**Experimental**

General

Melting points were determined in open capillaries and are uncorrected. $^1$H NMR spectra were recorded at 200 or 300 MHz and $^{13}$C NMR spectra at 62.5 or 75 MHz. EI or FAB mass spectra were recorded at The Ohio State University Chemical Instrument Center. MALDI-TOF spectrometry was performed using indoleacrylic acid as the matrix in tetrahydrofuran (THF). Gel permeation chromatography (gpc) was performed using three divinylbenzene columns arranged in series (500, $10^3$ and $10^4$ Å) with RI detection. All runs were carried out using THF as the carrier solvent at 40°C. All reactions were performed under an argon or nitrogen atmosphere. Dimethylformamide (DMF) was dried by distillation from barium oxide or magnesium sulfate; THF was distilled from sodium/benzophenone ketyl; acetone was distilled from $CaSO_4$ and dichloromethane was distilled from calcium hydride. Chromatographic separations were performed on silica gel 60 (230-400 mesh, 60 Å) using the indicated solvents.

**Dodecyl Anthranilate**. Dodecanol (2 mL) was treated with sodium metal (138 mg, 6 mmol) and was allowed to stir for *ca.* 5 min. until all the sodium metal was consumed. This solution was added to methyl anthranilate (9.0 g, 59.6 mmol) in THF (60 mL) and dodecanol (290 mL) and was heated to 80°C. After 16 h the reaction was cooled to ambient temperature and the solvent and excess dodecanol was removed in vacuo. The resultant residue was dispersed in $CH_2Cl_2$ (100 mL) washed with 1.2 N hydrochloric acid (2 x 50 mL). The organics layer was dried ($MgSO_4$), concentrated and purified by column chromatrography ($CH_2Cl_2$) affording dodecyl anthranilate as a clear oil (16.1 g, 53.0 mmol, 89%). $^1$H NMR (200 MHz, $CDCl_3$). δ 0.90 (m, 3H), 1.2-1.5 (m, 18H), 1.75 (m, 2H), 4.26 (t, *J*=6.60 Hz, 2H), 6.65 (td,

*J*=6.98, 1.21 Hz, 1H), 6.67 (d, *J*=7.71 Hz, 1H), 7.27 (td, *J*=7.68, 1.61 Hz, 1H), 7.85 (dd, *J*=8.59, 1.69 Hz, 1H); $^{13}$C NMR (50 MHz, $CDCl_3$) 14, 22, 27, 30-31(7 C), 32, 63, 111, 117.0 117.5, 131, 133, 149, 168 ppm; IR ($CHCl_3$) 3466, 3365, 1685, 1616 cm$^{-1}$; HRMS for $C_{19}H_{31}NO_2$ (FAB) (M+) Calcd. 305.2355; obsd. 305.2348.

**4-Chloro-pyridine-2,6-dicarbonyl chloride (2).** Chelidamic acid monohydrate (1.81 g, 9 mmol) was treated with phosphorous oxychloride ($POCl_3$) (20 mL) and heated at reflux for 24 h. The $POCl_3$ was removed by distillation at reduced pressure and the resultant residue was dissolved in 4 mL of $CH_2Cl_2$ and filtered to remove the insoluble components. Evaporation in vacuo afforded 4-chloro-pyridine-2,6-dicarbonyl chloride, **2**, as a pink solid which was used without further purification. Typically, **2** was stored as a solution in $CH_2Cl_2$. $^1$H NMR (250 MHz, $CDCl_3$). δ 8.31 (s, 2H).

**4-Chloro-2,6-bis-(2-(2-dodecanoxycarbonylphenylcarbamoyl)pyridine ($C_{12}H_{25}O_2C)_2$-[G1]-Cl. (3a)** Dodecyl anthranilate (18.4 g, 60.3 mmol) and 4-dimethylaminopyridine (DMAP) (736 mg, 6.03 mmol) was dissolved in a mixture of $CH_2Cl_2$ (40 mL) and pyridine (20 mL). A solution of 4-chloro-pyridine-2,6-dicarbonyl chloride, **2**, (7.92 g, 33.2 mmol) in 20 ml $CH_2Cl_2$ was then added dropwise via syringe over 5-10 min. resulting in a color change from light yellow to purple and the formation of a white precipitate. After stirring at rt for an additional hour, the mixture was taken up in $CH_2Cl_2$ (200 mL) and washed with water (200 mL) and the phases were separated. The aqueous phase was then extracted with $CH_2Cl_2$ (2 x 100 mL) and the combined organic layers were dried over $MgSO_4$ and concentrated to an orange waxy oil. Purification by flash chromatography ($SiO_2$) with $CH_2Cl_2$ afforded ($C_{12}H_{25}O_2C)_2$-[G1]-Cl (**3a**) (11.0 g, 14.2

mmol, 47%) as a clear waxy solid. $^1$H NMR (200 MHz, $CDCl_3$). δ 0.88 (bs, 6H), 1.24 (bs, 36 H), 1.58 (bs, 4H), 4.00 (t, *J*=6.8 Hz, 4H), 7.24 (td, *J*=8.24, 1.0 Hz, 2H), 7.67 (td, *J*=8.84, 1.86 Hz, 2H), 8.07 (dd, *J*=8.04, 1.62 Hz, 2H), 8.42 (s, 2H), 8.75 (d, *J*=7.4 Hz, 2H), 12.75 (s, 2H). $^{13}$C NMR (50 MHz, $CDCl_3$) 14, 23, 26, 27, 29-31(6 C), 32, 66, 118, 121, 123, 125, 131, 134, 140, 149, 151, 161, 166 ppm; IR ($CHCl_3$, 10 mM) 3358, 3239, 1686 cm$^{-1}$; HRMS for $C_{45}H_{62}ClN_3O_6$ (FAB) (M+H) Calcd. 776.4405; obsd. 776.4405. Anal. Calcd. for $C_{45}H_{61}ClN_3O_6$; C, 69.61; H, 8.05; N, 5.41; Cl, 4.57. Found: C, 69.45; H, 7.98; N, 5.38; Cl, 4.64

**4-Azido-2,6-bis-(2-(2-dodecanoxycarbonylphenylcarbamoyl)pyridine. (3b)** $(C_{12}H_{25}O_2C)_2$-**[G1]-$N_3$**. $(C_{12}H_{25}O_2C)_2$-[G1]-Cl (**3a**) (8.79 g, 11.31 mmol) and sodium azide (7.35 g, 113.1 mmol) were mixed in DMF (160 mL) then heated to 50°C. After 24 h, the DMF was removed by distillation under reduced pressure and the resultant residue was dispersed in $CH_2Cl_2$ (100 mL). The $CH_2Cl_2$ solution was washed with water (2 x 50 mL) then dried over $MgSO_4$ and concentrated in vacuo. Purification by flash chromatography ($SiO_2$) with 1% ether/$CH_2Cl_2$ afforded $(C_{12}H_{25}O_2C)_2$-[G1]-$N_3$ (**3b**) (8.35 g, 10.66 mmol, 94%) as a clear waxy solid. $^1$H NMR (200 MHz, $CDCl_3$). δ 0.88 (bm, 6H), 1.24 (bm, 36 H), 1.58 (bm, 4H), 4.01 (t, *J*=6.8 Hz, 4H), 7.20 (td, *J*=7.88, 1.0 Hz, 2H), 7.64 (td, *J*=8.58, 1.58 Hz, 2H), 8.07 (s, 2H), 8.08 (d, *J*=8.14 Hz, 2H), 8.75 (d, *J*=8.34 Hz, 2H), 12.76 (s, 2H). $^{13}$C NMR (50 MHz, $CDCl_3$) 14.01, 22.62, 25.81, 28.33, 29.11, 29.27 (2C), 29.44, 29.50, 29.58, 31.84, 65.37, 115.09, 117.92, 121.53, 123.51, 130.98, 134.06, 139.92, 151.22, 152.86, 161.33, 167.09 ppm; IR ($CHCl_3$, 10 mM) 3356, 3242, 2121, 1688 cm$^{-1}$; HRMS for $C_{45}H_{63}N_6O_6$ (FAB) (M+) calcd. 783.4809; obsd. 783.4807. Anal. Calcd. for $C_{45}H_{63}N_6O_6$; C, 69.03; H, 7.98; N, 10.73. Found: C, 69.04; H, 8.08; N, 10.85.

**4-Amino-2,6-bis-(2-(2-dodecanoxycarbonylphenylcarbamoyl)pyridine. (3c) $(C_{12}H_{25}O_2C)_2$-[G1]-$NH_2$.** $(C_{12}H_{25}O_2C)_2$-[G1]-$N_3$ **(3b)** (8.35 g, 10.66 mmol) was dissolved in 100 mL of THF-methanol (3:1) and the solution was degassed by sparging with argon for 10 min. 10% Pd-C (1.73 g) was added and the mixture was hydrogenated at 50 psi for 12 h at room temperature. The catalyst was then removed by filtration through a pad of celite with ethyl acetate. The ethyl acetate was removed in vacuo and the resultant solid was passed through a short plug of silica gel using ethyl acetate affording $(C_{12}H_{25}O_2C)_2$-[G1]-$NH_2$ **(3c)** as a white waxy solid (8.0 g, 10.57 mmol, 99%). $^1$H NMR (200 MHz, $CDCl_3$). δ 0.87 (bm, 6H), 1.24 (bm, 36 H), 1.57 (bm, 4H), 4.01 (t, *J*=6.7 Hz, 4H), 4.95 (bs, 2H) 7.16 (t, *J*=7.38 Hz, 2H), 7.60 (t, *J*=7.28 Hz, 2H), 7.68 (s, 2H), 8.06 (d, *J*=7.92 Hz, 2H), 8.72 (d, *J*=8.36 Hz, 2H), 12.67 (s, 2H). $^{13}$C NMR (50 MHz, $CDCl_3$) 14.04, 22.62, 25.82, 28.33, 29.12, 29.29 (2 C), 29.44, 29.50, 29.58, 31.85, 65.34, 109.97, 118.17, 121.59, 123.20, 130.99, 133.87, 140.07, 150.05, 155.91, 162.75, 167.10 ppm; IR ($CHCl_3$, 10 mM) 3479, 3364, 3238, 1690 cm$^{-1}$; HRMS for $C_{45}H_{65}N_4O_6$ (FAB) (M+H) calcd. 757.4903; obsd. 757.4888. Anal. Calcd. for $C_{45}H_{64}N_4O_6$; C, 71.40; H, 8.52; N, 7.40. Found: C, 71.66; H, 8.56; N, 7.55.

**$(C_{12}H_{25}O_2C)_4$-[G2]-Cl. (4a)** $(C_{12}H_{25}O_2C)_2$-[G1]-$NH_2$ **(3c)** (295 mg, 0.39 mmol) and 4-dimethylaminopyridine (DMAP) (8.8 mg, 0.072 mmol) was dissolved in a mixture of $CH_2Cl_2$ (2 mL) and pyridine (0.8 mL). 4-chloro-pyridine-2,6-dicarbonyl chloride (50.0 mg, 0.21 mmol) in 0.4 mL $CH_2Cl_2$ was then added dropwise via syringe to this mixture over 5-10 min. After stirring at rt for 16 h, the mixture was taken up in $CH_2Cl_2$ (10 mL) and washed with water (10 mL) and the phases were separated. The aqueous phase was then extracted with $CH_2Cl_2$ (2 x 10 mL) and the combined organic layers were dried over $MgSO_4$ and concentrated to an orange waxy oil.

Purification by flash chromatography ($SiO_2$) with 5% ether-$CH_2Cl_2$ afforded $(C_{12}H_{25}O_2C)_4$-[G2]-Cl (**4a**) (180 mg, 0.107 mmol, 55%) as a waxy solid. $^1$H NMR (200 MHz, $CDCl_3$). δ 0.87 (bm, 12H), 1.20 (bm, 72 H), 1.44 (bm, 8H), 3.90 (t, *J*=6.82 Hz, 8H), 6.89 (t, *J*=7.80Hz, 4H), 7.10(bm, 4H), 7.78 (d, *J*=7.46 Hz, 4H), 8.01 (s, 2H), 8.11 (bs, 4H), 9.27 (s, 4H), 11.16 (s, *ca.* 2H), 12.23 (bs, *ca.* 4H). $^{13}$C NMR (75 MHz, $CDCl_3$) 13.96, 22.54, 25.73, 28.22, 29.04, 29.21, 29.43 (2 C), 29.50, 29.53, 31.77, 65.35, 115.0, 115.1, 122.0, 123.0, 130.5, 133.0, 139.1, 148.1, 149.0, 149.5, 152.3, 160.5, 162.0, 163.1, 167 ppm; IR ($CHCl_3$, 10 mM) 3321, 3248, 1712, 1694 cm$^{-1}$; MALDI-TOF MS for $C_{97}H_{129}ClN_9O_{14}$ (MH) calcd. 1678; obsd. 1679; Anal. Calcd. for $C_{97}H_{128}ClN_9O_{14}$; C, 69.37; H, 7.68; N, 7.51. Found: C, 69.56; H, 7.69; N, 7.44.

**$(C_{12}H_{25}O_2C)_4$-[G2]-$N_3$.** (**4b**) $(C_{12}H_{25}O_2C)_4$-[G2]-Cl (**4a**) (688 mg, 0.41 mmol) and sodium azide (266 mg, 4.1 mmol) were mixed in DMF-THF (3:1) (12 mL) then heated to 50°C. After 24 h, the DMF was removed by distillation under reduced pressure and the resultant residue was dispersed in $CH_2Cl_2$ (20 mL). The $CH_2Cl_2$ was washed with water (2 x 20 mL) then dried over $MgSO_4$ and concentrated in vacuo. Purification by flash chromatography ($SiO_2$) with 1% ether/$CH_2Cl_2$ afforded $(C_{12}H_{25}O_2C)_4$-[G2]-$N_3$ (**4b**) (503 mg, 0.30 mmol, 73%) as a waxy solid. $^1$H NMR (200 MHz, $CDCl_3$). δ 0.83 (bm, 12H), 1.20 (bm, 72 H), 1.44 (bm, 8H), 3.89 (t, *J*=6.6 Hz, 8H), 6.87 (t, *J*=7.56 Hz, 4H), 7.10 (bm, 4H), 7.66 (s, 2H), 7.76 (d, *J*=7.30 Hz, 4H), 8.16 (bm, 4H), 9.23 (s, 4H), 11.18 (s, *ca.* 2H), 12.23 (bs, *ca.* 4H). $^{13}$C NMR (75 MHz, $CDCl_3$) (mult. overlapping carbons) 13.96, 22.54, 25.73, 28.22, 29.09, 29.21, 29.44 (2 C), 29.48, 29.53, 31.77, 65.35, 114.31, 114.89, 122.28, 123.04, 130.51, 132.66, 139.05, 147.91, 148.96, 149.54, 151.9, 160.34, 161.72, 166.56 ppm; IR ($CHCl_3$, 10 mM) 3323, 3234, 2114, 1693 cm$^{-1}$; MALDI-TOF

MS for $C_{97}H_{129}N_{12}O_{14}$ (MH) calcd. 1685; obsd. 1683; Anal. Calcd. for $C_{97}H_{128}N_{12}O_{14}$; C, 69.10; H, 7.65; N, 9.97. Found: C, 69.27; H, 7.63; N, 9.83.

**$(C_{12}H_{25}O_2C)_4$-[G2]-$NH_2$. (4c)** $(C_{12}H_{25}O_2C)_4$-[G2]-$N_3$ **(4b)** (492 mg, 0.292 mmol) was dissolved in 28 mL of THF-methanol (3:1) and the solution was degassed by sparging with argon for 10 min. 10% Pd-C (123 mg) was added and the mixture was hydrogenated at 50 psi for 12 h at room temperature. The catalyst was removed by filtration through a pad of celite with ethyl acetate. The solvent was removed in vacuo and the resultant solid was passed through a short plug of silica gel with ethyl acetate affording $(C_{12}H_{25}O_2C)_4$-[G2]-$NH_2$ **(4c)** as a white waxy solid (480 mg, 0.29 mmol, 100%). $^1$H NMR (200 MHz, $CDCl_3$) δ 0.83 (bm, 12H), 1.09 (bm, 72 H), 1.43 (bm, 8H), 3.89 (bt, *J*= *ca.* 5.0 Hz, 8H), 6.96 (bt, *J*=6.84 Hz, 4H), 7.13 (bm, 4H), 7.58 (s, 2H), 7.87 (d, *J*=6.02 Hz, 4H), 8.32 (bm, 4H), 9.31 (s, 4H), 11.38 (s, *ca.* 2H), 12.35 (bs, *ca.* 4H). $^{13}$C NMR (75 MHz, $CDCl_3$) (mult. overlapping carbons) 14.00, 22.59, 25.82, 28.31, 29.19, 29.27, 29.48, 29.52, 29.58, 30.22, 31.83, 65.30, 111.0, 115.1, 119.0, 120.0, 122.0, 124.1, 125.40, 128.1, 131, 134, 137, 139, 148, 149, 151.5, 162, 163, 167 ppm; IR ($CHCl_3$, 10 mM) 3374, 3252, 1711, 1693 cm$^{-1}$; MALDI-TOF MS for $C_{97}H_{131}N_{10}O_{14}$ (MH) calcd. 1659.98; obsd. 1658.65; Anal. Calcd. for $C_{97}H_{130}N_{12}O_{14}$; C, 70.18; H, 7.89; N, 8.44. Found: C, 70.38; H, 7.84; N, 8.45.

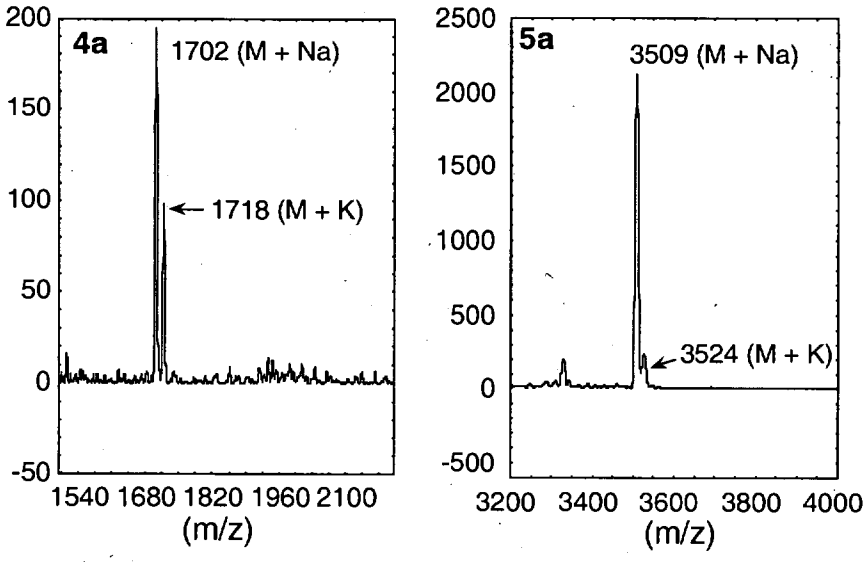
**$(C_{12}H_{25}O_2C)_8$-[G3]-Cl. (5a)** $(C_{12}H_{25}O_2C)_4$-[G2]-$NH_2$ **(4c)** (470 mg, 0.28 mmol) and 4-dimethylaminopyridine (DMAP) (8.8 mg, 0.072 mmol) was dissolved in a mixture of $CH_2Cl_2$ (4 mL) and pyridine (0.9 mL). 4-chloro-pyridine-2,6-dicarbonyl chloride (38.2 mg, 0.16 mmol) in 0.3 mL $CH_2Cl_2$ was then added dropwise via syringe to this mixture over 5-10 min. After stirring at rt for 16 h, the mixture was taken up in $CH_2Cl_2$ (10 mL) and washed with water (10 mL) and

the phases were separated. The aqueous phase was then extracted with $CH_2Cl_2$ (2 x 10 mL) and the combined organic layers were dried over $MgSO_4$ and concentrated to an orange waxy oil. Purification by flash chromatography ($SiO_2$) with 10-50% ether-$CH_2Cl_2$ afforded $(C_{12}H_{25}O_2C)_8$-[G3]-Cl (**5a**) (340 mg, 0.098 mmol, 70%) as a waxy solid. $^1$H NMR (250 MHz, 3:1 $CDCl_3$-DMSO-d$^6$, 50°C). δ 0.80 (bm, 24H), 1.18 (bm, 144 H), 1.51 (bm, 16H), 3.91 (bs, 16H), 7.04 (bt, 8H), 7.46 (bm, 8H), 7.91 (bm 10H), 8.60 (bd, *J*=6.80 Hz, 8H), 8.91 (bs, 12H), 11.22 (s, *ca.* 2H), 11.51 (bs, *ca.* 4H), 12.46 (bs, *ca.* 8H); $^{13}$C NMR (75 MHz, 3:1 $CDCl_3$-DMSO-d$^6$, 50°C) 11.97, 21.98, 25.30, 27.67, 28-29 (5 C), 30.00, 31.06, 64.6, 114.97, 117.55, 120.90, 122.47, 122.59, 130.04, 133.25, 139.44, 147.70, 148.79, 149.29, 149.56, 161.08, 162.22, 166.14 ppm; IR ($CHCl_3$, 1 mM) 3328, 3234, 1711, 1684 cm$^{-1}$; GPC Analysis ($M_{calc}$=3485; $M_w$=3418, $M_n$=3244, polydispersity index=1.05); MALDI-TOF MS for $C_{201}H_{260}ClN_{21}O_{30}Na$ (M+Na) calcd. 3508; obsd. 3509; Anal. Calcd. for $C_{201}H_{260}N_{21}O_{30}$; C, 69.26; H, 7.52; N, 8.44; Found: C, 69.50; H, 7.78; N, 7.98.

**$(C_{12}H_{25}O_2C)_8$-[G3]-$N_3$. (5b)** $(C_{12}H_{25}O_2C)_8$-[G3]-Cl (**5a**) (45 mg, 0.013 mmol) and sodium azide (8.4 mg, 0.13 mmol) were mixed in DMF-THF (3:1) (1.4 mL) then heated to 50°C. After 16 h, another portion of sodium azide (10 mg) was added. After 48h, the DMF was removed by distillation under reduced pressure and the resultant residue was dispersed in $CH_2Cl_2$ (10 mL). The $CH_2Cl_2$ was washed with water (2 x 10 mL) then dried over $MgSO_4$ and concentrated in vacuo. Purification by flash chromatography ($SiO_2$) with 1% ether/$CH_2Cl_2$ afforded $(C_{12}H_{25}O_2C)_8$-[G3]-$N_3$ (**5b**) (40 mg, 0.11 mmol, 88%) as a waxy solid. $^1$H NMR (250 MHz, 3:1 $CDCl_3$-DMSO-d$^6$, 50°C) δ 0.80 (bm, 24H), 1.18 (bm, 144 H), 1.50 (bm, 16H), 3.89 (bs, 16H), 7.06 (bm, 8H), 7.48 (bm, 8H), 7.92 (bm 10H), 8.62 (bd, 8H), 8.91 (bs, 12H), 11.29 (s, *ca.* 2H),

11.52 (bs, *ca.* 4H), 12.44 (bs, *ca.* 8H); $^{13}$C NMR (75 MHz, 3:1 $CDCl_3$-DMSO-$d^6$, 50°C) 13.3, 21.77, 25.10, 27.50, 28-29 (5 C), 30.46, 31.00, 64.4, (mult. overlapping carbons) 115, 122, 130., 132, 139, 149, 160, 162, 166. ppm; IR ($CHCl_3$, 1 mM) 3343, 3238, 2119, 1693 $cm^{-1}$; MALDI-TOF MS for $C_{201}H_{260}N_{24}O_{30}Na$ (M+Na) calcd. 3515; obsd. 3515.

**$(C_{12}H_{25}O_2C)_8$-[G3]-$NH_2$. (5c)** $(C_{12}H_{25}O_2C)_8$-[G3]-$N_3$ **(5b)** (35 mg, 0.010 mmol) was dissolved in 1.5 mL of THF-methanol (2:1) and the solution was degassed by sparging with argon for 10 min. 10% Pd-C (7 mg) was added and the mixture was placed under a balloon of $H_2$ for 24 h at room temperature. The catalyst was removed by filtration through a pad of celite with ethyl acetate. The solvent was removed in vacuo and the resultant solid was passed through a short plug of silica gel with ethyl acetate affording $(C_{12}H_{25}O_2C)_8$-[G3]-$NH_2$ (**5c**) as a white waxy solid (31 mg, 0.00895 mmol, 90%). $^1$H NMR (250 MHz, 3:1 $CDCl_3$-DMSO-$d^6$, 50°C) δ 0.80 (bm, 24H), 1.18 (bm, 144 H), 1.50 (bm, 16H), 3.89 (bs, 16H), 7.09 (bm, 8H), 7.52 (bm, 8H), 7.85-8.05 (bm 10H), 8.55-8.7 (bd, 8H), 9.05 (bm, ca. 12H), 11.37 (s, *ca.* 2H), 11.55 (bs, *ca.* 4H), 12.48 (bs, *ca.* 8H) $^{13}$C NMR (75 MHz, 3:1 $CDCl_3$-DMSO-$d^6$, 50°C) (mult. overlapping carbons) 12.6, 22.5, 22.6, 24.8, 26.7, 27-28 (4 C), 30.21, 31.91, 63.5, 105, 115, 122., 129, 132, 138, 149, 166. ppm; IR ($CHCl_3$, 1 mM) 3331, 3251, 1693 $cm^{-1}$; MALDI-TOF MS for $C_{201}H_{263}N_{22}O_{30}$ (MH) calcd. 3464; obsd. 3464.



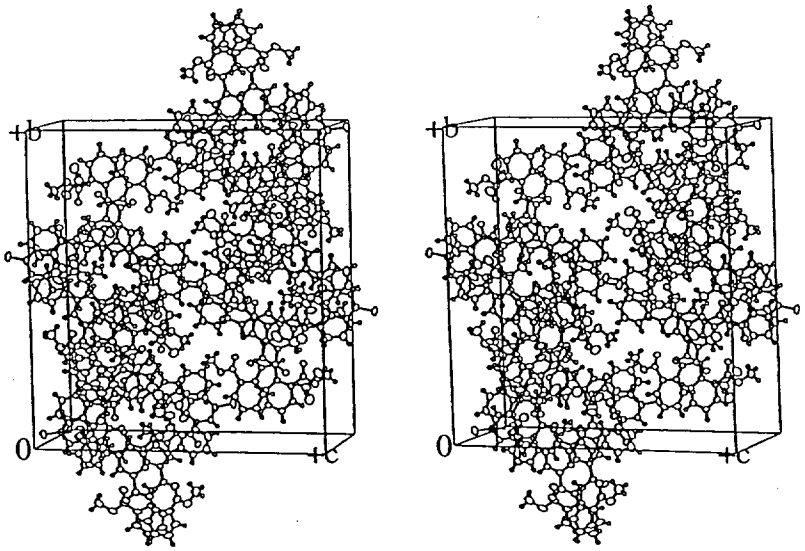

MALDI-TOF Plots for **4a** and **5a**.

**Table 1.** Spectroscopic Properties of NH Groups in **3-5a/c**

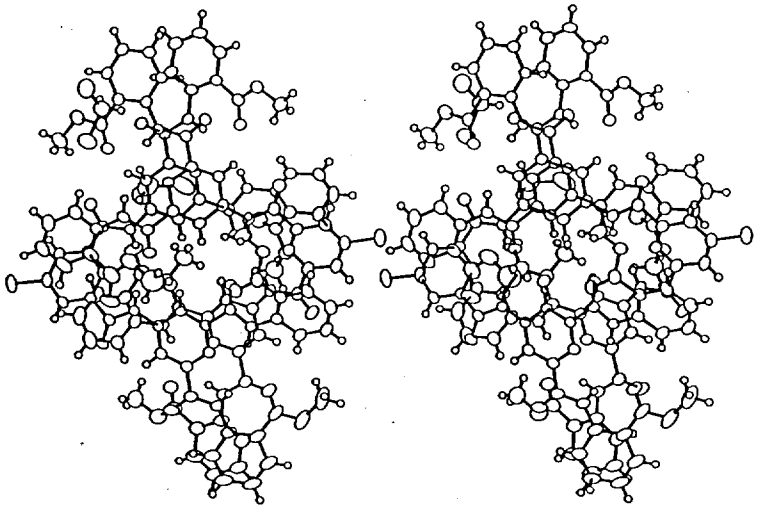
| Entry | Compound | δ (N-H)[a] (ppm) | IR[b] ($cm^{-1}$) |
|---|---|---|---|
| **1** | **3a**, [G1]-Cl | 12.75 | 3239, 3358 |
| **2** | **3b**, [G1]-$N_3$ | 12.76 | 3242, 3356 |
| **3** | **3c**, [G1]-$NH_2$ | 12.67 | 3238, 3364, 3479 |
| **4** | **4a**, [G2]-Cl | 12.23, 11.16 | 3248, 3321 |
| **5** | **4b**, [G2]-$N_3$ | 12.23, 11.18 | 3234, 3323 |
| **6** | **4c**, [G2]-$NH_2$ | 12.35, 11.38 | 3252, 3374 |
| **7** | **5a**, [G3]-Cl | 12.46, 11.51, 11.22 | 3234, 3328 |
| **8** | **5b**, [G3]-$N_3$ | 12.44, 11.52, 11.29 | 3343, 3238 |
| **9** | **5c**, [G3]-$NH_2$ | 12.48, 11.55, 11.37 | 3331, 3251 |

(a) Entries **1-6** in $CDCl_3$; **7-9** in 1:3 $d^6$-DMSO-$CDCl_3$, 50°C.
(b) Measured in $CDCl_3$ (1-10 mM).

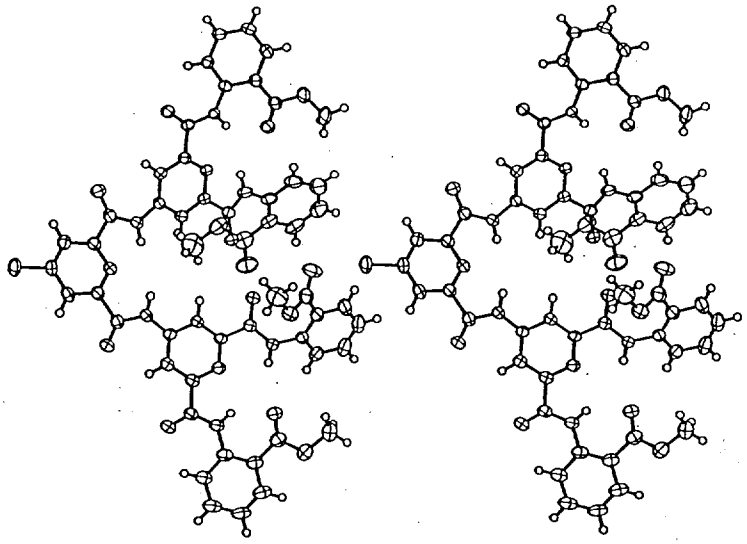
**Unit cell in stereo**



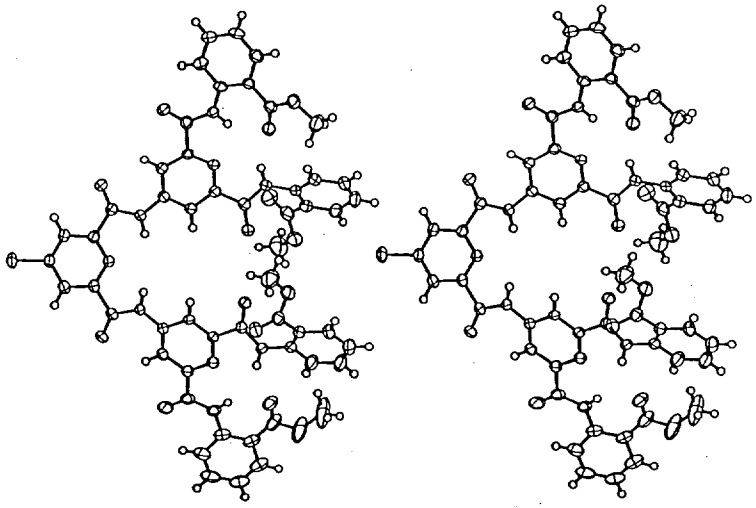
**Asymmetric unit in stereo**

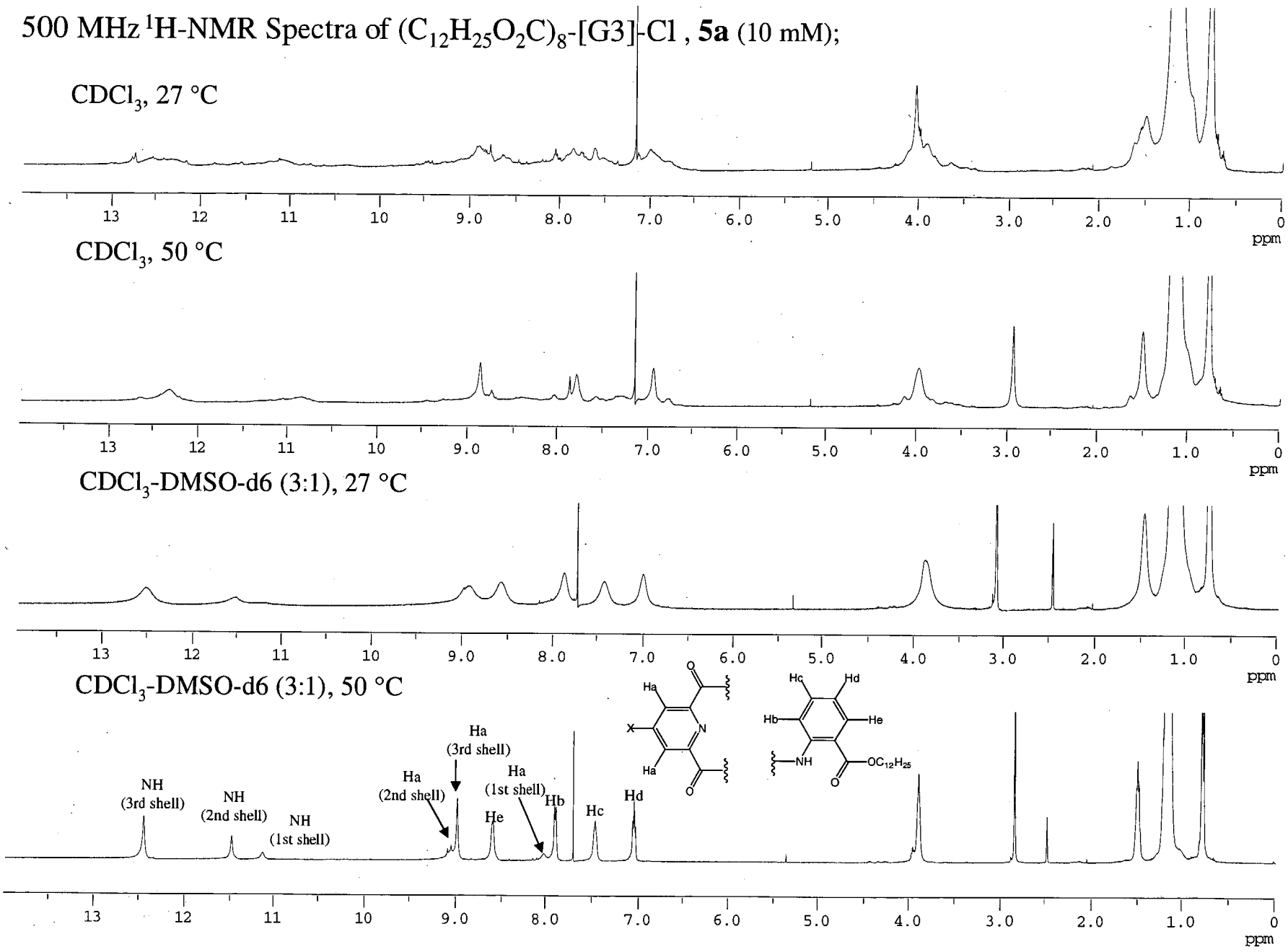


**Isolated dendron (A) in stereo**



**Isolated dendron (B) in stereo**





Crystal data and structure refinement for Turquette 073

| | |
|---|---|
| Empirical formula | C53 H40 Cl1 N9 O14 + CH2C12 + unidentified solvent |
| *Formula weight | 1147.32 |
| Temperature | 173(1) K |
| Wavelength | 0.71073 A |
| Crystal system | monoclinic |
| Space group | P2(sub1)/c (No. 14) |
| Unit cell dimensions | a = 13.5199(2) A<br>b = 29.2090(4) A<br>c = 27.1316(4) A<br>beta = 90.135(1) deg. |
| Volume | 10714.3(3) A^3 |
| Z | 8 |
| *Density (calculated) | 1.42 Mg/m^3 |
| *Absorption coefficient | 0.247 mm^-1 |
| Crystal size | 0.15 x 0.19 x 0.42 mm |
| Theta range for data collection | 2.12 to 25.03 deg. |
| Index ranges | 0<=h<=15, -34<=k<=34, -32<=l<=32 |
| Reflections collected | 97514 |
| Independent reflections | 18847 [R(int) = 0.047] |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 18847 / 0 / 1449 |
| Goodness-of-fit on F^2 | 1.060 |
| Final R indices [I>2sigma(I)] | R1 = 0.063, wR2 = 0.159 |
| R indices (all data) | R1 = 0.097, wR2 = 0.174 |
| Largest diff. peak and hole | 1.13 and -0.55 e/A^3 |

*Based on C53 H40 Cl1 N9 O14 + CH2Cl2

Bond lengths [A] and angles [deg] for Parquette 675

| | |
|---|---|
| Cl(1A)-C(1A) | 1.731(3) |
| Cl(1B)-C(1B) | 1.726(3) |
| Cl(3)-C(54) | 1.755(5) |
| Cl(4)-C(54) | 1.778(6) |
| Cl(5)-C(55) | 1.751(5) |
| Cl(6)-C(55) | 1.748(4) |
| O(1A)-C(6A) | 1.222(4) |
| O(2A)-C(12A) | 1.223(4) |
| O(3A)-C(19A) | 1.226(4) |
| O(4A)-C(19A) | 1.342(4) |
| O(4A)-C(20A) | 1.451(5) |
| O(5A)-C(21A) | 1.229(4) |
| O(6A)-C(28A) | 1.206(4) |
| O(7A)-C(28A) | 1.342(4) |
| O(7A)-C(29A) | 1.433(5) |
| O(8A)-C(30A) | 1.222(4) |
| O(9A)-C(36A) | 1.219(4) |
| O(10A)-C(43A) | 1.216(5) |
| O(11A)-C(43A) | 1.321(5) |
| O(11A)-C(44A) | 1.480(6) |
| O(12A)-C(45A) | 1.228(3) |
| O(13A)-C(52A) | 1.217(4) |
| O(14A)-C(52A) | 1.337(4) |
| O(14A)-C(53A) | 1.446(4) |
| O(1B)-C(6B) | 1.219(4) |
| O(2B)-C(12B) | 1.220(4) |
| O(3B)-C(19B) | 1.210(4) |
| O(4B)-C(19B) | 1.336(4) |
| O(4B)-C(20B) | 1.447(4) |
| O(5B)-C(21B) | 1.234(4) |
| O(6B)-C(28B) | 1.196(4) |
| O(7B)-C(28B) | 1.338(4) |
| O(7B)-C(29B) | 1.451(5) |
| O(8B)-C(30B) | 1.220(3) |
| O(9B)-C(36B) | 1.223(3) |
| O(10B)-C(43B) | 1.222(4) |
| O(11B)-C(43B) | 1.327(4) |
| O(11B)-C(44B) | 1.428(5) |
| O(12B)-C(45B) | 1.217(4) |
| O(13B)-C(52B) | 1.220(4) |
| O(14B)-C(52B) | 1.330(5) |
| O(14B)-C(53B) | 1.446(6) |
| N(1A)-C(3A) | 1.331(4) |
| N(1A)-C(4A) | 1.336(4) |
| N(2A)-C(6A) | 1.358(4) |
| N(2A)-C(7A) | 1.392(4) |
| N(2A)-H(2A) | 0.86 |
| N(3A)-C(9A) | 1.340(4) |
| N(3A)-C(10A) | 1.344(4) |
| N(4A)-C(12A) | 1.349(4) |
| N(4A)-C(13A) | 1.394(4) |
| N(4A)-H(4A) | 0.86 |
| N(5A)-C(21A) | 1.354(4) |
| N(5A)-C(22A) | 1.420(4) |
| N(5A)-H(5A) | 0.86 |
| N(6A)-C(30A) | 1.353(4) |
| N(6A)-C(31A) | 1.408(4) |
| N(6A)-H(6A) | 0.86 |
| N(7A)-C(34A) | 1.337(4) |
| N(7A)-C(33A) | 1.348(4) |
| N(8A)-C(36A) | 1.355(4) |
| N(8A)-C(37A) | 1.411(4) |

| | |
|---|---|
| N(9A)-C(45A) | 1.355(4) |
| N(9A)-C(46A) | 1.393(4) |
| N(9A)-H(9A) | 0.86 |
| N(1B)-C(3B) | 1.334(4) |
| N(1B)-C(4B) | 1.341(4) |
| N(2B)-C(6B) | 1.353(4) |
| N(2B)-C(7B) | 1.398(4) |
| N(2B)-H(2B) | 0.86 |
| N(3B)-C(10B) | 1.330(4) |
| N(3B)-C(9B) | 1.334(4) |
| N(4B)-C(12B) | 1.356(4) |
| N(4B)-C(13B) | 1.406(4) |
| N(4B)-H(4B) | 0.86 |
| N(5B)-C(21B) | 1.347(4) |
| N(5B)-C(22B) | 1.412(4) |
| N(5B)-H(5B) | 0.86 |
| N(6B)-C(30B) | 1.354(4) |
| N(6B)-C(31B) | 1.395(4) |
| N(6B)-H(6B) | 0.86 |
| N(7B)-C(34B) | 1.341(4) |
| N(7B)-C(33B) | 1.342(4) |
| N(8B)-C(36B) | 1.348(4) |
| N(8B)-C(37B) | 1.411(4) |
| N(8B)-H(8B) | 0.86 |
| N(9B)-C(45B) | 1.352(4) |
| N(9B)-C(46B) | 1.398(4) |
| N(9B)-H(9B) | 0.86 |
| C(1A)-C(5A) | 1.382(5) |
| C(1A)-C(2A) | 1.383(5) |
| C(2A)-C(3A) | 1.383(4) |
| C(2A)-H(2A1) | 0.93 |
| C(3A)-C(6A) | 1.503(5) |
| C(4A)-C(5A) | 1.393(4) |
| C(4A)-C(30A) | 1.505(4) |
| C(5A)-H(5A1) | 0.93 |
| C(7A)-C(8A) | 1.389(4) |
| C(7A)-C(11A) | 1.398(4) |
| C(8A)-C(9A) | 1.388(4) |
| C(8A)-H(8A1) | 0.93 |
| C(9A)-C(12A) | 1.518(4) |
| C(10A)-C(11A) | 1.375(4) |
| C(10A)-C(21A) | 1.496(4) |
| C(11A)-H(11A) | 0.93 |
| C(13A)-C(14A) | 1.398(5) |
| C(13A)-C(18A) | 1.410(5) |
| C(14A)-C(15A) | 1.388(5) |
| C(14A)-H(14A) | 0.93 |
| C(15A)-C(16A) | 1.377(6) |
| C(15A)-H(15A) | 0.93 |
| C(16A)-C(17A) | 1.366(5) |
| C(16A)-H(16A) | 0.93 |
| C(17A)-C(18A) | 1.401(5) |
| C(17A)-H(17A) | 0.93 |
| C(18A)-C(19A) | 1.479(5) |
| C(20A)-H(20A) | 0.96 |
| C(20A)-H(20B) | 0.96 |
| C(20A)-H(20C) | 0.96 |
| C(22A)-C(23A) | 1.382(5) |
| C(22A)-C(27A) | 1.406(5) |
| C(23A)-C(24A) | 1.387(5) |
| C(23A)-H(23A) | 0.93 |
| C(24A)-C(25A) | 1.382(6) |
| C(24A)-H(24A) | 0.93 |
| C(25A)-C(26A) | 1.374(6) |
| C(25A)-H(25A) | 0.93 |

| | |
|---|---|
| C(26A)-C(27A) | 1.391(5) |
| C(26A)-H(26A) | 0.93 |
| C(27A)-C(28A) | 1.485(5) |
| C(29A)-H(29A) | 0.96 |
| C(29A)-H(29B) | 0.96 |
| C(29A)-H(29C) | 0.96 |
| C(31A)-C(32A) | 1.381(4) |
| C(31A)-C(35A) | 1.395(4) |
| C(32A)-C(33A) | 1.374(4) |
| C(32A)-H(32A) | 0.93 |
| C(33A)-C(36A) | 1.507(4) |
| C(34A)-C(35A) | 1.384(4) |
| C(34A)-C(45A) | 1.513(4) |
| C(35A)-H(35A) | 0.93 |
| C(37A)-C(38A) | 1.383(5) |
| C(37A)-C(42A) | 1.402(5) |
| C(38A)-C(39A) | 1.387(5) |
| C(38A)-H(38A) | 0.93 |
| C(39A)-C(40A) | 1.375(6) |
| C(39A)-H(39A) | 0.93 |
| C(40A)-C(41A) | 1.360(6) |
| C(40A)-H(40A) | 0.93 |
| C(41A)-C(42A) | 1.398(5) |
| C(41A)-H(41A) | 0.93 |
| C(42A)-C(43A) | 1.490(6) |
| C(44A)-H(44A) | 0.96 |
| C(44A)-H(44B) | 0.96 |
| C(44A)-H(44C) | 0.96 |
| C(46A)-C(47A) | 1.405(4) |
| C(46A)-C(51A) | 1.411(4) |
| C(47A)-C(48A) | 1.367(4) |
| C(47A)-H(47A) | 0.93 |
| C(48A)-C(49A) | 1.379(4) |
| C(48A)-H(48A) | 0.93 |
| C(49A)-C(50A) | 1.375(4) |
| C(49A)-H(49A) | 0.93 |
| C(50A)-C(51A) | 1.402(4) |
| C(50A)-H(50A) | 0.93 |
| C(51A)-C(52A) | 1.482(4) |
| C(53A)-H(53A) | 0.96 |
| C(53A)-H(53B) | 0.96 |
| C(53A)-H(53C) | 0.96 |
| C(1B)-C(2B) | 1.376(4) |
| C(1B)-C(5B) | 1.387(4) |
| C(2B)-C(3B) | 1.381(4) |
| C(2B)-H(2B1) | 0.93 |
| C(3B)-C(30B) | 1.507(4) |
| C(4B)-C(5B) | 1.376(4) |
| C(4B)-C(6B) | 1.512(4) |
| C(5B)-H(5B1) | 0.93 |
| C(7B)-C(8B) | 1.391(4) |
| C(7B)-C(11B) | 1.396(4) |
| C(8B)-C(9B) | 1.380(4) |
| C(8B)-H(8B1) | 0.93 |
| C(9B)-C(21B) | 1.501(4) |
| C(10B)-C(11B) | 1.391(4) |
| C(10B)-C(12B) | 1.508(4) |
| C(11B)-H(11B) | 0.93 |
| C(13B)-C(14B) | 1.404(4) |
| C(13B)-C(18B) | 1.406(4) |
| C(14B)-C(15B) | 1.372(4) |
| C(14B)-H(14B) | 0.93 |
| C(15B)-C(16B) | 1.367(5) |
| C(15B)-H(15B) | 0.93 |
| C(16B)-C(17B) | 1.376(5) |
| C(16B)-H(16B) | 0.93 |

| | |
|---|---|
| C(17B)-H(17B) | 0.93 |
| C(18B)-C(19B) | 1.489(4) |
| C(20B)-H(20D) | 0.96 |
| C(20B)-H(20E) | 0.96 |
| C(20B)-H(20F) | 0.96 |
| C(22B)-C(23B) | 1.382(4) |
| C(22B)-C(27B) | 1.395(4) |
| C(23B)-C(24B) | 1.388(4) |
| C(23B)-H(23B) | 0.93 |
| C(24B)-C(25B) | 1.366(5) |
| C(24B)-H(24B) | 0.93 |
| C(25B)-C(26B) | 1.382(5) |
| C(25B)-H(25B) | 0.93 |
| C(26B)-C(27B) | 1.396(4) |
| C(26B)-H(26B) | 0.93 |
| C(27B)-C(28B) | 1.499(5) |
| C(29B)-H(29D) | 0.96 |
| C(29B)-H(29E) | 0.96 |
| C(29B)-H(29F) | 0.96 |
| C(31B)-C(35B) | 1.379(4) |
| C(31B)-C(32B) | 1.396(4) |
| C(32B)-C(33B) | 1.376(4) |
| C(32B)-H(32B) | 0.93 |
| C(33B)-C(36B) | 1.506(4) |
| C(34B)-C(35B) | 1.378(4) |
| C(34B)-C(45B) | 1.511(4) |
| C(35B)-H(35B) | 0.93 |
| C(37B)-C(38B) | 1.395(4) |
| C(37B)-C(42B) | 1.396(4) |
| C(38B)-C(39B) | 1.377(5) |
| C(38B)-H(38B) | 0.93 |
| C(39B)-C(40B) | 1.371(5) |
| C(39B)-H(39B) | 0.93 |
| C(40B)-C(41B) | 1.375(5) |
| C(40B)-H(40B) | 0.93 |
| C(41B)-C(42B) | 1.394(4) |
| C(41B)-H(41B) | 0.93 |
| C(42B)-C(43B) | 1.482(5) |
| C(44B)-H(44D) | 0.96 |
| C(44B)-H(44E) | 0.96 |
| C(44B)-H(44F) | 0.96 |
| C(46B)-C(47B) | 1.395(5) |
| C(46B)-C(51B) | 1.413(5) |
| C(47B)-C(48B) | 1.375(5) |
| C(47B)-H(47B) | 0.93 |
| C(48B)-C(49B) | 1.390(6) |
| C(48B)-H(48B) | 0.93 |
| C(49B)-C(50B) | 1.367(5) |
| C(49B)-H(49B) | 0.93 |
| C(50B)-C(51B) | 1.405(5) |
| C(50B)-H(50B) | 0.93 |
| C(51B)-C(52B) | 1.462(5) |
| C(53B)-H(53D) | 0.96 |
| C(53B)-H(53E) | 0.96 |
| C(53B)-H(53F) | 0.96 |
| C(54)-H(54A) | 0.97 |
| C(54)-H(54B) | 0.97 |
| C(55)-H(55A) | 0.97 |
| C(55)-H(55B) | 0.97 |

| | |
|---|---|
| C(19A)-O(4A)-C(20A) | 116.5(3) |
| C(28A)-O(7A)-C(29A) | 115.6(3) |
| C(43A)-O(11A)-C(44A) | 115.8(4) |
| C(52A)-O(14A)-C(53A) | 116.7(3) |
| C(19B)-O(4B)-C(20B) | 115.7(3) |

| | |
|---|---|
| C(28B)-O(7B)-C(29B) | 114.2(3) |
| C(43B)-O(11B)-C(44B) | 115.2(3) |
| C(52B)-O(14B)-C(53B) | 115.7(3) |
| C(3A)-N(1A)-C(4A) | 119.2(3) |
| C(6A)-N(2A)-C(7A) | 130.0(3) |
| C(6A)-N(2A)-H(2A) | 115.0(2) |
| C(7A)-N(2A)-H(2A) | 115.0(2) |
| C(9A)-N(3A)-C(10A) | 116.9(3) |
| C(12A)-N(4A)-C(13A) | 129.8(3) |
| C(12A)-N(4A)-H(4A) | 115.1(2) |
| C(13A)-N(4A)-H(4A) | 115.1(2) |
| C(21A)-N(5A)-C(22A) | 125.5(3) |
| C(21A)-N(5A)-H(5A) | 117.2(2) |
| C(22A)-N(5A)-H(5A) | 117.2(2) |
| C(30A)-N(6A)-C(31A) | 129.6(3) |
| C(30A)-N(6A)-H(6A) | 115.2(2) |
| C(31A)-N(6A)-H(6A) | 115.2(2) |
| C(34A)-N(7A)-C(33A) | 116.4(2) |
| C(36A)-N(8A)-C(37A) | 126.0(3) |
| C(36A)-N(8A)-H(8A) | 117.0(2) |
| C(37A)-N(8A)-H(8A) | 117.0(2) |
| C(45A)-N(9A)-C(46A) | 128.9(3) |
| C(45A)-N(9A)-H(9A) | 115.5(2) |
| C(46A)-N(9A)-H(9A) | 115.5(2) |
| C(3B)-N(1B)-C(4B) | 118.1(2) |
| C(6B)-N(2B)-C(7B) | 129.6(3) |
| C(6B)-N(2B)-H(2B) | 115.2(2) |
| C(7B)-N(2B)-H(2B) | 115.2(2) |
| C(10B)-N(3B)-C(9B) | 117.5(3) |
| C(12B)-N(4B)-C(13B) | 129.0(3) |
| C(12B)-N(4B)-H(4B) | 115.5(2) |
| C(13B)-N(4B)-H(4B) | 115.5(2) |
| C(21B)-N(5B)-C(22B) | 126.7(3) |
| C(21B)-N(5B)-H(5B) | 116.7(2) |
| C(22B)-N(5B)-H(5B) | 116.7(2) |
| C(30B)-N(6B)-C(31B) | 128.2(2) |
| C(30B)-N(6B)-H(6B) | 115.9(2) |
| C(31B)-N(6B)-H(6B) | 115.9(2) |
| C(34B)-N(7B)-C(33B) | 116.5(2) |
| C(36B)-N(8B)-C(37B) | 127.9(3) |
| C(36B)-N(8B)-H(8B) | 116.0(2) |
| C(37B)-N(8B)-H(8B) | 116.0(2) |
| C(45B)-N(9B)-C(46B) | 129.0(3) |
| C(45B)-N(9B)-H(9B) | 115.5(2) |
| C(46B)-N(9B)-H(9B) | 115.5(2) |
| C(5A)-C(1A)-C(2A) | 120.8(3) |
| C(5A)-C(1A)-Cl(1A) | 118.8(3) |
| C(2A)-C(1A)-Cl(1A) | 120.5(2) |
| C(1A)-C(2A)-C(3A) | 117.7(3) |
| C(1A)-C(2A)-H(2A1) | 121.1(2) |
| C(3A)-C(2A)-H(2A1) | 121.2(2) |
| N(1A)-C(3A)-C(2A) | 122.6(3) |
| N(1A)-C(3A)-C(6A) | 116.1(3) |
| C(2A)-C(3A)-C(6A) | 121.3(3) |
| N(1A)-C(4A)-C(5A) | 122.5(3) |
| N(1A)-C(4A)-C(30A) | 116.5(3) |
| C(5A)-C(4A)-C(30A) | 121.0(3) |
| C(1A)-C(5A)-C(4A) | 117.3(3) |
| C(1A)-C(5A)-H(5A1) | 121.4(2) |
| C(4A)-C(5A)-H(5A1) | 121.4(2) |
| O(1A)-C(6A)-N(2A) | 125.4(3) |
| O(1A)-C(6A)-C(3A) | 122.1(3) |
| N(2A)-C(6A)-C(3A) | 112.5(3) |
| C(8A)-C(7A)-N(2A) | 124.4(3) |
| C(8A)-C(7A)-C(11A) | 118.6(3) |
| N(2A)-C(7A)-C(11A) | 117.0(3) |

| | |
|---|---|
| C(9A)-C(8A)-C(7A) | 117.6(3) |
| C(9A)-C(8A)-H(8A1) | 121.2(2) |
| C(7A)-C(8A)-H(8A1) | 121.2(2) |
| N(3A)-C(9A)-C(8A) | 124.6(3) |
| N(3A)-C(9A)-C(12A) | 115.9(3) |
| C(8A)-C(9A)-C(12A) | 119.5(3) |
| N(3A)-C(10A)-C(11A) | 123.1(3) |
| N(3A)-C(10A)-C(21A) | 117.4(3) |
| C(11A)-C(10A)-C(21A) | 119.5(3) |
| C(10A)-C(11A)-C(7A) | 119.3(3) |
| C(10A)-C(11A)-H(11A) | 120.4(2) |
| C(7A)-C(11A)-H(11A) | 120.4(2) |
| O(2A)-C(12A)-N(4A) | 126.9(3) |
| O(2A)-C(12A)-C(9A) | 120.9(3) |
| N(4A)-C(12A)-C(9A) | 112.1(3) |
| N(4A)-C(13A)-C(14A) | 121.4(3) |
| N(4A)-C(13A)-C(18A) | 119.3(3) |
| C(14A)-C(13A)-C(18A) | 119.4(3) |
| C(15A)-C(14A)-C(13A) | 119.7(4) |
| C(15A)-C(14A)-H(14A) | 120.2(2) |
| C(13A)-C(14A)-H(14A) | 120.2(2) |
| C(16A)-C(15A)-C(14A) | 121.0(4) |
| C(16A)-C(15A)-H(15A) | 119.5(2) |
| C(14A)-C(15A)-H(15A) | 119.5(2) |
| C(17A)-C(16A)-C(15A) | 119.7(3) |
| C(17A)-C(16A)-H(16A) | 120.2(2) |
| C(15A)-C(16A)-H(16A) | 120.2(2) |
| C(16A)-C(17A)-C(18A) | 121.3(4) |
| C(16A)-C(17A)-H(17A) | 119.3(2) |
| C(18A)-C(17A)-H(17A) | 119.3(2) |
| C(17A)-C(18A)-C(13A) | 118.7(3) |
| C(17A)-C(18A)-C(19A) | 119.5(3) |
| C(13A)-C(18A)-C(19A) | 121.8(3) |
| O(3A)-C(19A)-O(4A) | 122.0(3) |
| O(3A)-C(19A)-C(18A) | 126.0(3) |
| O(4A)-C(19A)-C(18A) | 112.0(3) |
| O(4A)-C(20A)-H(20A) | 109.5(2) |
| O(4A)-C(20A)-H(20B) | 109.5(2) |
| H(20A)-C(20A)-H(20B) | 109.5 |
| O(4A)-C(20A)-H(20C) | 109.5(2) |
| H(20A)-C(20A)-H(20C) | 109.5 |
| H(20B)-C(20A)-H(20C) | 109.5 |
| O(5A)-C(21A)-N(5A) | 124.1(3) |
| O(5A)-C(21A)-C(10A) | 121.4(3) |
| N(5A)-C(21A)-C(10A) | 114.5(3) |
| C(23A)-C(22A)-C(27A) | 119.5(3) |
| C(23A)-C(22A)-N(5A) | 117.9(3) |
| C(27A)-C(22A)-N(5A) | 122.5(3) |
| C(22A)-C(23A)-C(24A) | 121.0(4) |
| C(22A)-C(23A)-H(23A) | 119.5(2) |
| C(24A)-C(23A)-H(23A) | 119.5(2) |
| C(25A)-C(24A)-C(23A) | 119.6(4) |
| C(25A)-C(24A)-H(24A) | 120.2(2) |
| C(23A)-C(24A)-H(24A) | 120.2(2) |
| C(26A)-C(25A)-C(24A) | 119.7(4) |
| C(26A)-C(25A)-H(25A) | 120.2(2) |
| C(24A)-C(25A)-H(25A) | 120.2(2) |
| C(25A)-C(26A)-C(27A) | 121.7(4) |
| C(25A)-C(26A)-H(26A) | 119.2(2) |
| C(27A)-C(26A)-H(26A) | 119.1(2) |
| C(26A)-C(27A)-C(22A) | 118.3(3) |
| C(26A)-C(27A)-C(28A) | 116.3(3) |
| C(22A)-C(27A)-C(28A) | 125.4(3) |
| O(6A)-C(28A)-O(7A) | 123.4(3) |
| O(6A)-C(28A)-C(27A) | 124.0(3) |
| O(7A)-C(28A)-C(27A) | 112.6(3) |

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| O(7A)-C(29A)-H(29B) | 109.5(2) |
| H(29A)-C(29A)-H(29B) | 109.5 |
| O(7A)-C(29A)-H(29C) | 109.5(2) |
| H(29A)-C(29A)-H(29C) | 109.5 |
| H(29B)-C(29A)-H(29C) | 109.5 |
| O(8A)-C(30A)-N(6A) | 125.9(3) |
| O(8A)-C(30A)-C(4A) | 122.1(3) |
| N(6A)-C(30A)-C(4A) | 112.0(3) |
| C(32A)-C(31A)-C(35A) | 118.9(3) |
| C(32A)-C(31A)-N(6A) | 116.7(3) |
| C(35A)-C(31A)-N(6A) | 124.4(3) |
| C(33A)-C(32A)-C(31A) | 119.3(3) |
| C(33A)-C(32A)-H(32A) | 120.3(2) |
| C(31A)-C(32A)-H(32A) | 120.3(2) |
| N(7A)-C(33A)-C(32A) | 123.2(3) |
| N(7A)-C(33A)-C(36A) | 117.1(3) |
| C(32A)-C(33A)-C(36A) | 119.6(3) |
| N(7A)-C(34A)-C(35A) | 124.8(3) |
| N(7A)-C(34A)-C(45A) | 116.0(3) |
| C(35A)-C(34A)-C(45A) | 119.2(3) |
| C(34A)-C(35A)-C(31A) | 117.3(3) |
| C(34A)-C(35A)-H(35A) | 121.3(2) |
| C(31A)-C(35A)-H(35A) | 121.3(2) |
| O(9A)-C(36A)-N(8A) | 125.1(3) |
| O(9A)-C(36A)-C(33A) | 121.4(3) |
| N(8A)-C(36A)-C(33A) | 113.4(3) |
| C(38A)-C(37A)-C(42A) | 120.1(3) |
| C(38A)-C(37A)-N(8A) | 116.1(3) |
| C(42A)-C(37A)-N(8A) | 123.8(3) |
| C(37A)-C(38A)-C(39A) | 120.1(4) |
| C(37A)-C(38A)-H(38A) | 119.9(2) |
| C(39A)-C(38A)-H(38A) | 120.0(3) |
| C(40A)-C(39A)-C(38A) | 120.3(4) |
| C(40A)-C(39A)-H(39A) | 119.8(3) |
| C(38A)-C(39A)-H(39A) | 119.8(3) |
| C(41A)-C(40A)-C(39A) | 119.6(4) |
| C(41A)-C(40A)-H(40A) | 120.2(2) |
| C(39A)-C(40A)-H(40A) | 120.2(3) |
| C(40A)-C(41A)-C(42A) | 122.1(4) |
| C(40A)-C(41A)-H(41A) | 119.0(2) |
| C(42A)-C(41A)-H(41A) | 119.0(2) |
| C(41A)-C(42A)-C(37A) | 117.7(4) |
| C(41A)-C(42A)-C(43A) | 116.4(3) |
| C(37A)-C(42A)-C(43A) | 125.8(3) |
| O(10A)-C(43A)-O(11A) | 124.0(4) |
| O(10A)-C(43A)-C(42A) | 121.4(4) |
| O(11A)-C(43A)-C(42A) | 114.6(3) |
| O(11A)-C(44A)-H(44A) | 109.5(3) |
| O(11A)-C(44A)-H(44B) | 109.5(2) |
| H(44A)-C(44A)-H(44B) | 109.5 |
| O(11A)-C(44A)-H(44C) | 109.5(2) |
| H(44A)-C(44A)-H(44C) | 109.5 |
| H(44B)-C(44A)-H(44C) | 109.5 |
| O(12A)-C(45A)-N(9A) | 125.7(3) |
| O(12A)-C(45A)-C(34A) | 120.8(3) |
| N(9A)-C(45A)-C(34A) | 113.6(3) |
| N(9A)-C(46A)-C(47A) | 122.3(3) |
| N(9A)-C(46A)-C(51A) | 119.5(3) |
| C(47A)-C(46A)-C(51A) | 118.3(3) |
| C(48A)-C(47A)-C(46A) | 121.1(3) |
| C(48A)-C(47A)-H(47A) | 119.5(2) |
| C(46A)-C(47A)-H(47A) | 119.5(2) |
| C(47A)-C(48A)-C(49A) | 120.8(3) |
| C(47A)-C(48A)-H(48A) | 119.6(2) |
| C(49A)-C(48A)-H(48A) | 119.6(2) |

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| C(50A)-C(49A)-H(49A) | 120.2(2) |
| C(48A)-C(49A)-H(49A) | 120.2(2) |
| C(49A)-C(50A)-C(51A) | 121.0(3) |
| C(49A)-C(50A)-H(50A) | 119.5(2) |
| C(51A)-C(50A)-H(50A) | 119.5(2) |
| C(50A)-C(51A)-C(46A) | 119.2(3) |
| C(50A)-C(51A)-C(52A) | 119.1(3) |
| C(46A)-C(51A)-C(52A) | 121.7(3) |
| O(13A)-C(52A)-O(14A) | 121.8(3) |
| O(13A)-C(52A)-C(51A) | 125.7(3) |
| O(14A)-C(52A)-C(51A) | 112.5(3) |
| O(14A)-C(53A)-H(53A) | 109.5(2) |
| O(14A)-C(53A)-H(53B) | 109.5(2) |
| H(53A)-C(53A)-H(53B) | 109.5 |
| O(14A)-C(53A)-H(53C) | 109.5(2) |
| H(53A)-C(53A)-H(53C) | 109.5 |
| H(53B)-C(53A)-H(53C) | 109.5 |
| C(2B)-C(1B)-C(5B) | 120.9(3) |
| C(2B)-C(1B)-Cl(1B) | 119.8(2) |
| C(5B)-C(1B)-Cl(1B) | 119.3(2) |
| C(1B)-C(2B)-C(3B) | 117.1(3) |
| C(1B)-C(2B)-H(2B1) | 121.4(2) |
| C(3B)-C(2B)-H(2B1) | 121.4(2) |
| N(1B)-C(3B)-C(2B) | 123.5(3) |
| N(1B)-C(3B)-C(30B) | 115.5(2) |
| C(2B)-C(3B)-C(30B) | 121.0(3) |
| N(1B)-C(4B)-C(5B) | 123.0(3) |
| N(1B)-C(4B)-C(6B) | 115.1(3) |
| C(5B)-C(4B)-C(6B) | 121.9(3) |
| C(4B)-C(5B)-C(1B) | 117.4(3) |
| C(4B)-C(5B)-H(5B1) | 121.3(2) |
| C(1B)-C(5B)-H(5B1) | 121.3(2) |
| O(1B)-C(6B)-N(2B) | 125.8(3) |
| O(1B)-C(6B)-C(4B) | 122.1(3) |
| N(2B)-C(6B)-C(4B) | 112.1(3) |
| C(8B)-C(7B)-C(11B) | 118.7(3) |
| C(8B)-C(7B)-N(2B) | 117.2(3) |
| C(11B)-C(7B)-N(2B) | 124.0(3) |
| C(9B)-C(8B)-C(7B) | 119.0(3) |
| C(9B)-C(8B)-H(8B1) | 120.5(2) |
| C(7B)-C(8B)-H(8B1) | 120.5(2) |
| N(3B)-C(9B)-C(8B) | 123.1(3) |
| N(3B)-C(9B)-C(21B) | 117.0(3) |
| C(8B)-C(9B)-C(21B) | 119.9(3) |
| N(3B)-C(10B)-C(11B) | 124.4(3) |
| N(3B)-C(10B)-C(12B) | 117.0(3) |
| C(11B)-C(10B)-C(12B) | 118.6(3) |
| C(10B)-C(11B)-C(7B) | 117.3(3) |
| C(10B)-C(11B)-H(11B) | 121.4(2) |
| C(7B)-C(11B)-H(11B) | 121.4(2) |
| O(2B)-C(12B)-N(4B) | 126.0(3) |
| O(2B)-C(12B)-C(10B) | 121.3(3) |
| N(4B)-C(12B)-C(10B) | 112.6(3) |
| C(14B)-C(13B)-N(4B) | 121.5(3) |
| C(14B)-C(13B)-C(18B) | 119.6(3) |
| N(4B)-C(13B)-C(18B) | 118.9(3) |
| C(15B)-C(14B)-C(13B) | 119.4(3) |
| C(15B)-C(14B)-H(14B) | 120.3(2) |
| C(13B)-C(14B)-H(14B) | 120.3(2) |
| C(16B)-C(15B)-C(14B) | 121.9(3) |
| C(16B)-C(15B)-H(15B) | 119.1(2) |
| C(14B)-C(15B)-H(15B) | 119.1(2) |
| C(15B)-C(16B)-C(17B) | 119.6(3) |
| C(15B)-C(16B)-H(16B) | 120.2(2) |
| C(17B)-C(16B)-H(16B) | 120.2(2) |

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| C(16B)-C(17B)-H(17B) | 119.5(2) |
| C(18B)-C(17B)-H(17B) | 119.5(2) |
| C(17B)-C(18B)-C(13B) | 118.6(3) |
| C(17B)-C(18B)-C(19B) | 119.6(3) |
| C(13B)-C(18B)-C(19B) | 121.8(3) |
| O(3B)-C(19B)-O(4B) | 122.3(3) |
| O(3B)-C(19B)-C(18B) | 125.7(3) |
| O(4B)-C(19B)-C(18B) | 112.0(3) |
| O(4B)-C(20B)-H(20D) | 109.5(2) |
| O(4B)-C(20B)-H(20E) | 109.5(2) |
| H(20D)-C(20B)-H(20E) | 109.5 |
| O(4B)-C(20B)-H(20F) | 109.5(2) |
| H(20D)-C(20B)-H(20F) | 109.5 |
| H(20E)-C(20B)-H(20F) | 109.5 |
| O(5B)-C(21B)-N(5B) | 124.0(3) |
| O(5B)-C(21B)-C(9B) | 122.1(3) |
| N(5B)-C(21B)-C(9B) | 113.9(3) |
| C(23B)-C(22B)-C(27B) | 119.8(3) |
| C(23B)-C(22B)-N(5B) | 117.5(3) |
| C(27B)-C(22B)-N(5B) | 122.7(3) |
| C(22B)-C(23B)-C(24B) | 120.7(3) |
| C(22B)-C(23B)-H(23B) | 119.7(2) |
| C(24B)-C(23B)-H(23B) | 119.7(2) |
| C(25B)-C(24B)-C(23B) | 120.1(3) |
| C(25B)-C(24B)-H(24B) | 120.0(2) |
| C(23B)-C(24B)-H(24B) | 120.0(2) |
| C(24B)-C(25B)-C(26B) | 119.8(3) |
| C(24B)-C(25B)-H(25B) | 120.1(2) |
| C(26B)-C(25B)-H(25B) | 120.1(2) |
| C(25B)-C(26B)-C(27B) | 121.1(3) |
| C(25B)-C(26B)-H(26B) | 119.5(2) |
| C(27B)-C(26B)-H(26B) | 119.4(2) |
| C(22B)-C(27B)-C(26B) | 118.5(3) |
| C(22B)-C(27B)-C(28B) | 121.6(3) |
| C(26B)-C(27B)-C(28B) | 119.3(3) |
| O(6B)-C(28B)-O(7B) | 123.9(3) |
| O(6B)-C(28B)-C(27B) | 124.8(3) |
| O(7B)-C(28B)-C(27B) | 111.2(3) |
| O(7B)-C(29B)-H(29D) | 109.5(2) |
| O(7B)-C(29B)-H(29E) | 109.5(2) |
| H(29D)-C(29B)-H(29E) | 109.5 |
| O(7B)-C(29B)-H(29F) | 109.5(2) |
| H(29D)-C(29B)-H(29F) | 109.5 |
| H(29E)-C(29B)-H(29F) | 109.5 |
| O(8B)-C(30B)-N(6B) | 125.7(3) |
| O(8B)-C(30B)-C(3B) | 121.9(3) |
| N(6B)-C(30B)-C(3B) | 112.4(2) |
| C(35B)-C(31B)-N(6B) | 124.5(3) |
| C(35B)-C(31B)-C(32B) | 118.3(3) |
| N(6B)-C(31B)-C(32B) | 117.0(3) |
| C(33B)-C(32B)-C(31B) | 119.0(3) |
| C(33B)-C(32B)-H(32B) | 120.5(2) |
| C(31B)-C(32B)-H(32B) | 120.5(2) |
| N(7B)-C(33B)-C(32B) | 123.4(3) |
| N(7B)-C(33B)-C(36B) | 117.4(2) |
| C(32B)-C(33B)-C(36B) | 119.2(3) |
| N(7B)-C(34B)-C(35B) | 124.2(3) |
| N(7B)-C(34B)-C(45B) | 116.9(3) |
| C(35B)-C(34B)-C(45B) | 118.8(3) |
| C(34B)-C(35B)-C(31B) | 118.5(3) |
| C(34B)-C(35B)-H(35B) | 120.7(2) |
| C(31B)-C(35B)-H(35B) | 120.7(2) |
| O(9B)-C(36B)-N(8B) | 125.1(3) |
| O(9B)-C(36B)-C(33B) | 121.8(3) |
| N(8B)-C(36B)-C(33B) | 113.1(3) |

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| C(38B)-C(37B)-N(8B) | 116.6(3) |
| C(42B)-C(37B)-N(8B) | 124.0(3) |
| C(39B)-C(38B)-C(37B) | 120.7(3) |
| C(39B)-C(38B)-H(38B) | 119.7(2) |
| C(37B)-C(38B)-H(38B) | 119.7(2) |
| C(40B)-C(39B)-C(38B) | 120.3(3) |
| C(40B)-C(39B)-H(39B) | 119.8(2) |
| C(38B)-C(39B)-H(39B) | 119.8(2) |
| C(39B)-C(40B)-C(41B) | 119.6(3) |
| C(39B)-C(40B)-H(40B) | 120.2(2) |
| C(41B)-C(40B)-H(40B) | 120.2(2) |
| C(40B)-C(41B)-C(42B) | 121.6(3) |
| C(40B)-C(41B)-H(41B) | 119.2(2) |
| C(42B)-C(41B)-H(41B) | 119.2(2) |
| C(41B)-C(42B)-C(37B) | 118.4(3) |
| C(41B)-C(42B)-C(43B) | 117.4(3) |
| C(37B)-C(42B)-C(43B) | 123.9(3) |
| O(10B)-C(43B)-O(11B) | 123.5(3) |
| O(10B)-C(43B)-C(42B) | 124.4(3) |
| O(11B)-C(43B)-C(42B) | 112.0(3) |
| O(11B)-C(44B)-H(44D) | 109.5(2) |
| O(11B)-C(44B)-H(44E) | 109.5(2) |
| H(44D)-C(44B)-H(44E) | 109.5 |
| O(11B)-C(44B)-H(44F) | 109.5(2) |
| H(44D)-C(44B)-H(44F) | 109.5 |
| H(44E)-C(44B)-H(44F) | 109.5 |
| O(12B)-C(45B)-N(9B) | 126.0(3) |
| O(12B)-C(45B)-C(34B) | 120.8(3) |
| N(9B)-C(45B)-C(34B) | 113.2(3) |
| C(47B)-C(46B)-N(9B) | 121.7(3) |
| C(47B)-C(46B)-C(51B) | 118.8(3) |
| N(9B)-C(46B)-C(51B) | 119.5(3) |
| C(48B)-C(47B)-C(46B) | 120.9(4) |
| C(48B)-C(47B)-H(47B) | 119.6(2) |
| C(46B)-C(47B)-H(47B) | 119.6(2) |
| C(47B)-C(48B)-C(49B) | 120.7(4) |
| C(47B)-C(48B)-H(48B) | 119.7(3) |
| C(49B)-C(48B)-H(48B) | 119.7(2) |
| C(50B)-C(49B)-C(48B) | 119.3(3) |
| C(50B)-C(49B)-H(49B) | 120.4(2) |
| C(48B)-C(49B)-H(49B) | 120.4(2) |
| C(49B)-C(50B)-C(51B) | 121.6(4) |
| C(49B)-C(50B)-H(50B) | 119.2(2) |
| C(51B)-C(50B)-H(50B) | 119.2(2) |
| C(50B)-C(51B)-C(46B) | 118.7(3) |
| C(50B)-C(51B)-C(52B) | 119.8(3) |
| C(46B)-C(51B)-C(52B) | 121.5(3) |
| O(13B)-C(52B)-O(14B) | 121.6(4) |
| O(13B)-C(52B)-C(51B) | 126.5(3) |
| O(14B)-C(52B)-C(51B) | 111.9(3) |
| O(14B)-C(53B)-H(53D) | 109.5(2) |
| O(14B)-C(53B)-H(53E) | 109.5(4) |
| H(53D)-C(53B)-H(53E) | 109.5 |
| O(14B)-C(53B)-H(53F) | 109.5(3) |
| H(53D)-C(53B)-H(53F) | 109.5 |
| H(53E)-C(53B)-H(53F) | 109.5 |
| Cl(3)-C(54)-Cl(4) | 111.3(3) |
| Cl(3)-C(54)-H(54A) | 109.4(2) |
| Cl(4)-C(54)-H(54A) | 109.4(2) |
| Cl(3)-C(54)-H(54B) | 109.4(2) |
| Cl(4)-C(54)-H(54B) | 109.4(2) |
| H(54A)-C(54)-H(54B) | 108.0 |
| Cl(6)-C(55)-Cl(5) | 111.1(2) |
| Cl(6)-C(55)-H(55A) | 109.4(2) |
| Cl(5)-C(55)-H(55A) | 109.41(14) |

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|---|---|
| Cl(6)-C(55)-H(55B) | 109.4(2) |
| Cl(5)-C(55)-H(55B) | 109.4(2) |
| H(55A)-C(55)-H(55B) | 108.0 |

Atomic coordinates ( x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Parquette 675

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Cl(1A) | 2573(1) | 5003(1) | 15664(1) | 55(1) |
| Cl(1B) | 1379(1) | 6004(1) | 9087(1) | 58(1) |
| Cl(3) | 7019(1) | 6573(1) | 11041(1) | 79(1) |
| Cl(4) | 6058(1) | 6570(1) | 12003(1) | 97(1) |
| Cl(5) | 4147(1) | 8667(1) | 11115(1) | 86(1) |
| Cl(6) | 4811(2) | 7802(1) | 10722(1) | 118(1) |
| O(1A) | 3304(2) | 4073(1) | 13968(1) | 52(1) |
| O(2A) | 3591(2) | 2988(1) | 12697(1) | 50(1) |
| O(3A) | 3779(2) | 3474(1) | 10936(1) | 51(1) |
| O(4A) | 4546(2) | 2997(1) | 10411(1) | 64(1) |
| O(5A) | 3261(2) | 5170(1) | 11616(1) | 38(1) |
| O(6A) | 4729(2) | 5826(1) | 10937(1) | 63(1) |
| O(7A) | 5213(2) | 5155(1) | 11259(1) | 47(1) |
| O(8A) | 1545(2) | 6310(1) | 14349(1) | 48(1) |
| O(9A) | 877(2) | 5867(1) | 11789(1) | 38(1) |
| O(10A) | -1021(2) | 5399(1) | 11117(1) | 76(1) |
| O(11A) | -1202(2) | 5915(1) | 11721(1) | 62(1) |
| O(12A) | 1496(2) | 7703(1) | 13430(1) | 41(1) |
| O(13A) | 1199(2) | 7709(1) | 11602(1) | 48(1) |
| O(14A) | 1655(2) | 8326(1) | 11174(1) | 61(1) |
| O(1B) | 2944(2) | 6830(1) | 10703(1) | 52(1) |
| O(2B) | 3700(2) | 7871(1) | 11969(1) | 47(1) |
| O(3B) | 3618(2) | 7387(1) | 13721(1) | 40(1) |
| O(4B) | 3189(2) | 7904(1) | 14287(1) | 51(1) |
| O(5B) | 3627(2) | 5661(1) | 12995(1) | 40(1) |
| O(6B) | 5801(2) | 5689(1) | 13213(1) | 59(1) |
| O(7B) | 5323(2) | 5032(1) | 13563(1) | 55(1) |
| O(8B) | 898(2) | 4638(1) | 10418(1) | 38(1) |
| O(9B) | 1029(2) | 5008(1) | 13013(1) | 36(1) |
| O(10B) | -977(2) | 5002(1) | 13353(1) | 44(1) |
| O(11B) | -268(2) | 5428(1) | 13945(1) | 47(1) |
| O(12B) | 1015(2) | 3259(1) | 11239(1) | 54(1) |
| O(13B) | 1216(2) | 3142(1) | 13056(1) | 52(1) |
| O(14B) | 1706(4) | 2490(1) | 13405(1) | 113(2) |
| N(1A) | 2426(2) | 5209(1) | 14031(1) | 35(1) |
| N(2A) | 3134(2) | 4634(1) | 13381(1) | 39(1) |
| N(3A) | 3463(2) | 4013(1) | 12003(1) | 35(1) |
| N(4A) | 3608(2) | 3130(1) | 11863(1) | 39(1) |
| N(5A) | 3635(2) | 4522(1) | 11185(1) | 35(1) |
| N(6A) | 1660(2) | 5932(1) | 13610(1) | 37(1) |
| N(7A) | 1063(2) | 6885(1) | 12492(1) | 31(1) |
| N(8A) | 339(2) | 6593(1) | 11625(1) | 41(1) |
| N(9A) | 1321(2) | 7778(1) | 12590(1) | 31(1) |
| N(1B) | 1891(2) | 5723(1) | 10687(1) | 32(1) |
| N(2B) | 2830(2) | 6264(1) | 11285(1) | 35(1) |
| N(3B) | 3757(2) | 6825(1) | 12624(1) | 31(1) |
| N(4B) | 3822(2) | 7714(1) | 12797(1) | 33(1) |
| N(5B) | 4087(2) | 6305(1) | 13410(1) | 36(1) |
| N(6B) | 1149(2) | 5015(1) | 11148(1) | 33(1) |
| N(7B) | 913(2) | 4022(1) | 12252(1) | 32(1) |
| N(8B) | 623(2) | 4268(1) | 13186(1) | 33(1) |
| N(9B) | 1028(2) | 3131(1) | 12072(1) | 37(1) |
| C(1A) | 2505(2) | 5076(1) | 15032(1) | 39(1) |
| C(2A) | 2815(2) | 4733(1) | 14717(1) | 38(1) |
| C(3A) | 2767(2) | 4817(1) | 14216(1) | 36(1) |
| C(4A) | 2115(2) | 5535(1) | 14338(1) | 36(1) |
| C(5A) | 2152(2) | 5487(1) | 14849(1) | 39(1) |

| | | | | |
|---|---|---|---|---|
| C(7A) | 3280(2) | 4408(1) | 12936(1) | 36(1) |
| C(8A) | 3357(2) | 3936(1) | 12887(1) | 37(1) |
| C(9A) | 3450(2) | 3760(1) | 12415(1) | 35(1) |
| C(10A) | 3395(2) | 4469(1) | 12059(1) | 32(1) |
| C(11A) | 3313(2) | 4678(1) | 12511(1) | 35(1) |
| C(12A) | 3554(2) | 3246(1) | 12343(1) | 37(1) |
| C(13A) | 3732(2) | 2701(1) | 11647(1) | 40(1) |
| C(14A) | 3662(3) | 2299(1) | 11924(2) | 48(1) |
| C(15A) | 3737(3) | 1877(1) | 11690(2) | 54(1) |
| C(16A) | 3893(3) | 1848(1) | 11190(2) | 57(1) |
| C(17A) | 4022(3) | 2239(1) | 10921(2) | 55(1) |
| C(18A) | 3930(3) | 2673(1) | 11138(1) | 45(1) |
| C(19A) | 4057(3) | 3087(1) | 10830(1) | 49(1) |
| C(20A) | 4695(4) | 3379(2) | 10078(2) | 75(1) |
| C(21A) | 3417(2) | 4756(1) | 11602(1) | 33(1) |
| C(22A) | 3656(2) | 4709(1) | 10702(1) | 38(1) |
| C(23A) | 3227(3) | 4459(1) | 10325(1) | 44(1) |
| C(24A) | 3178(3) | 4631(2) | 9850(1) | 55(1) |
| C(25A) | 3540(3) | 5065(2) | 9752(1) | 57(1) |
| C(26A) | 3989(3) | 5311(1) | 10122(1) | 50(1) |
| C(27A) | 4086(2) | 5136(1) | 10597(1) | 41(1) |
| C(28A) | 4683(3) | 5414(1) | 10947(1) | 46(1) |
| C(29A) | 5768(3) | 5400(2) | 11624(2) | 74(1) |
| C(30A) | 1743(2) | 5970(1) | 14106(1) | 37(1) |
| C(31A) | 1433(2) | 6269(1) | 13256(1) | 32(1) |
| C(32A) | 1192(2) | 6115(1) | 12790(1) | 34(1) |
| C(33A) | 1015(2) | 6428(1) | 12422(1) | 31(1) |
| C(34A) | 1289(2) | 7026(1) | 12947(1) | 31(1) |
| C(35A) | 1472(2) | 6739(1) | 13343(1) | 33(1) |
| C(36A) | 744(2) | 6264(1) | 11913(1) | 34(1) |
| C(37A) | 21(3) | 6539(1) | 11133(1) | 45(1) |
| C(38A) | 279(3) | 6886(1) | 10811(1) | 61(1) |
| C(39A) | 1(4) | 6860(2) | 10319(2) | 71(1) |
| C(40A) | -490(3) | 6481(2) | 10144(2) | 64(1) |
| C(41A) | -740(3) | 6139(2) | 10460(2) | 57(1) |
| C(42A) | -521(3) | 6161(1) | 10963(1) | 47(1) |
| C(43A) | -928(3) | 5786(2) | 11276(2) | 59(1) |
| C(44A) | -1523(4) | 5543(2) | 12055(2) | 98(2) |
| C(45A) | 1376(2) | 7538(1) | 13017(1) | 32(1) |
| C(46A) | 1433(2) | 8247(1) | 12515(1) | 31(1) |
| C(47A) | 1484(2) | 8560(1) | 12907(1) | 34(1) |
| C(48A) | 1615(2) | 9017(1) | 12822(1) | 37(1) |
| C(49A) | 1705(2) | 9184(1) | 12349(1) | 38(1) |
| C(50A) | 1656(2) | 8887(1) | 11956(1) | 38(1) |
| C(51A) | 1507(2) | 8417(1) | 12029(1) | 34(1) |
| C(52A) | 1439(3) | 8111(1) | 11595(1) | 40(1) |
| C(53A) | 1640(4) | 8053(2) | 10730(1) | 79(2) |
| C(1B) | 1599(2) | 5888(1) | 9701(1) | 36(1) |
| C(2B) | 1291(2) | 5479(1) | 9900(1) | 34(1) |
| C(3B) | 1448(2) | 5415(1) | 10398(1) | 31(1) |
| C(4B) | 2204(2) | 6114(1) | 10481(1) | 35(1) |
| C(5B) | 2070(2) | 6214(1) | 9990(1) | 37(1) |
| C(6B) | 2704(2) | 6445(1) | 10830(1) | 36(1) |
| C(7B) | 3194(2) | 6467(1) | 11715(1) | 32(1) |
| C(8B) | 3357(2) | 6183(1) | 12118(1) | 32(1) |
| C(9B) | 3628(2) | 6376(1) | 12562(1) | 32(1) |
| C(10B) | 3621(2) | 7094(1) | 12234(1) | 30(1) |
| C(11B) | 3349(2) | 6937(1) | 11769(1) | 32(1) |
| C(12B) | 3733(2) | 7602(1) | 12314(1) | 33(1) |
| C(13B) | 3873(2) | 8149(1) | 13015(1) | 33(1) |
| C(14B) | 4065(2) | 8543(1) | 12735(1) | 38(1) |
| C(15B) | 4128(2) | 8960(1) | 12966(1) | 42(1) |
| C(16B) | 4003(3) | 9005(1) | 13463(1) | 43(1) |
| C(17B) | 3799(3) | 8624(1) | 13744(1) | 40(1) |
| C(18B) | 3733(2) | 8189(1) | 13527(1) | 33(1) |

| | | | | |
|---|---|---|---|---|
| C(20B) | 3017(4) | 7532(1) | 14628(1) | 68(1) |
| C(21B) | 3783(2) | 6077(1) | 13006(1) | 34(1) |
| C(22B) | 4284(2) | 6117(1) | 13879(1) | 34(1) |
| C(23B) | 3962(3) | 6359(1) | 14286(1) | 39(1) |
| C(24B) | 4147(3) | 6199(1) | 14759(1) | 44(1) |
| C(25B) | 4628(3) | 5792(1) | 14826(1) | 50(1) |
| C(26B) | 4958(3) | 5548(1) | 14423(1) | 43(1) |
| C(27B) | 4817(2) | 5712(1) | 13944(1) | 38(1) |
| C(28B) | 5354(3) | 5488(1) | 13526(1) | 44(1) |
| C(29B) | 5887(4) | 4793(2) | 13188(2) | 85(2) |
| C(30B) | 1131(2) | 4979(1) | 10650(1) | 30(1) |
| C(31B) | 1020(2) | 4670(1) | 11497(1) | 29(1) |
| C(32B) | 973(2) | 4804(1) | 11990(1) | 29(1) |
| C(33B) | 918(2) | 4472(1) | 12349(1) | 28(1) |
| C(34B) | 959(2) | 3902(1) | 11775(1) | 30(1) |
| C(35B) | 1008(2) | 4208(1) | 11391(1) | 32(1) |
| C(36B) | 861(2) | 4615(1) | 12882(1) | 32(1) |
| C(37B) | 503(2) | 4282(1) | 13703(1) | 35(1) |
| C(38B) | 833(3) | 3901(1) | 13966(1) | 49(1) |
| C(39B) | 737(3) | 3882(1) | 14471(1) | 58(1) |
| C(40B) | 335(3) | 4244(1) | 14723(1) | 53(1) |
| C(41B) | 12(3) | 4622(1) | 14468(1) | 41(1) |
| C(42B) | 67(2) | 4645(1) | 13955(1) | 36(1) |
| C(43B) | -430(3) | 5036(1) | 13710(1) | 38(1) |
| C(44B) | -802(4) | 5813(1) | 13759(2) | 71(1) |
| C(45B) | 994(2) | 3395(1) | 11663(1) | 37(1) |
| C(46B) | 1129(2) | 2656(1) | 12109(1) | 39(1) |
| C(47B) | 1035(3) | 2371(1) | 11699(2) | 50(1) |
| C(48B) | 1167(3) | 1906(1) | 11740(2) | 58(1) |
| C(49B) | 1395(3) | 1708(1) | 12192(2) | 56(1) |
| C(50B) | 1461(3) | 1980(1) | 12601(2) | 52(1) |
| C(51B) | 1334(2) | 2457(1) | 12573(1) | 42(1) |
| C(52B) | 1406(3) | 2735(1) | 13020(1) | 54(1) |
| C(53B) | 1815(7) | 2740(2) | 13862(2) | 155(4) |
| C(54) | 5955(4) | 6727(2) | 11372(2) | 89(2) |
| C(55) | 5068(3) | 8246(1) | 11134(2) | 63(1) |

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Anisotropic displacement parameters (A^2 x 10^3) for Parquette 675.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [ h^2 a*^2 U11 + ... + 2 h k a* b* U12 ]

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Cl(1A) | 58(1) | 78(1) | 30(1) | 10(1) | 2(1) | 15(1) |
| Cl(1B) | 74(1) | 74(1) | 26(1) | 14(1) | -12(1) | -20(1) |
| Cl(3) | 66(1) | 85(1) | 85(1) | -6(1) | 3(1) | -5(1) |
| Cl(4) | 82(1) | 116(1) | 92(1) | -42(1) | 7(1) | -20(1) |
| Cl(5) | 115(1) | 86(1) | 58(1) | 4(1) | 10(1) | 10(1) |
| Cl(6) | 195(2) | 71(1) | 88(1) | -22(1) | -41(1) | 3(1) |
| O(1A) | 73(2) | 36(1) | 46(1) | 10(1) | 6(1) | 16(1) |
| O(2A) | 67(2) | 34(1) | 49(2) | 9(1) | 2(1) | 4(1) |
| O(3A) | 66(2) | 39(1) | 48(2) | -4(1) | 1(1) | 3(1) |
| O(4A) | 84(2) | 53(2) | 56(2) | -7(1) | 20(2) | 2(1) |
| O(5A) | 46(1) | 28(1) | 40(1) | 1(1) | 2(1) | 3(1) |
| O(6A) | 64(2) | 35(2) | 92(2) | 7(1) | 6(2) | -3(1) |
| O(7A) | 43(2) | 42(1) | 57(2) | 3(1) | 0(1) | -1(1) |
| O(8A) | 64(2) | 38(1) | 40(1) | -4(1) | -2(1) | 8(1) |
| O(9A) | 51(2) | 26(1) | 38(1) | -6(1) | 2(1) | 4(1) |
| O(10A) | 84(2) | 61(2) | 83(2) | -26(2) | -14(2) | -12(2) |
| O(11A) | 54(2) | 64(2) | 67(2) | -20(2) | 8(1) | -7(1) |
| O(12A) | 59(2) | 32(1) | 32(1) | -3(1) | -9(1) | -2(1) |
| O(13A) | 73(2) | 35(1) | 35(1) | -3(1) | -6(1) | -4(1) |
| O(14A) | 96(2) | 52(2) | 33(1) | 0(1) | 3(1) | -16(1) |
| O(1B) | 86(2) | 36(1) | 34(1) | 6(1) | -5(1) | -18(1) |
| O(2B) | 75(2) | 31(1) | 34(1) | 4(1) | 1(1) | -7(1) |
| O(3B) | 55(2) | 29(1) | 34(1) | -1(1) | 1(1) | 2(1) |
| O(4B) | 85(2) | 38(1) | 31(1) | -4(1) | 4(1) | 4(1) |
| O(5B) | 58(2) | 27(1) | 34(1) | 0(1) | -5(1) | -7(1) |
| O(6B) | 64(2) | 55(2) | 58(2) | -1(1) | 17(1) | 3(1) |
| O(7B) | 74(2) | 39(1) | 53(2) | -5(1) | -9(1) | 11(1) |
| O(8B) | 46(1) | 36(1) | 30(1) | -8(1) | -1(1) | -8(1) |
| O(9B) | 53(2) | 26(1) | 30(1) | -5(1) | 3(1) | -4(1) |
| O(10B) | 52(2) | 45(1) | 36(1) | -4(1) | -7(1) | 7(1) |
| O(11B) | 64(2) | 36(1) | 40(1) | -6(1) | -3(1) | 4(1) |
| O(12B) | 89(2) | 31(1) | 43(2) | -12(1) | 10(1) | -7(1) |
| O(13B) | 69(2) | 35(1) | 51(2) | 9(1) | 10(1) | 4(1) |
| O(14B) | 240(5) | 49(2) | 50(2) | 14(2) | 17(2) | 52(2) |
| N(1A) | 38(2) | 33(2) | 35(2) | 5(1) | -1(1) | -1(1) |
| N(2A) | 57(2) | 29(1) | 30(2) | 4(1) | -1(1) | 5(1) |
| N(3A) | 34(2) | 31(2) | 39(2) | -1(1) | 2(1) | 1(1) |
| N(4A) | 41(2) | 29(1) | 47(2) | 1(1) | 1(1) | 2(1) |
| N(5A) | 44(2) | 29(1) | 33(2) | 2(1) | 3(1) | 3(1) |
| N(6A) | 49(2) | 26(1) | 35(2) | 3(1) | -1(1) | 3(1) |
| N(7A) | 32(2) | 27(1) | 32(1) | -3(1) | -2(1) | 0(1) |
| N(8A) | 57(2) | 28(1) | 39(2) | -10(1) | -14(1) | 10(1) |
| N(9A) | 41(2) | 25(1) | 26(1) | -3(1) | -4(1) | 0(1) |
| N(1B) | 39(2) | 32(1) | 25(1) | 0(1) | 0(1) | -1(1) |
| N(2B) | 49(2) | 31(1) | 25(1) | -1(1) | -3(1) | -8(1) |
| N(3B) | 37(2) | 26(1) | 29(1) | -1(1) | 0(1) | -4(1) |
| N(4B) | 44(2) | 24(1) | 31(1) | 2(1) | 1(1) | 1(1) |
| N(5B) | 48(2) | 29(1) | 31(1) | 0(1) | -6(1) | -5(1) |
| N(6B) | 49(2) | 28(1) | 21(1) | -1(1) | 1(1) | -6(1) |
| N(7B) | 35(2) | 28(1) | 31(1) | -2(1) | 2(1) | -4(1) |
| N(8B) | 49(2) | 25(1) | 25(1) | 0(1) | 3(1) | -6(1) |
| N(9B) | 44(2) | 24(1) | 43(2) | -1(1) | 3(1) | 0(1) |
| C(1A) | 36(2) | 53(2) | 29(2) | 8(2) | 1(1) | -1(2) |
| C(2A) | 39(2) | 40(2) | 36(2) | 11(2) | -1(1) | 2(2) |
| C(3A) | 38(2) | 32(2) | 37(2) | 5(1) | 1(1) | 0(1) |
| C(4A) | 36(2) | 32(2) | 39(2) | 3(1) | 1(1) | -1(1) |

Calculated hydrogen coordinates ( x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Parquette 675

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2A) | 3052(2) | 4925(1) | 13358(1) | 46 |
| H(4A) | 3558(2) | 3354(1) | 11660(1) | 47 |
| H(5A) | 3773(2) | 4236(1) | 11215(1) | 42 |
| H(6A) | 1760(2) | 5662(1) | 13495(1) | 44 |
| H(8A) | 269(2) | 6860(1) | 11754(1) | 50 |
| H(9A) | 1201(2) | 7619(1) | 12330(1) | 37 |
| H(2B) | 2661(2) | 5981(1) | 11313(1) | 42 |
| H(4B) | 3852(2) | 7486(1) | 12998(1) | 39 |
| H(5B) | 4169(2) | 6596(1) | 13379(1) | 43 |
| H(6B) | 1253(2) | 5285(1) | 11263(1) | 39 |
| H(8B) | 533(2) | 4005(1) | 13049(1) | 40 |
| H(9B) | 980(2) | 3275(1) | 12347(1) | 44 |
| H(2A1) | 3047(2) | 4455(1) | 14838(1) | 46 |
| H(5A1) | 1947(2) | 5720(1) | 15057(1) | 46 |
| H(8A1) | 3346(2) | 3745(1) | 13161(1) | 45 |
| H(11A) | 3281(2) | 4995(1) | 12534(1) | 42 |
| H(14A) | 3566(3) | 2313(1) | 12263(2) | 57 |
| H(15A) | 3681(3) | 1610(1) | 11875(2) | 65 |
| H(16A) | 3910(3) | 1564(1) | 11036(2) | 68 |
| H(17A) | 4173(3) | 2217(1) | 10588(2) | 66 |
| H(20A) | 4070(5) | 3472(7) | 9943(9) | 112 |
| H(20B) | 5128(19) | 3288(4) | 9816(7) | 112 |
| H(20C) | 4986(22) | 3630(4) | 10255(3) | 112 |
| H(23A) | 2968(3) | 4171(1) | 10392(1) | 53 |
| H(24A) | 2903(3) | 4457(2) | 9598(1) | 66 |
| H(25A) | 3479(3) | 5189(2) | 9438(1) | 68 |
| H(26A) | 4234(3) | 5601(1) | 10053(1) | 60 |
| H(29A) | 6144(18) | 5187(2) | 11819(8) | 111 |
| H(29B) | 5322(4) | 5565(9) | 11834(7) | 111 |
| H(29C) | 6208(17) | 5611(8) | 11465(2) | 111 |
| H(32A) | 1150(2) | 5803(1) | 12725(1) | 40 |
| H(35A) | 1615(2) | 6855(1) | 13654(1) | 39 |
| H(38A) | 639(3) | 7136(1) | 10924(1) | 73 |
| H(39A) | 148(4) | 7101(2) | 10107(2) | 86 |
| H(40A) | -649(3) | 6459(2) | 9811(2) | 77 |
| H(41A) | -1067(3) | 5883(2) | 10338(2) | 68 |
| H(44A) | -2024(21) | 5656(4) | 12274(10) | 148 |
| H(44B) | -967(7) | 5438(10) | 12245(11) | 148 |
| H(44C) | -1785(28) | 5294(6) | 11864(2) | 148 |
| H(47A) | 1427(2) | 8454(1) | 13229(1) | 40 |
| H(48A) | 1644(2) | 9219(1) | 13087(1) | 44 |
| H(49A) | 1799(2) | 9495(1) | 12296(1) | 46 |
| H(50A) | 1723(2) | 9000(1) | 11637(1) | 46 |
| H(53A) | 1829(25) | 8239(3) | 10454(2) | 119 |
| H(53B) | 986(7) | 7935(9) | 10677(7) | 119 |
| H(53C) | 2096(18) | 7803(7) | 10763(5) | 119 |
| H(2B1) | 991(2) | 5255(1) | 9707(1) | 41 |
| H(5B1) | 2287(2) | 6490(1) | 9857(1) | 45 |
| H(8B1) | 3286(2) | 5867(1) | 12088(1) | 39 |
| H(11B) | 3273(2) | 7138(1) | 11505(1) | 38 |
| H(14B) | 4150(2) | 8522(1) | 12396(1) | 45 |
| H(15B) | 4258(2) | 9220(1) | 12779(1) | 50 |
| H(16B) | 4055(3) | 9291(1) | 13612(1) | 51 |
| H(17B) | 3703(3) | 8655(1) | 14081(1) | 48 |
| H(20D) | 2783(22) | 7652(2) | 14935(4) | 103 |
| H(20E) | 3624(6) | 7368(6) | 14682(9) | 103 |
| H(20F) | 2531(16) | 7328(6) | 14492(5) | 103 |

| | | | | |
|---|---|---|---|---|
| H(24B) | 3944(3) | 6369(1) | 15030(1) | 52 |
| H(25B) | 4733(3) | 5680(1) | 15143(1) | 60 |
| H(26B) | 5279(3) | 5270(1) | 14470(1) | 52 |
| H(29D) | 5837(21) | 4469(2) | 13240(8) | 127 |
| H(29E) | 6568(6) | 4885(9) | 13207(8) | 127 |
| H(29F) | 5628(17) | 4868(9) | 12868(2) | 127 |
| H(32B) | 979(2) | 5113(1) | 12075(1) | 34 |
| H(35B) | 1033(2) | 4106(1) | 11066(1) | 38 |
| H(38B) | 1120(3) | 3657(1) | 13799(1) | 59 |
| H(39B) | 946(3) | 3624(1) | 14641(1) | 69 |
| H(40B) | 281(3) | 4233(1) | 15064(1) | 63 |
| H(41B) | -250(3) | 4868(1) | 14641(1) | 49 |
| H(44D) | -630(17) | 6081(2) | 13946(7) | 107 |
| H(44E) | -1499(4) | 5757(5) | 13787(10) | 107 |
| H(44F) | -635(17) | 5860(6) | 13419(4) | 107 |
| H(47B) | 882(3) | 2498(1) | 11394(2) | 60 |
| H(48B) | 1102(3) | 1722(1) | 11462(2) | 69 |
| H(49B) | 1502(3) | 1395(1) | 12217(2) | 67 |
| H(50B) | 1592(3) | 1846(1) | 12905(2) | 62 |
| H(53D) | 2184(45) | 2558(10) | 14094(9) | 232 |
| H(53E) | 1173(7) | 2805(20) | 13996(13) | 232 |
| H(53F) | 2160(43) | 3021(11) | 13802(5) | 232 |
| H(54A) | 5384(4) | 6576(2) | 11228(2) | 107 |
| H(54B) | 5855(4) | 7055(2) | 11347(2) | 107 |
| H(55A) | 5701(3) | 8383(1) | 11052(2) | 76 |
| H(55B) | 5115(3) | 8124(1) | 11466(2) | 76 |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(6A) | 40(2) | 41(2) | 35(2) | 6(2) | 0(1) | 1(2) |
| C(7A) | 36(2) | 36(2) | 35(2) | 1(1) | 0(1) | 5(1) |
| C(8A) | 39(2) | 34(2) | 39(2) | 3(1) | -1(1) | 2(1) |
| C(9A) | 32(2) | 28(2) | 45(2) | 4(2) | -1(1) | 1(1) |
| C(10A) | 29(2) | 29(2) | 37(2) | 1(1) | -1(1) | 2(1) |
| C(11A) | 41(2) | 28(2) | 35(2) | 4(1) | 0(1) | 1(1) |
| C(12A) | 32(2) | 34(2) | 44(2) | 4(2) | 2(1) | 1(1) |
| C(13A) | 32(2) | 29(2) | 59(2) | -4(2) | -1(2) | -1(1) |
| C(14A) | 42(2) | 35(2) | 65(2) | 2(2) | 3(2) | 2(2) |
| C(15A) | 48(2) | 32(2) | 84(3) | 1(2) | 3(2) | 5(2) |
| C(16A) | 52(2) | 34(2) | 83(3) | -13(2) | 5(2) | 11(2) |
| C(17A) | 52(2) | 42(2) | 71(3) | -14(2) | 4(2) | 5(2) |
| C(18A) | 39(2) | 36(2) | 59(2) | -6(2) | 1(2) | 5(2) |
| C(19A) | 50(2) | 46(2) | 50(2) | -8(2) | -1(2) | -2(2) |
| C(20A) | 97(4) | 75(3) | 51(3) | 4(2) | 15(2) | 0(3) |
| C(21A) | 28(2) | 34(2) | 37(2) | 1(1) | 2(1) | -2(1) |
| C(22A) | 37(2) | 40(2) | 37(2) | 4(2) | 6(1) | 9(2) |
| C(23A) | 44(2) | 49(2) | 39(2) | -5(2) | 1(2) | 6(2) |
| C(24A) | 44(2) | 84(3) | 37(2) | -2(2) | 3(2) | 16(2) |
| C(25A) | 50(2) | 81(3) | 39(2) | 14(2) | 10(2) | 20(2) |
| C(26A) | 45(2) | 54(2) | 50(2) | 20(2) | 14(2) | 15(2) |
| C(27A) | 36(2) | 41(2) | 44(2) | 6(2) | 11(2) | 8(2) |
| C(28A) | 42(2) | 43(2) | 54(2) | 5(2) | 14(2) | 0(2) |
| C(29A) | 74(3) | 63(3) | 84(3) | -5(2) | -20(3) | -16(2) |
| C(30A) | 39(2) | 35(2) | 35(2) | 3(2) | -1(1) | -3(1) |
| C(31A) | 33(2) | 30(2) | 32(2) | 4(1) | 2(1) | 1(1) |
| C(32A) | 38(2) | 25(2) | 38(2) | -1(1) | 0(1) | 1(1) |
| C(33A) | 31(2) | 28(2) | 32(2) | -3(1) | -1(1) | 1(1) |
| C(34A) | 30(2) | 27(2) | 36(2) | 0(1) | 2(1) | 1(1) |
| C(35A) | 33(2) | 34(2) | 32(2) | -1(1) | 0(1) | 0(1) |
| C(36A) | 35(2) | 29(2) | 38(2) | -1(1) | -1(1) | -5(1) |
| C(37A) | 53(2) | 37(2) | 44(2) | -9(2) | -17(2) | 15(2) |
| C(38A) | 91(3) | 40(2) | 52(2) | -8(2) | -26(2) | 11(2) |
| C(39A) | 104(4) | 61(3) | 48(2) | 2(2) | -22(2) | 15(2) |
| C(40A) | 78(3) | 70(3) | 44(2) | -15(2) | -23(2) | 15(2) |
| C(41A) | 50(2) | 62(3) | 57(2) | -31(2) | -14(2) | 14(2) |
| C(42A) | 43(2) | 50(2) | 47(2) | -17(2) | -9(2) | 12(2) |
| C(43A) | 45(2) | 65(3) | 65(3) | -13(2) | -15(2) | 0(2) |
| C(44A) | 80(4) | 103(4) | 112(4) | 0(3) | 8(3) | -33(3) |
| C(45A) | 32(2) | 31(2) | 33(2) | -3(1) | -2(1) | 0(1) |
| C(46A) | 30(2) | 28(2) | 35(2) | 1(1) | -4(1) | 1(1) |
| C(47A) | 40(2) | 32(2) | 29(2) | -1(1) | -2(1) | 2(1) |
| C(48A) | 43(2) | 28(2) | 39(2) | -4(1) | -4(2) | 3(1) |
| C(49A) | 42(2) | 28(2) | 45(2) | 3(2) | -6(2) | -2(1) |
| C(50A) | 42(2) | 37(2) | 36(2) | 8(2) | -3(1) | -2(2) |
| C(51A) | 36(2) | 33(2) | 33(2) | -1(1) | -3(1) | 1(1) |
| C(52A) | 48(2) | 37(2) | 34(2) | 2(2) | -4(2) | 2(2) |
| C(53A) | 139(5) | 70(3) | 29(2) | -8(2) | 11(2) | -22(3) |
| C(1B) | 39(2) | 46(2) | 24(2) | 6(1) | -2(1) | -1(2) |
| C(2B) | 35(2) | 40(2) | 27(2) | -3(1) | -2(1) | -1(1) |
| C(3B) | 33(2) | 32(2) | 26(2) | -1(1) | 1(1) | 0(1) |
| C(4B) | 44(2) | 31(2) | 28(2) | 2(1) | 3(1) | 0(1) |
| C(5B) | 48(2) | 37(2) | 26(2) | 4(1) | 0(1) | -3(2) |
| C(6B) | 47(2) | 33(2) | 29(2) | 2(1) | 3(1) | -7(2) |
| C(7B) | 34(2) | 34(2) | 27(2) | -2(1) | 1(1) | -6(1) |
| C(8B) | 37(2) | 28(2) | 31(2) | -3(1) | 1(1) | -6(1) |
| C(9B) | 34(2) | 31(2) | 31(2) | 1(1) | 2(1) | -3(1) |
| C(10B) | 35(2) | 28(2) | 28(2) | 0(1) | 6(1) | -2(1) |
| C(11B) | 35(2) | 31(2) | 29(2) | 1(1) | 2(1) | -4(1) |
| C(12B) | 36(2) | 33(2) | 32(2) | 0(1) | 0(1) | 1(1) |
| C(13B) | 31(2) | 28(2) | 40(2) | -4(1) | -4(1) | 2(1) |
| C(14B) | 35(2) | 30(2) | 47(2) | 2(2) | 3(2) | 1(1) |
| C(15B) | 41(2) | 30(2) | 53(2) | 1(2) | 0(2) | -3(1) |
| C(16B) | 47(2) | 26(2) | 56(2) | -11(2) | -3(2) | -3(2) |
| C(17B) | 45(2) | 34(2) | 42(2) | -6(2) | -5(2) | 2(2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(19B) | 45(2) | 33(2) | 35(2) | -4(1) | -4(2) | 2(2) |
| C(20B) | 127(4) | 40(2) | 38(2) | 2(2) | 13(2) | 2(2) |
| C(21B) | 37(2) | 32(2) | 32(2) | -2(1) | 0(1) | -1(1) |
| C(22B) | 42(2) | 30(2) | 30(2) | 2(1) | -5(1) | -7(1) |
| C(23B) | 48(2) | 34(2) | 36(2) | -1(1) | -5(2) | -4(2) |
| C(24B) | 51(2) | 48(2) | 31(2) | -2(2) | -3(2) | -7(2) |
| C(25B) | 53(2) | 62(2) | 34(2) | 13(2) | -9(2) | -4(2) |
| C(26B) | 45(2) | 40(2) | 44(2) | 10(2) | -9(2) | 0(2) |
| C(27B) | 40(2) | 35(2) | 39(2) | 1(2) | -4(2) | -6(1) |
| C(28B) | 46(2) | 38(2) | 47(2) | -3(2) | -14(2) | 6(2) |
| C(29B) | 130(5) | 59(3) | 66(3) | -21(2) | -1(3) | 33(3) |
| C(30B) | 28(2) | 33(2) | 28(2) | -5(1) | -1(1) | 2(1) |
| C(31B) | 31(2) | 29(2) | 25(2) | 1(1) | -1(1) | -3(1) |
| C(32B) | 35(2) | 22(2) | 29(2) | 0(1) | 1(1) | -3(1) |
| C(33B) | 33(2) | 25(2) | 25(2) | -2(1) | 1(1) | -2(1) |
| C(34B) | 33(2) | 28(2) | 31(2) | -2(1) | 2(1) | -3(1) |
| C(35B) | 35(2) | 32(2) | 28(2) | -4(1) | 0(1) | -1(1) |
| C(36B) | 37(2) | 31(2) | 27(2) | 0(1) | 1(1) | -1(1) |
| C(37B) | 46(2) | 31(2) | 27(2) | 0(1) | 2(1) | -9(1) |
| C(38B) | 77(3) | 33(2) | 38(2) | 5(2) | 5(2) | 3(2) |
| C(39B) | 94(3) | 43(2) | 37(2) | 13(2) | 4(2) | 3(2) |
| C(40B) | 72(3) | 56(2) | 30(2) | 2(2) | 3(2) | -2(2) |
| C(41B) | 48(2) | 47(2) | 27(2) | -3(2) | 2(2) | 0(2) |
| C(42B) | 41(2) | 38(2) | 28(2) | 1(1) | 2(1) | -7(2) |
| C(43B) | 44(2) | 41(2) | 30(2) | -1(2) | 6(2) | 3(2) |
| C(44B) | 98(4) | 48(2) | 68(3) | 5(2) | 4(2) | 9(2) |
| C(45B) | 42(2) | 28(2) | 40(2) | -5(2) | 5(2) | -2(1) |
| C(46B) | 31(2) | 25(2) | 60(2) | -1(2) | 4(2) | -2(1) |
| C(47B) | 47(2) | 33(2) | 71(3) | -7(2) | -12(2) | -1(2) |
| C(48B) | 54(3) | 30(2) | 89(3) | -14(2) | -9(2) | 0(2) |
| C(49B) | 52(2) | 24(2) | 92(3) | -2(2) | 8(2) | 3(2) |
| C(50B) | 46(2) | 35(2) | 74(3) | 13(2) | 17(2) | 5(2) |
| C(51B) | 38(2) | 25(2) | 63(2) | 6(2) | 13(2) | 0(1) |
| C(52B) | 75(3) | 36(2) | 52(2) | 16(2) | 19(2) | 17(2) |
| C(53B) | 344(11) | 80(4) | 41(3) | 10(3) | 1(4) | 98(5) |
| C(54) | 73(3) | 78(3) | 116(4) | 13(3) | 10(3) | 6(3) |
| C(55) | 69(3) | 58(2) | 63(3) | -2(2) | 0(2) | -18(2) |