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SUPPORTING INFORMATION

Acid–Base Controllable Molecular Shuttles

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Supporting Information

Experimental Procedures

General Methods. Chemicals were purchased from Aldrich and used without further purification. Solvents were either used as purchased or dried (THF from Na–Ph_2CO, MeCN from CaH_2) according to procedures described[1] elsewhere. DBA·PF_6,[2] 3,5-Di-*tert*-butylbenzyl bromide[3] (**4**), 3,5-di-*tert*-butylbenzaldehyde[4] and 9-anthracenemethylamine[5] were prepared according to literature procedures. Reactions requiring ultrahigh pressures were performed in Teflon vessels using a custom-built ultrahigh pressure press manufactured by PSIKA Pressure Systems, Ltd., of Glossop, UK. Column chromatography was carried out utilizing silica 60 F (Merck 9385, 230–400 mesh). High performance liquid chromatography (HPLC) was performed on a Phenomenex Hypersil BDS C-18 column (250 × 4.6 mm), eluted using Gilson 305 and 306 HPLC pumps. The pumps were controlled by external Gilson 715 software running on a 486 PC, a Dynamax UV-1 ultraviolet detector being used. Melting points were determined on an Electrothermal 9200 apparatus and are uncorrected. ^{1}H And ^{13}C NMR spectra were recorded on a Bruker AC300 (at 300.1 and 75.5 MHz, respectively) spectrometer with either the solvent reference or TMS as the internal standard. Liquid secondary ion (LSI) mass spectra were obtained from a VG Zabspec mass spectrometer equipped with a cesium ion source and utilizing a *m*-nitrobenzylalcohol matrix. Microanalyses were performed by the University of North London Microanalytical Service.

3,5-Di-*tert*-butylbenzyl-4-carbomethoxybenzylamine. A solution of methyl 4-aminobenzoate (2.73 g, 16.0 mmol) and 3,5-di-*tert*-butylbenzaldehyde (3.52 g, 16.0 mmol) in MeOH (90 mL) was heated under reflux in the presence of 4 Å molecular sieves for 4 h. Upon cooling to 20 °C, the solvent was removed under reduced pressure and 3,5-di-*tert*-butylbenzylidene-4-carbomethoxybenzylamine was isolated as a white solid. This solid was dissolved in hot MeOH (70 mL), before being treated portionwise with $NaBH_4$ (4.10 g, 107.9 mmol). Thereupon, the reaction mixture was heated under reflux with stirring for 5 h and, after cooling to 20 °C, 2 N HCl was added (pH < 2) to generate a precipitate. The solvent was evaporated and the residual brown

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solid suspended in 8 N NaOH (30 mL), before being extracted with $CHCl_3$ (4 × 50 mL). The combined extracts were dried ($MgSO_4$), filtered and concentrated to furnish the title compound (5.63 g, 94%) as an oil that solidified eventually. This compound was used without further purification in the next step. ^{1}H NMR ($CDCl_3$): δ 1.33 (s, 18H), 3.79 (s, 2H), 3.89 (s, 2H), 3.91 (s, 3H), 7.17 (s, 2H), 7.33 (s, 1H), 7.54, 8.01 (AA'XX' system, 4H).

3,5-Di-*tert*-butylbenzyl-4-hydroxymethylbenzylammonium Chloride. A THF (50 mL) solution of 3,5-di-*tert*-butylbenzyl-4-carbomethoxybenzylamine (0.60 g, 1.6 mmol) was added dropwise to a suspension of $LiAlH_4$ (0.61 g, 16.1 mmol) in THF (50 mL) at 0 °C. After addition, the reaction mixture was allowed to warm up to 20 °C and was stirred overnight, before being treated sequentially with H_2O (1 mL), 5 N NaOH (1 mL) and H_2O (3 mL). The precipitated solid was filtered off through a celite pad, before being washed thoroughly with hot $CHCl_3$. The filtrate was concentrated under reduced pressure to yield 3,5-di-*tert*-butylbenzyl-4-hydroxymethylbenzylamine (0.54 g, 98%) as an oil that was dissolved in Et_2O (50 mL). HCl (g) Was bubbled through the solution until a precipitate appeared. Bubbling was continued for a further 15 min, then the solvent was evaporated off in vacuo to provide the title compound (0.60 g, 100%) as a white solid. ^{1}H NMR ($CDCl_3$): δ 1.32 (s, 18H), 2.48 (br s, 1H), 3.76 (br s, 2H), 3.92 (br s, 2H), 4.49 (s, 2H), 7.20 (d, J = 7.5 Hz, 2H), 7.38–7.41 (m, 5H); ^{13}C NMR ($CDCl_3$): δ 31.5, 35.0, 48.4, 49.8, 64.2, 123.2, 124.7, 127.4, 128.7, 129.1, 129.4, 130.0, 130.6, 142.4, 151.8; Anal. Calcd for $C_{23}H_{34}ClNO$: C, 73.47; H, 9.11; N, 3.73. Found: C, 73.13; H, 8.97; N, 3.49.

3,5-Di-*tert*-butylbenzyl-4-chloromethylbenzylammonium Hexafluorophosphate (2a-H·PF$_6$). A mixture of 3,5-di-*tert*-butylbenzyl-4-hydroxymethylbenzylammonium chloride (0.68 g, 1.8 mmol) and $SOCl_2$ (5 mL) was stirred for 24 h at 20 °C. The excess $SOCl_2$ was removed under reduced pressure and MeOH was added to generate a white precipitate that was collected and air-dried (Anal. Calcd for $C_{23}H_{33}Cl_2N$: C, 70.04; H, 8.43; N, 3.55. Found: C, 69.84; H, 8.54; N, 3.52). The hydrochloride salt **2a**-H·Cl was dissolved in Me_2CO (10 mL), before being treated with an aqueous NH_4PF_6 solution. The resulting solution was stirred for 15 min, before being treated with CH_2Cl_2. After separation of the two phases, the organic extracts were dried ($MgSO_4$) and concentrated to yield **2a**-H·PF$_6$ (0.64 g, 91%) as a white solid. ^{1}H NMR ($CDCl_3$): δ 1.33 (s, 18H), 4.16 (br s, 2H), 4.53 (br s, 4H), 7.18 (s, 2H), 7.35, 7.43 (AA′XX′ system, 4H), 7.48 (s, 1H); ^{13}C NMR ($CDCl_3$): δ 31.4, 34.9, 45.3, 47.8, 49.1, 123.1, 124.6, 129.0, 130.4, 138.5, 151.7; MS (LSI): *m/z* 358 $[M - PF_6]^+$.

3,5-Di-*tert*-butylbenzyl-4-[(4,4′-pyridylpyridinium)methyl]benzylammonium Bis-(hexafluorophosphate) (3a-H·2PF$_6$). A solution of **2a**-H·Cl (0.50 g, 1.3 mmol) in $CHCl_3$ (20 mL) was added dropwise to a refluxing solution of 4,4′-bipyridine (1.20 g, 7.7 mmol) in $CHCl_3$ (30 mL) with stirring over 3 h. After 3 d, the solvent was removed in vacuo and the crude product purified by column chromatography (CH_2Cl_2–MeOH, 9:1 followed by 7:1) to give **3a**-H·2Cl as a white solid (0.67 g, 67%). Thereupon, the solid was dissolved in Me_2CO (15 mL), before being treated with an aqueous NH_4PF_6 solution. The Me_2CO was removed in vacuo and the remainder treated with MeOH (10 mL). The white precipitate which formed was collected, washed thoroughly with H_2O and air-dried to furnish **3a**-H·2PF$_6$ (0.96 g, 98%). ^{1}H NMR (CD_3COCD_3): δ 1.29 (s, 18H), 4.62 (s, 2H), 4.69 (s, 2H), 6.15 (s, 2H), 7.43 (s, 2H), 7.55 (s, 1H), 7.72, 7.75 (AA′XX′ system, 4H), 7.96 (d, J = 6.0 Hz, 2H), 8.68 (d, J = 6.0 Hz, 2H), 8.85 (d, J = 6.0 Hz, 2H), 9.33 (d, J = 6.0 Hz, 2H); ^{13}C NMR (CD_3COCD_3): δ 31.5, 35.4, 52.1, 52.4, 64.5, 122.7, 123.8, 125.0, 127.2, 130.6, 131.3, 132.2, 133.2, 135.8, 142.0, 146.3, 152.0, 152.5, 155.4; Anal. Calcd for $C_{33}H_{41}F_{12}N_3P_2$: C, 51.50; H, 5.37; N, 5.46. Found: C, 51.61; H, 5.41; N, 5.41.

{[2]-[Dibenzo[24]crown-8]-[3,5-di-*tert*-butylbenzyl-4-[4,4′-(3,5-di-*tert*-butyl-benzylbipyridinium)methyl]benzylammonium]rotaxane} Bis(hexafluorophosphate) (1a-H·3PF$_6$). A $CHCl_3$ (5 mL) solution of 3,5-di-*tert*-butylbenzyl bromide (**4**, 300 mg, 1.1 mmol) was added to a stirred suspension of **3a**-H·2PF$_6$ (150 mg, 0.2 mmol) and DB24C8 (200 mg, 0.5 mmol) in $CHCl_3$ (15 mL), and the whole heated under reflux, for 4 d, until it became a clear solution. Upon cooling, the reaction mixture was concentrated in vacuo and the residual solid purified by column chromatography (CH_2Cl_2–MeOH, 1:0, then 9:1 and finally 7:1) to afford a pale yellow solid that was dissolved in Me_2CO (10 mL), before being treated with an aqueous NH_4PF_6 solution. The Me_2CO was removed in vacuo and the remaining solid precipitate collected, washed thoroughly with H_2O and air-dried to provide **1a**-H·3PF$_6$ (116 mg, 38%) as a beige solid. M.p. 169–173 °C; ^{1}H NMR (CD_3COCD_3): δ 1.23 (s, 18H), 1.30 (s, 18H), 3.58–4.22 (m, 24H), 4.85–4.87

(m, 4H), 5.88 (s, 2H), 6.14 (s, 2H), 6.83–6.86 (m, 8H), 7.21, 7.41 (AA'XX' system, 4H), 7.46 (s, 2H), 7.51 (s, 1H), 7.62 (s, 3H), 8.79–8.80 (m, 4H), 9.23 (d, J = 6.0 Hz, 2H), 9.56 (d, J = 6.0 Hz, 2H); ^{13}C NMR (CD_3COCD_3): δ 31.6, 35.5, 52.8, 54.0, 65.0, 66.5, 68.8, 69.6, 70.4, 71.1, 71.2, 71.4, 113.3, 122.1, 122.4, 124.3, 124.7, 125.0, 128.5, 129.6, 131.5, 134.3, 134.5, 146.6, 146.8; MS (LSI): *m/z* 1420 $[M - PF_6]^+$.

3,5-Di-*tert*-butylbenzyl-4-[4,4′-(3,5-di-*tert*-butylbenzylbipyridinium)methyl]benzylammonium Bis(hexafluorophosphate) (6a-H·3PF$_6$). An MeCN (10 mL) solution of **3a**-H·2PF$_6$ (50 mg, 0.1 mmol) and 3,5-di-*tert*-butylbenzyl bromide (**4**, 100 mg, 0.4 mmol) was subjected to ultrahigh pressure (12 kbar) for 5 d at 50 °C. After removal of the solvent, the reaction mixture was purified by column chromatography (CH_2Cl_2–MeOH, 9:1, then MeOH–2 M NH_4Cl–$MeNO_2$, 7:2:1). After counterion exchange (NH_4PF_6–H_2O–Me_2CO), **6a**-H·3PF$_6$ (48 mg, 66%) was isolated as a beige solid. M.p. 187–193 °C (dec.); ^{1}H NMR (CD_3COCD_3): δ 1.28 (s, 18H), 1.30 (s, 18H), 4.63 (s, 2H), 4.70 (s, 2H), 6.14 (s, 2H), 6.20 (s, 2H), 7.43 (s, 2H), 7.56 (s, 1H), 7.61 (s, 3H), 7.70, 7.74 (AA'XX' system, 4H), 8.76 (d, J = 6.0 Hz, 2H), 8.78 (d, J = 6.0 Hz, 2H), 9.42 (d, J = 6.0 Hz, 2H), 9.53 (d, J = 6.0 Hz, 2H); ^{13}C NMR (CD_3COCD_3): δ 31.6, 35.5, 35.6, 52.1, 53.4, 65.1, 66.4, 124.4, 124.7, 125.1, 128.4, 128.6, 130.7, 132.2, 133.3, 133.7, 146.6, 146.9, 151.6, 152.6, 153.3; MS (LSI): *m/z* 972 $[M - PF_6]^+$; Anal. Calcd for $C_{48}H_{64}F_{18}N_3P_3$: C, 51.57; H, 5.77; N, 3.76. Found: C, 51.56; H, 5.74; N, 3.52.

9-Anthracenemethyl-4-carbomethoxybenzylamine. A stirred solution of 9-anthracenemethylamine (1.70 g, 8.2 mmol) and methyl 4-formylbenzoate (1.35 g, 8.2 mmol) in PhMe (150 mL) was heated under reflux for 14 h, the H_2O liberated being collected in a Dean–Stark trap. Upon cooling to 20 °C, the solvent was removed under reduced pressure to furnish 4-carbomethoxybenzylidene-9-anthracenemethylamine as a brown solid that was dissolved in hot MeOH (150 mL). $NaBH_4$ (0.95 g, 25.0 mmol) Was added portionwise to the reaction mixture, over 2 h, which was then stirred and heated under reflux for a further 10 h. A precipitate appeared after cooling to 20 °C and careful addition of 2 N HCl (pH < 2). Thereupon, the solvent was evaporated off and the residual brown solid suspended in 8 N NaOH (60 mL), before being extracted with $CHCl_3$ (4 × 50 mL). The combined organic extracts were dried ($MgSO_4$), filtered and concentrated to yield the title compound

(2.41 g, 84%) as a brown solid that was used in the next reaction without further purification. M.p. 117–118 °C; ^{1}H NMR ($CDCl_3$): δ 3.91 (s, 3H), 4.05 (s, 2H), 4.68 (s, 2H), 7.40–7.50 (m, 8H), 7.96 (d, J = 9.0 Hz, 2H), 8.02 (d, J = 9.0 Hz, 2H), 8.39 (s, 1H); ^{13}C NMR ($CDCl_3$): δ 45.0, 52.1, 53.9, 124.1, 125.0, 126.2, 127.4, 128.2, 129.2, 129.8, 130.3, 131.6, 145.8, 165.3; MS (LSI): m/z 355 $[M]^+$; HRMS (LSI)—Calcd for $C_{24}H_{21}NO_2$: m/z 355.1572. Found: m/z 355.1576.

9-Anthracenemethyl-4-hydroxymethylbenzylammonium Chloride. $LiAlH_4$ (1.08 g, 28.0 mmol) was added portionwise to a stirred suspension of 9-anthracenemethyl-4-carbomethoxy-benzylamine (2.51 g, 7.1 mmol) in refluxing THF (150 mL) over 30 min. The reaction mixture was heated for a further 1 h and then allowed to cool down to 20 °C, before being treated sequentially with H_2O (1 mL), 5 N NaOH (1 mL) and H_2O (3 mL). The white precipitate that was formed was filtered off through a celite pad, before being washed thoroughly with hot $CHCl_3$. Thereupon, the filtrate was concentrated under reduced pressure to furnish 9-anthracenemethyl-4-hydroxymethylbenzylamine (2.21 g, 95%) as a brownish solid (M.p. 106–107 °C) that was dissolved in $CHCl_3$ (100 mL). HCl (g) Was bubbled through the solution until a precipitate appeared. Bubbling was continued for an additional 15 min, then the precipitated solid was collected and air-dried to yield the title compound (2.74 g, 100%). M.p. > 103 °C (dec.); ^{1}H NMR (CD_3SOCD_3): δ 4.48 (s, 2H), 4.57 (s, 2H), 5.12 (s, 2H), 7.44 (d, J = 6.0 Hz, 2H), 7.50–7.63 (m, 6H), 8.17 (d, J = 9.0 Hz, 2H), 8.22 (d, J = 9.0 Hz, 2H), 8.77 (s, 1H), 9.47 (br, 2H); MS (LSI): m/z 327 $[M - Cl]^+$; HRMS (LSI)—Calcd for $[C_{23}H_{22}NO_2]^+$: m/z 328.1701. Found: m/z 328.1717.

9-Anthracenemethyl-4-bromomethylbenzylammonium Bromide (2b-H·Br). 9-Anthracenemethyl-4-hydroxymethylbenzylammonium chloride (1.26 g, 3.1 mmol) was dissolved in a mixture of hot 48% aqueous HBr (25 mL) and H_2O (25 mL). For 24 h, the reaction mixture was stirred and heated to 100 °C, then the resulting precipitate was collected, washed thoroughly with H_2O and air-dried to yield **2b**-H·Br (1.10 g, 75%). It was used without further purification in the following reaction. M.p. > 209 °C (dec.); ^{1}H NMR ($CDCl_3$): δ 3.78 (s, 2H), 4.27 (s, 2H), 4.87 (s, 2H), 7.23 (d, J = 6.0 Hz, 2H), 7.32 (d, J = 6.0 Hz, 2H), 7.40–7.59 (m, 4H), 7.90 (d, J = 9.0 Hz, 2H), 8.06 (d, J = 9.0 Hz, 2H), 8.38 (s, 1H), 9.53 (br, 2H); ^{13}C NMR (CD_3SOCD_3): δ 34.0, 42.0, 50.6, 123.0, 124.3, 125.6, 127.0, 129.2, 129.6, 129.9, 130.6, 130.9, 131.0, 131.9, 139.2; MS

(LSI): *m/z* 390 [M – Br]$^+$; HRMS (LSI)—Calcd for $C_{23}H_{21}BrN^+$: *m/z* 390.0857. Found: *m/z* 390.0861.

9-Anthracenemethyl-4-[(4,4′-pyridylpyridinium)methyl]benzylammonium Bis(hexafluorophosphate) (3b-H·2PF$_6$). A DMF (60 mL) solution of **2b**-H·Br (1.10 g, 2.3 mmol) was added dropwise to a refluxing/stirring solution of 4,4′-bipyridine (2.93 g, 19.0 mmol) in DMF (100 mL) over 3 h. The reaction mixture was stirred and heated under reflux for a further 3 d, before being concentrated under reduced pressure. The solid residue was suspended in Me_2CO (50 mL), then an aqueous solution of NH_4PF_6 (1.20 g, 7.4 mmol) was added until complete dissolution was achieved. The Me_2CO was removed in vacuo and the solid residue collected and washed exhaustively with hot H_2O. The crude product was then purified by column chromatography (CH_2Cl_2–MeOH, 10:3) to afford a brownish solid that was, once again, suspended in Me_2CO (50 mL), before being treated with an aqueous solution of NH_4PF_6 (1.20 g, 7.4 mmol). The solid obtained after Me_2CO evaporation was collected, washed with H_2O and air-dried to yield **3b**-H·2PF$_6$ (450 mg, 25%). M.p. > 199 °C (dec.); ^1H NMR (CD_3COCD_3): δ 5.02 (s, 2H), 5.64 (s, 2H), 6.16 (s, 2H), 7.52–7.80 (m, 4H), 7.78, 7.90 (AA′XX′ system, 4H), 7.97 (d, J = 6.0 Hz, 2H), 8.19 (d, J = 9.0 Hz, 2H), 8.33 (d, J = 9.0 Hz, 2H), 8.73 (d, J = 6.0 Hz, 2H), 8.80 (s, 1H), 8.86 (d, J = 6.0 Hz, 2H), 8.96 (d, J = 6.0 Hz, 2H); ^{13}C NMR (CD_3COCD_3): δ 44.6, 52.7, 64.5, 122.6, 124.1, 126.4, 127.1, 128.3, 130.2, 130.6, 131.5, 131.8, 132.3, 133.7, 136.0, 141.9, 146.3, 151.9, 155.3; MS (LSI): *m/z* 612 [M – PF$_6$]$^+$; HRMS (LSI)—Calcd for $[C_{33}H_{29}F_6N_3P]^+$: *m/z* 612.2003. Found: *m/z* 612.2016.

3,5-Di-*tert*-butylbenzyl-4,4′-pyridylpyridinium Hexafluorophosphate (5·PF$_6$). A $CHCl_3$ (50 mL) solution of 3,5-di-*tert*-butylbenzyl bromide (**4**, 0.50 g, 1.8 mmol) was added dropwise with stirring to a refluxing solution of 4,4′-bipyridine (1.11 g, 7.1 mmol), in $CHCl_3$ (50 mL), over 2 h, then the whole was stirred and heated under reflux for 3 d. After evaporation of the solvent in vacuo, the residual solid was suspended in Me_2CO (30 mL), before being treated with an aqueous solution of NH_4PF_6 (0.86 g, 5.3 mmol) in order to effect complete dissolution. The Me_2CO was evaporated off, then the precipitate formed was collected, washed thoroughly with hot H_2O and air-dried to give **5**·PF$_6$ (0.69 g, 77%). M.p. > 197 °C (dec.); ^1H NMR (CD_3COCD_3): δ 1.32 (s, 18H), 6.10 (s, 2H), 7.61 (s, 3H), 7.96 (d, J = 6.0 Hz, 2H), 8.67 (d, J = 6.0 Hz, 2H), 8.86

(d, J = 6.0 Hz, 2H), 9.44 (d, J = 6.0 Hz, 2H); ^{13}C NMR (CD_3COCD_3): δ 31.5, 35.5, 65.7, 122.6, 124.6, 124.7, 127.0, 133.5, 142.0, 146.0, 151.9, 153.1, 155.0; MS (LSI): *m/z* 359 $[M - PF_6]^+$; HRMS (LSI)—Calcd for $[C_{25}H_{31}N_2]^+$: *m/z* 359.2487. Found: *m/z* 359.2491.

{[2]-[Dibenzo[24]crown-8]-[9-anthracenemethyl-4-[4,4′-(3,5-Di-*tert*-butylbenzylbipyridinium)methyl]benzylammonium]rotaxane} Bis(hexafluorophosphate) (1b-H·3PF$_6$). Method A. A stirred $CHCl_3$–MeCN (1:1, 26 mL) solution of **5**·PF_6 (564 mg, 1.1 mmol) and **2b**-H·PF_6 (300 mg, 0.6 mmol) was heated under reflux in the presence of DB24C8 (753 mg, 1.7 mmol) for 10 d. Upon cooling to 20 °C, the solvent was evaporated off and the crude product purified by column chromatography (CH_2Cl_2–MeOH, 20:1 until the rotaxane started to come off the column, followed by 9:1 and then 7:1). The pure [2]rotaxane **1b**-H·3PF_6 (240 mg, 30%) was isolated only after purification by HPLC (0.1% TFA in a gradient of 50% MeCN to 100% MeCN in H_2O over 25 min). ^{1}H NMR (CD_3COCD_3): δ 1.35 (s, 18H), 3.46–4.17 (m, 24H), 5.45 (br, 2H), 5.73 (s, 2H), 6.12 (s, 4H), 6.44–6.47 (m, 4H), 6.62–6.66 (m, 4H), 7.49–7.51 (m, 2H), 7.61–7.68 (m, 6H), 7.75 (s, 1H), 7.91–7.95 (m, 4H), 8.32 (s, 1H), 8.56–8.59 (d, J = 9.0 Hz, 2H), 8.73–8.77 (m, 4H), 9.36 (d, J = 6.0 Hz, 2H), 9.54 (d, J = 6.0 Hz, 2H); MS (LSI): *m/z* 1408 $[M - PF_6]^+$; HRMS (LSI)—Calcd for $[C_{72}H_{84}F_{12}N_3O_8P_2]^+$: *m/z* 1408.5542. Found: *m/z* 1408.5567.

Method B. **3b**-H·2PF_6 (150 mg, 0.2 mmol) And 3,5-di-*tert*-butylbenzyl bromide (**4**, 170 mg, 0.6 mmol) were stirred and heated under reflux in the presence of DB24C8 (267 mg, 0.6 mmol) for 10 d in $CHCl_3$–MeCN (1:1, 26 mL). The reaction mixture was worked-up as described in Method A to furnish pure **1b**-H·3PF_6 (62 mg, 30%).

9-Anthracenemethyl-4-[4,4′-(3,5-di-*tert*-butylbenzylbipyridinium)methyl]benzylammonium Bis(hexafluorophosphate) (6b-H·3PF$_6$). A solution of **3b**-H·2PF_6 (100 mg, 0.1 mmol) and 3,5-di-*tert*-butylbenzyl bromide (**4**, 56 mg, 0.2 mmol) in MeCN (10 mL) was subjected to a pressure of 12 kbar for 5 d at 50 °C. After solvent removal, the remainder was purified by column chromatography (CH_2Cl_2–MeOH, 9:1, then MeOH–2 M NH_4Cl–$MeNO_2$, 7:2:1). After counterion exchange (NH_4PF_6–H_2O–Me_2CO), **6b**-H·3PF_6 (146 mg, 65%) was isolated as a beige solid. M.p. > 200 °C (dec.); ^{1}H NMR (CD_3COCD_3): δ 1.31 (s, 18H), 4.51 (s, 2H), 5.25 (s, 2H), 5.75 (s, 2H), 5.85 (s, 2H), 7.39–7.41 (m, 2H), 7.53–7.69 (m, 9H), 8.13–8.17 (m, 4H), 8.35 (d, J

= 6 Hz, 2H), 8.38 (d, J = 6 Hz, 2H), 8.74 (s, 1H), 8.94–8.99 (m, 4H); ^{13}C NMR (CD_3COCD_3): δ 30.6, 35.4, 44.9, 65.7, 64.6, 124.0, 124.7, 126.5, 128.4, 130.3, 132.2.

X-Ray Crystallography. Single crystals, suitable for both X-ray analyses, were obtained by liquid diffusion of *i*-Pr_2O into Me_2CO–$CHCl_3$ (1:1) solutions of the appropriate compounds. Table 1 (*Journal*) provides a summary of the crystal data, data collection and refinement parameters for the structures [DB24C8·**3b**-H][PF_6]$_2$ and **1b**-H·3PF_6. Both structures were solved by direct methods and refined by full matrix least-squares (blocked for **1b**-H·3PF_6) based on F^2. In [DB24C8·**3b**-H][PF_6]$_2$, the structure was ordered and all non-hydrogen atoms were refined anisotropically. In **1b**-H·3PF_6, however, disorder was found in one of the *t*-Bu groups of each of the two crystallographically-independent molecules and in two of the six unique PF_6^- anions. In each case, two partial occupancy orientations were identified, with only the atoms of the major occupancy orientations being refined anisotropically. The solvent molecules were all ordered and were refined isotropically in this structure. In both structures, the C–H hydrogen atoms were placed in calculated positions, assigned isotropic thermal parameters, $U(H) = 1.2U_{eq}(C)$ [$U(H) = 1.5U_{eq}(C\text{–}Me)$], and allowed to ride on their parent atoms. The N–H hydrogen atoms in both structures could not be located from ΔF maps and were therefore placed in calculated positions. In [DB24C8·**3b**-H][PF_6]$_2$, these atoms were assigned isotropic thermal parameters, $U(H) = 1.2U_{eq}(N)$, and allowed to ride on their parent atoms, whereas in **1b**-H·3PF_6, they were refined isotropically subject to a distance constraint. Computations were carried out using the SHELXTL PC program system.[6]

Absorption and Emission Spectra. Absorption spectra were recorded in MeCN with a Perkin Elmer λ 6 spectrophotometer. Uncorrected emission spectra were obtained with a Perkin Elmer LS50 spectrofluorimeter. Luminescence quantum yields were determined using either naphthalene in degassed *c*-C_6H_{12} (Φ = 0.23)[7] or anthracene in degassed MeOH (Φ = 0.27)[8] as standards. The experimental error was ±15%.

Photochemistry. Photochemical experiments were carried out with a medium pressure Q400 Hanau Mercury lamp in aerated MeCN solution, the 365 nm wavelength being filtered with an

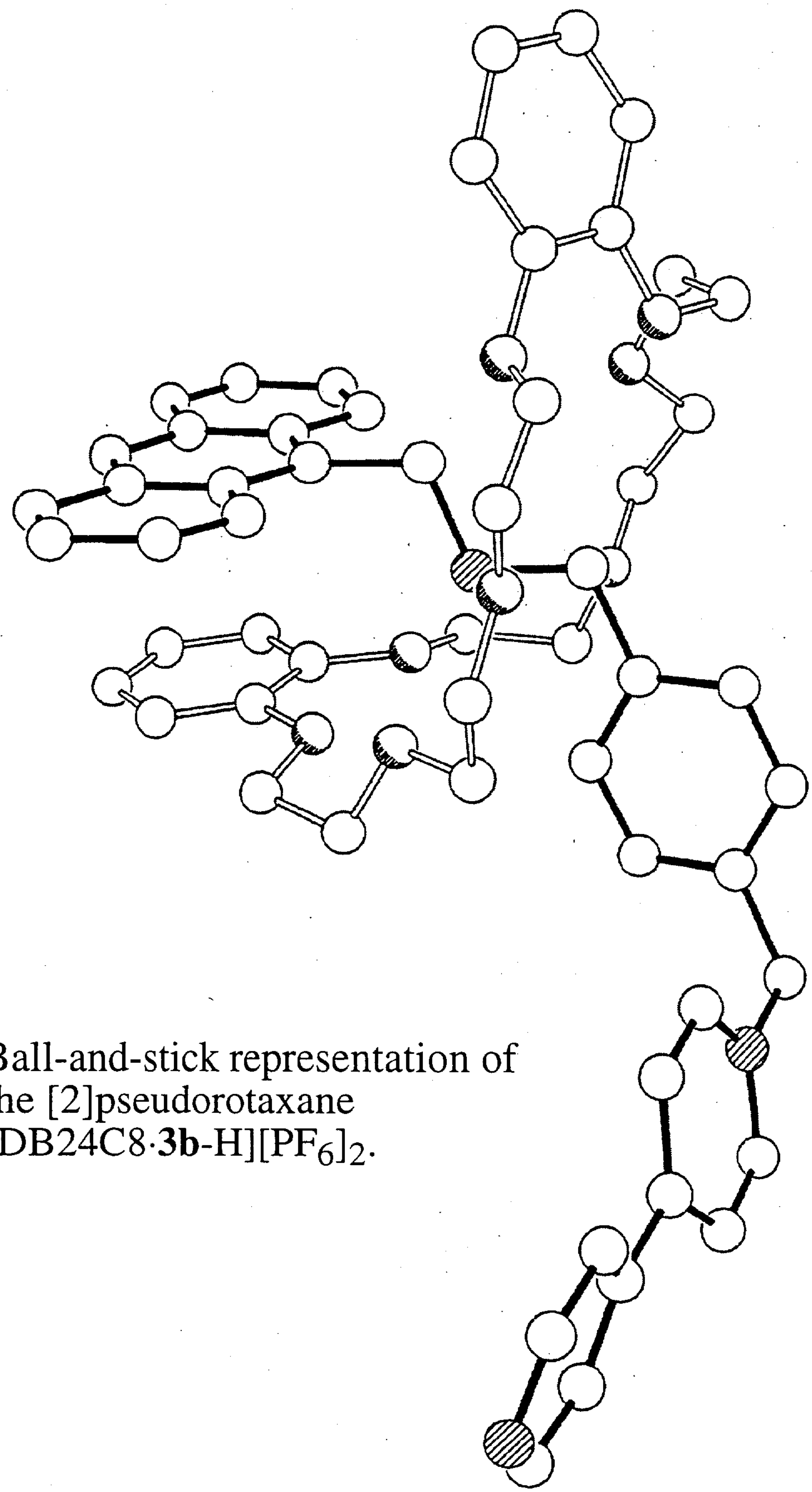
(6) SHELXTL PC Version 5.03, Siemens Analytical X-Ray Instruments, Inc., Madison, WI, 1994.
(7) Berlman, I. B. *Handbook of Fluorescence Spectra of Aromatic Compounds*; Academic: London, 1965.
(8) Dawson, W. R.; Windsor, M. W. *J. Phys. Chem.* **1968**, *72*, 3251–3260.

interference filter. The incident light intensity was measured using the ferric oxalate actinometer[9] and was of the order 10^{-7} Nhv/min. The experimental error on the photochemical quantum yields was ±20%.

Electrochemical Measurements. Electrochemical experiments were carried out in Ar-purged MeCN solutions with a Princeton Applied Research 273 multipurpose instrument interfaced to a PC, using cyclic voltammetry (CV) and differential pulse voltammetry (DPV) techniques. The working electrode was a glassy carbon electrode (0.08 cm^2, Amel); its surface was polished routinely with a 0.05 μm alumina–H_2O slurry on a felt surface immediately prior to use. The counter electrode was a Pt wire, while the reference electrode was a saturated calomel electrode (SCE) separated with a fine glass frit. The concentration of the compounds examined was 5.0×10^{-4} M, 0.05 M Et_4NPF_6 being added as supporting electrolyte and $FeCp_2$ as an internal reference. CVs Were obtained at sweep rates of 10, 20, 50, 200, 500 and 1000 mV s^{-1}. DPV Experiments were performed with scan rates of 20 mV s^{-1}, a pulse height of 75 mV and a duration of 40 ms. For reversible processes, the same halfwave potential values were obtained from the DPV peaks and an average of the cathodic and anodic CV peaks. The potential values for processes that were not fully reversible were estimated from the DPV peaks. Both CV and DPV techniques have been used[10] to measure the number of electrons exchanged in each redox process. To establish the reversibility of a process, we used the following criteria: (1) 60 mV separation between cathodic and anodic peaks, (2) cathodic and anodic currents' intensities have a ratio close to unity and (3) peak potential constancy on changing sweep rate in the CVs. The experimental errors on the reduction and oxidation potential values were estimated to be ±10 and ±30 mV, respectively.

(9) (a) Hatchard, C. G.; Parker, C. A. *Proc. R. Soc. London A* **1956**, *235*, 518–536. (b) Fisher, E. *EPA Newsletters* **1984** (July), 33.

(10) Flanagan, J. B.; Margel, S.; Bard, A. J.; Anson, F. C. *J. Am. Chem. Soc.* **1978**, *100*, 4248–4253.



Ball-and-stick representation of the [2]pseudorotaxane [DB24C8·**3b**-H][PF_6]$_2$.

Table 1. Crystal data and structure refinement for 1.

Identification code	fs9714
Empirical formula	$C_{59}H_{64}F_{12}N_4O_8P_2$
Formula weight	1247.08
Temperature	203(2) K
Diffractometer used	Siemens P4/RA
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 11.5513(9) Å alpha = 90°
	b = 26.3711(11) Å beta = 97.310(4)°
	c = 18.9108(6) Å gamma = 90°
Volume, Z	5713.8(5) $Å^3$, 4
Density (calculated)	1.450 Mg/m^3
Absorption coefficient	1.555 mm^{-1}
F(000)	2592
Crystal morphology/size	yellow needle, 0.50 x 0.13 x 0.12 mm
θ range for data collection	2.89 to 59.99°
Limiting indices	$0 \le h \le 12$, $0 \le k \le 29$, $-21 \le l \le 21$
Reflections collected	8554
Independent reflections	8387 (R_{int} = 0.0567)
Observed reflections	5771 [F>4σ(F)]
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7598 / 0 / 768
Goodness-of-fit on F^2	1.049
Final R indices [I>2σ(I)]	R1 = 0.1046, wR2 = 0.2631
R indices (all data)	R1 = 0.1401, wR2 = 0.3139
Largest diff. peak and hole	0.571 and -0.696 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	2341(3)	2972(2)	-4470(2)	44(1)
C(2)	3446(5)	2891(3)	-4733(3)	50(1)
C(3)	4050(5)	2463(2)	-4314(3)	48(1)
O(4)	4423(3)	2586(2)	-3588(2)	49(1)
C(5)	5545(5)	2823(3)	-3493(4)	57(2)
C(6)	5973(5)	2854(3)	-2714(4)	57(2)
O(7)	5317(4)	3230(2)	-2394(2)	52(1)
C(8)	5800(5)	3349(3)	-1687(3)	53(1)
C(9)	5333(6)	3024(3)	-1130(4)	56(2)
O(10)	4173(4)	3152(2)	-1024(2)	56(1)
C(11)	4009(5)	3573(2)	-631(3)	45(1)
C(12)	4906(5)	3877(2)	-299(3)	46(1)
C(13)	4631(6)	4302(2)	82(3)	52(1)
C(14)	3496(6)	4430(3)	140(3)	55(2)
C(15)	2599(6)	4121(3)	-183(3)	51(1)
C(16)	2855(5)	3692(3)	-561(3)	50(1)
O(17)	1936(5)	3421(3)	-911(3)	90(2)
C(18)	1325(9)	3124(4)	-530(4)	89(3)
C(19)	301(6)	2889(3)	-835(3)	61(2)
O(20)	347(3)	2654(2)	-1488(2)	47(1)
C(21)	-686(5)	2387(3)	-1731(3)	52(1)
C(22)	-591(6)	2148(2)	-2427(4)	55(2)
O(23)	-438(4)	2526(2)	-2950(2)	50(1)
C(24)	-1036(5)	2415(3)	-3637(3)	49(1)
C(25)	-994(5)	2860(3)	-4112(3)	50(1)
O(26)	207(3)	2933(2)	-4217(2)	45(1)
C(27)	428(5)	3285(2)	-4718(3)	42(1)
C(28)	-409(6)	3596(2)	-5084(3)	49(1)
C(29)	-69(6)	3928(3)	-5597(3)	55(2)
C(30)	1045(7)	3943(3)	-5740(3)	57(2)
C(31)	1894(6)	3633(2)	-5376(3)	51(1)
C(32)	1586(5)	3297(2)	-4865(3)	42(1)
C(33)	2307(5)	4137(2)	-3572(3)	45(1)
C(34)	3480(6)	4020(2)	-3654(4)	53(1)
C(35)	4048(7)	4282(3)	-4133(5)	70(2)
C(36)	3494(8)	4679(3)	-4559(4)	73(2)
C(37)	2389(7)	4801(3)	-4490(4)	61(2)
C(38)	1745(6)	4536(2)	-4016(3)	45(1)
C(39)	589(6)	4654(2)	-3962(3)	50(1)
C(40)	-60(5)	4405(2)	-3492(3)	45(1)
C(41)	-1243(6)	4536(3)	-3436(4)	60(2)
C(42)	-1848(6)	4302(3)	-2965(5)	66(2)
C(43)	-1289(6)	3924(3)	-2500(4)	61(2)
C(44)	-179(6)	3779(2)	-2549(3)	53(1)
C(45)	498(5)	4014(2)	-3044(3)	42(1)
C(46)	1660(5)	3881(2)	-3092(3)	39(1)
C(47)	2261(6)	3482(2)	-2606(3)	48(1)
N(48)	2010(4)	2945(2)	-2905(2)	39(1)
C(49)	2655(5)	2562(2)	-2432(3)	39(1)
C(50)	2391(4)	2017(2)	-2674(3)	39(1)
C(51)	1806(5)	1897(2)	-3332(3)	39(1)
C(52)	1533(5)	1393(2)	-3493(3)	42(1)

C(53)	1833(4)	1015(2)	-3010(3)	[illegible]
C(54)	2458(5)	1135(2)	-2360(3)	45(1)
C(55)	2728(5)	1636(2)	-2184(3)	42(1)
C(56)	1468(5)	469(2)	-3172(3)	46(1)
N(57)	226(4)	373(2)	-3042(2)	38(1)
C(58)	-323(5)	674(2)	-2618(3)	44(1)
C(59)	-1444(5)	584(2)	-2515(3)	44(1)
C(60)	-2072(5)	177(2)	-2856(3)	37(1)
C(61)	-1463(5)	-133(2)	-3275(3)	43(1)
C(62)	-335(5)	-30(2)	-3366(3)	42(1)
C(63)	-3314(5)	84(2)	-2775(3)	38(1)
C(64)	-3788(5)	252(2)	-2167(3)	47(1)
C(65)	-4949(6)	166(3)	-2126(4)	55(2)
N(66)	-5694(4)	-46(2)	-2643(3)	55(1)
C(67)	-5222(6)	-206(2)	-3223(4)	55(2)
C(68)	-4075(5)	-148(2)	-3308(3)	45(1)
P(1)	1519(1)	5790(1)	142(1)	49(1)
F(11)	1865(7)	6361(2)	178(5)	124(3)
F(12)	2431(7)	5681(3)	808(4)	134(3)
F(13)	617(7)	5864(3)	-512(4)	134(3)
F(14)	1209(5)	5202(2)	145(4)	102(2)
F(15)	2484(5)	5677(2)	-346(3)	96(2)
F(16)	538(5)	5893(2)	647(4)	95(2)
P(2)	-3920(2)	3536(1)	-5815(1)	59(1)
F(21)	-4832(7)	3980(3)	-5789(5)	139(3)
F(22)	-3611(9)	3560(4)	-4985(4)	145(3)
F(23)	-4244(6)	3515(4)	-6625(3)	146(3)
F(24)	-2909(6)	3929(3)	-5878(5)	138(3)
F(25)	-4945(5)	3144(2)	-5758(4)	98(2)
F(26)	-3010(5)	3085(2)	-5803(4)	98(2)
N(100)	-3045(9)	3462(4)	-8336(7)	121(4)
C(101)	-3987(7)	3572(3)	-8319(5)	69(2)
C(102)	-5163(7)	3711(3)	-8270(4)	66(2)

Table 3. Bond lengths [Å] and angles [°] for 1.

O(1)-C(32)	1.375(7)	O(1)-C(2)	1.444(7)
C(2)-C(3)	1.498(9)	C(3)-O(4)	1.423(7)
O(4)-C(5)	1.431(8)	C(5)-C(6)	1.494(9)
C(6)-O(7)	1.428(8)	O(7)-C(8)	1.418(7)
C(8)-C(9)	1.510(10)	C(9)-O(10)	1.420(8)
O(10)-C(11)	1.361(7)	C(11)-C(16)	1.392(9)
C(11)-C(12)	1.395(8)	C(12)-C(13)	1.393(9)
C(13)-C(14)	1.372(10)	C(14)-C(15)	1.396(10)
C(15)-C(16)	1.389(10)	C(16)-O(17)	1.378(8)
O(17)-C(18)	1.327(10)	C(18)-C(19)	1.394(11)
C(19)-O(20)	1.388(8)	O(20)-C(21)	1.412(7)
C(21)-C(22)	1.475(9)	C(22)-O(23)	1.432(7)
O(23)-C(24)	1.422(7)	C(24)-C(25)	1.480(9)
C(25)-O(26)	1.440(7)	O(26)-C(27)	1.374(7)
C(27)-C(28)	1.385(8)	C(27)-C(32)	1.401(8)
C(28)-C(29)	1.399(9)	C(29)-C(30)	1.350(10)
C(30)-C(31)	1.390(10)	C(31)-C(32)	1.389(9)
C(33)-C(34)	1.417(9)	C(33)-C(46)	1.418(8)
C(33)-C(38)	1.448(8)	C(34)-C(35)	1.371(11)
C(35)-C(36)	1.422(13)	C(36)-C(37)	1.338(12)
C(37)-C(38)	1.420(9)	C(38)-C(39)	1.387(9)
C(39)-C(40)	1.398(9)	C(40)-C(41)	1.427(9)
C(40)-C(45)	1.434(8)	C(41)-C(42)	1.349(11)
C(42)-C(43)	1.427(11)	C(43)-C(44)	1.352(10)
C(44)-C(45)	1.433(9)	C(45)-C(46)	1.402(8)
C(46)-C(47)	1.508(8)	C(47)-N(48)	1.536(7)
N(48)-C(49)	1.485(7)	C(49)-C(50)	1.525(7)
C(50)-C(51)	1.376(8)	C(50)-C(55)	1.389(8)
C(51)-C(52)	1.389(8)	C(52)-C(53)	1.366(8)
C(53)-C(54)	1.381(8)	C(53)-C(56)	1.521(8)
C(54)-C(55)	1.388(8)	C(56)-N(57)	1.509(7)
N(57)-C(58)	1.344(7)	N(57)-C(62)	1.349(7)
C(58)-C(59)	1.353(8)	C(59)-C(60)	1.405(8)
C(60)-C(61)	1.391(8)	C(60)-C(63)	1.482(8)
C(61)-C(62)	1.363(8)	C(63)-C(68)	1.392(8)
C(63)-C(64)	1.407(8)	C(64)-C(65)	1.373(9)
C(65)-N(66)	1.341(9)	N(66)-C(67)	1.353(10)
C(67)-C(68)	1.363(9)	P(1)-F(13)	1.524(5)
P(1)-F(11)	1.558(5)	P(1)-F(15)	1.562(5)
P(1)-F(12)	1.563(6)	P(1)-F(14)	1.591(5)
P(1)-F(16)	1.597(5)	P(2)-F(23)	1.531(6)
P(2)-F(22)	1.566(7)	P(2)-F(24)	1.577(6)
P(2)-F(21)	1.582(7)	P(2)-F(26)	1.583(6)
P(2)-F(25)	1.585(5)	N(100)-C(101)	1.131(12)
C(101)-C(102)	1.421(11)		
C(32)-O(1)-C(2)	115.6(4)	O(1)-C(2)-C(3)	107.6(5)
O(4)-C(3)-C(2)	113.7(5)	C(3)-O(4)-C(5)	112.3(5)
O(4)-C(5)-C(6)	109.2(6)	O(7)-C(6)-C(5)	109.2(5)
C(8)-O(7)-C(6)	112.7(5)	O(7)-C(8)-C(9)	113.6(5)
O(10)-C(9)-C(8)	113.0(5)	C(11)-O(10)-C(9)	118.0(5)
O(10)-C(11)-C(16)	116.0(5)	O(10)-C(11)-C(12)	124.5(6)
C(16)-C(11)-C(12)	119.5(6)	C(13)-C(12)-C(11)	119.4(6)
C(14)-C(13)-C(12)	121.5(6)	C(13)-C(14)-C(15)	119.1(6)
C(16)-C(15)-C(14)	120.3(6)	O(17)-C(16)-C(15)	117.9(6)
O(17)-C(16)-C(11)	121.6(6)	C(15)-C(16)-C(11)	120.2(5)
C(18)-O(17)-C(16)	118.4(6)	O(17)-C(18)-C(19)	121.4(7)
O(20)-C(19)-C(18)	116.1(7)	C(19)-O(20)-C(21)	112.7(5)
O(20)-C(21)-C(22)	110.4(5)	O(23)-C(22)-C(21)	110.4(5)

C(24)-O(23)-C(22)	113.6(5)	O(23)-C(24)-C(25)	110.0(5)
O(26)-C(25)-C(24)	107.3(5)	C(27)-O(26)-C(25)	117.0(4)
O(26)-C(27)-C(28)	124.4(5)	O(26)-C(27)-C(32)	114.8(5)
C(28)-C(27)-C(32)	120.7(5)	C(27)-C(28)-C(29)	118.5(6)
C(30)-C(29)-C(28)	121.1(6)	C(29)-C(30)-C(31)	120.9(6)
C(32)-C(31)-C(30)	119.5(6)	O(1)-C(32)-C(31)	125.1(5)
O(1)-C(32)-C(27)	115.7(5)	C(31)-C(32)-C(27)	119.2(5)
C(34)-C(33)-C(46)	123.7(6)	C(34)-C(33)-C(38)	117.4(5)
C(46)-C(33)-C(38)	118.9(5)	C(35)-C(34)-C(33)	120.5(7)
C(34)-C(35)-C(36)	121.7(7)	C(37)-C(36)-C(35)	119.2(7)
C(36)-C(37)-C(38)	121.8(7)	C(39)-C(38)-C(37)	121.6(6)
C(39)-C(38)-C(33)	119.0(5)	C(37)-C(38)-C(33)	119.4(6)
C(38)-C(39)-C(40)	122.7(5)	C(39)-C(40)-C(41)	121.9(6)
C(39)-C(40)-C(45)	118.5(6)	C(41)-C(40)-C(45)	119.5(6)
C(42)-C(41)-C(40)	121.4(7)	C(41)-C(42)-C(43)	119.5(6)
C(44)-C(43)-C(42)	120.9(7)	C(43)-C(44)-C(45)	121.6(7)
C(46)-C(45)-C(44)	122.8(5)	C(46)-C(45)-C(40)	120.2(5)
C(44)-C(45)-C(40)	117.0(6)	C(45)-C(46)-C(33)	120.7(5)
C(45)-C(46)-C(47)	120.3(5)	C(33)-C(46)-C(47)	118.9(5)
C(46)-C(47)-N(48)	111.7(4)	C(49)-N(48)-C(47)	110.5(4)
N(48)-C(49)-C(50)	113.3(4)	C(51)-C(50)-C(55)	119.9(5)
C(51)-C(50)-C(49)	123.0(5)	C(55)-C(50)-C(49)	117.0(5)
C(50)-C(51)-C(52)	119.4(5)	C(53)-C(52)-C(51)	121.3(5)
C(52)-C(53)-C(54)	119.2(5)	C(52)-C(53)-C(56)	121.1(5)
C(54)-C(53)-C(56)	119.7(5)	C(53)-C(54)-C(55)	120.4(5)
C(54)-C(55)-C(50)	119.7(5)	N(57)-C(56)-C(53)	111.8(4)
C(58)-N(57)-C(62)	120.0(5)	C(58)-N(57)-C(56)	122.0(4)
C(62)-N(57)-C(56)	118.1(5)	N(57)-C(58)-C(59)	121.0(5)
C(58)-C(59)-C(60)	121.0(5)	C(61)-C(60)-C(59)	116.2(5)
C(61)-C(60)-C(63)	121.8(5)	C(59)-C(60)-C(63)	122.0(5)
C(62)-C(61)-C(60)	121.0(5)	N(57)-C(62)-C(61)	120.8(5)
C(68)-C(63)-C(64)	117.0(5)	C(68)-C(63)-C(60)	122.0(5)
C(64)-C(63)-C(60)	120.9(5)	C(65)-C(64)-C(63)	118.6(6)
N(66)-C(65)-C(64)	124.7(6)	C(65)-N(66)-C(67)	115.7(5)
N(66)-C(67)-C(68)	123.9(6)	C(67)-C(68)-C(63)	119.9(6)
F(13)-P(1)-F(11)	93.2(5)	F(13)-P(1)-F(15)	90.7(4)
F(11)-P(1)-F(15)	90.7(3)	F(13)-P(1)-F(12)	176.8(5)
F(11)-P(1)-F(12)	90.0(5)	F(15)-P(1)-F(12)	89.0(4)
F(13)-P(1)-F(14)	89.8(5)	F(11)-P(1)-F(14)	176.9(5)
F(15)-P(1)-F(14)	89.7(3)	F(12)-P(1)-F(14)	87.0(4)
F(13)-P(1)-F(16)	90.0(4)	F(11)-P(1)-F(16)	90.4(3)
F(15)-P(1)-F(16)	178.7(3)	F(12)-P(1)-F(16)	90.3(4)
F(14)-P(1)-F(16)	89.2(3)	F(23)-P(2)-F(22)	179.0(5)
F(23)-P(2)-F(24)	92.1(5)	F(22)-P(2)-F(24)	88.4(5)
F(23)-P(2)-F(21)	88.8(5)	F(22)-P(2)-F(21)	90.4(5)
F(24)-P(2)-F(21)	91.0(5)	F(23)-P(2)-F(26)	93.7(5)
F(22)-P(2)-F(26)	87.1(4)	F(24)-P(2)-F(26)	89.9(4)
F(21)-P(2)-F(26)	177.3(5)	F(23)-P(2)-F(25)	87.5(4)
F(22)-P(2)-F(25)	92.0(5)	F(24)-P(2)-F(25)	179.4(3)
F(21)-P(2)-F(25)	88.5(4)	F(26)-P(2)-F(25)	90.6(3)
N(100)-C(101)-C(102)	177.8(11)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 1.

The anisotropic displacement factor exponent takes the form:
$-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

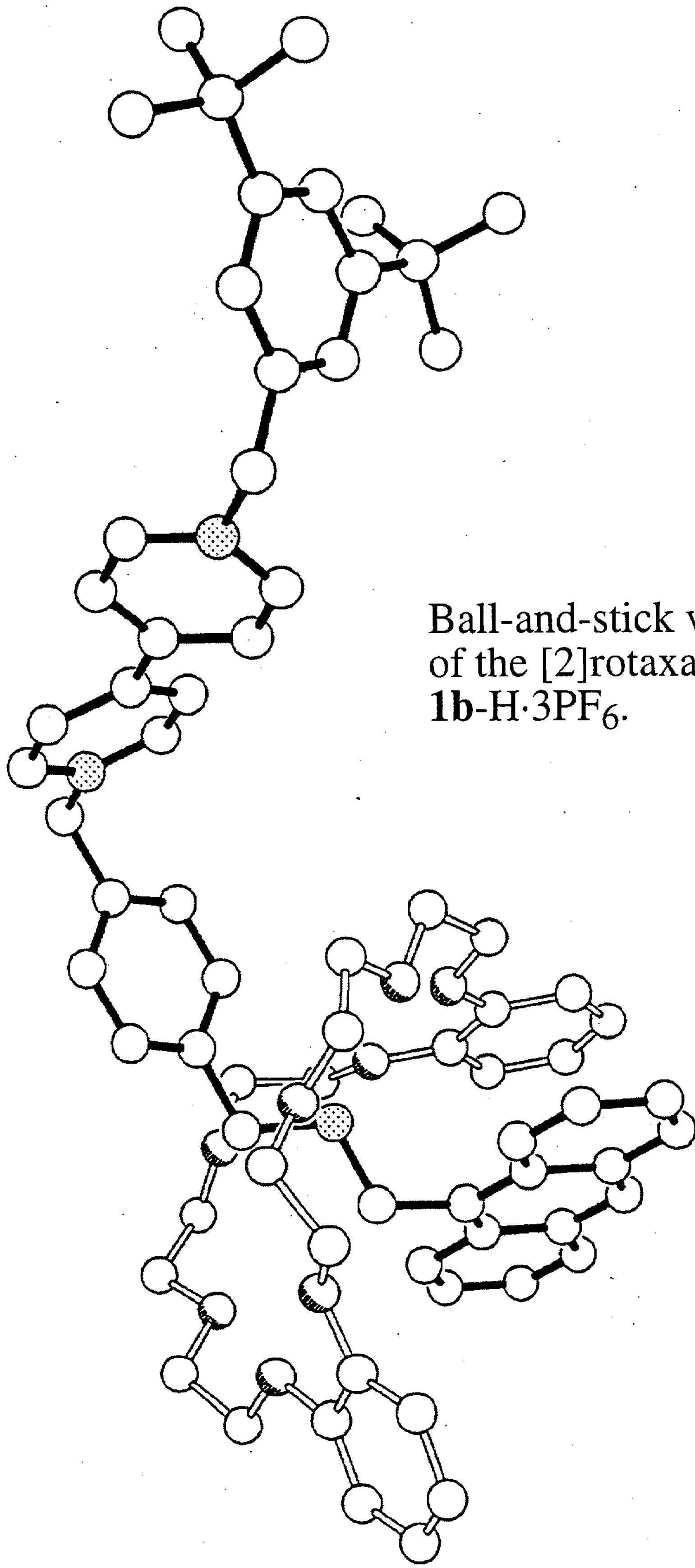
	U11	U22	U33	U23	U13	U12
O(1)	39(2)	55(2)	38(2)	1(2)	2(2)	-3(2)
C(2)	42(3)	65(4)	42(3)	-8(3)	6(2)	-3(3)
C(3)	47(3)	52(3)	44(3)	-12(2)	0(2)	2(2)
O(4)	38(2)	66(2)	39(2)	-7(2)	-4(2)	0(2)
C(5)	38(3)	80(4)	54(3)	-20(3)	5(3)	2(3)
C(6)	39(3)	69(4)	62(4)	-16(3)	-5(3)	9(3)
O(7)	45(2)	62(2)	48(2)	-14(2)	-2(2)	3(2)
C(8)	44(3)	61(4)	52(3)	-15(3)	1(3)	-6(3)
C(9)	65(4)	52(3)	50(3)	-6(3)	1(3)	4(3)
O(10)	60(3)	54(2)	54(2)	-13(2)	13(2)	-6(2)
C(11)	54(3)	50(3)	27(2)	-2(2)	-6(2)	-6(2)
C(12)	43(3)	55(3)	38(3)	-2(2)	-3(2)	1(2)
C(13)	53(3)	54(3)	45(3)	-5(3)	-7(3)	-5(3)
C(14)	65(4)	53(3)	44(3)	-7(3)	-4(3)	3(3)
C(15)	49(3)	72(4)	31(3)	1(3)	-2(2)	4(3)
C(16)	45(3)	75(4)	28(2)	-8(2)	-2(2)	-13(3)
O(17)	71(3)	150(6)	54(3)	-39(3)	21(3)	-57(4)
C(18)	105(7)	120(7)	40(3)	-13(4)	5(4)	-54(6)
C(19)	61(4)	78(4)	44(3)	-14(3)	8(3)	-20(3)
O(20)	41(2)	54(2)	43(2)	-2(2)	1(2)	-7(2)
C(21)	45(3)	60(3)	50(3)	1(3)	4(2)	-11(3)
C(22)	59(4)	51(3)	54(3)	1(3)	7(3)	-15(3)
O(23)	57(2)	53(2)	36(2)	3(2)	-5(2)	-15(2)
C(24)	36(3)	66(4)	41(3)	1(3)	-5(2)	-9(2)
C(25)	36(3)	74(4)	38(3)	9(3)	-5(2)	0(3)
O(26)	37(2)	57(2)	38(2)	9(2)	-8(2)	-5(2)
C(27)	49(3)	45(3)	29(2)	1(2)	-6(2)	-3(2)
C(28)	51(3)	51(3)	42(3)	-2(3)	-7(2)	1(3)
C(29)	70(4)	56(3)	36(3)	9(3)	-10(3)	3(3)
C(30)	78(5)	55(3)	36(3)	14(3)	-4(3)	-10(3)
C(31)	59(4)	51(3)	43(3)	2(3)	5(3)	-6(3)
C(32)	51(3)	48(3)	23(2)	-3(2)	-7(2)	-2(2)
C(33)	51(3)	41(3)	41(3)	-7(2)	3(2)	-8(2)
C(34)	55(3)	47(3)	55(3)	-12(3)	2(3)	-5(3)
C(35)	58(4)	75(5)	80(5)	-20(4)	25(4)	-16(3)
C(36)	95(6)	74(5)	52(4)	-10(3)	20(4)	-35(4)
C(37)	82(5)	53(3)	49(3)	2(3)	9(3)	-18(3)
C(38)	63(4)	40(3)	32(2)	-1(2)	2(2)	-4(2)
C(39)	69(4)	39(3)	41(3)	1(2)	0(3)	5(3)
C(40)	50(3)	42(3)	42(3)	-2(2)	-5(2)	0(2)
C(41)	52(4)	54(3)	71(4)	-11(3)	-4(3)	7(3)
C(42)	43(3)	68(4)	86(5)	-15(4)	5(3)	2(3)
C(43)	62(4)	62(4)	62(4)	-15(3)	23(3)	-13(3)
C(44)	59(4)	53(3)	47(3)	-5(3)	7(3)	-7(3)
C(45)	53(3)	37(3)	34(3)	-6(2)	-1(2)	-2(2)
C(46)	49(3)	32(2)	32(2)	-3(2)	-3(2)	-3(2)
C(47)	62(4)	42(3)	36(3)	-7(2)	-10(2)	-3(2)
N(48)	41(2)	38(2)	36(2)	-3(2)	-5(2)	-7(2)
C(49)	37(3)	42(3)	36(2)	0(2)	-9(2)	-2(2)
C(50)	32(2)	43(3)	39(3)	4(2)	-4(2)	-4(2)
C(51)	38(3)	42(3)	34(3)	9(2)	-5(2)	0(2)
C(52)	39(3)	49(3)	34(3)	-6(2)	-5(2)	-6(2)

C(53)	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
C(54)	39(3)	47(3)	46(3)	15(2)	-7(2)	1(2)
C(55)	36(3)	51(3)	36(3)	4(2)	-8(2)	-2(2)
C(56)	36(3)	43(3)	57(3)	0(2)	6(2)	-3(2)
N(57)	40(2)	33(2)	38(2)	0(2)	-6(2)	-2(2)
C(58)	44(3)	39(3)	48(3)	-14(2)	-1(2)	-4(2)
C(59)	38(3)	46(3)	47(3)	-12(2)	0(2)	-3(2)
C(60)	42(3)	37(2)	29(2)	1(2)	-9(2)	-1(2)
C(61)	47(3)	40(3)	40(3)	-8(2)	0(2)	-6(2)
C(62)	44(3)	42(3)	41(3)	-6(2)	5(2)	-2(2)
C(63)	39(3)	39(3)	33(2)	2(2)	-6(2)	1(2)
C(64)	45(3)	49(3)	46(3)	-6(2)	-1(2)	2(2)
C(65)	48(3)	66(4)	51(3)	6(3)	9(3)	3(3)
N(66)	40(3)	57(3)	66(3)	7(3)	0(2)	-3(2)
C(67)	46(3)	52(3)	63(4)	3(3)	-16(3)	-10(3)
C(68)	46(3)	49(3)	37(3)	0(2)	-10(2)	-2(2)
P(1)	40(1)	55(1)	48(1)	-4(1)	-6(1)	-1(1)
F(11)	155(6)	58(3)	174(7)	-18(3)	84(5)	-21(3)
F(12)	127(6)	169(7)	91(4)	-20(4)	-49(4)	25(5)
F(13)	118(5)	180(7)	85(4)	-19(4)	-54(4)	50(5)
F(14)	89(3)	63(3)	162(6)	-2(3)	49(4)	-6(2)
F(15)	86(3)	93(4)	118(4)	-10(3)	48(3)	-1(3)
F(16)	93(4)	73(3)	131(5)	0(3)	60(4)	9(3)
P(2)	54(1)	63(1)	58(1)	12(1)	-6(1)	-7(1)
F(21)	108(5)	100(5)	200(9)	-9(5)	-12(5)	29(4)
F(22)	182(8)	169(7)	71(4)	-11(4)	-30(4)	29(6)
F(23)	101(5)	267(11)	63(3)	7(5)	-20(3)	-29(6)
F(24)	84(4)	111(5)	200(8)	84(5)	-50(4)	-41(3)
F(25)	73(3)	89(3)	140(5)	16(3)	40(3)	-18(3)
F(26)	69(3)	86(3)	140(5)	-1(3)	21(3)	2(2)
N(100)	82(6)	120(8)	166(11)	9(7)	30(6)	36(5)
C(101)	59(4)	65(4)	82(5)	7(4)	10(4)	9(3)
C(102)	58(4)	67(4)	72(4)	9(3)	2(3)	0(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(2A)	3923(5)	3199(3)	-4672(3)	60
H(2B)	3321(5)	2805(3)	-5241(3)	60
H(3A)	3518(5)	2173(2)	-4333(3)	58
H(3B)	4731(5)	2361(2)	-4540(3)	58
H(5A)	5489(5)	3165(3)	-3699(4)	69
H(5B)	6095(5)	2626(3)	-3736(4)	69
H(6A)	5882(5)	2524(3)	-2489(4)	69
H(6B)	6803(5)	2944(3)	-2645(4)	69
H(8A)	5638(5)	3705(3)	-1592(3)	63
H(8B)	6649(5)	3308(3)	-1644(3)	63
H(9A)	5354(6)	2668(3)	-1274(4)	67
H(9B)	5842(6)	3061(3)	-677(4)	67
H(12A)	5690(5)	3795(2)	-332(3)	55
H(13A)	5237(6)	4507(2)	304(3)	62
H(14A)	3324(6)	4721(3)	394(3)	66
H(15A)	1817(6)	4204(3)	-145(3)	62
H(18A)	1125(9)	3327(4)	-129(4)	107
H(18B)	1852(9)	2855(4)	-328(4)	107
H(19A)	80(6)	2635(3)	-499(3)	73
H(19B)	-321(6)	3144(3)	-895(3)	73
H(21A)	-1351(5)	2621(3)	-1778(3)	62
H(21B)	-824(5)	2125(3)	-1383(3)	62
H(22A)	74(6)	1914(2)	-2380(4)	66
H(22B)	-1300(6)	1952(2)	-2580(4)	66
H(24A)	-1850(5)	2329(3)	-3597(3)	58
H(24B)	-671(5)	2123(3)	-3840(3)	58
H(25A)	-1473(5)	2798(3)	-4570(3)	60
H(25B)	-1293(5)	3161(3)	-3893(3)	60
H(28A)	-1188(6)	3585(2)	-4990(3)	59
H(29A)	-627(6)	4143(3)	-5847(3)	66
H(30A)	1251(7)	4167(3)	-6090(3)	69
H(31A)	2670(6)	3650(2)	-5475(3)	62
H(34A)	3871(6)	3761(2)	-3378(4)	63
H(35A)	4825(7)	4198(3)	-4180(5)	84
H(36A)	3898(8)	4853(3)	-4886(4)	87
H(37A)	2031(7)	5069(3)	-4763(4)	73
H(39A)	227(6)	4912(2)	-4254(3)	60
H(41A)	-1608(6)	4790(3)	-3733(4)	72
H(42A)	-2633(6)	4387(3)	-2943(5)	79
H(43A)	-1698(6)	3774(3)	-2156(4)	73
H(44A)	157(6)	3519(2)	-2252(3)	64
H(47A)	1992(6)	3507(2)	-2136(3)	58
H(47B)	3104(6)	3542(2)	-2546(3)	58
H(48A)	1231(4)	2882(2)	-2940(2)	47
H(48B)	2230(4)	2924(2)	-3349(2)	47
H(49A)	2453(5)	2604(2)	-1948(3)	47
H(49B)	3495(5)	2623(2)	-2417(3)	47
H(51A)	1593(5)	2152(2)	-3669(3)	47
H(52A)	1133(5)	1311(2)	-3942(3)	50
H(54A)	2702(5)	875(2)	-2034(3)	54
H(55A)	3136(5)	1716(2)	-1736(3)	50
H(56A)	1547(5)	393(2)	-3671(3)	55
H(56B)	1990(5)	241(2)	-2872(3)	55

H(58A)	77(5)	950(2)	-2389(3)	53
H(59A)	-1807(5)	798(2)	-2212(3)	53
H(61A)	-1834(5)	-419(2)	-3498(3)	51
H(62A)	56(5)	-241(2)	-3657(3)	50
H(64A)	-3319(5)	420(2)	-1796(3)	56
H(65A)	-5243(6)	263(3)	-1704(4)	66
H(67A)	-5714(6)	-367(2)	-3590(4)	66
H(68A)	-3798(5)	-265(2)	-3725(3)	54
H(10A)	-5616(14)	3686(25)	-8737(8)	99
H(10B)	-5187(9)	4056(9)	-8098(34)	99
H(10C)	-5487(19)	3484(16)	-7942(28)	99



Ball-and-stick view of the [2]rotaxane **1b**-H·3PF_6.

Table 1. Crystal data and structure refinement for 1.

Identification code	FS9722
Empirical formula	$C_{72}H_{84}N_3O_8 \cdot 3PF_6 \cdot 4Me_2CO$
Formula weight	1786.64
Temperature	203(2) K
Diffractometer Used	Siemens P4/RA
Wavelength	1.54178 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	*a* = 20.138(3) Å alpha = 115.28(2)°
	b = 21.696(5) Å beta = 101.73(2)°
	c = 23.916(4) Å gamma = 97.52(2)°
Volume, Z	8967(3) $Å^3$, 4
Density (calculated)	1.323 Mg/m^3
Absorption coefficient	1.445 mm^{-1}
F(000)	3744
Crystal morphology/size	Orange/red rhombs, 0.73 x 0.70 x 0.53 mm
θ range for data collection	2.13 to 57.49°
Limiting indices	$-13 \le h \le 16$, $-20 \le k \le 20$, $-23 \le l \le 26$
Reflections collected	21959
Independent reflections	21069 (R_{int} = 0.0916)
Observed reflections	12294 [$F > 4\sigma(F)$]
Absorption correction	None
Refinement method	Full-matrix-block least-squares on F^2
Data / restraints / parameters	21064 / 22 / 2094
Goodness-of-fit on F^2	1.015
Final R indices [$I>2\sigma(I)$]	R1 = 0.1014, wR2 = 0.2517
R indices (all data)	R1 = 0.1635, wR2 = 0.3133
Extinction coefficient	0.00018(5)
Largest diff. peak and hole	0.854 and -0.665 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4], equivalent isotropic displacement parameters [$Å^2$ x 10^3] and occupancies [K] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor, K is unity unless otherwise stated.

	x	y	z	U(eq)	K
O(1)	3516(3)	939(3)	8239(3)	52(2)	
C(2)	4030(5)	804(5)	7882(4)	60(3)	
C(3)	4037(5)	1258(5)	7577(4)	64(3)	
O(4)	4340(4)	1984(3)	8036(3)	56(2)	
C(5)	5063(5)	2196(5)	8174(4)	57(3)	
C(6)	5301(5)	2974(5)	8505(4)	57(3)	
O(7)	5238(3)	3257(3)	9146(2)	42(1)	
C(8)	5496(5)	3998(5)	9472(4)	50(2)	
C(9)	5562(5)	4297(5)	10179(4)	47(2)	
O(10)	4872(3)	4285(3)	10258(3)	41(1)	
C(11)	4845(4)	4626(4)	10886(4)	37(2)	
C(12)	5412(5)	4905(4)	11426(4)	44(2)	
C(13)	5306(6)	5252(5)	12036(4)	58(3)	
C(14)	4660(6)	5288(5)	12099(4)	54(2)	
C(15)	4086(5)	5013(4)	11562(4)	46(2)	
C(16)	4178(4)	4675(4)	10947(4)	38(2)	
O(17)	3652(3)	4412(3)	10384(3)	45(1)	
C(18)	2991(5)	4571(5)	10416(4)	50(2)	
C(19)	2563(5)	4335(5)	9738(5)	59(3)	
O(20)	2341(3)	3592(3)	9368(3)	53(2)	
C(21)	1644(5)	3315(5)	9309(5)	56(2)	
C(22)	1378(5)	2592(5)	8754(4)	54(2)	
O(23)	1755(3)	2128(3)	8884(3)	46(1)	
C(24)	1379(5)	1406(5)	8488(4)	52(2)	
C(25)	1743(5)	954(5)	8716(4)	58(3)	
O(26)	2390(3)	964(3)	8571(3)	52(2)	
C(27)	2768(5)	522(4)	8694(4)	52(2)	
C(28)	2576(6)	104(5)	8969(5)	68(3)	
C(29)	3008(8)	-311(5)	9070(6)	80(4)	
C(30)	3597(8)	-319(5)	8888(6)	83(4)	
C(31)	3791(6)	75(5)	8597(5)	73(3)	
C(32)	3375(5)	500(5)	8496(4)	55(3)	
C(33)	4361(4)	1888(4)	9935(3)	38(2)	
C(34)	4934(5)	1956(5)	9675(4)	50(2)	
C(35)	5413(5)	1573(5)	9687(4)	59(3)	
C(36)	5386(6)	1126(5)	9965(5)	62(3)	
C(37)	4870(5)	1050(5)	10219(5)	56(2)	
C(38)	4338(5)	1422(4)	10218(4)	42(2)	
C(39)	3799(5)	1324(5)	10464(4)	53(2)	
C(40)	3279(5)	1682(4)	10471(3)	42(2)	
C(41)	2713(5)	1576(5)	10718(4)	57(3)	
C(42)	2202(6)	1929(5)	10727(4)	58(3)	
C(43)	2223(5)	2413(5)	10467(4)	51(2)	
C(44)	2745(5)	2524(4)	10227(3)	45(2)	
C(45)	3285(5)	2160(4)	10200(3)	42(2)	
C(46)	3828(4)	2247(4)	9926(3)	36(2)	
C(47)	3818(4)	2730(4)	9622(3)	37(2)	
N(48)	3299(3)	2411(3)	8968(3)	34(2)	
C(49)	3375(4)	2881(4)	8665(3)	37(2)	
C(50)	2792(4)	2663(4)	8057(4)	35(2)	

C(51)	2427(4)	1967(4)	7641(4)	40(2)	
C(52)	1891(4)	1810(4)	7095(4)	43(2)	
C(53)	1716(4)	2333(4)	6955(3)	35(2)	
C(54)	2083(5)	3023(5)	7368(4)	47(2)	
C(55)	2612(5)	3180(4)	7919(4)	44(2)	
C(56)	1132(4)	2181(5)	6382(4)	46(2)	
N(57)	496(3)	2372(4)	6573(3)	39(2)	
C(58)	123(5)	1983(4)	6758(4)	44(2)	
C(59)	-444(4)	2139(4)	6949(4)	40(2)	
C(60)	-665(4)	2722(4)	6943(3)	37(2)	
C(61)	-285(4)	3120(4)	6739(4)	44(2)	
C(62)	305(4)	2933(4)	6549(4)	43(2)	
C(63)	-1297(4)	2902(4)	7150(3)	33(2)	
C(64)	-1474(4)	2727(4)	7607(4)	37(2)	
C(65)	-2070(4)	2869(4)	7773(4)	43(2)	
N(66)	-2488(3)	3152(3)	7496(3)	38(2)	
C(67)	-2322(4)	3339(4)	7067(3)	37(2)	
C(68)	-1723(4)	3222(4)	6887(4)	38(2)	
C(69)	-3160(4)	3241(4)	7645(4)	40(2)	
C(70)	-3750(4)	2590(4)	7192(3)	34(2)	
C(71)	-4365(4)	2681(4)	6891(3)	35(2)	
C(72)	-4938(4)	2107(4)	6483(4)	34(2)	
C(73)	-4855(4)	1447(4)	6391(4)	39(2)	
C(74)	-4241(4)	1339(4)	6687(4)	37(2)	
C(75)	-3694(4)	1921(4)	7085(4)	37(2)	
C(76)	-5624(5)	2201(5)	6158(5)	55(2)	
C(77)	-6161(6)	2065(9)	6446(8)	109(5)	
C(78)	-5547(6)	2888(6)	6142(7)	95(4)	
C(79)	-5887(7)	1621(7)	5436(6)	113(5)	
C(80)	-4187(5)	583(4)	6545(4)	47(2)	
C(81)	-4303(10)	137(7)	5825(7)	80(5)	0.70
C(82)	-3436(8)	577(7)	6869(9)	81(5)	0.70
C(83)	-4668(10)	271(8)	6785(9)	84(5)	0.70
C(81A)	-3666(18)	403(17)	6243(16)	56(8)	0.30
C(82A)	-4000(21)	662(19)	7232(16)	67(9)	0.30
C(83A)	-4903(20)	27(19)	6112(18)	72(10)	0.30
O(1')	8055(3)	1050(3)	3334(3)	46(1)	
C(2')	8602(5)	806(5)	3068(5)	58(2)	
C(3')	8782(6)	1186(5)	2725(4)	58(3)	
O(4')	9087(3)	1921(3)	3134(3)	57(2)	
C(5')	9815(6)	2115(6)	3269(5)	76(3)	
C(6')	10084(6)	2888(6)	3561(5)	80(3)	
O(7')	10051(3)	3224(3)	4209(3)	55(2)	
C(8')	10399(5)	3952(5)	4529(5)	59(3)	
C(9')	10507(5)	4232(5)	5238(5)	55(2)	
O(10')	9843(3)	4292(3)	5368(3)	47(2)	
C(11')	9842(5)	4549(4)	5997(4)	44(2)	
C(12')	10399(5)	4654(5)	6504(4)	53(2)	
C(13')	10329(5)	4894(5)	7123(5)	60(3)	
C(14')	9701(6)	5014(5)	7238(5)	67(3)	
C(15')	9149(5)	4907(5)	6735(4)	54(2)	
C(16')	9203(4)	4673(4)	6108(4)	40(2)	
O(17')	8696(3)	4577(3)	5586(3)	45(1)	
C(18')	8079(5)	4809(5)	5699(5)	58(3)	
C(19')	7640(5)	4719(5)	5088(5)	67(3)	
O(20')	7326(3)	3994(4)	4649(4)	83(2)	
C(21')	6610(5)	3823(5)	4412(5)	62(3)	
C(22')	6297(7)	3159(7)	3897(9)	141(8)	
O(23')	6523(3)	2613(3)	3862(3)	68(2)	
C(24')	6090(5)	1955(5)	3364(6)	73(3)	
C(25')	6198(5)	1407(6)	3566(5)	72(3)	
O(26')	6910(3)	1343(3)	3575(3)	51(2)	
C(27')	7106(5)	829(4)	3703(4)	52(2)	

C(28')	6745(5)	466(5)	3960(4)	61(3)	
C(29')	6985(8)	-32(6)	4084(5)	79(4)	
C(30')	7567(7)	-202(5)	3936(5)	73(3)	
C(31')	7954(5)	139(5)	3682(4)	59(3)	
C(32')	7712(5)	660(4)	3560(4)	47(2)	
C(33')	8925(5)	1944(4)	5021(3)	46(2)	
C(34')	9524(6)	2061(5)	4811(4)	63(3)	
C(35')	9981(6)	1647(7)	4765(5)	75(3)	
C(36')	9911(6)	1120(7)	4935(5)	75(3)	
C(37')	9377(6)	1002(5)	5166(5)	68(3)	
C(38')	8863(5)	1409(4)	5222(4)	49(2)	
C(39')	8308(5)	1292(4)	5442(4)	53(2)	
C(40')	7788(5)	1659(4)	5463(4)	48(2)	
C(41')	7207(6)	1514(5)	5674(4)	60(3)	
C(42')	6689(6)	1845(6)	5653(4)	62(3)	
C(43')	6724(5)	2363(5)	5446(4)	60(3)	
C(44')	7277(5)	2533(4)	5257(4)	46(2)	
C(45')	7828(5)	2188(4)	5246(4)	43(2)	
C(46')	8413(4)	2341(4)	5043(3)	39(2)	
C(47')	8481(5)	2897(4)	4838(4)	45(2)	
N(48')	8092(4)	2632(4)	4136(3)	42(2)	
C(49')	8325(4)	3134(4)	3901(4)	37(2)	
C(50')	7835(4)	2992(4)	3272(4)	38(2)	
C(51')	7527(5)	2324(4)	2781(4)	51(2)	
C(52')	7053(5)	2220(5)	2214(4)	54(2)	
C(53')	6887(5)	2765(5)	2134(4)	46(2)	
C(54')	7212(6)	3444(5)	2616(5)	64(3)	
C(55')	7671(6)	3539(5)	3174(5)	63(3)	
C(56')	6366(5)	2656(5)	1529(4)	58(3)	
N(57')	5701(4)	2803(4)	1665(3)	48(2)	
C(58')	5317(6)	2406(5)	1839(5)	58(3)	
C(59')	4712(5)	2535(5)	1989(4)	52(2)	
C(60')	4470(5)	3091(4)	1940(4)	44(2)	
C(61')	4877(5)	3488(5)	1750(4)	50(2)	
C(62')	5479(5)	3347(5)	1616(4)	54(2)	
C(63')	3823(5)	3242(4)	2090(4)	46(2)	
C(64')	3568(6)	3051(5)	2512(4)	56(2)	
C(65')	2957(6)	3167(5)	2618(4)	63(3)	
N(66')	2556(4)	3465(3)	2326(3)	49(2)	
C(67')	2809(5)	3675(4)	1940(4)	46(2)	
C(68')	3422(5)	3576(4)	1819(4)	43(2)	
C(69')	1844(5)	3524(5)	2405(5)	56(2)	
C(70')	1304(5)	2859(5)	1900(5)	55(2)	
C(71')	899(5)	2835(5)	1333(4)	50(2)	
C(72')	432(5)	2211(5)	843(5)	59(3)	
C(73')	397(5)	1623(5)	940(5)	60(3)	
C(74')	789(5)	1629(5)	1497(5)	57(2)	
C(75')	1237(5)	2261(5)	1976(4)	53(2)	
C(76')	-6(7)	2177(7)	219(6)	86(4)	
C(77')	-770(9)	1808(12)	78(9)	79(6)	0.60
C(78')	111(13)	2793(10)	153(10)	90(7)	0.60
C(79')	251(11)	1588(11)	-368(8)	87(6)	0.60
C(77B)	-480(15)	2805(15)	501(13)	75(7)	0.40
C(78B)	407(17)	2483(18)	-90(15)	78(9)	0.40
C(79B)	-536(24)	1483(22)	-234(21)	119(14)	0.40
C(80')	741(6)	931(5)	1537(5)	64(3)	
C(81')	1064(8)	447(6)	1037(7)	109(5)	
C(82')	1139(8)	1068(7)	2216(6)	98(4)	
C(83')	-21(7)	563(6)	1392(7)	97(4)	
P(10)	8514(1)	5154(1)	8692(1)	44(1)	
F(11)	8271(3)	5872(2)	8981(2)	57(1)	
F(12)	8566(4)	5131(4)	9349(3)	90(2)	
F(13)	7718(3)	4734(3)	8431(3)	76(2)	

F(14)	8443(4)	5178(4)	8033(3)	89(2)	
F(15)	9301(3)	5571(3)	8960(4)	91(2)	
F(16)	8745(3)	4432(3)	8401(3)	70(2)	
P(20)	-212(1)	227(1)	6920(1)	51(1)	
F(21)	-622(4)	366(4)	6366(3)	100(2)	
F(22)	505(4)	453(4)	6799(4)	99(2)	
F(23)	-109(3)	1022(3)	7420(3)	79(2)	
F(24)	-927(3)	3(4)	7032(4)	92(2)	
F(25)	-296(4)	-563(3)	6423(3)	92(2)	
F(26)	204(3)	97(3)	7478(3)	83(2)	
P(30)	7529(2)	4777(2)	1744(1)	64(1)	
F(31)	7898(4)	4631(6)	2307(4)	128(3)	
F(32)	7947(4)	4343(4)	1313(4)	121(3)	
F(33)	8156(4)	5442(4)	2007(4)	119(3)	
F(34)	7135(4)	5272(5)	2192(4)	122(3)	
F(35)	6900(4)	4141(4)	1505(5)	119(3)	
F(36)	7149(4)	4956(5)	1217(4)	117(3)	
P(40)	5745(2)	-460(2)	8215(1)	67(1)	
F(41)	6349(4)	-172(4)	8004(5)	121(3)	
F(42)	5440(6)	165(6)	8290(6)	168(5)	
F(43)	5364(5)	-872(6)	7498(4)	157(4)	
F(44)	6117(5)	-1062(5)	8206(5)	134(3)	
F(45)	6165(7)	-59(6)	8944(4)	179(5)	
F(46)	5155(5)	-780(6)	8416(6)	160(4)	
P(50)	3523(1)	5469(1)	3526(1)	46(1)	
F(51)	3083(4)	6007(3)	3849(3)	91(2)	
F(52)	4111(9)	5821(10)	4172(7)	143(7)	0.60
F(53)	3783(9)	6046(8)	3332(10)	133(6)	0.60
F(54)	2900(10)	5112(8)	2889(8)	158(9)	0.60
F(55)	3203(11)	4909(8)	3700(13)	145(8)	0.60
F(56)	3955(3)	4927(4)	3203(3)	82(2)	
F(52')	3726(11)	5439(12)	4158(9)	75(5)	0.40
F(53')	4213(12)	5990(11)	3721(12)	102(6)	0.40
F(54')	3337(10)	5472(11)	2870(8)	70(4)	0.40
F(55')	2875(10)	4906(10)	3293(9)	71(4)	0.40
P(60)	2438(2)	3178(2)	4221(2)	93(1)	
F(61)	2005(6)	3488(5)	3817(5)	147(4)	
F(62)	2164(21)	2494(16)	3672(13)	141(12)	0.50
F(63)	1911(16)	3145(23)	4581(17)	132(10)	0.50
F(64)	2911(17)	3950(10)	4861(9)	128(8)	0.50
F(65)	3171(12)	3261(24)	3973(14)	146(10)	0.50
F(66)	2894(5)	2871(5)	4620(4)	117(3)	
F(62')	1684(11)	2574(15)	4037(17)	128(7)	0.50
F(63')	2137(21)	3662(16)	4752(12)	134(11)	0.50
F(64')	2987(12)	3735(14)	4309(19)	152(10)	0.50
F(65')	2525(22)	2612(17)	3581(15)	122(13)	0.50
O(90)	1570(4)	3568(3)	6133(3)	60(2)	
C(91)	2178(5)	3832(5)	6196(4)	51(2)	
C(92)	2401(6)	4523(5)	6260(5)	65(3)	
C(93)	2707(6)	3404(6)	6186(5)	76(3)	
O(94)	95(5)	3332(5)	8387(4)	100(3)	
C(95)	135(6)	3907(6)	8817(5)	72(3)	
C(96)	-177(8)	3992(7)	9331(7)	101(4)	
C(97)	529(9)	4551(8)	8867(8)	127(5)	
O(98)	5515(8)	4206(8)	3276(8)	180(5)	
C(99)	5396(8)	4647(8)	3750(7)	95(4)	
C(100)	5003(9)	4439(9)	4082(8)	127(5)	
C(101)	5664(11)	5389(10)	3951(10)	157(7)	
O(102)	7083(9)	3262(9)	-974(9)	197(6)	
C(103)	7387(9)	3288(8)	-474(8)	104(4)	
C(104)	6982(10)	2988(10)	-165(9)	140(6)	
C(105)	8120(11)	3630(11)	-195(10)	161(7)	
O(106)	-1789(8)	-1146(8)	4718(7)	173(5)	

C(107)	-1963(7)	-1076(7)	5202(6)	87(3)
C(108)	-2288(8)	-491(7)	5523(7)	105(4)
C(109)	-1878(10)	-1565(10)	5423(9)	144(6)
O(110)	7785(9)	2182(9)	968(8)	195(6)
C(111)	8348(11)	2397(10)	1400(9)	131(6)
C(112)	8675(10)	1938(10)	1553(9)	147(7)
C(113)	8723(15)	3165(15)	1753(14)	234(13)
O(114)	4425(5)	2502(5)	3398(5)	116(3)
C(115)	4214(10)	2201(10)	3724(9)	195(9)
C(116)	3604(11)	1624(11)	3423(12)	230(12)
C(117)	4606(15)	2484(16)	4396(9)	323(18)
O(118)	-1893(9)	1954(10)	8480(8)	199(6)
C(119)	-2089(12)	1345(12)	8440(11)	153(7)
C(120)	-1781(17)	812(17)	7984(16)	272(16)
C(121)	-2504(18)	1266(17)	8904(16)	287(17)

Table 3. Bond lengths [Å] and angles [°] for 1.

O(1)-C(32)	1.366(11)	O(1)-C(2)	1.452(11)
C(2)-C(3)	1.453(14)	C(3)-O(4)	1.435(11)
O(4)-C(5)	1.393(12)	C(5)-C(6)	1.483(13)
C(6)-O(7)	1.429(9)	O(7)-C(8)	1.417(10)
C(8)-C(9)	1.499(12)	C(9)-O(10)	1.439(10)
O(10)-C(11)	1.378(9)	C(11)-C(12)	1.375(11)
C(11)-C(16)	1.394(12)	C(12)-C(13)	1.403(12)
C(13)-C(14)	1.348(14)	C(14)-C(15)	1.381(13)
C(15)-C(16)	1.400(11)	C(16)-O(17)	1.366(9)
O(17)-C(18)	1.427(11)	C(18)-C(19)	1.496(13)
C(19)-O(20)	1.418(11)	O(20)-C(21)	1.408(11)
C(21)-C(22)	1.490(12)	C(22)-O(23)	1.435(11)
O(23)-C(24)	1.435(10)	C(24)-C(25)	1.510(13)
C(25)-O(26)	1.413(12)	O(26)-C(27)	1.388(11)
C(27)-C(28)	1.386(14)	C(27)-C(32)	1.397(14)
C(28)-C(29)	1.39(2)	C(29)-C(30)	1.35(2)
C(30)-C(31)	1.38(2)	C(31)-C(32)	1.385(14)
C(33)-C(46)	1.408(12)	C(33)-C(34)	1.437(12)
C(33)-C(38)	1.437(11)	C(34)-C(35)	1.358(13)
C(35)-C(36)	1.389(14)	C(36)-C(37)	1.331(14)
C(37)-C(38)	1.423(13)	C(38)-C(39)	1.369(13)
C(39)-C(40)	1.382(13)	C(40)-C(41)	1.420(13)
C(40)-C(45)	1.441(11)	C(41)-C(42)	1.360(14)
C(42)-C(43)	1.431(13)	C(43)-C(44)	1.338(12)
C(44)-C(45)	1.421(12)	C(45)-C(46)	1.415(12)
C(46)-C(47)	1.508(10)	C(47)-N(48)	1.497(9)
N(48)-C(49)	1.492(10)	C(49)-C(50)	1.512(10)
C(50)-C(55)	1.369(11)	C(50)-C(51)	1.391(11)
C(51)-C(52)	1.392(11)	C(52)-C(53)	1.380(11)
C(53)-C(54)	1.384(12)	C(53)-C(56)	1.493(11)
C(54)-C(55)	1.392(11)	C(56)-N(57)	1.496(11)
N(57)-C(58)	1.326(11)	N(57)-C(62)	1.344(10)
C(58)-C(59)	1.345(12)	C(59)-C(60)	1.398(11)
C(60)-C(61)	1.382(11)	C(60)-C(63)	1.498(11)
C(61)-C(62)	1.403(12)	C(63)-C(68)	1.385(11)
C(63)-C(64)	1.395(11)	C(64)-C(65)	1.369(12)
C(65)-N(66)	1.334(10)	N(66)-C(67)	1.339(10)
N(66)-C(69)	1.484(11)	C(67)-C(68)	1.379(12)
C(69)-C(70)	1.520(10)	C(70)-C(71)	1.384(11)
C(70)-C(75)	1.386(11)	C(71)-C(72)	1.400(10)
C(72)-C(73)	1.392(11)	C(72)-C(76)	1.524(12)
C(73)-C(74)	1.395(11)	C(74)-C(75)	1.378(11)
C(74)-C(80)	1.549(11)	C(76)-C(77)	1.46(2)
C(76)-C(78)	1.498(14)	C(76)-C(79)	1.56(2)
C(80)-C(81A)	1.40(3)	C(80)-C(83)	1.45(2)
C(80)-C(81)	1.52(2)	C(80)-C(82A)	1.54(3)
C(80)-C(82)	1.56(2)	C(80)-C(83A)	1.57(4)
O(1')-C(32')	1.369(10)	O(1')-C(2')	1.432(11)
C(2')-C(3')	1.453(13)	C(3')-O(4')	1.429(10)
O(4')-C(5')	1.401(13)	C(5')-C(6')	1.49(2)
C(6')-O(7')	1.423(11)	O(7')-C(8')	1.425(11)
C(8')-C(9')	1.492(13)	C(9')-O(10')	1.445(11)
O(10')-C(11')	1.361(10)	C(11')-C(12')	1.389(12)
C(11')-C(16')	1.402(12)	C(12')-C(13')	1.387(13)
C(13')-C(14')	1.38(2)	C(14')-C(15')	1.375(14)
C(15')-C(16')	1.396(12)	C(16')-O(17')	1.358(10)
O(17')-C(18')	1.435(10)	C(18')-C(19')	1.463(14)
C(19')-O(20')	1.426(11)	O(20')-C(21')	1.374(11)
C(21')-C(22')	1.39(2)	C(22')-O(23')	1.298(14)

O(23')-C(24')	1.421(11)	C(24')-C(25')	1.49(2)
C(25')-O(26')	1.455(12)	O(26')-C(27')	1.362(11)
C(27')-C(32')	1.385(13)	C(27')-C(28')	1.404(13)
C(28')-C(29')	1.36(2)	C(29')-C(30')	1.34(2)
C(30')-C(31')	1.40(2)	C(31')-C(32')	1.403(13)
C(33')-C(46')	1.422(12)	C(33')-C(34')	1.431(14)
C(33')-C(38')	1.434(13)	C(34')-C(35')	1.36(2)
C(35')-C(36')	1.37(2)	C(36')-C(37')	1.35(2)
C(37')-C(38')	1.436(14)	C(38')-C(39')	1.368(14)
C(39')-C(40')	1.391(13)	C(40')-C(41')	1.415(14)
C(40')-C(45')	1.449(12)	C(41')-C(42')	1.348(14)
C(42')-C(43')	1.41(2)	C(43')-C(44')	1.349(13)
C(44')-C(45')	1.416(12)	C(45')-C(46')	1.414(12)
C(46')-C(47')	1.486(11)	C(47')-N(48')	1.512(10)
N(48')-C(49')	1.487(10)	C(49')-C(50')	1.503(10)
C(50')-C(51')	1.370(11)	C(50')-C(55')	1.371(12)
C(51')-C(52')	1.399(12)	C(52')-C(53')	1.349(12)
C(53')-C(54')	1.386(12)	C(53')-C(56')	1.509(12)
C(54')-C(55')	1.374(13)	C(56')-N(57')	1.485(12)
N(57')-C(58')	1.330(12)	N(57')-C(62')	1.358(11)
C(58')-C(59')	1.369(14)	C(59')-C(60')	1.401(12)
C(60')-C(61')	1.387(12)	C(60')-C(63')	1.460(13)
C(61')-C(62')	1.354(14)	C(63')-C(68')	1.394(12)
C(63')-C(64')	1.401(12)	C(64')-C(65')	1.341(14)
C(65')-N(66')	1.361(12)	N(66')-C(67')	1.345(11)
N(66')-C(69')	1.497(12)	C(67')-C(68')	1.348(13)
C(69')-C(70')	1.514(13)	C(70')-C(75')	1.381(13)
C(70')-C(71')	1.407(13)	C(71')-C(72')	1.398(13)
C(72')-C(73')	1.388(14)	C(72')-C(76')	1.54(2)
C(73')-C(74')	1.397(14)	C(74')-C(75')	1.385(13)
C(74')-C(80')	1.548(13)	C(76')-C(78')	1.41(2)
C(76')-C(78B)	1.48(3)	C(76')-C(79B)	1.52(4)
C(76')-C(77')	1.54(2)	C(76')-C(79')	1.68(2)
C(76')-C(77B)	1.74(3)	C(80')-C(83')	1.53(2)
C(80')-C(82')	1.54(2)	C(80')-C(81')	1.54(2)

C(32)-O(1)-C(2)	116.1(7)	O(1)-C(2)-C(3)	107.7(7)
O(4)-C(3)-C(2)	112.4(7)	C(5)-O(4)-C(3)	114.7(7)
O(4)-C(5)-C(6)	110.6(8)	O(7)-C(6)-C(5)	110.3(7)
C(8)-O(7)-C(6)	110.3(6)	O(7)-C(8)-C(9)	111.6(7)
O(10)-C(9)-C(8)	108.3(7)	C(11)-O(10)-C(9)	115.6(6)
C(12)-C(11)-O(10)	125.2(8)	C(12)-C(11)-C(16)	120.2(7)
O(10)-C(11)-C(16)	114.6(7)	C(11)-C(12)-C(13)	118.7(9)
C(14)-C(13)-C(12)	121.3(9)	C(13)-C(14)-C(15)	120.7(9)
C(14)-C(15)-C(16)	119.2(9)	O(17)-C(16)-C(11)	116.2(7)
O(17)-C(16)-C(15)	123.9(8)	C(11)-C(16)-C(15)	119.8(8)
C(16)-O(17)-C(18)	118.4(6)	O(17)-C(18)-C(19)	107.0(7)
O(20)-C(19)-C(18)	112.9(7)	C(21)-O(20)-C(19)	113.7(7)
O(20)-C(21)-C(22)	110.1(8)	O(23)-C(22)-C(21)	109.7(7)
C(24)-O(23)-C(22)	111.6(6)	O(23)-C(24)-C(25)	109.2(7)
O(26)-C(25)-C(24)	108.2(7)	C(27)-O(26)-C(25)	116.0(7)
C(28)-C(27)-O(26)	125.3(10)	C(28)-C(27)-C(32)	120.0(9)
O(26)-C(27)-C(32)	114.6(8)	C(27)-C(28)-C(29)	119.4(12)
C(30)-C(29)-C(28)	120.1(12)	C(29)-C(30)-C(31)	121.7(11)
C(30)-C(31)-C(32)	119.5(12)	O(1)-C(32)-C(31)	125.7(11)
O(1)-C(32)-C(27)	114.9(8)	C(31)-C(32)-C(27)	119.3(10)
C(46)-C(33)-C(34)	124.0(7)	C(46)-C(33)-C(38)	118.9(8)
C(34)-C(33)-C(38)	117.2(7)	C(35)-C(34)-C(33)	120.0(8)
C(34)-C(35)-C(36)	122.2(10)	C(37)-C(36)-C(35)	120.3(9)
C(36)-C(37)-C(38)	121.4(9)	C(39)-C(38)-C(37)	120.8(8)
C(39)-C(38)-C(33)	120.1(8)	C(37)-C(38)-C(33)	119.0(8)
C(38)-C(39)-C(40)	121.9(8)	C(39)-C(40)-C(41)	122.2(8)
C(39)-C(40)-C(45)	119.8(8)	C(41)-C(40)-C(45)	117.9(8)

C(42)-C(41)-C(40)	122.2(9)	C(41)-C(42)-C(43)	119.2(9)
C(44)-C(43)-C(42)	120.4(9)	C(43)-C(44)-C(45)	122.3(8)
C(46)-C(45)-C(44)	123.6(7)	C(46)-C(45)-C(40)	118.5(8)
C(44)-C(45)-C(40)	117.9(8)	C(33)-C(46)-C(45)	120.7(7)
C(33)-C(46)-C(47)	121.1(7)	C(45)-C(46)-C(47)	118.3(7)
N(48)-C(47)-C(46)	113.5(6)	C(49)-N(48)-C(47)	110.6(6)
N(48)-C(49)-C(50)	113.9(6)	C(55)-C(50)-C(51)	118.9(7)
C(55)-C(50)-C(49)	117.8(7)	C(51)-C(50)-C(49)	123.3(7)
C(50)-C(51)-C(52)	119.8(7)	C(53)-C(52)-C(51)	121.1(8)
C(52)-C(53)-C(54)	118.9(7)	C(52)-C(53)-C(56)	122.2(7)
C(54)-C(53)-C(56)	118.9(7)	C(53)-C(54)-C(55)	119.9(7)
C(50)-C(55)-C(54)	121.4(8)	C(53)-C(56)-N(57)	111.2(6)
C(58)-N(57)-C(62)	120.8(7)	C(58)-N(57)-C(56)	119.9(7)
C(62)-N(57)-C(56)	119.4(7)	N(57)-C(58)-C(59)	122.4(8)
C(58)-C(59)-C(60)	119.7(8)	C(61)-C(60)-C(59)	118.0(8)
C(61)-C(60)-C(63)	121.4(7)	C(59)-C(60)-C(63)	120.5(7)
C(60)-C(61)-C(62)	119.6(8)	N(57)-C(62)-C(61)	119.5(8)
C(68)-C(63)-C(64)	119.1(7)	C(68)-C(63)-C(60)	121.8(7)
C(64)-C(63)-C(60)	119.2(7)	C(65)-C(64)-C(63)	118.5(7)
N(66)-C(65)-C(64)	121.6(8)	C(65)-N(66)-C(67)	120.9(7)
C(65)-N(66)-C(69)	120.1(7)	C(67)-N(66)-C(69)	118.9(7)
N(66)-C(67)-C(68)	120.4(7)	C(67)-C(68)-C(63)	119.4(7)
N(66)-C(69)-C(70)	111.3(6)	C(71)-C(70)-C(75)	119.8(7)
C(71)-C(70)-C(69)	117.9(7)	C(75)-C(70)-C(69)	122.3(7)
C(70)-C(71)-C(72)	121.1(7)	C(73)-C(72)-C(71)	116.9(7)
C(73)-C(72)-C(76)	121.4(7)	C(71)-C(72)-C(76)	121.7(7)
C(72)-C(73)-C(74)	123.3(7)	C(75)-C(74)-C(73)	117.4(7)
C(75)-C(74)-C(80)	122.6(7)	C(73)-C(74)-C(80)	120.0(7)
C(74)-C(75)-C(70)	121.5(8)	C(77)-C(76)-C(78)	114.0(10)
C(77)-C(76)-C(72)	109.5(8)	C(78)-C(76)-C(72)	113.1(8)
C(77)-C(76)-C(79)	105.2(11)	C(78)-C(76)-C(79)	105.7(10)
C(72)-C(76)-C(79)	108.8(8)	C(83)-C(80)-C(81)	111.9(12)
C(81A)-C(80)-C(82A)	113(2)	C(81A)-C(80)-C(74)	111(2)
C(83)-C(80)-C(74)	111.7(8)	C(81)-C(80)-C(74)	109.6(8)
C(82A)-C(80)-C(74)	101(2)	C(83)-C(80)-C(82)	107.3(12)
C(81)-C(80)-C(82)	104.8(11)	C(74)-C(80)-C(82)	111.3(8)
C(81A)-C(80)-C(83A)	110(2)	C(82A)-C(80)-C(83A)	111(2)
C(74)-C(80)-C(83A)	112(2)	C(32')-O(1')-C(2')	117.4(7)
O(1')-C(2')-C(3')	108.5(8)	O(4')-C(3')-C(2')	113.8(8)
C(5')-O(4')-C(3')	114.1(7)	O(4')-C(5')-C(6')	111.8(9)
O(7')-C(6')-C(5')	110.6(9)	C(6')-O(7')-C(8')	111.6(7)
O(7')-C(8')-C(9')	109.0(8)	O(10')-C(9')-C(8')	108.7(8)
C(11')-O(10')-C(9')	117.0(7)	O(10')-C(11')-C(12')	125.2(8)
O(10')-C(11')-C(16')	114.9(7)	C(12')-C(11')-C(16')	119.9(8)
C(13')-C(12')-C(11')	120.2(9)	C(14')-C(13')-C(12')	120.6(9)
C(15')-C(14')-C(13')	119.2(9)	C(14')-C(15')-C(16')	121.8(9)
O(17')-C(16')-C(15')	126.0(8)	O(17')-C(16')-C(11')	115.5(7)
C(15')-C(16')-C(11')	118.4(8)	C(16')-O(17')-C(18')	117.2(7)
O(17')-C(18')-C(19')	108.0(8)	O(20')-C(19')-C(18')	111.2(9)
C(21')-O(20')-C(19')	115.3(7)	O(20')-C(21')-C(22')	116.9(9)
O(23')-C(22')-C(21')	121.5(11)	C(22')-O(23')-C(24')	115.3(8)
O(23')-C(24')-C(25')	108.4(9)	O(26')-C(25')-C(24')	106.4(9)
C(27')-O(26')-C(25')	116.3(8)	O(26')-C(27')-C(32')	115.8(8)
O(26')-C(27')-C(28')	125.3(10)	C(32')-C(27')-C(28')	118.9(9)
C(29')-C(28')-C(27')	121.4(11)	C(30')-C(29')-C(28')	119.5(11)
C(29')-C(30')-C(31')	122.1(11)	C(30')-C(31')-C(32')	118.5(10)
O(1')-C(32')-C(27')	116.2(8)	O(1')-C(32')-C(31')	124.2(9)
C(27')-C(32')-C(31')	119.5(9)	C(46')-C(33')-C(34')	122.4(8)
C(46')-C(33')-C(38')	120.5(8)	C(34')-C(33')-C(38')	117.1(8)
C(35')-C(34')-C(33')	120.5(11)	C(34')-C(35')-C(36')	122.6(12)
C(37')-C(36')-C(35')	119.9(11)	C(36')-C(37')-C(38')	121.2(11)
C(39')-C(38')-C(33')	118.9(8)	C(39')-C(38')-C(37')	122.5(9)
C(33')-C(38')-C(37')	118.6(10)	C(38')-C(39')-C(40')	122.7(8)

C(39')-C(40')-C(41')	121.7(9)	C(39')-C(40')-C(45')	119.5(9)
C(41')-C(40')-C(45')	118.8(9)	C(42')-C(41')-C(40')	120.6(9)
C(41')-C(42')-C(43')	121.0(10)	C(44')-C(43')-C(42')	120.4(9)
C(43')-C(44')-C(45')	121.5(9)	C(46')-C(45')-C(44')	123.5(8)
C(46')-C(45')-C(40')	118.9(8)	C(44')-C(45')-C(40')	117.5(9)
C(45')-C(46')-C(33')	119.4(8)	C(45')-C(46')-C(47')	120.2(7)
C(33')-C(46')-C(47')	120.4(8)	C(46')-C(47')-N(48')	112.8(6)
C(49')-N(48')-C(47')	111.1(6)	N(48')-C(49')-C(50')	112.7(6)
C(51')-C(50')-C(55')	117.5(8)	C(51')-C(50')-C(49')	122.2(7)
C(55')-C(50')-C(49')	120.3(7)	C(50')-C(51')-C(52')	120.0(8)
C(53')-C(52')-C(51')	121.5(8)	C(52')-C(53')-C(54')	119.1(8)
C(52')-C(53')-C(56')	121.8(8)	C(54')-C(53')-C(56')	119.1(8)
C(55')-C(54')-C(53')	118.7(8)	C(50')-C(55')-C(54')	123.1(9)
N(57')-C(56')-C(53')	110.0(7)	C(58')-N(57')-C(62')	119.3(9)
C(58')-N(57')-C(56')	120.6(8)	C(62')-N(57')-C(56')	120.1(8)
N(57')-C(58')-C(59')	122.7(8)	C(58')-C(59')-C(60')	119.2(9)
C(61')-C(60')-C(59')	116.6(9)	C(61')-C(60')-C(63')	122.5(8)
C(59')-C(60')-C(63')	120.8(8)	C(62')-C(61')-C(60')	122.0(9)
C(61')-C(62')-N(57')	120.2(9)	C(68')-C(63')-C(64')	116.3(9)
C(68')-C(63')-C(60')	122.0(8)	C(64')-C(63')-C(60')	121.7(8)
C(65')-C(64')-C(63')	120.4(8)	C(64')-C(65')-N(66')	122.6(9)
C(67')-N(66')-C(65')	117.5(9)	C(67')-N(66')-C(69')	121.2(8)
C(65')-N(66')-C(69')	121.3(8)	N(66')-C(67')-C(68')	122.5(8)
C(67')-C(68')-C(63')	120.7(8)	N(66')-C(69')-C(70')	109.7(7)
C(75')-C(70')-C(71')	119.7(9)	C(75')-C(70')-C(69')	119.8(9)
C(71')-C(70')-C(69')	120.4(8)	C(72')-C(71')-C(70')	121.0(8)
C(73')-C(72')-C(71')	116.7(9)	C(73')-C(72')-C(76')	121.9(9)
C(71')-C(72')-C(76')	121.4(9)	C(72')-C(73')-C(74')	123.7(9)
C(75')-C(74')-C(73')	117.6(9)	C(75')-C(74')-C(80')	123.0(9)
C(73')-C(74')-C(80')	119.2(9)	C(70')-C(75')-C(74')	121.1(9)
C(78B)-C(76')-C(79B)	116(2)	C(78')-C(76')-C(77')	117(2)
C(78')-C(76')-C(72')	116.9(12)	C(78B)-C(76')-C(72')	114(2)
C(79B)-C(76')-C(72')	115(2)	C(77')-C(76')-C(72')	108.9(10)
C(78')-C(76')-C(79')	105(2)	C(77')-C(76')-C(79')	102.8(13)
C(72')-C(76')-C(79')	104.3(11)	C(78B)-C(76')-C(77B)	101(2)
C(79B)-C(76')-C(77B)	107(2)	C(72')-C(76')-C(77B)	103.0(12)
C(83')-C(80')-C(82')	108.0(9)	C(83')-C(80')-C(81')	109.3(10)
C(82')-C(80')-C(81')	109.4(11)	C(83')-C(80')-C(74')	110.9(10)
C(82')-C(80')-C(74')	110.7(9)	C(81')-C(80')-C(74')	108.6(8)

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 1.

The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2U_{11} + ... + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
O(1)	60(4)	48(3)	44(3)	18(3)	8(3)	20(3)
C(2)	60(7)	55(6)	46(5)	6(4)	9(4)	26(5)
C(3)	62(7)	73(7)	36(5)	3(5)	12(4)	26(5)
O(4)	54(5)	62(4)	47(3)	16(3)	23(3)	20(3)
C(5)	55(8)	76(7)	39(5)	15(4)	24(4)	33(5)
C(6)	59(7)	79(7)	44(5)	30(5)	32(4)	20(5)
O(7)	52(4)	49(3)	37(3)	25(3)	21(3)	16(3)
C(8)	52(6)	54(6)	62(6)	35(5)	30(5)	18(4)
C(9)	30(6)	51(5)	59(5)	22(4)	19(4)	10(4)
O(10)	31(4)	45(3)	50(3)	24(3)	15(2)	8(2)
C(11)	41(6)	26(4)	43(5)	15(3)	12(4)	12(3)
C(12)	44(6)	35(4)	46(5)	14(4)	7(4)	10(4)
C(13)	57(8)	57(6)	41(5)	11(4)	1(4)	14(5)
C(14)	67(8)	45(5)	45(5)	17(4)	16(5)	12(5)
C(15)	47(6)	33(4)	62(6)	18(4)	29(5)	12(4)
C(16)	33(6)	29(4)	50(5)	17(4)	11(4)	7(3)
O(17)	36(4)	49(3)	53(3)	22(3)	17(3)	15(3)
C(18)	38(6)	45(5)	73(6)	29(4)	22(4)	16(4)
C(19)	44(6)	71(7)	83(7)	52(6)	18(5)	27(5)
O(20)	32(4)	58(4)	62(4)	23(3)	9(3)	14(3)
C(21)	35(7)	59(6)	76(6)	28(5)	21(5)	17(5)
C(22)	37(6)	57(6)	55(5)	21(4)	5(4)	3(4)
O(23)	41(4)	49(3)	43(3)	17(3)	7(3)	11(3)
C(24)	31(5)	63(6)	40(5)	10(4)	9(4)	0(4)
C(25)	64(8)	49(5)	44(5)	16(4)	4(5)	0(5)
O(26)	46(4)	57(4)	50(3)	24(3)	13(3)	10(3)
C(27)	59(7)	27(4)	54(5)	14(4)	-4(5)	1(4)
C(28)	75(8)	47(6)	61(6)	15(5)	8(5)	1(5)
C(29)	93(10)	48(6)	87(8)	34(6)	2(7)	4(6)
C(30)	93(11)	38(6)	83(8)	14(5)	-10(7)	12(6)
C(31)	76(8)	51(6)	72(7)	20(5)	-1(6)	16(6)
C(32)	58(7)	41(5)	44(5)	9(4)	-4(4)	8(4)
C(33)	45(6)	35(4)	29(4)	15(3)	-2(3)	11(4)
C(34)	46(6)	58(6)	45(5)	27(4)	9(4)	7(5)
C(35)	45(7)	71(7)	59(6)	27(5)	15(4)	20(5)
C(36)	65(8)	64(6)	61(6)	34(5)	2(5)	34(5)
C(37)	59(7)	51(6)	60(6)	32(5)	7(5)	18(5)
C(38)	38(6)	38(5)	40(4)	14(4)	-1(4)	9(4)
C(39)	56(7)	52(5)	56(5)	35(4)	6(5)	11(5)
C(40)	46(6)	42(5)	30(4)	17(3)	1(4)	-1(4)
C(41)	67(7)	58(6)	43(5)	26(4)	13(5)	6(5)
C(42)	60(7)	66(6)	43(5)	20(5)	22(4)	11(5)
C(43)	55(7)	48(5)	41(5)	10(4)	16(4)	16(4)
C(44)	55(6)	44(5)	27(4)	14(3)	4(4)	8(4)
C(45)	50(6)	34(4)	27(4)	7(3)	-2(4)	5(4)
C(46)	44(6)	27(4)	23(4)	8(3)	-3(3)	-5(4)
C(47)	42(5)	30(4)	28(4)	12(3)	0(3)	0(3)
N(48)	29(4)	39(4)	30(3)	16(3)	6(3)	6(3)
C(49)	32(5)	46(5)	38(4)	27(4)	7(3)	11(4)
C(50)	30(5)	46(5)	40(4)	25(4)	11(3)	17(4)
C(51)	41(5)	44(5)	42(4)	24(4)	11(4)	23(4)
C(52)	38(5)	49(5)	40(4)	19(4)	9(4)	18(4)

C(53)	28(5)	51(5)	30(4)	17(4)	15(3)	19(4)
C(54)	45(6)	59(6)	53(5)	39(5)	11(4)	28(4)
C(55)	49(6)	45(5)	45(5)	29(4)	8(4)	11(4)
C(56)	41(6)	66(6)	44(5)	30(4)	21(4)	31(4)
N(57)	30(4)	54(4)	37(3)	23(3)	11(3)	20(3)
C(58)	42(6)	47(5)	50(5)	26(4)	17(4)	17(4)
C(59)	36(6)	40(5)	53(5)	27(4)	18(4)	12(4)
C(60)	33(5)	39(5)	35(4)	16(3)	7(3)	9(4)
C(61)	36(6)	42(5)	57(5)	23(4)	15(4)	17(4)
C(62)	38(6)	55(5)	48(5)	30(4)	20(4)	19(4)
C(63)	23(5)	35(4)	36(4)	11(3)	6(3)	13(3)
C(64)	20(5)	50(5)	51(5)	31(4)	10(4)	10(4)
C(65)	30(6)	50(5)	50(5)	26(4)	8(4)	8(4)
N(66)	33(5)	35(4)	39(3)	11(3)	8(3)	9(3)
C(67)	30(5)	40(4)	39(4)	17(3)	6(4)	12(4)
C(68)	41(6)	38(4)	35(4)	15(3)	9(4)	14(4)
C(69)	17(5)	48(5)	44(4)	12(4)	9(3)	9(3)
C(70)	28(5)	33(4)	37(4)	12(3)	9(3)	9(3)
C(71)	31(5)	30(4)	41(4)	14(3)	8(3)	12(3)
C(72)	23(5)	37(4)	43(4)	21(3)	7(3)	7(3)
C(73)	40(5)	32(4)	39(4)	14(3)	8(4)	5(4)
C(74)	35(5)	36(4)	41(4)	16(3)	17(4)	12(4)
C(75)	29(5)	41(5)	51(5)	26(4)	19(4)	15(4)
C(76)	34(6)	51(5)	75(6)	32(5)	2(5)	10(4)
C(77)	45(8)	166(14)	166(14)	119(13)	28(8)	43(8)
C(78)	61(8)	83(8)	154(12)	84(9)	-5(7)	18(6)
C(79)	106(11)	102(10)	81(8)	24(7)	-37(8)	36(8)
C(80)	45(6)	38(5)	72(6)	34(4)	21(4)	19(4)
C(81)	134(16)	39(8)	63(9)	13(7)	37(10)	37(9)
C(82)	47(10)	47(8)	139(16)	40(9)	4(9)	23(7)
C(83)	123(16)	47(9)	131(15)	63(10)	72(13)	45(10)
O(1′)	39(4)	46(3)	48(3)	16(3)	13(3)	17(3)
C(2′)	50(7)	47(5)	67(6)	19(5)	15(5)	13(4)
C(3′)	66(7)	48(5)	56(5)	12(4)	31(5)	20(5)
O(4′)	49(5)	46(4)	71(4)	18(3)	28(3)	16(3)
C(5′)	72(9)	76(7)	67(7)	12(6)	38(6)	22(6)
C(6′)	64(8)	88(8)	69(7)	20(6)	36(6)	-3(6)
O(7′)	40(4)	60(4)	61(4)	19(3)	27(3)	16(3)
C(8′)	47(6)	55(6)	68(6)	20(5)	27(5)	9(5)
C(9′)	29(6)	61(6)	71(6)	23(5)	26(4)	10(4)
O(10′)	21(4)	58(4)	61(4)	23(3)	14(3)	15(3)
C(11′)	40(6)	37(4)	48(5)	14(4)	13(4)	5(4)
C(12′)	31(6)	50(5)	68(6)	23(5)	4(4)	10(4)
C(13′)	47(7)	67(6)	59(6)	28(5)	4(5)	17(5)
C(14′)	80(9)	68(7)	51(6)	23(5)	17(5)	32(6)
C(15′)	55(7)	48(5)	60(6)	17(4)	27(5)	24(4)
C(16′)	37(6)	28(4)	59(5)	17(4)	21(4)	18(4)
O(17′)	30(4)	49(3)	56(3)	19(3)	16(3)	25(3)
C(18′)	44(7)	62(6)	78(7)	29(5)	29(5)	39(5)
C(19′)	40(6)	48(6)	100(8)	20(5)	17(5)	26(4)
O(20′)	26(4)	71(5)	105(6)	7(4)	-5(4)	27(3)
C(21′)	35(7)	61(6)	86(7)	27(5)	16(5)	22(5)
C(22′)	51(9)	87(10)	201(17)	24(10)	-40(9)	26(7)
O(23′)	34(4)	60(4)	77(5)	10(3)	-2(3)	14(3)
C(24′)	33(6)	59(6)	92(8)	15(6)	-7(5)	14(5)
C(25′)	23(7)	89(8)	69(7)	9(6)	5(4)	10(5)
O(26′)	43(5)	46(4)	59(4)	23(3)	11(3)	9(3)
C(27′)	52(7)	37(5)	47(5)	7(4)	10(4)	-8(4)
C(28′)	55(7)	51(6)	49(5)	12(4)	6(4)	-15(5)
C(29′)	112(11)	54(7)	58(6)	24(5)	15(7)	-3(7)
C(30′)	108(10)	41(6)	56(6)	20(5)	8(6)	1(6)
C(31′)	61(7)	46(5)	55(5)	19(4)	2(5)	10(5)
C(32′)	63(7)	38(5)	33(4)	12(4)	11(4)	9(4)

C(33′)	43(6)	53(5)	25(4)	6(4)	2(4)	12(4)
C(34′)	68(8)	63(6)	41(5)	12(4)	2(5)	26(5)
C(35′)	63(8)	103(9)	45(6)	19(6)	16(5)	31(7)
C(36′)	62(9)	98(9)	49(6)	18(6)	6(5)	40(7)
C(37′)	74(8)	65(6)	50(6)	20(5)	-4(5)	31(6)
C(38′)	53(7)	38(5)	37(4)	6(4)	-7(4)	23(4)
C(39′)	60(7)	40(5)	51(5)	20(4)	-2(5)	16(5)
C(40′)	60(7)	33(4)	31(4)	11(3)	-4(4)	-5(4)
C(41′)	61(8)	57(6)	52(5)	28(5)	6(5)	-4(5)
C(42′)	50(7)	74(7)	44(5)	15(5)	14(4)	-2(5)
C(43′)	35(7)	72(7)	53(5)	13(5)	5(4)	14(5)
C(44′)	43(6)	40(5)	44(5)	14(4)	2(4)	14(4)
C(45′)	49(6)	37(4)	31(4)	10(3)	-1(4)	7(4)
C(46′)	37(6)	36(4)	32(4)	12(3)	0(3)	7(4)
C(47′)	42(6)	40(5)	42(4)	18(4)	0(4)	3(4)
N(48′)	37(5)	42(4)	41(4)	17(3)	3(3)	8(3)
C(49′)	23(5)	43(5)	45(4)	22(4)	7(3)	8(3)
C(50′)	29(5)	45(5)	45(4)	24(4)	11(3)	14(4)
C(51′)	54(6)	42(5)	56(5)	22(4)	5(4)	29(4)
C(52′)	60(7)	47(5)	44(5)	13(4)	6(4)	22(4)
C(53′)	45(6)	52(5)	50(5)	30(4)	11(4)	19(4)
C(54′)	79(8)	46(6)	69(6)	38(5)	1(5)	16(5)
C(55′)	76(7)	41(5)	63(6)	27(5)	0(5)	8(5)
C(56′)	56(7)	75(7)	50(5)	33(5)	14(4)	29(5)
N(57′)	47(5)	50(4)	44(4)	27(3)	0(3)	5(4)
C(58′)	56(7)	48(6)	74(6)	36(5)	5(5)	18(5)
C(59′)	49(7)	49(5)	69(6)	41(5)	9(5)	13(5)
C(60′)	37(6)	47(5)	43(4)	23(4)	1(4)	8(4)
C(61′)	58(7)	48(5)	56(5)	36(4)	12(4)	10(5)
C(62′)	51(7)	61(6)	64(6)	42(5)	12(5)	17(5)
C(63′)	61(7)	37(5)	33(4)	18(4)	1(4)	4(4)
C(64′)	64(8)	62(6)	61(6)	40(5)	16(5)	31(5)
C(65′)	92(9)	66(6)	48(5)	42(5)	15(5)	24(6)
N(66′)	58(6)	37(4)	39(4)	10(3)	7(3)	9(3)
C(67′)	64(7)	37(5)	36(4)	18(4)	6(4)	15(4)
C(68′)	50(7)	43(5)	44(5)	26(4)	10(4)	17(4)
C(69′)	62(7)	47(5)	63(6)	24(4)	27(5)	19(5)
C(70′)	58(7)	42(5)	64(6)	20(4)	27(5)	14(4)
C(71′)	52(6)	45(5)	59(5)	29(4)	19(4)	9(4)
C(72′)	50(7)	60(6)	63(6)	26(5)	16(5)	10(5)
C(73′)	51(7)	54(6)	75(7)	28(5)	27(5)	4(5)
C(74′)	64(7)	52(6)	74(6)	38(5)	36(5)	22(5)
C(75′)	62(7)	52(6)	55(5)	27(5)	30(5)	22(5)
C(76′)	79(9)	100(9)	71(7)	48(7)	5(6)	-4(7)
C(77′)	47(13)	124(17)	58(11)	42(11)	7(9)	7(11)
C(78′)	124(20)	72(13)	71(12)	45(11)	-2(12)	21(13)
C(79′)	89(16)	112(16)	43(9)	21(10)	21(9)	24(12)
C(80′)	81(8)	54(6)	73(7)	35(5)	43(6)	16(5)
C(81′)	152(14)	63(8)	146(13)	52(8)	98(11)	35(8)
C(82′)	118(12)	81(9)	111(10)	65(8)	20(8)	24(8)
C(83′)	113(12)	70(8)	120(11)	49(8)	58(9)	6(7)
P(10)	40(1)	41(1)	42(1)	14(1)	5(1)	16(1)
F(11)	58(4)	45(3)	72(3)	25(2)	25(3)	26(2)
F(12)	131(6)	101(5)	55(3)	46(3)	22(4)	57(4)
F(13)	42(4)	59(3)	88(4)	5(3)	12(3)	0(3)
F(14)	106(5)	133(6)	74(4)	65(4)	49(4)	79(5)
F(15)	37(4)	62(4)	131(6)	16(4)	7(3)	7(3)
F(16)	62(4)	47(3)	70(3)	2(3)	4(3)	28(3)
P(20)	49(2)	47(1)	51(1)	22(1)	6(1)	8(1)
F(21)	91(5)	117(5)	83(4)	66(4)	-21(4)	-2(4)
F(22)	66(5)	109(5)	122(6)	53(5)	42(4)	4(4)
F(23)	100(5)	47(3)	73(4)	20(3)	5(3)	27(3)
F(24)	68(5)	101(5)	130(6)	67(5)	50(4)	24(4)

F(25)	96(5)	57(4)	82(4)	2(3)	18(4)	6(3)
F(26)	87(5)	71(4)	80(4)	42(3)	-9(3)	13(3)
P(30)	53(2)	86(2)	84(2)	58(2)	28(1)	35(2)
F(31)	93(6)	215(10)	143(7)	132(7)	39(5)	69(6)
F(32)	107(6)	128(6)	104(6)	21(5)	49(5)	46(5)
F(33)	70(5)	105(6)	161(8)	51(5)	13(5)	22(4)
F(34)	86(6)	145(7)	123(6)	38(5)	47(5)	55(5)
F(35)	73(5)	113(6)	199(9)	110(6)	19(5)	11(4)
F(36)	97(6)	155(7)	135(6)	116(6)	1(5)	21(5)
P(40)	82(2)	65(2)	66(2)	45(1)	17(1)	13(1)
F(41)	105(6)	117(6)	206(9)	118(7)	73(6)	32(5)
F(42)	234(12)	189(10)	256(12)	181(10)	179(11)	159(9)
F(43)	133(8)	180(10)	101(6)	59(6)	-30(6)	-18(7)
F(44)	164(8)	130(7)	191(9)	124(7)	85(7)	76(6)
F(45)	251(14)	150(9)	92(6)	46(6)	-3(7)	35(9)
F(46)	141(8)	196(10)	262(13)	182(10)	118(9)	64(7)
P(50)	38(1)	46(1)	51(1)	19(1)	12(1)	16(1)
F(51)	109(6)	67(4)	120(5)	42(4)	62(4)	54(4)
F(52)	115(12)	143(13)	69(8)	-14(9)	-41(8)	43(11)
F(53)	142(13)	103(10)	261(19)	145(13)	124(14)	51(10)
F(54)	131(13)	89(9)	127(12)	-13(9)	-93(10)	54(9)
F(55)	180(16)	101(10)	314(23)	168(15)	190(18)	104(12)
F(56)	82(5)	106(5)	69(4)	33(3)	36(3)	62(4)
P(60)	152(4)	89(2)	67(2)	42(2)	55(2)	66(3)
F(61)	232(12)	163(8)	136(7)	113(7)	89(8)	125(8)
F(62)	163(33)	93(15)	97(20)	-10(13)	16(16)	39(18)
F(63)	121(22)	213(31)	143(26)	127(27)	72(20)	93(25)
F(64)	164(22)	113(14)	84(12)	29(10)	7(12)	72(15)
F(65)	114(18)	277(34)	138(18)	152(22)	75(15)	80(23)
F(66)	148(8)	138(7)	96(5)	71(5)	42(5)	68(6)
F(62')	116(17)	124(16)	165(21)	103(16)	17(16)	0(14)
F(63')	187(31)	156(21)	78(11)	41(15)	75(15)	99(23)
F(64')	118(19)	111(16)	242(34)	86(20)	89(21)	8(14)
F(65')	193(38)	114(19)	115(16)	65(16)	101(23)	91(24)

Table 5. Hydrogen coordinates (x 10^4), isotropic displacement parameters ($Å^2$ x 10^3) and occupancies [K] for 1. K is unity unless otherwise stated.

	x	y	z	U(eq)	K
H(2A)	3904(5)	310(5)	7553(4)	72	
H(2B)	4494(5)	906(5)	8175(4)	72	
H(3A)	4303(5)	1109(5)	7262(4)	77	
H(3B)	3556(5)	1205(5)	7343(4)	77	
H(5A)	5195(5)	2003(5)	7772(4)	69	
H(5B)	5292(5)	2012(5)	8451(4)	69	
H(6A)	5790(5)	3114(5)	8521(4)	69	
H(6B)	5019(5)	3162(5)	8261(4)	69	
H(8A)	5179(5)	4208(5)	9280(4)	61	
H(8B)	5955(5)	4119(5)	9415(4)	61	
H(9A)	5786(5)	4018(5)	10354(4)	57	
H(9B)	5852(5)	4781(5)	10411(4)	57	
H(12A)	5862(5)	4865(4)	11388(4)	53	
H(13A)	5693(6)	5463(5)	12407(4)	70	
H(14A)	4600(6)	5504(5)	12514(4)	65	
H(15A)	3639(5)	5052(4)	11608(4)	56	
H(18A)	3054(5)	5078(5)	10679(4)	60	
H(18B)	2758(5)	4325(5)	10611(4)	60	
H(19A)	2151(5)	4530(5)	9749(5)	71	
H(19B)	2841(5)	4521(5)	9528(5)	71	
H(21A)	1351(5)	3618(5)	9242(5)	68	
H(21B)	1618(5)	3299(5)	9708(5)	68	
H(22A)	878(5)	2423(5)	8685(4)	65	
H(22B)	1439(5)	2601(5)	8361(4)	65	
H(24A)	1361(5)	1263(5)	8036(4)	62	
H(24B)	898(5)	1346(5)	8516(4)	62	
H(25A)	1822(5)	1136(5)	9182(4)	69	
H(25B)	1453(5)	470(5)	8496(4)	69	
H(28A)	2157(6)	102(5)	9085(5)	82	
H(29A)	2888(8)	-586(5)	9266(6)	96	
H(30A)	3885(8)	-601(5)	8961(6)	99	
H(31A)	4202(6)	57(5)	8468(5)	88	
H(34A)	4976(5)	2265(5)	9497(4)	59	
H(35A)	5776(5)	1611(5)	9502(4)	71	
H(36A)	5733(6)	877(5)	9973(5)	75	
H(37A)	4857(5)	744(5)	10403(5)	67	
H(39A)	3783(5)	1004(5)	10633(4)	64	
H(41A)	2692(5)	1250(5)	10881(4)	69	
H(42A)	1840(6)	1857(5)	10902(4)	69	
H(43A)	1868(5)	2654(5)	10464(4)	62	
H(44A)	2756(5)	2855(4)	10071(3)	54	
H(47A)	3708(4)	3161(4)	9908(3)	44	
H(47B)	4285(4)	2861(4)	9586(3)	44	
H(48A)	2871(13)	2346(31)	9023(28)	12(15)	
H(48B)	3419(34)	2013(20)	8738(27)	23(15)	
H(49A)	3821(4)	2890(4)	8561(3)	44	
H(49B)	3391(4)	3360(4)	8979(3)	44	
H(51A)	2541(4)	1605(4)	7729(4)	48	
H(52A)	1645(4)	1340(4)	6816(4)	51	
H(54A)	1975(5)	3386(5)	7277(4)	56	
H(55A)	2851(5)	3652(4)	8203(4)	53	

H(56A)	1016(4)	1680(5)	6073(4)	55	
H(56B)	1283(4)	2449(5)	6168(4)	55	
H(58A)	259(5)	1584(4)	6755(4)	53	
H(59A)	-691(4)	1857(4)	7085(4)	48	
H(61A)	-420(4)	3513(4)	6727(4)	53	
H(62A)	564(4)	3198(4)	6405(4)	51	
H(64A)	-1191(4)	2515(4)	7798(4)	45	
H(65A)	-2186(4)	2765(4)	8089(4)	52	
H(67A)	-2615(4)	3551(4)	6886(3)	44	
H(68A)	-1604(4)	3358(4)	6589(4)	46	
H(69A)	-3277(4)	3647(4)	7605(4)	47	
H(69B)	-3110(4)	3333(4)	8092(4)	47	
H(71A)	-4399(4)	3135(4)	6962(3)	42	
H(73A)	-5232(4)	1054(4)	6115(4)	47	
H(75A)	-3272(4)	1863(4)	7288(4)	44	
H(77A)	-6181(6)	1613(9)	6440(8)	163	
H(77B)	-6611(6)	2060(9)	6201(8)	163	
H(77C)	-6049(6)	2432(9)	6888(8)	163	
H(78A)	-5182(6)	2942(6)	5945(7)	142	
H(78B)	-5424(6)	3270(6)	6579(7)	142	
H(78C)	-5986(6)	2898(6)	5891(7)	142	
H(79A)	-5550(7)	1681(7)	5215(6)	170	
H(79B)	-6334(7)	1662(7)	5230(6)	170	
H(79C)	-5939(7)	1160(7)	5416(6)	170	
H(81A)	-3974(10)	361(7)	5683(7)	120	0.70
H(81B)	-4777(10)	89(7)	5592(7)	120	0.70
H(81C)	-4233(10)	-325(7)	5741(7)	120	0.70
H(82A)	-3101(8)	782(7)	6719(9)	122	0.70
H(82B)	-3412(8)	96(7)	6756(9)	122	0.70
H(82C)	-3328(8)	848(7)	7334(9)	122	0.70
H(83A)	-4578(10)	570(8)	7245(9)	126	0.70
H(83B)	-4601(10)	-189(8)	6710(9)	126	0.70
H(83C)	-5145(10)	225(8)	6561(9)	126	0.70
H(81G)	-3810(18)	359(17)	5813(16)	84	0.30
H(81H)	-3594(18)	-42(17)	6213(16)	84	0.30
H(81I)	-3234(18)	765(17)	6494(16)	84	0.30
H(82G)	-4377(21)	788(19)	7420(16)	101	0.30
H(82H)	-3572(21)	1028(19)	7495(16)	101	0.30
H(82I)	-3932(21)	220(19)	7215(16)	101	0.30
H(83G)	-5264(20)	154(19)	6323(18)	108	0.30
H(83H)	-4857(20)	-435(19)	6052(18)	108	0.30
H(83I)	-5030(20)	20(19)	5696(18)	108	0.30
H(2'A)	8445(5)	300(5)	2772(5)	69	
H(2'B)	9013(5)	887(5)	3415(5)	69	
H(3'A)	9111(6)	979(5)	2494(4)	70	
H(3'B)	8358(6)	1127(5)	2401(4)	70	
H(5'A)	9945(6)	1886(6)	2869(5)	92	
H(5'B)	10035(6)	1950(6)	3567(5)	92	
H(6'A)	10570(6)	2997(6)	3555(5)	95	
H(6'B)	9805(6)	3067(6)	3306(5)	95	
H(8'A)	10116(5)	4210(5)	4369(5)	70	
H(8'B)	10851(5)	4014(5)	4442(5)	70	
H(9'A)	10698(5)	3913(5)	5381(5)	66	
H(9'B)	10841(5)	4693(5)	5473(5)	66	
H(12B)	10824(5)	4562(5)	6429(4)	63	
H(13B)	10713(5)	4976(5)	7466(5)	72	
H(14B)	9652(6)	5167(5)	7656(5)	80	
H(15B)	8724(5)	4994(5)	6815(4)	65	
H(18C)	8206(5)	5304(5)	6025(5)	70	
H(18D)	7824(5)	4531(5)	5856(5)	70	
H(19C)	7273(5)	4972(5)	5170(5)	80	
H(19D)	7926(5)	4921(5)	4892(5)	80	
H(21C)	6479(5)	4170(5)	4278(5)	75	

H(21D)	6412(5)	3869(5)	4765(5)	75	
H(22C)	5802(7)	3057(7)	3878(9)	169	
H(22D)	6314(7)	3190(7)	3503(9)	169	
H(24C)	6213(5)	1843(5)	2961(6)	87	
H(24D)	5598(5)	1973(5)	3289(6)	87	
H(25C)	6137(5)	1546(6)	3996(5)	87	
H(25D)	5862(5)	957(6)	3260(5)	87	
H(28B)	6327(5)	571(5)	4048(4)	73	
H(29B)	6747(8)	-256(6)	4273(5)	95	
H(30B)	7718(7)	-562(5)	4005(5)	88	
H(31B)	8368(5)	22(5)	3594(4)	70	
H(34B)	9601(6)	2429(5)	4703(4)	76	
H(35B)	10360(6)	1724(7)	4609(5)	90	
H(36B)	10236(6)	840(7)	4892(5)	90	
H(37B)	9339(6)	646(5)	5291(5)	81	
H(39B)	8276(5)	949(4)	5584(4)	64	
H(41B)	7183(6)	1184(5)	5831(4)	72	
H(42B)	6297(6)	1729(6)	5778(4)	75	
H(43B)	6359(5)	2592(5)	5440(4)	72	
H(44B)	7297(5)	2888(4)	5131(4)	55	
H(47C)	8977(5)	3086(4)	4909(4)	54	
H(47D)	8300(5)	3282(4)	5107(4)	54	
H(48C)	7629(8)	2539(38)	4089(35)	34(18)	
H(48D)	8141(37)	2209(17)	3868(26)	27(16)	
H(49C)	8791(4)	3103(4)	3847(4)	44	
H(49D)	8363(4)	3614(4)	4228(4)	44	
H(51B)	7635(5)	1936(4)	2826(4)	61	
H(52B)	6845(5)	1759(5)	1882(4)	65	
H(54B)	7121(6)	3833(5)	2563(5)	77	
H(55B)	7881(6)	4001(5)	3504(5)	76	
H(56C)	6558(5)	2970(5)	1373(4)	70	
H(56D)	6278(5)	2170(5)	1191(4)	70	
H(58B)	5468(6)	2022(5)	1859(5)	70	
H(59B)	4462(5)	2253(5)	2124(4)	63	
H(61B)	4732(5)	3867(5)	1713(4)	61	
H(62B)	5744(5)	3627(5)	1489(4)	65	
H(64B)	3828(6)	2840(5)	2721(4)	68	
H(65B)	2799(6)	3036(5)	2905(4)	76	
H(67B)	2548(5)	3900(4)	1748(4)	56	
H(68B)	3581(5)	3735(4)	1548(4)	52	
H(69C)	1732(5)	3929(5)	2359(5)	67	
H(69D)	1838(5)	3597(5)	2838(5)	67	
H(71B)	942(5)	3244(5)	1285(4)	60	
H(73B)	92(5)	1196(5)	613(5)	72	
H(75B)	1499(5)	2282(5)	2360(4)	63	
H(77D)	-784(9)	1394(12)	140(9)	119	0.60
H(77E)	-1023(9)	1671(12)	-365(9)	119	0.60
H(77F)	-984(9)	2127(12)	370(9)	119	0.60
H(78D)	610(13)	2977(10)	253(10)	135	0.60
H(78E)	-78(13)	3141(10)	446(10)	135	0.60
H(78F)	-117(13)	2685(10)	-288(10)	135	0.60
H(79D)	185(11)	1147(11)	-349(8)	130	0.60
H(79E)	741(11)	1763(11)	-311(8)	130	0.60
H(79F)	-26(11)	1513(11)	-785(8)	130	0.60
H(77G)	-779(15)	2669(15)	721(13)	112	0.40
H(77H)	-766(15)	2836(15)	140(13)	112	0.40
H(77I)	-160(15)	3259(15)	800(13)	112	0.40
H(78G)	731(17)	2923(18)	238(15)	117	0.40
H(78H)	94(17)	2567(18)	-400(15)	117	0.40
H(78I)	668(17)	2157(18)	-308(15)	117	0.40
H(79G)	-777(24)	1327(22)	12(21)	178	0.40
H(79H)	-298(24)	1134(22)	-457(21)	178	0.40
H(79I)	-873(24)	1544(22)	-548(21)	178	0.40

H(81D)	1547(8)	680(6)	1127(7)	164
H(81E)	803(8)	347(6)	607(7)	164
H(81F)	1045(8)	11(6)	1062(7)	164
H(82D)	1625(8)	1303(7)	2318(6)	147
H(82E)	1114(8)	625(7)	2227(6)	147
H(82F)	930(8)	1365(7)	2529(6)	147
H(83D)	-283(7)	470(6)	965(7)	146
H(83E)	-223(7)	862(6)	1711(7)	146
H(83F)	-39(7)	122(6)	1409(7)	146
H(92A)	2006(6)	4728(5)	6256(5)	98
H(92B)	2759(6)	4810(5)	6662(5)	98
H(92C)	2579(6)	4494(5)	5909(5)	98
H(93A)	2491(6)	2956(6)	6138(5)	114
H(93B)	2896(6)	3336(6)	5832(5)	114
H(93C)	3077(6)	3652(6)	6585(5)	114
H(96A)	-429(8)	3542(7)	9253(7)	151
H(96B)	180(8)	4206(7)	9738(7)	151
H(96C)	-494(8)	4288(7)	9342(7)	151
H(97A)	729(9)	4461(8)	8516(8)	190
H(97B)	221(9)	4855(8)	8872(8)	190
H(97C)	896(9)	4773(8)	9268(8)	190
H(10A)	4871(9)	3935(9)	3887(8)	190
H(10B)	5272(9)	4626(9)	4525(8)	190
H(10C)	4590(9)	4615(9)	4064(8)	190
H(10D)	5927(11)	5436(10)	3672(10)	235
H(10E)	5280(11)	5605(10)	3926(10)	235
H(10F)	5962(11)	5616(10)	4387(10)	235
H(10G)	6514(10)	2790(10)	-449(9)	211
H(10H)	7168(10)	2625(10)	-110(9)	211
H(10I)	6979(10)	3344(10)	247(9)	211
H(10J)	8251(11)	3774(11)	-493(10)	241
H(10K)	8204(11)	4036(11)	215(10)	241
H(10L)	8393(11)	3317(11)	-142(10)	241
H(10M)	-2294(8)	-183(7)	5331(7)	158
H(10N)	-2759(8)	-699(7)	5481(7)	158
H(10O)	-2030(8)	-229(7)	5972(7)	158
H(10P)	-1652(10)	-1902(10)	5175(9)	216
H(10Q)	-1610(10)	-1332(10)	5870(9)	216
H(10R)	-2339(10)	-1802(10)	5378(9)	216
H(11A)	8376(10)	1473(10)	1286(9)	221
H(11B)	9117(10)	1954(10)	1461(9)	221
H(11C)	8746(10)	2054(10)	1999(9)	221
H(11D)	8438(15)	3420(15)	1609(14)	351
H(11E)	8795(15)	3333(15)	2209(14)	351
H(11F)	9166(15)	3232(15)	1670(14)	351
H(11G)	3424(11)	1424(11)	2962(12)	345
H(11H)	3775(11)	1283(11)	3529(12)	345
H(11I)	3238(11)	1754(11)	3617(12)	345
H(11J)	4463(15)	2292(16)	4660(9)	485
H(11K)	5094(15)	2507(16)	4435(9)	485
H(11L)	4530(15)	2948(16)	4536(9)	485
H(12C)	-1581(17)	1008(17)	7747(16)	407
H(12D)	-1425(17)	691(17)	8224(16)	407
H(12E)	-2146(17)	397(17)	7689(16)	407
H(12F)	-2648(18)	1682(17)	9144(16)	430
H(12G)	-2906(18)	875(17)	8662(16)	430
H(12H)	-2186(18)	1170(17)	9197(16)	430

Cyclic voltammetric patterns for **1b**$^{2+}$ at different scan rates. Ar-Purged MeCN solution, 293 K, 5×10^{-4} M **1b**$^{2+}$, 5×10^{-2} M Et_4NPF_6 as supporting electrode, glassy carbon as working electrode.