

Excitation of **5**, **7**, and **8** ( $10^{-4}$  M in degassed  $\text{CH}_2\text{Cl}_2$  at room temperature) by a 20-ps laser pulse at 530 nm was used for transient absorption measurements at 820 nm (triplet state absorption; see Ref. [11]) with an apparatus already described.<sup>[12]</sup> Simultaneously, time-resolved emission measurements were performed. In **5**, emission at 600 nm is completely quenched whereas emission at 660 nm is enhanced as compared to **7** under the same conditions. The formation rate of the triplet state localized on the non-metallated subunit ( $10^8 \text{ s}^{-1}$  at room temperature in degassed  $\text{CH}_2\text{Cl}_2$ ) is similar to the decay rate of the singlet state (non-metallated ring). Furthermore, the emission quantum yield at 660 nm and the quantum yield of triplet state generation (absorption at 820 nm) for **5** are roughly twice those for **7**, corroborating the data of Table 2 obtained by classical emission spectroscopy. No evidence was obtained for light-induced electron transfer. These observations are in full agreement with the postulated reaction of efficient intramolecular singlet energy transfer from the zinc porphyrin part to the non-metallated ring.

The present oblique bis-porphyrin may be related to the hypothetical mechanism of the photosynthetic bacterial reaction center. Energy migration from the special pair to the isolated bacteriochlorophyll followed by electron transfer or initial electron transfer from the special pair may be operative.<sup>[12]</sup>

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**1**, 116287-98-0; **2**, 120085-98-5; **3**, 120085-99-6; **4**, 120086-00-2; **5**, 120086-01-3; **6**, 120086-02-4; **7**, 89372-90-7; **8**, 116123-17-2; pyrrole, 109-97-7; 3,5-di-*tert*-butylbenzaldehyde, 17610-00-3.

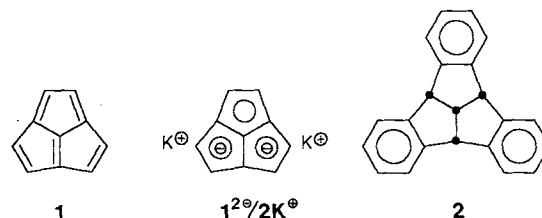
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## Towards Tribenzoaceptalene: Tribenzotriquinacene, Dihydrotribenzoaceptalenediide, and the Tribenzoaceptalene Radical Anion\*\*

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Dedicated to Professor Kurt Heyns on the occasion of his 80th birthday

Benzoannulation can increase the stability of cyclically conjugated, nonaromatic hydrocarbons that, owing to unfavorable electron configuration and/or unfavorable HOMO energies, are unstable and therefore highly reactive. To explore this possibility for aceptalene **1**, only the dianion of which,  $1^{2-}$ , is so far known,<sup>[1]</sup> we synthesized tribenzotriquinacene (tetrahydrotribenzoaceptalene) **2** and investigated its deprotonation-dehydrogenation both in solution and in the gas phase.

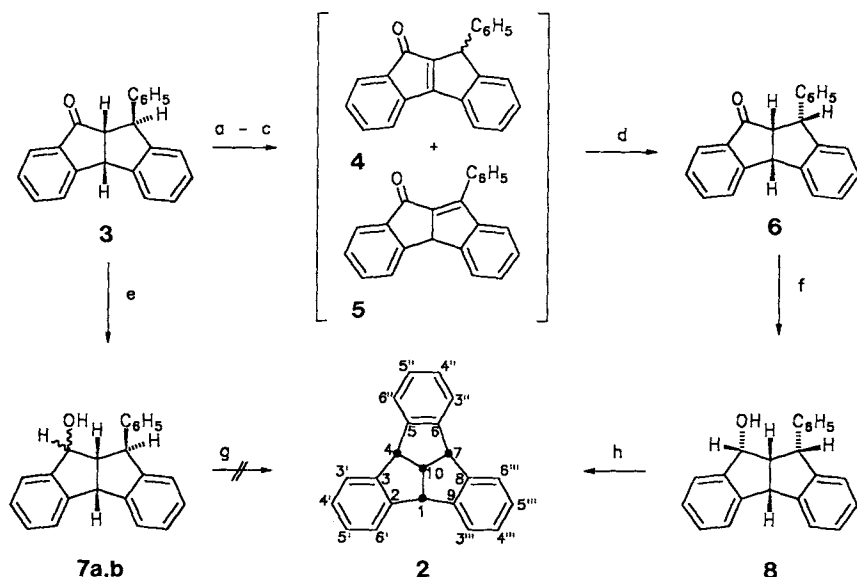


Tribenzotriquinacenes with substituents on the central C atom are accessible by double cyclodehydration of the correspondingly substituted 2-benzhydryl-1,3-indandiol.<sup>[2]</sup> The unsubstituted hydrocarbon **2**, however, could be obtained only in low yields via this route. Starting from cinnamic acid, Baker et al.<sup>[3]</sup> synthesized the diquinane ketone **3** in three steps; bromination/dehydrobromination then gave the enone **4** in moderate yield. In our attempts to synthesize **2** and higher benzoannulated centropolyquinanes,<sup>[4]</sup> the ketone **3** and the alcohols **7a**, **b**<sup>[5]</sup> derived therefrom were identified as 8-*exo*-phenyl stereoisomers on the basis of their mass spectra;<sup>[5]</sup> thus, the cyclodehydration **7** → **2** attempted by Baker et al.<sup>[3]</sup> was doomed to failure for steric reasons. The enone **4**, together with the isomer **5**,<sup>[8]</sup> is accessible on a preparative scale (overall yield 25%, Scheme 1) by an alternative route involving phenylsulfenylation of **3**, oxidation, and thermal elimination of the phenylsulfinyl derivative.<sup>[6, 7]</sup> Subsequently, **4** and **5** can be rehydrogenated with palladium on charcoal in dioxane to afford the isomeric diquinane ketone **6** with high selectivity. After reduction to the alcohol **8**, bearing an *endo*-phenyl group, the cyclodehydration to the tricyclic compound **2** occurs readily, as expected. Compound **2** crystallizes from hot xylene as sparingly soluble, colorless, long, hard needles having an unusually high melting point (390 °C). The identity of **2** was established on the basis of its analytical<sup>[9]</sup> and spectroscopic data.<sup>[10]</sup>

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Scheme 1. a)  $\text{LiNiPr}_2/\text{THF}$ ,  $-40^\circ\text{C} \rightarrow 0^\circ\text{C}$ ,  $(\text{PhS})_2/\text{THF}$ , room temperature (RT), 1 h (76%); b) *m*-chloroperoxybenzoic acid/ $\text{CH}_2\text{Cl}_2$ ,  $-30^\circ\text{C} \rightarrow \text{RT}$ , then 10 h (91%); c)  $\Delta/\text{toluene}$ ,  $110^\circ\text{C}$ . 4 d (36%); d)  $\text{H}_2/\text{Pd,C/dioxane}$ , RT (71% [9]); e)  $\text{LiAlH}_4/\text{Et}_2\text{O}$  [3] or  $\text{Al}(\text{O}i\text{Pr})_3/i\text{PrOH/toluene}$  [3]; f)  $\text{LiAlH}_4/\text{Et}_2\text{O}$ , 3 h,  $36^\circ\text{C}$  (95%); g)  $\text{CuSO}_4/\text{xylene}$  [3]; h)  $\text{H}_3\text{PO}_4/\text{xylene}$ ,  $135^\circ\text{C}$ , 4 h (58%). The numbering in **2** is unsystematic; the numbers 1–10 refer to the triquinacene.

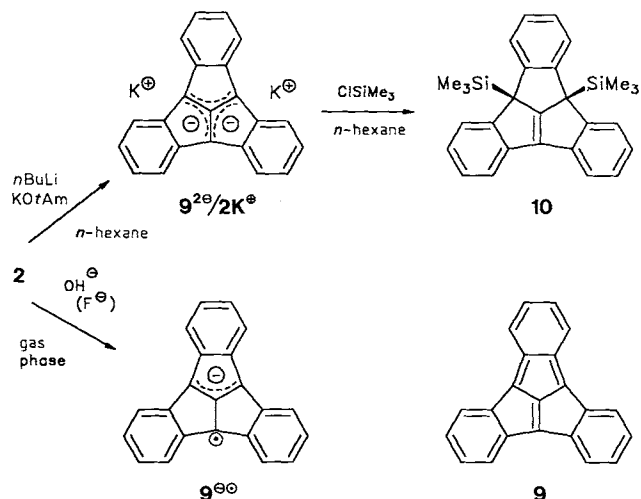
Upon treatment of a suspension of **2** in *n*-hexane with *n*-butyllithium and potassium *tert*-amyl alkoxide (molar ratio 1:4.7:2.5), the mixture turns carmine red within 30 min. After 24 h at room temperature and an additional 24 h at reflux temperature, the reaction mixture was filtered under argon. The red-brown solid was washed four times with *n*-hexane and once with diethyl ether and then dried at  $40^\circ\text{C}/0.1$  torr. In addition to dipotassium dihydrotribenzoacepentalediide ( $\mathbf{9}^{2\ominus}/2\text{K}^\oplus$ ),<sup>[11]</sup> the pyrophoric solid contained lithium and potassium as the hydrides and *tert*-amyl alkoxides, as well as, possibly, butyllithium. Despite the impurities,  $\mathbf{9}^{2\ominus}$  could be unambiguously characterized by NMR spectroscopy in  $[\text{D}_{10}]$ dimethoxyethane (Table 1). Particularly surprising is the position of the signal of the central C atom (C-10) at extremely high field ( $\delta = 173.17$ ); its assignment is confirmed by the unchanged half-width ( $\nu_{1/2} = 5.5$  Hz) in the broadband- and “gated”-decoupled  $^{13}\text{C}$  NMR spectrum. This  $^{13}\text{C}$  chemical shift and those of the peripheral acepentalene C atoms (C-2,3,5,6,8,9) indicate that, for  $\mathbf{9}^{2\ominus}$ , another resonance structure besides that with Y-like delocalization<sup>[12]</sup> of the negative charges, shown here, contributes even less to the resonance hybrid than for  $\mathbf{1}^{2\ominus}$ .

Table 1. Characteristic NMR data for dipotassium dihydrotribenzoacepentalediide  $\mathbf{9}^{2\ominus}/2\text{K}^\oplus$  and its trapping product **10**. For numbering, see Scheme 1. The cross peaks of magnetically equivalent atoms are not listed separately.

$\mathbf{9}^{2\ominus}$ :  $^1\text{H}$  NMR (400 MHz,  $[\text{D}_{10}]$ DME, 293 K):  $\delta = 6.69$  (AA'BB',  $^3J = 5.57$  Hz, 6H, 4',5',4'',5'',5''',5''',H), 7.74 (AA'BB',  $^3J = 5.57$  Hz, 6H, 3',6',3'',6'',3''',6''',H),  $^{13}\text{C}$  NMR (100.62 MHz,  $[\text{D}_{10}]$ DME, 273 K, “gated”):  $\delta = 99.86$  (s,  $\nu_{1/2} = 9$  Hz, C-1,4,7), 113.95 (d, C-4',5',4'',5'',4''',5''',  $^1J_{\text{CH}} = 146$  Hz), 119.59 (d, C-3',6',3'',6'',3''',6''',  $^1J_{\text{CH}} = 146$  Hz), 137.77 (s, C-2,3,5,6,8,9), 173.17 (s,  $\nu_{1/2} = 5.5$  Hz, C-10). In the H,C-COLOC spectrum<sup>[13]</sup> (SF(2) = 100.62 MHz, SF(1) = 400.14 MHz), the following cross peaks were found: C-1/3',6'-H, C-2/3',5',6'-H, C-3'/4',5'-H, C-4'/3',6'-H

**10**:  $^1\text{H}$  NMR (400 MHz,  $[\text{D}_8]$ THF, 297 K):  $\delta = 0.22$  (s, 18H,  $\text{Si}(\text{CH}_3)_3$ ), 7.10 (AA'BB',  $^3J = 5.8$  Hz, 2H, 4',5''-H), 7.14 (dt,  $^3J = 7.6$ ,  $^4J = 1.1$  Hz, 2H, 3',6'-H), 7.27 (dt,  $^3J = 7.6$ ,  $^4J = 1.1$  Hz, 2H, 5',4''-H); 7.42 (AA'BB',  $^3J = 5.8$  Hz, 2H, 3'',6''-H), 7.69 (dd,  $^3J = 7.4$  Hz, 2H, 6',3''-H), 7.72 (dd,  $^3J = 7.6$  Hz, 2H, 4',5''-H). Assignment of the protons was made from the H,H COSY spectrum:  $^{13}\text{C}$  NMR (100.62 MHz,  $[\text{D}_8]$ THF, 297 K):  $\delta = 0.49$  (–,  $\text{Si}(\text{CH}_3)_3$ ), 61.60 (0, C-4,7), 121.60 (–, C-3',6''), 124.50 (–, C-4',5'''), 125.88 (–, C-6',3''), 125.91 (–, C-3'',6''), 128.86 (–, C-4',5''), 127.10 (–, C-5',4''), 143.66 (0, C-2,9), 148.76 (0, C-5,6), 156.46 (0, C-1), 159.4 (0, C-3,8), 182.32 (0, C-10). The assignment was made from the DEPT spectrum with  $135^\circ$  pulse (+ = positive signal for  $\text{CH}_2$ ; – = negative signal for CH,  $\text{CH}_3$ ; 0 = no signal for quart. C) and a C-H correlation.—In the H,C-COLOC spectrum<sup>[13]</sup> (SF2 = 100.62 MHz, SF1 = 400.14 MHz), the following cross peaks were found: C-1/6'-H, C-2/3',5',6'-H, C-3'/3',4',6'-H, C-4'/ $\text{CH}_3$ ,3',6'-H, C-5'/5'',6''-H

The chemical proof for the constitution of  $\mathbf{9}^{2\ominus}$  was accomplished, as for  $\mathbf{1}^{2\ominus}$ ,<sup>[11]</sup> by trapping with chlorotrimethylsilane in *n*-hexane. The bis(trimethylsilyl)dihydrotribenzoacepentalediide **10** (colorless crystals, m.p.  $191^\circ\text{C}$  (dec.); for spectroscopic data, see Table 1), isolated in 97% yield (based on **2**), was much easier to purify than the corresponding parent compound; in addition,  $\mathbf{9}^{2\ominus}/2\text{K}^\oplus$  is markedly more stable than  $\mathbf{1}^{2\ominus}/2\text{K}^\oplus$ . The special stabilization of  $\mathbf{9}^{2\ominus}$  is also supported by the fact that it is formed from 10-methyltribenzotriquinacene<sup>[12]</sup> with formal expulsion of methane under the same conditions as it is formed from **2**.



In the gas phase, compound **2** also undergoes ready deprotonation to give the monoanion  $[\mathbf{2}-\text{H}]^\ominus$  under the conditions of negative chemical ionization (NCI).<sup>[14, 15]</sup> Moreover, at low pressure of the reactant gas (i.e., for a higher average excitation of the  $[\mathbf{2}-\text{H}]^\ominus$  ions), predominant formation of  $[\mathbf{2}-2\text{H}]^{2\ominus}$  and  $[\mathbf{2}-4\text{H}]^{2\ominus}$  ions ( $\cong \mathbf{9}^{2\ominus}$ ) is observed, indicating elimination or abstraction of up to three hydrogen atoms (see Fig. 1). Correspondingly, the NCI spectrum of 10-methyltribenzotriquinacene<sup>[2]</sup> is governed by the  $[\text{M}-2\text{H}-\text{CH}_4]^\ominus$  peak at low reactant gas pressures. Apparently, therefore, the (unsolvated!) radical anion  $\mathbf{9}^{2\ominus}$  of

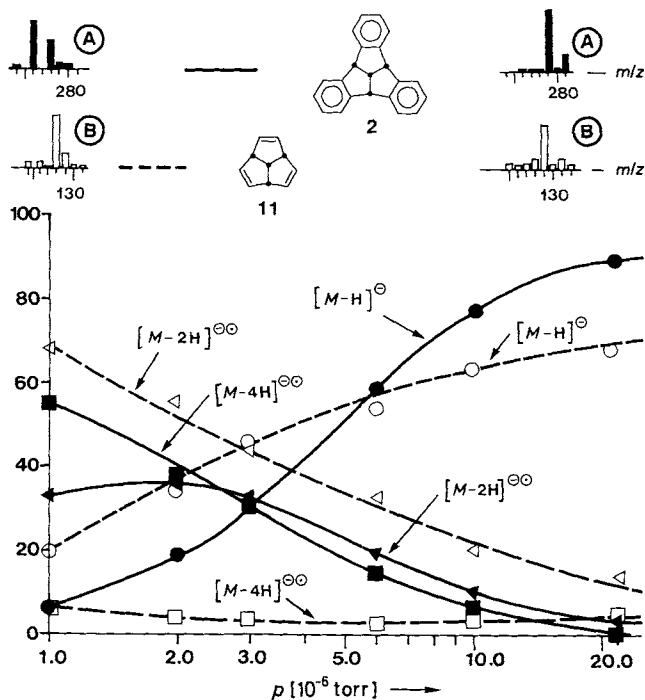


Fig. 1. Relative ion abundances in the NCI ( $N_2O/CH_4$ ) mass spectra [15] of triquinacene **11** (---) and tribenzotriquinacene **2** (—) as a function of the (nominal) pressure of the reactant gas. (The values are  $^{13}C$ -corrected and normalized with respect to  $\Sigma[C_{22}H_4]^\ominus$  and  $\Sigma[C_{10}H_2]^\ominus$ , respectively.) (A) and (B): the  $[M-nH]^\ominus$  region of the NCI-MS of **2** ( $M = 280$ ) and **11** ( $M = 130$ ), respectively.

tribenzoacentalene **9** is very stable—in marked contrast to **1**. Under identical conditions, triquinacene **11** is deprotonated to the monoanion  $[11-H]^\ominus$ , but, at lower pressure of the reactant gas, only  $[11-2H]^{2-}$  along with a small amount of  $[11-4H]^{2-}$  ( $\cong 1^\ominus$ , see Fig. 1) is formed. Accordingly, the neutral tribenzoacentalene **9** must also be appreciably more stable than the parent system **1** and might even be detectable in pure form.

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**2**, 120022-86-8; **3**, 120057-05-8; **4**, 116665-59-9; **5**, 120022-87-9; **6**, 120057-06-9; **8**, 120057-07-0; **9** $^\ominus$ , 120022-88-0; **9** $^{2-}$ , 120022-90-4; **10**, 120022-89-1.

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[8] Compound **4** is also formed as a mixture with **5** by the route described by Baker et al. [3]; D. Kuck, E. Neumann, unpublished.  
[9] All new compounds, except for **6** and **9** $^{2-}/2K^\oplus$ , which were used as crude products, gave satisfactory elemental analyses.  
[10] Spectroscopic data for **2**:  $^1H$  NMR (300 MHz,  $CDCl_3$ ):  $\delta = 4.49$  (q,  $^3J = 9.7$  Hz, 1H), 4.97 (d,  $^3J = 9.7$  Hz, 3H), 7.18, 7.46 (AA'BB', 12H).  $^{13}C$  NMR (75.5 MHz,  $CDCl_3$ ):  $\delta = 51.2$  (d), 56.0 (d), 124.3 (d), 127.4 (d), 145.9 (s). MS (EI, 70 eV):  $m/z$  280 ( $M^\ominus$ , 100%), 279 (32), 278 (13),

277 (12), 276 (16), 203 (23), 202 (22). IR (KBr) [ $cm^{-1}$ ]:  $\bar{\nu} = 3070$  (w); 3020 (w), 2980 (w), 2900 (w), 1482 (m), 1476 (m), 1458 (m), 754 (s), 746 (s), 713 (m), 575 (s). UV ( $n-C_7H_{16}$ ,  $c = 8 \times 10^{-5}$  mol  $L^{-1}$ ) [nm]:  $\lambda_{max}(c) = 276.5$  (4850), 269 (3840), 263 (2350).

- [11] All experimental findings indicate the presence of the dipotassium salt  $9^{2-}/2K^\oplus$ ; cf. D. Wilhelm, T. Clark, P. von R. Schleyer, J. L. Courtneidge, A. G. Davies, *J. Organomet. Chem.* 273 (1984) C 1.  
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[15] Measuring conditions: ZAB-2F mass spectrometer (Vacuum Generators); reactant gases  $CF_4$  or  $CH_4/N_2O$  (1:1); reactant ions  $F^\ominus$  and  $OH^\ominus$ , respectively; acceleration voltage 5.6 eV; electron energy 100 eV; emission 500  $\mu A$ ; source pressure, see Fig. 1; source temperature 190  $^\circ C$ . Comparative measurements (Fig. 1) were carried out with simultaneous admission of **2** and **11** (direct inlet system, 110  $^\circ C$ , and injection system, 150  $^\circ C$ , respectively).

## Electron Densities, Deformation Densities, and Chemical Bonding\*\*

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The frequently postulated relationship between electron density and chemical bonding has so far been investigated in two different, although fundamentally related, ways. According to the older method,<sup>[1, 21]</sup> one uses the difference density  $\Delta \rho = \rho_{molecule} - \sum \rho_{atoms}$ , where  $\rho_{molecule}$  is the electron density of the molecule and  $\rho_{atom}$  the spherically averaged density of an unperturbed, correctly positioned atom. A chemical bond should be characterized by a positive  $\Delta \rho$  between the atoms. According to the more recent method,<sup>[3, 4]</sup> instead of  $\Delta \rho$  one uses the second derivative of the molecular density  $\nabla^2 \rho_{molecule}$ . Large negative values of  $\nabla^2 \rho_{molecule}$  between two atoms, especially in comparison with the spherically averaged atomic densities, are regarded as an indication of chemical bonding.

The ground states of most atoms with open valence shells, however, are degenerate (e.g.,  $^2P$  states for  $C(1s^2 2s^2 2p^2)$  and  $F(1s^2 2s^2 2p^5)$ ); that is, their electron density is anisotropic. The electron density of the free atoms can be oriented (e.g., F in the  $^2P_z$  state, see Fig. 1c) without any increase in energy. Thus, molecules and crystals can be envisioned as consisting of suitably positioned and oriented atoms (whereby, owing to the Heisenberg uncertainty principle, even the positioning of noninteracting atoms requires the zero-point vibrational energy). The positions of the atomic cores along with their

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