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Synthesis and Homo-Diels-Alder Cleavage of the Epoxy-azoalkane *exo*-3-Oxa-6,7-diazatricyclo[3.2.1.$0^{2,4}$]oct-6-ene

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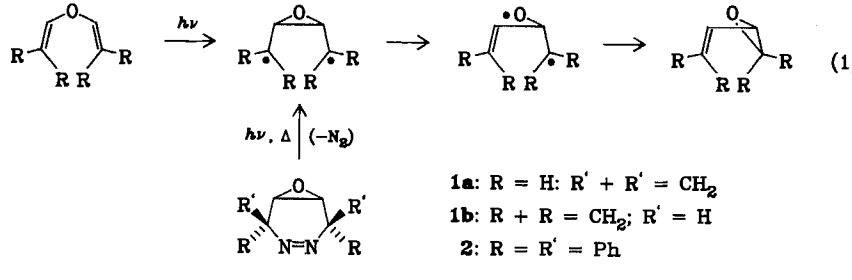
Synthese und Homo-Diels-Alder-Spaltung des Epoxy-azoalkans *exo*-3-Oxa-6,7-diazatricyclo[3.2.1.$0^{2,4}$]oct-6-en

exo-3-Oxa-6,7-diazatricyclo[3.2.1.$0^{2,4}$]oct-6-en (**1a**) wurde durch Epoxidierung des Diels-Alder-Addukts **3** und nachfolgende reduktive Verseifung und Oxidation synthetisiert. Das Epoxy-azoalkan **1a** spaltete über −20°C leicht Stickstoff ab, und 4*H*-Pyran bildete sich als einziges Produkt. Die Versuche, das *endo*-Isomere **1b** durch basenkatalysierte Cyclisierung von Bis(2,2,2-trichlorethyl)-*endo*-5-acetoxy-*exo*-6-brom-2,3-diazabicyclo[2.2.1]heptan-2,3-dicarboxylat (**5**) oder *endo*-5-Acetoxy-*exo*-6-brom-*N*-phenyl-2,3-diazabicyclo[2.2.1]heptan-2,3-dicarboximid (**6**) darzustellen, schlugen fehl. Addition von 4-Phenyl-4*H*-1,2,4-triazol-3,5-dion (PTAD) an 1,1,4,4-Tetraphenyl-1,3-butadien ergab das 2:1-Addukt 2-H_{endo}-5-(2,2-Diphenylvinyl)-*N,N'*,6-triphenyl-3,4,9,10-tetraazatricyclo[6.2.2.$0^{2,7}$]dodeca-6,11-dien-3,4:9,10-bisdicarboximid (**10**) anstelle des erwarteten 1,2,3,6-Tetrahydro-*N*,3,3,6,6-pentaphenylpyridazin-1,2-carboximids (**9**).

In pursuit of our interest in the 3-oxadi-π-methane rearrangement[1] of divinyl ethers to vinyl epoxides [Eq. (1)], we required the hitherto unknown epoxy-azoalkanes *exo,endo*-3-oxa-6,7-diazatricyclo[3.2.1.$0^{2,4}$]oct-6-enes (**1a, b**) and 2,2,5,5-tetraphenyl-7-oxa-3,4-diazabicyclo[4.1.0]hept-3-ene (**2**) for the independent generation of the oxiranyldicarbinyl diradicals[2] by thermal and/or photochemical denitrogenation. Presently we report on the preparation of the tricyclic *exo*-isomer **1a** and our unsuccessful experiences with the *endo*-isomer **1b** and the bicyclic derivative **2**.

Our synthetic efforts on the *exo,endo*-isomers **1a, b** are summarized in Eq. (2). Thus, the *exo*-isomer **1a** was obtained by epoxidation of the diazanorbornene **3**, the Diels-Alder adduct



(1)

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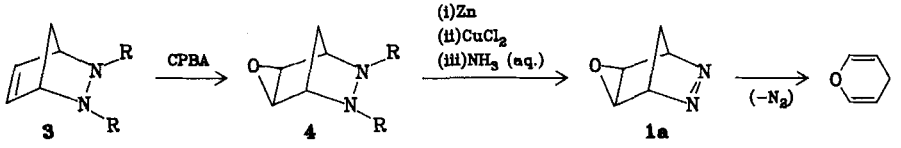
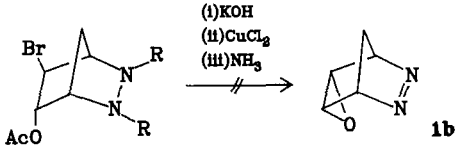
derived from 2,2,2-trichloroethyl azodicarboxylate and cyclopentadiene, followed by reductive saponification and oxidation of the *exo*-epoxide **4**. The ^{1}H NMR spectrum of the crude epoxidation product of **3** indicated that only the *exo*-epoxide **4** was formed, isolated in 34% yield and fully characterized. The thermally labile *exo*-epoxy-azoalkane **1a**, detected at ca. −40°C by ^{1}H and ^{13}C NMR (cf. Experimental Part; *exo*-oxirane ring[3] suggested by the W-coupling of J = 1.8 Hz for the 2,4-H_{endo} protons), quantitatively denitrogenated into 4*H*-pyran (identified by ^{1}H NMR)[4] on warming above −20°C.





(2)

5: R = −CO−OCH$_2$CCl$_3$

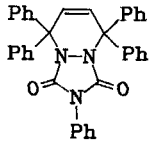
6: R + R = −CO−N(Ph)−CO−

The great ease of nitrogen loss of the *exo*-epoxide **1a** parallels closely the behaviour of the corresponding *exo*-cyclopropane **7**, which also readily extrudes nitrogen above −20°C by homo-Diels-Alder cleavage[5]. Thus, the *exo*-isomer **7** denitrogenates by ca. eleven orders of magnitude faster than its parent azoalkane **8**[6].

It was hoped to prepare the presumably more stable *endo*-epoxide **1b** for our mechanistic investigations on the 3-ODPM reaction. The synthesis of the *endo*-epoxide **1b** commenced with the preparation of the *trans*-acetoxy-bromide **5** by addition of acetyl hypobromite to the diazanorbornene **3** [Eq. (2)]. The structure of **5** is based on spectral data and elemental composition (cf. Experimental Part). Attempts to cyclize the *trans*-acetoxy-bromide **5** into the desired *endo*-epoxide **1b** by treatment with base under a variety of conditions led to undefined tarry material. No copper complex could be precipitated from the hydrolysates by addition of copper(II) chloride. Similar failures were made with the *trans*-acetoxy-bromide **6**, the acetyl hypobromite adduct of *N*-phenyl-2,3-diazabicyclo[2.2.1]hept-5-ene-2,3-carboximide. Unfortunately this synthetic pathway precluded access to the *endo*-epoxide **1b**.

For the alternative epoxy-azoalkane **2**, the urazole **9** was required as precursor. Diels-Alder reaction of PTAD with 1,1,4,4-tetraphenyl-1,3-butadiene afforded instead the 2:1 adduct **10**. Its structure was assigned on the basis of its ^{1}H and ^{13}C NMR data (cf. Experimental Part) and by comparison of this NMR data with the related bicyclo[2.2.2]oct-2-

ene[7]. Rather than adding the azo-dienophile across the 1,3-butadiene moiety, as is the case with 1,4-diphenyl-1,3-butadiene and PTAD[8], steric congestion obliged participation of the benzene double bond in the tetraphenylbutadiene[9].



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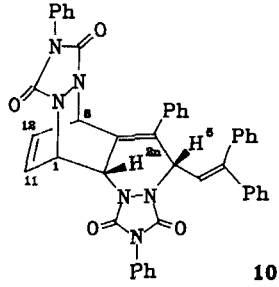

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We thank the *Deutsche Forschungsgemeinschaft* and the *Fonds der Chemischen Industrie* for generous financial support.

Experimental Part

Melting points are uncorrected. – IR spectra: Beckman Acculab 4. – ^{1}H NMR spectra: At 90 MHz on a Varian EM 390 or at 400 MHz on a Bruker WM 400. – ^{13}C NMR spectra: At 100.61 MHz on a Bruker WM 400. – Mass spectra: Varian MAT CH 7. – The elemental analyses were kindly run for us by Professor *G. Maier's* staff of the Universität Gießen. – Known compounds used in this research were either purchased from standard suppliers or prepared according to literature procedures and purified to match the reported physical and spectral data. Only the experimental details of hitherto unknown compounds are provided.

Bis(2,2,2-trichloroethyl) 2,3-Diazabicyclo[2.2.1]hept-5-ene-2,3-dicarboxylate (**3**): A solution of 5.00 g (13.1 mmol) of bis(2,2,2-trichloroethyl) azodicarboxylate in 50 ml of carbon tetrachloride was placed into a 250 ml, round-bottomed flask, equipped with a dropping funnel. A solution of 870 mg (13.2 mmol) of cyclopentadiene in 20 ml of carbon tetrachloride was dropped into the stirred solution at ca. 20°C within 15 min. The colourless solution was rota-evaporated at 30–40°C/15 Torr and the crude product recrystallized from methanol, affording 5.30 g (90%) of colourless needles, m. p. 120–121°C. – IR (KBr): 2995, 2960, 1765, 1736, 1392, 1341, 1305, 1173, 1128, 1046, 799, 749, 722 cm^{-1}. – ^{1}H NMR ($CDCl_3$, 90 MHz): δ = 1.8–1.9 (m; 2H, 7-H), 4.84 (s; 4H, $CO_2CH_2CCl_3$), 5.2–5.5 (m; 2H, 1,4-H), 6.6–6.8 (m; 2H, 5,6-H). – ^{13}C NMR ($CDCl_3$, 100.6 MHz): δ = 48.36 (t; C-7), 66.00 (br. d; C-1,4), 75.30 (t; $CO_2CH_2CCl_3$), 94.95 (s; CCl_3), 136.4 (br. s; C-5,6), 156.37 (br. s; $CO_2CH_2CCl_3$). – MS (70 eV): *m/e* = 446 (3%, M^+, Cl_6-pattern), 131 (18, $C_2H_2Cl_3^+$, Cl_3-pattern), 66 (100, $C_5H_6^+$).

$C_{11}H_{10}Cl_6N_2O_4$ (446.9) Calcd. C 29.56 H 2.26 N 6.27
Found C 29.60 H 1.88 N 6.22

Bis(2,2,2-trichloroethyl) exo-3-Oxa-6,7-diazatricyclo[3.2.1.0^{2,4}]octane-6,7-dicarboxylate (**4**): A sample of 2.00 g (4.47 mmol) of **3**, 3.70 g (18.2 mmol) of 85% *m*-chloroperbenzoic acid, and 40.0 mg (0.182 mmol) of 2,6-di-*tert*-butyl-4-methylphenol were suspended in 10 ml of 1,2-dichloroethane, sealed in a glass tube and heated in an autoclave at 90–100°C for 3.5 h. The tube was carefully opened after cooling to ca. 20°C (CAUTION), the contents taken up in 50 ml of chloroform and the suspension extracted with 15% aq. sodium hydro-

gensulfite (50 ml). The aq. layer was separated, neutralized with sodium hydrogencarbonate and extracted with chloroform (2 × 25 ml). The chloroform phases were combined, filtered, extracted with 15% aq. sodium hydrogensulfite (25 ml) and saturated aq. sodium hydrogen carbonate (2 × 25 ml), dried over anhydrous sodium sulfate and rota-evaporated at 20–30°C/15 Torr. The remaining yellow oil was taken up in 5 ml of methanol and allowed to crystallize at 0°C. Repeated recrystallization of the crude product from methanol afforded 700 mg (34%) of colourless prisms, m. p. 100°C. – IR (KBr): 3022, 2962, 1718, 1449, 1395, 1331, 1196, 1130, 1068, 1026, 861, 731 cm^{-1}. – ^1H NMR ($CDCl_3$, 90 MHz): δ = 1.3–2.1 (m; 2H, 8-H), 3.63 (br. s; 2H, 2,4-H), 4.8–5.1 (m; 6H, 1,5-H, $CO_2CH_2CCl_3$). – ^{13}C NMR ($CDCl_3$, 100.6 MHz): δ = 26.49 (t; C-8), 47.21 (br. d; C-2,4), 61.91 (br. d; C-1,5), 75.31 (br. t; $CO_2CH_2CCl_3$), 94.75 (s; CCl_3), 155.28 (br. s; $CO_2CH_2CCl_3$). – MS (70 eV): *m/e* = 462 (6%, M^+, Cl_6-pattern), 131 (52, $C_2H_2Cl_3^+$, Cl_3-pattern), 81 (100%, $C_5H_5O^+$).

$C_{11}H_{10}Cl_6N_2O_5$ (462.9) Calcd. C 28.54 H 2.18 N 6.05
Found C 28.93 H 2.14 N 6.05

exo-3-Oxa-6,7-diazatricyclo[3.2.1.$0^{2,4}$]oct-6-ene (**1a**): A Schlenk tube was charged with 1.12 g (17.1 mmol) of zinc dust under nitrogen. The zinc was activated with 5% aq. HCl (4 × 2 ml, 1 min), washed with distilled water (5 × 1.5 ml), absol. ethanol (4 × 1.5 ml), and absol. ether (5 × 1.5 ml) and dried at 20°C/0.01 Torr. A sample of 125 mg (0.270 mmol) of **4** was dissolved in 10 ml of a 1:1 acetic acid/absol. THF and added to the activated zinc. The suspension was ultrasonicated under nitrogen for 1 h at 0°C. The reaction mixture was filtered under nitrogen into a 50-ml, round-bottomed flask and the excess zinc washed with distilled water (3 × 5 ml). The flask was placed into an ice bath and the pH of the filtrate adjusted to 7–8 by addition of conc. aq. ammonia. 2 M $CuCl_2$ (3 ml) was added and the brick-red copper complex precipitated. Acetic acid was added dropwise until precipitation was complete. The copper complex was isolated by centrifugation, washed with water (2 × 5 ml), absol. ethanol (2 × 5 ml), and absol. ether (2 × 5 ml) and dried at 0°C/0.01 Torr to afford 50.0 mg (89%) of a brick-red crystalline powder (CAUTION: At ca. 20°C, spontaneous decomposition of the copper complex was observed in several cases). A sample of 30.0 mg (0.123 mmol) of the copper complex was placed into a Schlenk tube under nitrogen and cooled by means of a dry ice/methanol bath, 1 ml of $CDCl_3$ and 2 ml of 25% aq. ammonia were added. The temperature was kept just above the freezing point of the aq. layer and the mixture was shaken until the copper complex was completely dissolved. The $CDCl_3$ phase was removed by means of a pipet and filtered rapidely through anhydrous magnesium sulfate into a precooled NMR tube. – ^1H NMR ($CDCl_3$, 400 MHz, –40°C): δ = 1.09 (td, $J_{8anti,\ 2,4\text{-H}}$ = 1.8 Hz, $J_{8anti,8syn}$ = 11.0 Hz; 1H, 8-H_{anti}), 1.52 (d, $J_{8syn,8anti}$ = 11.0 Hz; 1H, 8-H_{syn}), 3.49 (br. s; 2H, 2,4-H), 5.63 (br. s; 2H, 1,5-H). – ^{13}C NMR ($CDCl_3$, 100 MHz, –40°C): δ = 32.93 (t; C-8), 52.99 (d; C-2,4), 82.01 (d; C-1,5).

On warming of the epoxy-azoalkane **1a** above –20°C, the ^1H and ^{13}C NMR signals were replaced by those of 4*H-pyran*. – ^{13}C NMR ($CDCl_3$, 100.6 MHz, –40°C): δ = 18.58 (t; C-4), 101.14 (d; C-3,5), 140.61 (d; C-2,6).

Bis(2,2,2-trichloroethyl) endo-5-Acetoxy-exo-6-bromo-2,3-diazabicyclo[2.2.1]heptane-2,3-dicarboxylate (**5**): A 25 ml, round-bottomed flask, equipped with a magnetic stirrer, was charged with a suspension of 1.50 g (8.99 mmol) of finely powdered silver acetate in 10 ml of absol. carbon tetrachloride. The suspension was stirred under protection of light and cooled to –15°C. A solution of 957 mg (5.99 mmol) of bromine in 5 ml of absol. carbon tetrachloride was cooled to 0°C and added to the suspension within 5 min. Stirring was continued at –15°C for 10 min and the mixture was filtered into a precooled (0°C) stirred solution of 1.00 g (2.24 mmol) of **3** in 10 ml of absol. carbon tetrachloride. The reaction

mixture was allowed to warm up to ca. 20°C and stirring was continued for 15 min. The solvent was then rota-evaporated (ca. 20°C/15 Torr) and the remaining colourless oil taken up in 3 ml of absol. methanol. On storing for 2 d at −30°C, the product crystallized, affording 1.12 g (85%) of colourless needles, m. p. 104°C. An analytically pure sample was obtained by recrystallization from hexane, m. p. 104°C. – IR (KBr): 3002, 2960, 1778, 1752, 1441, 1371, 1338, 1229, 1213, 1144, 822, 715 cm^{-1}. – ^1H NMR ($CDCl_3$, 90 MHz): δ = 2.10 (s; 3H, CH_3CO_2), 2.2–2.9 (m; 2H, 7-H), 4.1–4.4 (m; 1H, 6-H_{endo}), 4.7–5.2 (m; 7H, $CO_2CH_2CCl_3$, 1,4-H, 5-H_{exo}). – ^{13}C NMR ($CDCl_3$, 100.6 MHz): δ = 20.84 (q; CH_3CO_2), 35.87 (br. t; C-7), 43.91 (d; C-6), 64.12 (br. d; C-1), 65.20 (br. d; C-4), 72.13 (d; C-5), 75.58 (t; $CO_2CH_2CCl_3$), 94.58 (s; $CO_2CH_2CCl_3$), 155.02 (br. s; $CO_2CH_2CCl_3$), 169.65 (s; CH_3CO_2). – MS (70 eV): *m/e* = 586 (7%, M^+, Cl_6Br-pattern), 131 (84%, $C_2H_2Cl_3^+$, Cl_3-pattern), 43 (100%, CH_3CO^+).

$C_{13}H_{13}BrCl_6N_2O_6$ (585.9) Calcd. C 26.65 H 2.24 N 4.78
Found C 26.78 H 2.19 N 4.65

endo-5-Acetoxy-exo-6-bromo-N-phenyl-2,3-diazabicyclo[2.2.1]heptane-2,3-dicarboximide (**6**): Analogous to the synthesis of **5**, 540 mg (2.24 mmol) of *N*-phenyl-2,3-diazabicyclo-[2.2.1]hept-5-ene-2,3-dicarboximide[10] were treated with acetyl hypobromite. After rota-evaporation of the solvent (ca. 20°C/15 Torr), a nearly colourless solid remained, which was recrystallized from hexane/ethyl acetate to afford 400 mg (33%) of colourless plates, m. p. 185–186°C. – IR (KBr): 3059, 2970, 1725, 1600, 1502, 1417, 1229, 1143, 1084, 886, 822, 773, 701, 685 cm^{-1}. – ^1H NMR ($CDCl_3$, 90 MHz): δ = 2.10 (s; 3H, CH_3CO_2), 2.2–2.7 (m; 2H, 7-H), 3.9–4.1 (m; 1H, 6-H_{endo}), 4.6–4.9 (m; 2H, 1,4-H), 5.1–5.3 (m; 1H, 5-H_{exo}), 7.4–7.6 (m; 5H, C_6H_5). – ^{13}C NMR ($CDCl_3$, 100.6 MHz): δ = 20.82 (q; CH_3CO_2), 35.74 (t; C-7), 45.15 (d; C-6), 63.18 (d; C-1), 64.10 (d; C-4), 75.52 (d; C-5), 125.34 (d; C_6H_5, C_{ortho}), 128.72 (d; C_6H_5, C_{para}), 129.30 (d; C_6H_5, C_{meta}), 131.15 (s; C_6H_5, C_{ipso}), 156.05, 156.70 (s; imide-CO), 169.74 (s; CH_3CO_2). – MS (70 eV): 379 (14%, M^+, Br-pattern), 119 (59, $PhNCO^+$), 43 (100, CH_3CO^+).

$C_{15}H_{14}BrN_3O_4$ (380.2) Calcd. C 47.39 H 3.71 N 11.05
Found C 47.66 H 3.60 N 10.73

Hydrolysis/Oxidation of the Acetoxy-bromides **5** *and* **6**: Samples of 100–200 mg of the acetoxy-bromides were refluxed under nitrogen in ca. 10 ml of 2-propanol with varying amounts of potassium hydroxide (up to 25-fold excess of base), the reaction times ranging from 30 min to 7 h. The solutions were then cooled to ca. 20°C and adjusted to pH 3–6 by dropwise addition of conc. hydrochloric acid. The addition of 2 M aq. copper(II) chloride did not result in the precipitation of a copper complex under any of the reaction conditions used. Only tarry, intractable product was obtained.

2-H_{endo}-5-(2,2-Diphenylvinyl)-N,N',6-triphenyl-3,4,9,10-tetraazatricyclo[6.2.2.0^{2,7}]dodeca-6,11-diene-3,4:9,10-bisdicarboximide (**10**): A solution of 500 mg (1.39 mmol) of 1,1,4,4-tetraphenyl-1,3-butadiene in 20 ml of dichloromethane was placed into a 50 ml, round-bottomed flask, 700 mg (4.00 mmol) of 4-phenyl-4*H*-1,2,4-triazole-3,5-dione were added and the reaction mixture stirred for 20 h at ca. 20°C. The solvent was rota-evaporated (ca. 20°C/15 Torr) and silica gel chromatography of the brown solid residue (adsorbant-substrate ratio 50:1), eluting with 7:3 dichloromethane/ethyl acetate mixture, gave 480 mg (49%) of a colourless solid. An analytically pure sample was obtained by recrystallization from toluene, m. p. 229°C (dec.). – IR (KBr): 3082, 3050, 3025, 1780, 1730, 1601, 1503, 1404, 1270, 1148, 1130, 770, 731, 703, 689 cm^{-1}. – ^1H NMR ($CDCl_3$, 400 MHz): δ = 4.12 (dd, $J_{2\text{-Hn},1\text{-H}}$ = 1.5 Hz, $J_{2\text{-Hn},5\text{-H}}$ = 2.0 Hz; 1H, 2-H_n), 5.37 (dd, $J_{8\text{-H},11\text{-H}}$ = 1.5 Hz, $J_{8\text{-H},12\text{-H}}$ = 5.5 Hz; 1H, 8-H), 5.45 (dd, $J_{5\text{-H},2\text{-Hn}}$ = 2.0 Hz, $J_{5\text{-H,vinyl-H}}$ = 10.0 Hz; 1H, 5-H), 5.91 (d, $J_{\text{vinyl-H},5\text{-H}}$ =

10.0 Hz; 1H, vinyl-H), 6.47 (ddd, $J_{1\text{-H},2\text{-Hn}}$ = 1.5 Hz, $J_{1\text{-H},11\text{-H}}$ = 6.0 Hz, $J_{1\text{-H},12\text{-H}}$ = 1.5 Hz; 1H, 1-H), 6.49 (ddd, $J_{12\text{-H},1\text{-H}}$ = 1.5 Hz, $J_{12\text{-H},8\text{-H}}$ = 5.5 Hz, $J_{12\text{-H},11\text{-H}}$ = 8.0 Hz; 1H, 12-H), 6.62 (ddd, $J_{11\text{-H},1\text{-H}}$ = 6.0 Hz, $J_{11\text{-H},8\text{-H}}$ = 1.5 Hz, $J_{11\text{-H},12\text{-H}}$ = 8.0 Hz; 1H, 11-H), 7.0–7.6 (m; 25H, C_6H_5). [Chemical shifts and coupling constants were optimized by computer simulation (LAOCOON III)[11].] – ^{13}C NMR ($CDCl_3$, 100.6 MHz): δ = 51.19, 54.19, 56.54, 95.39 (d; C-1,2,5,8), 120.16, 122.20, 125.42, 125.57, 127.39, 127.49, 127.88, 128.13, 128.18, 128.37, 128.45, 128.55, 128.69, 128.97, 129.17, 129.27, 129.52, 129.66, 130.88, 131.54, 134.76, 136.97, 137.88, 140.97, 147.83 (C_6H_5, vinyl-C, vinyl-CH), 150.87, 154.33, 155.94, 156.79 (s; CO). – MS (70 eV): *m/e* = 531 (4%, $M^+ - C_8H_7N_3O_2$), 358 (100%, $C_{28}H_{22}^+$), 267 (31), 167 (96).

$C_{44}H_{32}N_6O_4$ (708.8) Calcd. C 74.56 H 4.55 N 11.86
Found C 74.83 H 4.52 N 11.76

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[1] To distinguish between the various heterosubstituted di-π-methane rearrangements, we suggest to use the usual IUPAC rule for specifying the replaced carbon atom by the appropriate numeric prefix, e. g. the common oxadi-π-methane rearrangement (ODPM) would herewith be called the 1-ODPM and the present case the 3-ODPM. This nomenclature replaces the previously suggested oxydi-π-methane designation for the present 3-ODPM rearrangement (cf. Ref.[2]).

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[91/85]