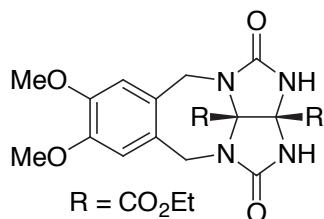


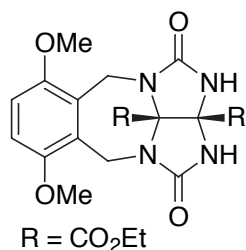
Diastereoselective Formation of Methylene Bridged Glycoluril Dimers – Supporting Information

by Dariusz Witt^{a,b}, Jason Lagona^a, Fehmi Damkaci^a,
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General. Starting materials were purchased from Alfa-Aesar, Acros, and Aldrich and were used without further purification. Compounds **3**, **5**, **6**, and **7** were prepared according to the literature procedures.¹¹ THF and toluene were distilled from sodium benzophenone ketyl and methylene chloride was distilled from CaH₂ immediately before use. TLC analysis was performed using pre-coated glass plates from Analtech or Merck. Column chromatography was performed using silica gel (230 - 400 mesh, 0.040-0.063 μ m) from E. Merck using eluents in the indicated v:v ratio. Melting points were measured on a Meltemp apparatus in open capillary tubes and are uncorrected. NMR spectra were measured on Bruker AM-400 and DRX-400 instruments operating at 400 MHz for ¹H and 100 MHz for ¹³C. Mass spectrometry was performed using a VG 7070E magnetic sector instrument by electron impact (EI) or by fast atom bombardment (FAB) using the indicated matrix. The matrix “magic bullet” is a 5:1 (w:w) mixture of dithiothreitol:dithioerythritol.

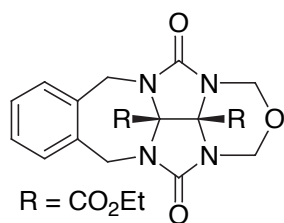


4,5-Dimethoxyxylylene glycoluril (8). Glycoluril **3** (4.58 g, 16.00 mmol) was dissolved in anh. DMSO (50 mL) under N₂ and *t*-BuOK (3.6 g, 32.0 mmol) was added. After stirring for 15 min., 1,2-bis(bromomethyl)-4,5-dimethoxybenzene (1.17 g, 3.60 mmol) was added in one portion and stirring was continued for 3 h. The reaction mixture was poured into 0.1 N HCl (1L) and extracted with EtOAc (3 x 400 mL). The extracts were washed with brine (2 x 300 mL) and dried over anh. MgSO₄. After filtration and rotary evaporation the residue was purified by flash chromatography (SiO₂, CHCl₃/MeOH, 50:1) to give **8** (0.72 g, 1.60 mmol, 45%). M.p. 284-285 °C. TLC (CHCl₃/MeOH 50:1) *R*_f 0.13. IR (KBr, cm⁻¹): 3426m, 3318s, 3020w, 2980w, 2940w, 2837w, 1726s, 1715s, 1710s, 1460s, 1260s, 1142s, 1096m, 1029m. ¹H NMR (400 MHz, DMSO-*d*₆): 8.39 (s, 2H), 6.85 (s, 2H), 4.50 (d, *J* = 15.9, 2H), 4.30 (d, *J* = 15.9, 2H), 4.17 (q, *J* = 7.1, 2H), 4.09 (q, *J* = 7.1, 2H), 3.68 (s, 6H), 1.18 (t, *J* = 7.1, 3H), 1.15 (t, *J* = 7.1, 3H). ¹³C NMR (100 MHz, DMSO-*d*₆): 166.6, 166.2, 157.1, 147.4, 129.8, 113.7, 82.5, 74.0, 62.7, 62.6, 55.8, 43.5, 13.8, 13.8. MS (FAB, Magic Bullet): *m/z* 449 (44, [M + H]⁺), 206 (100, [C₁₁H₁₂NO₃]⁺). HR-MS (FAB, Magic Bullet): *m/z* 449.1690 ([M + H]⁺, C₂₀H₂₅N₄O₈, calcd 449.1672).



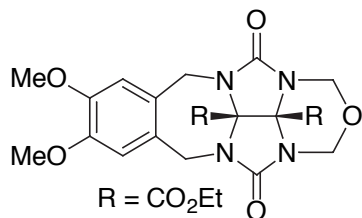
3,6-Dimethoxylylene glycoluril (9): Compound **7** (4.58 g, 16.0 mmol) was dissolved in anh. DMSO (50 mL) under N₂ and *t*-BuOK (3.60 g, 32.0 mmol) was added. After stirring for 15 min., **6** (1.17 g, 3.60 mmol) was added in one portion and stirring was continued for 3 h. The reaction mixture was poured into 0.1 N HCl (1L) and extracted with EtOAc (3 x 400 mL). The extracts were washed with brine (2 x 300 mL) and dried over anh. MgSO₄. After filtration and rotary evaporation the residue was purified by

flash chromatography (SiO₂, CHCl₃/MeOH, 50:1) to give **9** (0.72 g, 1.60 mmol, 45%). M.p. 232-235 °C. TLC (CHCl₃/MeOH 25:1) *R*_f 0.20. IR (KBr, cm⁻¹): 3396w, 3196m, 2987w, 2940w, 2835w, 1745s, 1707s, 1465s, 1260s, 1075s, 1023m. ¹H NMR (400 MHz, DMSO-*d*₆): 8.38 (s, 2H), 6.92 (s, 2H), 5.24 (d, *J* = 15.8, 2H), 4.30 4.17 (q, *J* = 7.1, 2H), 4.12 (q, *J* = 7.1, 2H), 4.00 (d, *J* = 15.8, 2H), 3.74 (s, 6H), 1.20 (t, *J* = 7.1, 3H), 1.19 (t, *J* = 7.1, 3H). ¹³C NMR (100 MHz, DMSO-*d*₆): 166.6, 166.2, 157.0, 150.7, 127.3, 112.6, 82.6, 73.9, 62.6, 62.6, 56.9, 35.5, 13.8. (only 13 of the 14 expected resonances were observed). MS (FAB, Magic Bullet): *m/z* 449 (100, [M + H]⁺). HR-MS (FAB, Magic Bullet): *m/z* 449.1664 ([M + H]⁺, C₂₀H₂₅N₄O₈, calcd 449.1672).



Xylylene cyclic ether (10). Compound **7** (0.58 g, 1.50 mmol) was dissolved in TFA (10 mL) and paraformaldehyde (0.18 g, 6.00 mmol of CH₂O) was added in one portion. The reaction mixture was stirred and heated at reflux for 6 h. After rotary evaporation the residue was dissolved in EtOAc (100 mL), washed with sat. Na₂CO₃, dried over anh.

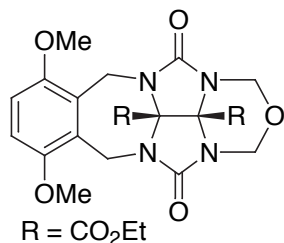
MgSO₄ and concentrated. Flash chromatography (SiO₂, Hexanes/EtOAc, 2:1) yielded **10** (0.28 g, 0.66 mmol, 44%). M.p. 188-189 °C. TLC (Hexanes/EtOAc, 2:1) *R*_f 0.23. IR (CHCl₃, cm⁻¹): 3044s, 2997m, 2934m, 2901m, 2868m, 1755s, 1735s, 1465s, 1417s, 1165s, 1013s. ¹H NMR (400 MHz, CDCl₃): δ 7.45-7.35 (m, 2H), 7.30-7.20 (m, 2H), 5.37 (d, *J* = 11.2, 2H), 4.80 (d, *J* = 16.0, 2H), 4.68 (d, *J* = 11.2, 2H), 4.54 (d, *J* = 16.0, 2H), 4.32 (q, *J* = 7.1, 2H), 4.29 (q, *J* = 7.1, 2H), 1.33 (t, *J* = 7.1, 3H), 1.32 (t, *J* = 7.1, 3H). ¹³C NMR (100 MHz, CDCl₃): δ 165.3, 165.0, 156.2, 136.1, 129.7, 128.2, 80.2, 74.1, 72.2, 63.4, 45.6, 13.9, 13.8. MS (FAB, Magic Bullet): *m/z* 431 (100, [M + H]⁺), 91 (48, C₇H₇⁺). HR-MS (FAB, Magic Bullet): *m/z* 431.1588 ([M + H]⁺, C₂₀H₂₃O₇N₄, calcd 431.1567). X-ray crystal structure.



4,5-Dimethoxyxylylene cyclic ether (11). Compound **8** (0.27 g, 0.60 mmol) was dissolved in TFA (10 mL) and paraformaldehyde (0.078 g, 2.500 mmol of CH₂O) was added in one portion. The reaction mixture was stirred and heated at reflux for 6 h. After rotary evaporation the residue was chromatographed on SiO₂ (CHCl₃) to give **11** (0.15 g, 0.31 mmol, 52%). M.p. 227-228 °C.

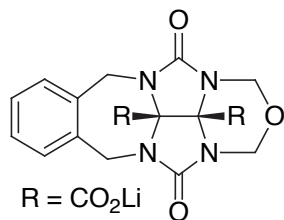
TLC (CHCl₃/MeOH, 100:1) *R*_f 0.30. IR (KBr, cm⁻¹): 2993w, 2959w, 2940w, 2910w, 1730s,

1472m, 1450m, 1420s, 1276m, 1254m, 1097m, 1010m. ^1H NMR (400 MHz, CDCl_3): 6.85 (s, 2H), 5.37 (d, $J = 11.1$, 2H), 4.69 (d, $J = 16.0$, 2H), 4.68 (d, $J = 11.1$, 2H), 4.49 (d, $J = 16.0$, 2H), 4.35-4.25 (m, 4H), 3.84 (s, 6H), 1.35-1.25 (m, 6H). ^{13}C NMR (100 MHz, CDCl_3): 165.3, 165.1, 156.3, 147.9, 128.7, 113.2, 80.3, 74.1, 72.2, 63.4, 55.9, 45.3, 13.9, 13.8, (only 14 of the 15 expected resonances were observed). MS (FAB, Magic Bullet): m/z 491 (45, $[\text{M} + \text{H}]^+$), 206 (100, $[\text{C}_{11}\text{H}_{12}\text{NO}_3]^+$). HR-MS (FAB, Magic Bullet): m/z 491.1748 ($[\text{M} + \text{H}]^+$, $\text{C}_{22}\text{H}_{27}\text{N}_4\text{O}_9$, calcd 491.1778).



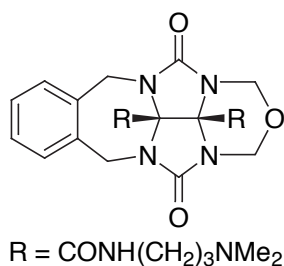
3,6-Dimethoxyxylylene cyclic ether (12). Compound **9** (0.27 g, 0.60 mmol) was dissolved in TFA (10 mL) and paraformaldehyde (0.078 g, 2.50 mmol of CH_2O) was added in one portion. The reaction mixture was stirred and heated at reflux for 6 h. After rotary evaporation the residue was chromatographed on SiO_2 ($\text{CHCl}_3/\text{EtOAc}$, 5:1) to give **12** (0.17 g, 0.34 mmol, 56%). M.p. 234-235 °C. TLC ($\text{CHCl}_3/\text{EtOAc}$, 5:1)

R_f 0.38. IR (KBr, cm^{-1}): 2982w, 2954w, 2930w, 2830w, 1745s, 1726s, 1474m, 1417s, 1260s, 1089s, 1018m. ^1H NMR (400 MHz, CDCl_3): 6.84 (s, 2H), 5.58 (d, $J = 16.0$, 2H), 5.40 (d, $J = 11.1$, 2H), 4.70 (d, $J = 11.1$, 2H), 4.30-4.20 (m, 4H), 4.13 (d, $J = 16.0$, 2H), 3.86 (s, 6H), 1.35-1.25 (m, 6H). ^{13}C NMR (100 MHz, CDCl_3): 165.4, 165.2, 156.2, 151.4, 126.7, 112.8, 80.4, 74.1, 72.3, 63.4, 63.3, 57.2, 37.3, 13.9, 13.9. MS (FAB, Magic Bullet): m/z 491 (25, $[\text{M} + \text{H}]^+$), 206 (100, $[\text{C}_{11}\text{H}_{12}\text{NO}_3]^+$). HR-MS (FAB, Magic Bullet): m/z 491.1789 ($[\text{M} + \text{H}]^+$, $\text{C}_{22}\text{H}_{27}\text{N}_4\text{O}_9$, calcd 491.1778).



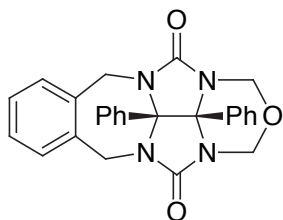
Cyclic Ether (13). Compound **10** (0.215 g, 0.500 mmol) was suspended in a mixture of MeOH (20 mL) and water (2 mL). After addition of LiOH (0.024 g, 1.000 mmol) the resulting suspension was heated at 45 °C for 48 h. The solvent was evaporated and the residue was dried under high vacuum to yield **13** (0.19 g, 0.49 mmol, 98%). M.p. > 320 °C (dec.) IR (KBr, cm^{-1}): 3430s, 2976w, 2920w, 1707s, 1673s, 1480s, 1380s,

1311m, 1280m, 931s. ^1H NMR (400 MHz, $\text{DMSO}-d_6$): 7.30-7.15 (m, 4H), 4.99 (d, $J = 10.5$, 2H), 4.62 (d, $J = 10.5$, 2H), 4.50-4.40 (m, 4H). ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): 167.5, 167.1, 157.3, 138.5, 129.4, 127.1, 82.6, 75.2, 71.1, 45.1. MS (FAB, Glycerol): m/z 393 (11, $[\text{M} + \text{Li}]^+$), 57 (100). HR-MS (FAB, Glycerol): m/z 393.1167 ($[\text{M} + \text{Li}]^+$, $\text{C}_{16}\text{H}_{12}\text{Li}_3\text{N}_4\text{O}_7$ calcd 393.1186).

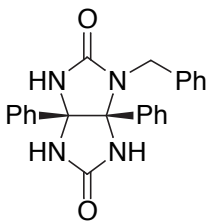


Xylylene cyclic ether diamide (14). Compound **10** (0.108 g, 0.250 mmol) was heated at 80 °C with 3(dimethylamino)propylamine (5 mL) for 24 h. The excess of amine was evaporated and resulting residue was washed with Et_2O and dried under high vacuum to give **14** (0.126 g,

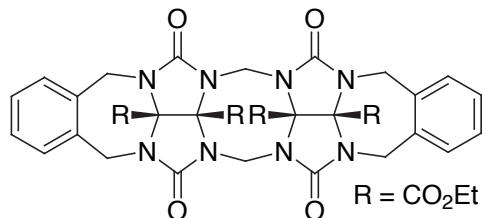
0.230 mmol, 92%). M.p. 203-204 °C. IR (KBr, cm^{-1}): 3408m, 3317m, 2944m, 2866m, 2817m, 2764m, 1730s, 1702s, 1520,m, 1470s, 1448s, 1415s, 1023w. ^1H NMR (400 MHz, CDCl_3): 9.74 (br, 1H), 9.51 (br, 1H), 7.40-7.35 (m, 2H), 7.30-7.20 (m, 2H), 5.38 (d, $J = 11.2$, 2H), 4.75 (d, $J = 15.8$, 2H), 4.49 (d, $J = 11.2$, 2H), 4.43 (d, $J = 15.8$, 2H), 3.45-3.30 (m, 4H), 2.52-2.40 (m, 4H), 2.29 (s, 6H), 2.22 (s, 6H), 1.75-1.60 (m, 4H). ^{13}C NMR (100 MHz, CDCl_3): 162.7, 162.2, 156.6, 137.2, 129.6, 127.6, 81.4, 74.6, 71.7, 57.2, 57.1, 45.1, 45.0, 26.0, 25.9, (only 15 of the 18 expected resonances were observed). MS (FAB, Magic Bullet): m/z 543 (76, $[\text{M} + \text{H}]^+$), 129 (100, $[\text{C}_6\text{H}_{13}\text{N}_2\text{O}]^+$). HR-MS (FAB, Magic Bullet): m/z 543.3007 ($[\text{M} + \text{H}]^+$, $\text{C}_{26}\text{H}_{39}\text{N}_8\text{O}_5$, calcd 543.3043).



Xylylene cyclic ether diphenyl glycoluril (15). A mixture of (+/-)-**16** (7.00 g, 18.2 mmol), paraformaldehyde (5.47 g, 182 mmol of CH_2O), and TFA was heated at 95 °C for 18 h. The reaction mixture was cooled to RT and allowed to crystallize. The solid residue was filtered, stirred with Et_2O (100 mL) for 30 min, filtered again, and dried under vacuum giving **15** (5.0 g, 63%). M.p. 317-318 °C (dec.). TLC (hexanes/EtOAc 2:1) R_f 0.28. IR (KBr, cm^{-1}): 3062w, 3027w, 3008w, 2916w, 2869w, 1734s, 1718s, 1465m, 1445s, 1420s, 1009m. ^1H NMR (400 MHz, CDCl_3): δ 7.40-7.00 (m, 14H), 5.47 (d, $J = 11.1$, 2H), 4.83 (d, $J = 15.6$, 2H), 4.39 (d, $J = 11.1$, 2H), 4.28 (d, $J = 15.6$, 2H). ^{13}C NMR (100 MHz, CDCl_3): δ 157.9, 136.5, 133.6, 132.8, 129.6, 129.0, 128.9, 128.7, 128.2, 128.0, 127.9, 127.7, 85.5, 78.8, 71.6, 45.4. MS (FAB, Magic Bullet): m/z 439 (100, $[\text{M} + \text{H}]^+$). HR-MS (FAB, Magic Bullet): m/z 439.1770 ($[\text{M} + \text{H}]^+$, $\text{C}_{26}\text{H}_{23}\text{N}_4\text{O}_3$, calcd 439.1770).



Benzyl diphenylglycoluril ((+/-)-16). A mixture of benzyl urea (9.01 g, 60 mmol), urea (3.6 g, 60 mmol), benzil (12.62 g, 60 mmol), TFA (10 mL), and benzene (150 mL) was heated at reflux for 20 h using a Dean-Stark trap for removal of H_2O . After concentration, the residue was stirred with a mixture of EtOH (100 mL) and acetone (10 mL). The remaining solid was collected by filtration, heated with a mixture of CHCl_3 (900 mL) and MeOH (100mL), and filtered while hot. After the solid was heated with acetone (500 mL), it was filtered while still warm, and dried under vacuum giving (+/-)-**16** (8.19 g, 36%) as a white solid. M.p. 290-292 °C. IR (KBr, cm^{-1}): 3247s, 3089m, 3062m, 3034m, 2924w, 2847w, 1714s, 1695s, 1473s, 1450s, 1384m. ^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 8.31(s, 1H), 8.15 (s, 1H), 8.08 (s, 1H), 7.25-7.00 (m, 11H), 6.90 (br. s, 4H), 4.34 (d, $J = 16.0$, 1H), 3.96 (d, $J = 16.0$, 1H). ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ 160.4, 159.7, 139.1, 137.9, 135.7, 128.1, 128.0, 127.6, 127.5, 127.3, 127.1, 126.4, 85.9, 80.6, 44.2 (15 peaks out of 17 expected). MS (FAB, Magic Bullet): m/z 385 (100, $[\text{M} + \text{H}]^+$), 91 (90, C_7H_7^+). HR-MS (FAB, Magic Bullet): m/z 385.1665 ($[\text{M} + \text{H}]^+$, $\text{C}_{23}\text{H}_{21}\text{N}_4\text{O}_2$, calcd 385.1664).



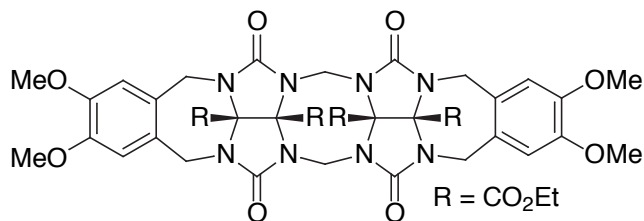
Xylylene dimer (C_{2v} -17). Method 1: A mixture of PTSA (0.48 g 2.50 mmol) in $\text{ClCH}_2\text{CH}_2\text{Cl}$ (20 mL) was heated under N_2 at reflux for 30 min. under a Soxhlet apparatus filled with molecular sieves ($4\text{\AA}$). Compound **10** (0.215 g, 0.500 mmol) was added in one portion and reflux was continued for 24 h. The reaction mixture was

diluted with EtOAc (100 mL), washed with sat. Na_2CO_3 , dried over anh. MgSO_4 , and concentrated. Flash chromatography (SiO_2 , EtOAc/ CHCl_3 , 1:1) gave C_{2v} -17 (0.184 g, 0.230 mmol, 92%).

Method 2: A mixture of PTSA (0.38 g 2.00 mmol) in $\text{ClCH}_2\text{CH}_2\text{Cl}$ (20 mL) was heated under N_2 at reflux for 30 min. under a Soxhlet apparatus filled with molecular sieves ($4\text{\AA}$). Compound **7** (0.194 g, 0.500 mmol) and paraformaldehyde (0.045 g, 1.500 mmol) were added and reflux was continued for 48 h. The reaction mixture was diluted with EtOAc (100 mL), washed with sat. Na_2CO_3 , dried over anh. MgSO_4 , and concentrated. Flash chromatography (SiO_2 , EtOAc/ CHCl_3 , 1:1) gave C_{2v} -17 (0.175 g, 0.220 mmol, 88%).

Method 3: A mixture of PTSA (0.238 g, 1.250 mmol) in $\text{ClCH}_2\text{CH}_2\text{Cl}$ (10 mL) was heated under N_2 at reflux for 30 min. under a Soxhlet apparatus filled with molecular sieves ($4\text{\AA}$). Compound **7** (0.097 g, 0.250 mmol) and **10** (0.108 g, 0.250 mmol) were added and reflux was continued for 24 h. The reaction mixture was diluted with EtOAc (100 mL), washed with sat. Na_2CO_3 , dried over anh. MgSO_4 , and concentrated. Flash chromatography (SiO_2 , EtOAc/ CHCl_3 , 1:1) gave C_{2v} -17 (0.182 g, 0.230 mmol, 92%).

C_{2v} -17: M.p. 267-268 °C. TLC ($\text{CH}_2\text{Cl}_2/\text{MeOH}$ 25:1) R_f 0.43. IR (CHCl_3 , cm^{-1}): 3092w, 3068w, 2959w, 2940w, 2901w, 1755s, 1735s, 1456s, 1417s, 1085m, 1013s. ^1H NMR (400 MHz, CDCl_3): δ 7.25-7.15 (m, 4H), 7.15-7.05 (m, 4H), 6.01 (d, $J = 16.1$, 2H), 4.82 (d, $J = 16.0$, 4H), 4.58 (d, $J = 16.1$, 2H), 4.38 (d, $J = 16.0$, 4H), 4.21 (q, $J = 7.1$, 4H), 4.17 (q, $J = 7.1$, 4H), 1.29 (t, $J = 7.1$, 6H), 1.24 (t, $J = 7.1$, 6H). ^{13}C NMR (100 MHz, CDCl_3): δ 165.6, 164.9, 154.6, 136.0, 129.7, 128.3, 80.0, 78.8, 63.7, 63.3, 47.8, 45.4, 13.9, 13.8. MS (FAB, Magic Bullet): m/z 801 (100, $[\text{M} + \text{H}]^+$). HR-MS (FAB, Magic Bullet): m/z 801.2825 ($[\text{M} + \text{H}]^+$, $\text{C}_{38}\text{H}_{41}\text{O}_{12}\text{N}_8$, calcd 801.2844). X-ray crystal structure.



Dimethoxyxylylene dimer tetraethyl ester (C_{2v} -18). Method 1: A mixture of PTSA (0.190 g, 1.00 mmol) in $\text{ClCH}_2\text{CH}_2\text{Cl}$ (10 mL) was heated under nitrogen at reflux for

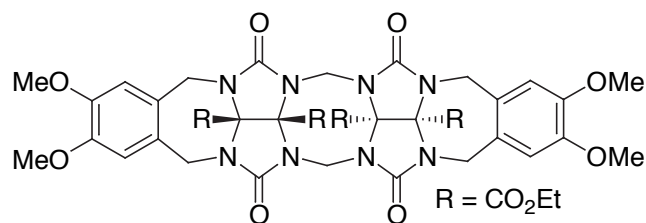
30 min. under a Soxhlet apparatus filled with molecular sieves (4Å). Compound **11** (0.1 g, 0.2 mmol) was added and heating was continued for 24h. The reaction mixture was diluted with EtOAc (100 mL), washed with sat. Na₂CO₃, and dried over anh. MgSO₄. After concentration, the residue was purified by flash chromatography (SiO₂, EtOAc) to yield C_{2v}-**18** (0.086 g, 0.093 mmol, 93%).

Method 2: A mixture of PTSA (0.38 g 2.00 mmol) and ClCH₂CH₂Cl (20 mL) was heated under N₂ at reflux for 30 min. under a Soxhlet apparatus filled with molecular sieves (4Å). Compound **8** (0.22 g, 0.50 mmol) and paraformaldehyde (0.045 g, 1.500 mmol) were added and reflux was continued for 48 h. The reaction mixture was diluted with EtOAc (100 mL), washed with sat. Na₂CO₃, dried over anh. MgSO₄, and concentrated. Flash chromatography (SiO₂, CH₃CN/CHCl₃, 1:4) gave C_{2v}-**18** (0.200 g, 0.217 mmol, 87%).

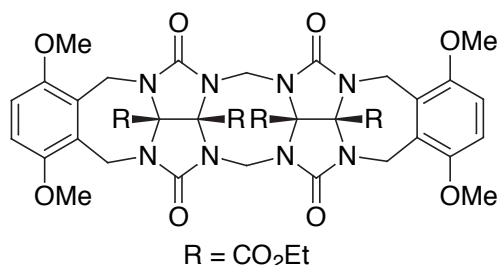
Method 3: A mixture of PTSA (0.38 g, 2.00 mmol) and ClCH₂CH₂Cl (20 mL) was heated under N₂ at reflux for 30 min. under a Soxhlet apparatus filled with molecular sieves (4Å). Compound **8** (0.179 g, 0.400 mmol) and **11** (0.196 g, 0.400 mmol) were added and reflux was continued for 24 h. The reaction mixture was diluted with EtOAc (100 mL), washed with sat. Na₂CO₃, dried over anh. MgSO₄, and concentrated. Flash chromatography (SiO₂, CH₃CN/CHCl₃, 1:4) gave C_{2v}-**18** (0.276 g, 0.300 mmol, 75%) and C_{2h}-**18** (0.070 g, 0.076 mmol, 19%).

Method 4: A mixture of PTSA (0.042 g, 0.220 mmol) and compound C_{2h}-**18** (0.020 g, 0.022 mmol) and ClCH₂CH₂Cl (10 mL) was heated under N₂ at reflux for 24 h under a Soxhlet apparatus filled with molecular sieves (4Å). The reaction mixture was diluted with EtOAc (100 mL), washed with sat. Na₂CO₃, dried over anh. MgSO₄, and concentrated. Flash chromatography (SiO₂, CH₃CN/CHCl₃, 1:4) gave C_{2v}-**18** (0.018 g, 0.018 mmol, 80%).

C_{2v}-**18**: M.p. 284-286 °C. TLC (CHCl₃/MeOH, 50:1) R_f 0.33. IR (KBr, cm⁻¹): 2980m, 2925m, 2868w, 2834w, 1741s, 1455s, 1422s, 1256s, 1103s, 1018s. ¹H NMR (400 MHz, CDCl₃): 6.76 (s, 4H), 6.06 (d, *J* = 16.0, 2H), 4.79 (d, *J* = 16.0, 4H), 4.61 (d, *J* = 16.0, 2H), 4.37 (d, *J* = 16.0, 4H), 4.22 (q, *J* = 7.1, 4H), 4.20 (q, *J* = 7.1, 4H), 3.80 (s, 12H), 1.31 (t, *J* = 7.1, 6H), 1.26 (t, *J* = 7.1, 6H). ¹³C NMR (100 MHz, CDCl₃): 165.6, 164.9, 154.6, 148.0, 128.6, 113.0, 80.1, 78.8, 63.7, 63.3, 55.8, 47.9, 45.0, 13.9, 13.8. MS (FAB, Magic Bullet): *m/z* 921 (7, [M + H]⁺), 206 (100, [C₁₁H₁₂NO₃]⁺). HR-MS (FAB, Magic Bullet): *m/z* 921.3314 ([M + H]⁺, C₄₂H₄₉N₈O₁₆, calcd 921.3267).



4,5-Dimethoxyxylylene dimer tetraethyl ester (C_{2h} -18**).** A mixture of compound **11** (0.1 g, 0.2 mmol) and PTSA (0.19 g, 1.00 mmol) in $\text{ClCH}_2\text{CH}_2\text{Cl}$ (10 mL) was heated under nitrogen at 110 °C (bath temperature) for 12 h under a Soxhlet apparatus filled with molecular sieves (4Å). The reaction mixture was diluted with EtOAc (100 mL), washed with sat. Na_2CO_3 , dried over anh. MgSO_4 , and concentrated. Flash chromatography (SiO_2 , EtOAc) gave **11** (0.040 g, 0.082 mmol, 41%), C_{2h} -**18** (0.020 g, 0.022 mmol, 22%), and C_{2v} -**18** (0.030 g, 0.033 mmol, 33%). C_{2h} -**18**: M.p. 282-283 °C. TLC ($\text{CHCl}_3/\text{MeOH}$, 50:1) R_f 0.45. IR (KBr, cm^{-1}): 2982w, 2934w, 2863w, 2830w, 1727s, 1456s, 1422s, 1384s, 1263s, 1099m, 1018m. ^1H NMR (400 MHz, CDCl_3): 6.84 (s, 4H), 5.04 (s, 4H), 4.75 (d, $J = 16.0$, 4H), 4.32 (d, $J = 16.0$, 4H), 4.22 (q, $J = 7.1$, 4H), 3.86 (s, 12H), 3.70 (q, $J = 7.1$, 4H), 1.28 (t, $J = 7.1$, 6H), 1.12 (t, $J = 7.1$, 6H). ^{13}C NMR (100 MHz, CDCl_3): 165.3, 164.1, 155.3, 148.0, 128.7, 113.0, 81.6, 78.6, 63.8, 63.6, 56.0, 51.9, 44.9, 14.0, 13.6. MS (FAB, Magic Bullet): m/z 921 (10, $[\text{M} + \text{H}]^+$), 206 (100, $[\text{C}_{11}\text{H}_{12}\text{NO}_3]^+$). HR-MS (FAB, Magic Bullet): m/z 921.3267 ($[\text{M} + \text{H}]^+$, $\text{C}_{42}\text{H}_{49}\text{N}_8\text{O}_{16}$, calcd 921.3267).



1,4-Dimethoxyxylylene Dimer (C_{2v} -19**).** Method 1: Method 1: A mixture of PTSA (0.48 g 2.50 mmol) and $\text{ClCH}_2\text{CH}_2\text{Cl}$ (20 mL) was heated under N_2 at reflux for 30 min. under a Soxhlet apparatus filled with molecular sieves (4Å). Compound **12** (0.245 g, 0.500 mmol) was added in one portion and reflux was continued for 24 h. The reaction mixture was diluted with EtOAc (100 mL),

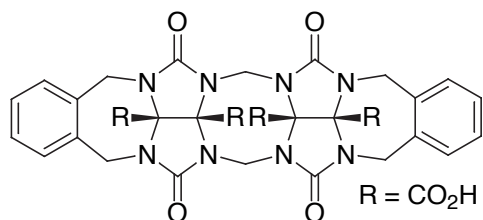
washed with sat. Na_2CO_3 , dried over anh. MgSO_4 , and concentrated. Compound C_{2v} -**19** could not be detected by TLC or NMR.

Method 2: A mixture of PTSA (0.38 g 2.00 mmol) and $\text{ClCH}_2\text{CH}_2\text{Cl}$ (20 mL) was heated under N_2 at reflux for 30 min. under a Soxhlet apparatus filled with molecular sieves (4Å). Compound **9** (0.22 g, 0.50 mmol) and paraformaldehyde (0.045 g, 1.500 mmol) were added and reflux was continued for 48 h. The reaction mixture was diluted with EtOAc (100 mL), washed with sat. Na_2CO_3 , dried over anh. MgSO_4 , and concentrated. Compound C_{2v} -**19** could not be detected by TLC or NMR.

Method 3: A mixture of PTSA (0.48 g, 2.50 mmol) and $\text{ClCH}_2\text{CH}_2\text{Cl}$ (20 mL) was heated under N_2 at reflux for 30 min. under a Soxhlet apparatus filled with molecular sieves ($4\text{\AA}$). Compound **9** (0.224 g, 0.500 mmol) and **12** (0.245 g, 0.500 mmol) were added and reflux was continued for 24 h. The reaction mixture was diluted with EtOAc (100 mL), washed with sat. Na_2CO_3 , dried over anhydrous MgSO_4 , and concentrated. Flash chromatography (SiO_2 , $\text{CH}_3\text{CN}/\text{CHCl}_3$, 1:2) gave C_{2v} -**19** (0.258 g, 0.28 mmol, 56%).

C_{2v} -**19**: M.p. $>310\text{ }^\circ\text{C}$. TLC ($\text{CH}_3\text{CN}/\text{CHCl}_3$, 1:4) R_f 0.21. IR (KBr, cm^{-1}): 2982m, 2935m, 2901w, 2840w, 1745s, 1489s, 1437s, 1256s, 1084s, 1013s.

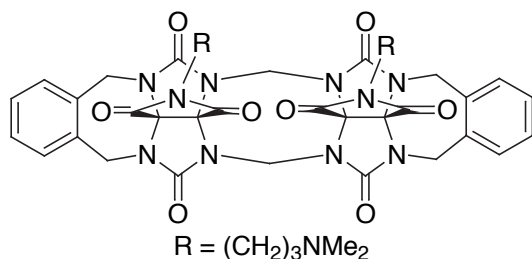
^1H NMR (400 MHz, CDCl_3): 6.05 (d, $J = 16.1$, 2H), 6.02 (s, 4H), 5.51 (d, $J = 16.2$, 4H), 4.57 (d, $J = 16.1$, 2H), 4.20 (q, $J = 7.1$, 4H), 4.16 (q, $J = 7.1$, 4H), 3.88 (d, $J = 16.2$, 4H), 3.58 (s, 12H), 1.29 (t, $J = 7.1$, 6H), 1.22 (t, $J = 7.1$, 6H). ^{13}C NMR (100 MHz, CDCl_3): 165.8, 165.1, 154.5, 150.0, 125.5, 111.1, 80.0, 78.7, 63.5, 63.1, 56.0, 47.9, 36.7, 13.9, 13.8. MS (FAB, Magic Bullet): m/z 921 (15, $[\text{M} + \text{H}]^+$), 206 (100, $[\text{C}_{11}\text{H}_{12}\text{NO}_3]^+$). HR-MS (FAB, Magic Bullet): m/z 921.3289 ($[\text{M} + \text{H}]^+$, $\text{C}_{42}\text{H}_{49}\text{N}_8\text{O}_{16}$, calcd 921.3267).



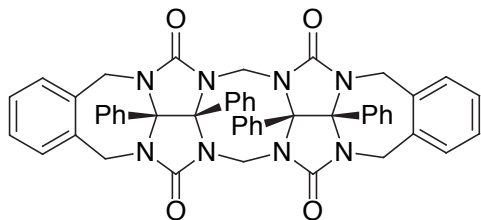
Xylylene dimer tetracarboxylic acid (C_{2v} -20**).**

Compound **13** (0.10 g, 0.26 mmol) and PTSA (0.346 g, 1.820 mmol) in $\text{ClCH}_2\text{CH}_2\text{Cl}$ (10 mL) was heated under nitrogen at reflux for 24 h under a Soxhlet apparatus filled with molecular sieves ($4\text{\AA}$). The solvent was evaporated and the residue was washed with acetone (20

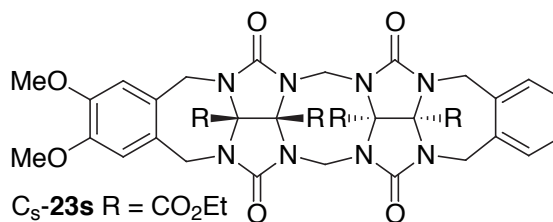
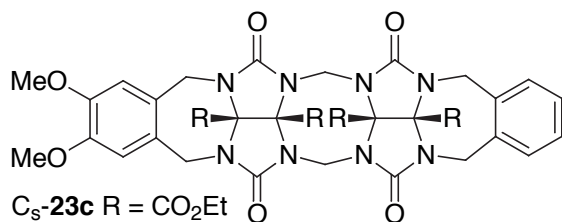
mL). Filtration yielded C_{2v} -**20** (0.078 g, 0.110 mmol, 85%). M.p. $>270\text{ }^\circ\text{C}$. IR (KBr, cm^{-1}): 3425s, 1734s, 1464s, 1424m, 1280m, 906s. ^1H NMR (400 MHz, $\text{DMSO}-d_6$): 7.30-7.00 (m, 8H), 5.66 (d, $J = 15.7$, 2H), 4.64 (d, $J = 15.7$, 2H), 4.61 (d, $J = 15.9$, 4H), 4.43 (d, $J = 15.9$, 4H). ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): 166.7, 165.8, 154.7, 138.8, 128.5, 127.9, 80.3, 79.0, 47.5, 44.7. MS (FAB, Glycerol): m/z 689 (6, $[\text{M} + \text{H}]^+$), 167 (100). HR-MS (FAB, Glycerol): m/z 689.1554 ($[\text{M} + \text{H}]^+$, $\text{C}_{30}\text{H}_{25}\text{N}_8\text{O}_{12}$, calcd 689.1592).



Xylylene dimer diimide (C_{2v} -21**).** A mixture of PTSA (0.19 g, 1.00 mmol) in $\text{ClCH}_2\text{CH}_2\text{Cl}$ (10 mL) was heated under nitrogen at reflux for 30 min. under a Soxhlet apparatus filled with molecular sieves ($4\text{\AA}$). Compound **14** (0.108 g, 0.200 mmol) was added and heating was continued for 24h. The reaction mixture was diluted with EtOAc (100 mL), washed with sat. Na_2CO_3 , dried over anh. MgSO_4 , and concentrated. The residue was washed with Et_2O (20 mL) and dried under high vacuum to yield C_{2v} -**21** (0.070 g, 0.085 mmol, 85%). M.p. >275 dec. $^\circ\text{C}$. TLC ($\text{CHCl}_3/\text{MeOH}$, 1:1) R_f 0.15. IR (thin film, cm^{-1}): 2927w, 2816w, 1751s, 1710s, 1445m, 1420m, 1296m. ^1H NMR (400 MHz, CDCl_3): 7.30-7.15 (m, 8H), 5.74 (d, $J = 15.4$, 2H), 5.20 (d, $J = 15.4$, 2H), 4.94 (d, $J = 15.9$, 4H), 4.80 (d, $J = 15.9$, 4H), 3.75-3.65 (m, 4H), 2.35-2.30 (m, 4H), 2.04 (s, 12H), 1.85-1.75 (m, 4H). ^{13}C NMR (100 MHz, CDCl_3): 168.3, 167.1, 136.6, 129.9, 128.4, 73.3, 70.7, 58.0, 45.8, 45.5, 44.9, 39.0, 29.7, 23.3. MS (FAB, Magic Bullet): m/z 821 (42, $[\text{M} + \text{H}]^+$), 214 (100). HR-MS (FAB, Magic Bullet): m/z 821.3483 ($[\text{M} + \text{H}]^+$, $\text{C}_{40}\text{H}_{45}\text{N}_{12}\text{O}_8$, calcd 821.3462).



Attempted synthesis of xylylene diphenylglycoluril dimer (C_{2v} -22**).** A mixture of PTSA (433 mg, 2.28 mmol) and $\text{ClCH}_2\text{CH}_2\text{Cl}$ (5 mL) was heated under N_2 at reflux for 30 min under a Soxhlet apparatus filled with molecular sieves ($4\text{\AA}$). After cooling, **15** (250 mg, 0.570 mmol) was added and reflux was continued for 96 h. The reaction mixture was diluted with EtOAc (150 mL), washed with sat. aq. Na_2CO_3 (150 mL), brine (150 mL), and dried over anh. MgSO_4 . The crude ^1H NMR did not show the pair of diastereotopic methylene resonances expected for the bridging methylene groups.



Dimethoxyxylylene xylylene dimers (C_{2v} -23c** and C_{2v} -**23s**).** Method 1: A mixture of PTSA (0.19 g, 1.00 mmol) in $\text{ClCH}_2\text{CH}_2\text{Cl}$ (15 mL) was heated under nitrogen at reflux for 30 min.

under a Soxhlet apparatus filled with molecular sieves (4Å). Compound **10** (0.086 g, 0.200 mmol) and **8** (0.090 g, 0.200 mmol) were added and heating was continued for 24 h. The reaction mixture was diluted with EtOAc (100 mL), washed with sat. Na₂CO₃, dried over anh. MgSO₄, and concentrated. Flash chromatography (SiO₂, CHCl₃/ EtOAc, 1:1) gave C_{2v}-**23s** (0.027 g, 0.031 mmol, 16%), C_{2v}-**17** (0.006 g, 0.007 mmol, 8%), C_{2v}-**23c** (0.223 g, 0.260 mmol, 65%), C_{2v}-**18** (0.013 g, 0.014 mmol, 14%).

C_s-**23s**: M.p. 229-230 °C. TLC (EtOAc/Hexanes, 1:1) R_f 0.49. IR (KBr, cm⁻¹): 2982m, 2935m, 2868w, 2830w, 1736s, 1455s, 1384s, 1313s, 1270s, 1018m. ¹H NMR (400 MHz, CDCl₃): 7.35-7.30 (m, 2H), 7.25-7.20 (m, 2H), 6.83 (s, 2H), 5.01 (AB q, 4H), 4.82 (d, *J* = 16.0, 2H), 4.72 (d, *J* = 16.0, 2H), 4.35 (d, *J* = 16.0, 2H), 4.30 (d, *J* = 16.0, 2H), 4.25-4.15 (m, 4H), 3.84 (s, 6H), 3.71 (q, *J* = 7.1, 2H), 3.60 (q, *J* = 7.1, 2H), 1.30-1.20 (m, 6H), 1.15-1.05 (m, 6H). ¹³C NMR (100 MHz, CDCl₃): 165.3, 165.2, 164.0, 155.3, 155.2, 148.0, 136.2, 129.7, 128.6, 128.2, 113.0, 81.7, 81.5, 78.6, 78.5, 63.8, 63.7, 63.7, 63.6, 56.0, 51.8, 45.1, 44.9, 13.9, 13.6, (only 25 of the 28 expected resonances were observed). MS (FAB, Magic Bullet): *m/z* 861 (24, [M + H]⁺), 206 (100, [C₁₁H₁₂NO₃]⁺). HR-MS (FAB, Magic Bullet): *m/z* 861.3126 ([M + H]⁺, C₄₀H₄₅N₈O₁₄, calcd 861.3055). X-ray crystal structure.

C_s-**23c**: M.p. 288-289 °C. TLC (EtOAc/Hexanes, 1:1) R_f 0.10. IR (KBr, cm⁻¹): 2982w, 2940w, 2900w, 2840w, 1740s, 1450s, 1422m, 1256s, 1013m, 913m. ¹H NMR (400 MHz, CDCl₃): 7.30-7.15 (m, 4H), 6.74 (s, 2H), 6.04 (d, *J* = 16.1, 2H), 4.87 (d, *J* = 16.1, 2H), 4.77 (d, *J* = 16.1, 2H), 4.61 (d, *J* = 16.1, 2H), 4.41 (d, *J* = 16.1, 2H), 4.36 (d, *J* = 16.1, 2H), 4.30-4.15 (m, 8H), 3.79 (s, 6H), 1.31 (t, *J* = 7.1, 6H), 1.26 (t, *J* = 7.1, 2H). ¹³C NMR (100 MHz, CDCl₃): 165.6, 165.5, 164.9, 154.6, 147.9, 136.2, 129.7, 128.5, 128.4, 113.0, 80.1, 80.0, 78.7, 63.7, 63.4, 63.3, 55.8, 47.8, 45.3, 45.0, 13.9, 13.8, (only 22 of the 28 expected resonances were observed). MS (FAB, Magic Bullet): *m/z* 861 (22, [M + H]⁺), 206 (100, [C₁₁H₁₂NO₃]⁺). HR-MS (FAB, Magic Bullet): *m/z* 861.3091 ([M + H]⁺, C₄₀H₄₅N₈O₁₄, calcd 861.3055).

Details of the x-ray structural determination of **17**.

Experimental: An orange, hexagonal block, with dimensions 0.50 x 0.45 x 0.38 mm was placed and optically centered on the Enraf-Nonius CAD-4 diffractometer that was controlled by a Digital Equipment Corporation MicroVAX II (MVII) computer and the Enraf-Nonius VAX\VMS CAD4 Express control program¹. The crystals' final cell parameters and crystal orientation matrix were determined from 25 reflections in the range 17.9 < θ < 19.1°; these constants were confirmed with axial photographs. Data were collected [MoKα] with ω scans over the range 2.3 < θ < 25.0° with a scan width of (0.59+0.45tanθ)° and fixed scan speed of 3.3°min.⁻¹ with each scan recorded in 96 steps with the outermost 16 steps on each end of the scan being used for background determination. Three standard reflections well dispersed in reciprocal space were monitored at 60-minute intervals of X-ray exposure. Minor variations in intensity were observed; data were not corrected. Eleven ψ-scan reflections were collected twice

over the range $6.0 < \theta < 13.7^\circ$; the absorption correction was applied with transmission factors ranging from 0.9529-0.9644. One form of data was collected, indices $hk\pm l$ resulting in the measurement of 8815 reflections; 8332 unique [$R(\text{int}) = 0.0129$].

Structural determination and Refinement: All crystallographic calculations were performed on a Personal computer (PC) with dual Pentium 450MHz processors and 256MB of extended memory. Data were corrected for Lorentz and polarization factors and reduced to F_o^2 and $\bar{F}_o^2$ using the program XCAD4². Systematic absences clearly determined the centrosymmetric monoclinic space group $P2_1/c$ (no. 14). The SHELXTL³ program package was now implemented to confirm the monoclinic centric space group $P2_1/c$, to apply the absorption correction, and set up the initial files. The structure was determined by direct methods with the successful location of nearly all non-hydrogen atoms using the program XS⁴ that also included two full occupancy benzene solvent molecules. The structure was refined with XL⁵. The remaining non-hydrogen atoms were located directly from an initial difference-Fourier map. After several cycles of refinement, all of the non-hydrogen atoms were refined anisotropically. Hydrogen atoms were initially placed in calculated positions but later allowed to refine freely (xyzU). The final structure was refined to convergence [$\Delta/\sigma \leq 0.001$] with $R(F)=6.98\%$, $wR(F^2)=10.95\%$ and $GOF=1.023$ for all 8332 unique reflections [$R(F)=4.38\%$, $wR(F^2)=9.69\%$ for those 6096 data with $F_o > 4\sigma(F_o)$]. A final difference-Fourier map was featureless with the largest peak, $|\Delta\rho| \leq 0.33\text{e}\text{\AA}^{-3}$, indicating that the structure is both correct and complete.

The function minimized during the full-matrix least-squares refinement was $\Sigma w(F_o^2 - F_c^2)^2$ where $w = 1/[\sigma^2(F_o^2) + (0.0467 \cdot P)^2 + 2.1939 \cdot P]$ and $P = (\max(F_o^2, 0) + 2 \cdot F_c^2)/3$. An empirical correction for extinction was also attempted but found to be negative and therefore not applied.

References:

1. Enraf-Nonius(1994). CAD-4 EXPRESS. Version 5.1/1.2 Enraf-Nonius, Delft, The Netherlands.
2. Harms K., XCAD4 (1997). Program for the Lp-correction of Nonius-CAD-4 diffractometer data, University of Marburg, Germany.
3. Sheldrick, G.M., (1994). SHELXTL. Version 5.03. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
4. Sheldrick, G.M., (1990). Acta Cryst. A46, 467-473.
5. Sheldrick, G.M., (1993). Shelxl93 Program for the Refinement of Crystal Structures. University of Göttingen, Germany.

Table 1. Crystal data and structure refinement for $[\text{C}_{38}\text{H}_{40}\text{N}_8\text{O}_{12}][\text{C}_6\text{H}_6]_2$.

Identification code	d
Empirical formula	$\text{C}_{50}\text{H}_{52}\text{N}_8\text{O}_{12}$
Formula weight	957.00

Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 10.5520(6) Å	$\alpha = 90^\circ$.
	b = 26.114(3) Å	$\beta = 95.048(7)^\circ$.
	c = 17.2513(11) Å	$\gamma = 90^\circ$.
Volume	4735.3(7) Å ³	
Z	4	
Density (calculated)	1.342 Mg/m ³	
Absorption coefficient	0.098 mm ⁻¹	
F(000)	2016	
Crystal size	0.50 x 0.45 x 0.38 mm ³	
Theta range for data collection	2.32 to 25.00°.	
Index ranges	0 ≤ h ≤ 12, 0 ≤ k ≤ 31, -20 ≤ l ≤ 20	
Reflections collected	8815	
Independent reflections	8332 [R(int) = 0.0129]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9644 and 0.9529	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	8332 / 0 / 839	
Goodness-of-fit on F ²	1.023	
Final R indices [I > 2sigma(I)]	R1 = 0.0438, wR2 = 0.0969 [6096 Data]	
R indices (all data)	R1 = 0.0698, wR2 = 0.1095	
Largest diff. peak and hole	0.333 and -0.206 e.Å ⁻³	

Table 2. Atomic coordinates (× 10⁴) and equivalent isotropic displacement parameters (Å² × 10³) for [C₃₈H₄₀N₈O₁₂][C₆H₆]₂. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	5697(2)	7936(1)	2626(1)	35(1)

C(2)	4849(2)	7597(1)	2923(1)	40(1)
C(3)	4053(2)	7309(1)	2422(1)	38(1)
C(4A)	4943(2)	7692(1)	1315(1)	27(1)
C(4)	4104(2)	7355(1)	1623(1)	32(1)
C(5)	4913(2)	7751(1)	443(1)	29(1)
N(5A)	6135(2)	7663(1)	117(1)	25(1)
C(6)	6510(2)	7181(1)	-75(1)	26(1)
N(6A)	7815(2)	7189(1)	-137(1)	25(1)
O(6)	5828(1)	6811(1)	-190(1)	35(1)
N(7A)	9274(2)	6461(1)	-109(1)	25(1)
C(7)	8388(2)	6785(1)	-569(1)	25(1)
N(8A)	9986(2)	5750(1)	497(1)	26(1)
O(8)	7925(1)	5763(1)	-66(1)	32(1)
C(8)	8945(2)	5969(1)	99(1)	26(1)
C(9A)	9529(2)	5343(1)	1744(1)	29(1)
C(9)	9913(2)	5272(1)	928(1)	29(1)
C(10)	8442(2)	5102(1)	1962(1)	35(1)
C(11)	8098(3)	5149(1)	2717(2)	42(1)
C(12)	8818(2)	5441(1)	3256(2)	43(1)
C(13A)	10271(2)	5640(1)	2291(1)	31(1)
C(13)	9891(2)	5686(1)	3040(1)	38(1)
N(14A)	11269(2)	6259(1)	1440(1)	28(1)
C(14)	11469(2)	5895(1)	2083(1)	32(1)
N(15A)	10553(2)	6973(1)	848(1)	27(1)
O(15)	11105(1)	6985(1)	2174(1)	32(1)
C(15)	10981(2)	6759(1)	1557(1)	26(1)
C(15C)	11032(2)	6099(1)	644(1)	26(1)
C(15B)	10533(2)	6608(1)	212(1)	25(1)
N(16A)	9266(2)	7750(1)	656(1)	27(1)
C(16)	10524(2)	7525(1)	751(1)	29(1)
O(16E)	12156(2)	5688(1)	-333(1)	43(1)
C(16E)	12227(2)	5877(1)	304(1)	29(1)
O(16D)	12461(1)	6955(1)	-191(1)	37(1)
C(16D)	11433(2)	6785(1)	-395(1)	27(1)
N(17A)	7550(2)	8136(1)	1028(1)	27(1)
C(17B)	7180(2)	8014(1)	228(1)	26(1)

C(17C)	8359(2)	7699(1)	-19(1)	25(1)
C(17)	8750(2)	7983(1)	1276(1)	27(1)
O(17)	9282(1)	8047(1)	1921(1)	36(1)
C(17E)	14456(2)	5763(1)	478(2)	50(1)
O(17E)	13262(1)	5933(1)	774(1)	39(1)
O(17D)	10941(1)	6721(1)	-1111(1)	40(1)
C(17D)	11749(3)	6872(1)	-1730(2)	51(1)
C(18A)	5750(2)	7989(1)	1829(1)	29(1)
C(18)	6669(2)	8368(1)	1531(1)	30(1)
O(18B)	7768(2)	8855(1)	-177(1)	43(1)
C(18B)	6977(2)	8524(1)	-226(1)	31(1)
C(18C)	8919(2)	7891(1)	-760(1)	29(1)
O(18C)	10018(2)	7989(1)	-787(1)	54(1)
C(18E)	15452(3)	5807(3)	1130(3)	97(2)
C(18D)	12607(4)	6438(2)	-1897(2)	71(1)
O(19B)	5867(1)	8548(1)	-638(1)	39(1)
C(19B)	5589(3)	9030(1)	-1050(2)	51(1)
C(19C)	8502(3)	8021(1)	-2114(1)	45(1)
O(19C)	8035(1)	7909(1)	-1350(1)	33(1)
C(20B)	4348(4)	8971(1)	-1495(3)	74(1)
C(20C)	7485(3)	8272(1)	-2625(2)	48(1)
C(21)	2635(4)	4417(1)	1946(2)	59(1)
C(22)	3381(4)	4644(1)	2567(2)	68(1)
C(23)	2871(4)	4695(1)	3267(2)	60(1)
C(24)	1651(3)	4519(1)	3367(2)	62(1)
C(25)	948(3)	4299(1)	2758(2)	62(1)
C(26)	1445(3)	4246(1)	2042(2)	61(1)
C(31)	2626(4)	5281(1)	5240(2)	73(1)
C(32)	3567(3)	5496(1)	5721(2)	68(1)
C(33)	3376(4)	5957(1)	6055(2)	70(1)
C(34)	2280(5)	6208(1)	5919(2)	88(1)
C(35)	1312(4)	5994(2)	5430(3)	91(1)
C(36)	1492(4)	5523(2)	5084(2)	76(1)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for $[\text{C}_{38}\text{H}_{40}\text{N}_8\text{O}_{12}][\text{C}_6\text{H}_6]_2$.

C(1)-C(18A)	1.387(3)	C(10)-C(11)	1.389(3)
C(1)-C(2)	1.389(3)	C(10)-H(10)	0.97(2)
C(1)-H(1)	1.00(2)	C(11)-C(12)	1.376(4)
C(2)-C(3)	1.375(3)	C(11)-H(11)	0.93(2)
C(2)-H(2)	0.99(2)	C(12)-C(13)	1.381(3)
C(3)-C(4)	1.389(3)	C(12)-H(12)	0.99(3)
C(3)-H(3)	0.96(3)	C(13A)-C(13)	1.393(3)
C(4A)-C(4)	1.386(3)	C(13A)-C(14)	1.501(3)
C(4A)-C(18A)	1.407(3)	C(13)-H(13)	0.98(3)
C(4A)-C(5)	1.511(3)	N(14A)-C(15)	1.360(3)
C(4)-H(4)	0.95(2)	N(14A)-C(15C)	1.436(3)
C(5)-N(5A)	1.469(3)	N(14A)-C(14)	1.460(3)
C(5)-H(5A)	0.97(2)	C(14)-H(14A)	0.99(2)
C(5)-H(5B)	0.98(2)	C(14)-H(14B)	0.96(2)
N(5A)-C(6)	1.370(3)	N(15A)-C(15)	1.385(3)
N(5A)-C(17B)	1.434(3)	N(15A)-C(16)	1.450(3)
C(6)-O(6)	1.209(2)	N(15A)-C(15B)	1.452(3)
C(6)-N(6A)	1.391(3)	O(15)-C(15)	1.213(2)
N(6A)-C(7)	1.455(3)	C(15C)-C(16E)	1.549(3)
N(6A)-C(17C)	1.458(2)	C(15C)-C(15B)	1.590(3)
N(7A)-C(8)	1.386(3)	C(15B)-C(16D)	1.545(3)
N(7A)-C(7)	1.445(3)	N(16A)-C(17)	1.384(3)
N(7A)-C(15B)	1.446(2)	N(16A)-C(17C)	1.447(2)
C(7)-H(7A)	0.96(2)	N(16A)-C(16)	1.448(3)
C(7)-H(7B)	0.97(2)	C(16)-H(16A)	0.99(2)
N(8A)-C(8)	1.368(3)	C(16)-H(16B)	1.00(2)
N(8A)-C(15C)	1.436(3)	O(16E)-C(16E)	1.202(3)
N(8A)-C(9)	1.459(3)	C(16E)-O(17E)	1.310(3)
O(8)-C(8)	1.215(2)	O(16D)-C(16D)	1.197(2)
C(9A)-C(10)	1.388(3)	C(16D)-O(17D)	1.309(2)
C(9A)-C(13A)	1.405(3)	N(17A)-C(17)	1.361(3)
C(9A)-C(9)	1.510(3)	N(17A)-C(17B)	1.437(3)
C(9)-H(9A)	0.99(2)	N(17A)-C(18)	1.457(3)
C(9)-H(9B)	0.96(2)	C(17B)-C(18B)	1.549(3)

C(17B)-C(17C)	1.580(3)	C(20C)-H(20E)	0.98(3)
C(17C)-C(18C)	1.539(3)	C(20C)-H(20F)	0.97(3)
C(17)-O(17)	1.213(2)	C(21)-C(26)	1.356(5)
C(17E)-O(17E)	1.469(3)	C(21)-C(22)	1.403(4)
C(17E)-C(18E)	1.474(5)	C(21)-H(21)	0.99(3)
C(17E)-H(17C)	1.02(3)	C(22)-C(23)	1.370(5)
C(17E)-H(17D)	0.94(3)	C(22)-H(22)	1.09(3)
O(17D)-C(17D)	1.477(3)	C(23)-C(24)	1.391(5)
C(17D)-C(18D)	1.493(5)	C(23)-H(23)	0.97(3)
C(17D)-H(17A)	1.02(3)	C(24)-C(25)	1.360(4)
C(17D)-H(17B)	0.93(3)	C(24)-H(24)	1.14(3)
C(18A)-C(18)	1.507(3)	C(25)-C(26)	1.390(4)
C(18)-H(18A)	0.99(2)	C(25)-H(25)	1.14(4)
C(18)-H(18B)	0.97(2)	C(26)-H(26)	1.04(3)
O(18B)-C(18B)	1.200(3)	C(31)-C(36)	1.359(5)
C(18B)-O(19B)	1.316(3)	C(31)-C(32)	1.359(5)
C(18C)-O(18C)	1.193(3)	C(31)-H(31)	0.98(4)
C(18C)-O(19C)	1.319(2)	C(32)-C(33)	1.358(5)
C(18E)-H(18F)	0.90(9)	C(32)-H(32)	1.08(4)
C(18E)-H(18G)	0.96(4)	C(33)-C(34)	1.331(5)
C(18E)-H(18H)	1.05(5)	C(33)-H(33)	1.06(4)
C(18D)-H(18C)	1.01(4)	C(34)-C(35)	1.384(6)
C(18D)-H(18D)	0.99(3)	C(34)-H(34)	0.94(5)
C(18D)-H(18E)	0.98(4)	C(35)-C(36)	1.387(6)
O(19B)-C(19B)	1.465(3)	C(35)-H(35)	0.85(5)
C(19B)-C(20B)	1.467(4)	C(36)-H(36)	0.83(4)
C(19B)-H(19A)	0.98(3)		
C(19B)-H(19B)	1.07(4)	C(18A)-C(1)-C(2)	120.8(2)
C(19C)-O(19C)	1.476(3)	C(18A)-C(1)-H(1)	118.0(13)
C(19C)-C(20C)	1.481(4)	C(2)-C(1)-H(1)	121.2(13)
C(19C)-H(19C)	0.95(3)	C(3)-C(2)-C(1)	119.7(2)
C(19C)-H(19D)	1.02(3)	C(3)-C(2)-H(2)	119.9(14)
C(20B)-H(20A)	1.05(5)	C(1)-C(2)-H(2)	120.4(14)
C(20B)-H(20B)	1.05(4)	C(2)-C(3)-C(4)	120.0(2)
C(20B)-H(20C)	1.01(3)	C(2)-C(3)-H(3)	120.0(15)
C(20C)-H(20D)	0.96(3)	C(4)-C(3)-H(3)	120.0(15)

C(4)-C(4A)-C(18A)	118.7(2)	C(10)-C(9A)-C(13A)	119.5(2)
C(4)-C(4A)-C(5)	119.23(19)	C(10)-C(9A)-C(9)	119.5(2)
C(18A)-C(4A)-C(5)	121.98(19)	C(13A)-C(9A)-C(9)	120.95(19)
C(4A)-C(4)-C(3)	121.1(2)	N(8A)-C(9)-C(9A)	113.59(17)
C(4A)-C(4)-H(4)	118.1(13)	N(8A)-C(9)-H(9A)	105.3(13)
C(3)-C(4)-H(4)	120.8(13)	C(9A)-C(9)-H(9A)	112.7(12)
N(5A)-C(5)-C(4A)	115.04(17)	N(8A)-C(9)-H(9B)	108.1(13)
N(5A)-C(5)-H(5A)	105.8(12)	C(9A)-C(9)-H(9B)	109.2(13)
C(4A)-C(5)-H(5A)	110.3(12)	H(9A)-C(9)-H(9B)	107.7(18)
N(5A)-C(5)-H(5B)	107.2(12)	C(9A)-C(10)-C(11)	120.3(2)
C(4A)-C(5)-H(5B)	110.6(12)	C(9A)-C(10)-H(10)	120.5(13)
H(5A)-C(5)-H(5B)	107.5(17)	C(11)-C(10)-H(10)	119.2(13)
C(6)-N(5A)-C(17B)	112.65(16)	C(12)-C(11)-C(10)	120.5(2)
C(6)-N(5A)-C(5)	121.14(17)	C(12)-C(11)-H(11)	119.9(15)
C(17B)-N(5A)-C(5)	122.68(17)	C(10)-C(11)-H(11)	119.5(15)
O(6)-C(6)-N(5A)	126.40(19)	C(11)-C(12)-C(13)	119.5(2)
O(6)-C(6)-N(6A)	125.38(19)	C(11)-C(12)-H(12)	120.7(15)
N(5A)-C(6)-N(6A)	108.20(17)	C(13)-C(12)-H(12)	119.8(15)
C(6)-N(6A)-C(7)	119.11(17)	C(13)-C(13A)-C(9A)	118.9(2)
C(6)-N(6A)-C(17C)	112.60(16)	C(13)-C(13A)-C(14)	120.0(2)
C(7)-N(6A)-C(17C)	123.99(17)	C(9A)-C(13A)-C(14)	121.09(19)
C(8)-N(7A)-C(7)	121.34(17)	C(12)-C(13)-C(13A)	121.2(2)
C(8)-N(7A)-C(15B)	112.87(16)	C(12)-C(13)-H(13)	120.6(14)
C(7)-N(7A)-C(15B)	125.72(16)	C(13A)-C(13)-H(13)	118.2(15)
N(7A)-C(7)-N(6A)	114.94(16)	C(15)-N(14A)-C(15C)	113.47(16)
N(7A)-C(7)-H(7A)	107.0(12)	C(15)-N(14A)-C(14)	122.03(18)
N(6A)-C(7)-H(7A)	104.6(12)	C(15C)-N(14A)-C(14)	122.63(17)
N(7A)-C(7)-H(7B)	109.5(12)	N(14A)-C(14)-C(13A)	113.67(18)
N(6A)-C(7)-H(7B)	109.5(12)	N(14A)-C(14)-H(14A)	105.5(14)
H(7A)-C(7)-H(7B)	111.2(17)	C(13A)-C(14)-H(14A)	110.4(14)
C(8)-N(8A)-C(15C)	113.18(16)	N(14A)-C(14)-H(14B)	107.8(12)
C(8)-N(8A)-C(9)	122.47(17)	C(13A)-C(14)-H(14B)	110.7(12)
C(15C)-N(8A)-C(9)	121.86(17)	H(14A)-C(14)-H(14B)	108.5(18)
O(8)-C(8)-N(8A)	126.07(19)	C(15)-N(15A)-C(16)	120.38(17)
O(8)-C(8)-N(7A)	125.87(19)	C(15)-N(15A)-C(15B)	112.57(16)
N(8A)-C(8)-N(7A)	108.01(17)	C(16)-N(15A)-C(15B)	124.48(17)

O(15)-C(15)-N(14A)	126.11(19)	N(5A)-C(17B)-C(17C)	104.25(15)
O(15)-C(15)-N(15A)	125.42(19)	N(17A)-C(17B)-C(17C)	102.76(15)
N(14A)-C(15)-N(15A)	108.45(17)	C(18B)-C(17B)-C(17C)	112.77(16)
N(14A)-C(15C)-N(8A)	114.79(17)	N(16A)-C(17C)-N(6A)	114.89(16)
N(14A)-C(15C)-C(16E)	113.03(16)	N(16A)-C(17C)-C(18C)	111.30(16)
N(8A)-C(15C)-C(16E)	109.50(16)	N(6A)-C(17C)-C(18C)	110.85(16)
N(14A)-C(15C)-C(15B)	103.20(16)	N(16A)-C(17C)-C(17B)	102.50(16)
N(8A)-C(15C)-C(15B)	103.30(15)	N(6A)-C(17C)-C(17B)	101.74(15)
C(16E)-C(15C)-C(15B)	112.51(16)	C(18C)-C(17C)-C(17B)	115.09(16)
N(7A)-C(15B)-N(15A)	114.58(16)	O(17)-C(17)-N(17A)	126.2(2)
N(7A)-C(15B)-C(16D)	114.71(16)	O(17)-C(17)-N(16A)	126.00(19)
N(15A)-C(15B)-C(16D)	110.30(16)	N(17A)-C(17)-N(16A)	107.78(17)
N(7A)-C(15B)-C(15C)	102.32(15)	O(17E)-C(17E)-C(18E)	106.7(3)
N(15A)-C(15B)-C(15C)	102.30(15)	O(17E)-C(17E)-H(17C)	105.9(19)
C(16D)-C(15B)-C(15C)	111.65(16)	C(18E)-C(17E)-H(17C)	105.2(19)
C(17)-N(16A)-C(17C)	112.61(16)	O(17E)-C(17E)-H(17D)	108.1(15)
C(17)-N(16A)-C(16)	120.72(17)	C(18E)-C(17E)-H(17D)	114.0(15)
C(17C)-N(16A)-C(16)	126.07(17)	H(17C)-C(17E)-H(17D)	116(2)
N(16A)-C(16)-N(15A)	115.26(17)	C(16E)-O(17E)-C(17E)	116.47(19)
N(16A)-C(16)-H(16A)	110.2(12)	C(16D)-O(17D)-C(17D)	116.22(18)
N(15A)-C(16)-H(16A)	108.5(12)	O(17D)-C(17D)-C(18D)	109.6(3)
N(16A)-C(16)-H(16B)	104.7(14)	O(17D)-C(17D)-H(17A)	105.5(15)
N(15A)-C(16)-H(16B)	105.7(14)	C(18D)-C(17D)-H(17A)	111.4(15)
H(16A)-C(16)-H(16B)	112.5(18)	O(17D)-C(17D)-H(17B)	102.4(19)
O(16E)-C(16E)-O(17E)	126.4(2)	C(18D)-C(17D)-H(17B)	114(2)
O(16E)-C(16E)-C(15C)	120.85(19)	H(17A)-C(17D)-H(17B)	114(3)
O(17E)-C(16E)-C(15C)	112.74(18)	C(1)-C(18A)-C(4A)	119.6(2)
O(16D)-C(16D)-O(17D)	126.8(2)	C(1)-C(18A)-C(18)	119.1(2)
O(16D)-C(16D)-C(15B)	120.54(18)	C(4A)-C(18A)-C(18)	121.24(19)
O(17D)-C(16D)-C(15B)	112.70(17)	N(17A)-C(18)-C(18A)	113.22(17)
C(17)-N(17A)-C(17B)	113.77(16)	N(17A)-C(18)-H(18A)	106.4(12)
C(17)-N(17A)-C(18)	124.06(17)	C(18A)-C(18)-H(18A)	109.0(12)
C(17B)-N(17A)-C(18)	122.01(17)	N(17A)-C(18)-H(18B)	108.4(13)
N(5A)-C(17B)-N(17A)	114.31(16)	C(18A)-C(18)-H(18B)	110.4(13)
N(5A)-C(17B)-C(18B)	114.22(16)	H(18A)-C(18)-H(18B)	109.3(18)
N(17A)-C(17B)-C(18B)	108.00(16)	O(18B)-C(18B)-O(19B)	125.8(2)

O(18B)-C(18B)-C(17B)	121.23(19)	H(20B)-C(20B)-H(20C)	114(3)
O(19B)-C(18B)-C(17B)	112.98(18)	C(19C)-C(20C)-H(20D)	114.3(18)
O(18C)-C(18C)-O(19C)	125.9(2)	C(19C)-C(20C)-H(20E)	109.7(16)
O(18C)-C(18C)-C(17C)	123.20(19)	H(20D)-C(20C)-H(20E)	108(2)
O(19C)-C(18C)-C(17C)	110.83(17)	C(19C)-C(20C)-H(20F)	112.6(18)
C(17E)-C(18E)-H(18F)	110(5)	H(20D)-C(20C)-H(20F)	104(2)
C(17E)-C(18E)-H(18G)	105(2)	H(20E)-C(20C)-H(20F)	108(2)
H(18F)-C(18E)-H(18G)	125(6)	C(26)-C(21)-C(22)	120.5(3)
C(17E)-C(18E)-H(18H)	99(2)	C(26)-C(21)-H(21)	134.0(16)
H(18F)-C(18E)-H(18H)	113(6)	C(22)-C(21)-H(21)	105.0(17)
H(18G)-C(18E)-H(18H)	101(3)	C(23)-C(22)-C(21)	118.4(4)
C(17D)-C(18D)-H(18C)	109(2)	C(23)-C(22)-H(22)	126.6(18)
C(17D)-C(18D)-H(18D)	110.3(19)	C(21)-C(22)-H(22)	114.6(18)
H(18C)-C(18D)-H(18D)	107(3)	C(22)-C(23)-C(24)	121.1(3)
C(17D)-C(18D)-H(18E)	107(2)	C(22)-C(23)-H(23)	117.2(19)
H(18C)-C(18D)-H(18E)	117(3)	C(24)-C(23)-H(23)	121.7(19)
H(18D)-C(18D)-H(18E)	107(3)	C(25)-C(24)-C(23)	119.5(3)
C(18B)-O(19B)-C(19B)	115.69(19)	C(25)-C(24)-H(24)	118.3(17)
O(19B)-C(19B)-C(20B)	107.2(2)	C(23)-C(24)-H(24)	122.1(17)
O(19B)-C(19B)-H(19A)	106.3(17)	C(24)-C(25)-C(26)	120.3(3)
C(20B)-C(19B)-H(19A)	114.9(17)	C(24)-C(25)-H(25)	122.5(19)
O(19B)-C(19B)-H(19B)	109.8(18)	C(26)-C(25)-H(25)	117.0(19)
C(20B)-C(19B)-H(19B)	107.0(18)	C(21)-C(26)-C(25)	120.2(3)
H(19A)-C(19B)-H(19B)	112(2)	C(21)-C(26)-H(26)	121.1(17)
O(19C)-C(19C)-C(20C)	109.7(2)	C(25)-C(26)-H(26)	118.6(18)
O(19C)-C(19C)-H(19C)	105.3(16)	C(36)-C(31)-C(32)	120.8(4)
C(20C)-C(19C)-H(19C)	113.9(16)	C(36)-C(31)-H(31)	120(2)
O(19C)-C(19C)-H(19D)	109.0(16)	C(32)-C(31)-H(31)	120(2)
C(20C)-C(19C)-H(19D)	112.2(16)	C(33)-C(32)-C(31)	119.9(4)
H(19C)-C(19C)-H(19D)	106(2)	C(33)-C(32)-H(32)	117(2)
C(18C)-O(19C)-C(19C)	115.24(18)	C(31)-C(32)-H(32)	123(2)
C(19B)-C(20B)-H(20A)	104(3)	C(34)-C(33)-C(32)	121.3(4)
C(19B)-C(20B)-H(20B)	105.8(19)	C(34)-C(33)-H(33)	119(2)
H(20A)-C(20B)-H(20B)	109(3)	C(32)-C(33)-H(33)	120(2)
C(19B)-C(20B)-H(20C)	108.6(17)	C(33)-C(34)-C(35)	119.5(4)
H(20A)-C(20B)-H(20C)	114(3)	C(33)-C(34)-H(34)	119(3)

C(35)-C(34)-H(34)	121(3)	C(31)-C(36)-C(35)	118.6(4)
C(34)-C(35)-C(36)	119.9(4)	C(31)-C(36)-H(36)	124(3)
C(34)-C(35)-H(35)	119(3)	C(35)-C(36)-H(36)	117(3)
C(36)-C(35)-H(35)	121(3)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{C}_{38}\text{H}_{40}\text{N}_8\text{O}_{12}][\text{C}_6\text{H}_6]_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	28(1)	45(1)	31(1)	-6(1)	-1(1)	2(1)
C(2)	34(1)	55(2)	31(1)	2(1)	5(1)	2(1)
C(3)	30(1)	46(1)	39(1)	8(1)	6(1)	-3(1)
C(4A)	23(1)	27(1)	31(1)	-1(1)	0(1)	5(1)
C(4)	23(1)	35(1)	37(1)	-1(1)	1(1)	-1(1)
C(5)	22(1)	32(1)	33(1)	-2(1)	1(1)	-1(1)
N(5A)	21(1)	27(1)	28(1)	-1(1)	0(1)	-1(1)
C(6)	25(1)	27(1)	25(1)	2(1)	-2(1)	-3(1)
N(6A)	23(1)	23(1)	29(1)	-1(1)	-1(1)	-2(1)
O(6)	28(1)	31(1)	45(1)	-4(1)	1(1)	-6(1)
N(7A)	22(1)	24(1)	28(1)	1(1)	-2(1)	-2(1)
C(7)	24(1)	26(1)	25(1)	-2(1)	-3(1)	-2(1)
N(8A)	27(1)	25(1)	27(1)	4(1)	0(1)	-2(1)
O(8)	28(1)	31(1)	37(1)	1(1)	-2(1)	-8(1)
C(8)	27(1)	26(1)	24(1)	-2(1)	4(1)	-1(1)
C(9A)	32(1)	25(1)	30(1)	6(1)	4(1)	7(1)
C(9)	32(1)	25(1)	30(1)	2(1)	3(1)	0(1)
C(10)	36(1)	30(1)	39(1)	7(1)	7(1)	1(1)
C(11)	41(1)	44(2)	45(2)	10(1)	16(1)	5(1)
C(12)	52(2)	45(2)	33(1)	6(1)	16(1)	8(1)
C(13A)	34(1)	28(1)	29(1)	6(1)	1(1)	9(1)
C(13)	47(1)	38(1)	28(1)	2(1)	4(1)	8(1)

N(14A)	29(1)	30(1)	24(1)	0(1)	-2(1)	1(1)
C(14)	35(1)	35(1)	26(1)	3(1)	-3(1)	4(1)
N(15A)	29(1)	24(1)	27(1)	-2(1)	-3(1)	0(1)
O(15)	32(1)	38(1)	27(1)	-7(1)	1(1)	-1(1)
C(15)	18(1)	33(1)	28(1)	-2(1)	0(1)	-2(1)
C(15C)	26(1)	27(1)	24(1)	1(1)	0(1)	-1(1)
C(15B)	25(1)	25(1)	26(1)	-1(1)	-1(1)	-2(1)
N(16A)	24(1)	26(1)	28(1)	-3(1)	-4(1)	-1(1)
C(16)	27(1)	26(1)	34(1)	-4(1)	-2(1)	-2(1)
O(16E)	42(1)	44(1)	44(1)	-13(1)	12(1)	-4(1)
C(16E)	32(1)	23(1)	33(1)	2(1)	4(1)	0(1)
O(16D)	27(1)	43(1)	40(1)	-4(1)	2(1)	-9(1)
C(16D)	26(1)	24(1)	29(1)	2(1)	-2(1)	-1(1)
N(17A)	27(1)	28(1)	27(1)	-3(1)	1(1)	-2(1)
C(17B)	25(1)	27(1)	26(1)	0(1)	0(1)	-2(1)
C(17C)	23(1)	23(1)	28(1)	0(1)	0(1)	-1(1)
C(17)	28(1)	21(1)	31(1)	-1(1)	-1(1)	-3(1)
O(17)	37(1)	34(1)	33(1)	-8(1)	-9(1)	2(1)
C(17E)	30(1)	64(2)	58(2)	14(2)	15(1)	13(1)
O(17E)	25(1)	54(1)	39(1)	5(1)	2(1)	8(1)
O(17D)	30(1)	66(1)	25(1)	6(1)	2(1)	-9(1)
C(17D)	36(1)	89(2)	29(1)	13(1)	4(1)	-7(2)
C(18A)	26(1)	28(1)	34(1)	-4(1)	3(1)	4(1)
C(18)	31(1)	29(1)	32(1)	-7(1)	2(1)	-1(1)
O(18B)	49(1)	31(1)	48(1)	8(1)	1(1)	-9(1)
C(18B)	31(1)	29(1)	33(1)	1(1)	5(1)	2(1)
C(18C)	28(1)	26(1)	32(1)	-1(1)	3(1)	-2(1)
O(18C)	32(1)	85(1)	45(1)	15(1)	3(1)	-16(1)
C(18E)	32(2)	183(5)	77(3)	35(3)	8(2)	30(2)
C(18D)	77(2)	82(2)	61(2)	-17(2)	40(2)	-25(2)
O(19B)	35(1)	34(1)	46(1)	12(1)	-2(1)	5(1)
C(19B)	55(2)	41(2)	54(2)	16(1)	-3(1)	13(1)
C(19C)	53(2)	52(2)	30(1)	7(1)	12(1)	3(1)
O(19C)	32(1)	41(1)	26(1)	3(1)	2(1)	-2(1)
C(20B)	76(2)	49(2)	91(3)	10(2)	-34(2)	13(2)
C(20C)	54(2)	54(2)	36(2)	12(1)	0(1)	-10(2)

C(21)	90(2)	46(2)	38(2)	3(1)	-6(2)	5(2)
C(22)	92(3)	46(2)	64(2)	9(2)	2(2)	-4(2)
C(23)	92(2)	39(2)	46(2)	-5(1)	-10(2)	2(2)
C(24)	79(2)	45(2)	62(2)	-1(2)	2(2)	15(2)
C(25)	71(2)	46(2)	67(2)	-1(2)	-8(2)	23(2)
C(26)	82(2)	41(2)	55(2)	-2(1)	-18(2)	13(2)
C(31)	116(3)	57(2)	45(2)	-4(2)	6(2)	11(2)
C(32)	58(2)	80(2)	67(2)	0(2)	18(2)	6(2)
C(33)	77(2)	59(2)	73(2)	9(2)	-1(2)	-25(2)
C(34)	126(4)	46(2)	88(3)	-3(2)	-11(3)	24(2)
C(35)	85(3)	92(3)	95(3)	25(3)	-2(2)	37(3)
C(36)	97(3)	73(3)	52(2)	20(2)	-24(2)	-24(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for $[\text{C}_{38}\text{H}_{40}\text{N}_8\text{O}_{12}][\text{C}_6\text{H}_6]_2$.

	x	y	z	U(eq)
H(1)	6280(20)	8150(9)	2976(13)	37(6)
H(2)	4800(20)	7567(9)	3494(14)	41(7)
H(3)	3440(20)	7082(10)	2625(14)	49(7)
H(4)	3560(20)	7156(9)	1270(13)	32(6)
H(5A)	4322(19)	7508(8)	184(12)	25(5)
H(5B)	4625(19)	8095(9)	283(12)	28(6)
H(7A)	7690(20)	6572(8)	-759(12)	24(5)
H(7B)	8808(19)	6934(8)	-995(12)	21(5)
H(9A)	10760(20)	5112(8)	918(12)	32(6)
H(9B)	9300(20)	5053(9)	642(13)	34(6)
H(10)	7930(20)	4891(9)	1594(13)	34(6)
H(11)	7390(20)	4975(9)	2862(13)	40(7)
H(12)	8580(20)	5472(9)	3793(15)	48(7)
H(13)	10410(20)	5897(10)	3413(14)	46(7)
H(14A)	11860(20)	6098(9)	2531(14)	43(7)
H(14B)	12080(20)	5646(8)	1943(11)	24(5)

H(16A)	11009(19)	7614(8)	301(12)	23(5)
H(16B)	10920(20)	7668(9)	1251(14)	44(7)
H(17C)	14360(30)	5380(14)	379(19)	87(11)
H(17D)	14600(20)	5967(10)	45(15)	46(7)
H(17A)	12250(30)	7182(10)	-1516(15)	54(8)
H(17B)	11150(30)	6950(12)	-2142(19)	79(10)
H(18A)	6180(20)	8630(8)	1213(12)	27(6)
H(18B)	7160(20)	8534(9)	1960(13)	37(6)
H(18F)	15380(80)	6110(30)	1370(50)	290(50)
H(18G)	16210(40)	5677(15)	930(20)	107(13)
H(18H)	15190(40)	5497(17)	1460(30)	130(17)
H(18C)	13240(30)	6383(14)	-1430(20)	93(12)
H(18D)	13100(30)	6523(12)	-2344(19)	79(10)
H(18E)	12050(30)	6147(15)	-2060(20)	94(12)
H(19A)	6300(30)	9092(11)	-1365(17)	62(9)
H(19B)	5490(30)	9331(14)	-640(20)	91(11)
H(19C)	8770(20)	7699(11)	-2303(15)	54(8)
H(19D)	9300(30)	8240(11)	-2033(16)	65(9)
H(20A)	4500(50)	8680(20)	-1900(30)	160(20)
H(20B)	4170(30)	9319(14)	-1790(20)	93(11)
H(20C)	3690(30)	8877(11)	-1123(17)	61(9)
H(20D)	6710(30)	8083(12)	-2689(17)	69(9)
H(20E)	7780(20)	8327(10)	-3140(16)	55(8)
H(20F)	7240(30)	8602(13)	-2426(18)	71(10)
H(21)	3210(30)	4384(11)	1525(17)	60(9)
H(22)	4360(30)	4721(13)	2452(19)	88(11)
H(23)	3390(30)	4861(12)	3685(19)	78(10)
H(24)	1240(30)	4529(13)	3950(20)	93(11)
H(25)	-90(40)	4184(14)	2790(20)	111(13)
H(26)	870(30)	4094(12)	1579(19)	79(10)
H(31)	2760(40)	4948(16)	5000(20)	107(13)
H(32)	4490(30)	5317(14)	5850(20)	102(12)
H(33)	4090(30)	6112(14)	6460(20)	100(12)
H(34)	2210(40)	6545(18)	6100(20)	133(16)
H(35)	610(50)	6154(18)	5350(30)	139(19)
H(36)	880(40)	5401(15)	4810(20)	98(14)

Details of the x-ray structural determination of C_{2h} -18.

Experimental: A colorless crystalline parallelepiped with dimensions 0.30 x 0.15 x 0.10mm³ was placed and optically centered on the Bruker SMART CCD X-ray diffractometer at -100 °C. The initial unit cell was indexed using a least-squares analysis of a random set of reflections collected from three series of 0.3° wide ω scans (25 frames/series) that were well distributed in reciprocal space. Data frames were collected [MoK α] with 0.3° wide ω scans, 40 seconds/frame, 606 frames per series, 5 complete series and an additional 60 frames of the first series for decay purposes, a crystal to detector distance of 4.94cm, providing a complete sphere of data to $2\theta_{\max}=45.0^\circ$. A total of 31983 reflections were collected and corrected for Lorentz and polarization effects and absorption using Blessing's method as incorporated into the program SADABS^{1,2} with 21797 unique [R(int)=0.0317].

Structural determination and Refinement: All crystallographic calculations were performed on a Personal computer (PC) with dual Pentium 450MHz processors and 256MB of extended memory. The SHELXTL³ program package was now implemented, XPREP, to determine the probable space group and set up the initial files. System symmetry and lack of systematic absences indicated the possible space groups to be either the non-centrosymmetric triclinic space group P1 (no.1) or the centrosymmetric space group P-1 (no.2) with intensity statistics clearly favoring the centric case. The structure was determined by direct methods with the successful location of nearly all non-hydrogen atoms using the program XS⁴ in the centrosymmetric possibility P-1. The structure was refined with XL⁵. After several refinement difference-Fourier cycles it became clear, due to the disordered nature of the side chains on the ensemble and lack of convergence, that the space group P1 was more likely so this new model was now constructed and refined. Several refinement difference-Fourier cycles were performed in order to locate all of the missing non-hydrogen atoms. Hydrogen atoms were placed in calculated positions. All of the non-hydrogen atoms were refined isotropically, then anisotropically initially but several were found to refine to non-positive-definite thermal parameters so these atoms were further refined isotropically. The final structure was refined to convergence [$\Delta/\sigma \leq 0.001$] with R(F)=9.60%, wR(F²)=11.56%, GOF=0.877 for all 21797 unique reflections [R(F)=4.69%, wR(F²)=10.16% for those 12912 data with $F_o > 4\sigma(F_o)$]. A final difference-Fourier map was featureless, with the largest peak $|\Delta\rho| \leq 0.38\text{e}\text{\AA}^{-3}$, while the absolute structure parameter, Flack(x)⁶, refined to a value of -0.7(15) indicating that the structure is complete but correct enantiomorph cannot be determined with any confidence.

The function minimized during the full-matrix least-squares refinement was $\Sigma w(F_o^2 - F_c^2)^2$ where $w = 1/[\sigma^2(F_o^2) + (0.0524 \cdot P)^2 + 0.0 \cdot P]$ and $P = (\max(F_o^2, 0) + 2 \cdot F_c^2)/3$. An empirical correction for extinction was also applied to the data in the form $(F_c^2, \text{corr}) = k[1 + 0.001 \cdot x \cdot F_c^2 \cdot \lambda^3/\sin(2\theta)]^{(-1/4)}$ where $k=0.06550$ is the overall scale factor. The value determined for x was 0.00003(5).

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Table 1. Crystal data and structure refinement for C₄₂H₄₈N₈O₁₆.

Identification code	548c	
Empirical formula	C ₄₂ H ₄₈ N ₈ O ₁₆	
Formula weight	920.88	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P1	
Unit cell dimensions	a = 15.1085(18) Å	α = 78.438(2)°.
	b = 15.883(2) Å	β = 81.985(2)°.
	c = 18.321(2) Å	γ = 88.302(2)°.
Volume	4265.1(9) Å ³	
Z	4	
Density (calculated)	1.434 Mg/m ³	
Absorption coefficient	0.112 mm ⁻¹	
F(000)	1936	
Crystal size	0.10 x 0.15 x 0.3 mm ³	
Theta range for data collection	1.31 to 22.50°.	
Index ranges	-16 ≤ h ≤ 16, -17 ≤ k ≤ 17, -19 ≤ l ≤ 19	
Reflections collected	31983	
Independent reflections	21797 [R(int) = 0.0317]	
Completeness to theta = 22.50°	99.9 %	
Absorption correction	Empirical, SADABS	
Refinement method	Full-matrix-block least-squares on F ²	
Data / restraints / parameters	21797 / 3 / 2313	

Goodness-of-fit on F^2	0.877
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0469$, $wR2 = 0.1016$ [12912 Data]
R indices (all data)	$R1 = 0.0960$, $wR2 = 0.1156$
Absolute structure parameter	-0.7(15)
Extinction coefficient	0.00003(5)
Largest diff. peak and hole	0.381 and -0.371 e. $\text{\AA}^{-3}$

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for C₄₂H₄₈N₈O₁₆. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
C(1)	4051(7)	8773(6)	2350(5)	36(3)
C(2)	4397(7)	9281(6)	2813(5)	32(3)
O(2)	3898(4)	9775(4)	3229(4)	37(2)
C(2A)	2969(6)	9711(6)	3314(6)	57(3)
C(3)	5283(6)	9258(6)	2846(5)	35(3)
O(3)	5597(4)	9723(4)	3311(4)	40(2)
C(3A)	6490(7)	9623(7)	3441(6)	68(3)
C(4)	5845(6)	8717(6)	2439(5)	27(2)
C(4A)	5492(7)	8211(6)	2032(5)	33(3)
C(5)	6117(5)	7647(6)	1629(5)	26(2)
N(5A)	5922(5)	6725(5)	1864(4)	26(2)
C(6)	6171(6)	6254(6)	2514(5)	32(3)
N(6A)	5693(4)	5510(5)	2714(4)	27(2)
O(6)	6771(4)	6446(4)	2851(3)	32(2)
C(7)	5966(5)	4836(6)	3310(5)	27(2)
N(7A)	5598(5)	4015(5)	3301(4)	32(2)
C(8)	6142(6)	3400(6)	3028(5)	30(3)
N(8A)	5631(5)	2646(5)	3180(4)	28(2)
O(8)	6902(4)	3498(4)	2715(4)	42(2)
C(9)	5902(6)	1917(7)	2796(6)	35(3)
C(9A)	5431(6)	1839(6)	2156(6)	34(3)
C(10)	5961(6)	1726(6)	1475(5)	32(3)

C(11A)	6963(7)	1641(7)	84(6)	53(3)
O(11A)	6044(4)	1407(4)	231(4)	38(2)
C(11)	5557(6)	1557(6)	888(5)	28(2)
C(12)	4637(6)	1486(6)	938(5)	29(2)
O(12A)	4312(4)	1302(4)	349(3)	40(2)
C(12A)	3390(6)	996(7)	449(5)	62(4)
C(13A)	4496(6)	1803(6)	2193(5)	23(2)
C(13)	4115(6)	1627(6)	1594(6)	38(3)
C(14)	3860(6)	1930(6)	2879(6)	34(3)
N(14A)	4024(5)	2704(5)	3164(4)	29(2)
O(15D)	4003(6)	4089(5)	4823(4)	95(3)
O(15E)	5425(4)	3429(4)	4808(3)	51(2)
C(15)	3590(6)	3456(6)	3037(5)	28(2)
C(15B)	4765(5)	3662(5)	3708(5)	28(2)
N(15A)	3990(5)	4013(5)	3371(4)	31(2)
O(15)	2923(4)	3608(4)	2709(4)	39(2)
C(15D)	4670(7)	3752(6)	4557(5)	48(3)
O(15G)	5185(5)	1500(5)	4443(4)	56(2)
C(15C)	4786(6)	2721(6)	3583(5)	33(3)
O(15C)	3872(5)	2129(5)	4739(4)	48(2)
C(15G)	4547(5)	2097(5)	4334(5)	26(2)
C(15I)	4339(7)	168(6)	4930(6)	55(3)
C(15H)	4971(7)	802(6)	5092(6)	55(3)
C(15F)	5650(7)	2797(7)	5979(6)	143(4)
C(15E)	5027(8)	3227(8)	5762(6)	155(5)
C(16)	3722(6)	4944(5)	3261(5)	31(2)
N(16A)	4120(5)	5464(5)	2542(4)	29(2)
O(17D)	4699(4)	5980(4)	576(3)	38(2)
O(17E)	6058(4)	6580(4)	453(3)	28(2)
C(17I)	7158(4)	4084(4)	670(3)	47(2)
O(17C)	4692(4)	4195(4)	1752(3)	39(2)
O(17G)	6090(4)	4742(4)	1468(4)	41(2)
C(17G)	5229(6)	4718(6)	1810(5)	26(2)
C(17)	3737(6)	6280(6)	2380(5)	26(2)
C(17B)	5157(6)	6369(6)	1666(5)	24(2)
C(17C)	5052(6)	5467(6)	2211(5)	24(2)

C(17D)	5277(6)	6283(6)	820(5)	24(2)
N(17A)	4326(5)	6771(5)	1836(4)	30(2)
O(17)	3042(4)	6486(4)	2667(4)	38(2)
C(17E)	6139(6)	6580(7)	-359(5)	42(3)
C(17H)	6159(3)	4109(4)	925(3)	37(1)
C(17F)	7049(6)	6972(8)	-665(5)	55(3)
C(18)	4190(6)	7659(5)	1543(5)	33(2)
C(18A)	4596(6)	8244(6)	1977(5)	24(2)
C(21)	9048(6)	-3742(6)	2502(5)	30(2)
C(22)	9590(6)	-4243(6)	2129(5)	28(2)
C(22A)	8391(6)	-4686(6)	1591(6)	55(3)
O(22)	9320(4)	-4748(4)	1675(4)	42(2)
C(23A)	11981(6)	-4730(7)	1711(5)	52(3)
C(23)	10520(6)	-4276(6)	2179(5)	28(2)
O(23)	11028(5)	-4766(5)	1723(4)	43(2)
C(24)	10869(6)	-3805(6)	2598(5)	24(2)
C(24A)	10314(6)	-3265(6)	2990(5)	28(3)
C(25)	10757(6)	-2707(5)	3413(5)	26(2)
N(25A)	10589(5)	-1769(5)	3128(4)	22(2)
C(26)	11145(6)	-1281(6)	2582(6)	33(3)
N(26A)	10796(5)	-466(5)	2412(4)	27(2)
O(26)	11883(4)	-1508(4)	2284(4)	44(2)
C(27)	11152(5)	97(6)	1692(5)	39(3)
N(27A)	10928(5)	948(5)	1625(4)	29(2)
C(28)	11331(6)	1554(7)	1943(6)	34(3)
N(28A)	10849(5)	2295(5)	1823(4)	27(2)
O(28)	11991(4)	1412(4)	2230(4)	39(2)
C(29A)	10403(6)	3186(6)	2778(6)	32(3)
C(29)	11037(6)	3063(6)	2085(5)	27(2)
C(30)	10789(6)	3384(6)	3381(4)	23(2)
C(31)	10249(6)	3541(6)	4011(5)	31(3)
C(31A)	11481(6)	3991(6)	4498(5)	50(3)
O(31)	10597(4)	3729(4)	4641(4)	38(2)
C(32)	9343(6)	3485(6)	4073(5)	31(3)
C(32A)	7967(6)	3348(8)	4897(6)	45(3)
O(32)	8867(4)	3611(4)	4741(4)	41(2)

C(33A)	9505(6)	3152(6)	2827(5)	23(2)
C(33)	8979(6)	3287(6)	3475(6)	32(3)
C(34)	9026(6)	3086(6)	2160(5)	30(3)
N(34A)	9269(5)	2346(5)	1817(4)	31(2)
C(35C)	10163(6)	2257(6)	1398(5)	29(2)
C(35)	8798(6)	1637(6)	1946(5)	30(2)
C(35B)	10190(6)	1296(5)	1286(5)	35(2)
C(35G)	10320(7)	2952(6)	643(5)	49(3)
C(35I)	10590(8)	4843(7)	-14(5)	70(4)
N(35A)	9308(5)	990(5)	1667(4)	30(2)
O(35)	8035(4)	1513(4)	2244(4)	43(2)
O(35D)	10818(5)	863(4)	112(3)	58(2)
O(35G)	9727(4)	3514(4)	542(4)	38(2)
O(35C)	11040(5)	2885(5)	232(4)	50(2)
C(35H)	9928(7)	4225(7)	-122(6)	63(4)
C(35E)	9366(3)	1550(3)	-612(2)	20(1)
O(35E)	9615(5)	1605(4)	134(3)	84(2)
C(35F)	10037(5)	2193(4)	-1149(3)	58(2)
C(35D)	10274(7)	1230(5)	459(5)	52(3)
C(36)	8982(7)	175(6)	1635(5)	44(3)
N(36A)	9221(5)	-500(5)	2236(4)	27(2)
C(37C)	9879(6)	-430(6)	2740(5)	23(2)
C(37)	8714(5)	-1251(6)	2454(5)	20(2)
C(37B)	9753(6)	-1340(6)	3304(5)	24(2)
N(37A)	8992(4)	-1727(5)	3077(4)	22(2)
O(37)	8137(4)	-1428(4)	2118(4)	34(2)
C(37I)	8022(4)	567(4)	4609(4)	67(2)
O(37D)	10227(4)	-1004(5)	4394(4)	55(2)
O(37C)	10243(5)	811(5)	3205(4)	57(2)
O(37G)	8858(4)	284(4)	3482(3)	35(2)
C(37G)	9676(7)	319(6)	3179(5)	30(2)
C(37D)	9635(7)	-1281(6)	4127(5)	32(3)
O(37E)	8869(4)	-1581(4)	4505(3)	34(2)
C(37F)	7849(6)	-1977(6)	5657(5)	43(3)
C(37H)	8431(4)	940(4)	3853(4)	53(2)
C(37E)	8723(6)	-1589(6)	5313(5)	35(3)

C(38A)	9402(6)	-3235(6)	2953(5)	23(2)
C(38)	8762(6)	-2645(6)	3327(5)	31(3)
C(41)	5870(6)	1142(5)	7492(5)	20(1)
C(42)	5431(6)	659(6)	7129(5)	27(2)
O(42)	5862(4)	179(4)	6616(3)	33(2)
C(42A)	6835(5)	188(7)	6506(6)	47(3)
C(43)	4508(6)	678(6)	7175(5)	23(2)
O(43)	4134(4)	162(4)	6778(4)	35(2)
C(43A)	3199(6)	237(6)	6786(6)	38(3)
C(44)	4019(6)	1173(6)	7621(5)	33(3)
C(44A)	4467(6)	1690(6)	7996(5)	23(2)
C(45)	3924(6)	2286(6)	8455(5)	30(2)
N(45A)	4147(5)	3172(5)	8193(4)	28(2)
C(46)	3745(6)	3681(5)	7629(5)	22(2)
N(46A)	4171(4)	4490(5)	7470(4)	22(2)
O(46)	3133(4)	3509(4)	7342(4)	30(2)
C(47)	4087(6)	5031(5)	6734(4)	27(2)
N(47A)	4353(4)	5902(5)	6636(4)	21(2)
C(48)	3790(6)	6523(6)	6944(5)	26(2)
N(48A)	4274(4)	7237(5)	6825(4)	23(2)
O(48)	3035(4)	6398(4)	7232(4)	30(2)
C(49)	3944(6)	8051(6)	7054(5)	24(2)
C(49A)	4355(6)	8234(6)	7718(5)	22(2)
C(50)	3783(6)	8422(6)	8326(5)	35(3)
C(51)	4141(6)	8612(6)	8940(5)	31(3)
C(51A)	2687(7)	8945(10)	9543(7)	102(5)
O(51A)	3589(5)	8743(5)	9588(4)	53(2)
C(52)	5032(6)	8656(6)	8925(5)	33(3)
O(52A)	5407(4)	8804(5)	9552(4)	50(2)
C(52A)	5237(7)	9659(7)	9685(6)	73(4)
C(53A)	5264(6)	8272(6)	7705(5)	26(2)
C(53)	5629(6)	8466(6)	8340(5)	33(2)
C(54)	5929(6)	8150(5)	7037(5)	29(2)
N(54A)	5863(5)	7362(5)	6770(4)	27(2)
O(55E)	6322(4)	6518(4)	5322(4)	38(2)
C(55)	6294(6)	6638(6)	7062(5)	22(2)

C(55B)	5236(5)	6210(5)	6381(5)	23(2)
N(55A)	5892(5)	5946(5)	6851(4)	23(2)
O(55)	6928(4)	6593(4)	7408(4)	33(2)
C(55D)	5574(6)	6058(6)	5576(5)	22(2)
O(55G)	4571(4)	7496(4)	5250(4)	43(2)
C(55C)	5152(6)	7202(6)	6413(4)	25(2)
C(55H)	4561(7)	7854(5)	4453(5)	46(3)
O(55C)	5659(4)	8385(4)	5346(4)	42(2)
O(55D)	5238(4)	5623(4)	5249(3)	41(2)
C(55G)	5163(6)	7811(6)	5597(5)	29(2)
C(55E)	6765(6)	6473(6)	4566(5)	44(3)
C(55I)	3971(4)	7330(5)	4165(4)	72(2)
C(56)	6339(5)	5172(5)	6911(5)	28(2)
N(56A)	5785(4)	4424(4)	7318(4)	22(2)
O(57D)	5581(4)	3376(5)	9501(4)	40(2)
O(57E)	4134(4)	3731(5)	9498(4)	39(2)
C(57I)	3186(6)	6238(7)	9170(6)	52(3)
O(57C)	5671(4)	5258(4)	8566(4)	32(2)
O(57G)	4225(4)	5549(4)	8402(3)	31(2)
C(57G)	5019(6)	5176(6)	8295(5)	27(2)
C(57)	6237(6)	3631(6)	7467(6)	34(3)
C(57B)	4920(5)	3543(6)	8363(5)	24(2)
C(57C)	4984(5)	4460(6)	7835(5)	20(2)
C(57D)	4946(6)	3550(5)	9185(5)	31(3)
N(57A)	5745(5)	3134(5)	8084(4)	25(2)
O(57)	6933(4)	3452(4)	7108(4)	34(2)
C(57E)	3983(4)	3749(5)	10304(4)	34(2)
C(57H)	4132(6)	6123(6)	8945(6)	37(3)
C(57F)	3076(6)	3602(7)	10619(6)	55(3)
C(58)	5914(6)	2201(5)	8316(5)	26(2)
C(58A)	5401(6)	1673(6)	7938(5)	27(2)
C(93)	7415(7)	5716(7)	4626(6)	58(3)
C(61)	10870(6)	13801(5)	7341(5)	19(2)
O(62)	10784(4)	14816(4)	8191(3)	28(2)
C(62)	10401(6)	14341(6)	7780(5)	27(2)
C(62A)	11738(6)	14739(7)	8186(6)	49(3)

O(63)	9042(4)	14831(4)	8330(4)	31(2)
C(63A)	8115(6)	14799(6)	8457(5)	39(3)
C(63)	9463(6)	14338(6)	7875(5)	27(2)
C(64)	9025(7)	13853(6)	7469(6)	37(3)
C(64A)	9521(6)	13353(6)	7016(5)	21(2)
N(65A)	9165(5)	11867(5)	6903(4)	24(2)
C(65)	9003(6)	12779(6)	6640(5)	28(2)
O(66)	7983(4)	11535(4)	7827(4)	40(2)
N(66A)	9101(4)	10583(5)	7646(4)	27(2)
C(66)	8695(6)	11361(6)	7485(5)	20(2)
N(67A)	9029(4)	9051(5)	8082(4)	22(2)
C(67)	8544(6)	9884(5)	8073(5)	32(2)
O(68)	8011(4)	8430(4)	7540(4)	36(2)
N(68A)	9028(4)	7625(5)	8220(4)	19(2)
C(68)	8619(6)	8366(6)	7914(5)	31(3)
C(69A)	9608(6)	6718(6)	7264(5)	26(2)
C(69)	8960(6)	6799(5)	7953(5)	27(2)
C(70)	9322(5)	6520(6)	6665(5)	25(2)
O(71)	9497(4)	6215(5)	5420(4)	44(2)
C(71)	9863(6)	6385(6)	6021(5)	32(3)
C(71A)	9659(7)	5359(6)	5276(6)	67(4)
O(72)	11305(4)	6258(5)	5395(4)	46(2)
C(72)	10796(6)	6417(7)	6016(6)	36(3)
C(72A)	12218(7)	6037(8)	5477(6)	75(4)
C(73A)	10541(6)	6758(6)	7260(5)	25(2)
C(73)	11117(6)	6615(6)	6625(5)	26(2)
N(74A)	10633(5)	7737(5)	8140(4)	24(2)
C(74)	10948(6)	6963(6)	7914(5)	32(3)
O(75)	11889(4)	8611(4)	7741(4)	30(2)
O(75D)	9672(4)	9428(4)	9715(4)	39(2)
O(75G)	10380(4)	7502(4)	9702(3)	38(2)
O(75C)	9280(4)	6620(5)	9618(4)	40(2)
N(75A)	10578(4)	9093(5)	8312(4)	22(2)
C(75C)	9782(5)	7786(5)	8602(4)	20(2)
C(75)	11107(6)	8499(6)	8030(5)	22(2)
C(75B)	9691(5)	8764(6)	8611(4)	23(2)

O(75E)	8577(4)	8518(4)	9628(3)	31(2)
C(75E)	8116(6)	8587(6)	10379(5)	43(3)
C(75G)	9756(6)	7243(5)	9366(5)	27(2)
C(75F)	7514(7)	9316(7)	10333(6)	59(4)
C(75H)	10380(9)	7074(7)	10506(5)	84(4)
C(75I)	10559(4)	7791(4)	10922(4)	45(2)
C(75D)	9320(6)	8950(7)	9396(6)	33(3)
N(76A)	10734(4)	10515(5)	7487(4)	24(2)
C(76)	10850(5)	9991(6)	8224(5)	29(3)
O(77)	11768(4)	11500(4)	7627(4)	32(2)
O(77C)	9248(4)	9738(4)	6392(4)	38(2)
O(77G)	10679(4)	9473(4)	6567(3)	27(2)
O(77D)	9322(5)	11617(5)	5456(4)	47(2)
O(77E)	10774(4)	11281(4)	5455(4)	38(2)
N(77A)	10785(4)	11811(5)	6751(4)	20(2)
C(77C)	9935(6)	10537(6)	7149(5)	26(2)
C(77)	11149(5)	11299(6)	7308(5)	23(2)
C(77B)	9959(6)	11483(6)	6627(5)	24(2)
C(77H)	10748(6)	8895(6)	6030(5)	33(3)
C(77D)	9985(6)	11483(6)	5757(5)	26(2)
C(77I)	11748(6)	8755(6)	5806(5)	47(3)
C(77F)	11808(7)	11403(8)	4337(6)	71(4)
C(77G)	9912(6)	9858(5)	6669(5)	21(2)
C(77E)	10790(5)	11218(6)	4655(5)	47(2)
C(78A)	10442(6)	13309(6)	6953(5)	27(2)
C(78)	10995(6)	12752(5)	6502(5)	26(2)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for $\text{C}_{42}\text{H}_{48}\text{N}_8\text{O}_{16}$.

C(1)-C(18A)	1.372(12)	C(8)-N(8A)	1.404(11)
C(1)-C(2)	1.438(12)	N(8A)-C(15C)	1.396(11)
C(1)-H(1A)	0.9500	N(8A)-C(9)	1.490(12)
C(2)-O(2)	1.344(11)	C(9)-C(9A)	1.482(13)
C(2)-C(3)	1.347(12)	C(9)-H(9A)	0.9900
O(2)-C(2A)	1.396(10)	C(9)-H(9B)	0.9900
C(2A)-H(2AA)	0.9800	C(9A)-C(13A)	1.406(12)
C(2A)-H(2AB)	0.9800	C(9A)-C(10)	1.425(13)
C(2A)-H(2AC)	0.9800	C(10)-C(11)	1.382(12)
C(3)-O(3)	1.373(10)	C(10)-H(10A)	0.9500
C(3)-C(4)	1.432(12)	C(11A)-O(11A)	1.423(11)
O(3)-C(3A)	1.401(10)	C(11A)-H(11A)	0.9800
C(3A)-H(3AA)	0.9800	C(11A)-H(11B)	0.9800
C(3A)-H(3AB)	0.9800	C(11A)-H(11C)	0.9800
C(3A)-H(3AC)	0.9800	O(11A)-C(11)	1.379(10)
C(4)-C(4A)	1.366(12)	C(11)-C(12)	1.387(12)
C(4)-H(4A)	0.9500	C(12)-O(12A)	1.332(10)
C(4A)-C(18A)	1.370(12)	C(12)-C(13)	1.396(12)
C(4A)-C(5)	1.502(13)	O(12A)-C(12A)	1.464(9)
C(5)-N(5A)	1.467(11)	C(12A)-H(12A)	0.9800
C(5)-H(5A)	0.9900	C(12A)-H(12B)	0.9800
C(5)-H(5B)	0.9900	C(12A)-H(12C)	0.9800
N(5A)-C(6)	1.368(11)	C(13A)-C(13)	1.388(12)
N(5A)-C(17B)	1.423(10)	C(13A)-C(14)	1.515(12)
C(6)-O(6)	1.241(10)	C(13)-H(13A)	0.9500
C(6)-N(6A)	1.363(11)	C(14)-N(14A)	1.468(11)
N(6A)-C(17C)	1.439(11)	C(14)-H(14A)	0.9900
N(6A)-C(7)	1.463(11)	C(14)-H(14B)	0.9900
C(7)-N(7A)	1.437(11)	N(14A)-C(15)	1.339(11)
C(7)-H(7A)	0.9900	N(14A)-C(15C)	1.475(11)
C(7)-H(7B)	0.9900	O(15D)-C(15D)	1.215(12)
N(7A)-C(8)	1.383(11)	O(15E)-C(15D)	1.340(10)
N(7A)-C(15B)	1.437(11)	O(15E)-C(15E)	1.735(13)
C(8)-O(8)	1.209(9)	C(15)-O(15)	1.237(10)

C(15)-N(15A)	1.370(11)	C(17G)-C(17C)	1.516(13)
C(15B)-N(15A)	1.445(10)	C(17)-O(17)	1.176(9)
C(15B)-C(15C)	1.554(12)	C(17)-N(17A)	1.370(11)
C(15B)-C(15D)	1.578(12)	C(17B)-N(17A)	1.416(11)
N(15A)-C(16)	1.504(10)	C(17B)-C(17D)	1.569(12)
O(15G)-C(15G)	1.339(10)	C(17B)-C(17C)	1.571(12)
O(15G)-C(15H)	1.460(11)	N(17A)-C(18)	1.424(11)
C(15C)-C(15G)	1.531(12)	C(17E)-C(17F)	1.512(12)
O(15C)-C(15G)	1.180(9)	C(17E)-H(17D)	0.9900
C(15I)-C(15H)	1.507(13)	C(17E)-H(17E)	0.9900
C(15I)-H(15A)	0.9800	C(17H)-H(17F)	0.9900
C(15I)-H(15B)	0.9800	C(17H)-H(17G)	0.9900
C(15I)-H(15C)	0.9800	C(17F)-H(17G)	0.9800
C(15H)-H(15D)	0.9900	C(17F)-H(17H)	0.9800
C(15H)-H(15E)	0.9900	C(17F)-H(17I)	0.9800
C(15F)-C(15E)	1.212(12)	C(18)-C(18A)	1.529(12)
C(15F)-H(15F)	0.9800	C(18)-H(18A)	0.9900
C(15F)-H(15G)	0.9800	C(18)-H(18B)	0.9900
C(15F)-H(15H)	0.9800	C(21)-C(22)	1.340(12)
C(15E)-H(15I)	0.9900	C(21)-C(38A)	1.426(11)
C(15E)-H(15J)	0.9900	C(21)-H(21A)	0.9500
C(16)-N(16A)	1.467(11)	C(22)-O(22)	1.372(11)
C(16)-H(16A)	0.9900	C(22)-C(23)	1.420(11)
C(16)-H(16B)	0.9900	C(22A)-O(22)	1.431(10)
N(16A)-C(17)	1.396(11)	C(22A)-H(22A)	0.9800
N(16A)-C(17C)	1.454(10)	C(22A)-H(22B)	0.9800
O(17D)-C(17D)	1.189(9)	C(22A)-H(22C)	0.9800
O(17E)-C(17D)	1.323(9)	C(23A)-O(23)	1.439(10)
O(17E)-C(17E)	1.477(10)	C(23A)-H(23A)	0.9800
C(17I)-C(17H)	1.519(7)	C(23A)-H(23B)	0.9800
C(17I)-H(17A)	0.9800	C(23A)-H(23C)	0.9800
C(17I)-H(17B)	0.9800	C(23)-C(24)	1.339(11)
C(17I)-H(17C)	0.9800	C(23)-O(23)	1.393(10)
O(17C)-C(17G)	1.208(10)	C(24)-C(24A)	1.412(12)
O(17G)-C(17G)	1.361(9)	C(24)-H(24A)	0.9500
O(17G)-C(17H)	1.542(8)	C(24A)-C(38A)	1.387(11)

C(24A)-C(25)	1.512(11)	C(32A)-H(32B)	0.9800
C(25)-N(25A)	1.504(10)	C(32A)-H(32C)	0.9800
C(25)-H(25A)	0.9900	C(33A)-C(33)	1.384(12)
C(25)-H(25B)	0.9900	C(33A)-C(34)	1.527(12)
N(25A)-C(26)	1.341(11)	C(33)-H(33A)	0.9500
N(25A)-C(37B)	1.444(11)	C(34)-N(34A)	1.456(11)
C(26)-O(26)	1.248(10)	C(34)-H(34A)	0.9900
C(26)-N(26A)	1.377(11)	C(34)-H(34B)	0.9900
N(26A)-C(37C)	1.436(10)	N(34A)-C(35)	1.313(11)
N(26A)-C(27)	1.479(11)	N(34A)-C(35C)	1.475(10)
C(27)-N(27A)	1.370(11)	C(35C)-C(35B)	1.579(12)
C(27)-H(27A)	0.9900	C(35C)-C(35G)	1.581(13)
C(27)-H(27B)	0.9900	C(35)-O(35)	1.209(10)
N(27A)-C(35B)	1.397(11)	C(35)-N(35A)	1.402(11)
N(27A)-C(28)	1.412(12)	C(35B)-N(35A)	1.463(11)
C(28)-O(28)	1.184(10)	C(35B)-C(35D)	1.527(12)
C(28)-N(28A)	1.363(12)	C(35G)-O(35C)	1.248(11)
N(28A)-C(35C)	1.390(11)	C(35G)-O(35G)	1.251(11)
N(28A)-C(29)	1.445(11)	C(35I)-C(35H)	1.482(14)
C(29A)-C(33A)	1.349(11)	C(35I)-H(35A)	0.9800
C(29A)-C(30)	1.411(12)	C(35I)-H(35B)	0.9800
C(29A)-C(29)	1.522(12)	C(35I)-H(35C)	0.9800
C(29)-H(29A)	0.9900	N(35A)-C(36)	1.414(11)
C(29)-H(29B)	0.9900	O(35D)-C(35D)	1.182(10)
C(30)-C(31)	1.379(12)	O(35G)-C(35H)	1.487(11)
C(30)-H(30A)	0.9500	C(35H)-H(35D)	0.9900
C(31)-C(32)	1.362(12)	C(35H)-H(35E)	0.9900
C(31)-O(31)	1.420(10)	C(35E)-O(35E)	1.486(7)
C(31A)-O(31)	1.385(10)	C(35E)-C(35F)	1.555(7)
C(31A)-H(31A)	0.9800	C(35E)-H(35F)	0.9900
C(31A)-H(31B)	0.9800	C(35E)-H(35G)	0.9900
C(31A)-H(31C)	0.9800	O(35E)-C(35D)	1.299(11)
C(32)-O(32)	1.379(11)	C(35F)-H(35H)	0.9800
C(32)-C(33)	1.384(13)	C(35F)-H(35I)	0.9800
C(32A)-O(32)	1.409(11)	C(35F)-H(35J)	0.9800
C(32A)-H(32A)	0.9800	C(36)-N(36A)	1.451(11)

C(36)-H(36A)	0.9900	C(42)-O(42)	1.404(10)
C(36)-H(36B)	0.9900	O(42)-C(42A)	1.455(9)
N(36A)-C(37)	1.395(10)	C(42A)-H(42A)	0.9800
N(36A)-C(37C)	1.468(10)	C(42A)-H(42B)	0.9800
C(37C)-C(37G)	1.565(12)	C(42A)-H(42C)	0.9800
C(37C)-C(37B)	1.598(12)	C(43)-C(44)	1.375(12)
C(37)-O(37)	1.204(9)	C(43)-O(43)	1.379(10)
C(37)-N(37A)	1.348(10)	O(43)-C(43A)	1.414(10)
C(37B)-N(37A)	1.467(10)	C(43A)-H(43A)	0.9800
C(37B)-C(37D)	1.515(13)	C(43A)-H(43B)	0.9800
N(37A)-C(38)	1.475(11)	C(43A)-H(43C)	0.9800
C(37I)-C(37H)	1.452(9)	C(44)-C(44A)	1.411(12)
C(37I)-H(37A)	0.9800	C(44)-H(44A)	0.9500
C(37I)-H(37B)	0.9800	C(44A)-C(58A)	1.399(11)
C(37I)-H(37C)	0.9800	C(44A)-C(45)	1.536(11)
O(37D)-C(37D)	1.210(10)	C(45)-N(45A)	1.427(11)
O(37C)-C(37G)	1.188(10)	C(45)-H(45A)	0.9900
O(37G)-C(37G)	1.281(10)	C(45)-H(45B)	0.9900
O(37G)-C(37H)	1.444(8)	N(45A)-C(46)	1.380(10)
C(37D)-O(37E)	1.313(10)	N(45A)-C(57B)	1.423(10)
O(37E)-C(37E)	1.463(10)	C(46)-O(46)	1.189(9)
C(37F)-C(37E)	1.478(12)	C(46)-N(46A)	1.413(11)
C(37F)-H(37D)	0.9800	N(46A)-C(47)	1.466(10)
C(37F)-H(37E)	0.9800	N(46A)-C(57C)	1.474(10)
C(37F)-H(37F)	0.9800	C(47)-N(47A)	1.421(11)
C(37H)-H(37G)	0.9900	C(47)-H(47A)	0.9900
C(37H)-H(37H)	0.9900	C(47)-H(47B)	0.9900
C(37E)-H(37H)	0.9900	N(47A)-C(55B)	1.417(10)
C(37E)-H(37I)	0.9900	N(47A)-C(48)	1.433(11)
C(38A)-C(38)	1.517(12)	C(48)-O(48)	1.193(9)
C(38)-H(38A)	0.9900	C(48)-N(48A)	1.332(11)
C(38)-H(38B)	0.9900	N(48A)-C(55C)	1.438(10)
C(41)-C(42)	1.353(12)	N(48A)-C(49)	1.488(10)
C(41)-C(58A)	1.400(12)	C(49)-C(49A)	1.523(12)
C(41)-H(41A)	0.9500	C(49)-H(49A)	0.9900
C(42)-C(43)	1.386(12)	C(49)-H(49B)	0.9900

C(49A)-C(53A)	1.373(11)	C(55H)-C(55I)	1.455(10)
C(49A)-C(50)	1.388(12)	C(55H)-H(55A)	0.9900
C(50)-C(51)	1.401(12)	C(55H)-H(55B)	0.9900
C(50)-H(50A)	0.9500	O(55C)-C(55G)	1.175(9)
C(51)-C(52)	1.346(12)	C(55E)-C(93)	1.527(12)
C(51)-O(51A)	1.399(10)	C(55E)-H(55C)	0.9900
C(51A)-O(51A)	1.401(11)	C(55E)-H(55D)	0.9900
C(51A)-H(51A)	0.9800	C(55I)-H(55E)	0.9800
C(51A)-H(51B)	0.9800	C(55I)-H(55F)	0.9800
C(51A)-H(51C)	0.9800	C(55I)-H(55G)	0.9800
C(52)-C(53)	1.378(12)	C(56)-N(56A)	1.483(10)
C(52)-O(52A)	1.412(11)	C(56)-H(56A)	0.9900
O(52A)-C(52A)	1.436(11)	C(56)-H(56B)	0.9900
C(52A)-H(52A)	0.9800	N(56A)-C(57)	1.411(11)
C(52A)-H(52B)	0.9800	N(56A)-C(57C)	1.436(10)
C(52A)-H(52C)	0.9800	O(57D)-C(57D)	1.188(10)
C(53A)-C(53)	1.443(11)	O(57E)-C(57D)	1.329(10)
C(53A)-C(54)	1.512(12)	O(57E)-C(57E)	1.467(9)
C(53)-H(53A)	0.9500	C(57I)-C(57H)	1.449(11)
C(54)-N(54A)	1.442(11)	C(57I)-H(57A)	0.9800
C(54)-H(54A)	0.9900	C(57I)-H(57B)	0.9800
C(54)-H(54B)	0.9900	C(57I)-H(57C)	0.9800
N(54A)-C(55)	1.356(11)	O(57C)-C(57G)	1.185(9)
N(54A)-C(55C)	1.387(10)	O(57G)-C(57G)	1.329(10)
O(55E)-C(55D)	1.340(10)	O(57G)-C(57H)	1.469(10)
O(55E)-C(55E)	1.467(10)	C(57G)-C(57C)	1.551(12)
C(55)-O(55)	1.213(9)	C(57)-O(57)	1.218(10)
C(55)-N(55A)	1.416(10)	C(57)-N(57A)	1.377(12)
C(55B)-N(55A)	1.404(10)	C(57B)-N(57A)	1.464(10)
C(55B)-C(55D)	1.556(12)	C(57B)-C(57D)	1.514(12)
C(55B)-C(55C)	1.588(12)	C(57B)-C(57C)	1.576(12)
N(55A)-C(56)	1.377(10)	N(57A)-C(58)	1.482(10)
C(55D)-O(55D)	1.169(10)	C(57E)-C(57F)	1.419(11)
O(55G)-C(55G)	1.330(9)	C(57E)-H(57D)	0.9900
O(55G)-C(55H)	1.458(10)	C(57E)-H(57E)	0.9900
C(55C)-C(55G)	1.608(12)	C(57H)-H(57F)	0.9900

C(57H)-H(57G)	0.9900	N(66A)-C(67)	1.441(11)
C(57F)-H(57H)	0.9800	N(66A)-C(77C)	1.458(10)
C(57F)-H(57I)	0.9800	N(67A)-C(68)	1.375(11)
C(57F)-H(57J)	0.9800	N(67A)-C(75B)	1.486(10)
C(58)-C(58A)	1.486(12)	N(67A)-C(67)	1.492(10)
C(58)-H(58A)	0.9900	C(67)-H(67A)	0.9900
C(58)-H(58B)	0.9900	C(67)-H(67B)	0.9900
C(93)-H(93A)	0.9800	O(68)-C(68)	1.211(10)
C(93)-H(93B)	0.9800	N(68A)-C(68)	1.367(11)
C(93)-H(93C)	0.9800	N(68A)-C(75C)	1.472(10)
C(61)-C(78A)	1.384(12)	N(68A)-C(69)	1.498(10)
C(61)-C(62)	1.402(12)	C(69A)-C(70)	1.330(11)
C(61)-H(61A)	0.9500	C(69A)-C(73A)	1.411(11)
O(62)-C(62)	1.359(10)	C(69A)-C(69)	1.511(12)
O(62)-C(62A)	1.441(10)	C(69)-H(69A)	0.9900
C(62)-C(63)	1.402(12)	C(69)-H(69B)	0.9900
C(62A)-H(62A)	0.9800	C(70)-C(71)	1.390(12)
C(62A)-H(62B)	0.9800	C(70)-H(70A)	0.9500
C(62A)-H(62C)	0.9800	O(71)-C(71)	1.375(10)
O(63)-C(63)	1.339(10)	O(71)-C(71A)	1.445(11)
O(63)-C(63A)	1.388(9)	C(71)-C(72)	1.411(12)
C(63A)-H(63A)	0.9800	C(71A)-H(71A)	0.9800
C(63A)-H(63B)	0.9800	C(71A)-H(71B)	0.9800
C(63A)-H(63C)	0.9800	C(71A)-H(71C)	0.9800
C(63)-C(64)	1.409(12)	O(72)-C(72)	1.345(11)
C(64)-C(64A)	1.390(13)	O(72)-C(72A)	1.434(11)
C(64)-H(64A)	0.9500	C(72)-C(73)	1.369(12)
C(64A)-C(78A)	1.382(12)	C(72A)-H(72A)	0.9800
C(64A)-C(65)	1.538(11)	C(72A)-H(72B)	0.9800
N(65A)-C(66)	1.328(11)	C(72A)-H(72C)	0.9800
N(65A)-C(77B)	1.407(10)	C(73A)-C(73)	1.405(12)
N(65A)-C(65)	1.457(11)	C(73A)-C(74)	1.514(12)
C(65)-H(65A)	0.9900	C(73)-H(73A)	0.9500
C(65)-H(65B)	0.9900	N(74A)-C(75)	1.390(11)
O(66)-C(66)	1.222(9)	N(74A)-C(74)	1.424(11)
N(66A)-C(66)	1.359(11)	N(74A)-C(75C)	1.446(10)

C(74)-H(74A)	0.9900	O(77D)-C(77D)	1.203(10)
C(74)-H(74B)	0.9900	O(77E)-C(77D)	1.303(10)
O(75)-C(75)	1.227(9)	O(77E)-C(77E)	1.486(10)
O(75D)-C(75D)	1.221(11)	N(77A)-C(77)	1.342(10)
O(75G)-C(75G)	1.314(10)	N(77A)-C(77B)	1.430(10)
O(75G)-C(75H)	1.494(11)	N(77A)-C(78)	1.502(10)
O(75C)-C(75G)	1.214(9)	C(77C)-C(77G)	1.526(12)
N(75A)-C(75)	1.353(11)	C(77C)-C(77B)	1.609(12)
N(75A)-C(75B)	1.447(10)	C(77B)-C(77D)	1.589(11)
N(75A)-C(76)	1.466(11)	C(77H)-C(77I)	1.530(12)
C(75C)-C(75G)	1.485(11)	C(77H)-H(77A)	0.9900
C(75C)-C(75B)	1.559(12)	C(77H)-H(77B)	0.9900
C(75B)-C(75D)	1.551(12)	C(77I)-H(77C)	0.9800
O(75E)-C(75D)	1.307(10)	C(77I)-H(77D)	0.9800
O(75E)-C(75E)	1.475(10)	C(77I)-H(77E)	0.9800
C(75E)-C(75F)	1.448(13)	C(77F)-C(77E)	1.582(12)
C(75E)-H(75A)	0.9900	C(77F)-H(77F)	0.9800
C(75E)-H(75B)	0.9900	C(77F)-H(77G)	0.9800
C(75F)-H(75C)	0.9800	C(77F)-H(77H)	0.9800
C(75F)-H(75D)	0.9800	C(77E)-H(77I)	0.9900
C(75F)-H(75E)	0.9800	C(77E)-H(77J)	0.9900
C(75H)-C(75I)	1.540(11)	C(78A)-C(78)	1.489(12)
C(75H)-H(75F)	0.9900	C(78)-H(78A)	0.9900
C(75H)-H(75G)	0.9900	C(78)-H(78B)	0.9900
C(75I)-H(75H)	0.9800		
C(75I)-H(75I)	0.9800	C(18A)-C(1)-C(2)	121.3(9)
C(75I)-H(75J)	0.9800	C(18A)-C(1)-H(1A)	119.3
N(76A)-C(77)	1.370(10)	C(2)-C(1)-H(1A)	119.3
N(76A)-C(77C)	1.427(10)	O(2)-C(2)-C(3)	116.9(9)
N(76A)-C(76)	1.469(11)	O(2)-C(2)-C(1)	124.8(9)
C(76)-H(76A)	0.9900	C(3)-C(2)-C(1)	118.3(9)
C(76)-H(76B)	0.9900	C(2)-O(2)-C(2A)	119.0(8)
O(77)-C(77)	1.250(9)	O(2)-C(2A)-H(2AA)	109.5
O(77C)-C(77G)	1.222(9)	O(2)-C(2A)-H(2AB)	109.5
O(77G)-C(77G)	1.301(10)	H(2AA)-C(2A)-H(2AB)	109.5
O(77G)-C(77H)	1.467(10)	O(2)-C(2A)-H(2AC)	109.5

H(2AA)-C(2A)-H(2AC)	109.5	N(7A)-C(7)-H(7B)	109.2
H(2AB)-C(2A)-H(2AC)	109.5	N(6A)-C(7)-H(7B)	109.2
C(2)-C(3)-O(3)	117.5(9)	H(7A)-C(7)-H(7B)	107.9
C(2)-C(3)-C(4)	119.6(9)	C(8)-N(7A)-C(15B)	112.3(8)
O(3)-C(3)-C(4)	122.8(8)	C(8)-N(7A)-C(7)	119.5(8)
C(3)-O(3)-C(3A)	119.1(8)	C(15B)-N(7A)-C(7)	126.5(8)
O(3)-C(3A)-H(3AA)	109.5	O(8)-C(8)-N(7A)	126.8(9)
O(3)-C(3A)-H(3AB)	109.5	O(8)-C(8)-N(8A)	127.1(9)
H(3AA)-C(3A)-H(3AB)	109.5	N(7A)-C(8)-N(8A)	106.1(8)
O(3)-C(3A)-H(3AC)	109.5	C(15C)-N(8A)-C(8)	113.8(8)
H(3AA)-C(3A)-H(3AC)	109.5	C(15C)-N(8A)-C(9)	123.8(8)
H(3AB)-C(3A)-H(3AC)	109.5	C(8)-N(8A)-C(9)	121.1(8)
C(4A)-C(4)-C(3)	120.8(9)	C(9A)-C(9)-N(8A)	116.7(8)
C(4A)-C(4)-H(4A)	119.6	C(9A)-C(9)-H(9A)	108.1
C(3)-C(4)-H(4A)	119.6	N(8A)-C(9)-H(9A)	108.1
C(4)-C(4A)-C(18A)	120.2(10)	C(9A)-C(9)-H(9B)	108.1
C(4)-C(4A)-C(5)	118.1(8)	N(8A)-C(9)-H(9B)	108.1
C(18A)-C(4A)-C(5)	121.6(8)	H(9A)-C(9)-H(9B)	107.3
N(5A)-C(5)-C(4A)	114.4(7)	C(13A)-C(9A)-C(10)	117.8(9)
N(5A)-C(5)-H(5A)	108.7	C(13A)-C(9A)-C(9)	124.3(9)
C(4A)-C(5)-H(5A)	108.7	C(10)-C(9A)-C(9)	117.7(8)
N(5A)-C(5)-H(5B)	108.7	C(11)-C(10)-C(9A)	120.2(9)
C(4A)-C(5)-H(5B)	108.7	C(11)-C(10)-H(10A)	119.9
H(5A)-C(5)-H(5B)	107.6	C(9A)-C(10)-H(10A)	119.9
C(6)-N(5A)-C(17B)	111.6(7)	O(11A)-C(11A)-H(11A)	109.5
C(6)-N(5A)-C(5)	121.5(7)	O(11A)-C(11A)-H(11B)	109.5
C(17B)-N(5A)-C(5)	120.8(7)	H(11A)-C(11A)-H(11B)	109.5
O(6)-C(6)-N(6A)	124.8(9)	O(11A)-C(11A)-H(11C)	109.5
O(6)-C(6)-N(5A)	125.8(9)	H(11A)-C(11A)-H(11C)	109.5
N(6A)-C(6)-N(5A)	109.2(8)	H(11B)-C(11A)-H(11C)	109.5
C(6)-N(6A)-C(17C)	112.0(7)	C(11)-O(11A)-C(11A)	117.9(7)
C(6)-N(6A)-C(7)	118.4(7)	O(11A)-C(11)-C(10)	122.2(8)
C(17C)-N(6A)-C(7)	128.9(7)	O(11A)-C(11)-C(12)	115.9(8)
N(7A)-C(7)-N(6A)	111.8(7)	C(10)-C(11)-C(12)	121.9(9)
N(7A)-C(7)-H(7A)	109.2	O(12A)-C(12)-C(11)	117.5(8)
N(6A)-C(7)-H(7A)	109.2	O(12A)-C(12)-C(13)	124.5(8)

C(11)-C(12)-C(13)	118.0(9)	O(15D)-C(15D)-O(15E)	135.2(9)
C(12)-O(12A)-C(12A)	118.8(7)	O(15D)-C(15D)-C(15B)	118.9(8)
O(12A)-C(12A)-H(12A)	109.5	O(15E)-C(15D)-C(15B)	105.9(8)
O(12A)-C(12A)-H(12B)	109.5	C(15G)-O(15G)-C(15H)	115.2(8)
H(12A)-C(12A)-H(12B)	109.5	N(8A)-C(15C)-N(14A)	115.7(8)
O(12A)-C(12A)-H(12C)	109.5	N(8A)-C(15C)-C(15G)	117.9(7)
H(12A)-C(12A)-H(12C)	109.5	N(14A)-C(15C)-C(15G)	105.8(7)
H(12B)-C(12A)-H(12C)	109.5	N(8A)-C(15C)-C(15B)	103.7(7)
C(13)-C(13A)-C(9A)	120.3(9)	N(14A)-C(15C)-C(15B)	102.4(7)
C(13)-C(13A)-C(14)	116.8(8)	C(15G)-C(15C)-C(15B)	110.2(8)
C(9A)-C(13A)-C(14)	122.9(8)	O(15C)-C(15G)-O(15G)	125.6(8)
C(13A)-C(13)-C(12)	121.7(9)	O(15C)-C(15G)-C(15C)	123.7(8)
C(13A)-C(13)-H(13A)	119.2	O(15G)-C(15G)-C(15C)	110.5(7)
C(12)-C(13)-H(13A)	119.2	C(15H)-C(15I)-H(15A)	109.5
N(14A)-C(14)-C(13A)	114.9(7)	C(15H)-C(15I)-H(15B)	109.5
N(14A)-C(14)-H(14A)	108.5	H(15A)-C(15I)-H(15B)	109.5
C(13A)-C(14)-H(14A)	108.5	C(15H)-C(15I)-H(15C)	109.5
N(14A)-C(14)-H(14B)	108.5	H(15A)-C(15I)-H(15C)	109.5
C(13A)-C(14)-H(14B)	108.5	H(15B)-C(15I)-H(15C)	109.5
H(14A)-C(14)-H(14B)	107.5	O(15G)-C(15H)-C(15I)	111.2(8)
C(15)-N(14A)-C(14)	126.9(8)	O(15G)-C(15H)-H(15D)	109.4
C(15)-N(14A)-C(15C)	113.5(8)	C(15I)-C(15H)-H(15D)	109.4
C(14)-N(14A)-C(15C)	119.4(7)	O(15G)-C(15H)-H(15E)	109.4
C(15D)-O(15E)-C(15E)	97.7(6)	C(15I)-C(15H)-H(15E)	109.4
O(15)-C(15)-N(14A)	126.3(9)	H(15D)-C(15H)-H(15E)	108.0
O(15)-C(15)-N(15A)	126.1(9)	C(15E)-C(15F)-H(15F)	109.5
N(14A)-C(15)-N(15A)	107.5(8)	C(15E)-C(15F)-H(15G)	109.5
N(7A)-C(15B)-N(15A)	113.9(7)	H(15F)-C(15F)-H(15G)	109.5
N(7A)-C(15B)-C(15C)	103.7(7)	C(15E)-C(15F)-H(15H)	109.5
N(15A)-C(15B)-C(15C)	102.5(7)	H(15F)-C(15F)-H(15H)	109.5
N(7A)-C(15B)-C(15D)	111.1(7)	H(15G)-C(15F)-H(15H)	109.5
N(15A)-C(15B)-C(15D)	110.6(7)	C(15F)-C(15E)-O(15E)	97.7(10)
C(15C)-C(15B)-C(15D)	114.8(7)	C(15F)-C(15E)-H(15I)	112.2
C(15)-N(15A)-C(15B)	114.0(8)	O(15E)-C(15E)-H(15I)	112.2
C(15)-N(15A)-C(16)	120.7(8)	C(15F)-C(15E)-H(15J)	112.2
C(15B)-N(15A)-C(16)	124.4(7)	O(15E)-C(15E)-H(15J)	112.2

H(15I)-C(15E)-H(15J)	109.8	O(17D)-C(17D)-O(17E)	127.4(8)
N(16A)-C(16)-N(15A)	113.9(7)	O(17D)-C(17D)-C(17B)	120.3(8)
N(16A)-C(16)-H(16A)	108.8	O(17E)-C(17D)-C(17B)	112.3(7)
N(15A)-C(16)-H(16A)	108.8	C(17)-N(17A)-C(17B)	114.6(8)
N(16A)-C(16)-H(16B)	108.8	C(17)-N(17A)-C(18)	123.7(8)
N(15A)-C(16)-H(16B)	108.8	C(17B)-N(17A)-C(18)	121.1(8)
H(16A)-C(16)-H(16B)	107.7	O(17E)-C(17E)-C(17F)	103.6(7)
C(17)-N(16A)-C(17C)	111.4(7)	O(17E)-C(17E)-H(17D)	111.0
C(17)-N(16A)-C(16)	113.3(7)	C(17F)-C(17E)-H(17D)	111.0
C(17C)-N(16A)-C(16)	126.7(7)	O(17E)-C(17E)-H(17E)	111.0
C(17D)-O(17E)-C(17E)	112.6(6)	C(17F)-C(17E)-H(17E)	111.0
C(17H)-C(17I)-H(17A)	109.5	H(17D)-C(17E)-H(17E)	109.0
C(17H)-C(17I)-H(17B)	109.5	C(17I)-C(17H)-O(17G)	102.3(4)
H(17A)-C(17I)-H(17B)	109.5	C(17I)-C(17H)-H(17F)	111.3
C(17H)-C(17I)-H(17C)	109.5	O(17G)-C(17H)-H(17F)	111.3
H(17A)-C(17I)-H(17C)	109.5	C(17I)-C(17H)-H(17G)	111.3
H(17B)-C(17I)-H(17C)	109.5	O(17G)-C(17H)-H(17G)	111.3
C(17G)-O(17G)-C(17H)	107.0(6)	H(17F)-C(17H)-H(17G)	109.2
O(17C)-C(17G)-O(17G)	123.1(8)	C(17E)-C(17F)-H(17G)	109.5
O(17C)-C(17G)-C(17C)	126.8(8)	C(17E)-C(17F)-H(17H)	109.5
O(17G)-C(17G)-C(17C)	110.0(7)	H(17G)-C(17F)-H(17H)	109.5
O(17)-C(17)-N(17A)	127.9(9)	C(17E)-C(17F)-H(17I)	109.5
O(17)-C(17)-N(16A)	125.3(8)	H(17G)-C(17F)-H(17I)	109.5
N(17A)-C(17)-N(16A)	106.8(8)	H(17H)-C(17F)-H(17I)	109.5
N(17A)-C(17B)-N(5A)	116.8(8)	N(17A)-C(18)-C(18A)	112.5(7)
N(17A)-C(17B)-C(17D)	108.8(7)	N(17A)-C(18)-H(18A)	109.1
N(5A)-C(17B)-C(17D)	112.6(7)	C(18A)-C(18)-H(18A)	109.1
N(17A)-C(17B)-C(17C)	103.0(7)	N(17A)-C(18)-H(18B)	109.1
N(5A)-C(17B)-C(17C)	103.5(7)	C(18A)-C(18)-H(18B)	109.1
C(17D)-C(17B)-C(17C)	111.6(7)	H(18A)-C(18)-H(18B)	107.8
N(6A)-C(17C)-N(16A)	115.5(7)	C(4A)-C(18A)-C(1)	119.6(9)
N(6A)-C(17C)-C(17G)	112.3(7)	C(4A)-C(18A)-C(18)	120.6(8)
N(16A)-C(17C)-C(17G)	109.7(7)	C(1)-C(18A)-C(18)	119.7(8)
N(6A)-C(17C)-C(17B)	102.5(7)	C(22)-C(21)-C(38A)	120.2(8)
N(16A)-C(17C)-C(17B)	102.9(7)	C(22)-C(21)-H(21A)	119.9
C(17G)-C(17C)-C(17B)	113.5(7)	C(38A)-C(21)-H(21A)	119.9

C(21)-C(22)-O(22)	124.8(8)	O(26)-C(26)-N(26A)	124.1(9)
C(21)-C(22)-C(23)	120.5(8)	N(25A)-C(26)-N(26A)	109.6(8)
O(22)-C(22)-C(23)	114.7(8)	C(26)-N(26A)-C(37C)	111.7(7)
O(22)-C(22A)-H(22A)	109.5	C(26)-N(26A)-C(27)	118.3(8)
O(22)-C(22A)-H(22B)	109.5	C(37C)-N(26A)-C(27)	122.1(7)
H(22A)-C(22A)-H(22B)	109.5	N(27A)-C(27)-N(26A)	115.6(8)
O(22)-C(22A)-H(22C)	109.5	N(27A)-C(27)-H(27A)	108.4
H(22A)-C(22A)-H(22C)	109.5	N(26A)-C(27)-H(27A)	108.4
H(22B)-C(22A)-H(22C)	109.5	N(27A)-C(27)-H(27B)	108.4
C(22)-O(22)-C(22A)	115.1(7)	N(26A)-C(27)-H(27B)	108.4
O(23)-C(23A)-H(23A)	109.5	H(27A)-C(27)-H(27B)	107.4
O(23)-C(23A)-H(23B)	109.5	C(27)-N(27A)-C(35B)	122.0(8)
H(23A)-C(23A)-H(23B)	109.5	C(27)-N(27A)-C(28)	125.9(8)
O(23)-C(23A)-H(23C)	109.5	C(35B)-N(27A)-C(28)	111.8(7)
H(23A)-C(23A)-H(23C)	109.5	O(28)-C(28)-N(28A)	129.1(10)
H(23B)-C(23A)-H(23C)	109.5	O(28)-C(28)-N(27A)	123.4(9)
C(24)-C(23)-O(23)	123.8(8)	N(28A)-C(28)-N(27A)	107.5(8)
C(24)-C(23)-C(22)	120.5(8)	C(28)-N(28A)-C(35C)	113.3(8)
O(23)-C(23)-C(22)	115.5(8)	C(28)-N(28A)-C(29)	124.3(8)
C(23)-O(23)-C(23A)	115.7(7)	C(35C)-N(28A)-C(29)	122.4(8)
C(23)-C(24)-C(24A)	120.1(8)	C(33A)-C(29A)-C(30)	119.3(9)
C(23)-C(24)-H(24A)	120.0	C(33A)-C(29A)-C(29)	123.5(9)
C(24A)-C(24)-H(24A)	120.0	C(30)-C(29A)-C(29)	117.2(8)
C(38A)-C(24A)-C(24)	119.9(8)	N(28A)-C(29)-C(29A)	112.9(7)
C(38A)-C(24A)-C(25)	122.5(9)	N(28A)-C(29)-H(29A)	109.0
C(24)-C(24A)-C(25)	117.5(8)	C(29A)-C(29)-H(29A)	109.0
N(25A)-C(25)-C(24A)	111.4(7)	N(28A)-C(29)-H(29B)	109.0
N(25A)-C(25)-H(25A)	109.3	C(29A)-C(29)-H(29B)	109.0
C(24A)-C(25)-H(25A)	109.3	H(29A)-C(29)-H(29B)	107.8
N(25A)-C(25)-H(25B)	109.3	C(31)-C(30)-C(29A)	119.9(8)
C(24A)-C(25)-H(25B)	109.3	C(31)-C(30)-H(30A)	120.0
H(25A)-C(25)-H(25B)	108.0	C(29A)-C(30)-H(30A)	120.0
C(26)-N(25A)-C(37B)	112.5(8)	C(32)-C(31)-C(30)	121.1(9)
C(26)-N(25A)-C(25)	122.7(8)	C(32)-C(31)-O(31)	116.3(9)
C(37B)-N(25A)-C(25)	123.9(7)	C(30)-C(31)-O(31)	122.5(8)
O(26)-C(26)-N(25A)	126.2(9)	O(31)-C(31A)-H(31A)	109.5

O(31)-C(31A)-H(31B)	109.5	C(35B)-C(35C)-C(35G)	114.5(7)
H(31A)-C(31A)-H(31B)	109.5	O(35)-C(35)-N(34A)	128.6(9)
O(31)-C(31A)-H(31C)	109.5	O(35)-C(35)-N(35A)	121.5(8)
H(31A)-C(31A)-H(31C)	109.5	N(34A)-C(35)-N(35A)	109.9(8)
H(31B)-C(31A)-H(31C)	109.5	N(27A)-C(35B)-N(35A)	116.8(7)
C(31A)-O(31)-C(31)	114.7(7)	N(27A)-C(35B)-C(35D)	112.6(8)
C(31)-C(32)-O(32)	116.4(9)	N(35A)-C(35B)-C(35D)	109.5(8)
C(31)-C(32)-C(33)	117.9(9)	N(27A)-C(35B)-C(35C)	103.5(7)
O(32)-C(32)-C(33)	125.7(9)	N(35A)-C(35B)-C(35C)	101.3(7)
O(32)-C(32A)-H(32A)	109.5	C(35D)-C(35B)-C(35C)	112.5(7)
O(32)-C(32A)-H(32B)	109.5	O(35C)-C(35G)-O(35G)	128.1(10)
H(32A)-C(32A)-H(32B)	109.5	O(35C)-C(35G)-C(35C)	115.3(9)
O(32)-C(32A)-H(32C)	109.5	O(35G)-C(35G)-C(35C)	116.5(9)
H(32A)-C(32A)-H(32C)	109.5	C(35H)-C(35I)-H(35A)	109.5
H(32B)-C(32A)-H(32C)	109.5	C(35H)-C(35I)-H(35B)	109.5
C(32)-O(32)-C(32A)	117.3(8)	H(35A)-C(35I)-H(35B)	109.5
C(29A)-C(33A)-C(33)	119.6(9)	C(35H)-C(35I)-H(35C)	109.5
C(29A)-C(33A)-C(34)	122.9(9)	H(35A)-C(35I)-H(35C)	109.5
C(33)-C(33A)-C(34)	117.0(8)	H(35B)-C(35I)-H(35C)	109.5
C(33A)-C(33)-C(32)	122.1(9)	C(35)-N(35A)-C(36)	125.1(8)
C(33A)-C(33)-H(33A)	118.9	C(35)-N(35A)-C(35B)	112.3(7)
C(32)-C(33)-H(33A)	118.9	C(36)-N(35A)-C(35B)	121.8(8)
N(34A)-C(34)-C(33A)	115.3(7)	C(35G)-O(35G)-C(35H)	116.3(8)
N(34A)-C(34)-H(34A)	108.4	C(35I)-C(35H)-O(35G)	113.0(8)
C(33A)-C(34)-H(34A)	108.4	C(35I)-C(35H)-H(35D)	109.0
N(34A)-C(34)-H(34B)	108.4	O(35G)-C(35H)-H(35D)	109.0
C(33A)-C(34)-H(34B)	108.4	C(35I)-C(35H)-H(35E)	109.0
H(34A)-C(34)-H(34B)	107.5	O(35G)-C(35H)-H(35E)	109.0
C(35)-N(34A)-C(34)	124.6(8)	H(35D)-C(35H)-H(35E)	107.8
C(35)-N(34A)-C(35C)	112.4(8)	O(35E)-C(35E)-C(35F)	101.3(5)
C(34)-N(34A)-C(35C)	122.0(7)	O(35E)-C(35E)-H(35F)	111.5
N(28A)-C(35C)-N(34A)	112.8(7)	C(35F)-C(35E)-H(35F)	111.5
N(28A)-C(35C)-C(35B)	103.8(7)	O(35E)-C(35E)-H(35G)	111.5
N(34A)-C(35C)-C(35B)	104.1(7)	C(35F)-C(35E)-H(35G)	111.5
N(28A)-C(35C)-C(35G)	109.9(8)	H(35F)-C(35E)-H(35G)	109.3
N(34A)-C(35C)-C(35G)	111.4(7)	C(35D)-O(35E)-C(35E)	128.5(7)

C(35E)-C(35F)-H(35H)	109.5	C(37H)-C(37I)-H(37A)	109.5
C(35E)-C(35F)-H(35I)	109.5	C(37H)-C(37I)-H(37B)	109.5
H(35H)-C(35F)-H(35I)	109.5	H(37A)-C(37I)-H(37B)	109.5
C(35E)-C(35F)-H(35J)	109.5	C(37H)-C(37I)-H(37C)	109.5
H(35H)-C(35F)-H(35J)	109.5	H(37A)-C(37I)-H(37C)	109.5
H(35I)-C(35F)-H(35J)	109.5	H(37B)-C(37I)-H(37C)	109.5
O(35D)-C(35D)-O(35E)	118.8(8)	C(37G)-O(37G)-C(37H)	123.5(7)
O(35D)-C(35D)-C(35B)	128.8(9)	O(37C)-C(37G)-O(37G)	129.2(8)
O(35E)-C(35D)-C(35B)	112.3(8)	O(37C)-C(37G)-C(37C)	121.1(8)
N(35A)-C(36)-N(36A)	112.8(7)	O(37G)-C(37G)-C(37C)	109.7(8)
N(35A)-C(36)-H(36A)	109.0	O(37D)-C(37D)-O(37E)	125.1(9)
N(36A)-C(36)-H(36A)	109.0	O(37D)-C(37D)-C(37B)	120.7(9)
N(35A)-C(36)-H(36B)	109.0	O(37E)-C(37D)-C(37B)	114.1(8)
N(36A)-C(36)-H(36B)	109.0	C(37D)-O(37E)-C(37E)	117.4(7)
H(36A)-C(36)-H(36B)	107.8	C(37E)-C(37F)-H(37D)	109.5
C(37)-N(36A)-C(36)	119.8(7)	C(37E)-C(37F)-H(37E)	109.5
C(37)-N(36A)-C(37C)	113.5(7)	H(37D)-C(37F)-H(37E)	109.5
C(36)-N(36A)-C(37C)	125.9(7)	C(37E)-C(37F)-H(37F)	109.5
N(26A)-C(37C)-N(36A)	115.0(7)	H(37D)-C(37F)-H(37F)	109.5
N(26A)-C(37C)-C(37G)	113.5(7)	H(37E)-C(37F)-H(37F)	109.5
N(36A)-C(37C)-C(37G)	113.4(7)	O(37G)-C(37H)-C(37I)	110.6(6)
N(26A)-C(37C)-C(37B)	102.1(7)	O(37G)-C(37H)-H(37G)	109.5
N(36A)-C(37C)-C(37B)	100.7(7)	C(37I)-C(37H)-H(37G)	109.5
C(37G)-C(37C)-C(37B)	110.5(7)	O(37G)-C(37H)-H(37H)	109.5
O(37)-C(37)-N(37A)	127.4(8)	C(37I)-C(37H)-H(37H)	109.5
O(37)-C(37)-N(36A)	123.8(8)	H(37G)-C(37H)-H(37H)	108.1
N(37A)-C(37)-N(36A)	108.8(7)	O(37E)-C(37E)-C(37F)	110.6(7)
N(25A)-C(37B)-N(37A)	113.0(7)	O(37E)-C(37E)-H(37H)	109.5
N(25A)-C(37B)-C(37D)	108.9(8)	C(37F)-C(37E)-H(37H)	109.5
N(37A)-C(37B)-C(37D)	114.0(7)	O(37E)-C(37E)-H(37I)	109.5
N(25A)-C(37B)-C(37C)	102.6(7)	C(37F)-C(37E)-H(37I)	109.5
N(37A)-C(37B)-C(37C)	104.0(7)	H(37H)-C(37E)-H(37I)	108.1
C(37D)-C(37B)-C(37C)	113.8(7)	C(24A)-C(38A)-C(21)	118.8(9)
C(37)-N(37A)-C(37B)	112.6(7)	C(24A)-C(38A)-C(38)	123.5(8)
C(37)-N(37A)-C(38)	121.5(7)	C(21)-C(38A)-C(38)	117.6(8)
C(37B)-N(37A)-C(38)	122.8(7)	N(37A)-C(38)-C(38A)	113.5(7)

N(37A)-C(38)-H(38A)	108.9	C(44A)-C(45)-H(45A)	108.9
C(38A)-C(38)-H(38A)	108.9	N(45A)-C(45)-H(45B)	108.9
N(37A)-C(38)-H(38B)	108.9	C(44A)-C(45)-H(45B)	108.9
C(38A)-C(38)-H(38B)	108.9	H(45A)-C(45)-H(45B)	107.7
H(38A)-C(38)-H(38B)	107.7	C(46)-N(45A)-C(57B)	114.2(7)
C(42)-C(41)-C(58A)	120.7(8)	C(46)-N(45A)-C(45)	121.7(7)
C(42)-C(41)-H(41A)	119.6	C(57B)-N(45A)-C(45)	122.7(7)
C(58A)-C(41)-H(41A)	119.6	O(46)-C(46)-N(45A)	128.3(8)
C(41)-C(42)-C(43)	121.6(8)	O(46)-C(46)-N(46A)	125.0(8)
C(41)-C(42)-O(42)	123.5(8)	N(45A)-C(46)-N(46A)	106.7(7)
C(43)-C(42)-O(42)	114.5(8)	C(46)-N(46A)-C(47)	116.2(7)
C(42)-O(42)-C(42A)	116.8(7)	C(46)-N(46A)-C(57C)	111.6(7)
O(42)-C(42A)-H(42A)	109.5	C(47)-N(46A)-C(57C)	123.2(7)
O(42)-C(42A)-H(42B)	109.5	N(47A)-C(47)-N(46A)	115.8(7)
H(42A)-C(42A)-H(42B)	109.5	N(47A)-C(47)-H(47A)	108.3
O(42)-C(42A)-H(42C)	109.5	N(46A)-C(47)-H(47A)	108.3
H(42A)-C(42A)-H(42C)	109.5	N(47A)-C(47)-H(47B)	108.3
H(42B)-C(42A)-H(42C)	109.5	N(46A)-C(47)-H(47B)	108.3
C(44)-C(43)-O(43)	123.9(8)	H(47A)-C(47)-H(47B)	107.4
C(44)-C(43)-C(42)	119.6(9)	C(55B)-N(47A)-C(47)	124.9(7)
O(43)-C(43)-C(42)	116.4(8)	C(55B)-N(47A)-C(48)	112.1(7)
C(43)-O(43)-C(43A)	115.7(7)	C(47)-N(47A)-C(48)	121.7(7)
O(43)-C(43A)-H(43A)	109.5	O(48)-C(48)-N(48A)	129.0(9)
O(43)-C(43A)-H(43B)	109.5	O(48)-C(48)-N(47A)	124.7(9)
H(43A)-C(43A)-H(43B)	109.5	N(48A)-C(48)-N(47A)	106.3(8)
O(43)-C(43A)-H(43C)	109.5	C(48)-N(48A)-C(55C)	115.6(8)
H(43A)-C(43A)-H(43C)	109.5	C(48)-N(48A)-C(49)	124.3(7)
H(43B)-C(43A)-H(43C)	109.5	C(55C)-N(48A)-C(49)	120.0(7)
C(43)-C(44)-C(44A)	119.5(9)	N(48A)-C(49)-C(49A)	113.0(7)
C(43)-C(44)-H(44A)	120.3	N(48A)-C(49)-H(49A)	109.0
C(44A)-C(44)-H(44A)	120.3	C(49A)-C(49)-H(49A)	109.0
C(58A)-C(44A)-C(44)	120.3(9)	N(48A)-C(49)-H(49B)	109.0
C(58A)-C(44A)-C(45)	120.2(8)	C(49A)-C(49)-H(49B)	109.0
C(44)-C(44A)-C(45)	119.5(8)	H(49A)-C(49)-H(49B)	107.8
N(45A)-C(45)-C(44A)	113.3(7)	C(53A)-C(49A)-C(50)	120.1(9)
N(45A)-C(45)-H(45A)	108.9	C(53A)-C(49A)-C(49)	121.7(8)

C(50)-C(49A)-C(49)	118.0(8)	C(55)-N(54A)-C(55C)	113.2(7)
C(49A)-C(50)-C(51)	119.5(9)	C(55)-N(54A)-C(54)	121.4(7)
C(49A)-C(50)-H(50A)	120.3	C(55C)-N(54A)-C(54)	121.9(7)
C(51)-C(50)-H(50A)	120.3	C(55D)-O(55E)-C(55E)	117.4(7)
C(52)-C(51)-O(51A)	118.3(9)	O(55)-C(55)-N(54A)	126.9(8)
C(52)-C(51)-C(50)	120.4(9)	O(55)-C(55)-N(55A)	126.3(8)
O(51A)-C(51)-C(50)	121.4(8)	N(54A)-C(55)-N(55A)	106.7(7)
O(51A)-C(51A)-H(51A)	109.5	N(55A)-C(55B)-N(47A)	117.9(7)
O(51A)-C(51A)-H(51B)	109.5	N(55A)-C(55B)-C(55D)	109.7(7)
H(51A)-C(51A)-H(51B)	109.5	N(47A)-C(55B)-C(55D)	111.9(7)
O(51A)-C(51A)-H(51C)	109.5	N(55A)-C(55B)-C(55C)	101.1(7)
H(51A)-C(51A)-H(51C)	109.5	N(47A)-C(55B)-C(55C)	103.2(6)
H(51B)-C(51A)-H(51C)	109.5	C(55D)-C(55B)-C(55C)	112.5(7)
C(51)-O(51A)-C(51A)	118.8(8)	C(56)-N(55A)-C(55B)	125.1(7)
C(51)-C(52)-C(53)	122.4(9)	C(56)-N(55A)-C(55)	118.3(7)
C(51)-C(52)-O(52A)	121.3(9)	C(55B)-N(55A)-C(55)	113.2(7)
C(53)-C(52)-O(52A)	116.0(8)	O(55D)-C(55D)-O(55E)	125.9(9)
C(52)-O(52A)-C(52A)	112.5(7)	O(55D)-C(55D)-C(55B)	126.4(8)
O(52A)-C(52A)-H(52A)	109.5	O(55E)-C(55D)-C(55B)	107.6(7)
O(52A)-C(52A)-H(52B)	109.5	C(55G)-O(55G)-C(55H)	117.6(7)
H(52A)-C(52A)-H(52B)	109.5	N(54A)-C(55C)-N(48A)	116.3(7)
O(52A)-C(52A)-H(52C)	109.5	N(54A)-C(55C)-C(55B)	104.7(7)
H(52A)-C(52A)-H(52C)	109.5	N(48A)-C(55C)-C(55B)	101.4(6)
H(52B)-C(52A)-H(52C)	109.5	N(54A)-C(55C)-C(55G)	112.5(7)
C(49A)-C(53A)-C(53)	120.1(9)	N(48A)-C(55C)-C(55G)	108.3(6)
C(49A)-C(53A)-C(54)	123.3(8)	C(55B)-C(55C)-C(55G)	113.0(7)
C(53)-C(53A)-C(54)	116.6(8)	C(55I)-C(55H)-O(55G)	108.1(7)
C(52)-C(53)-C(53A)	117.3(8)	C(55I)-C(55H)-H(55A)	110.1
C(52)-C(53)-H(53A)	121.3	O(55G)-C(55H)-H(55A)	110.1
C(53A)-C(53)-H(53A)	121.3	C(55I)-C(55H)-H(55B)	110.1
N(54A)-C(54)-C(53A)	116.6(7)	O(55G)-C(55H)-H(55B)	110.1
N(54A)-C(54)-H(54A)	108.1	H(55A)-C(55H)-H(55B)	108.4
C(53A)-C(54)-H(54A)	108.1	O(55C)-C(55G)-O(55G)	127.4(9)
N(54A)-C(54)-H(54B)	108.1	O(55C)-C(55G)-C(55C)	125.0(8)
C(53A)-C(54)-H(54B)	108.1	O(55G)-C(55G)-C(55C)	107.4(7)
H(54A)-C(54)-H(54B)	107.3	O(55E)-C(55E)-C(93)	108.7(7)

O(55E)-C(55E)-H(55C) 109.9
 C(93)-C(55E)-H(55C) 109.9
 O(55E)-C(55E)-H(55D) 109.9
 C(93)-C(55E)-H(55D) 109.9
 H(55C)-C(55E)-H(55D) 108.3
 C(55H)-C(55I)-H(55E) 109.5
 C(55H)-C(55I)-H(55F) 109.5
 H(55E)-C(55I)-H(55F) 109.5
 C(55H)-C(55I)-H(55G) 109.5
 H(55E)-C(55I)-H(55G) 109.5
 H(55F)-C(55I)-H(55G) 109.5
 N(55A)-C(56)-N(56A) 114.0(7)
 N(55A)-C(56)-H(56A) 108.8
 N(56A)-C(56)-H(56A) 108.8
 N(55A)-C(56)-H(56B) 108.8
 N(56A)-C(56)-H(56B) 108.8
 H(56A)-C(56)-H(56B) 107.7
 C(57)-N(56A)-C(57C) 112.8(7)
 C(57)-N(56A)-C(56) 116.1(7)
 C(57C)-N(56A)-C(56) 125.6(7)
 C(57D)-O(57E)-C(57E) 119.1(7)
 C(57H)-C(57I)-H(57A) 109.5
 C(57H)-C(57I)-H(57B) 109.5
 H(57A)-C(57I)-H(57B) 109.5
 C(57H)-C(57I)-H(57C) 109.5
 H(57A)-C(57I)-H(57C) 109.5
 H(57B)-C(57I)-H(57C) 109.5
 C(57G)-O(57G)-C(57H) 115.9(7)
 O(57C)-C(57G)-O(57G) 128.8(8)
 O(57C)-C(57G)-C(57C) 119.5(8)
 O(57G)-C(57G)-C(57C) 111.0(7)
 O(57)-C(57)-N(57A) 128.5(9)
 O(57)-C(57)-N(56A) 124.8(9)
 N(57A)-C(57)-N(56A) 106.7(8)
 N(45A)-C(57B)-N(57A) 112.1(7)
 N(45A)-C(57B)-C(57D) 116.1(7)

N(57A)-C(57B)-C(57D) 107.5(7)
 N(45A)-C(57B)-C(57C) 104.1(7)
 N(57A)-C(57B)-C(57C) 102.0(7)
 C(57D)-C(57B)-C(57C) 114.3(7)
 N(56A)-C(57C)-N(46A) 112.3(7)
 N(56A)-C(57C)-C(57G) 112.4(7)
 N(46A)-C(57C)-C(57G) 113.5(7)
 N(56A)-C(57C)-C(57B) 104.3(6)
 N(46A)-C(57C)-C(57B) 102.3(7)
 C(57G)-C(57C)-C(57B) 111.1(7)
 O(57D)-C(57D)-O(57E) 126.0(9)
 O(57D)-C(57D)-C(57B) 124.9(9)
 O(57E)-C(57D)-C(57B) 109.0(8)
 C(57)-N(57A)-C(57B) 114.1(8)
 C(57)-N(57A)-C(58) 122.0(8)
 C(57B)-N(57A)-C(58) 122.2(7)
 C(57F)-C(57E)-O(57E) 112.4(7)
 C(57F)-C(57E)-H(57D) 109.1
 O(57E)-C(57E)-H(57D) 109.1
 C(57F)-C(57E)-H(57E) 109.1
 O(57E)-C(57E)-H(57E) 109.1
 H(57D)-C(57E)-H(57E) 107.9
 C(57I)-C(57H)-O(57G) 107.6(7)
 C(57I)-C(57H)-H(57F) 110.2
 O(57G)-C(57H)-H(57F) 110.2
 C(57I)-C(57H)-H(57G) 110.2
 O(57G)-C(57H)-H(57G) 110.2
 H(57F)-C(57H)-H(57G) 108.5
 C(57E)-C(57F)-H(57H) 109.5
 C(57E)-C(57F)-H(57I) 109.5
 H(57H)-C(57F)-H(57I) 109.5
 C(57E)-C(57F)-H(57J) 109.5
 H(57H)-C(57F)-H(57J) 109.5
 H(57I)-C(57F)-H(57J) 109.5
 N(57A)-C(58)-C(58A) 112.5(7)
 N(57A)-C(58)-H(58A) 109.1

C(58A)-C(58)-H(58A)	109.1	C(64A)-C(64)-C(63)	119.9(9)
N(57A)-C(58)-H(58B)	109.1	C(64A)-C(64)-H(64A)	120.1
C(58A)-C(58)-H(58B)	109.1	C(63)-C(64)-H(64A)	120.1
H(58A)-C(58)-H(58B)	107.8	C(78A)-C(64A)-C(64)	122.0(9)
C(41)-C(58A)-C(44A)	118.2(9)	C(78A)-C(64A)-C(65)	120.3(8)
C(41)-C(58A)-C(58)	118.8(8)	C(64)-C(64A)-C(65)	117.5(8)
C(44A)-C(58A)-C(58)	123.0(9)	C(66)-N(65A)-C(77B)	113.2(8)
C(55E)-C(93)-H(93A)	109.5	C(66)-N(65A)-C(65)	125.7(8)
C(55E)-C(93)-H(93B)	109.5	C(77B)-N(65A)-C(65)	120.1(7)
H(93A)-C(93)-H(93B)	109.5	N(65A)-C(65)-C(64A)	112.6(7)
C(55E)-C(93)-H(93C)	109.5	N(65A)-C(65)-H(65A)	109.1
H(93A)-C(93)-H(93C)	109.5	C(64A)-C(65)-H(65A)	109.1
H(93B)-C(93)-H(93C)	109.5	N(65A)-C(65)-H(65B)	109.1
C(78A)-C(61)-C(62)	122.2(8)	C(64A)-C(65)-H(65B)	109.1
C(78A)-C(61)-H(61A)	118.9	H(65A)-C(65)-H(65B)	107.8
C(62)-C(61)-H(61A)	118.9	C(66)-N(66A)-C(67)	116.4(7)
C(62)-O(62)-C(62A)	117.2(7)	C(66)-N(66A)-C(77C)	112.0(7)
O(62)-C(62)-C(63)	115.9(8)	C(67)-N(66A)-C(77C)	128.1(7)
O(62)-C(62)-C(61)	124.6(8)	O(66)-C(66)-N(65A)	126.5(9)
C(63)-C(62)-C(61)	119.2(8)	O(66)-C(66)-N(66A)	122.9(8)
O(62)-C(62A)-H(62A)	109.5	N(65A)-C(66)-N(66A)	110.6(8)
O(62)-C(62A)-H(62B)	109.5	C(68)-N(67A)-C(75B)	111.7(7)
H(62A)-C(62A)-H(62B)	109.5	C(68)-N(67A)-C(67)	120.0(7)
O(62)-C(62A)-H(62C)	109.5	C(75B)-N(67A)-C(67)	121.2(7)
H(62A)-C(62A)-H(62C)	109.5	N(66A)-C(67)-N(67A)	110.2(7)
H(62B)-C(62A)-H(62C)	109.5	N(66A)-C(67)-H(67A)	109.6
C(63)-O(63)-C(63A)	117.5(7)	N(67A)-C(67)-H(67A)	109.6
O(63)-C(63A)-H(63A)	109.5	N(66A)-C(67)-H(67B)	109.6
O(63)-C(63A)-H(63B)	109.5	N(67A)-C(67)-H(67B)	109.6
H(63A)-C(63A)-H(63B)	109.5	H(67A)-C(67)-H(67B)	108.1
O(63)-C(63A)-H(63C)	109.5	C(68)-N(68A)-C(75C)	112.6(7)
H(63A)-C(63A)-H(63C)	109.5	C(68)-N(68A)-C(69)	122.6(7)
H(63B)-C(63A)-H(63C)	109.5	C(75C)-N(68A)-C(69)	121.0(7)
O(63)-C(63)-C(62)	117.1(8)	O(68)-C(68)-N(68A)	127.0(9)
O(63)-C(63)-C(64)	124.1(8)	O(68)-C(68)-N(67A)	124.3(9)
C(62)-C(63)-C(64)	118.7(9)	N(68A)-C(68)-N(67A)	108.7(8)

C(70)-C(69A)-C(73A)	117.4(8)	C(72)-C(73)-H(73A)	119.2
C(70)-C(69A)-C(69)	120.8(8)	C(73A)-C(73)-H(73A)	119.2
C(73A)-C(69A)-C(69)	121.4(8)	C(75)-N(74A)-C(74)	126.6(8)
N(68A)-C(69)-C(69A)	114.6(6)	C(75)-N(74A)-C(75C)	111.0(7)
N(68A)-C(69)-H(69A)	108.6	C(74)-N(74A)-C(75C)	122.1(7)
C(69A)-C(69)-H(69A)	108.6	N(74A)-C(74)-C(73A)	114.7(8)
N(68A)-C(69)-H(69B)	108.6	N(74A)-C(74)-H(74A)	108.6
C(69A)-C(69)-H(69B)	108.6	C(73A)-C(74)-H(74A)	108.6
H(69A)-C(69)-H(69B)	107.6	N(74A)-C(74)-H(74B)	108.6
C(69A)-C(70)-C(71)	125.4(8)	C(73A)-C(74)-H(74B)	108.6
C(69A)-C(70)-H(70A)	117.3	H(74A)-C(74)-H(74B)	107.6
C(71)-C(70)-H(70A)	117.3	C(75G)-O(75G)-C(75H)	115.3(7)
C(71)-O(71)-C(71A)	115.0(7)	C(75)-N(75A)-C(75B)	111.8(7)
O(71)-C(71)-C(70)	120.8(8)	C(75)-N(75A)-C(76)	122.9(7)
O(71)-C(71)-C(72)	121.8(9)	C(75B)-N(75A)-C(76)	124.8(7)
C(70)-C(71)-C(72)	117.4(8)	N(74A)-C(75C)-N(68A)	112.0(6)
O(71)-C(71A)-H(71A)	109.5	N(74A)-C(75C)-C(75G)	112.5(7)
O(71)-C(71A)-H(71B)	109.5	N(68A)-C(75C)-C(75G)	113.0(7)
H(71A)-C(71A)-H(71B)	109.5	N(74A)-C(75C)-C(75B)	102.7(6)
O(71)-C(71A)-H(71C)	109.5	N(68A)-C(75C)-C(75B)	102.9(6)
H(71A)-C(71A)-H(71C)	109.5	C(75G)-C(75C)-C(75B)	113.0(7)
H(71B)-C(71A)-H(71C)	109.5	O(75)-C(75)-N(75A)	125.3(8)
C(72)-O(72)-C(72A)	115.4(8)	O(75)-C(75)-N(74A)	125.5(8)
O(72)-C(72)-C(73)	125.0(8)	N(75A)-C(75)-N(74A)	109.2(7)
O(72)-C(72)-C(71)	116.1(9)	N(75A)-C(75B)-N(67A)	112.5(6)
C(73)-C(72)-C(71)	118.8(9)	N(75A)-C(75B)-C(75D)	115.0(8)
O(72)-C(72A)-H(72A)	109.5	N(67A)-C(75B)-C(75D)	109.4(7)
O(72)-C(72A)-H(72B)	109.5	N(75A)-C(75B)-C(75C)	103.4(7)
H(72A)-C(72A)-H(72B)	109.5	N(67A)-C(75B)-C(75C)	102.5(6)
O(72)-C(72A)-H(72C)	109.5	C(75D)-C(75B)-C(75C)	113.2(7)
H(72A)-C(72A)-H(72C)	109.5	C(75D)-O(75E)-C(75E)	116.7(7)
H(72B)-C(72A)-H(72C)	109.5	C(75F)-C(75E)-O(75E)	111.1(8)
C(73)-C(73A)-C(69A)	119.2(8)	C(75F)-C(75E)-H(75A)	109.4
C(73)-C(73A)-C(74)	118.5(8)	O(75E)-C(75E)-H(75A)	109.4
C(69A)-C(73A)-C(74)	122.3(8)	C(75F)-C(75E)-H(75B)	109.4
C(72)-C(73)-C(73A)	121.7(9)	O(75E)-C(75E)-H(75B)	109.4

H(75A)-C(75E)-H(75B)	108.0	C(77)-N(77A)-C(77B)	112.6(7)
O(75C)-C(75G)-O(75G)	125.3(9)	C(77)-N(77A)-C(78)	123.1(7)
O(75C)-C(75G)-C(75C)	125.5(9)	C(77B)-N(77A)-C(78)	120.2(7)
O(75G)-C(75G)-C(75C)	109.0(7)	N(76A)-C(77C)-N(66A)	115.9(7)
C(75E)-C(75F)-H(75C)	109.5	N(76A)-C(77C)-C(77G)	113.4(8)
C(75E)-C(75F)-H(75D)	109.5	N(66A)-C(77C)-C(77G)	112.6(7)
H(75C)-C(75F)-H(75D)	109.5	N(76A)-C(77C)-C(77B)	102.9(7)
C(75E)-C(75F)-H(75E)	109.5	N(66A)-C(77C)-C(77B)	100.5(7)
H(75C)-C(75F)-H(75E)	109.5	C(77G)-C(77C)-C(77B)	110.0(7)
H(75D)-C(75F)-H(75E)	109.5	O(77)-C(77)-N(77A)	125.8(8)
O(75G)-C(75H)-C(75I)	105.9(7)	O(77)-C(77)-N(76A)	124.4(8)
O(75G)-C(75H)-H(75F)	110.6	N(77A)-C(77)-N(76A)	109.8(7)
C(75I)-C(75H)-H(75F)	110.6	N(65A)-C(77B)-N(77A)	117.5(7)
O(75G)-C(75H)-H(75G)	110.6	N(65A)-C(77B)-C(77D)	110.3(7)
C(75I)-C(75H)-H(75G)	110.6	N(77A)-C(77B)-C(77D)	109.4(7)
H(75F)-C(75H)-H(75G)	108.7	N(65A)-C(77B)-C(77C)	103.7(7)
C(75H)-C(75I)-H(75H)	109.5	N(77A)-C(77B)-C(77C)	101.8(6)
C(75H)-C(75I)-H(75I)	109.5	C(77D)-C(77B)-C(77C)	113.9(7)
H(75H)-C(75I)-H(75I)	109.5	O(77G)-C(77H)-C(77I)	106.3(7)
C(75H)-C(75I)-H(75J)	109.5	O(77G)-C(77H)-H(77A)	110.5
H(75H)-C(75I)-H(75J)	109.5	C(77I)-C(77H)-H(77A)	110.5
H(75I)-C(75I)-H(75J)	109.5	O(77G)-C(77H)-H(77B)	110.5
O(75D)-C(75D)-O(75E)	127.9(10)	C(77I)-C(77H)-H(77B)	110.5
O(75D)-C(75D)-C(75B)	124.7(9)	H(77A)-C(77H)-H(77B)	108.7
O(75E)-C(75D)-C(75B)	107.4(8)	O(77D)-C(77D)-O(77E)	126.9(8)
C(77)-N(76A)-C(77C)	111.3(7)	O(77D)-C(77D)-C(77B)	121.4(8)
C(77)-N(76A)-C(76)	115.8(7)	O(77E)-C(77D)-C(77B)	111.6(7)
C(77C)-N(76A)-C(76)	124.1(7)	C(77H)-C(77I)-H(77C)	109.5
N(75A)-C(76)-N(76A)	113.2(7)	C(77H)-C(77I)-H(77D)	109.5
N(75A)-C(76)-H(76A)	108.9	H(77C)-C(77I)-H(77D)	109.5
N(76A)-C(76)-H(76A)	108.9	C(77H)-C(77I)-H(77E)	109.5
N(75A)-C(76)-H(76B)	108.9	H(77C)-C(77I)-H(77E)	109.5
N(76A)-C(76)-H(76B)	108.9	H(77D)-C(77I)-H(77E)	109.5
H(76A)-C(76)-H(76B)	107.8	C(77E)-C(77F)-H(77F)	109.5
C(77G)-O(77G)-C(77H)	115.7(7)	C(77E)-C(77F)-H(77G)	109.5
C(77D)-O(77E)-C(77E)	112.1(6)	H(77F)-C(77F)-H(77G)	109.5

C(77E)-C(77F)-H(77H)	109.5	H(77I)-C(77E)-H(77J)	109.3
H(77F)-C(77F)-H(77H)	109.5	C(64A)-C(78A)-C(61)	117.8(9)
H(77G)-C(77F)-H(77H)	109.5	C(64A)-C(78A)-C(78)	123.7(9)
O(77C)-C(77G)-O(77G)	125.6(8)	C(61)-C(78A)-C(78)	118.5(8)
O(77C)-C(77G)-C(77C)	122.0(8)	C(78A)-C(78)-N(77A)	113.9(7)
O(77G)-C(77G)-C(77C)	112.3(7)	C(78A)-C(78)-H(78A)	108.8
O(77E)-C(77E)-C(77F)	101.4(6)	N(77A)-C(78)-H(78A)	108.8
O(77E)-C(77E)-H(77I)	111.5	C(78A)-C(78)-H(78B)	108.8
C(77F)-C(77E)-H(77I)	111.5	N(77A)-C(78)-H(78B)	108.8
O(77E)-C(77E)-H(77J)	111.5	H(78A)-C(78)-H(78B)	107.7
C(77F)-C(77E)-H(77J)	111.5		

Symmetry transformations used to generate equivalent atoms.

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for C₄₂H₄₈N₈O₁₆. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(1)	46(7)	32(6)	33(6)	-8(5)	-11(5)	-10(5)
C(2)	54(7)	18(6)	23(6)	2(5)	-12(5)	15(5)
O(2)	35(4)	32(5)	46(5)	-15(4)	-4(4)	7(3)
C(2A)	68(8)	28(6)	73(7)	-9(5)	0(6)	5(5)
C(3)	55(7)	32(7)	26(6)	-18(5)	-14(5)	12(5)
O(3)	58(5)	34(4)	38(4)	-23(4)	-15(4)	4(4)
C(3A)	76(8)	87(9)	60(7)	-46(6)	-31(6)	-11(6)
C(4)	24(5)	29(6)	25(6)	-4(5)	8(4)	-2(4)
C(4A)	51(7)	28(6)	16(5)	2(5)	-5(5)	-6(5)
C(5)	13(5)	27(6)	35(6)	2(5)	-7(4)	-7(4)
N(5A)	34(5)	30(5)	15(4)	1(4)	-11(4)	-7(4)
C(6)	40(6)	35(7)	20(6)	-7(5)	-3(5)	20(5)
N(6A)	26(5)	23(5)	30(5)	2(4)	1(4)	-18(4)
O(6)	34(4)	41(5)	29(4)	-21(3)	-12(3)	1(3)
C(7)	24(5)	25(6)	36(6)	-12(5)	-5(4)	-1(4)
N(7A)	50(6)	28(6)	23(5)	-13(4)	-14(4)	0(4)

C(8)	25(6)	38(7)	30(6)	-4(5)	-24(5)	5(5)
N(8A)	43(5)	19(5)	22(5)	-5(4)	1(4)	-3(4)
O(8)	27(4)	44(5)	52(5)	-5(4)	2(4)	9(3)
C(9)	34(6)	37(7)	37(7)	-9(6)	-11(5)	1(5)
C(9A)	42(7)	30(7)	30(6)	-7(5)	-6(5)	-1(5)
C(10)	39(6)	32(7)	31(6)	-17(5)	-6(5)	6(5)
C(11A)	46(7)	57(8)	53(8)	-23(6)	16(6)	-7(6)
O(11A)	33(4)	50(5)	32(4)	-17(4)	9(4)	-8(4)
C(11)	43(7)	21(6)	19(6)	-5(5)	5(5)	-10(5)
C(12)	32(6)	32(7)	23(6)	-11(5)	-1(5)	7(5)
O(12A)	45(4)	51(5)	26(4)	-12(4)	1(3)	-17(4)
C(12A)	54(7)	93(9)	38(7)	-2(6)	-5(5)	-52(6)
C(13A)	30(6)	27(6)	11(5)	1(4)	-5(4)	-2(5)
C(13)	37(6)	17(6)	53(8)	-2(5)	6(5)	-14(5)
C(14)	36(6)	28(6)	39(7)	-12(5)	3(5)	-15(5)
N(14A)	41(5)	19(5)	28(5)	-7(4)	-3(4)	5(4)
O(15D)	164(7)	65(5)	33(4)	-5(4)	50(4)	25(5)
O(15E)	68(4)	54(5)	28(4)	-1(3)	-12(3)	8(3)
C(15)	31(6)	21(6)	23(6)	5(5)	17(5)	-7(5)
C(15B)	29(5)	31(6)	19(5)	5(4)	-1(4)	-4(4)
N(15A)	33(5)	20(5)	36(5)	-6(4)	13(4)	-6(4)
O(15)	28(4)	34(5)	51(5)	-6(4)	-1(4)	-4(3)
C(15D)	73(7)	45(7)	34(6)	-10(5)	-23(6)	-19(6)
O(15G)	100(6)	41(5)	23(4)	-5(4)	-2(4)	11(4)
C(15C)	49(6)	18(6)	32(6)	-3(5)	-9(5)	-5(5)
O(15C)	57(5)	43(5)	36(5)	2(4)	12(4)	3(4)
C(15G)	25(5)	23(5)	26(6)	7(4)	-3(4)	3(4)
C(15I)	93(9)	17(6)	48(7)	10(5)	-3(6)	1(6)
C(15H)	73(8)	41(7)	45(7)	13(6)	-14(6)	-24(5)
C(16)	62(6)	8(5)	18(5)	0(4)	5(5)	1(4)
N(16A)	22(5)	30(6)	29(5)	3(4)	4(4)	-3(4)
O(17D)	52(4)	41(4)	22(4)	-4(3)	-7(3)	-16(3)
O(17E)	42(4)	30(4)	15(4)	-11(3)	-2(3)	-2(3)
O(17C)	47(4)	45(5)	22(4)	-10(4)	16(3)	-14(4)
O(17G)	52(4)	37(4)	34(4)	-16(3)	4(3)	-6(3)
C(17G)	22(5)	32(6)	20(6)	2(5)	0(4)	-12(4)

C(17)	22(5)	20(6)	33(6)	-6(5)	11(5)	-12(4)
C(17B)	22(5)	32(6)	18(6)	-7(5)	-2(5)	4(5)
C(17C)	20(5)	29(6)	24(6)	-14(5)	4(4)	-3(4)
C(17D)	24(6)	38(7)	16(5)	-16(5)	-2(4)	-5(5)
N(17A)	27(5)	32(6)	32(5)	-9(4)	-9(4)	7(4)
O(17)	25(4)	38(5)	43(5)	-1(4)	5(3)	10(3)
C(17E)	46(6)	70(8)	8(5)	-8(5)	8(5)	-11(6)
C(17F)	57(7)	94(10)	16(6)	-15(6)	2(5)	-26(7)
C(18)	34(6)	24(5)	42(7)	-12(5)	-6(5)	-1(4)
C(18A)	28(6)	18(6)	21(6)	-2(5)	10(5)	1(4)
C(21)	44(6)	18(6)	32(6)	-6(5)	-17(5)	-9(5)
C(22)	30(6)	18(6)	34(6)	-1(5)	1(5)	-14(4)
C(22A)	48(7)	51(7)	83(8)	-43(6)	-25(6)	17(5)
O(22)	42(4)	43(5)	47(5)	-24(4)	-9(4)	-6(3)
C(23A)	33(6)	76(8)	61(7)	-54(6)	-9(5)	21(5)
C(23)	29(6)	31(6)	27(6)	-17(5)	6(5)	-3(5)
O(23)	59(5)	35(5)	38(5)	-18(4)	0(4)	8(4)
C(24)	24(5)	28(6)	17(5)	1(4)	0(4)	13(4)
C(24A)	45(7)	19(6)	22(6)	2(5)	-17(5)	-5(5)
C(25)	46(6)	14(5)	20(5)	1(4)	-12(5)	0(4)
N(25A)	33(5)	12(5)	20(5)	-1(4)	2(4)	-10(4)
C(26)	32(6)	30(7)	45(7)	-14(5)	-25(5)	9(5)
N(26A)	25(5)	26(5)	29(5)	-7(4)	7(4)	4(4)
O(26)	28(4)	30(4)	73(6)	-16(4)	8(4)	-5(3)
C(27)	16(5)	49(7)	48(7)	-14(6)	16(5)	-4(5)
N(27A)	36(5)	20(5)	29(5)	-4(4)	-5(4)	3(4)
C(28)	27(6)	49(8)	27(6)	-10(5)	-4(5)	5(5)
N(28A)	28(4)	31(5)	21(5)	-8(4)	0(4)	-3(4)
O(28)	31(4)	36(5)	45(5)	-5(4)	6(4)	-1(3)
C(29A)	35(6)	19(6)	42(7)	-15(5)	7(5)	-3(5)
C(29)	39(6)	27(6)	12(5)	0(5)	-1(5)	1(5)
C(30)	21(5)	34(6)	13(5)	-6(4)	-7(4)	12(4)
C(31)	41(6)	32(6)	20(6)	-5(5)	-4(5)	-13(5)
C(31A)	51(6)	66(8)	49(7)	-45(6)	-12(5)	16(5)
O(31)	35(4)	54(5)	31(4)	-24(4)	-4(3)	-1(3)
C(32)	36(6)	26(6)	30(7)	-7(5)	-1(5)	9(5)

C(32A)	28(6)	76(9)	35(7)	-19(6)	-7(5)	14(5)
O(32)	45(5)	47(5)	32(5)	-20(4)	5(4)	7(4)
C(33A)	27(6)	16(6)	26(6)	-8(5)	-4(5)	3(4)
C(33)	28(6)	18(6)	44(7)	4(5)	4(5)	-6(4)
C(34)	39(6)	23(6)	26(6)	-8(5)	0(5)	8(5)
N(34A)	33(5)	29(6)	34(5)	-14(4)	-3(4)	-2(4)
C(35C)	38(6)	31(6)	15(5)	-4(5)	8(5)	-1(5)
C(35)	45(6)	28(6)	15(6)	0(5)	0(5)	-2(5)
C(35B)	58(7)	21(5)	29(6)	-17(4)	2(5)	-4(5)
C(35G)	86(8)	41(7)	28(7)	-29(6)	-3(6)	1(6)
C(35I)	137(11)	45(8)	30(6)	-23(5)	2(7)	-17(7)
N(35A)	27(5)	21(5)	40(5)	-1(4)	-2(4)	-2(4)
O(35)	37(4)	26(4)	65(6)	-6(4)	-13(4)	-7(3)
O(35D)	114(5)	26(4)	33(4)	-9(3)	-9(4)	11(4)
O(35G)	40(4)	38(5)	32(4)	5(4)	-6(3)	11(3)
O(35C)	67(6)	40(5)	39(5)	-5(4)	5(4)	-3(4)
C(35H)	101(9)	56(8)	22(6)	9(5)	-6(6)	47(6)
O(35E)	214(7)	33(4)	16(4)	-12(3)	-46(4)	6(4)
C(35F)	88(5)	43(4)	40(4)	-22(3)	20(3)	-20(4)
C(35D)	124(9)	12(5)	13(5)	0(4)	8(5)	19(5)
C(36)	83(7)	25(6)	28(6)	5(5)	-27(6)	-11(5)
N(36A)	42(5)	26(5)	20(5)	-11(4)	-21(4)	12(4)
C(37C)	27(5)	20(5)	21(6)	4(4)	-8(5)	-7(4)
C(37)	17(5)	23(6)	21(6)	-11(5)	3(4)	-8(4)
C(37B)	28(6)	20(6)	24(6)	-4(5)	-4(5)	-10(4)
N(37A)	26(4)	19(5)	22(5)	-10(4)	5(4)	-4(4)
O(37)	34(4)	28(4)	40(5)	2(3)	-12(3)	-8(3)
O(37D)	50(5)	94(6)	25(4)	-24(4)	2(4)	-36(4)
O(37C)	92(6)	47(5)	38(5)	-26(4)	2(4)	-39(4)
O(37G)	38(4)	18(4)	41(4)	-12(3)	21(3)	13(3)
C(37G)	51(7)	20(6)	19(6)	-13(5)	3(5)	2(5)
C(37D)	47(7)	17(6)	28(6)	7(5)	-6(5)	-5(5)
O(37E)	33(4)	48(5)	19(4)	-7(4)	2(3)	-8(3)
C(37F)	28(6)	53(7)	44(7)	-14(6)	13(5)	4(5)
C(37E)	43(6)	39(7)	29(6)	-18(5)	-7(5)	-3(5)
C(38A)	25(5)	18(5)	21(5)	-6(4)	12(4)	-7(4)

C(38)	53(6)	31(6)	10(5)	-10(5)	8(4)	-9(5)
C(41)	20(3)	16(3)	21(3)	-3(2)	0(2)	6(2)
C(42)	39(6)	20(6)	17(5)	-4(4)	10(5)	13(5)
O(42)	42(4)	26(4)	29(4)	-1(3)	-6(3)	0(3)
C(42A)	24(5)	53(7)	60(7)	-24(6)	25(5)	-11(5)
C(43)	32(6)	22(6)	16(6)	-4(5)	-3(5)	0(5)
O(43)	37(4)	35(4)	37(4)	-16(4)	-11(4)	-7(3)
C(43A)	41(6)	35(6)	47(7)	-28(6)	-13(5)	8(5)
C(44)	39(6)	29(6)	28(6)	-5(5)	4(5)	-2(5)
C(44A)	27(6)	15(6)	26(6)	-9(5)	5(5)	5(4)
C(45)	35(6)	38(6)	16(5)	-14(5)	11(4)	5(5)
N(45A)	35(5)	20(5)	28(5)	-8(4)	0(4)	2(4)
C(46)	31(6)	19(5)	15(5)	-2(4)	0(4)	16(4)
N(46A)	25(5)	15(5)	30(5)	-12(4)	-12(4)	2(3)
O(46)	35(4)	27(4)	33(4)	-10(3)	-14(3)	-4(3)
C(47)	58(6)	20(6)	7(5)	-7(4)	-9(5)	-6(5)
N(47A)	22(4)	20(5)	22(5)	-7(4)	-5(4)	7(4)
C(48)	30(6)	36(6)	12(5)	-2(5)	-13(5)	15(5)
N(48A)	19(4)	21(5)	26(5)	-4(4)	2(4)	1(4)
O(48)	18(4)	31(4)	39(5)	-7(4)	3(3)	-2(3)
C(49)	32(6)	15(6)	27(6)	-10(5)	-1(5)	8(4)
C(49A)	22(6)	15(6)	29(6)	2(4)	-9(5)	-3(4)
C(50)	28(6)	38(7)	34(7)	1(5)	0(5)	1(5)
C(51)	36(6)	34(7)	26(6)	-20(5)	5(5)	3(5)
C(51A)	26(7)	223(17)	82(9)	-96(11)	-4(6)	17(8)
O(51A)	48(5)	78(6)	40(5)	-36(4)	4(4)	15(4)
C(52)	48(7)	26(6)	31(6)	-13(5)	-14(5)	4(5)
O(52A)	57(5)	55(5)	49(5)	-30(4)	-28(4)	22(4)
C(52A)	72(7)	80(9)	80(9)	-65(7)	17(6)	-18(6)
C(53A)	32(6)	15(6)	31(6)	-7(5)	4(5)	-12(4)
C(53)	42(6)	30(6)	37(6)	-25(5)	-15(5)	8(5)
C(54)	22(5)	34(6)	28(6)	-2(4)	2(4)	1(4)
N(54A)	27(5)	22(5)	34(5)	-7(4)	-7(4)	-2(4)
O(55E)	49(4)	37(4)	28(4)	-16(3)	13(3)	-12(3)
C(55)	28(6)	21(6)	20(5)	-8(5)	-9(5)	-4(4)
C(55B)	19(5)	12(5)	40(6)	-12(4)	3(5)	-4(4)

N(55A)	25(4)	20(5)	24(5)	-5(4)	-1(4)	6(4)
O(55)	20(4)	30(4)	46(5)	-5(3)	-2(3)	-3(3)
C(55D)	26(4)	22(4)	18(3)	-6(2)	5(2)	-6(2)
O(55G)	53(4)	47(5)	27(4)	7(4)	-18(4)	-12(4)
C(55C)	26(5)	27(6)	19(5)	-3(4)	3(4)	-1(4)
C(55H)	88(7)	21(5)	31(6)	3(4)	-23(6)	-8(5)
O(55C)	65(5)	22(4)	34(5)	10(4)	-8(4)	-18(4)
O(55D)	69(5)	35(4)	20(4)	-12(3)	3(4)	-19(3)
C(55G)	24(5)	44(6)	23(6)	-12(5)	-7(5)	-4(5)
C(55E)	60(6)	55(6)	10(5)	-2(5)	12(5)	25(5)
C(56)	20(5)	43(6)	23(5)	-15(5)	1(4)	-7(4)
N(56A)	28(5)	11(4)	28(5)	-7(4)	-6(4)	3(3)
O(57D)	43(4)	51(5)	36(5)	-23(4)	-23(4)	10(4)
O(57E)	43(4)	58(5)	17(4)	-17(4)	5(3)	-1(4)
C(57I)	28(6)	72(9)	69(8)	-44(7)	-12(6)	14(5)
O(57C)	31(4)	40(5)	30(4)	-13(3)	-12(3)	-9(3)
O(57G)	35(4)	37(4)	29(4)	-24(3)	-4(3)	8(3)
C(57G)	32(6)	21(6)	29(6)	-13(5)	0(5)	-3(5)
C(57)	29(6)	29(7)	44(7)	-2(5)	-16(6)	4(5)
C(57B)	19(5)	22(6)	36(6)	-16(5)	-3(4)	11(4)
C(57C)	13(5)	28(6)	21(5)	-15(5)	4(4)	9(4)
C(57D)	45(7)	7(5)	36(6)	-1(4)	3(5)	-1(5)
N(57A)	25(5)	16(5)	32(5)	-1(4)	4(4)	3(4)
O(57)	16(4)	36(4)	45(4)	-10(4)	13(3)	11(3)
C(57H)	49(7)	29(6)	39(7)	-28(5)	3(5)	-6(5)
C(58)	35(6)	10(5)	29(6)	1(4)	-4(5)	11(4)
C(58A)	39(6)	18(6)	24(6)	-4(5)	-10(5)	13(5)
C(93)	70(8)	49(8)	44(7)	-9(6)	28(6)	5(6)
C(61)	22(5)	16(5)	20(5)	-2(4)	-6(4)	-1(4)
O(62)	30(4)	26(4)	30(4)	-14(3)	1(3)	4(3)
C(62)	38(6)	16(6)	27(6)	-4(5)	-6(5)	-6(5)
C(62A)	32(6)	65(8)	54(8)	-21(6)	-1(6)	-17(5)
O(63)	30(4)	36(4)	34(4)	-26(3)	0(3)	10(3)
C(63A)	53(6)	33(6)	39(6)	-20(5)	-21(5)	18(5)
C(63)	34(6)	23(6)	27(5)	-9(5)	-7(5)	-1(5)
C(64)	39(7)	31(7)	40(7)	-1(6)	-14(6)	-3(5)

C(64A)	25(5)	16(5)	19(6)	-7(4)	6(4)	-5(4)
N(65A)	32(5)	22(5)	21(5)	-9(4)	-12(4)	8(4)
C(65)	36(6)	32(6)	22(6)	-13(5)	-8(5)	-4(5)
O(66)	41(4)	25(4)	49(5)	-4(4)	-1(4)	4(3)
N(66A)	18(4)	29(5)	29(5)	-2(4)	12(4)	-1(4)
C(66)	25(6)	19(6)	20(6)	-15(5)	1(5)	-2(4)
N(67A)	20(4)	18(5)	30(5)	-9(4)	-7(4)	-1(3)
C(67)	32(6)	12(5)	48(7)	2(4)	-2(5)	11(4)
O(68)	41(4)	39(5)	31(4)	-6(3)	-19(3)	-2(3)
N(68A)	26(4)	17(5)	18(4)	-12(4)	-3(4)	2(3)
C(68)	17(5)	39(7)	29(6)	0(5)	13(5)	0(5)
C(69A)	28(6)	21(6)	30(6)	-9(5)	-5(5)	11(4)
C(69)	36(6)	14(5)	35(6)	-14(4)	-7(5)	-11(4)
C(70)	11(4)	33(6)	29(5)	-1(4)	-1(4)	1(4)
O(71)	50(5)	60(5)	31(4)	-35(4)	-4(4)	4(4)
C(71)	30(6)	45(7)	26(6)	-16(5)	-8(5)	10(5)
C(71A)	100(8)	46(7)	83(9)	-38(6)	-75(7)	42(6)
O(72)	36(4)	69(6)	36(5)	-23(4)	0(4)	2(4)
C(72)	30(6)	48(7)	31(7)	-11(6)	-4(5)	9(5)
C(72A)	47(8)	116(11)	77(9)	-71(8)	9(6)	16(7)
C(73A)	38(6)	20(6)	20(6)	-11(5)	0(5)	6(5)
C(73)	26(6)	28(6)	32(6)	-23(5)	-5(5)	10(4)
N(74A)	28(5)	20(5)	29(5)	-14(4)	-5(4)	4(4)
C(74)	29(6)	37(7)	29(6)	-4(5)	-8(5)	2(5)
O(75)	30(4)	30(4)	32(4)	-10(3)	-3(3)	2(3)
O(75D)	37(4)	48(4)	38(4)	-25(4)	1(3)	-7(3)
O(75G)	66(5)	27(4)	24(4)	-4(3)	-19(4)	-8(4)
O(75C)	40(4)	48(5)	29(4)	-3(4)	2(3)	-6(4)
N(75A)	19(4)	19(5)	27(5)	-4(4)	3(4)	0(4)
C(75C)	23(5)	19(5)	22(5)	-12(4)	-10(4)	2(4)
C(75)	18(5)	22(6)	27(6)	-8(5)	2(5)	-10(4)
C(75B)	25(5)	39(6)	4(4)	-1(4)	-2(4)	1(4)
O(75E)	27(4)	40(4)	24(4)	-10(3)	9(3)	-5(3)
C(75E)	46(6)	48(6)	35(6)	-18(5)	18(5)	-34(5)
C(75G)	41(6)	9(5)	27(6)	-2(4)	6(5)	8(4)
C(75F)	49(7)	91(10)	42(7)	-30(7)	-9(6)	29(6)

C(75H)	177(12)	63(7)	19(6)	6(5)	-50(7)	-30(7)
N(76A)	25(5)	29(5)	13(4)	2(4)	2(4)	-5(4)
C(76)	16(5)	29(6)	44(7)	-8(5)	-4(5)	2(4)
O(77)	25(4)	33(4)	37(4)	-6(4)	-1(3)	0(3)
O(77C)	37(4)	45(5)	39(5)	-26(4)	-1(4)	6(3)
O(77G)	32(4)	28(4)	23(4)	-9(3)	-9(3)	12(3)
O(77D)	57(5)	52(5)	31(5)	-7(4)	-6(4)	3(4)
O(77E)	56(5)	40(5)	19(4)	-9(3)	-5(4)	14(4)
N(77A)	20(4)	22(5)	16(4)	-2(4)	1(3)	-1(3)
C(77C)	31(6)	18(6)	26(6)	-1(5)	-2(5)	-6(4)
C(77)	18(5)	27(6)	27(6)	-18(5)	9(4)	-10(4)
C(77B)	35(6)	22(6)	12(5)	2(4)	-5(4)	-5(4)
C(77H)	52(7)	35(6)	18(6)	-11(5)	-16(5)	18(5)
C(77D)	27(6)	41(6)	15(5)	-14(5)	-7(4)	0(5)
C(77I)	76(8)	37(7)	28(6)	-19(5)	11(5)	-1(6)
C(77F)	78(6)	96(7)	31(4)	-21(4)	21(3)	31(4)
C(77G)	31(6)	20(5)	8(5)	7(4)	-6(4)	5(4)
C(78A)	40(6)	21(6)	17(6)	2(5)	2(5)	0(5)
C(78)	37(6)	5(5)	36(6)	5(4)	-11(5)	-12(4)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for C₄₂H₄₈N₈O₁₆.

	x	y	z	U(eq)
H(1A)	3432	8805	2301	43
H(2AA)	2701	10096	3641	86
H(2AB)	2790	9117	3540	86
H(2AC)	2763	9874	2821	86
H(3AA)	6615	10002	3775	102
H(3AB)	6884	9772	2961	102
H(3AC)	6595	9025	3676	102
H(4A)	6472	8711	2453	33

H(5A)	6091	7820	1083	31
H(5B)	6734	7748	1714	31
H(7A)	6626	4795	3248	33
H(7B)	5765	4992	3804	33
H(9A)	6550	1970	2613	42
H(9B)	5813	1376	3175	42
H(10A)	6593	1768	1425	39
H(11A)	7222	1518	-404	79
H(11B)	7281	1310	479	79
H(11C)	7019	2256	76	79
H(12A)	3244	898	-32	94
H(12B)	2983	1428	624	94
H(12C)	3327	457	821	94
H(13A)	3482	1602	1630	45
H(14A)	3242	1957	2752	41
H(14B)	3899	1422	3286	41
H(15A)	4192	-283	5379	83
H(15B)	4623	-91	4513	83
H(15C)	3790	465	4793	83
H(15D)	4695	1044	5528	66
H(15E)	5528	503	5224	66
H(15F)	5584	2691	6530	215
H(15G)	6210	3105	5772	215
H(15H)	5660	2248	5812	215
H(15I)	4950	3761	5966	186
H(15J)	4460	2900	5878	186
H(16A)	3063	4984	3293	37
H(16B)	3899	5189	3675	37
H(17A)	7290	3643	365	71
H(17B)	7475	3948	1111	71
H(17C)	7355	4646	369	71
H(17D)	5662	6931	-592	51
H(17E)	6109	5988	-450	51
H(17F)	5929	3534	1186	45
H(17G)	5827	4323	495	45
H(17G)	7169	6988	-1208	83

H(17H)	7508	6624	-415	83
H(17I)	7061	7557	-572	83
H(18A)	3540	7775	1564	39
H(18B)	4460	7796	1009	39
H(21A)	8427	-3724	2466	36
H(22A)	8262	-5057	1251	83
H(22B)	8245	-4090	1381	83
H(22C)	8032	-4869	2083	83
H(23A)	12275	-5103	1384	77
H(23B)	12128	-4925	2222	77
H(23C)	12187	-4138	1519	77
H(24A)	11492	-3834	2631	29
H(25A)	10524	-2861	3955	32
H(25B)	11409	-2818	3355	32
H(27A)	11811	49	1624	46
H(27B)	10935	-120	1278	46
H(29A)	10993	3569	1676	32
H(29B)	11658	3032	2204	32
H(30A)	11421	3409	3353	27
H(31A)	11664	4121	4956	75
H(31B)	11546	4507	4099	75
H(31C)	11859	3531	4338	75
H(32A)	7698	3490	5376	68
H(32B)	7936	2726	4930	68
H(32C)	7640	3644	4494	68
H(33A)	8349	3241	3511	38
H(34A)	8374	3067	2330	36
H(34B)	9150	3614	1771	36
H(35A)	10690	5301	-463	105
H(35B)	11155	4544	69	105
H(35C)	10364	5094	423	105
H(35D)	10159	3978	-567	76
H(35E)	9367	4536	-225	76
H(35F)	8739	1731	-653	24
H(35G)	9452	961	-713	24
H(35H)	9925	2232	-1669	86

H(35I)	10649	1992	-1100	86
H(35J)	9958	2761	-1016	86
H(36A)	9225	29	1145	53
H(36B)	8323	203	1664	53
H(37A)	7899	1021	4901	100
H(37B)	8429	143	4850	100
H(37C)	7461	285	4585	100
H(37D)	7770	-1992	6200	64
H(37E)	7826	-2564	5568	64
H(37F)	7370	-1633	5432	64
H(37G)	7969	1235	3560	63
H(37H)	8880	1373	3875	63
H(37H)	8744	-993	5396	42
H(37I)	9206	-1922	5554	42
H(38A)	8151	-2734	3220	38
H(38B)	8758	-2805	3879	38
H(41A)	6504	1120	7444	23
H(42A)	7060	-189	6159	70
H(42B)	7053	-16	6990	70
H(42C)	7047	775	6295	70
H(43A)	3000	-145	6481	57
H(43B)	3046	832	6578	57
H(43C)	2901	74	7304	57
H(44A)	3384	1168	7678	40
H(45A)	3280	2210	8436	36
H(45B)	4026	2115	8987	36
H(47A)	4448	4772	6342	33
H(47B)	3455	5023	6648	33
H(49A)	3286	8019	7187	29
H(49B)	4081	8534	6621	29
H(50A)	3154	8421	8327	42
H(51A)	2391	9027	10035	153
H(51B)	2397	8474	9394	153
H(51C)	2642	9474	9169	153
H(52A)	5517	9733	10119	109
H(52B)	4590	9749	9787	109

H(52C)	5486	10077	9240	109
H(53A)	6255	8463	8353	39
H(54A)	5862	8637	6616	35
H(54B)	6538	8183	7170	35
H(55A)	4344	8455	4386	56
H(55B)	5173	7851	4177	56
H(55C)	7093	7014	4339	53
H(55D)	6315	6396	4240	53
H(55E)	3928	7579	3637	107
H(55F)	3376	7313	4459	107
H(55G)	4212	6745	4205	107
H(56A)	6863	5204	7174	33
H(56B)	6565	5079	6399	33
H(57A)	3102	6625	9529	78
H(57B)	2913	5680	9407	78
H(57C)	2901	6487	8727	78
H(57D)	4360	3304	10572	40
H(57E)	4169	4315	10378	40
H(57F)	4426	5867	9388	44
H(57G)	4416	6684	8711	44
H(57H)	3002	3646	11150	83
H(57I)	2900	3026	10578	83
H(57J)	2698	4032	10347	83
H(58A)	5749	2028	8867	31
H(58B)	6560	2087	8197	31
H(93A)	7708	5672	4123	87
H(93B)	7087	5184	4856	87
H(93C)	7868	5804	4938	87
H(61A)	11503	13772	7309	23
H(62A)	11934	15118	8493	73
H(62B)	12037	14903	7668	73
H(62C)	11890	14143	8392	73
H(63A)	7893	15160	8819	58
H(63B)	7922	14204	8659	58
H(63C)	7877	15010	7983	58
H(64A)	8391	13866	7504	44

H(65A)	8355	12897	6745	34
H(65B)	9180	12927	6089	34
H(67A)	7988	9870	7845	39
H(67B)	8376	9972	8594	39
H(69A)	8345	6745	7842	32
H(69B)	9063	6316	8367	32
H(70A)	8695	6467	6679	30
H(71A)	9383	5297	4836	101
H(71B)	9400	4937	5715	101
H(71C)	10305	5261	5179	101
H(72A)	12536	5946	4996	112
H(72B)	12238	5510	5858	112
H(72C)	12503	6505	5635	112
H(73A)	11744	6656	6617	32
H(74A)	10822	6480	8349	38
H(74B)	11605	7002	7775	38
H(75A)	7775	8053	10603	52
H(75B)	8565	8650	10710	52
H(75C)	7200	9334	10835	88
H(75D)	7077	9260	9997	88
H(75E)	7856	9847	10136	88
H(75F)	10853	6629	10553	101
H(75G)	9795	6799	10716	101
H(75H)	10542	7550	11460	67
H(75I)	10101	8238	10850	67
H(75J)	11150	8041	10720	67
H(76A)	11486	10006	8296	35
H(76B)	10493	10246	8622	35
H(77A)	10464	9156	5583	40
H(77B)	10450	8341	6265	40
H(77C)	11830	8376	5440	70
H(77D)	12018	8490	6254	70
H(77E)	12035	9309	5581	70
H(77F)	11904	11400	3797	106
H(77G)	12180	10957	4598	106
H(77H)	11973	11966	4418	106

H(77I)	10395	11653	4397	56
H(77J)	10611	10638	4608	56
H(78A)	11633	12841	6533	32
H(78B)	10903	12935	5968	32
