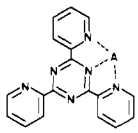
with the frequency of the exchange of the metal ion between sites A and A′.

In order to make the concept as clear as possible, we want to extend the designation and we define the following subclasses: *Isoalterdentate ligands* can bind a metal ion at two or more symmetrically equivalent positions. If one of the sites is occupied, the others are still available for coordination. The number of sites can be included as a prefix. Nin$^-$ (I) and all$^-$ (II) are accordingly diisoalterdentate ligands. Sometimes, it depends on the nature of the metal ion whether a ligand acts as a *chelate* or as an *alterdentate*. In most cases en is a chelate, whereas for Ag^+ it is an alterdentate in the complex $Ag(en)_2^+$, owing to the linear coordination of the silver ion.[4] *S*-Triazine (III) is triisoalterdentate, and the cyclopentadienyl anion (IV) is pentaisoalterdentate in some $(\eta^1\text{-}C_5H_5)M$ species.

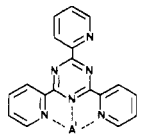
(III)

(IV)

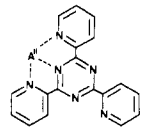
There is another type of ligand, exemplified by TPTZ (V),



(Va)



(Vb)

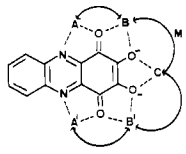


(Vc)

which can offer equivalent coordination sites. The metal can change from A to A′ to A″ (Va to Vc) only if the ligand itself rearranges simultaneously, however, and the same type of coordination sites is no longer available if one metal is bound. This class is called *anisoalterdentate*, and TPTZ is therefore trianisoalterdentate. $\Delta G°$ for the rearrangement is still 0.

Ambidentate ligands offer nonequivalent coordination sites to the metal, and, generally, $\Delta G° \neq 0$ for the exchange between sites. Of the three different isotopic species $^{15}N^{14}N^{14}N^-$, $^{14}N^{15}N^{14}N^-$, and $^{14}N^{14}N^{14}N^-$, having natural abundances of 0.74%, 0.37%, and 98.89%, the first is ambidentate and the second and the third are isoalterdentate.

The two types can be combined and the phenazine (VI)



(VI)

derivative with five sites AA′BB′C, of which AA′ and BB′ are pairwise equivalent, can be disignated as isoalterambidentate.

The proposed classification scheme emphasizes a possible nonrigidity in metal complexes, which has not been very often considered, so far, in coordination chemistry. Many alterdentate ligands are known, and many more could be designed. Experimental observation of rearrangements will, in most cases, be possible by NMR spectroscopy with diamagnetic ligands or with ESR in the case of radical ligands if the metals are sufficiently labile. For substitution-inert complexes, other methods such as isotopic labelling might be used.

Complicated polyfunctional ligands in biochemical systems could, in principal, exchange metal ions between several equivalent coordination sites, and alterdenticity may play an important role in some bioinorganic reactions, including the transport of metal ions over considerable distances.

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The Complexities of Ascorbate as a Reducing Agent

Sir:

Aqueous solutions of ascorbic acid (H_2A, vitamin C) have been widely used by inorganic chemists because of the convenience of ascorbate as a reducing agent.[1-3] We have recently utilized this reductant as a source of reducing equivalents in a multicomponent system that promotes the photoreduction of water.[4] In connection with this work information on the redox characteristics of the various species generated in the oxidation of ascorbate in water was sought. Here a summary of these findings is presented.

The structures I, II, and V shown in Figure 1 are generally given[5] for ascorbic acid, ascorbate ion (HA^-), and dehydroascorbic acid (A), respectively, but it has recently been established that VI is actually that appropriate to dehydroascorbic acid in aqueous solutions.[6] On the basis of EPR results Schuler and co-workers[7] have concluded that IV is the structure of ascorbate radical ($A^{-}\cdot$), the one-electron oxidation product of ascorbic acid or of ascorbate ion; its structure is invariant in the pH range 0–13, but at lower pH, $A^{-}\cdot$ protonates to give III.[7]

Ascorbic acid is a weak acid,[8] while the radical $HA\cdot$ is a very strong acid.[7] Observations by Ball suggest that dehydroascorbic acid undergoes proton loss with a pK_a of ~8.[9] Data relevant to the various protonation equilibria are summarized in Table I.

Thermodynamic data bearing on redox equilibria between the various species come from several sources. By recourse to mediators Ball performed potentiometric measurements on the ascorbic acid/dehydroascorbic acid couple (eq 1) in

$$A + 2H^+ + 2e^- = H_2A \qquad (1)$$

aqueous solutions ranging from pH 1 to 8.57 at 30 °C.[9] The reduction potential for the couple was determined to be +0.39 V in 1 N acid at 30 °C.[9] The A/H_2A couple was found to be chemically reversible in a practical sense up to about pH 7; above pH 7, the decomposition of the oxidized form became rapid, with the half-life for its decomposition decreasing from ~40 min at pH 6.7 to ~0.5 min at pH 8.6. Foerster, Weis, and Staudinger[10] used an ESR method to evaluate the con-

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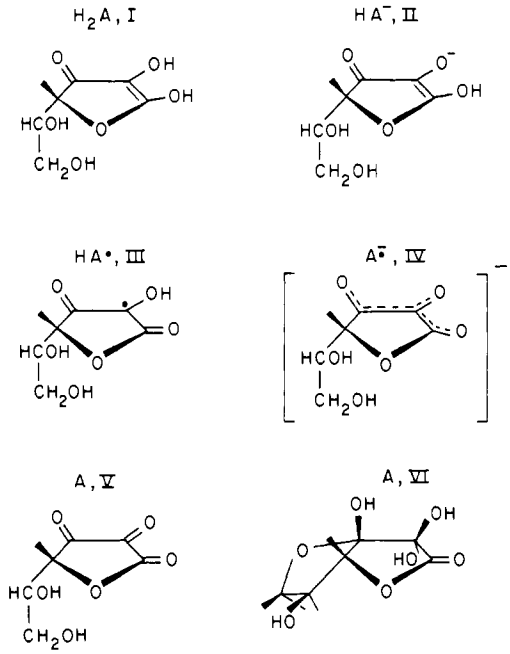

Figure 1. Structure of ascorbic acid (I, H_2A), ascorbate ion, (II, HA^-), protonated ascorbate radical (III, HA·), ascorbate radical (IV, $A^{-}\cdot$), and dehydroascorbic acid (V and VI, A).

Table I. Dissociation Constants for Ascorbic Acid, Ascorbate Radical, and Dehydroascorbic Acid

equilibrium	pK_a	ref
Ascorbic Acid		
$H_2A \rightleftharpoons H^+ + HA^-$	$pK_1 = 4.0^a$	8
$HA^- \rightleftharpoons H^+ + A^{2-}$	$pK_2 = 11.3^a$	
Ascorbate Radical		
$HA\cdot \rightleftharpoons H^+ + A^{-}\cdot$	$pK = -0.45$	7
Dehydroascorbic Acid[b]		
$A \rightleftharpoons H^+ + (A-H)^-$	$pK = \sim 8$	9

[a] At 25 °C and 0.1 M ionic strength. [b] The formula $(A-H)^-$ denotes the conjugate base of A.

centration of ascorbate radical resulting when ascorbate and dehydroascorbic acid are mixed at 25 °C, pH ≤ 6.4 (ionic strength ≈ (3×10^{-3})–(3×10^{-1}) M). Bielski has recently used their data to evaluate an equilibrium constant of 2×10^{-15} M for eq 2.[11] The results obtained by Ball and by Bielski may

$$A + HA^- \rightleftharpoons 2A^{-}\cdot + H^+ \quad (2)$$

be combined with values determined for the acidity constants of the various species (Table I) to give reduction potentials for several one- and two-electron couples important to the reactions of ascorbate species. Data for these couples are presented in Table II. Also presented in Table II are estimates based on the E° value obtained by Steenken and Neta for the $A^{-}\cdot/A^{2-}$ couple.[12] As is evident from the table, values obtained for the radical couples on the basis of EPR and pulse radiolysis methods are in reasonably good agreement. The 40-mV difference between the two data sets may reflect the differing media used in the two experiments and/or the accumulated effects of experimental errors.

Having addressed the thermodynamic aspects of the ascorbate system, we turn now to the kinetics of ascorbate oxidation reactions. Pelizetti and co-workers have compiled extensive data on outer-sphere oxidation of HA^- and H_2A by such oxidants as FeL_3^{3+} (L = a 2,2′-bipyridine or 1,10-phenanthroline derivative) and found the rate law for these reactions in ~0.1–1 M acid to be of the form given by eq 3.[14,15]

$$\frac{d[FeL_3^{2+}]}{dt} = k'[FeL_3^{3+}][HA^-] \quad (3)$$

(For some very strong oxidants, a term first order in oxidant and first order in H_2A was also important but will not be discussed further here.) The rate law eq 3 was interpreted in terms of Scheme I where the first step is rate determining

Table II. Reduction Potentials for Ascorbate Species in Aqueous Solution[a]

	couple	E°, V
(i)	$A + 2H^+ + 2e^- = H_2A$	+0.40
(ii)	$A + H^+ + 2e^- = HA^-$	+0.28
(iii)	$A + 2e^- = A^{2-}$	−0.05
(iv)	$A + e^- = A^{-}\cdot$	-0.16,[a,b] -0.12[a,c]
(v)	$A^{-}\cdot + e^- = A^{2-}$	$+0.05$,[a,b] $+0.015$[c]
(vi)	$HA\cdot + e^- = HA^-$	$+0.70$,[a,b] $+0.66$[a,c]

[a] Dissociation constants summarized in Table I have been used in these calculations. The value chosen as E° for the A/H_2A couple (entry i) represents a compromise between 0.39 V determined by Ball[9] at 30 °C and other values of ~0.41 V at 25 °C.[13] [b] The one-electron reduction potentials were calculated from the ascorbate radical disproportionation equilibrium data obtained by Foerster et al.[10] and evaluated by Bielski.[11] [c] Based on the $A^{-}\cdot/A^{2-}$ E° value determined by Steenken and Neta at pH 13.5 from the reaction of ascorbate with catechol.[12]

Scheme I

$$HA^- + FeL_3^{3+} \rightleftharpoons HA\cdot + FeL_3^{2+} \quad k_1, \text{ slow}$$

$$HA\cdot + FeL_3^{3+} \rightarrow A + H^+ + FeL_3^{2+} \quad k_2$$

so that $k' = 2k_1$. Values determined for k_1 ranged from 10^7 to $>10^9$ M^{-1} s^{-1}. Added FeL_3^{2+} did not alter the observed kinetics, which were well-behaved under pseudo-first-order conditions ($[H_2A] > 10[FeL_3^{3+}]$). The possible effects of HA· deprotonation (eq 4) and ascorbate radical disproportionation (eq 5) were not addressed. Either or both could however be

$$HA\cdot \rightleftharpoons H^+ + A^{-}\cdot \quad (4)$$

$$A^{-}\cdot + A^{-}\cdot \xrightarrow{H^+} HA^- + A \quad (5)$$

relevant since $A^{-}\cdot$ is half protonated only at ~2.8 M H^+ (the acidity range encompassed was 0.1–1.0 M), and the effective second-order rate constant for eq 5 is probably $\geq 10^8$ M^{-1} s^{-1} in the acidity range used.[11] In a very recent study of the oxidation of ascorbate in acidic solution both forward and reverse rate constants for ascorbate radical production were directly measured[16] with the oxidant used being the chloropromazine cation radical ($ClPMZ^+$).

Scheme II

$$HA^- + Fe^{III}(\text{cyt } c) \rightarrow HA\cdot + Fe^{II}(\text{cyt } c) \quad k_1$$

$$HA\cdot \rightleftharpoons H^+ + A^{-}\cdot$$

$$A^{-}\cdot + Fe^{III}(\text{cyt } c) \rightarrow A + Fe^{II}(\text{cyt } c) \quad k_2$$

$$A^{2-} + Fe^{III}(\text{cyt } c) \rightarrow A^{-}\cdot + Fe^{II}(\text{cyt } c) \quad k_3$$

$$2A^{-}\cdot + H^+ \rightarrow HA^- + A \quad k_4$$

By contrast, studies of the oxidation of ascorbate by the milder oxidant ferricytochrome c (Fe^{III}(cyt c), E° = 0.26 V[17])

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in neutral solution have implicated the mechanism given in Scheme II,[18] where $k_1 \sim 1\ M^{-1}\ s^{-1}$,[18b] $k_2 \sim 10^4\ M^{-1}\ s^{-1}$,[18] and $k_3 \sim 5 \times 10^5\ M^{-1}\ s^{-1}$.[18] Depending upon the conditions used, the ascorbate radical decayed through oxidation by Fe^{III}(cyt *c*) or through the disproportionation reaction eq 5 for which the effective value of k_4 was $(1-2) \times 10^5\ M^{-1}\ s^{-1}$. Both Scheme I and Scheme II lead to the stoichiometry given in eq 6.

$$HA^- + 2Fe^{III} \rightarrow A + H^+ + 2Fe^{II} \quad (6)$$

The results of these studies illustrate some of the complexities of ascorbate as a reductant. Depending upon the pH and the properties of the oxidant, H_2A, HA^-, and/or A^{2-} may be the kinetically significant reducing agent(s). The cytochrome *c* work shows that, depending upon the H^+ ion and reactant concentrations, the ascorbate radical may be consumed via eq 5 or through reaction with the added oxidant. On the other hand, the assumptions used in treating the FeL_3^{3+} kinetics require that oxidation of HA· or A^{-}· by FeL_3^{3+} predominate. While these assumptions are probably valid under many conditions, a recent reinvestigation[16] of the chloropromazine cation reduction by ascorbate[19] suggests that oxidation of ascorbate radical can be relatively slow in acid as well as in neutral solution. The reinvestigation indicates that, in 0.25–1.0 M H^+, an equilibrium between $ClPMZ^+$, ascorbic acid, ClPMZ, and the ascorbate radical is rapidly set up and that reaction of the ascorbate radical with $ClPMZ^+$, itself, or impurities is rate determining.[16] Clearly the kinetics of ascorbate reactions in acid (as well as in neutral solution) merit further attention. In any case the above studies do provide some information bearing on the general kinetic reactivity of the various ascorbate couples. This subject is considered in the following paragraphs.

It is worthwhile to discuss the reactivity of species toward outer-sphere redox reactions in terms of the driving force for the electron-transfer reaction and the intrinsic electron-transfer barrier associated with each of the reactants. This dichotomy is embodied in the Marcus cross-relation,[20] $k_{12} = (k_{11}k_{22}K_{12})^{1/2}$, where k_{12} and K_{12} are respectively the rate and equilibrium constant for the electron-transfer reaction and k_{11} and k_{22} are self-exchange rate constants for the reactant species involved (see below). In Table II are one-electron $E°$ values, which may be used to evaluate K_{12} for outer-sphere reactions involving ascorbate species. The next focus of discussion is the intrinsic electron-transfer barrier (reflected in the magnitude of k_{11}) relevant to each of the ascorbate couples. First the ascorbate/ascorbate radical self-exchange processes eq 7–9

$$HA^- + HA\cdot \rightleftharpoons HA\cdot + HA^- \quad (7)$$

$$H_2A + H_2A^{+}\cdot \rightleftharpoons H_2A^{+}\cdot + H_2A \quad (8)$$

$$A^{2-} + A^{-}\cdot \rightleftharpoons A^{-}\cdot + A^{2-} \quad (9)$$

are considered. Pelizetti and co-workers have attempted to systematically characterize the reactivity of the $HA^-/HA\cdot$ and $H_2A/H_2A^{+}\cdot$ couples with outer-sphere oxidants.[14,15] From the free energy dependences of HA^- and H_2A oxidation rate constants with characterized outer-sphere reagents $E°$ estimates for these couples were extracted by assuming that the intrinsic barriers to electron transfer are not large for these couples. By this means an $E°$ estimate of 0.85–1.0 V was obtained for the $HA\cdot/HA^-$ couple. Since that estimate is at least 150 mV more positive than the value derived from the thermodynamic experiments (Table II), it is likely that the driving force for the oxidation reactions was underestimated. Consequently, it is likely that the intrinsic electron-transfer barrier is significant for the couple. When the lower $E°$ value ($+0.68 \pm 0.02$ V) is used for the $HA\cdot/HA^-$ couple and the self-exchange rates for the FeL_3^{3+}/FeL_3^{2+} couples are taken as $\sim 10^9\ M^{-1}\ s^{-1}$, the self-exchange rate for this ascorbate couple (eq 7) is calculated from the Marcus cross-relation to lie in the range 10^2–$10^4\ M^{-1}\ s^{-1}$. This value for the exchange rate is also consistent with that ($10^4\ M^{-1}\ s^{-1}$) calculated from the Fe^{III}(cyt *c*)/HA^- rate constant by using $1 \times 10^3\ M^{-1}\ s^{-1}$ for the cytochrome *c* self-exchange process.[21] These considerations thus implicate a much less than diffusion controlled rate constant for the self-exchange of the $HA^-/HA\cdot$ couple. Undoubtedly part of the barrier to this electron-exchange process derives from the differences in C–O (and to a smaller extent C–C) bond lengths in structures II and III in Figure 1. While eq 7 describes the self-exchange process relevant to the bulk of reactions in which ascorbate is oxidized, the related processes eq 8 and 9 may be the crucial ones at low and high pH, respectively. As mentioned earlier, rate constants for outer-sphere oxidation of H_2A are available. Unfortunately these cannot be interpreted in the Marcus framework without an independent measure of $E°$ for the $H_2A^{+}\cdot/H_2A$ couple. At this time the $E°$ evaluation cannot be made since the second pK_a of the ascorbate radical (i.e., for $H_2A^{+}\cdot \rightleftharpoons HA\cdot + H^+$) is not known. By contrast, for the $A^{-}\cdot/A^{2-}$ couple the $E°$ ($+0.03 \pm 0.02$ V) is known but kinetic data are sparse. A measure of the reactivity of this couple may, however, be obtained through the cytochrome *c* results. With use of the rate constant ($k_3 = k_{12} = 5 \times 10^5\ M^{-1}\ s^{-1}$) for the A^{2-}/Fe^{III}(cyt *c*) reaction discussed above, $k_{22} = 1 \times 10^3\ M^{-1}\ s^{-1}$ for Fe^{II}(cyt *c*)/Fe^{III}(cyt *c*), and $K_{12} = 7.9 \times 10^3$ (calculated from the $E°$ in Table II) a self-exchange rate $k_{11} \sim 10^5\ M^{-1}\ s^{-1}$ is obtained for eq 9. From these considerations the intrinsic electron-transfer barrier for the $A^{2-}/A^{-}\cdot$ couple thus appears comparable to or smaller than that for the $HA^-/A^{-}\cdot$ couple. This conclusion is, of course, tentative since it rests on a single rate constant. It is possible that some of the rate constants measured for reduction of the ascorbate radical (for example, that for ClPMZ and ascorbate radical in ref 16) reflect a pathway involving the $A^{-}\cdot/A^{2-}$ (as opposed to the $HA\cdot/HA^-$) couple. In general, however, these data cannot be interpreted since no acid dependence (permitting disentangling of the HA· and $A^{-}\cdot$ reduction pathways) was carried out. Again, further detailed kinetic studies could clarify some of these points.

In the previous paragraph, the reactivities of the ascorbate radical/ascorbate couples were addressed. We turn now to the process relevant to *oxidation* of the radical or reduction of dehydroascorbic acid (eq 10). No studies of the kinetics

$$A^{-}\cdot + A \rightleftharpoons A + A^{-}\cdot \quad (10)$$

of the reduction of dehydroascorbic acid appear to have been made, and few bearing on the oxidation of the radical are available. In fact the only quantitative information bearing directly on this question are the rate constants for ascorbate radical disproportionation at high pH ($\sim 10^5\ M^{-1}\ s^{-1}$, depending upon the medium[11]), an upper limit ($5 \times 10^2\ M^{-1}\ s^{-1}$ [11]) for oxidation of ascorbate radical by O_2, and that for oxidation of $A^{-}\cdot$ by ferricytochrome *c*. All of these seem rather slow in light of the -0.14 ± 0.02 V $E°$ for the $A/A^{-}\cdot$ couple. The cytochrome *c* results provide a useful basis for quantitative comparisons. As mentioned earlier rate constants for oxidation of A^{2-} by Fe^{III}(cyt *c*) ($k_3 = 5 \times 10^5\ M^{-1}\ s^{-1}$) and for oxidation of $A^{-}\cdot$ by Fe^{III}(cyt *c*) ($k_2 \sim 10^4\ M^{-1}\ s^{-1}$) have been determined

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(Scheme II). Oxidation of A^{2-} involves the $A^{-}\cdot/A^{2-}$ couple for which $E^\circ = +0.03 \pm 0.02$ V while oxidation of $A^{-}\cdot$ involves the $A/A^{-}\cdot$ couple for which $E^\circ = -0.14 \pm 0.02$ V. Thus the rate constant for the oxidation of the radical is smaller despite the fact that the driving force for this reaction is greater than for the oxidation of A^{2-}. As above, the self-exchange rate (eq 10) is estimated from the $A^{-}\cdot/Fe^{III}$(cyt *c*) reaction rate constant; a rate constant $k_{22} \leq 10^{-1}$ M^{-1} s^{-1} is thus obtained. Thus we arrive at the conclusion that the $A^{-}\cdot/A$ couple has a rather high intrinsic electron-transfer barrier. While the evidence is limited, sluggish redox properties for this couple might have been predicted on the basis of the structures IV and VI shown in Figure 1. The water-equilibrated form of dehydroascorbic acid (whose properties Ball's thermodynamic measurements should reflect) has a bicyclic monoketo structure. It seems likely that oxidation of $A^{-}\cdot$, a monocyclic species with extensive radical delocalization over three >C=O groups, yields initially the monocyclic triketo form of dehydroascorbic acid V. Rearrangement of V to the stable form VI would then ensue. Alternatively, rearrangement of the radical to a species more strongly resembling VI could precede the electron-transfer step. These alternative mechanisms are summarized in Schemes III and IV where A(V) and A(VI) depict dehydroascorbic acid in forms V and VI, respectively, and $A^{-}\cdot'$ depicts a form of ascorbate radical that is structurally similar to VI rather than to V. Neither thermodynamic nor kinetic data bearing on the equilibrium between structures V and VI are available; nor is there any indication that $A^{-}\cdot'$ exists. Thus the mechanism of ascorbate radical oxidation cannot be clarified to any greater extent at this time. It is worth noting, however, that, on the basis of Scheme III or IV, neither the self-exchange estimate obtained above nor the overall E° given in Table II is for the simple process implied by eq 10 and that far from simple kinetic behavior may be anticipated for reactions involving the $A^{-}\cdot/A$ couple.

Scheme III

$$A^{-}\cdot \rightarrow A(V) + e^{-}$$

$$A(V) \rightleftharpoons A(VI)$$

Scheme IV

$$A^{-}\cdot \rightleftharpoons A^{-}\cdot'$$

$$A^{-}\cdot' + e^{-} \rightarrow A(VI)$$

We mention one other complicating feature in passing. While in most reactions involving ascorbate as a reductant eq 11 is likely to represent the initial step, it is worth reiterating

$$HA^{-} + OX \rightarrow HA\cdot + RED \qquad (11)$$

that at pH 0–13 the stable form of the ascorbate radical is the anionic species $A^{-}\cdot$. Thus above pH ~0 eq 11 is expected to be followed by very rapid deprotonation of HA·, eq 4. With

$$HA\cdot \underset{k_{-5}}{\overset{k_5}{\rightleftharpoons}} H^{+} + A^{-}\cdot \qquad (4)$$

the assumption that k_{-5} is nearly diffusion controlled ($k_{-5} = 10^{9}$ M^{-1} s^{-1}), proton dissociation could proceed with $k_5 = 3.5 \times 10^{8}$ s^{-1}; thus the lifetime of HA· may in some instances be less than 10 ns. The rapid deprotonation of HA· introduces an additional subtlety into the behavior of ascorbate systems: while the rate of production of ascorbate radicals is related to the properties (E°, k_{11}) of the $HA\cdot/HA^{-}$ couple, subsequent reactions are determined by the properties of the $A^{-}\cdot/A^{2-}$ and $A/A^{-}\cdot$ couples discussed above. The rapid deprotonation of HA· (as well as the sluggishness of the $A^{-}\cdot/A$ couple) may be of particular importance in the photochemical systems[4] where it may provide a "switching" mechanism, effectively slowing down some of the reactions that destroy reactive intermediates. In the thermal reactions reviewed in this paper these interesting complications may also play an important, if infrequently recognized, role. We hope that further detailed studies of ascorbate reactions will lead to a fuller understanding of these questions.

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Electron Correlation Effects in B_4H_{10} Structures

Sir:

The experimental geometry of B_4H_{10} is well established[1] as a molecule of C_{2v} symmetry of *styx* topology 4012 in which each of the two BH_2 groups is joined by bridged hydrogens to a singly bonded pair of BH units. An early proposal,[2] also of topology 4012, is the bis(diborane) structure, in which two B_2H_5 units are joined by a single bond. Here, we address the question, "What level of theoretical accuracy yields the observed structure in preference to the bis(diborane) structure?"

In two previous calculations the observed structure is not preferred. A 4-31G* study showed that bis(diborane) is more stable than the observed structure by 16.5 kcal/mol. Neither the addition of configuration interaction nor modification of this basis set altered this conclusion.[3] A study by Kleier,[4] who used the PRDDO method,[5] yielded the gauche form of bis(diborane) as more stable than the trans form by about 1 kcal/mol, and more stable than the cis form by about 3 kcal/mol. The observed structure of C_{2v} symmetry was about 5 kcal/mol less stable than the gauche form of bis(diborane).[4]

In the present study geometries were optimized[6] with use of a double-ζ basis set (3-21G),[7] assuming symmetry C_{2v} for the observed structure, C_{2h} for *trans*-bis(diborane), C_{2v} for *cis*-bis(diborane), and C_1 for *gauche*-bis(diborane). The gauche form optimized to C_2 symmetry. These optimized geometries (Table I) yielded the energies listed in Table II at the levels 6-31G and 6-31G* (polarization added) and Møller–Plesset (MP) corrections[8] to third order[9] for the 6-31G basis (configuration interaction). In Table II we add the

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