b reports a MINDO/3 value of 544.4 kcal/mol for a lower symmetry nonplanar structure. [d] Reference 12. [e] Reference 15. [f] Reference 9. [g] Reference 8.

minimum. Although the mass spectroscopic species possesses excess energy under the conditions of observation, knowledge of the ground-state potential-energy surface may facilitate interpretation. Table I summarizes the results. Both the minimal STO-3G and the split-valence 3-21G basis sets were used with complete geometry optimization within the symmetries indicated.[7] Also included are dications **6**, **7**, and **10** (Chart I), which should readily loose a methyl cation to give likely $C_5H_3^+$ isomers (**11**–**13**). Two groups have reported related theoretical examinations recently at the semiempirical MINDO/3 calculational level.[4,5] Unfortunately, our own extensive experience indicates that MINDO/3[8] generally gives unsatisfactory energies for carbodications and misleading results. As is shown in the table, MNDO[9] is a more satisfactory semiempirical method for this purpose, but it, too, has limitations.

The fulvene dication (**1**) and the two allylcyclopropenium ions (**2** and **3**) are the most likely candidates for the global $C_6H_6^{2+}$ energy minimum. The Hückel π energy of **1**[10] is particularly favorable. Despite ring strain, cyclopropenium ions are quite stable thermodynamically;[11] the perpendicular conformations of **2** and **3** facilitate hyperconjugation. Since d-type polarization functions are needed to describe small ring compounds accurately,[11] the ab initio relative energies of **2** and **3** are expected to be even more favorable than indicated in the table. This is also true of **6** and of **5**, a nido structure[12] closely related to Hogeveen's $(CCH_3)_6^{2+}$ dication, a species directly observable in solution in superacid media.[13]

Since the π HOMO of benzene is doubly degenerate, the most stable $C_6H_6^{2+}$ dication *in D_{6h} symmetry* is, as expected, a triplet. This is shown in the table for singlet and triplet species constrained to the benzene geometry (r_{CC} = 1.385 Å at 3-21G//3-21G). Full optimization of the triplet leads to the D_{6h} structure **4** (r_{CC} = 1.420 Å), only 4.6 kcal/mol lower in energy. However, the singlet undergoes a more pronounced Jahn–Teller distortion upon optimization, and a D_{2h}, elongated, double-allyl cation geometry[4] results (r_{CC} = 1.418 (4×) and 1.525 Å (2×) at 3-21G//3-21G). The energy lowering, 19.7 kcal, is much larger than with the triplet. While triplet **4** is indicated at both UHF/STO-3G/STO-3G and UHF/3-21G//3-21G levels to be the lowest energy $C_6H_6^{2+}$ isomer, this is a computational artifact. Triplets are favored by about 20 kcal/mol over singlets at the Hartree–Fock levels employed (due to electron correlation differences).[14] The relative energies in the table are corrected roughly for this effect. Taking this correction into account, it is not clear if the lowest energy benzene-like $C_6H_6^{2+}$ species is a D_{6h} triplet or a distorted, lower symmetry singlet.

The experimentally observed *vertical* double ionization of benzene, which should lead to a dication with negligible geometry alteration, requires 26 eV or 600 kcal/mol.[3] The calculated 3-21G energy difference between benzene and the singlet $C_6H_6^{2+}$ with the benzene geometry is in reasonable agreement, after electron correlation correction is made (C_6H_6 and $C_6H_6^{2+}$ have different numbers of electron pairs). The experimentally generated $C_6H_6^{2+}$ species, whatever its nature may be, has excess energy that suffices for rearrangement, fragmentation etc.[4a]

The members of the second set of $C_6H_6^{2+}$ isomers, **6**–**10**, have methyl groups, a structural feature assumed to be necessary in the metastable dication undergoing fragmentation into CH_3^+ and $C_5H_3^+$. The often-proposed dimethyldiacetylene dication, $CH_3C_4CH_3^{2+}$ (**9**), is unfavorable energetically. Like **4**, **9** should have a triplet ground state; direct comparison reveals **9** to be about 50 kcal/mol less stable than triplet **4**. Moreover, loss of a methyl group from **9** would give $CH_3C_3C^+$, a very unfavorable, high-energy species.[5] Similarly, loss of a methyl cation from **8** would not give a stable $C_5H_3^+$ cation directly.

The energetically most likely $C_5H_3^+$ fragmentation products are **11**–**13**. The ethynylcyclopropenium ion, **11**, is probably the $C_5H_3^+$ global energy minimum. Already indicated to be the most stable isomer at 3-21G, **11** will have an even more favorable relative energy at higher theoretical levels.[11] This is also shown by the heats of formation, 311 kcal/mol for **11** vs. 326 kcal/mol

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[7] A modified GAUSSIAN 76 program was used: Binkley, J. S.; Whiteside, R. A.; Hariharan, P.; Seeger, R.; Pople, J. A.; Hehre, W. J.; Newton, M. D. *QCPE* **1979**, *11*, 368. For the 3-21G basis set, see: Binkley, J. S.; Pople, J. A.; Hehre, W. J. *J. Am. Chem. Soc.* **1980**, *102*, 939–947.

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for **12**, evaluated by means of isodesmic reactions, eq 1 and 2 (with $\Delta H_f°_{298}$ values in kcal/mol given in parentheses), which tend to

$$\underset{\substack{\text{cyclopropenium}\\ \text{ion}\\ (257^{16})}}{(CH)_3^+} + \underset{(44.3^{16})}{CH_3C{\equiv}CH} \rightarrow \underset{\substack{\mathbf{11}\\ (311\text{ calcd})}}{(CH)_2CC{\equiv}CH^+} + \underset{(-17.9^{16})}{CH_4} \qquad -8.2\text{ kcal/mol (3-21G//3-21G)} \tag{1}$$

$$\underset{\substack{\text{propargyl}\\ \text{cation}\\ (281^{16})}}{HC{\equiv}CCH_2^+} + \underset{(44.3^{16})}{CH_3C{\equiv}CH} \rightarrow \underset{\substack{\mathbf{12}\\ (326\text{ calcd})}}{HC{\equiv}CC{\equiv}CCH_2^+} + \underset{(-17.9^{16})}{CH_4} \qquad -17.6\text{ kcal/mol (3-21G//3-21G)} \tag{2}$$

cancel errors. An experimental upper limit of 342 kcal/mol for the heat of formation of $C_5H_3^+$ of unknown structure[17] is in general agreement.

Based on the estimated $\Delta H_f°$ for **11**, the experimental value for CH_3^+, and the calculated energy of eq 3, $\Delta H_f° = 601$ kcal/mol for the geometry-optimized D_{2h} singlet benzene dication is obtained as shown in eq 3 ($\Delta H_f°_{298}$ values in kcal/mol given in parentheses).

$$\underset{\substack{\mathbf{4}\text{, singlet,}\\ D_{2h}\\ (601\text{ calcd})}}{C_6H_6^{2+}} \rightarrow \underset{(262^{16})}{CH_3^+} + \underset{\substack{\mathbf{11}\\ (311\text{ calcd,}\\ \text{eq 1)}}}{C_5H_3^+} \qquad -28.0\text{ kcal/mol} \tag{3}$$

Like **11**, **12** and **13** can also be formed by CH_3^+ elimination from $C_6H_6^{2+}$ precursors, e.g., **11** from **6**, **12** from **7**, and **13** from **10**. Both **7** and **10** have unbranched carbon skeletons which might have been formed by opening of the benzene dication ring followed by hydrogen migrations. Likewise, **2** might give **6** prior to fragmentation. Three-membered rings are often produced in carbocationic processes, and **2** might arise via cleavage of a bicyclo[3.1.0]hexenediyl dication intermediate. There is some precedent in the mechanism of the photochemical rearrangements of benzene.[18]

Since **10** is a rather unstable $C_6H_6^{2+}$ isomer, we regard **6** and **7** to be more likely metastable fragmentation precursors. The energetically more favorable process, exothermic by 47 kcal/mol (3-21G), involves fragmentation of **6** into **11** and CH_3^+. This is related to, but does not correspond directly to, the experimental process which releases 2.6 eV (60 kcal/mol) of translational energy. The energy difference between the fragmentation transition state (e.g., $\mathbf{6}^‡$ rather than **6**) and the products (e.g., **11** and CH_3^+) may be involved. Decomposition of dications into two monocations typically requires activation, even though such transformations may be very favorable thermodynamically.[1] Assuming this also to be true for the decomposition of **6**, the 47 kcal/mol exothermicity would only have to be augmented by a modest activation energy to agree with the experimental energy release value of 60 kcal/mol.

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Registry No. 1, 84253-83-8; **2**, 84237-96-7; **3**, 84237-97-8; **4**, 15157-23-0; **5**, 55574-89-5; **6**, 84237-98-9; **7**, 84237-94-5; **8**, 84237-99-0; **9**, 81932-71-0; **10**, 84237-95-6; **11**, 84238-00-6; **12**, 81932-80-1; **13**, 79530-50-0.

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Bis(borane)-Cyclenphosphorane: A Stable Adduct in Which Two Phosphorus(V)-Bonded Nitrogen Atoms Display Donor Character

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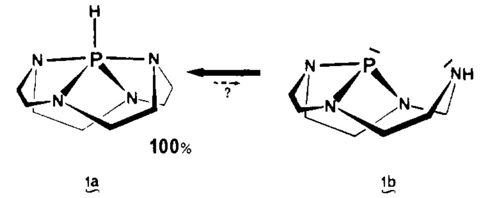
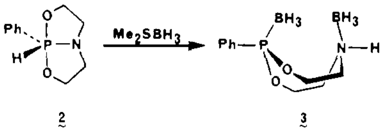
Phosphorus-bonded tricoordinated Nitrogen atoms usually show little donor capacity. The few known BH_3 adducts derive from constrained structures and are usually unstable.[1] The unique behavior reported here of cyclenphosphorane **1a** toward diborane is therefore remarkable. It provides the first example of a stable H_3B-N-P-N-BH_3 sequence and adds a new facet to the already rich chemistry of phosphoranes derived from macrocyclic tetraamines.[2-4]



1a **1b** (1)

Aside from homocyclen, cyclenphosphorane is the only member of the family of tetracyclic tetraaminophosphoranes for which the open-form phosphane tautomer **1b** has not been detected in solution. It was therefore of interest to investigate the possibility of revealing such an open form and of displacing the tautomeric equilibrium 1 under the action of a Lewis acid capable of coordinating the phosphane and/or amine sites of **1b**. Such behavior has previously been observed in the case of bicyclic aminophosphoranes of type **2**, for which the open form is usually not present either and which, under the action of transition-metal derivatives[5] or diborane,[6] convert to adducts such as **3**. The coordination of the nitrogen site in the phosphorus-bound form **2** has never been observed.



2 **3**

Cyclenphosphorane was found to react readily with diborane on the vacuum line and to add 2 equiv of BH_3. The reaction product, which was isolated in near-quantitative yield as a white crystalline powder, proved, quite unexpectedly, not to be the open-form analogue of **3** but the bis-adduct **4**, in which no rearrangement of the initial structure had occurred.

Even more surprising is the outstanding stability of **4**, as illustrated by its high melting point (with decomposition) at 200

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