

Supporting Information

Macrocyclisation and Molecular Interlocking via Mitsunobu Alkylation: Highlighting the Role of C–H $\cdots$ O Interactions in Templating

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Experimental Details

All solvents were distilled prior to use. THF was dried over sodium/benzophenone, DMF was dried by standing over freshly activated molecular sieves for three days. DCM was distilled from CaH₂. All chemicals were purchased from the Aldrich Chemical Co. and were used without further purification. Preparative and analytical Thin Layer Chromatography (TLC) were performed using glass plates coated with Merck 5554 Kieselgel 60 F254. Column chromatography was performed using Kieselgel 60 (0.040-0.063mm, Merck 9385). Melting points were measured on a Gallenkamp melting point apparatus and are uncorrected. ¹H and ¹³C NMR were performed either on Bruker AC/DPX 250 (250MHz) or AM 400 (400MHz) spectrometers. Elemental analyses were performed by the Cambridge University Microanalytical Service. Tetraethyleneglycol monotosylate, tetraethyleneglycol monoazide (2-(2-(2-(2-Azidoethoxy)ethoxy)ethoxy)ethanol), and 2-(2-(2-(2-aminoethoxy)ethoxy)ethoxy)-ethanol were prepared according to literature procedures.^{4,5}

Bis-N, N'-(2-(2-(2-(2-Hydroxyethoxy)ethoxy)ethoxy)ethyl)pyromellitic diimide 7.

Pyromellitic dianhydride (0.87 g, 4 mmol) was suspended in dry DMF (15 mL) containing 2-(2-(2-(2-aminoethoxy)ethoxy)ethoxy)ethanol (1.93 g, 10 mmol) and the mixture was heated to 150 °C for 16 hours under an atmosphere of argon. The DMF was subsequently evaporated *in vacuo* and the residue dissolved in DCM (30 mL), washed with water (30 mL), dried (MgSO₄) and purified by column chromatography (SiO₂; DCM:MeOH 19:1) to yield the product as a white solid (0.63 g, 28 %). Mp. 72-74 °C. ¹H NMR (CDCl₃, 400 MHz): δ 8.23 (s, 2 H, H_{Ar}), 3.93 (t, 4 H, J = 5.5 Hz, CH₂N), 3.61 (t, 4 H, J = 5.5 Hz, OCH₂CH₂N), 3.57 (m, 24 H, CH₂O), 2.70 (t, 2 H, J = 6.1 Hz, OH). ¹³C NMR (CDCl₃, 100 MHz): δ 166.22 (0), 137.25 (0), 118.21 (1), 72.48 (2), 70.60 (2), 70.50 (2), 70.28 (2), 70.05 (2), 67.65 (2), 61.66 (2), 37.94 (2). MS(ES): m/z: 569.29 ([M+H]⁺). Calcd. for C₂₆H₃₆N₂O₁₂ (568.58): C 54.92, H 6.38, N 4.93 %. Found: C 54.62, H 6.36, N 4.97 %.

Bis-N, N'-(2-(2-(2-(2-Hydroxyethoxy)ethoxy)ethoxy)ethyl)naphthalenetetracarboxylic diimide 8.

Naphthalenetetracarboxylic dianhydride (1.07 g, 4 mmol) was suspended in dry

DMF (15 mL) and (2-(2-(2-aminoethoxy)ethoxy)ethoxy)ethanol (1.93 g, 10 mmol) was added. The mixture was heated to 150 °C under argon for 16 h after which the DMF was evaporated under reduced pressure. Repeated column chromatography afforded the product as a tan solid (1.81g, 73 %; each column yielded an analytically pure fraction and a fraction contaminated with a strongly coloured unidentified compound). Mp. 75-76 °C. ^1H NMR (CDCl_3 , 400 MHz): δ 8.71 (s, 4 H, H_{Ar}), 4.43 (t, 4 H, $J = 5.8$ Hz, $\text{NCH}_2\text{CH}_2\text{O}$), 3.83 (t, 4 H, $J = 5.8$ Hz, $\text{NCH}_2\text{CH}_2\text{O}$), 3.71, 3.53, 3.47 (m, 24 H, CH_2O), 2.71 (t, 2 H, $J = 6.1$ Hz, OH). ^{13}C NMR (CDCl_3 , 100 MHz): δ 162.92 (0), 130.96 (1), 126.73 (0), 126.62 (0), 72.46 (2), 70.58 (2), 70.27 (2), 70.12 (2), 67.85 (2), 61.65 (2), 39.62 (2). MS(ES): m/z : 619.39 ($[\text{M}+\text{H}]^+$). Calcd. for $\text{C}_{30}\text{H}_{38}\text{N}_2\text{O}_{12}$ (618.64): C 58.25, H 6.19, N 4.53 %. Found: C 58.09, H 6.12, N 4.41 %.

Bis-pyromelliticdiimide macrocycle 4. Diol 7 (200 mg, 0.35 mmol) was dissolved in dry THF (50 mL) and pyromellitic diimide 9 (76 mg, 0.35 mmol) and PPh_3 (230 mg, 0.88 mmol) were added. The solution was stirred under Ar and DEAD (152 mg, 0.88 mmol, 0.14 mL) was added *via* syringe and the reaction mixture was stirred overnight. After evaporating the solvent the residue was recrystallized from $\text{CHCl}_3/\text{MeOH}$. The solid thus obtained was purified by preparative TLC (SiO_2 ; DCM:MeOH 19:1) to yield the analytically pure product as a white solid (86 mg, 33 %). Mp 255-257 °C. ^1H NMR (CDCl_3 , 400 MHz): δ 8.22 (s, 4 H, H_{Ar}), 3.90 (t, 8 H, $J = 5.5$ Hz, NCH_2), 3.71 (t, 8 H, $J = 5.5$ Hz, $\text{NCH}_2\text{CH}_2\text{O}$), 3.54 (m, 8 H, CH_2O), 3.49 (m, 8 H, CH_2O). ^{13}C NMR (CDCl_3 , 100 MHz): δ 166.16 (0), 137.23 (0), 118.24 (1), 70.44 (2), 70.04 (2), 67.55 (2), 37.92 (2). MS(ES): m/z 766 ($[\text{M}+\text{H}_2\text{O}]^+$), 749 ($[\text{M}+\text{H}]^+$). Calcd. for $\text{C}_{36}\text{H}_{36}\text{N}_4\text{O}_{14}$ (748.70): C 57.75, H 4.85, N 7.48 %. Found: C 57.45, H 4.83, N 7.32 %.

Mixed pyromellitic/naphthalene diimide macrocycle 10. Diol 8 (200 mg, 0.32 mmol), pyromellitic diimide 9 (70 mg, 0.32 mmol) and PPh_3 (210 mg, 0.8 mmol) were dissolved in dry THF (50 mL) and DEAD (139 mg, 0.8 mmol) was added via syringe. The mixture was stirred overnight after which time the solvent was evaporated. The residue was recrystallized from $\text{CHCl}_3/\text{MeOH}$ to remove $\text{Ph}_3\text{P}=\text{O}$ and then purified by preparative TLC (SiO_2 ; DCM:MeOH 19:1, eluted twice) to afford a white solid (81 mg, 32%). Mp. 277-279 °C. ^1H NMR (CDCl_3 , 400 MHz): δ 8.71 (s, 4 H, naphthalene- H_{Ar}), 8.15 (s, 2 H, pyromellitic- H_{Ar}), 4.40 (t, 4 H, $J = 5.7$ Hz, CH_2N), 3.80-3.40 (m, 28 H, CH_2O). ^{13}C NMR (CDCl_3 , 100 MHz): δ 166.02 (0), 162.88 (0), 137.15 (0), 130.99 (1), 126.73 (0), 126.62 (0), 118.16 (1), 70.46 (2), 70.39 (2), 70.14 (2), 69.91 (2), 67.66 (2), 67.46 (2), 37.78 (2), 39.55 (2). MS(ES): m/z 799.14 ($[\text{M}+\text{H}]^+$).

Naphthalenetetracarboxylic diimide 11. Naphthalenetetracarboxylic dianhydride (2.50 g, 9.32 mmol) was heated to 60 °C for 1h in concentrated ammonia (35 mL) until an even suspension was obtained. The mixture was cooled to room temperature and filtered under

suction. The solid thus obtained was heated to 200 °C under high vacuum in a Kugelrohr apparatus for 4 h yielding the product as a yellow powder (2.20g, 89%). Mp: > 320 °C. MS(FAB): m/z: 267.3 ([M+H]⁺) Calcd. for C₁₄H₆N₂O₄ (266.21): C 63.17, H 2.27, N 10.52 %. Found: C 62.25, H 2.35, N 10.34 %.

Bis-naphthalene diimide macrocycle 12. Diol **8** (200 mg, 0.32 mmol), diimide **11** (172 mg, 0.65 mmol) and PPh₃ (254 mg, 0.97mmol) were dissolved/suspended in dry THF (60 mL). The suspension was sonicated for 2 min before DEAD (169 mg, 0.97 mmol) was added. The mixture was sonicated for a further 45 min before the solvent was evaporated *in vacuo*. Recrystallisation from CHCl₃/MeOH yielded a crude product which was subjected to preparative TLC (SiO₂; DCM:MeOH 19:1) to yield an off-white solid (14 mg, 5 %). Mp. 305-310 °C. ¹H NMR (CDCl₃, 400 MHz): δ 8.67 (s, 8 H, H_{Ar}), 4.27 (t, 8 H, J = 5.8 Hz, NCH₂), 3.71 (t, 8 H, J = 5.8 Hz, NCH₂CH₂O), 3.52 (s, 16 H, CH₂O). ¹³C NMR (CDCl₃, 100 MHz): δ 162.66 (0), 130.98 (1), 126.62 (0), 126.47 (0), 70.46 (2), 70.04 (2), 67.55 (2), 39.43 (2). MS(ES): m/z 849.18 ([M+H]⁺).

[2]Catenane 13. Dinaphtho crown **1** (26 mg, 0.04 mmol), diol **8** (25 mg, 0.04 mmol), pyromellitic diimide **9** (9 mg, 0.04 mmol) and PPh₃ (26 mg, 0.10 mmol) were added to dry DCM (8 mL) under an atmosphere of Ar giving a red solution/suspension. DEAD (17 mg, 0.10 mmol) was added *via* syringe and the reaction mixture was stirred for 5 h after which time no diimide remained suspended. The solvent was evaporated *in vacuo* and the residue purified by preparative TLC to afford the [2]catenane as a red solid (10 mg, 16%). ¹H NMR (CDCl₃, 400 MHz): δ 8.11 (s, 4H, H_{Ar}), 7.10 (s, 2 H, H_{Ar}), 6.57 (d, 4 H, J = 8.0 Hz, H_{Ar}), 6.52 (t, 4 H, J = 7.8 Hz, H_{Ar}), 5.97 (d, 4 H, J = 7.8 Hz, H_{Ar}), 4.22 (t, 4 H, J = 5.7 Hz, NCH₂), 3.77 (m, 60 H, CH₂O). ¹³C NMR (100 MHz, CDCl₃) δ: 165.99 (0), 163.06 (0), 152.70 (0), 134.66 (0), 130.36 (1), 124.91 (0), 124.21 (0), 123.81 (1), 115.79 (1), 113.94 (1), 103.63 (1), 71.27 (2), 71.11 (2), 70.86 (2), 70.45 (2), 70.02 (2), 69.83 (2), 68.30 (2), 68.03 (2), 67.29 (2), 38.99 (2), 37.72 (2). MS(ES): m/z 1436.19 ([M+H]⁺), 1435.30 (M⁺).

Crystal X-ray data collection and structural refinement

General Information. Single crystals of **13** were grown by slow diffusion of methanol into a chloroform solution of the catenane. Diffraction data were collected on a RAXIS diffractometer, corrections were applied for incident beam decay and the structure was solved by direct methods and refined by full-matrix least-squares analysis on F^2 . Atomic coordinates, bond lengths and angles, and thermal parameters have been deposited at the Cambridge Crystallographic Data Centre (CCDC). Any request to the CCDC for this material should quote the full literature citation and the reference number ??????.

Table 1. Crystal data and structure refinement for **13**.

Empirical formula	$C_{78}H_{84}Cl_6N_4O_{24}$	
Formula weight	1674.19	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	$a = 13.1740(10)$ Å	$\alpha = 90^\circ$.
	$b = 29.8510(10)$ Å	$\beta = 105.270(10)^\circ$.
	$c = 20.3590(10)$ Å	$\gamma = 90^\circ$.
Volume	$7723.7(7)$ Å ³	
Z	4	
Density (calculated)	1.440 g/cm ³	
Absorption coefficient	0.304 mm ⁻¹	
F(000)	3496	
Crystal size	$0.35 \times 0.35 \times 0.15$ mm	
Theta range for data collection	3.55 to 25.19° .	
Index ranges	$0 \leq h \leq 15$, $0 \leq k \leq 35$, $-24 \leq l \leq 23$	
Reflections collected	21666	
Independent reflections	12702 [R(int) = 0.0664]	
Completeness to theta = 25.19°	91.3 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12702 / 106 / 1043	
Goodness-of-fit on F^2	0.987	
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0711$, $wR2 = 0.1304$	
R indices (all data)	$R1 = 0.1566$, $wR2 = 0.1583$	
Largest diff. peak and hole	0.467 and -0.406 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **13**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
C(77)	-3043(4)	5156(2)	4687(3)	64(2)
Cl(1)	-3973(2)	5515(1)	4173(1)	109(1)
Cl(2)	-1893(1)	5451(1)	5066(1)	92(1)
Cl(3)	-3558(1)	4910(1)	5315(1)	78(1)
C(78)	-1151(4)	5222(2)	8187(2)	51(1)
Cl(4)	-2062(1)	5491(1)	7513(1)	88(1)
Cl(5)	-79(1)	5574(1)	8503(1)	75(1)
Cl(6)	-1747(1)	5071(1)	8828(1)	71(1)
O(1)	1761(3)	3456(1)	10163(2)	49(1)
O(2)	-1430(3)	3619(1)	8601(2)	53(1)
O(3)	1263(3)	1447(1)	9981(2)	52(1)
O(4)	-1851(2)	1603(1)	8343(2)	56(1)
O(5)	3592(2)	1224(1)	7115(2)	46(1)
O(6)	5419(2)	2428(1)	8201(2)	52(1)
O(7)	1529(2)	3847(1)	6229(2)	51(1)
O(8)	-408(3)	2630(1)	5308(2)	59(1)
O(9)	930(2)	748(1)	8600(2)	52(1)
O(10)	2995(2)	495(1)	8806(2)	54(1)
O(11)	4645(2)	1120(1)	8773(1)	43(1)
O(12)	-1047(2)	3855(1)	6102(2)	43(1)
O(13)	-236(3)	4668(1)	7116(2)	54(1)
O(14)	372(2)	4380(1)	8511(2)	57(1)
O(15)	2473(2)	3113(1)	8714(1)	32(1)
O(16)	-457(2)	1746(1)	7134(1)	37(1)
O(17)	-649(2)	1070(1)	6132(2)	48(1)
O(18)	1210(3)	594(1)	6058(2)	65(1)
O(19)	1351(3)	985(1)	4750(2)	62(1)
O(20)	2629(2)	1827(1)	4862(2)	45(1)
O(24)	3693(2)	3864(1)	8628(2)	41(1)
N(1)	180(3)	3651(2)	9411(2)	44(1)
N(2)	-300(3)	1410(1)	9129(2)	39(1)
N(3)	4514(3)	1825(1)	7663(2)	35(1)
N(4)	566(3)	3232(2)	5754(2)	36(1)

C(1)	936(4)	3353(2)	9753(3)	42(1)
C(2)	-661(4)	3437(2)	8966(3)	41(1)
C(3)	-429(4)	2949(2)	9033(2)	36(1)
C(4)	-1023(4)	2586(2)	8735(2)	44(1)
C(5)	-595(3)	2169(2)	8942(2)	36(1)
C(6)	-1027(4)	1715(2)	8746(3)	43(1)
C(7)	558(4)	1632(2)	9571(2)	39(1)
C(8)	366(3)	2115(2)	9431(2)	36(1)
C(9)	967(3)	2480(2)	9728(2)	37(1)
C(10)	544(4)	2898(2)	9519(2)	36(1)
C(11)	-455(4)	929(2)	9120(3)	49(1)
C(12)	-189(4)	700(2)	8522(3)	56(2)
C(13)	1241(4)	544(2)	8078(3)	59(2)
C(14)	2378(3)	616(2)	8145(2)	49(1)
C(15)	4039(4)	372(2)	8844(3)	53(2)
C(16)	4642(4)	687(2)	8495(3)	47(1)
C(17)	5491(3)	1394(2)	8688(2)	45(1)
C(18)	5427(3)	1532(2)	7966(2)	42(1)
C(19)	3623(4)	1625(2)	7222(2)	37(1)
C(20)	2763(3)	1926(2)	6887(2)	33(1)
C(21)	1845(3)	1749(2)	6477(2)	41(1)
C(22)	1068(3)	2030(2)	6101(2)	39(1)
C(23)	1194(4)	2486(2)	6137(2)	34(1)
C(24)	388(4)	2777(2)	5702(2)	40(1)
C(25)	1437(4)	3440(2)	6205(2)	39(1)
C(26)	2233(3)	3141(2)	6631(2)	32(1)
C(27)	3137(4)	3321(2)	7065(2)	39(1)
C(28)	3912(4)	3040(2)	7449(2)	39(1)
C(29)	3801(3)	2584(2)	7393(2)	32(1)
C(30)	4638(4)	2286(2)	7794(2)	39(1)
C(31)	2893(3)	2390(2)	6961(2)	31(1)
C(32)	2101(3)	2679(2)	6576(2)	33(1)
C(33)	-210(4)	3522(2)	5285(2)	48(1)
C(34)	-1201(3)	3587(2)	5508(2)	44(1)
C(35)	-982(4)	4318(2)	5977(3)	56(2)
C(36)	-1156(4)	4586(2)	6566(3)	55(2)
C(37)	359(4)	4284(2)	7375(2)	56(2)

C(38)	1012(4)	4366(2)	8070(2)	49(1)
C(39)	877(4)	4389(2)	9219(3)	58(2)
C(40)	224(4)	4128(2)	9574(3)	54(2)
C(41)	2180(3)	2684(2)	8534(2)	26(1)
C(42)	1210(3)	2648(2)	8022(2)	25(1)
C(43)	623(3)	3029(2)	7724(2)	31(1)
C(44)	-324(3)	2974(2)	7238(2)	33(1)
C(45)	-724(3)	2554(2)	7031(2)	31(1)
C(46)	-160(3)	2177(2)	7303(2)	33(1)
C(47)	825(3)	2217(2)	7815(2)	26(1)
C(48)	1407(3)	1832(2)	8105(2)	32(1)
C(49)	2351(3)	1885(2)	8587(2)	33(1)
C(50)	2748(3)	2309(2)	8802(2)	30(1)
C(51)	-1389(3)	1675(2)	6594(2)	40(1)
C(52)	-1444(3)	1179(2)	6452(2)	45(1)
C(53)	-600(4)	609(2)	6044(3)	52(1)
C(54)	203(4)	494(2)	5668(3)	60(2)
C(55)	1988(4)	493(2)	5688(3)	71(2)
C(56)	2223(4)	868(2)	5279(3)	69(2)
C(57)	1507(4)	1266(2)	4221(3)	57(2)
C(58)	1625(3)	1754(2)	4383(2)	49(1)
C(59)	2922(3)	2255(2)	5054(2)	37(1)
C(60)	3915(3)	2286(2)	5556(2)	31(1)
C(61)	4494(3)	1901(2)	5825(2)	34(1)
C(62)	5447(3)	1944(2)	6289(2)	39(1)
C(63)	5864(3)	2366(2)	6512(2)	44(1)
C(64)	5309(3)	2743(2)	6259(2)	40(1)
C(65)	4305(3)	2716(2)	5769(2)	32(1)
C(66)	3728(3)	3103(2)	5501(2)	39(1)
C(67)	2776(4)	3059(2)	5028(2)	43(1)
C(68)	2364(4)	2634(2)	4797(2)	44(1)
O(21)	5621(2)	3173(1)	6435(2)	51(1)
C(69)	6594(7)	3219(4)	6991(5)	46(4)
C(70)	6850(8)	3684(4)	7087(5)	37(2)
O(22)	6133(4)	3874(2)	7389(4)	35(1)
C(71)	6171(8)	4359(3)	7398(6)	43(2)
C(72)	5533(8)	4522(4)	7723(5)	43(2)

C(69')	6692(10)	3279(7)	6772(8)	61(6)
C(70')	6790(13)	3805(6)	6710(9)	58(5)
O(22')	6105(8)	4100(5)	6925(6)	86(3)
C(71')	6334(15)	4160(8)	7546(9)	80(4)
C(72')	5404(14)	4480(7)	7999(8)	80(4)
O(23)	4556(3)	4331(2)	7639(2)	92(2)
C(73)	3840(4)	4515(2)	7987(3)	62(2)
C(74)	3914(4)	4332(2)	8679(3)	46(1)
C(75)	3700(3)	3667(2)	9266(2)	37(1)
C(76)	3503(3)	3179(2)	9172(2)	34(1)

Table 3. Bond lengths [Å] and angles [°] for **13**.

C(77)-Cl(2)	1.747(6)
C(77)-Cl(1)	1.752(6)
C(77)-Cl(3)	1.759(5)
C(77)-H(77)	1.0000
C(78)-Cl(5)	1.741(5)
C(78)-Cl(6)	1.749(4)
C(78)-Cl(4)	1.761(5)
C(78)-H(78)	1.0000
O(1)-C(1)	1.224(6)
O(2)-C(2)	1.216(6)
O(3)-C(7)	1.206(5)
O(4)-C(6)	1.222(6)
O(5)-C(19)	1.218(6)
O(6)-C(30)	1.215(5)
O(7)-C(25)	1.221(6)
O(8)-C(24)	1.222(5)
O(9)-C(13)	1.377(5)
O(9)-C(12)	1.447(5)
O(10)-C(15)	1.407(5)
O(10)-C(14)	1.423(5)
O(11)-C(16)	1.410(6)
O(11)-C(17)	1.430(5)
O(12)-C(35)	1.413(6)
O(12)-C(34)	1.419(5)

O(13)-C(37)	1.408(6)
O(13)-C(36)	1.438(6)
O(14)-C(38)	1.385(5)
O(14)-C(39)	1.419(6)
O(15)-C(41)	1.362(5)
O(15)-C(76)	1.443(5)
O(16)-C(46)	1.363(5)
O(16)-C(51)	1.431(5)
O(17)-C(53)	1.392(6)
O(17)-C(52)	1.410(5)
O(18)-C(54)	1.387(6)
O(18)-C(55)	1.457(6)
O(19)-C(56)	1.396(6)
O(19)-C(57)	1.422(6)
O(20)-C(59)	1.360(6)
O(20)-C(58)	1.439(5)
O(24)-C(75)	1.424(5)
O(24)-C(74)	1.424(5)
N(1)-C(1)	1.380(6)
N(1)-C(2)	1.388(6)
N(1)-C(40)	1.462(6)
N(2)-C(6)	1.400(6)
N(2)-C(7)	1.411(6)
N(2)-C(11)	1.448(6)
N(3)-C(30)	1.402(6)
N(3)-C(19)	1.408(6)
N(3)-C(18)	1.485(5)
N(4)-C(24)	1.376(6)
N(4)-C(25)	1.411(6)
N(4)-C(33)	1.480(6)
C(1)-C(10)	1.486(7)
C(2)-C(3)	1.487(7)
C(3)-C(4)	1.379(7)
C(3)-C(10)	1.407(6)
C(4)-C(5)	1.385(7)
C(4)-H(4A)	0.9500
C(5)-C(8)	1.399(6)

C(5)-C(6)	1.485(7)
C(7)-C(8)	1.478(7)
C(8)-C(9)	1.390(6)
C(9)-C(10)	1.385(6)
C(9)-H(9A)	0.9500
C(11)-C(12)	1.516(6)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.484(6)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.522(6)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.507(6)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(20)	1.465(6)
C(20)-C(21)	1.380(6)
C(20)-C(31)	1.398(6)
C(21)-C(22)	1.388(6)
C(21)-H(21A)	0.9500
C(22)-C(23)	1.370(7)
C(22)-H(22A)	0.9500
C(23)-C(32)	1.412(6)
C(23)-C(24)	1.473(6)
C(25)-C(26)	1.472(6)
C(26)-C(27)	1.391(6)
C(26)-C(32)	1.390(6)

C(27)-C(28)	1.393(6)
C(27)-H(27A)	0.9500
C(28)-C(29)	1.370(6)
C(28)-H(28A)	0.9500
C(29)-C(31)	1.409(6)
C(29)-C(30)	1.484(6)
C(31)-C(32)	1.422(6)
C(33)-C(34)	1.504(5)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900
C(35)-C(36)	1.507(6)
C(35)-H(35A)	0.9900
C(35)-H(35B)	0.9900
C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900
C(37)-C(38)	1.468(6)
C(37)-H(37A)	0.9900
C(37)-H(37B)	0.9900
C(38)-H(38A)	0.9900
C(38)-H(38B)	0.9900
C(39)-C(40)	1.481(6)
C(39)-H(39A)	0.9900
C(39)-H(39B)	0.9900
C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900
C(41)-C(50)	1.375(6)
C(41)-C(42)	1.424(6)
C(42)-C(47)	1.407(6)
C(42)-C(43)	1.417(6)
C(43)-C(44)	1.383(6)
C(43)-H(43A)	0.9500
C(44)-C(45)	1.381(6)
C(44)-H(44A)	0.9500
C(45)-C(46)	1.381(6)
C(45)-H(45A)	0.9500

C(46)-C(47)	1.439(6)
C(47)-C(48)	1.419(6)
C(48)-C(49)	1.376(6)
C(48)-H(48A)	0.9500
C(49)-C(50)	1.395(6)
C(49)-H(49A)	0.9500
C(50)-H(50A)	0.9500
C(51)-C(52)	1.506(6)
C(51)-H(51A)	0.9900
C(51)-H(51B)	0.9900
C(52)-H(52A)	0.9900
C(52)-H(52B)	0.9900
C(53)-C(54)	1.499(6)
C(53)-H(53A)	0.9900
C(53)-H(53B)	0.9900
C(54)-H(54A)	0.9900
C(54)-H(54B)	0.9900
C(55)-C(56)	1.476(7)
C(55)-H(55A)	0.9900
C(55)-H(55B)	0.9900
C(56)-H(56A)	0.9900
C(56)-H(56B)	0.9900
C(57)-C(58)	1.491(7)
C(57)-H(57A)	0.9900
C(57)-H(57B)	0.9900
C(58)-H(58A)	0.9900
C(58)-H(58B)	0.9900
C(59)-C(68)	1.375(7)
C(59)-C(60)	1.435(6)
C(60)-C(65)	1.407(6)
C(60)-C(61)	1.407(6)
C(61)-C(62)	1.364(6)
C(61)-H(61A)	0.9500
C(62)-C(63)	1.400(7)
C(62)-H(62A)	0.9500
C(63)-C(64)	1.369(7)
C(63)-H(63A)	0.9500

C(64)-O(21)	1.365(6)
C(64)-C(65)	1.434(6)
C(65)-C(66)	1.412(6)
C(66)-C(67)	1.372(6)
C(66)-H(66A)	0.9500
C(67)-C(68)	1.412(7)
C(67)-H(67A)	0.9500
C(68)-H(68A)	0.9500
O(21)-C(69')	1.432(10)
O(21)-C(69)	1.476(8)
C(69)-C(70)	1.428(16)
C(69)-H(69A)	0.9900
C(69)-H(69B)	0.9900
C(70)-O(22)	1.378(11)
C(70)-H(70A)	0.9900
C(70)-H(70B)	0.9900
O(22)-C(71)	1.451(11)
C(71)-C(72)	1.294(12)
C(71)-H(71A)	0.9900
C(71)-H(71B)	0.9900
C(72)-O(23)	1.376(10)
C(72)-H(72A)	0.9900
C(72)-H(72B)	0.9900
C(69')-C(70')	1.58(3)
C(69')-H(69C)	0.9900
C(69')-H(69D)	0.9900
C(70')-O(22')	1.411(19)
C(70')-H(70C)	0.9900
C(70')-H(70D)	0.9900
O(22')-C(71')	1.23(2)
C(71')-C(72')	1.96(3)
C(71')-H(71C)	0.9900
C(71')-H(71D)	0.9900
C(72')-O(23)	1.246(17)
C(72')-H(72C)	0.9900
C(72')-H(72D)	0.9900
O(23)-C(73)	1.431(5)

C(73)-C(74)	1.491(6)
C(73)-H(73A)	0.9900
C(73)-H(73B)	0.9900
C(74)-H(74A)	0.9900
C(74)-H(74B)	0.9900
C(75)-C(76)	1.483(6)
C(75)-H(75A)	0.9900
C(75)-H(75B)	0.9900
C(76)-H(76A)	0.9900
C(76)-H(76B)	0.9900
Cl(2)-C(77)-Cl(1)	110.1(4)
Cl(2)-C(77)-Cl(3)	110.1(3)
Cl(1)-C(77)-Cl(3)	110.3(3)
Cl(2)-C(77)-H(77)	108.8
Cl(1)-C(77)-H(77)	108.7
Cl(3)-C(77)-H(77)	108.8
Cl(5)-C(78)-Cl(6)	111.1(3)
Cl(5)-C(78)-Cl(4)	109.5(3)
Cl(6)-C(78)-Cl(4)	110.5(2)
Cl(5)-C(78)-H(78)	108.5
Cl(6)-C(78)-H(78)	108.5
Cl(4)-C(78)-H(78)	108.5
C(13)-O(9)-C(12)	111.9(4)
C(15)-O(10)-C(14)	115.1(3)
C(16)-O(11)-C(17)	113.3(3)
C(35)-O(12)-C(34)	113.6(4)
C(37)-O(13)-C(36)	115.2(4)
C(38)-O(14)-C(39)	117.2(4)
C(41)-O(15)-C(76)	117.0(3)
C(46)-O(16)-C(51)	117.8(4)
C(53)-O(17)-C(52)	110.6(4)
C(54)-O(18)-C(55)	110.9(4)
C(56)-O(19)-C(57)	118.5(4)
C(59)-O(20)-C(58)	118.6(4)
C(75)-O(24)-C(74)	112.8(3)
C(1)-N(1)-C(2)	112.2(5)
C(1)-N(1)-C(40)	122.3(5)

C(2)-N(1)-C(40)	125.1(4)
C(6)-N(2)-C(7)	111.4(5)
C(6)-N(2)-C(11)	124.3(4)
C(7)-N(2)-C(11)	124.1(4)
C(30)-N(3)-C(19)	125.0(4)
C(30)-N(3)-C(18)	117.2(4)
C(19)-N(3)-C(18)	117.6(4)
C(24)-N(4)-C(25)	125.2(4)
C(24)-N(4)-C(33)	116.9(4)
C(25)-N(4)-C(33)	117.9(4)
O(1)-C(1)-N(1)	125.0(5)
O(1)-C(1)-C(10)	128.4(5)
N(1)-C(1)-C(10)	106.6(5)
O(2)-C(2)-N(1)	125.9(5)
O(2)-C(2)-C(3)	127.7(5)
N(1)-C(2)-C(3)	106.4(5)
C(4)-C(3)-C(10)	122.0(5)
C(4)-C(3)-C(2)	130.5(5)
C(10)-C(3)-C(2)	107.3(5)
C(3)-C(4)-C(5)	115.7(5)
C(3)-C(4)-H(4A)	122.2
C(5)-C(4)-H(4A)	122.1
C(4)-C(5)-C(8)	122.7(5)
C(4)-C(5)-C(6)	130.0(5)
C(8)-C(5)-C(6)	107.2(5)
O(4)-C(6)-N(2)	123.6(5)
O(4)-C(6)-C(5)	129.7(5)
N(2)-C(6)-C(5)	106.7(4)
O(3)-C(7)-N(2)	124.6(5)
O(3)-C(7)-C(8)	129.9(5)
N(2)-C(7)-C(8)	105.5(4)
C(9)-C(8)-C(5)	121.6(5)
C(9)-C(8)-C(7)	129.2(5)
C(5)-C(8)-C(7)	109.1(4)
C(10)-C(9)-C(8)	115.8(4)
C(10)-C(9)-H(9A)	122.1
C(8)-C(9)-H(9A)	122.1

C(9)-C(10)-C(3)	122.2(5)
C(9)-C(10)-C(1)	130.2(5)
C(3)-C(10)-C(1)	107.5(5)
N(2)-C(11)-C(12)	113.2(4)
N(2)-C(11)-H(11A)	108.9
C(12)-C(11)-H(11A)	108.9
N(2)-C(11)-H(11B)	109.0
C(12)-C(11)-H(11B)	109.0
H(11A)-C(11)-H(11B)	107.8
O(9)-C(12)-C(11)	108.2(4)
O(9)-C(12)-H(12A)	110.0
C(11)-C(12)-H(12A)	110.1
O(9)-C(12)-H(12B)	110.1
C(11)-C(12)-H(12B)	110.1
H(12A)-C(12)-H(12B)	108.4
O(9)-C(13)-C(14)	111.3(4)
O(9)-C(13)-H(13A)	109.5
C(14)-C(13)-H(13A)	109.4
O(9)-C(13)-H(13B)	109.3
C(14)-C(13)-H(13B)	109.3
H(13A)-C(13)-H(13B)	108.0
O(10)-C(14)-C(13)	111.2(4)
O(10)-C(14)-H(14A)	109.4
C(13)-C(14)-H(14A)	109.4
O(10)-C(14)-H(14B)	109.4
C(13)-C(14)-H(14B)	109.3
H(14A)-C(14)-H(14B)	108.0
O(10)-C(15)-C(16)	115.8(4)
O(10)-C(15)-H(15A)	108.3
C(16)-C(15)-H(15A)	108.3
O(10)-C(15)-H(15B)	108.3
C(16)-C(15)-H(15B)	108.4
H(15A)-C(15)-H(15B)	107.4
O(11)-C(16)-C(15)	109.1(4)
O(11)-C(16)-H(16A)	109.9
C(15)-C(16)-H(16A)	109.8
O(11)-C(16)-H(16B)	109.9

C(15)-C(16)-H(16B)	109.9
H(16A)-C(16)-H(16B)	108.3
O(11)-C(17)-C(18)	115.4(4)
O(11)-C(17)-H(17A)	108.4
C(18)-C(17)-H(17A)	108.3
O(11)-C(17)-H(17B)	108.5
C(18)-C(17)-H(17B)	108.5
H(17A)-C(17)-H(17B)	107.5
N(3)-C(18)-C(17)	113.4(3)
N(3)-C(18)-H(18A)	108.9
C(17)-C(18)-H(18A)	108.9
N(3)-C(18)-H(18B)	108.9
C(17)-C(18)-H(18B)	108.9
H(18A)-C(18)-H(18B)	107.7
O(5)-C(19)-N(3)	121.0(5)
O(5)-C(19)-C(20)	122.3(5)
N(3)-C(19)-C(20)	116.7(5)
C(21)-C(20)-C(31)	120.4(5)
C(21)-C(20)-C(19)	119.6(5)
C(31)-C(20)-C(19)	119.9(4)
C(20)-C(21)-C(22)	120.3(5)
C(20)-C(21)-H(21A)	119.8
C(22)-C(21)-H(21A)	119.9
C(23)-C(22)-C(21)	120.6(5)
C(23)-C(22)-H(22A)	119.6
C(21)-C(22)-H(22A)	119.7
C(22)-C(23)-C(32)	120.6(5)
C(22)-C(23)-C(24)	119.7(5)
C(32)-C(23)-C(24)	119.7(5)
O(8)-C(24)-N(4)	120.3(5)
O(8)-C(24)-C(23)	122.7(5)
N(4)-C(24)-C(23)	117.0(5)
O(7)-C(25)-N(4)	121.2(5)
O(7)-C(25)-C(26)	122.2(5)
N(4)-C(25)-C(26)	116.6(5)
C(27)-C(26)-C(32)	120.2(5)
C(27)-C(26)-C(25)	119.8(5)

C(32)-C(26)-C(25)	119.9(4)
C(26)-C(27)-C(28)	120.1(5)
C(26)-C(27)-H(27A)	119.9
C(28)-C(27)-H(27A)	120.0
C(29)-C(28)-C(27)	120.4(5)
C(29)-C(28)-H(28A)	119.8
C(27)-C(28)-H(28A)	119.8
C(28)-C(29)-C(31)	121.1(5)
C(28)-C(29)-C(30)	120.1(5)
C(31)-C(29)-C(30)	118.8(5)
O(6)-C(30)-N(3)	120.6(5)
O(6)-C(30)-C(29)	122.6(5)
N(3)-C(30)-C(29)	116.8(4)
C(20)-C(31)-C(29)	122.3(5)
C(20)-C(31)-C(32)	119.5(4)
C(29)-C(31)-C(32)	118.2(5)
C(26)-C(32)-C(23)	121.5(4)
C(26)-C(32)-C(31)	120.0(4)
C(23)-C(32)-C(31)	118.5(5)
N(4)-C(33)-C(34)	112.9(4)
N(4)-C(33)-H(33A)	109.0
C(34)-C(33)-H(33A)	109.0
N(4)-C(33)-H(33B)	109.0
C(34)-C(33)-H(33B)	109.0
H(33A)-C(33)-H(33B)	107.8
O(12)-C(34)-C(33)	112.9(4)
O(12)-C(34)-H(34A)	109.0
C(33)-C(34)-H(34A)	109.0
O(12)-C(34)-H(34B)	109.0
C(33)-C(34)-H(34B)	109.0
H(34A)-C(34)-H(34B)	107.8
O(12)-C(35)-C(36)	110.3(4)
O(12)-C(35)-H(35A)	109.6
C(36)-C(35)-H(35A)	109.6
O(12)-C(35)-H(35B)	109.6
C(36)-C(35)-H(35B)	109.6
H(35A)-C(35)-H(35B)	108.1

O(13)-C(36)-C(35)	115.8(4)
O(13)-C(36)-H(36A)	108.3
C(35)-C(36)-H(36A)	108.4
O(13)-C(36)-H(36B)	108.3
C(35)-C(36)-H(36B)	108.3
H(36A)-C(36)-H(36B)	107.4
O(13)-C(37)-C(38)	110.8(4)
O(13)-C(37)-H(37A)	109.6
C(38)-C(37)-H(37A)	109.6
O(13)-C(37)-H(37B)	109.4
C(38)-C(37)-H(37B)	109.4
H(37A)-C(37)-H(37B)	108.1
O(14)-C(38)-C(37)	109.2(4)
O(14)-C(38)-H(38A)	109.8
C(37)-C(38)-H(38A)	109.8
O(14)-C(38)-H(38B)	109.9
C(37)-C(38)-H(38B)	109.8
H(38A)-C(38)-H(38B)	108.3
O(14)-C(39)-C(40)	108.0(4)
O(14)-C(39)-H(39A)	110.1
C(40)-C(39)-H(39A)	110.1
O(14)-C(39)-H(39B)	110.1
C(40)-C(39)-H(39B)	110.1
H(39A)-C(39)-H(39B)	108.4
N(1)-C(40)-C(39)	113.3(4)
N(1)-C(40)-H(40A)	108.9
C(39)-C(40)-H(40A)	108.9
N(1)-C(40)-H(40B)	109.0
C(39)-C(40)-H(40B)	108.9
H(40A)-C(40)-H(40B)	107.7
O(15)-C(41)-C(50)	124.9(4)
O(15)-C(41)-C(42)	113.8(4)
C(50)-C(41)-C(42)	121.3(4)
C(47)-C(42)-C(43)	119.5(4)
C(47)-C(42)-C(41)	118.0(4)
C(43)-C(42)-C(41)	122.5(4)
C(44)-C(43)-C(42)	120.0(4)

C(44)-C(43)-H(43A)	120.0
C(42)-C(43)-H(43A)	120.0
C(43)-C(44)-C(45)	121.7(4)
C(43)-C(44)-H(44A)	119.1
C(45)-C(44)-H(44A)	119.2
C(46)-C(45)-C(44)	119.7(4)
C(46)-C(45)-H(45A)	120.2
C(44)-C(45)-H(45A)	120.2
O(16)-C(46)-C(45)	125.4(4)
O(16)-C(46)-C(47)	113.9(4)
C(45)-C(46)-C(47)	120.8(4)
C(42)-C(47)-C(48)	120.2(4)
C(42)-C(47)-C(46)	118.5(4)
C(48)-C(47)-C(46)	121.4(4)
C(49)-C(48)-C(47)	119.4(4)
C(49)-C(48)-H(48A)	120.3
C(47)-C(48)-H(48A)	120.3
C(48)-C(49)-C(50)	121.4(4)
C(48)-C(49)-H(49A)	119.3
C(50)-C(49)-H(49A)	119.3
C(41)-C(50)-C(49)	119.6(4)
C(41)-C(50)-H(50A)	120.2
C(49)-C(50)-H(50A)	120.2
O(16)-C(51)-C(52)	106.4(4)
O(16)-C(51)-H(51A)	110.4
C(52)-C(51)-H(51A)	110.5
O(16)-C(51)-H(51B)	110.4
C(52)-C(51)-H(51B)	110.4
H(51A)-C(51)-H(51B)	108.6
O(17)-C(52)-C(51)	108.1(4)
O(17)-C(52)-H(52A)	110.1
C(51)-C(52)-H(52A)	110.1
O(17)-C(52)-H(52B)	110.1
C(51)-C(52)-H(52B)	110.0
H(52A)-C(52)-H(52B)	108.4
O(17)-C(53)-C(54)	110.9(4)
O(17)-C(53)-H(53A)	109.5

C(54)-C(53)-H(53A)	109.5
O(17)-C(53)-H(53B)	109.4
C(54)-C(53)-H(53B)	109.4
H(53A)-C(53)-H(53B)	108.0
O(18)-C(54)-C(53)	110.8(4)
O(18)-C(54)-H(54A)	109.5
C(53)-C(54)-H(54A)	109.5
O(18)-C(54)-H(54B)	109.5
C(53)-C(54)-H(54B)	109.4
H(54A)-C(54)-H(54B)	108.1
O(18)-C(55)-C(56)	114.5(5)
O(18)-C(55)-H(55A)	108.7
C(56)-C(55)-H(55A)	108.5
O(18)-C(55)-H(55B)	108.6
C(56)-C(55)-H(55B)	108.7
H(55A)-C(55)-H(55B)	107.6
O(19)-C(56)-C(55)	111.9(5)
O(19)-C(56)-H(56A)	109.2
C(55)-C(56)-H(56A)	109.2
O(19)-C(56)-H(56B)	109.3
C(55)-C(56)-H(56B)	109.2
H(56A)-C(56)-H(56B)	107.9
O(19)-C(57)-C(58)	115.8(4)
O(19)-C(57)-H(57A)	108.3
C(58)-C(57)-H(57A)	108.3
O(19)-C(57)-H(57B)	108.4
C(58)-C(57)-H(57B)	108.3
H(57A)-C(57)-H(57B)	107.4
O(20)-C(58)-C(57)	108.9(4)
O(20)-C(58)-H(58A)	109.9
C(57)-C(58)-H(58A)	109.9
O(20)-C(58)-H(58B)	109.9
C(57)-C(58)-H(58B)	109.9
H(58A)-C(58)-H(58B)	108.3
O(20)-C(59)-C(68)	125.4(4)
O(20)-C(59)-C(60)	113.7(5)
C(68)-C(59)-C(60)	120.9(5)

C(65)-C(60)-C(61)	120.5(4)
C(65)-C(60)-C(59)	118.0(5)
C(61)-C(60)-C(59)	121.5(5)
C(62)-C(61)-C(60)	119.9(5)
C(62)-C(61)-H(61A)	120.0
C(60)-C(61)-H(61A)	120.1
C(61)-C(62)-C(63)	121.3(5)
C(61)-C(62)-H(62A)	119.3
C(63)-C(62)-H(62A)	119.4
C(64)-C(63)-C(62)	119.5(4)
C(64)-C(63)-H(63A)	120.3
C(62)-C(63)-H(63A)	120.2
O(21)-C(64)-C(63)	125.5(4)
O(21)-C(64)-C(65)	113.3(5)
C(63)-C(64)-C(65)	121.2(5)
C(60)-C(65)-C(66)	120.8(4)
C(60)-C(65)-C(64)	117.5(5)
C(66)-C(65)-C(64)	121.7(5)
C(67)-C(66)-C(65)	119.5(5)
C(67)-C(66)-H(66A)	120.2
C(65)-C(66)-H(66A)	120.2
C(66)-C(67)-C(68)	121.3(5)
C(66)-C(67)-H(67A)	119.3
C(68)-C(67)-H(67A)	119.4
C(59)-C(68)-C(67)	119.5(5)
C(59)-C(68)-H(68A)	120.2
C(67)-C(68)-H(68A)	120.2
C(64)-O(21)-C(69')	121.6(9)
C(64)-O(21)-C(69)	115.5(6)
C(69')-O(21)-C(69)	20.8(10)
C(70)-C(69)-O(21)	108.8(10)
C(70)-C(69)-H(69A)	110.0
O(21)-C(69)-H(69A)	109.9
C(70)-C(69)-H(69B)	109.8
O(21)-C(69)-H(69B)	109.8
H(69A)-C(69)-H(69B)	108.5
O(22)-C(70)-C(69)	107.2(8)

O(22)-C(70)-H(70A)	110.2
C(69)-C(70)-H(70A)	110.8
O(22)-C(70)-H(70B)	110.3
C(69)-C(70)-H(70B)	109.9
H(70A)-C(70)-H(70B)	108.5
C(70)-O(22)-C(71)	113.0(6)
C(72)-C(71)-O(22)	110.9(6)
C(72)-C(71)-H(71A)	109.4
O(22)-C(71)-H(71A)	110.2
C(72)-C(71)-H(71B)	109.9
O(22)-C(71)-H(71B)	108.4
H(71A)-C(71)-H(71B)	108.0
C(71)-C(72)-O(23)	119.5(9)
C(71)-C(72)-H(72A)	107.0
O(23)-C(72)-H(72A)	106.4
C(71)-C(72)-H(72B)	107.8
O(23)-C(72)-H(72B)	108.6
H(72A)-C(72)-H(72B)	107.0
O(21)-C(69')-C(70')	105.8(14)
O(21)-C(69')-H(69C)	110.9
C(70')-C(69')-H(69C)	110.6
O(21)-C(69')-H(69D)	110.8
C(70')-C(69')-H(69D)	110.2
H(69C)-C(69')-H(69D)	108.5
O(22')-C(70')-C(69')	121.5(14)
O(22')-C(70')-H(70C)	107.3
C(69')-C(70')-H(70C)	106.6
O(22')-C(70')-H(70D)	106.9
C(69')-C(70')-H(70D)	107.0
H(70C)-C(70')-H(70D)	106.8
C(71')-O(22')-C(70')	113.8(15)
O(22')-C(71')-C(72')	122.5(13)
O(22')-C(71')-H(71C)	106.3
C(72')-C(71')-H(71C)	106.9
O(22')-C(71')-H(71D)	106.9
C(72')-C(71')-H(71D)	106.7
H(71C)-C(71')-H(71D)	106.7

O(23)-C(72')-C(71')	97.0(11)
O(23)-C(72')-H(72C)	112.5
C(71')-C(72')-H(72C)	112.2
O(23)-C(72')-H(72D)	113.0
C(71')-C(72')-H(72D)	111.9
H(72C)-C(72')-H(72D)	109.7
C(72')-O(23)-C(72)	27.8(8)
C(72')-O(23)-C(73)	100.2(9)
C(72)-O(23)-C(73)	119.7(6)
O(23)-C(73)-C(74)	116.1(5)
O(23)-C(73)-H(73A)	108.2
C(74)-C(73)-H(73A)	108.0
O(23)-C(73)-H(73B)	108.3
C(74)-C(73)-H(73B)	108.5
H(73A)-C(73)-H(73B)	107.4
O(24)-C(74)-C(73)	109.1(4)
O(24)-C(74)-H(74A)	109.7
C(73)-C(74)-H(74A)	109.6
O(24)-C(74)-H(74B)	110.0
C(73)-C(74)-H(74B)	110.1
H(74A)-C(74)-H(74B)	108.3
O(24)-C(75)-C(76)	109.3(4)
O(24)-C(75)-H(75A)	109.8
C(76)-C(75)-H(75A)	109.8
O(24)-C(75)-H(75B)	109.9
C(76)-C(75)-H(75B)	109.9
H(75A)-C(75)-H(75B)	108.2
O(15)-C(76)-C(75)	108.7(4)
O(15)-C(76)-H(76A)	110.0
C(75)-C(76)-H(76A)	110.0
O(15)-C(76)-H(76B)	110.0
C(75)-C(76)-H(76B)	109.9
H(76A)-C(76)-H(76B)	108.4

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **13**. The anisotropic displacement factor exponent takes the form: $-2_{-2} [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(77)	54(3)	75(5)	55(4)	-12(3)	2(3)	7(3)
Cl(1)	115(2)	106(2)	85(1)	6(1)	-10(1)	29(1)
Cl(2)	88(1)	104(2)	76(1)	4(1)	8(1)	-34(1)
Cl(3)	67(1)	72(1)	97(1)	-4(1)	24(1)	1(1)
C(78)	51(3)	51(4)	52(3)	-7(3)	14(3)	8(3)
Cl(4)	62(1)	130(2)	66(1)	4(1)	5(1)	42(1)
Cl(5)	60(1)	68(1)	92(1)	6(1)	13(1)	-12(1)
Cl(6)	67(1)	66(1)	90(1)	5(1)	42(1)	7(1)
O(1)	54(2)	52(3)	43(2)	-1(2)	14(2)	-5(2)
O(2)	48(2)	59(3)	53(2)	12(2)	17(2)	20(2)
O(3)	43(2)	63(3)	48(2)	13(2)	7(2)	8(2)
O(4)	33(2)	74(3)	59(2)	-12(2)	9(2)	-7(2)
O(5)	52(2)	44(3)	40(2)	-1(2)	10(2)	0(2)
O(6)	40(2)	61(3)	44(2)	-7(2)	-5(2)	-9(2)
O(7)	48(2)	52(3)	58(2)	3(2)	22(2)	2(2)
O(8)	55(2)	70(3)	39(2)	-2(2)	-10(2)	-1(2)
O(9)	39(2)	67(3)	49(2)	-14(2)	11(2)	5(2)
O(10)	41(2)	69(3)	50(2)	16(2)	8(2)	5(2)
O(11)	47(2)	50(2)	31(2)	-3(2)	10(2)	-3(2)
O(12)	41(2)	32(2)	53(2)	0(2)	9(2)	2(2)
O(13)	63(2)	46(3)	46(2)	-2(2)	5(2)	8(2)
O(14)	42(2)	82(3)	51(2)	18(2)	18(2)	5(2)
O(15)	26(2)	34(2)	32(2)	3(2)	-1(1)	-2(2)
O(16)	29(2)	41(2)	35(2)	-1(2)	-3(1)	2(2)
O(17)	50(2)	35(2)	61(2)	-2(2)	21(2)	2(2)
O(18)	49(2)	65(3)	76(3)	1(2)	9(2)	-7(2)
O(19)	45(2)	84(3)	55(2)	-4(2)	10(2)	-15(2)
O(20)	30(2)	57(3)	43(2)	-11(2)	3(2)	-7(2)
O(24)	46(2)	31(2)	47(2)	5(2)	13(2)	-7(2)
N(1)	47(3)	40(3)	47(3)	4(2)	17(2)	6(2)
N(2)	38(2)	37(3)	48(3)	-2(2)	19(2)	2(2)
N(3)	26(2)	48(3)	29(2)	0(2)	4(2)	5(2)

N(4)	30(2)	50(3)	27(2)	6(2)	7(2)	7(2)
C(1)	45(3)	53(4)	35(3)	5(3)	22(3)	-1(3)
C(2)	43(3)	48(4)	40(3)	5(3)	26(3)	7(3)
C(3)	37(3)	46(4)	30(3)	2(3)	19(2)	-1(3)
C(4)	35(3)	63(4)	40(3)	5(3)	19(2)	12(3)
C(5)	33(3)	46(4)	32(3)	-2(3)	14(2)	4(3)
C(6)	28(3)	62(4)	46(3)	1(3)	20(3)	6(3)
C(7)	29(3)	56(4)	36(3)	3(3)	15(2)	-3(3)
C(8)	36(3)	41(3)	36(3)	-6(3)	19(2)	-3(2)
C(9)	30(3)	58(4)	26(3)	2(3)	12(2)	-4(3)
C(10)	36(3)	40(3)	37(3)	5(3)	21(2)	4(3)
C(11)	34(3)	63(4)	52(3)	4(3)	18(3)	0(3)
C(12)	46(3)	58(4)	58(4)	-15(3)	5(3)	1(3)
C(13)	57(3)	63(4)	55(3)	4(3)	13(3)	-2(3)
C(14)	48(3)	53(4)	43(3)	-7(3)	9(3)	5(3)
C(15)	43(3)	54(4)	58(3)	13(3)	8(3)	14(3)
C(16)	48(3)	48(4)	49(3)	1(3)	18(3)	7(3)
C(17)	33(3)	56(4)	40(3)	3(3)	0(2)	-1(3)
C(18)	30(2)	56(4)	40(3)	9(3)	10(2)	6(3)
C(19)	42(3)	42(4)	29(3)	-2(3)	16(2)	-3(3)
C(20)	31(3)	46(4)	25(3)	2(2)	11(2)	3(2)
C(21)	36(3)	45(4)	43(3)	-5(3)	11(2)	-5(3)
C(22)	32(3)	48(4)	33(3)	-1(3)	1(2)	-3(3)
C(23)	39(3)	40(3)	25(3)	2(2)	12(2)	5(2)
C(24)	48(3)	44(4)	27(3)	2(3)	8(2)	-3(3)
C(25)	46(3)	38(4)	42(3)	5(3)	24(3)	2(3)
C(26)	32(3)	44(4)	23(2)	-4(2)	12(2)	-4(2)
C(27)	50(3)	32(3)	40(3)	-7(3)	19(3)	-2(3)
C(28)	41(3)	46(4)	28(3)	-6(3)	7(2)	1(3)
C(29)	26(2)	48(4)	24(2)	-2(2)	8(2)	6(2)
C(30)	34(3)	51(4)	34(3)	-1(3)	13(2)	1(3)
C(31)	26(2)	44(4)	24(2)	-4(2)	9(2)	2(2)
C(32)	34(3)	43(4)	24(3)	-1(2)	14(2)	-1(3)
C(33)	60(3)	51(4)	33(3)	9(3)	11(2)	12(3)
C(34)	41(3)	48(4)	35(3)	-1(3)	-5(2)	10(3)
C(35)	65(4)	53(4)	45(3)	-2(3)	6(3)	1(3)
C(36)	59(3)	47(4)	52(3)	-3(3)	5(3)	6(3)

C(37)	61(4)	54(4)	46(3)	-6(3)	2(3)	19(3)
C(38)	41(3)	46(4)	57(3)	-12(3)	8(3)	9(3)
C(39)	58(3)	56(4)	53(4)	2(3)	5(3)	8(3)
C(40)	73(4)	42(4)	56(3)	5(3)	31(3)	11(3)
C(41)	26(2)	28(3)	25(2)	-3(2)	8(2)	-4(2)
C(42)	27(2)	26(3)	23(2)	4(2)	9(2)	1(2)
C(43)	35(3)	20(3)	40(3)	2(2)	13(2)	-3(2)
C(44)	33(3)	33(3)	34(3)	12(2)	7(2)	11(2)
C(45)	24(2)	31(3)	35(3)	0(2)	1(2)	6(2)
C(46)	31(3)	36(3)	36(3)	-2(2)	15(2)	-1(2)
C(47)	23(2)	33(3)	21(2)	3(2)	4(2)	3(2)
C(48)	34(3)	27(3)	33(3)	1(2)	8(2)	4(2)
C(49)	31(3)	37(3)	29(3)	3(2)	6(2)	10(2)
C(50)	27(2)	31(3)	27(2)	-1(2)	-1(2)	-2(2)
C(51)	30(3)	39(3)	46(3)	-6(3)	1(2)	0(2)
C(52)	35(3)	48(4)	47(3)	-11(3)	1(2)	-14(3)
C(53)	54(3)	56(4)	45(3)	-4(3)	9(3)	-5(3)
C(54)	60(4)	35(4)	76(4)	-5(3)	3(3)	-7(3)
C(55)	48(3)	55(4)	109(5)	8(4)	18(3)	0(3)
C(56)	44(3)	79(5)	90(5)	0(4)	30(4)	3(3)
C(57)	43(3)	80(5)	49(3)	-15(3)	12(3)	-17(3)
C(58)	36(3)	64(4)	45(3)	-8(3)	7(2)	-13(3)
C(59)	33(3)	49(4)	33(3)	-8(3)	15(2)	-7(3)
C(60)	24(2)	47(3)	24(2)	-2(2)	9(2)	-2(2)
C(61)	33(3)	40(3)	33(3)	-6(2)	14(2)	-8(2)
C(62)	36(3)	46(4)	37(3)	2(3)	12(2)	3(3)
C(63)	24(2)	68(4)	39(3)	-11(3)	6(2)	4(3)
C(64)	30(3)	53(4)	42(3)	-22(3)	16(2)	-6(3)
C(65)	27(2)	39(3)	33(3)	-5(2)	12(2)	-1(2)
C(66)	34(3)	43(4)	44(3)	-11(3)	18(3)	-7(3)
C(67)	47(3)	47(4)	40(3)	5(3)	21(3)	9(3)
C(68)	32(3)	63(4)	38(3)	-1(3)	10(2)	4(3)
O(21)	27(2)	59(3)	66(2)	-29(2)	9(2)	-8(2)
C(69)	18(5)	63(8)	58(7)	-27(6)	13(5)	-9(5)
C(70)	34(5)	43(6)	33(6)	-5(5)	9(5)	-4(4)
O(22)	49(3)	20(4)	46(4)	-7(3)	28(3)	-6(3)
C(71)	57(4)	25(4)	61(5)	-11(4)	43(4)	-20(3)

C(72)	57(4)	25(4)	61(5)	-11(4)	43(4)	-20(3)
C(69')	22(7)	112(15)	57(11)	-46(11)	25(7)	-19(8)
C(70')	29(7)	67(12)	81(11)	-49(10)	19(9)	-11(8)
O(22')	57(6)	95(9)	92(8)	-40(8)	-4(6)	8(7)
C(71')	72(8)	58(9)	77(8)	-39(8)	-36(6)	3(7)
C(72')	72(8)	58(9)	77(8)	-39(8)	-36(6)	3(7)
O(23)	75(3)	104(4)	110(4)	-4(3)	44(3)	-8(3)
C(73)	58(3)	55(4)	81(4)	18(3)	35(3)	8(3)
C(74)	36(3)	41(4)	58(4)	1(3)	8(3)	-3(3)
C(75)	25(2)	36(3)	45(3)	-3(3)	-2(2)	-2(2)
C(76)	31(2)	34(3)	31(3)	4(2)	1(2)	0(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **13**.

	x	y	z	U(eq)
H(77)	-2871	4913	4395	77
H(78)	-896	4944	8007	62
H(4A)	-1682	2620	8409	53
H(9A)	1627	2446	10054	45
H(11A)	-1199	866	9104	58
H(11B)	-11	800	9548	58
H(12A)	-380	379	8510	67
H(12B)	-587	840	8090	67
H(13A)	827	667	7637	70
H(13B)	1096	219	8081	70
H(14A)	2597	434	7799	58
H(14B)	2502	935	8058	58
H(15A)	4033	71	8640	63
H(15B)	4428	348	9330	63
H(16A)	5374	580	8565	57
H(16B)	4304	695	8000	57
H(17A)	6159	1230	8870	54
H(17B)	5519	1668	8966	54
H(18A)	6082	1692	7957	50
H(18B)	5382	1259	7682	50
H(21A)	1745	1434	6453	50

H(22A)	443	1906	5816	47
H(27A)	3226	3637	7099	47
H(28A)	4522	3165	7752	46
H(33A)	-391	3386	4825	58
H(33B)	115	3817	5255	58
H(34A)	-1738	3731	5133	53
H(34B)	-1475	3291	5596	53
H(35A)	-1520	4401	5555	67
H(35B)	-281	4389	5913	67
H(36A)	-1467	4878	6391	66
H(36B)	-1679	4426	6751	66
H(37A)	817	4205	7077	67
H(37B)	-120	4029	7378	67
H(38A)	1537	4123	8207	59
H(38B)	1393	4653	8087	59
H(39A)	949	4702	9386	69
H(39B)	1588	4256	9307	69
H(40A)	512	4166	10071	65
H(40B)	-500	4251	9449	65
H(43A)	879	3321	7859	37
H(44A)	-710	3231	7041	40
H(45A)	-1383	2525	6703	38
H(48A)	1148	1541	7966	38
H(49A)	2741	1628	8779	39
H(50A)	3406	2339	9130	36
H(51A)	-1352	1844	6183	48
H(51B)	-2018	1775	6733	48
H(52A)	-1338	1009	6883	54
H(52B)	-2143	1100	6152	54
H(53A)	-1298	498	5785	63
H(53B)	-414	460	6494	63
H(54A)	157	171	5556	72
H(54B)	55	665	5236	72
H(55A)	1734	236	5381	86
H(55B)	2649	400	6018	86
H(56A)	2449	1131	5578	83
H(56B)	2811	783	5086	83

H(57A)	903	1227	3816	69
H(57B)	2145	1163	4095	69
H(58A)	1581	1927	3962	59
H(58B)	1053	1854	4580	59
H(61A)	4221	1612	5683	41
H(62A)	5836	1683	6464	47
H(63A)	6528	2389	6837	53
H(66A)	3997	3392	5648	47
H(67A)	2386	3320	4852	51
H(68A)	1706	2609	4466	53
H(69A)	6488	3090	7416	55
H(69B)	7176	3056	6874	55
H(70A)	7574	3721	7382	44
H(70B)	6808	3829	6644	44
H(71A)	6897	4459	7620	51
H(71B)	5978	4474	6925	51
H(72A)	5422	4842	7596	51
H(72B)	5896	4512	8215	51
H(69C)	7178	3124	6551	74
H(69D)	6861	3187	7256	74
H(70C)	7515	3887	6965	70
H(70D)	6727	3872	6225	70
H(71C)	7017	4319	7669	95
H(71D)	6461	3860	7760	95
H(72C)	5528	4393	8484	95
H(72D)	5457	4809	7961	95
H(73A)	3114	4466	7702	74
H(73B)	3956	4843	8027	74
H(74A)	4629	4383	8979	55
H(74B)	3403	4487	8881	55
H(75A)	3149	3806	9448	45
H(75B)	4390	3718	9596	45
H(76A)	4045	3040	8980	40
H(76B)	3537	3036	9616	40

Table 6. Torsion angles [°] for **13**.

C(2)-N(1)-C(1)-O(1)	178.6(4)
C(40)-N(1)-C(1)-O(1)	-8.5(6)
C(2)-N(1)-C(1)-C(10)	-1.1(4)
C(40)-N(1)-C(1)-C(10)	171.8(3)
C(1)-N(1)-C(2)-O(2)	-179.7(4)
C(40)-N(1)-C(2)-O(2)	7.7(7)
C(1)-N(1)-C(2)-C(3)	0.6(4)
C(40)-N(1)-C(2)-C(3)	-172.1(4)
O(2)-C(2)-C(3)-C(4)	-3.4(7)
N(1)-C(2)-C(3)-C(4)	176.3(4)
O(2)-C(2)-C(3)-C(10)	-179.6(4)
N(1)-C(2)-C(3)-C(10)	0.2(4)
C(10)-C(3)-C(4)-C(5)	-0.4(6)
C(2)-C(3)-C(4)-C(5)	-176.1(4)
C(3)-C(4)-C(5)-C(8)	1.2(6)
C(3)-C(4)-C(5)-C(6)	177.9(4)
C(7)-N(2)-C(6)-O(4)	-177.7(4)
C(11)-N(2)-C(6)-O(4)	-3.1(6)
C(7)-N(2)-C(6)-C(5)	1.5(4)
C(11)-N(2)-C(6)-C(5)	176.1(3)
C(4)-C(5)-C(6)-O(4)	2.1(7)
C(8)-C(5)-C(6)-O(4)	179.1(4)
C(4)-C(5)-C(6)-N(2)	-177.1(4)
C(8)-C(5)-C(6)-N(2)	-0.1(4)
C(6)-N(2)-C(7)-O(3)	175.8(4)
C(11)-N(2)-C(7)-O(3)	1.2(6)
C(6)-N(2)-C(7)-C(8)	-2.3(4)
C(11)-N(2)-C(7)-C(8)	-176.9(3)
C(4)-C(5)-C(8)-C(9)	-1.8(6)
C(6)-C(5)-C(8)-C(9)	-179.0(3)
C(4)-C(5)-C(8)-C(7)	175.9(4)
C(6)-C(5)-C(8)-C(7)	-1.3(4)
O(3)-C(7)-C(8)-C(9)	1.7(7)
N(2)-C(7)-C(8)-C(9)	179.7(4)
O(3)-C(7)-C(8)-C(5)	-175.8(4)

N(2)-C(7)-C(8)-C(5)	2.2(4)
C(5)-C(8)-C(9)-C(10)	1.3(5)
C(7)-C(8)-C(9)-C(10)	-175.9(4)
C(8)-C(9)-C(10)-C(3)	-0.5(5)
C(8)-C(9)-C(10)-C(1)	176.3(4)
C(4)-C(3)-C(10)-C(9)	0.0(6)
C(2)-C(3)-C(10)-C(9)	176.6(3)
C(4)-C(3)-C(10)-C(1)	-177.4(3)
C(2)-C(3)-C(10)-C(1)	-0.8(4)
O(1)-C(1)-C(10)-C(9)	4.3(7)
N(1)-C(1)-C(10)-C(9)	-176.0(4)
O(1)-C(1)-C(10)-C(3)	-178.6(4)
N(1)-C(1)-C(10)-C(3)	1.2(4)
C(6)-N(2)-C(11)-C(12)	81.9(5)
C(7)-N(2)-C(11)-C(12)	-104.2(5)
C(13)-O(9)-C(12)-C(11)	179.5(4)
N(2)-C(11)-C(12)-O(9)	65.8(5)
C(12)-O(9)-C(13)-C(14)	177.0(4)
C(15)-O(10)-C(14)-C(13)	154.7(4)
O(9)-C(13)-C(14)-O(10)	51.7(6)
C(14)-O(10)-C(15)-C(16)	48.1(6)
C(17)-O(11)-C(16)-C(15)	157.2(4)
O(10)-C(15)-C(16)-O(11)	57.2(6)
C(16)-O(11)-C(17)-C(18)	68.5(5)
C(30)-N(3)-C(18)-C(17)	84.8(5)
C(19)-N(3)-C(18)-C(17)	-100.3(5)
O(11)-C(17)-C(18)-N(3)	64.6(6)
C(30)-N(3)-C(19)-O(5)	177.2(4)
C(18)-N(3)-C(19)-O(5)	2.7(5)
C(30)-N(3)-C(19)-C(20)	-1.0(5)
C(18)-N(3)-C(19)-C(20)	-175.5(3)
O(5)-C(19)-C(20)-C(21)	5.3(6)
N(3)-C(19)-C(20)-C(21)	-176.5(3)
O(5)-C(19)-C(20)-C(31)	-171.9(4)
N(3)-C(19)-C(20)-C(31)	6.3(5)
C(31)-C(20)-C(21)-C(22)	4.0(6)
C(19)-C(20)-C(21)-C(22)	-173.2(4)

C(20)-C(21)-C(22)-C(23)	-0.8(6)
C(21)-C(22)-C(23)-C(32)	-2.2(6)
C(21)-C(22)-C(23)-C(24)	176.4(3)
C(25)-N(4)-C(24)-O(8)	177.9(4)
C(33)-N(4)-C(24)-O(8)	-3.7(6)
C(25)-N(4)-C(24)-C(23)	-2.3(6)
C(33)-N(4)-C(24)-C(23)	176.1(3)
C(22)-C(23)-C(24)-O(8)	0.7(6)
C(32)-C(23)-C(24)-O(8)	179.3(4)
C(22)-C(23)-C(24)-N(4)	-179.1(4)
C(32)-C(23)-C(24)-N(4)	-0.5(5)
C(24)-N(4)-C(25)-O(7)	-178.7(4)
C(33)-N(4)-C(25)-O(7)	3.0(6)
C(24)-N(4)-C(25)-C(26)	2.6(6)
C(33)-N(4)-C(25)-C(26)	-175.8(3)
O(7)-C(25)-C(26)-C(27)	-1.7(6)
N(4)-C(25)-C(26)-C(27)	177.1(3)
O(7)-C(25)-C(26)-C(32)	-178.8(4)
N(4)-C(25)-C(26)-C(32)	-0.1(5)
C(32)-C(26)-C(27)-C(28)	-0.3(6)
C(25)-C(26)-C(27)-C(28)	-177.5(3)
C(26)-C(27)-C(28)-C(29)	1.3(6)
C(27)-C(28)-C(29)-C(31)	-1.7(6)
C(27)-C(28)-C(29)-C(30)	178.9(3)
C(19)-N(3)-C(30)-O(6)	177.4(4)
C(18)-N(3)-C(30)-O(6)	-8.1(6)
C(19)-N(3)-C(30)-C(29)	-5.2(5)
C(18)-N(3)-C(30)-C(29)	169.3(3)
C(28)-C(29)-C(30)-O(6)	3.1(6)
C(31)-C(29)-C(30)-O(6)	-176.4(4)
C(28)-C(29)-C(30)-N(3)	-174.3(4)
C(31)-C(29)-C(30)-N(3)	6.3(5)
C(21)-C(20)-C(31)-C(29)	177.7(3)
C(19)-C(20)-C(31)-C(29)	-5.1(6)
C(21)-C(20)-C(31)-C(32)	-4.1(6)
C(19)-C(20)-C(31)-C(32)	173.1(3)
C(28)-C(29)-C(31)-C(20)	179.3(4)

C(30)-C(29)-C(31)-C(20)	-1.3(6)
C(28)-C(29)-C(31)-C(32)	1.0(6)
C(30)-C(29)-C(31)-C(32)	-179.5(3)
C(27)-C(26)-C(32)-C(23)	-179.7(3)
C(25)-C(26)-C(32)-C(23)	-2.6(6)
C(27)-C(26)-C(32)-C(31)	-0.3(6)
C(25)-C(26)-C(32)-C(31)	176.9(3)
C(22)-C(23)-C(32)-C(26)	-178.6(4)
C(24)-C(23)-C(32)-C(26)	2.9(6)
C(22)-C(23)-C(32)-C(31)	2.0(6)
C(24)-C(23)-C(32)-C(31)	-176.5(3)
C(20)-C(31)-C(32)-C(26)	-178.3(3)
C(29)-C(31)-C(32)-C(26)	0.0(5)
C(20)-C(31)-C(32)-C(23)	1.1(5)
C(29)-C(31)-C(32)-C(23)	179.4(3)
C(24)-N(4)-C(33)-C(34)	78.2(5)
C(25)-N(4)-C(33)-C(34)	-103.3(5)
C(35)-O(12)-C(34)-C(33)	77.7(5)
N(4)-C(33)-C(34)-O(12)	69.9(6)
C(34)-O(12)-C(35)-C(36)	162.5(4)
C(37)-O(13)-C(36)-C(35)	-51.9(6)
O(12)-C(35)-C(36)-O(13)	86.9(5)
C(36)-O(13)-C(37)-C(38)	-158.3(4)
C(39)-O(14)-C(38)-C(37)	170.9(5)
O(13)-C(37)-C(38)-O(14)	72.0(6)
C(38)-O(14)-C(39)-C(40)	-144.5(4)
C(1)-N(1)-C(40)-C(39)	85.5(6)
C(2)-N(1)-C(40)-C(39)	-102.5(5)
O(14)-C(39)-C(40)-N(1)	66.3(6)
C(76)-O(15)-C(41)-C(50)	6.1(5)
C(76)-O(15)-C(41)-C(42)	-173.1(3)
O(15)-C(41)-C(42)-C(47)	-178.3(3)
C(50)-C(41)-C(42)-C(47)	2.5(5)
O(15)-C(41)-C(42)-C(43)	0.9(5)
C(50)-C(41)-C(42)-C(43)	-178.3(3)
C(47)-C(42)-C(43)-C(44)	0.4(5)
C(41)-C(42)-C(43)-C(44)	-178.8(3)

C(42)-C(43)-C(44)-C(45)	0.2(6)
C(43)-C(44)-C(45)-C(46)	-1.4(6)
C(51)-O(16)-C(46)-C(45)	5.0(5)
C(51)-O(16)-C(46)-C(47)	-175.7(3)
C(44)-C(45)-C(46)-O(16)	-178.8(3)
C(44)-C(45)-C(46)-C(47)	1.9(6)
C(43)-C(42)-C(47)-C(48)	179.6(3)
C(41)-C(42)-C(47)-C(48)	-1.2(5)
C(43)-C(42)-C(47)-C(46)	0.2(5)
C(41)-C(42)-C(47)-C(46)	179.3(3)
O(16)-C(46)-C(47)-C(42)	179.4(3)
C(45)-C(46)-C(47)-C(42)	-1.3(5)
O(16)-C(46)-C(47)-C(48)	-0.1(5)
C(45)-C(46)-C(47)-C(48)	179.3(4)
C(42)-C(47)-C(48)-C(49)	-0.1(5)
C(46)-C(47)-C(48)-C(49)	179.3(3)
C(47)-C(48)-C(49)-C(50)	0.3(6)
O(15)-C(41)-C(50)-C(49)	178.4(3)
C(42)-C(41)-C(50)-C(49)	-2.5(5)
C(48)-C(49)-C(50)-C(41)	1.0(6)
C(46)-O(16)-C(51)-C(52)	172.3(3)
C(53)-O(17)-C(52)-C(51)	174.6(4)
O(16)-C(51)-C(52)-O(17)	-71.5(4)
C(52)-O(17)-C(53)-C(54)	176.8(4)
C(55)-O(18)-C(54)-C(53)	-178.5(4)
O(17)-C(53)-C(54)-O(18)	66.9(6)
C(54)-O(18)-C(55)-C(56)	90.2(6)
C(57)-O(19)-C(56)-C(55)	-165.8(5)
O(18)-C(55)-C(56)-O(19)	-65.1(7)
C(56)-O(19)-C(57)-C(58)	-78.9(6)
C(59)-O(20)-C(58)-C(57)	176.7(4)
O(19)-C(57)-C(58)-O(20)	71.3(5)
C(58)-O(20)-C(59)-C(68)	-4.1(6)
C(58)-O(20)-C(59)-C(60)	177.3(3)
O(20)-C(59)-C(60)-C(65)	177.7(3)
C(68)-C(59)-C(60)-C(65)	-0.9(5)
O(20)-C(59)-C(60)-C(61)	-1.5(5)

C(68)-C(59)-C(60)-C(61)	179.9(4)
C(65)-C(60)-C(61)-C(62)	-0.8(5)
C(59)-C(60)-C(61)-C(62)	178.4(3)
C(60)-C(61)-C(62)-C(63)	0.6(6)
C(61)-C(62)-C(63)-C(64)	-0.2(6)
C(62)-C(63)-C(64)-O(21)	179.7(4)
C(62)-C(63)-C(64)-C(65)	0.0(6)
C(61)-C(60)-C(65)-C(66)	-180.0(3)
C(59)-C(60)-C(65)-C(66)	0.8(5)
C(61)-C(60)-C(65)-C(64)	0.6(5)
C(59)-C(60)-C(65)-C(64)	-178.6(3)
O(21)-C(64)-C(65)-C(60)	-179.9(3)
C(63)-C(64)-C(65)-C(60)	-0.2(6)
O(21)-C(64)-C(65)-C(66)	0.7(5)
C(63)-C(64)-C(65)-C(66)	-179.6(4)
C(60)-C(65)-C(66)-C(67)	0.0(6)
C(64)-C(65)-C(66)-C(67)	179.4(4)
C(65)-C(66)-C(67)-C(68)	-0.6(6)
O(20)-C(59)-C(68)-C(67)	-178.1(4)
C(60)-C(59)-C(68)-C(67)	0.3(6)
C(66)-C(67)-C(68)-C(59)	0.5(6)
C(63)-C(64)-O(21)-C(69')	16.7(10)
C(65)-C(64)-O(21)-C(69')	-163.6(9)
C(63)-C(64)-O(21)-C(69)	-5.9(7)
C(65)-C(64)-O(21)-C(69)	173.8(6)
C(64)-O(21)-C(69)-C(70)	176.5(6)
C(69')-O(21)-C(69)-C(70)	64(3)
O(21)-C(69)-C(70)-O(22)	72.5(10)
C(69)-C(70)-O(22)-C(71)	-168.8(9)
C(70)-O(22)-C(71)-C(72)	-176.0(8)
O(22)-C(71)-C(72)-O(23)	-40.2(13)
C(64)-O(21)-C(69')-C(70')	165.5(8)
C(69)-O(21)-C(69')-C(70')	-116(4)
O(21)-C(69')-C(70')-O(22')	53.7(19)
C(69')-C(70')-O(22')-C(71')	79(2)
C(70')-O(22')-C(71')-C(72')	-170.6(15)
O(22')-C(71')-C(72')-O(23)	38(3)

C(71')-C(72')-O(23)-C(72)	-48(2)
C(71')-C(72')-O(23)-C(73)	174.3(9)
C(71)-C(72)-O(23)-C(72')	132(3)
C(71)-C(72)-O(23)-C(73)	-178.8(8)
C(72')-O(23)-C(73)-C(74)	-68.2(12)
C(72)-O(23)-C(73)-C(74)	-89.4(8)
C(75)-O(24)-C(74)-C(73)	-177.3(4)
O(23)-C(73)-C(74)-O(24)	-61.1(6)
C(74)-O(24)-C(75)-C(76)	-178.0(4)
C(41)-O(15)-C(76)-C(75)	176.1(3)
O(24)-C(75)-C(76)-O(15)	-62.1(4)