Inert Carbon Free Radicals. 6. Perchloro-2-phenyldiphenylmethyl (PODM), a New Radical of the Perchlorodiphenylmethyl Series, and Products Therefrom

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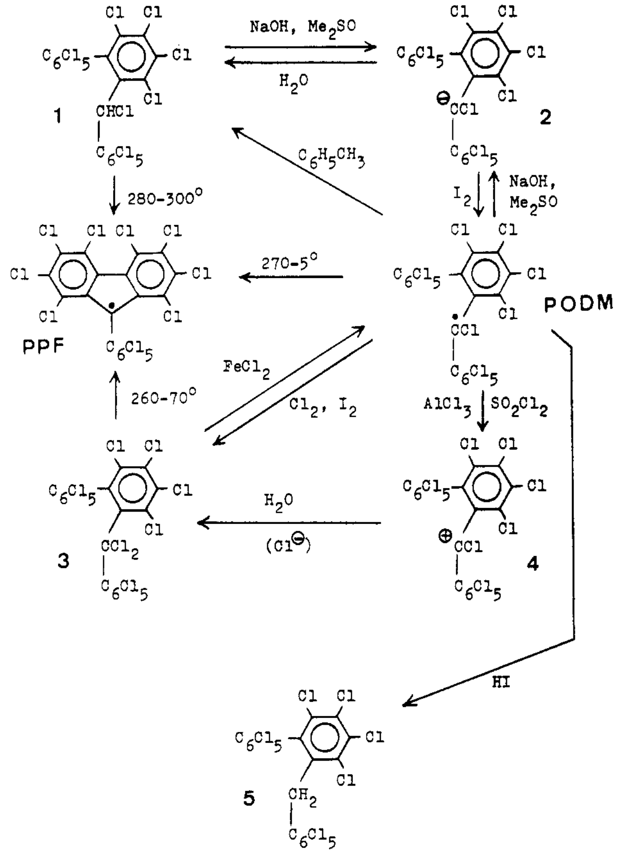
In order to determine the effect of replacing an *o*-chlorine with a bulky pentachlorophenyl group on the stability of the perchlorodiphenylmethyl radical (PDM), a new perchlorinated radical, perchloro-2-phenyldiphenylmethyl (PODM), was examined. PODM was synthesized from αH-pentadecachloro-2-phenyldiphenylmethane (1) and isolated as a pure, completely disassociated radical. Its stabilities toward O_2 and concentrated HNO_3 are significantly higher than those of the radical PDM. PODM chlorinates to perchloro-2-phenyldiphenylmethane (3), which may be reduced back to PODM. Chlorocarbon 3, as well as PODM, undergoes cyclization at 260–270 °C to perchloro-9-phenylfluorenyl radical (PPF). PODM may be oxidized to perchloro-3-phenyl-4-benzylidenecyclohexa-2,5-dienone (8) and perchloro-4-(2-biphenylylmethylene)cyclohexa-2,5-dienone (9). Reductions of PODM to either α,α-di-H-tetradecachloro-2-phenyldiphenylmethane (5) or αH-compound 1 are described. The mechanisms of some unusual reactions here reported, as well as the ESR and other spectra of the PODM, are discussed.

Most of the inert trivalent carbon free radicals described so far belong to the so-called PTM (perchlorotriphenylmethyl) series.[1-4] Their exceptionally high chemical passivity and thermal stability are due to shielding of the trivalent carbon (where most of the *spin* density resides) by three pentachlorophenyl groups, which confer on those radicals a propeller-like conformation.[1] If the trivalent carbon is protected by only two perchlorinated rings and one α chlorine, some reactivity appears. For example, although the perchlorodiphenylmethyl radical (PDM)[1] withstands typical radical reagents, e.g., hydroquinone, nitric oxide, etc., and strong chemical species such as concentrated H_2SO_4, it does react with boiling toluene and concentrated HNO_3. It also reacts with O_2 in solution, its half-life being about 3 days at room temperature. In view of these results, it seemed appropriate to investigate the effect of partly restoring the shielding of the trivalent carbon by introducing a third perchlorinated ring in one of the ortho positions of the radical PDM, as in the perchloro-2-phenyldiphenylmethyl radical. The present paper presents a study of the synthesis and properties of such a radical.

Results and Discussion

Synthesis of Perchloro-2-phenyldiphenylmethyl (PODM) (Scheme I). It has been found[5] that treatment of αH-pentadecachloro-2-phenyldiphenylmethane (1) with a mixture of NaOH, ether, and Me_2SO gives a solution of the perchloro-2-phenyldiphenylcarbanion (2), which undergoes spontaneous cyclization to the perchloro-9-phenylfluorenyl anion. However, this cyclization can be largely avoided by treating carbanion 2 quickly with I_2. The resulting product is the expected radical PODM, which is crystalline, fluorescent, orange-red, and according to magnetic susceptibility measurements, is completely disassociated even in solid form.[1]

Scheme I



Although solid radical PODM is fluorescent, PDM is not. Space-filling models suggest that the two pentachlorophenyl rings of PODM are juxtaposed forming an internal π-complex, as shown in Figure 1. This would confer an additional degree of molecular rigidity to which the fluorescence is tentatively attributed. However, no differential UV–vis absorption traceable to such a complexing is observed, possibly because it is completely swamped in the long wave absorption of the radical.[1] The radical PODM is not fluorescent in solution, a fact which is consistent with the suggested internal association.

Stability of the Radical PODM. As measured by UV–vis spectroscopy, the half-life of the radical PODM in cyclohexane solution, in air, and at room temperature is much longer than that of PDM[1] (over 2 months vs. 2–3

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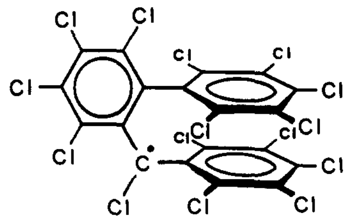
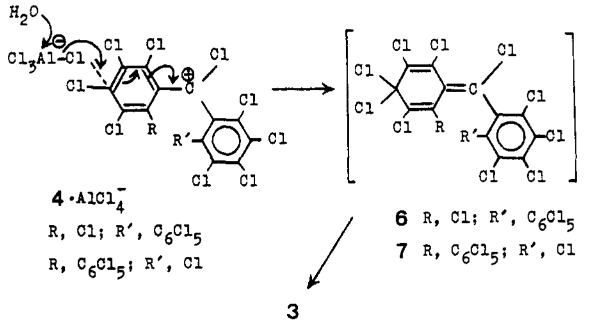


Figure 1.

Scheme II



days). This is attributed to the already mentioned increased shielding of the trivalent carbon. Its inertness to NaOH (ether, 2 days, 85% recovery), hydroquinone (ether, 7 days, 94%), *p*-quinone (ether, 7 days, 92%), chlorine in the dark (CCl_4, 2 days, 79%), bromine in the dark (CCl_4, 3 days, 83%), nitric oxide (CCl_4, 2 h, 83%), and concentrated H_2SO_4 (2 days, 94%) is similar to that of the radical PDM, and it appears less reactive toward concentrated HNO_3 (2 days, 94%).[1] However, it oxidizes in fuming concentrated HNO_3 and reacts with boiling toluene, as does the radical PDM.[1] It is stable up to its melting point of 244–246 °C.

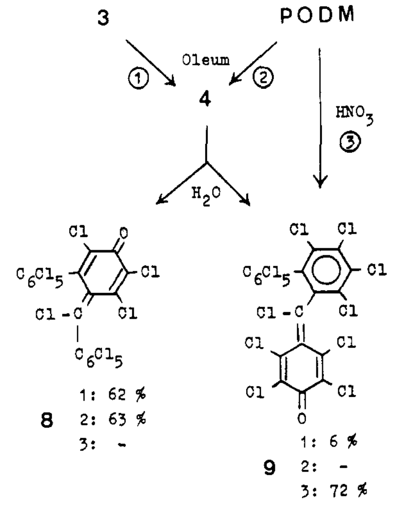
Chlorinations of the Radical PODM (Scheme I). (1) Although the PODM is stable toward Cl_2 in the dark, in the presence of I_2 it chlorinates readily to the perchloro-2-phenyldiphenylmethane (**3**).

(2) The radical PODM reacts with anhydrous $AlCl_3$ in SO_2Cl_2 giving a dark blue solution of the perchloro-2-phenyldiphenylcarbenium ion (**4**) (Scheme II), which by hydrolysis affords chlorocarbon **3**. A similar result is obtained with the radical PDM.[6] The formation of the chlorocarbon **3** probably takes place through the intermediacy of the thermodynamically less stable isomeric chlorocarbon **6** (or **7**), which would derive from "tight ion pairs",[5] where the $AlCl_4^-$ (or $Al_2Cl_7^-$) is presumably anchored to a peripheral position of the carbenium ion **4**.

The chlorocarbon **3** decomposes at about 260–270 °C giving the perchloro-9-phenylfluorenyl radical (PPF)[5] (75%), presumably by way of the radical PODM. Consistent with this hypothesis, PODM cyclizes to the radical PPF (94%) when heated at 260–270 °C. The chlorocarbon **3** reverts almost quantitatively to the radical PODM with $FeCl_2$ in ether.

Oxidative Hydrolysis of the Radical PODM (Scheme III). (1) The radical PODM, when treated with oleum and then with H_2O, gives predominantly perchloro-3-phenyl-4-benzylidenecyclohexa-2,5-dienone (**8**) and perchloro-4-(2-biphenylylmethylene)cyclohexa-2,5-dienone (**9**). A reasonable mechanism involves the formation of the perchloro-2-phenyldiphenylcarbenium ion (**4**) which is attacked at a peripheral position to give a protonated perchloro ketone with elimination of $HClSO_3$.[5] Similarly the chlorocarbon **3**, with oleum, gives the benzylidene dienone **8**. The less hindered perchlorodiphenylmethane affords the perchlorobenzophenone instead.[1]

Scheme III



To account for the preferred formation from PODM of dienone **8** over **9**, an internal π complexation between the two pentachlorophenyl rings in the carbenium ion **4**, analogous to that suggested above for PODM, is proposed (Figure 1). Models show that in such a complex the pentachlorophenyl groups are almost perpendicular to the plane of the trigonal α-carbon, thus disfavoring delocalization of the positive charge into these rings and enhancing it into the tetrachlorophenyl ring. This configuration should thus favor attack upon the para position of that ring and consequent formation of dienone **8** (Scheme II).

(2) The reaction between solid radical PODM and fuming concentrated HNO_3 takes place very quickly. It is unlikely that this reaction occurs via carbenium ion **4**, since no blue color is observed. This circumstantial evidence supports the assumption that the reacting species is the NO_2 radical. For unknown reasons, the attack on PODM takes place predominantly at the 4′-position of the latter giving the dienone **9**.

Reductions of the Radical PODM (Scheme I). (1) **With HI.** PODM reacts with HI (refluxing acetic acid/water) to give an excellent yield of α,α-di-*H*-tetradecachloro-2-phenyldiphenylmethane (**5**). This reaction probably proceeds through the αH-compound **1**.[5]

(2) **With Toluene.** The PODM, like PDM,[1] extracts hydrogen from boiling toluene to give the αH-compound **1**.

(3) **With NaOH/Ether/Me$_2$SO.** Reaction of PODM with this mixture gives a dark blue solution, which on treatment with water affords an excellent yield of the αH-compound **1** (Scheme I). The color is attributed to intermediate carbanion **2**. This is a well established reaction for related radicals.[1-3,5]

(4) **With Potassium.** The reaction of PODM with potassium gives the carbanion **2**, which is then hydrolyzed to the αH-compound **1**. This reaction takes place also with the radicals PDM and PTM.[1]

Structural Assignments for the Perchloro Ketones 8 and 9. The UV–vis spectra of the ketones **8** and **9** (Figure 2) (**8** 322 nm (ϵ 16600), **9** 323 (11 200)) rule out a benzophenone structure (perchlorobenzophenone[1] 316, 2460) and fully agrees with a methylenecyclohexadiene (*p*-quinomethane) structure (perchloro-4-benzylidenecyclohexadienone (**10**)[7] 325, 15 800). The structural assignment for dienone **9** is based on the positions of the IR peaks due to the quinomethane system (1680 and 1585 cm^{-1}), which are almost coincident with those of dienone

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[7] Ballester, M.; Riera, J.; Castañer, J., unpublished results.

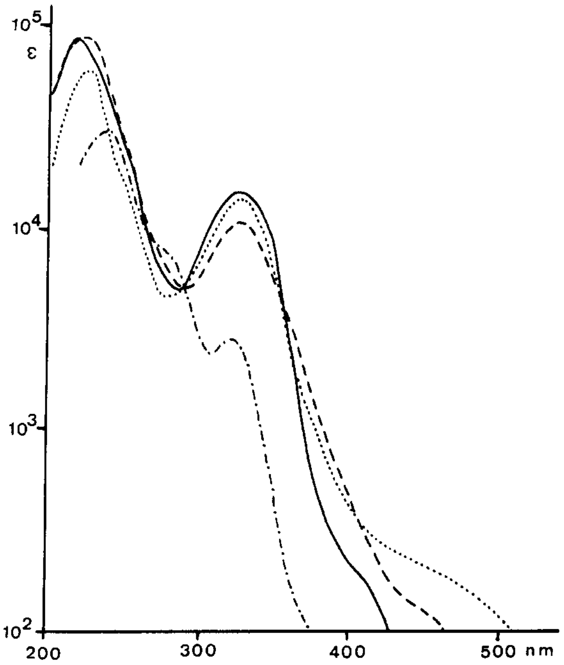

Figure 2. UV-vis of perchlorobenzophenone (-·-), dienone **8** (--), dienone **9** (—), dienone **10** (··).

10 (1677 and 1585) and quite different from those of dienone **8** (1693). Consequently, the structure of the latter is also established.

UV-Vis Spectra. The spectra of the perchloro ketones **8** and **9** are given in Figure 2, and have been discussed in the preceding paragraph. The spectrum of the radical PODM is similar to that of the radical PDM (PODM 294 nm, 370 (sh), 384, 485 (sh), and 525; PDM 300 nm, 368 (sh), 380, 485 (sh), 510 (sh)[1]). The spectra of the highly chlorinated compounds described here are regarded as normal.[1-3,5]

ESR Spectrum of the Radical PODM. The *g* value (2.0055) and the ESR hyperfine structure of the radical PODM are similar to those of the radical PDM.[1] The spectrum consists of the expected four main lines due to coupling with the α-chlorine (7.0 MHz) and two weak pairs of satellite quadruplets due to the α-^{13}C (104 MHz) and the aromatic ^{13}C (34 MHz).

Magnetic Susceptibility of the Radical PODM. The variation of the magnetic susceptibility of PODM with temperature indicates the existence of a slight antiferromagnetism at low temperatures.[5,8,9] From the relevant data, the radical puritiy has been calculated to be ~100%.

Experimental Section

General Methods. The IR, UV-vis, and ESR spectra were recorded with Perkin-Elmer 457, Perkin-Elmer 350, and Varian E4 spectrometers, respectively. The magnetic susceptibilities were measured in helium with a Varian 4-in. magnet with constant force caps, and a Cahn RG electrobalance.

The handling of radicals in solution was performed in the dark. Since the locations of the IR peaks of perchloroorganic compounds differ markedly from those of their non-chlorinated counterparts, they are included in this section.

Perchloro-2-phenyldiphenylmethyl Radical (PODM). (1) **From the αH-Compound 1.** A mixture of **1**[4] (0.515 g), powdered NaOH (1.50 g), ethyl ether (300 mL), and Me_2SO (60 mL) was shaken for 2.5 h under argon. The resulting dark blue solution was filtered onto I_2 (1.50 g) under argon. It was left undisturbed for 2 h, and then washed with aqueous $NaHSO_3$ and with water, dried, and concentrated to ~6 mL. The precipitate (0.471 g) was collected by filtration and purified through silica gel (hexane–CCl_4) giving the radical PODM (0.257 g, 50.0%), as orange-red, fluorescent crystals melting at 244 °C dec: UV-vis (C_6H_{12}) 213 nm, 294, 370 (sh), 384, 485 (sh), 525 (ϵ 94 800, 6020, 10 200, 10 300, 326, 218); IR (KBr) 1358 (w), 1336 (s), 1268 (m), 1097 (m), 1005 (m), 833 (m), 700 (m), 670 (m), 522 (m) cm^{-1}; ESR g = 2.0055, no. of lines = 4 (1:1:1:1), $a_{\alpha\text{-Cl}} = 7.0$ MHz, $a_{\alpha\text{-}^{13}C} = 104$ MHz, $a_{\text{arom}^{13}C} = 34.0$ MHz; magnetic susceptibility $\chi_{\text{dia}} = -0.514 \times 10^{-6}$ emu,[10] $J = -23$ °K, $\mu = 1.71$, spins/mole = 5.9×10^{23}. Anal. Calcd for $C_{19}Cl_{15}$: C, 30.0; Cl, 70.0. Found: C, 30.0; Cl, 70.1. From the mother liquors 0.047 g (9.1%) of starting material was recovered.

(2) **From Perchloro-2-phenyldiphenylmethane (3).** A mixture of **3** (0.083 g) (see below), $FeCl_2{\cdot}2H_2O$ (0.080 g) and ethyl ether (25 mL) was refluxed for 8 h under argon. The resulting solution was washed with water, dried, and evaporated giving a residue (0.080 g), which by purification through alumina (CCl_4) yielded the radical PODM (0.076 g, 96%).

Perchloro-2-phenyldiphenylmethane (3) from the Radical PODM. (1) **With Cl_2 and I_2.** Dry Cl_2 was passed for 1.5 h through a solution of the radical PODM (0.100 g) and I_2 (0.100 g) in CCl_4 (5 mL). By evaporation of the solvent a solid was obtained, which on recrystallization from hexane yielded the chlorocarbon **3** (0.092 g, 88%): mp 215 °C dec; UV (C_6H_{12}) 219 nm, 300 (sh), 308 (ϵ 106 100, 3650, 3700); IR (KBr) 1510 (w), 1350 (s), 1332 (s), 1320 (s), 1308 (m), 1110 (m), 810 (m), 790 (s), 755 (m), 695 (s), 688 (m), 655 (m), 559 (s), 532 (s) cm^{-1}. Anal. Calcd for $C_{19}Cl_{16}$: C, 28.7; Cl, 71.3. Found: C, 28.7; Cl, 71.4.

(2) **With SO_2Cl_2 and $AlCl_3$.** Radical PODM (0.100 g) was added to a cooled (−15 °C) solution of anhydrous $AlCl_3$ (0.13 g) in SO_2Cl_2 (15 mL), and the resulting mixture was stirred for 1.5 h at the same temperature. The resulting dark blue solution was poured onto cracked ice, and the SO_2Cl_2 was removed by evaporation in vacuo. The residue was treated with cold aqueous $NaHCO_3$, acidified with aqueous HCl, and extracted with ethyl ether. The organic layer was washed with water, dried, and evaporated giving a solid which on recrystallization from hexane yielded the chlorocarbon **3** (0.064 g, 61%).

Reductions of the Radical PODM. (1) **With HI.** A mixture of the radical PODM (0.200 g), 51% aqueous HI (1 mL), and acetic acid (10 mL) was refluxed for 48 h under argon. The resulting solution was poured into aqueous $NaHSO_3$ and the resulting mixture was extracted with ether. The ethereal layer was washed with aqueous $NaHCO_3$ and with water, dried, and evaporated giving a solid (0.185 g), which by purification through alumina (CCl_4) yielded α,α-di-H-tetradecachloro-2-phenyldiphenylmethane (**5**) (0.165 g, 86%): mp 255–258 °C; UV (C_6H_{12}) 213 nm, 250 (sh), 288–298 (ϵ 112 000, 22 000, 1300); IR (KBr) 2910 (w), 1425 (w), 1370 (m), 1355 (s), 1345 (s), 1327 (m), 1300 (m), 920 (m), 830 (m), 800 (m), 690 (m), 675 (m), 570 (m), 500 (m) cm^{-1}; ^1H NMR (CCl_4) τ 5.3 (s). Anal. Calcd for $C_{19}H_2Cl_{14}$: C, 31.4; H, 0.3; Cl, 68.3. Found: C, 31.5; H, 0.3; Cl, 68.4.

(2) **With Toluene.** A solution of the radical PODM (0.051 g) in toluene (20 mL) was refluxed for 24 h under argon. By evaporation of the solvent, a residue (0.070 g) was obtained, which on purification as described above gave the αH-compound **1** (0.034 g, 67%).

(3) **With NaOH–Ether–Me_2SO.** A mixture of the radical PODM (0.100 g), powdered NaOH (0.40 g), ethyl ether (75 mL), and Me_2SO (15 mL) was shaken for 2.5 h under argon. The resulting dark blue solution was filtered and poured into water. The organic layer was decanted, washed with water, dried, and evaporated. The residue (0.092 g) on purification through alumina (CCl_4) gave the αH-compound **1** (0.084 g, 84%).

(4) **With Potassium.** A mixture of the radical PODM (0.080 g), potassium (0.8 g), and ethyl ether (50 mL) was shaken vigorously for 1.25 h under argon. The resulting dark blue solution was worked up as described above to give the αH-compound **1** (0.071 g, 89%).

Perchloro-4-(2-biphenylylmethylene)cyclohexa-2,5-dienone (9) and Perchloro-3-phenyl-4-benzylidenecyclohexa-2,5-dienone (8). (1) **From the Radical PODM and Oleum.**

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(10) Calculated independently from modified Pascal's data.[3]

A mixture of the radical PODM (0.100 g) and 20% oleum (50 mL) was stirred for 24 h, and the resulting dark blue solution was poured onto cracked ice and extracted with ether. The ethereal layer was washed with water, dried, and evaporated. The resulting solid (0.069 g), after digestion with CCl_4, gave a residue of the dienone 9 (0.006 g, 6%) as yellow crystals: mp 208–212 °C; UV–vis (C_6H_{12}) 213 nm, 322, 400 (sh) (ϵ 91700, 16600, 240); IR (KBr) 1680 (s), 1585 (w), 1545 (m), 1350 (s), 1335 (s), 1232 (m), 1150 (m), 1102 (m), 1012 (m), 810 (s), 730 (s), 692 (m), 678 (m), 670 (m), 542 (m) cm^{-1}. Anal. Calcd for $C_{19}Cl_{14}O$: C, 30.8; Cl, 67.0. Found: C, 30.5; Cl, 66.9. Evaporation of the CCl_4 extract gave a solid which on recrystallization from hexane yielded the dienone 8 (0.060 g, 62%) as yellow crystals: mp 321–362 °C dec; UV–vis (C_6H_{12}) 215 nm, 323, 400 (sh) (ϵ 93400, 11200, 540); IR (KBr) 1693 (s), 1530 (m), 1405 (w), 1345 (s), 1330 (s), 1232 (s), 1155 (m), 1090 (m), 1012 (m), 838 (m), 802 (m), 775 (m), 745 (m), 738 (m), 698 (m), 688 (m), 671 (m), 650 (m), 540 (s) cm^{-1}. Anal. Calcd for $C_{19}Cl_{14}O$: C, 30.8; Cl, 67.0. Found: C, 30.5; Cl, 67.1.

(2) **From the Radical PODM with Fuming HNO_3.** Radical PODM (0.300 g) was added with stirring to fuming concentrated HNO_3 (100 mL). A yellow solid was formed immediately, which was filtered, washed with water, dried, and digested with hexane to give the dienone 9 (0.211 g, 72%).

(3) **From the Chlorocarbon 3 with Oleum.** A mixture of the chlorocarbon 3 (0.090 g) and 20% oleum (50 mL) was stirred for 15 h at room temperature. The resulting dark blue solution was poured onto cracked ice and extracted with ether. The ethereal layer was washed with water, dried, and evaporated. The resulting residue (0.070 g), on recrystallization from hexane, afforded the dienone 8 (0.053 g, 63%).

Preparation of the Radical Perchloro-9-phenylfluorenyl (PPF). (1) From the Radical PODM. PODM (0.100 g) was heated (270–275 °C, 1 h) under argon. When the resulting mass was worked up as usual, radical PPF (0.076 g, 84%) was obtained.

(2) **From the Perchloro-2-phenyldiphenylmethane (3).** Heating the chlorocarbon 3 (0.100 g) at 260–270 °C for 30 min under argon gave radical PPF (0.065 g, 75%).

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Application of Linear Free Energy Relationships to the Curtin–Hammett Principle: Correlation between Conformational Equilibrium, Chemical Reactivity, and Product Ratios

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The Curtin–Hammett principle (CHP) was originally derived to deter relating the product ratio $[A_4]/[A_1]$ to the equilibrium distribution $k_{23}/k_{32} = K$ for the kinetic system $A_1 \leftarrow A_2 \rightleftarrows A_3 \rightarrow A_4$ (Scheme I). By use of linear free energy relationships, it is herein shown that the product ratio $[A_4]/[A_1]$ for a Scheme I system is equal to $K^{1-\alpha}$, where α is a parameter which indicates the relative sensitivity of the ratio of reaction rate constants k_{34}/k_{21} and the equilibrium constant K to substituent effects. This result then permits estimation of equilibrium constants from experimental product ratios. Applications to steric effects and conformational equilibria and to electronic effects and tautomeric equilibria are discussed.

Introduction

The Curtin–Hammett principle (CHP) is one of the most valuable concepts in conformational analysis.[1,2] Historically, it was developed in the early 1950's to discourage attempts to determine conformational equilibrium constants from product ratios. According to the CHP, in a reaction (Scheme I) involving two rapidly interconverting conformers each of which yields a different product, the product composition is not solely dependent on the relative proportions of the two conformers, and it is determined by the difference in standard Gibbs free energies of the two reaction transition states ($\Delta G^{\ddagger}_{TS}$) (eq 1).[2] However,

Scheme I

$$A_1 \xleftarrow{k_{21}} A_2 \underset{k_{32}}{\overset{k_{23}}{\rightleftarrows}} A_3 \xrightarrow{k_{34}} A_4$$

$$k_{23}, k_{32} >> k_{21}, k_{34}$$

$$[A_4]/[A_1] = e^{-\Delta G^{\ddagger}_{TS}/RT} \qquad (1)$$

we herein wish to demonstrate that the applicability of linear free energy relationships (LFERs)[3-5] can permit a qualitative or semiquantitative determination of conformational equilibria from product ratios.

The Curtin–Hammett principle applies to the kinetic system of Scheme I. Here A_2 and A_3 are rapidly interconverting isomers in equilibrium, with the equilibrium constant given by eq 2. Originally A_2 and A_3 were considered to be conformational isomers, but for generality we also allow for tautomers, especially since it has often

$$[A_3]/[A_2] = k_{23}/k_{32} = K = e^{-\Delta G^{\circ}/RT} \qquad (2)$$

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