Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary Information for

Capsule Voided Nanospace Confinement in a π-Stacked Supramolecular Organic Solid

Abhijeet K. Chaudhari, Amitosh Sharma, Soumya Mukherjee, Biplab Joarder and Sujit K. Ghosh*

Indian Institute of Science Education and Research (IISER), Dr. Homi Bhabha Road, Pashan, Pune-411008, India
Tel: +91-20-2590 8076; Fax: +91-20-2590 8186; E-mail: sghosh@iiserpune.ac.in

Homepage: http://www.iiserpune.ac.in/~sghosh/

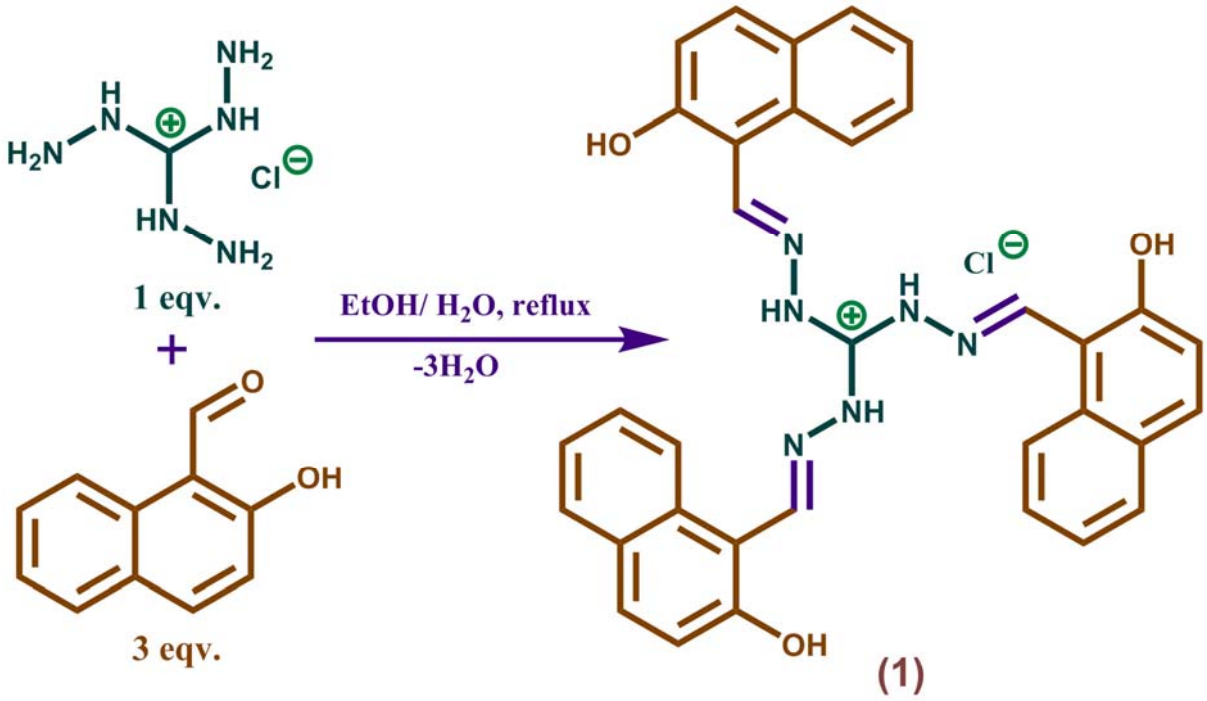
Table of Contents

General Methods.

All chemicals and solvents were commercially available and used without further purification. TGA was performed using a Perkin Elmer STA 6000 simultaneous thermal analyser; all sample were heated from 30 ^{0}C to 500 ^{0}C at the rate of 10 ^{0}C min^{-1}. The powder X-ray diffraction (PXRD) patterns were measured using a Bruker D8 Advance in the range of 5 to 40 of 2θ value with the scan rate 0.5 deg/min. Solid state UV measurements recorded using Perkin Elmer Lambda 950 UV/Vis spectrometer. Solid state luminescence measured using HORIBA JOBIN YVON Fluorolog-3 spectrofluorometer. FT-IR were measured in Nicolet 6700 FT-IR using solid sample containing KBR pellets. All samples were exposed to air before and during XRD data collection. PXRD and TGA were used to identify the phase transitions and the stabilities of the product respectively in solid state.

Experimental Section:

Detailed synthesis of tris (2-hydroxynapthalidene) triaminoguanidinium chloride (1):-



Scheme S1: Ligand Synthesis protocol

Triaminoguanidinium chloride (2g, 0.019mol) was dissolved in a hot mixture of ethanol (30mL) and water (15mL). After adjusting the pH to the value of 3 with HCl(aq), the solution of 2-hydroxynapthaldehyde (10.4g, 0.060mol) in methanol (10mL) was added slowly. The solubility of 2-hydroxynapthaldehyde in methanol was a problem, therefore addition of 2-hydroxynapthaldehyde was done at high temperature and its solution in methanol was directly added from high temperature. The resulting solution was heated under reflux at 90°C for 6 hours having nitrogen

atmosphere. The suspension formed, was then allowed to cool to room temperature. The reaction mixture then kept for overnight stirring and the crude product was then washed with aqueous methanol solution, collected, and dried under reduced pressure to give pure product **1**.

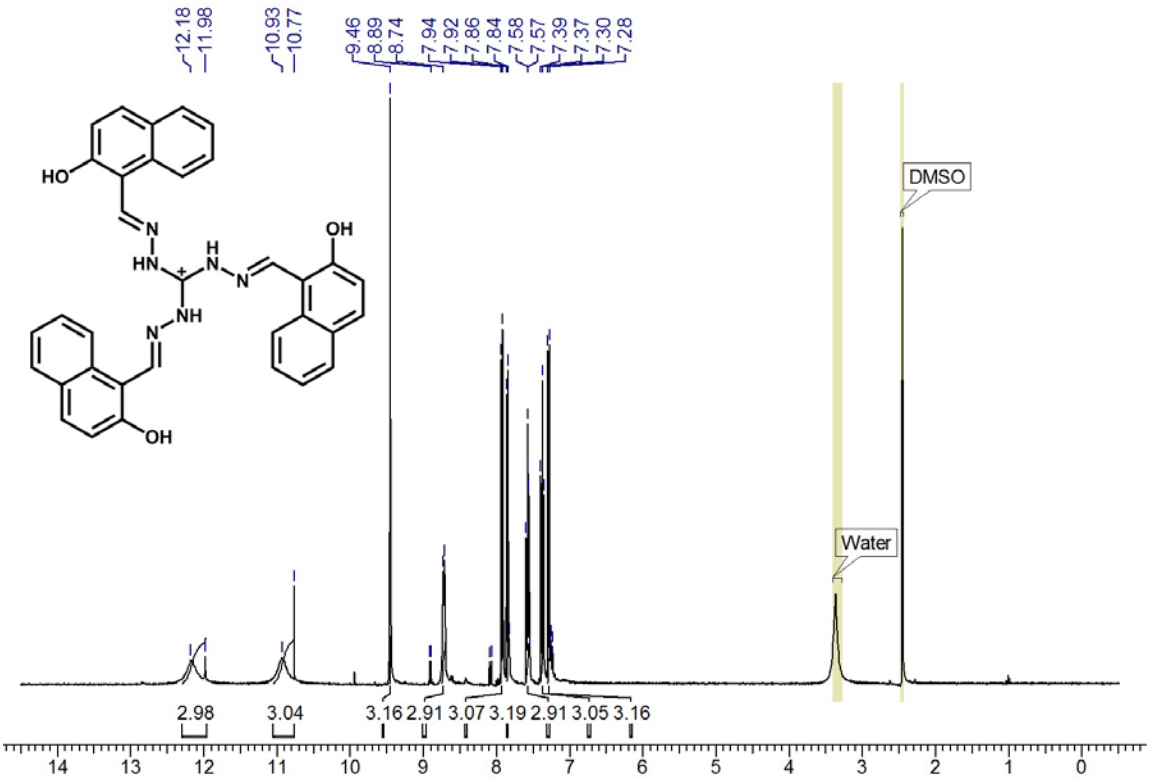


Figure S1: ^{1}H NMR spectrum for as-synthesized 1.

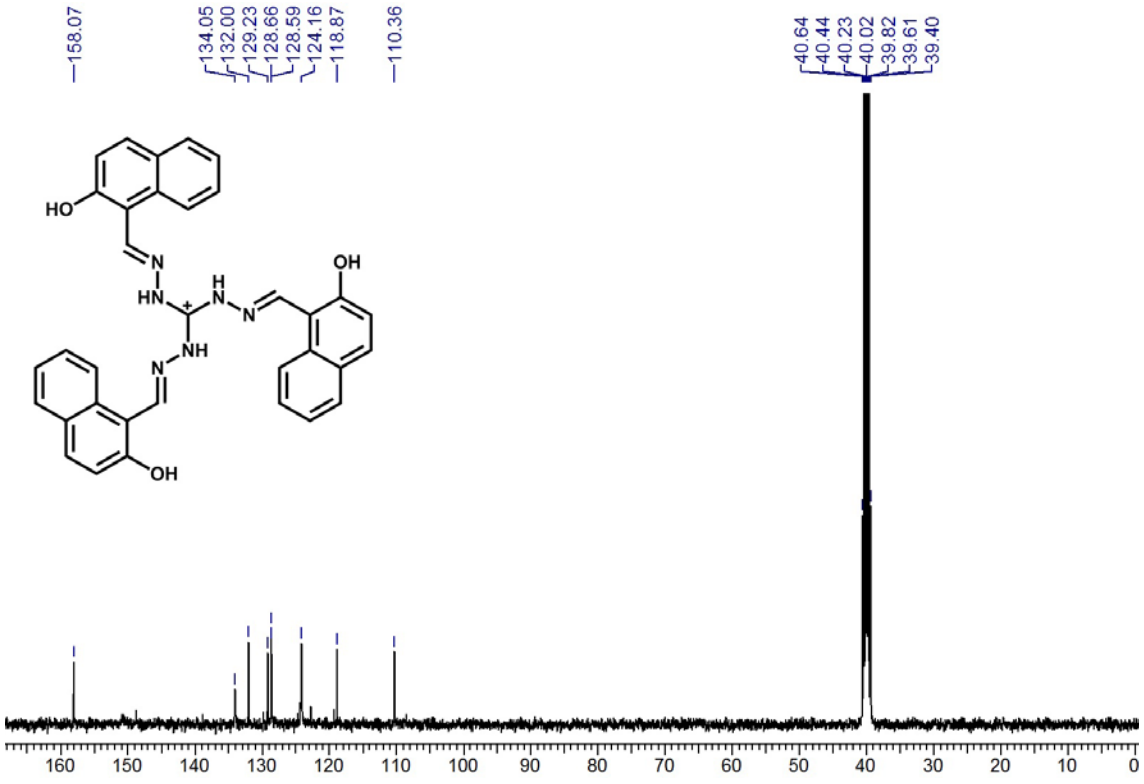


Figure S2: ^{13}C NMR spectrum for as synthesized 1.

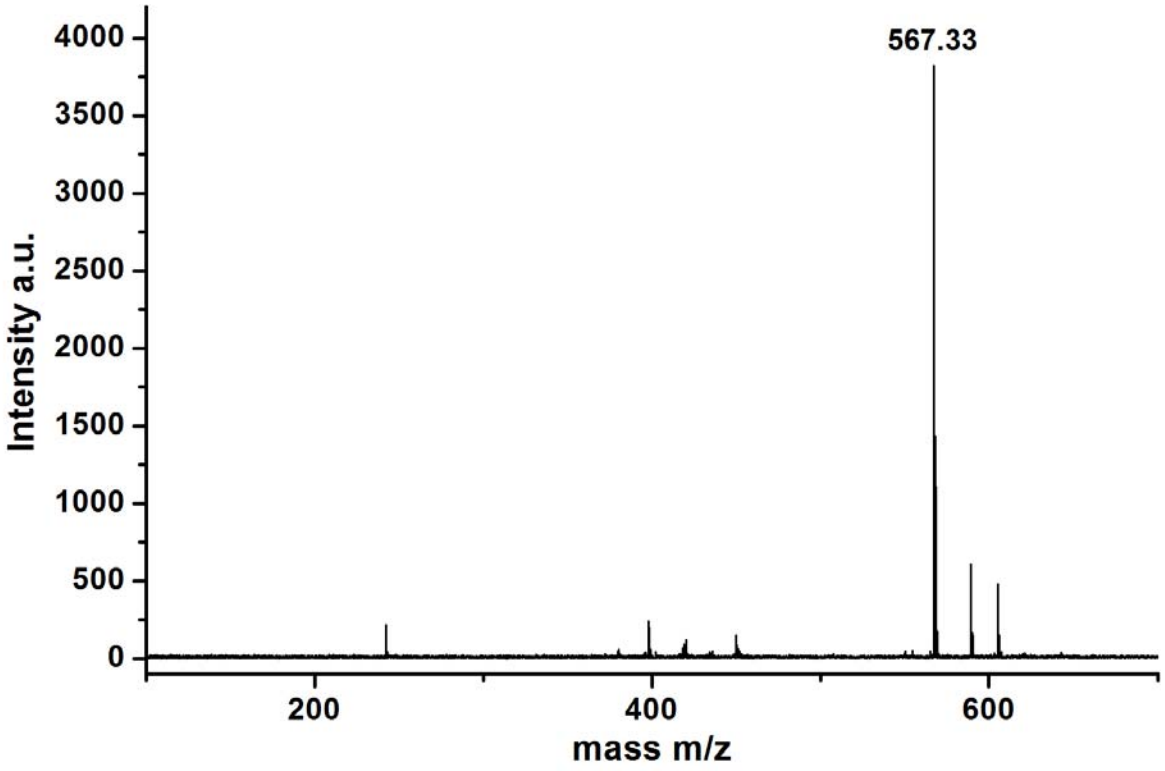


Figure S3: MALDI-TOF Mass spectrum for as-synthesized 1.

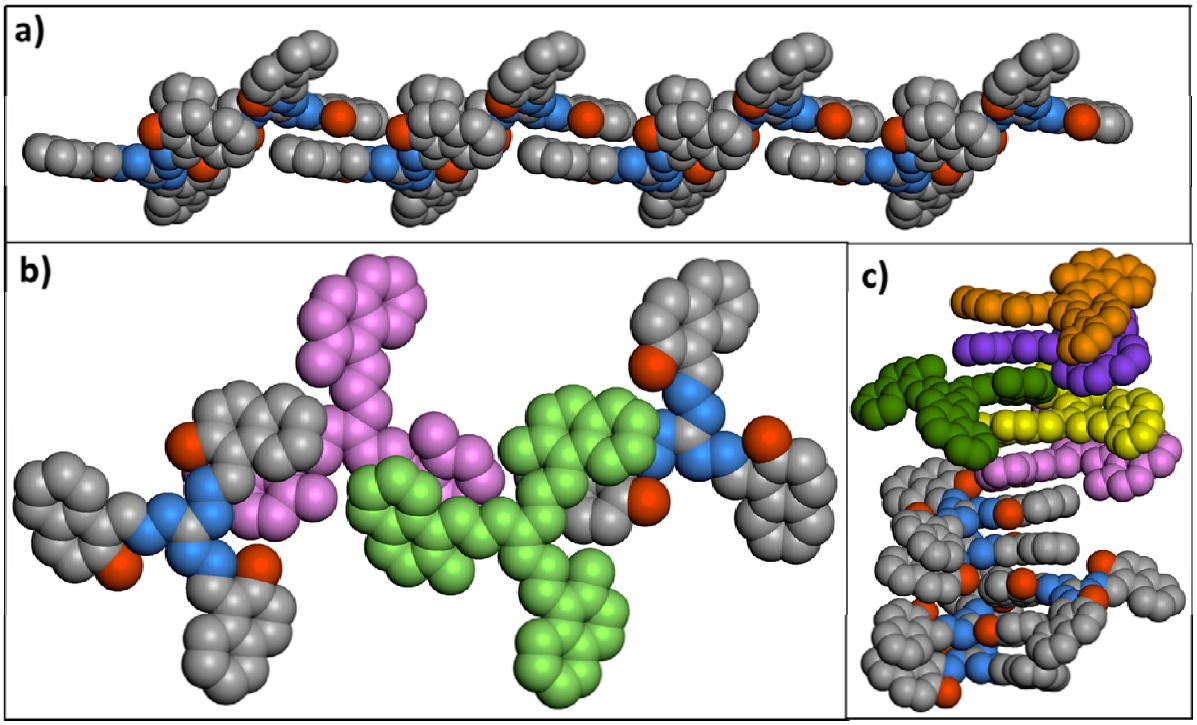


Figure S4: π-stacking in the molecular architecture along different directions in extended assembly.

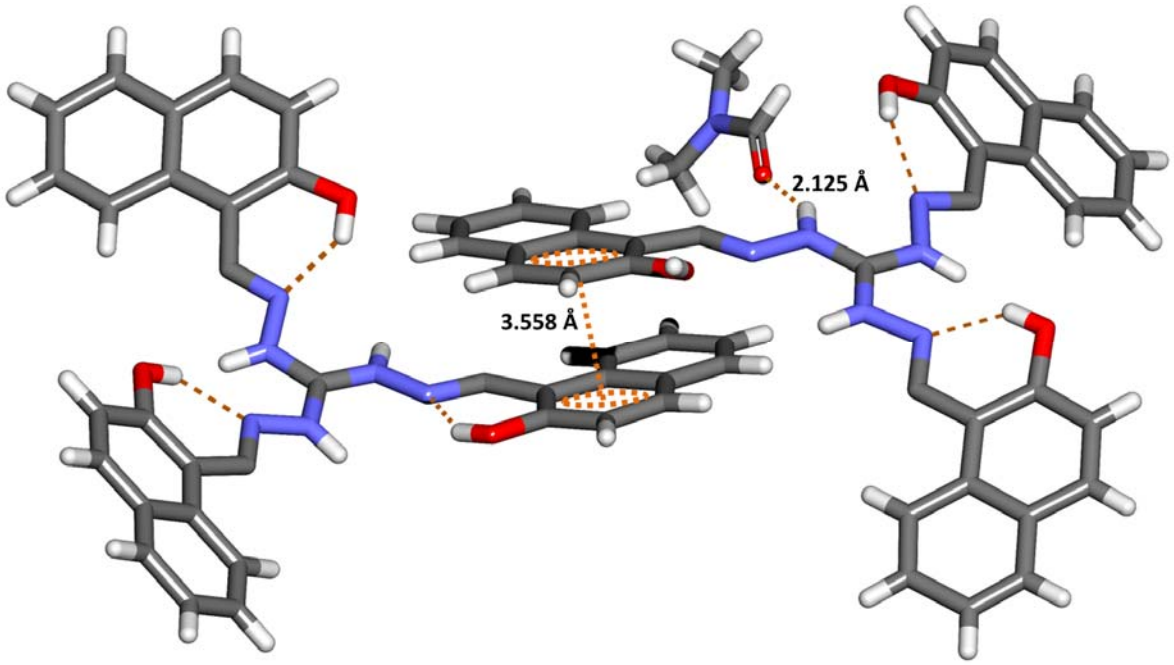


Figure S5: Hydrogen bonding present between the DMF molecule and the host molecule and pi-pi interaction between two hosts.

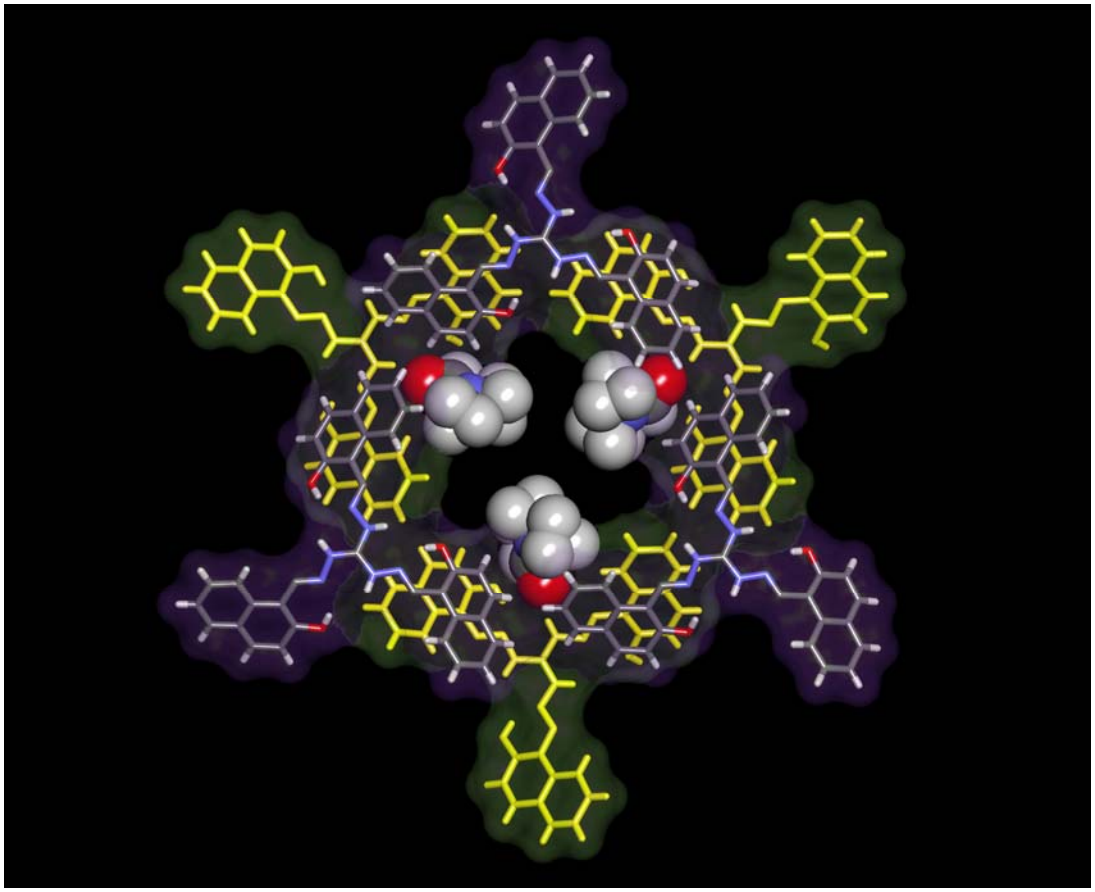


Figure S6: Arrangement of hydrogen bonded guest molecules inside the bilayered host molecules shown in two different surface colors.

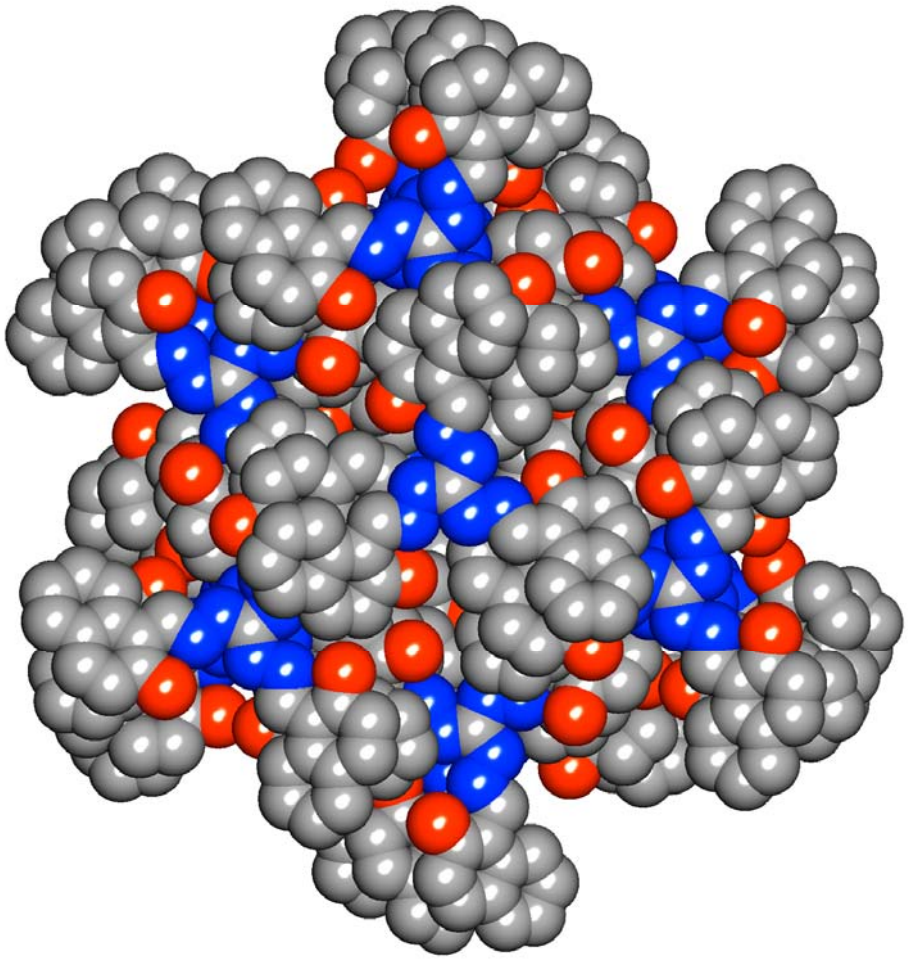


Figure S7: A single multi-molecular capsule showing along c-axis in space fill model, color code: grey: carbon, red: oxygen, blue: nitrogen; hydrogen atoms are omitted for clarity.

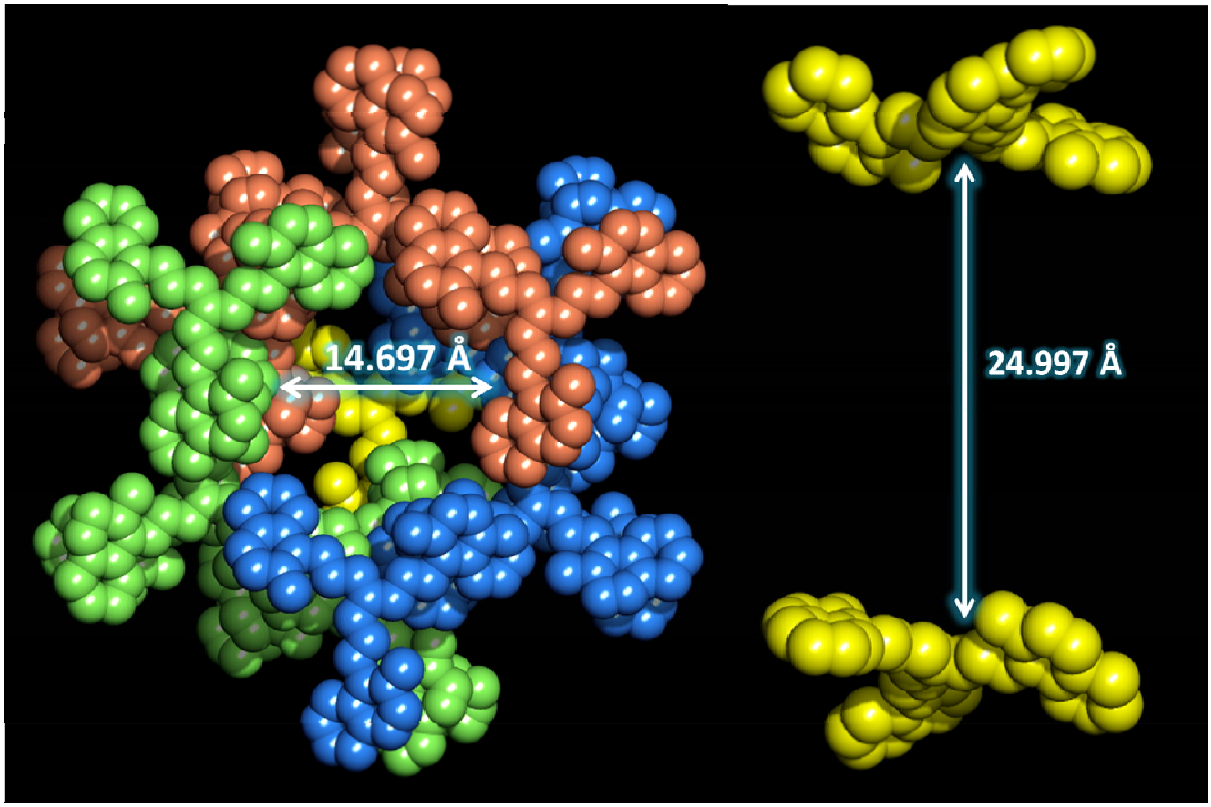


Figure S8: Cross section of a molecular capsule showing its dimensions: left: diameter; right: distance between two caps of the void.

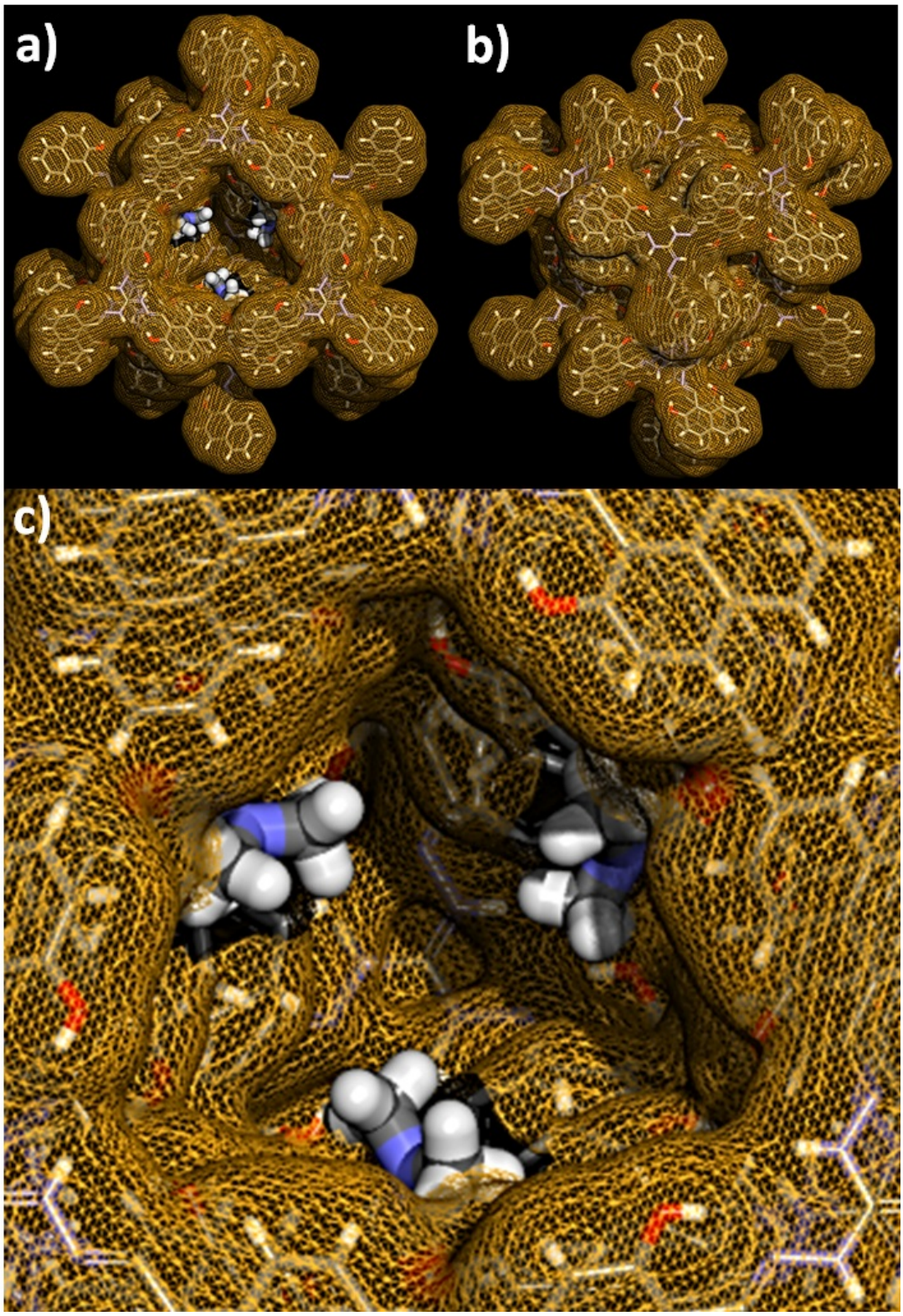


Figure S9: Cross section of a molecular capsule with molecular mesh surface showing encapsulated solvent molecules inside it, a) front view b) back view c) enlarged view.

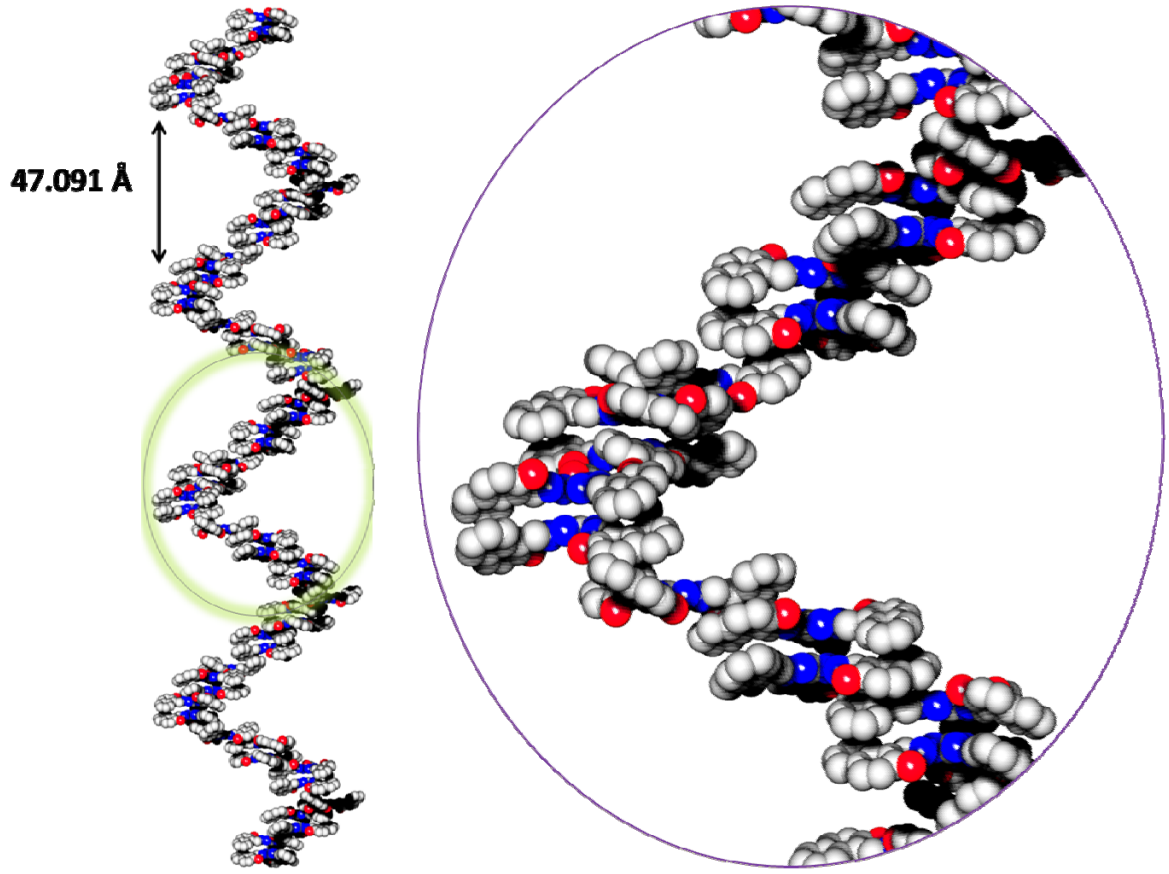


Figure S10: A single helix and its enlarged view assembled by molecular pi-pi interaction with pitch height of 47.091Å, color code: grey: carbon, red: oxygen, blue: nitrogen; hydrogen atoms are omitted for clarity.

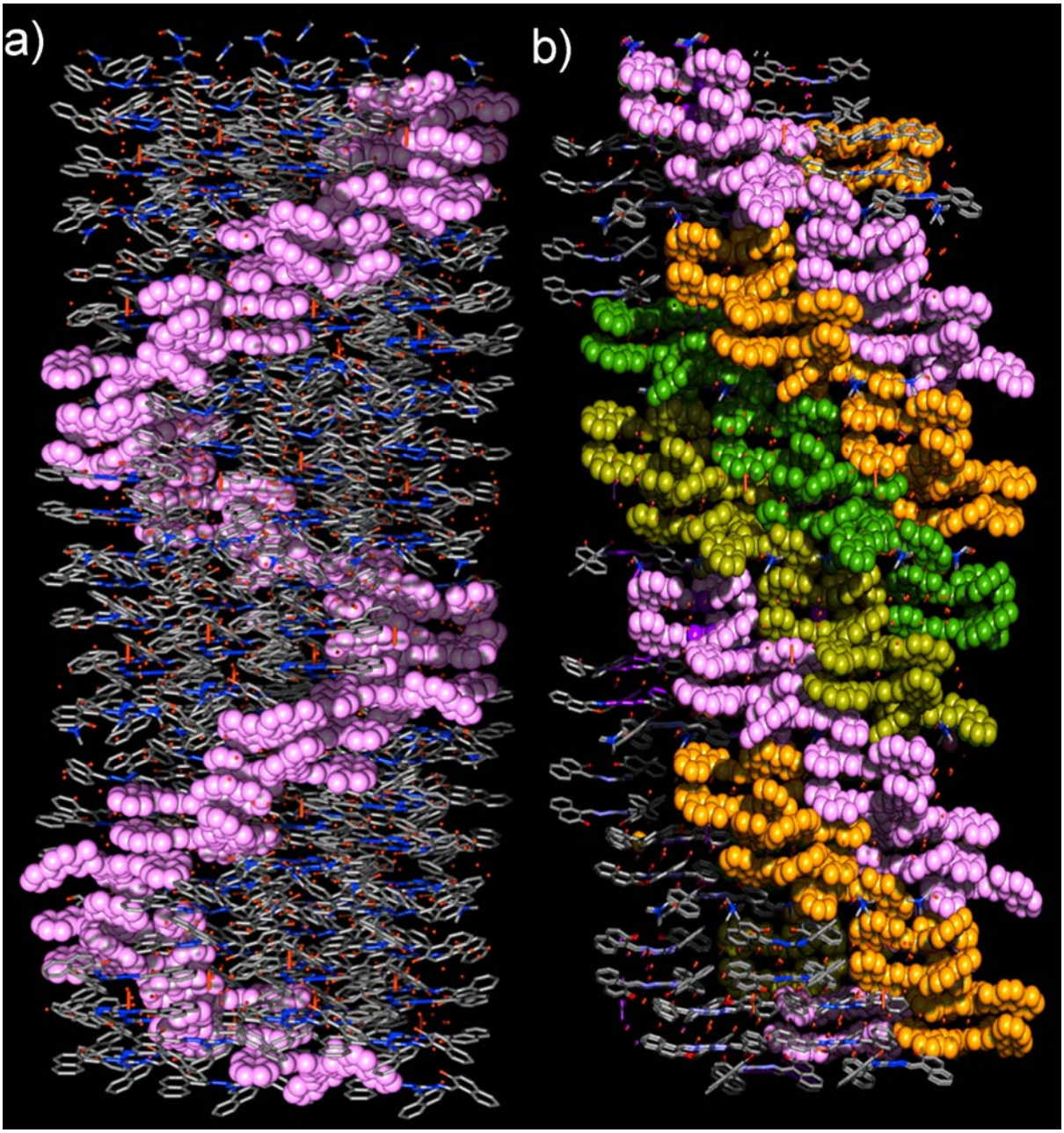


Figure S11: a) The progression of a single helix brought together by molecular pi-pi interactions, b) the simultaneous progression of four strands of similar helices; hydrogen atoms are omitted for clarity.

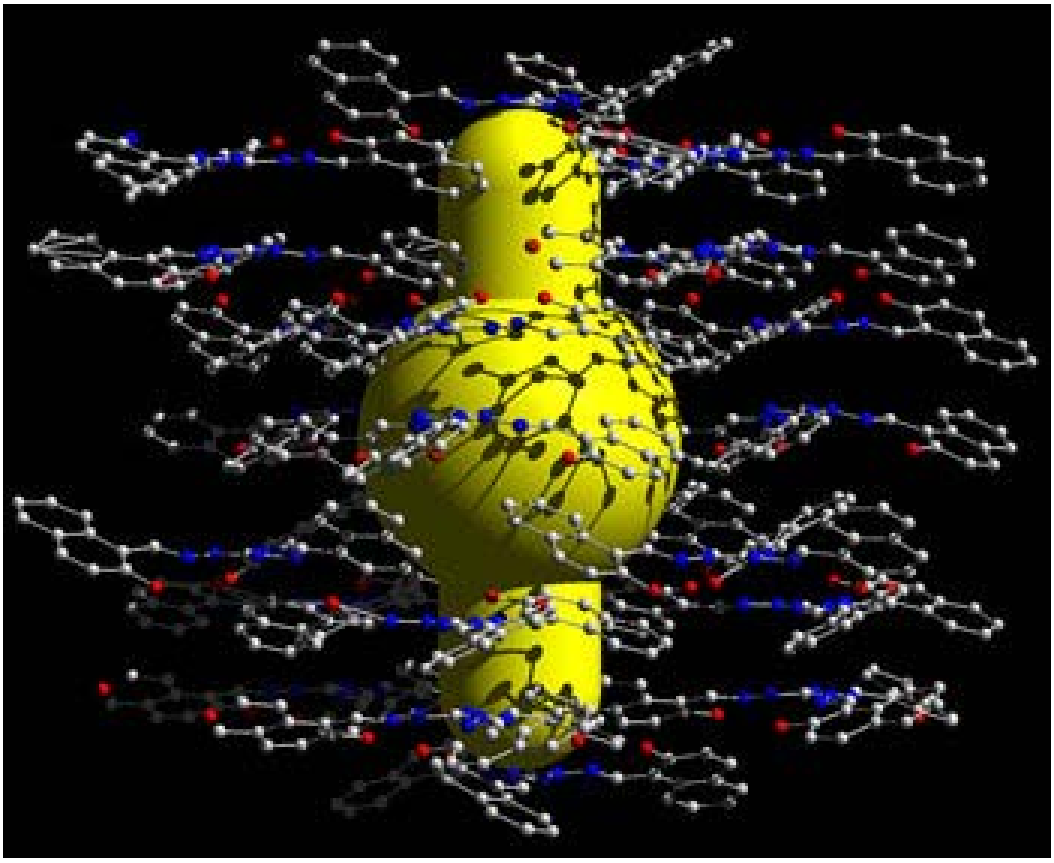


Figure S12: a) The capsule void created in the nanospace confinement of the π-Stacked Supramolecular arrangement for compound 1a. Hydrogen atoms are omitted for clarity.

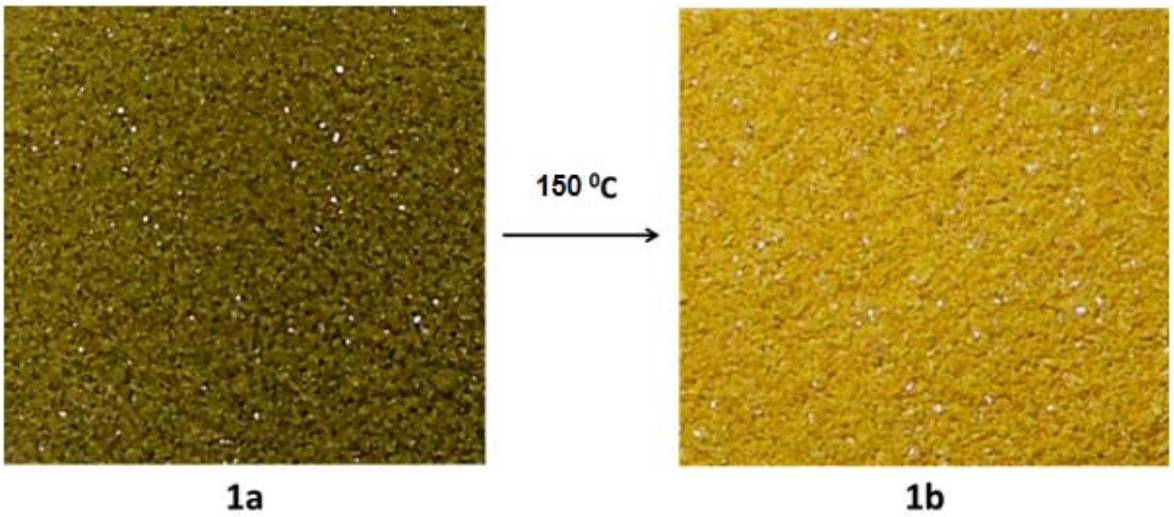


Figure S13: Visual color change from dark yellow to yellow of bulk crystals in transformation of supramolecular assembly from 1a to 1b.

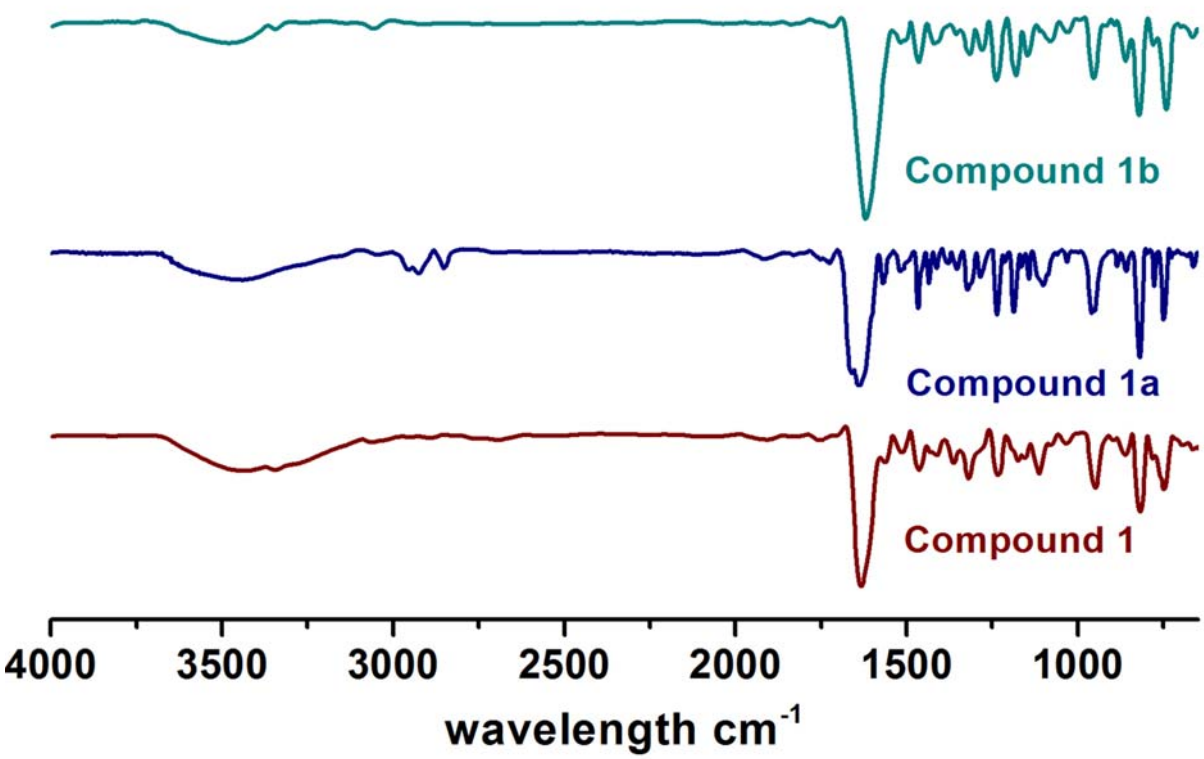


Figure S14: FTIR spectra of three different compounds.

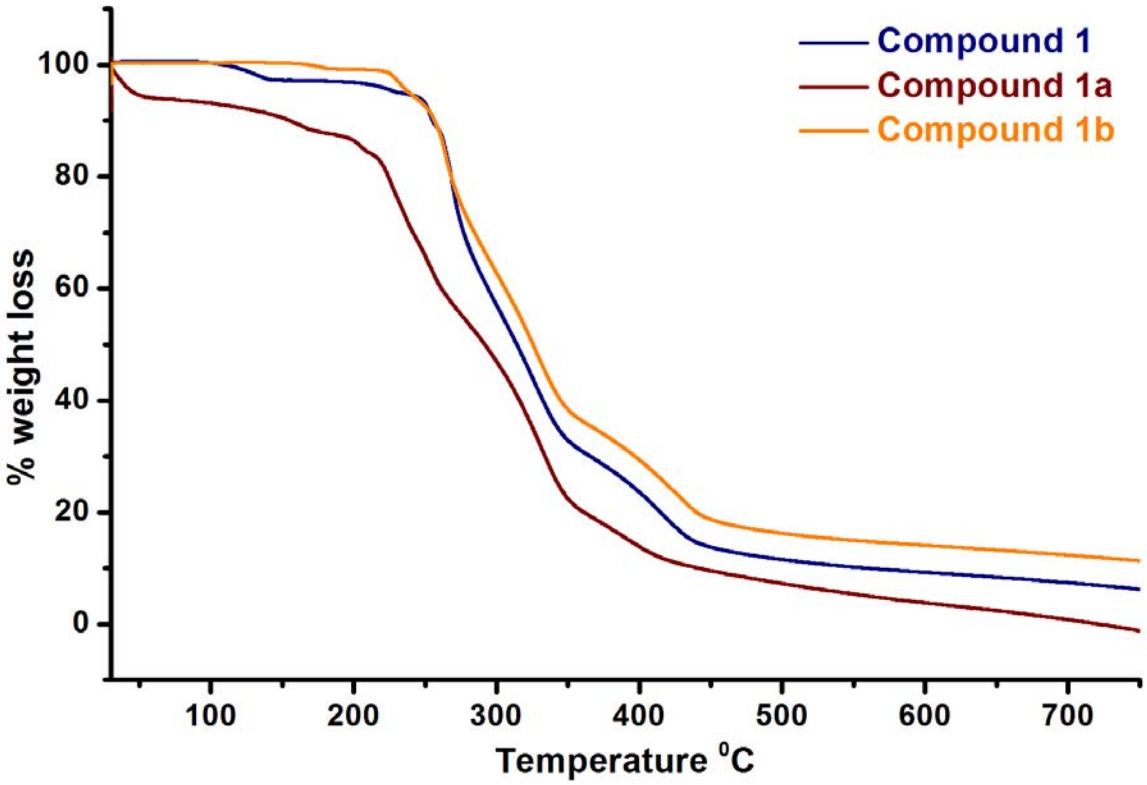


Figure S15: Thermogravimetric analysis plot for three compounds.

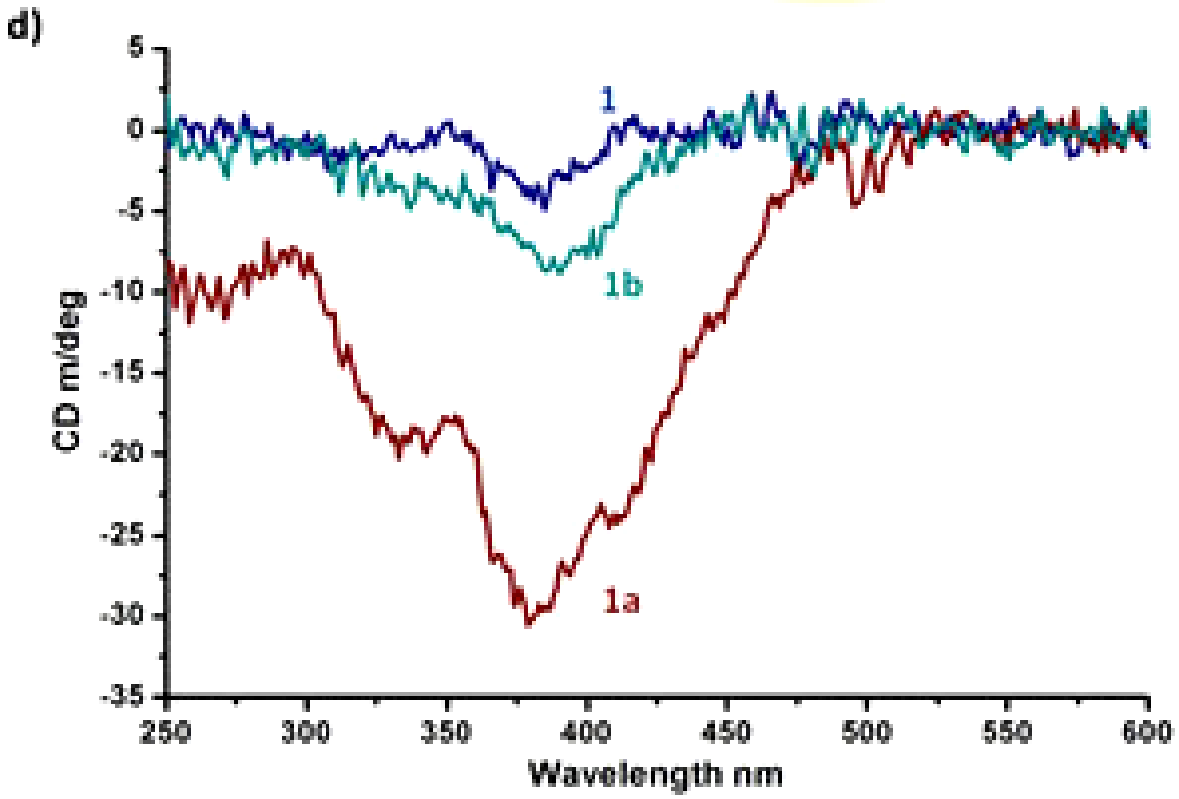


Figure S16: Circular dichroism spectra for three different phases.

Single crystal X-ray diffraction studies and details:

Single crystal data was collected on a Bruker SMART APEX-II Duo diffractometer equipped with a CCD area detector and operated at 1350 W power (45 kV, 30 mA) to generate Mo Kα radiation (λ=0.71073 Å). Crystal of the compound reported in the paper was mounted on nylon CryoLoops (Hampton Research). Structure was solved by direct methods and refined using the *SHELXTL 97* Software suite. Final models was refined anisotropically (if the number of data permitted) until full convergence was achieved. Hydrogen atoms associated with carbon atoms were fixed in geometrically constrained positions. Structure was examined using the *Adsym* subroutine of PLATON to assure that no additional symmetry could be applied to the model. Asymmetric unit of the self-assembly contains complete five molecules with cationic centres which are neutralised by five Cl^- ions, while four water molecules, three DMF molecules and a protonated chloride are encapsulated within the framework as a neutral species. Formula is $[L_5Cl_5]\cdot HCl, 4H_2O, 3DMF$.

Table 1. Crystal data and structure refinement for 1a.

Identification code	**1a**	
Empirical formula	C179 H165 Cl6 N33 O22	
Formula weight	3343.14	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C c	
Unit cell dimensions	a = 31.788(2) Å	α= 90°.
	b = 18.353(2) Å	β= 107.82°.
	c = 34.619(4) Å	γ= 90°.
Volume	19228(4) Å3	
Z	4	
Density (calculated)	1.124 Mg/m3	
Absorption coefficient	0.158 mm-1	
F(000)	6992	
Crystal size	0.20 x 0.16 x 0.14 mm3	
Theta range for data collection	1.30 to 28.76°.	
Index ranges	-36<=h<=42, -24<=k<=24, -46<=l<=39	
Reflections collected	62182	
Independent reflections	35000 [R(int) = 0.0909]	
Completeness to theta = 28.76°	97.50%	
Max. and min. transmission	Semi-empirical from equivalents	
Refinement method	0.9782 and 0.9691	
Data / restraints / parameters	Full-matrix least-squares on F2	
Goodness-of-fit on F2	35000 / 2 / 2107	
Final R indices [I>2sigma(I)]	0.998	
R indices (all data)	R1 = 0.1279, wR2 = 0.3014	
Absolute structure parameter	R1 = 0.2711, wR2 = 0.3864	
Extinction coefficient	0	
Largest diff. peak and hole	0.00144(14)	

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

	x	y	z	U(eq)
C(1)	2578(3)	2514(6)	4243(3)	29(2)
C(2)	1883(4)	3940(6)	4187(3)	33(2)
C(3)	1855(4)	4745(6)	4226(3)	38(3)
C(4)	2224(4)	5145(6)	4411(3)	41(3)
C(5)	2199(4)	5892(7)	4467(3)	53(3)
C(6)	1798(4)	6243(7)	4330(3)	51(3)
C(7)	1406(4)	5840(7)	4128(3)	45(3)
C(8)	994(5)	6226(7)	4010(3)	63(4)
C(9)	612(5)	5820(8)	3832(4)	67(4)
C(10)	634(4)	5098(7)	3773(3)	52(3)
C(11)	1017(4)	4728(7)	3900(3)	39(3)
C(12)	1425(4)	5099(6)	4075(3)	38(3)
C(13)	3612(4)	2796(6)	4190(3)	35(3)
C(14)	4052(4)	2471(6)	4227(3)	37(3)
C(15)	4167(4)	1811(6)	4417(3)	40(3)
C(16)	4590(4)	1526(8)	4472(4)	58(4)
C(17)	4876(4)	1859(7)	4324(3)	45(3)
C(18)	4781(3)	2548(7)	4132(3)	41(3)
C(19)	5106(4)	2927(8)	4003(3)	56(3)
C(20)	5007(4)	3588(9)	3832(4)	62(4)
C(21)	4623(4)	3888(7)	3787(4)	57(4)
C(22)	4296(4)	3565(6)	3900(3)	39(3)
C(23)	4373(3)	2858(6)	4080(3)	34(3)
C(24)	2176(4)	759(6)	4191(3)	35(3)
C(25)	1808(4)	309(6)	4229(3)	35(3)
C(26)	1519(4)	559(6)	4413(3)	40(3)
C(27)	1187(4)	99(6)	4468(3)	48(3)
C(28)	1138(4)	-583(6)	4328(3)	40(3)
C(29)	1436(4)	-861(6)	4130(3)	41(3)
C(30)	1389(5)	-1607(7)	4004(4)	64(4)
C(31)	1692(5)	-1890(8)	3828(4)	60(4)
C(32)	2009(5)	-1484(7)	3774(4)	54(3)

C(33)	2067(4)	-773(6)	3888(3)	44(3)
C(34)	1766(4)	-447(6)	4077(3)	38(3)
C(35)	2256(3)	2517(6)	3284(3)	37(2)
C(36)	3293(4)	2366(6)	3185(3)	41(3)
C(37)	3638(4)	2719(6)	3042(3)	38(3)
C(38)	3559(4)	3399(7)	2871(3)	45(3)
C(39)	3850(4)	3709(7)	2684(3)	50(3)
C(40)	4229(4)	3313(6)	2679(3)	43(3)
C(41)	4311(4)	2654(7)	2851(3)	44(3)
C(42)	4698(4)	2263(9)	2835(4)	61(4)
C(43)	4783(4)	1574(9)	3020(4)	73(4)
C(44)	4496(4)	1290(7)	3204(4)	56(4)
C(45)	4125(4)	1626(7)	3218(3)	46(3)
C(46)	4025(4)	2329(6)	3045(3)	36(3)
C(47)	1625(4)	964(6)	3183(3)	40(3)
C(48)	1558(4)	197(6)	3040(3)	32(2)
C(49)	1848(4)	-123(7)	2871(3)	41(3)
C(50)	1768(4)	-809(6)	2679(3)	49(3)
C(51)	1381(4)	-1162(6)	2677(3)	44(3)
C(52)	1088(4)	-875(6)	2847(3)	41(3)
C(53)	697(4)	-1242(7)	2838(3)	56(4)
C(54)	405(4)	-958(8)	3016(4)	69(4)
C(55)	483(4)	-279(8)	3201(4)	64(4)
C(56)	851(4)	106(7)	3214(3)	54(4)
C(57)	1169(4)	-180(6)	3038(3)	34(3)
C(58)	1758(4)	4185(7)	3179(3)	43(3)
C(59)	1347(3)	4579(6)	3039(3)	31(2)
C(60)	949(4)	4217(6)	2873(3)	49(3)
C(61)	553(4)	4593(7)	2691(3)	54(3)
C(62)	563(4)	5359(6)	2678(3)	44(3)
C(63)	938(4)	5745(6)	2850(3)	37(3)
C(64)	940(5)	6509(7)	2841(3)	56(4)
C(65)	1322(5)	6879(7)	3016(4)	76(4)
C(66)	1703(5)	6507(7)	3194(5)	63(4)
C(67)	1737(4)	5764(7)	3224(3)	44(3)
C(68)	1348(4)	5361(6)	3039(3)	41(3)
C(69)	77(4)	7507(6)	1749(3)	41(3)

C(70)	-971(4)	7161(6)	1826(3)	34(3)
C(71)	-1388(4)	7513(6)	1802(3)	38(3)
C(72)	-1503(4)	8192(6)	1619(3)	45(3)
C(73)	-1907(4)	8534(6)	1613(3)	43(3)
C(74)	-2186(4)	8213(7)	1794(3)	48(3)
C(75)	-2086(4)	7525(7)	1970(3)	44(3)
C(76)	-2380(4)	7176(7)	2138(3)	48(3)
C(77)	-2293(5)	6538(9)	2314(4)	65(4)
C(78)	-1880(5)	6151(7)	2322(3)	57(4)
C(79)	-1574(5)	6456(7)	2160(3)	51(3)
C(80)	-1673(4)	7151(6)	1978(3)	39(3)
C(81)	466(4)	9273(6)	1822(3)	38(3)
C(82)	837(4)	9723(6)	1795(3)	38(3)
C(83)	1146(4)	9468(7)	1607(3)	44(3)
C(84)	1508(4)	9890(7)	1602(4)	53(3)
C(85)	1581(4)	10566(7)	1798(3)	53(3)
C(86)	1271(4)	10859(6)	1969(3)	45(3)
C(87)	1330(5)	11541(7)	2147(3)	50(3)
C(88)	1054(6)	11829(7)	2305(4)	67(5)
C(89)	676(5)	11419(7)	2319(3)	58(4)
C(90)	589(4)	10721(6)	2150(3)	47(3)
C(91)	893(4)	10416(6)	1975(3)	35(3)
C(92)	806(4)	6070(6)	1821(3)	38(3)
C(93)	835(4)	5267(6)	1796(3)	36(3)
C(94)	467(4)	4848(7)	1612(3)	42(3)
C(95)	495(4)	4079(6)	1610(4)	50(3)
C(96)	891(4)	3739(6)	1796(3)	48(3)
C(97)	1267(4)	4143(6)	1972(3)	39(3)
C(98)	1670(4)	3784(7)	2142(3)	53(3)
C(99)	2038(5)	4156(9)	2310(3)	61(4)
C(100)	2021(4)	4937(9)	2315(3)	63(4)
C(101)	1638(4)	5334(8)	2160(3)	49(3)
C(102)	1249(4)	4918(6)	1971(3)	38(3)
C(103)	1516(4)	2508(6)	1054(3)	37(3)
C(104)	2528(4)	1877(7)	1038(3)	45(3)
C(105)	2817(3)	1219(7)	1081(3)	39(3)
C(106)	2721(4)	561(7)	1216(3)	48(3)

C(107)	3024(5)	-37(7)	1292(4)	60(4)
C(108)	3420(4)	69(7)	1217(4)	58(4)
C(109)	3534(4)	719(9)	1062(4)	61(4)
C(110)	3948(4)	836(10)	980(4)	73(5)
C(111)	4036(5)	1472(12)	806(5)	88(5)
C(112)	3742(5)	2039(10)	719(4)	70(4)
C(113)	3353(5)	1944(9)	808(3)	67(4)
C(114)	3236(3)	1312(6)	990(3)	31(2)
C(115)	1317(4)	4331(7)	1036(3)	46(3)
C(116)	1518(4)	5076(6)	1076(3)	40(3)
C(117)	1972(4)	5197(6)	1221(3)	47(3)
C(118)	2149(5)	5917(8)	1298(4)	66(4)
C(119)	1834(7)	6496(7)	1220(4)	73(5)
C(120)	1386(6)	6410(7)	1051(3)	57(4)
C(121)	1101(6)	7015(7)	976(5)	72(5)
C(122)	647(6)	6970(8)	812(4)	75(4)
C(123)	469(6)	6238(8)	719(4)	76(5)
C(124)	758(5)	5677(8)	806(4)	63(4)
C(125)	1216(4)	5704(6)	982(3)	37(3)
C(126)	686(4)	1288(6)	1044(3)	41(3)
C(127)	229(4)	1200(6)	1083(3)	38(3)
C(128)	22(4)	1735(6)	1226(3)	42(3)
C(129)	-402(5)	1595(9)	1291(4)	60(4)
C(130)	-581(4)	953(9)	1216(4)	59(4)
C(131)	-379(5)	383(8)	1063(3)	57(4)
C(132)	-585(5)	-317(8)	970(4)	69(4)
C(133)	-406(6)	-866(9)	806(4)	89(6)
C(134)	19(5)	-757(8)	720(4)	70(4)
C(135)	198(4)	-89(7)	810(3)	54(3)
C(136)	23(4)	481(6)	988(3)	43(3)
C(137)	11190(3)	7506(6)	5089(3)	31(2)
C(138)	10159(3)	8198(6)	5054(3)	31(2)
C(139)	9866(3)	8788(6)	4991(3)	32(3)
C(140)	9961(4)	9452(6)	4824(3)	44(3)
C(141)	9646(5)	9988(7)	4703(4)	54(3)
C(142)	9264(5)	9932(8)	4734(4)	65(4)
C(143)	9140(4)	9308(7)	4901(3)	51(3)

C(144)	8717(5)	9241(8)	4936(4)	66(4)
C(145)	8579(5)	8635(9)	5117(4)	73(4)
C(146)	8895(4)	8084(7)	5244(4)	57(3)
C(147)	9322(4)	8126(8)	5211(3)	51(3)
C(148)	9453(4)	8743(6)	5035(3)	45(3)
C(149)	12043(4)	8672(6)	5061(3)	33(3)
C(150)	12451(4)	8785(6)	4989(3)	36(3)
C(151)	12647(4)	8228(8)	4828(3)	50(3)
C(152)	13007(4)	8355(7)	4700(4)	51(3)
C(153)	13190(5)	8995(9)	4715(4)	69(4)
C(154)	13027(4)	9598(7)	4896(3)	49(3)
C(155)	13221(4)	10277(9)	4939(4)	65(4)
C(156)	13065(5)	10876(9)	5111(4)	74(5)
C(157)	12703(4)	10755(6)	5239(4)	51(3)
C(158)	12488(5)	10098(7)	5209(3)	58(4)
C(159)	12654(4)	9482(7)	5036(3)	44(3)
C(160)	11347(4)	5628(5)	5058(3)	32(2)
C(161)	11156(4)	4926(6)	4983(3)	36(3)
C(162)	10707(4)	4816(6)	4827(3)	42(3)
C(163)	10524(4)	4151(7)	4698(4)	51(3)
C(164)	10756(5)	3578(8)	4721(4)	66(4)
C(165)	11232(5)	3617(7)	4896(4)	50(3)
C(166)	11489(6)	3007(8)	4943(4)	63(4)
C(167)	11926(6)	3006(8)	5104(4)	77(5)
C(168)	12149(5)	3698(7)	5244(4)	61(4)
C(169)	11899(4)	4339(7)	5217(3)	51(3)
C(170)	11419(4)	4280(7)	5032(3)	46(3)
C(171)	8776(10)	-639(16)	7040(11)	244(19)
C(172)	9525(8)	-554(13)	7481(8)	173(12)
C(173)	9281(7)	264(10)	6956(5)	93(5)
C(174)	1718(6)	7676(11)	1960(6)	101(6)
C(175)	2452(9)	7938(14)	2079(8)	165(9)
C(176)	2249(8)	7169(14)	2494(8)	172(12)
C(177)	4293(13)	8790(13)	2083(9)	270(20)
C(178)	4216(10)	9776(12)	2491(9)	181(13)
C(179)	4453(6)	10080(9)	1984(6)	97(6)
Cl(01)	1358(1)	502(2)	556(1)	66(1)

Cl(02)	2339(1)	3509(2)	555(1)	64(1)
Cl(03)	347(1)	3482(2)	557(1)	66(1)
Cl(04)	3041(1)	804(2)	3724(1)	56(1)
Cl(05)	1238(1)	2396(2)	3725(1)	56(1)
Cl(06)	2936(1)	4302(2)	3725(1)	56(1)
N(1)	2219(3)	2859(5)	4234(3)	39(2)
N(2)	2237(3)	3615(5)	4271(2)	39(2)
N(3)	2938(3)	2852(5)	4234(3)	35(2)
N(4)	3309(3)	2466(5)	4267(3)	35(2)
N(5)	2572(3)	1791(5)	4240(3)	41(2)
N(6)	2203(3)	1436(5)	4265(3)	36(2)
N(7)	2640(3)	2220(4)	3279(3)	36(2)
N(8)	2939(3)	2673(5)	3181(3)	41(2)
N(9)	1917(3)	2060(4)	3278(3)	39(2)
N(10)	1951(3)	1350(5)	3183(3)	36(2)
N(11)	2210(3)	3218(4)	3275(2)	35(2)
N(12)	1785(3)	3487(5)	3180(3)	40(2)
N(13)	-287(3)	7139(5)	1756(3)	40(2)
N(14)	-667(3)	7533(5)	1725(2)	40(2)
N(15)	86(3)	8247(4)	1763(3)	37(2)
N(16)	460(3)	8589(5)	1722(2)	37(2)
N(17)	451(3)	7129(5)	1753(3)	38(2)
N(18)	419(3)	6377(4)	1722(2)	34(2)
N(19)	1942(3)	2474(5)	1059(2)	40(2)
N(20)	2150(3)	1810(4)	1087(2)	31(2)
N(21)	1286(3)	1876(5)	1059(2)	38(2)
N(22)	874(3)	1906(5)	1087(2)	34(2)
N(23)	1316(3)	3158(5)	1059(2)	34(2)
N(24)	1557(3)	3768(5)	1083(2)	31(2)
N(25)	10776(3)	7536(5)	5081(2)	31(2)
N(26)	10564(3)	8212(5)	5038(2)	36(2)
N(27)	11415(3)	8107(4)	5081(2)	33(2)
N(28)	11839(3)	8063(5)	5037(2)	36(2)
N(29)	11379(3)	6862(4)	5084(2)	34(2)
N(30)	11126(3)	6217(5)	5035(2)	33(2)
N(31)	9219(6)	-315(8)	7178(5)	103(5)
N(32)	2133(5)	7571(9)	2174(5)	101(4)

N(33)	4313(5)	9586(8)	2175(4)	91(4)
O(1)	2626(3)	4866(4)	4560(3)	50(2)
O(2)	3896(3)	1418(4)	4556(3)	54(2)
O(3)	1534(3)	1243(4)	4558(3)	51(2)
O(4)	3201(3)	3821(4)	2858(3)	58(2)
O(5)	2225(3)	208(4)	2856(2)	54(2)
O(6)	905(3)	3464(4)	2853(2)	57(2)
O(7)	-1253(3)	8569(4)	1418(2)	54(2)
O(8)	1119(3)	8823(4)	1416(2)	55(2)
O(9)	54(3)	5152(5)	1426(2)	60(2)
O(10)	2360(3)	436(5)	1310(3)	65(3)
O(11)	183(3)	2375(5)	1306(3)	63(2)
O(12)	2249(3)	4674(5)	1297(3)	65(3)
O(13)	10380(3)	9594(4)	4793(2)	54(2)
O(14)	12497(3)	7517(4)	4791(3)	56(2)
O(15)	10404(3)	5388(4)	4786(3)	55(2)
O(16)	9576(3)	655(5)	7005(3)	69(3)
O(17)	4534(3)	10683(5)	2013(3)	67(2)
O(18)	1392(3)	7460(5)	2010(3)	66(2)
OW1	8099(12)	360(20)	5647(12)	366(19)
OW2	1556(10)	-1220(17)	654(10)	319(15)
OW3	4205(10)	8612(15)	1010(10)	276(12)
OW4	-539(11)	4222(18)	532(11)	328(16)

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

C(1)-N(1)	1.296(13)
C(1)-N(3)	1.310(13)
C(1)-N(5)	1.327(12)
C(2)-N(2)	1.227(13)
C(2)-C(3)	1.488(15)
C(3)-C(4)	1.365(15)
C(3)-C(12)	1.460(15)
C(4)-O(1)	1.326(13)
C(4)-C(5)	1.390(15)
C(5)-C(6)	1.376(17)
C(5)-H(5A)	0.9300
C(6)-C(7)	1.434(17)
C(6)-H(6)	0.9300
C(7)-C(12)	1.376(15)
C(7)-C(8)	1.434(17)
C(8)-C(9)	1.397(19)
C(8)-H(8)	0.9300
C(9)-C(10)	1.346(17)
C(9)-H(9)	0.9300
C(10)-C(11)	1.344(16)
C(10)-H(10A)	0.9300
C(11)-C(12)	1.424(15)
C(11)-H(11A)	0.9300
C(13)-N(4)	1.234(13)
C(13)-C(14)	1.488(15)
C(14)-C(15)	1.372(15)
C(14)-C(23)	1.458(15)
C(15)-O(2)	1.322(13)
C(15)-C(16)	1.399(16)
C(16)-C(17)	1.319(17)
C(16)-H(16)	0.9300
C(17)-C(18)	1.417(16)
C(17)-H(17)	0.9300
C(18)-C(23)	1.375(15)
C(18)-C(19)	1.428(16)

C(19)-C(20)	1.345(19)
C(19)-H(19A)	0.9300
C(20)-C(21)	1.304(18)
C(20)-H(20)	0.9300
C(21)-C(22)	1.354(17)
C(21)-H(21A)	0.9300
C(22)-C(23)	1.428(15)
C(22)-H(22)	0.9300
C(24)-N(6)	1.266(12)
C(24)-C(25)	1.470(15)
C(25)-C(26)	1.348(15)
C(25)-C(34)	1.477(15)
C(26)-O(3)	1.348(13)
C(26)-C(27)	1.409(15)
C(27)-C(28)	1.335(15)
C(27)-H(27A)	0.9300
C(28)-C(29)	1.422(16)
C(28)-H(28)	0.9300
C(29)-C(34)	1.354(15)
C(29)-C(30)	1.431(17)
C(30)-C(31)	1.390(19)
C(30)-H(30)	0.9300
C(31)-C(32)	1.312(18)
C(31)-H(31)	0.9300
C(32)-C(33)	1.360(16)
C(32)-H(32)	0.9300
C(33)-C(34)	1.443(16)
C(33)-H(33)	0.9300
C(35)-N(11)	1.294(12)
C(35)-N(7)	1.342(13)
C(35)-N(9)	1.361(13)
C(36)-N(8)	1.253(14)
C(36)-C(37)	1.482(15)
C(37)-C(38)	1.370(15)
C(37)-C(46)	1.422(13)
C(38)-O(4)	1.367(14)
C(38)-C(39)	1.400(16)

C(39)-C(40)	1.413(16)
C(39)-H(39)	0.9300
C(40)-C(41)	1.337(16)
C(40)-H(40)	0.9300
C(41)-C(46)	1.418(16)
C(41)-C(42)	1.438(17)
C(42)-C(43)	1.406(19)
C(42)-H(42)	0.9300
C(43)-C(44)	1.366(18)
C(43)-H(43)	0.9300
C(44)-C(45)	1.344(16)
C(44)-H(44)	0.9300
C(45)-C(46)	1.417(15)
C(45)-H(45)	0.9300
C(47)-N(10)	1.255(13)
C(47)-C(48)	1.486(14)
C(48)-C(49)	1.365(15)
C(48)-C(57)	1.417(12)
C(49)-O(5)	1.359(13)
C(49)-C(50)	1.410(15)
C(50)-C(51)	1.390(16)
C(50)-H(50)	0.9300
C(51)-C(52)	1.352(16)
C(51)-H(51)	0.9300
C(52)-C(53)	1.406(16)
C(52)-C(57)	1.424(15)
C(53)-C(54)	1.363(18)
C(53)-H(53)	0.9300
C(54)-C(55)	1.388(19)
C(54)-H(54)	0.9300
C(55)-C(56)	1.357(17)
C(55)-H(55)	0.9300
C(56)-C(57)	1.428(17)
C(56)-H(56)	0.9300
C(58)-N(12)	1.282(14)
C(58)-C(59)	1.442(15)
C(59)-C(60)	1.388(15)

C(59)-C(68)	1.434(12)
C(60)-O(6)	1.389(13)
C(60)-C(61)	1.404(16)
C(61)-C(62)	1.407(16)
C(61)-H(61)	0.9300
C(62)-C(63)	1.358(15)
C(62)-H(62)	0.9300
C(63)-C(64)	1.403(16)
C(63)-C(68)	1.448(15)
C(64)-C(65)	1.362(19)
C(64)-H(64)	0.9300
C(65)-C(66)	1.362(18)
C(65)-H(65)	0.9300
C(66)-C(67)	1.370(16)
C(66)-H(66)	0.9300
C(67)-C(68)	1.416(16)
C(67)-H(67)	0.9300
C(69)-N(13)	1.345(14)
C(69)-N(15)	1.360(13)
C(69)-N(17)	1.374(14)
C(70)-N(14)	1.315(13)
C(70)-C(71)	1.453(15)
C(71)-C(72)	1.396(15)
C(71)-C(80)	1.403(16)
C(72)-O(7)	1.387(14)
C(72)-C(73)	1.426(16)
C(73)-C(74)	1.367(16)
C(73)-H(73)	0.9300
C(74)-C(75)	1.397(17)
C(74)-H(74)	0.9300
C(75)-C(76)	1.398(16)
C(75)-C(80)	1.474(17)
C(76)-C(77)	1.309(18)
C(76)-H(76)	0.9300
C(77)-C(78)	1.484(19)
C(77)-H(77)	0.9300
C(78)-C(79)	1.381(17)

C(78)-H(78)	0.9300
C(79)-C(80)	1.416(16)
C(79)-H(79)	0.9300
C(81)-N(16)	1.301(13)
C(81)-C(82)	1.466(15)
C(82)-C(91)	1.404(14)
C(82)-C(83)	1.414(16)
C(83)-O(8)	1.346(13)
C(83)-C(84)	1.392(16)
C(84)-C(85)	1.399(17)
C(84)-H(84)	0.9300
C(85)-C(86)	1.402(17)
C(85)-H(85)	0.9300
C(86)-C(87)	1.384(16)
C(86)-C(91)	1.456(16)
C(87)-C(88)	1.279(19)
C(87)-H(87)	0.9300
C(88)-C(89)	1.43(2)
C(88)-H(88)	0.9300
C(89)-C(90)	1.399(16)
C(89)-H(89)	0.9300
C(90)-C(91)	1.404(16)
C(90)-H(90)	0.9300
C(92)-N(18)	1.299(13)
C(92)-C(93)	1.481(14)
C(93)-C(94)	1.381(15)
C(93)-C(102)	1.422(14)
C(94)-O(9)	1.390(13)
C(94)-C(95)	1.413(16)
C(95)-C(96)	1.375(16)
C(95)-H(95)	0.9300
C(96)-C(97)	1.382(16)
C(96)-H(96)	0.9300
C(97)-C(98)	1.398(16)
C(97)-C(102)	1.423(15)
C(98)-C(99)	1.327(18)
C(98)-H(98)	0.9300

C(99)-C(100)	1.434(19)
C(99)-H(99)	0.9300
C(100)-C(101)	1.378(17)
C(100)-H(100)	0.9300
C(101)-C(102)	1.430(16)
C(101)-H(101)	0.9300
C(103)-N(19)	1.351(14)
C(103)-N(23)	1.354(13)
C(103)-N(21)	1.372(13)
C(104)-N(20)	1.269(14)
C(104)-C(105)	1.497(16)
C(105)-C(106)	1.364(17)
C(105)-C(114)	1.470(15)
C(106)-O(10)	1.302(15)
C(106)-C(107)	1.433(16)
C(107)-C(108)	1.372(19)
C(107)-H(107)	0.9300
C(108)-C(109)	1.402(19)
C(108)-H(108)	0.9300
C(109)-C(114)	1.413(16)
C(109)-C(110)	1.44(2)
C(110)-C(111)	1.38(2)
C(110)-H(110)	0.9300
C(111)-C(112)	1.37(2)
C(111)-H(111)	0.9300
C(112)-C(113)	1.370(19)
C(112)-H(112)	0.9300
C(113)-C(114)	1.423(18)
C(113)-H(113)	0.9300
C(115)-N(24)	1.266(14)
C(115)-C(116)	1.499(16)
C(116)-C(117)	1.394(16)
C(116)-C(125)	1.469(15)
C(117)-O(12)	1.274(13)
C(117)-C(118)	1.429(17)
C(118)-C(119)	1.43(2)
C(118)-H(118)	0.9300

C(119)-C(120)	1.37(2)
C(119)-H(119)	0.9300
C(120)-C(125)	1.397(17)
C(120)-C(121)	1.406(18)
C(121)-C(122)	1.38(2)
C(121)-H(121)	0.9300
C(122)-C(123)	1.45(2)
C(122)-H(122)	0.9300
C(123)-C(124)	1.350(18)
C(123)-H(123)	0.9300
C(124)-C(125)	1.399(18)
C(124)-H(124)	0.9300
C(126)-N(22)	1.270(13)
C(126)-C(127)	1.508(16)
C(127)-C(128)	1.358(16)
C(127)-C(136)	1.463(15)
C(128)-O(11)	1.277(12)
C(128)-C(129)	1.453(18)
C(129)-C(130)	1.299(18)
C(129)-H(129)	0.9300
C(130)-C(131)	1.414(19)
C(130)-H(130)	0.9300
C(131)-C(136)	1.391(18)
C(131)-C(132)	1.435(18)
C(132)-C(133)	1.36(2)
C(132)-H(132)	0.9300
C(133)-C(134)	1.48(2)
C(133)-H(133)	0.9300
C(134)-C(135)	1.347(17)
C(134)-H(134)	0.9300
C(135)-C(136)	1.411(17)
C(135)-H(135)	0.9300
C(137)-N(25)	1.308(12)
C(137)-N(27)	1.320(13)
C(137)-N(29)	1.328(12)
C(138)-N(26)	1.308(13)
C(138)-C(139)	1.401(14)

C(139)-C(148)	1.369(16)
C(139)-C(140)	1.421(15)
C(140)-C(141)	1.376(16)
C(140)-O(13)	1.393(14)
C(141)-C(142)	1.254(18)
C(141)-H(141)	0.9300
C(142)-C(143)	1.394(19)
C(142)-H(142)	0.9300
C(143)-C(144)	1.392(18)
C(143)-C(148)	1.413(16)
C(144)-C(145)	1.41(2)
C(144)-H(144)	0.9300
C(145)-C(146)	1.399(18)
C(145)-H(145)	0.9300
C(146)-C(147)	1.398(17)
C(146)-H(146)	0.9300
C(147)-C(148)	1.409(17)
C(147)-H(147)	0.9300
C(149)-N(28)	1.281(12)
C(149)-C(150)	1.408(15)
C(150)-C(151)	1.399(16)
C(150)-C(159)	1.421(16)
C(151)-C(152)	1.366(17)
C(151)-O(14)	1.382(15)
C(152)-C(153)	1.305(17)
C(152)-H(152)	0.9300
C(153)-C(154)	1.444(19)
C(153)-H(153)	0.9300
C(154)-C(155)	1.378(18)
C(154)-C(159)	1.427(17)
C(155)-C(156)	1.41(2)
C(155)-H(155)	0.9300
C(156)-C(157)	1.371(19)
C(156)-H(156)	0.9300
C(157)-C(158)	1.374(16)
C(157)-H(157)	0.9300
C(158)-C(159)	1.453(18)

C(158)-H(158)	0.9300
C(160)-N(30)	1.278(12)
C(160)-C(161)	1.413(15)
C(161)-C(162)	1.377(15)
C(161)-C(170)	1.431(16)
C(162)-C(163)	1.367(16)
C(162)-O(15)	1.403(14)
C(163)-C(164)	1.272(16)
C(163)-H(163)	0.9300
C(164)-C(165)	1.450(18)
C(164)-H(164)	0.9300
C(165)-C(166)	1.365(18)
C(165)-C(170)	1.373(16)
C(166)-C(167)	1.33(2)
C(166)-H(166)	0.9300
C(167)-C(168)	1.46(2)
C(167)-H(167)	0.9300
C(168)-C(169)	1.407(16)
C(168)-H(168)	0.9300
C(169)-C(170)	1.467(17)
C(169)-H(169)	0.9300
C(171)-N(31)	1.47(3)
C(171)-H(17H)	0.9600
C(171)-H(17I)	0.9600
C(171)-H(17J)	0.9600
C(172)-N(31)	1.27(2)
C(172)-H(17N)	0.9600
C(172)-H(17O)	0.9600
C(172)-H(17P)	0.9600
C(173)-O(16)	1.151(18)
C(173)-N(31)	1.36(2)
C(173)-H(173)	0.9300
C(174)-O(18)	1.171(17)
C(174)-N(32)	1.32(2)
C(174)-H(174)	0.9300
C(175)-N(32)	1.34(3)
C(175)-H(17B)	0.9600

C(175)-H(17C)	0.9600
C(175)-H(17D)	0.9600
C(176)-N(32)	1.28(2)
C(176)-H(17K)	0.9600
C(176)-H(17L)	0.9600
C(176)-H(17M)	0.9600
C(177)-N(33)	1.49(3)
C(177)-H(17E)	0.9600
C(177)-H(17F)	0.9600
C(177)-H(17G)	0.9600
C(178)-N(33)	1.27(2)
C(178)-H(17Q)	0.9600
C(178)-H(17R)	0.9600
C(178)-H(17S)	0.9600
C(179)-O(17)	1.133(15)
C(179)-N(33)	1.28(2)
C(179)-H(179)	0.9300
N(1)-N(2)	1.394(12)
N(1)-H(1A)	0.8600
N(3)-N(4)	1.353(11)
N(3)-H(3)	0.8600
N(5)-N(6)	1.367(12)
N(5)-H(5)	0.8600
N(7)-N(8)	1.382(12)
N(7)-H(7)	0.8600
N(9)-N(10)	1.356(11)
N(9)-H(9A)	0.8600
N(11)-N(12)	1.382(12)
N(11)-H(11B)	0.8600
N(13)-N(14)	1.384(12)
N(13)-H(13A)	0.8600
N(15)-N(16)	1.389(12)
N(15)-H(15A)	0.8600
N(17)-N(18)	1.385(11)
N(17)-H(17A)	0.8600
N(19)-N(20)	1.377(11)
N(19)-H(19)	0.8600

N(21)-N(22)	1.343(12)
N(21)-H(21)	0.8600
N(23)-N(24)	1.346(11)
N(23)-H(23)	0.8600
N(25)-N(26)	1.397(11)
N(25)-H(25)	0.8600
N(27)-N(28)	1.406(12)
N(27)-H(27)	0.8600
N(29)-N(30)	1.410(11)
N(29)-H(29)	0.8600
O(1)-H(1)	0.8200
O(2)-H(2)	0.8200
O(3)-H(3A)	0.8200
O(4)-H(4)	0.8200
O(5)-H(5B)	0.8200
O(6)-H(6A)	0.8200
O(7)-H(7A)	0.8200
O(8)-H(8A)	0.8200
O(9)-H(9B)	0.8200
O(10)-H(10)	0.8200
O(11)-H(11)	0.8200
O(12)-H(12)	0.8200
O(13)-H(13)	0.8200
O(14)-H(14)	0.8200
O(15)-H(15)	0.8200

N(1)-C(1)-N(3)	122.4(10)
N(1)-C(1)-N(5)	118.5(10)
N(3)-C(1)-N(5)	118.9(10)
N(2)-C(2)-C(3)	122.4(10)
C(4)-C(3)-C(12)	120.4(10)
C(4)-C(3)-C(2)	120.7(10)
C(12)-C(3)-C(2)	118.9(10)
O(1)-C(4)-C(3)	124.2(10)
O(1)-C(4)-C(5)	114.5(10)
C(3)-C(4)-C(5)	121.2(11)
C(6)-C(5)-C(4)	120.0(12)

C(6)-C(5)-H(5A)	120.0
C(4)-C(5)-H(5A)	120.0
C(5)-C(6)-C(7)	120.2(12)
C(5)-C(6)-H(6)	119.9
C(7)-C(6)-H(6)	119.9
C(12)-C(7)-C(8)	121.6(12)
C(12)-C(7)-C(6)	120.5(11)
C(8)-C(7)-C(6)	117.8(12)
C(9)-C(8)-C(7)	117.2(12)
C(9)-C(8)-H(8)	121.4
C(7)-C(8)-H(8)	121.4
C(10)-C(9)-C(8)	120.9(13)
C(10)-C(9)-H(9)	119.6
C(8)-C(9)-H(9)	119.6
C(11)-C(10)-C(9)	122.1(12)
C(11)-C(10)-H(10A)	118.9
C(9)-C(10)-H(10A)	118.9
C(10)-C(11)-C(12)	120.9(11)
C(10)-C(11)-H(11A)	119.6
C(12)-C(11)-H(11A)	119.6
C(7)-C(12)-C(11)	117.2(11)
C(7)-C(12)-C(3)	117.8(11)
C(11)-C(12)-C(3)	124.9(10)
N(4)-C(13)-C(14)	123.9(10)
C(15)-C(14)-C(23)	118.9(10)
C(15)-C(14)-C(13)	120.2(10)
C(23)-C(14)-C(13)	120.9(10)
O(2)-C(15)-C(14)	123.0(10)
O(2)-C(15)-C(16)	117.0(10)
C(14)-C(15)-C(16)	120.0(11)
C(17)-C(16)-C(15)	121.3(12)
C(17)-C(16)-H(16)	119.3
C(15)-C(16)-H(16)	119.3
C(16)-C(17)-C(18)	121.4(11)
C(16)-C(17)-H(17)	119.3
C(18)-C(17)-H(17)	119.3
C(23)-C(18)-C(17)	119.2(11)

C(23)-C(18)-C(19)	120.1(12)
C(17)-C(18)-C(19)	120.7(11)
C(20)-C(19)-C(18)	118.9(13)
C(20)-C(19)-H(19A)	120.5
C(18)-C(19)-H(19A)	120.5
C(21)-C(20)-C(19)	121.1(13)
C(21)-C(20)-H(20)	119.4
C(19)-C(20)-H(20)	119.4
C(20)-C(21)-C(22)	123.7(13)
C(20)-C(21)-H(21A)	118.1
C(22)-C(21)-H(21A)	118.1
C(21)-C(22)-C(23)	118.6(11)
C(21)-C(22)-H(22)	120.7
C(23)-C(22)-H(22)	120.7
C(18)-C(23)-C(22)	117.5(11)
C(18)-C(23)-C(14)	119.0(10)
C(22)-C(23)-C(14)	123.4(10)
N(6)-C(24)-C(25)	122.7(10)
C(26)-C(25)-C(24)	121.9(10)
C(26)-C(25)-C(34)	119.3(10)
C(24)-C(25)-C(34)	118.8(10)
O(3)-C(26)-C(25)	122.7(10)
O(3)-C(26)-C(27)	116.7(10)
C(25)-C(26)-C(27)	120.5(11)
C(28)-C(27)-C(26)	121.3(12)
C(28)-C(27)-H(27A)	119.3
C(26)-C(27)-H(27A)	119.3
C(27)-C(28)-C(29)	119.5(11)
C(27)-C(28)-H(28)	120.3
C(29)-C(28)-H(28)	120.3
C(34)-C(29)-C(28)	121.5(11)
C(34)-C(29)-C(30)	120.6(12)
C(28)-C(29)-C(30)	117.8(11)
C(31)-C(30)-C(29)	117.9(13)
C(31)-C(30)-H(30)	121.0
C(29)-C(30)-H(30)	121.0
C(32)-C(31)-C(30)	121.1(13)

C(32)-C(31)-H(31)	119.4
C(30)-C(31)-H(31)	119.4
C(31)-C(32)-C(33)	123.1(13)
C(31)-C(32)-H(32)	118.4
C(33)-C(32)-H(32)	118.4
C(32)-C(33)-C(34)	118.6(12)
C(32)-C(33)-H(33)	120.7
C(34)-C(33)-H(33)	120.7
C(29)-C(34)-C(33)	118.7(11)
C(29)-C(34)-C(25)	117.8(11)
C(33)-C(34)-C(25)	123.5(11)
N(11)-C(35)-N(7)	120.0(10)
N(11)-C(35)-N(9)	122.0(9)
N(7)-C(35)-N(9)	117.9(9)
N(8)-C(36)-C(37)	123.6(11)
C(38)-C(37)-C(46)	120.3(10)
C(38)-C(37)-C(36)	119.1(11)
C(46)-C(37)-C(36)	120.3(9)
O(4)-C(38)-C(37)	124.8(11)
O(4)-C(38)-C(39)	114.5(11)
C(37)-C(38)-C(39)	120.7(12)
C(38)-C(39)-C(40)	118.8(11)
C(38)-C(39)-H(39)	120.6
C(40)-C(39)-H(39)	120.6
C(41)-C(40)-C(39)	120.8(11)
C(41)-C(40)-H(40)	119.6
C(39)-C(40)-H(40)	119.6
C(40)-C(41)-C(46)	121.6(11)
C(40)-C(41)-C(42)	119.2(12)
C(46)-C(41)-C(42)	119.2(12)
C(43)-C(42)-C(41)	118.6(12)
C(43)-C(42)-H(42)	120.7
C(41)-C(42)-H(42)	120.7
C(44)-C(43)-C(42)	119.6(12)
C(44)-C(43)-H(43)	120.2
C(42)-C(43)-H(43)	120.2
C(45)-C(44)-C(43)	124.0(13)

C(45)-C(44)-H(44)	118.0
C(43)-C(44)-H(44)	118.0
C(44)-C(45)-C(46)	119.3(12)
C(44)-C(45)-H(45)	120.4
C(46)-C(45)-H(45)	120.4
C(45)-C(46)-C(41)	119.4(11)
C(45)-C(46)-C(37)	122.9(10)
C(41)-C(46)-C(37)	117.7(9)
N(10)-C(47)-C(48)	124.6(11)
C(49)-C(48)-C(57)	119.4(9)
C(49)-C(48)-C(47)	120.4(10)
C(57)-C(48)-C(47)	119.9(9)
O(5)-C(49)-C(48)	122.8(10)
O(5)-C(49)-C(50)	114.5(11)
C(48)-C(49)-C(50)	122.7(11)
C(51)-C(50)-C(49)	116.6(11)
C(51)-C(50)-H(50)	121.7
C(49)-C(50)-H(50)	121.7
C(52)-C(51)-C(50)	122.9(10)
C(52)-C(51)-H(51)	118.5
C(50)-C(51)-H(51)	118.5
C(51)-C(52)-C(53)	121.7(11)
C(51)-C(52)-C(57)	120.1(10)
C(53)-C(52)-C(57)	118.3(12)
C(54)-C(53)-C(52)	121.6(12)
C(54)-C(53)-H(53)	119.2
C(52)-C(53)-H(53)	119.2
C(53)-C(54)-C(55)	120.3(12)
C(53)-C(54)-H(54)	119.9
C(55)-C(54)-H(54)	119.9
C(56)-C(55)-C(54)	120.7(14)
C(56)-C(55)-H(55)	119.6
C(54)-C(55)-H(55)	119.6
C(55)-C(56)-C(57)	120.7(12)
C(55)-C(56)-H(56)	119.6
C(57)-C(56)-H(56)	119.6
C(48)-C(57)-C(52)	118.3(9)

C(48)-C(57)-C(56)	123.4(9)
C(52)-C(57)-C(56)	118.3(11)
N(12)-C(58)-C(59)	123.7(11)
C(60)-C(59)-C(68)	118.6(9)
C(60)-C(59)-C(58)	121.0(10)
C(68)-C(59)-C(58)	120.1(9)
C(59)-C(60)-O(6)	124.2(11)
C(59)-C(60)-C(61)	121.9(10)
O(6)-C(60)-C(61)	113.8(11)
C(60)-C(61)-C(62)	118.7(11)
C(60)-C(61)-H(61)	120.6
C(62)-C(61)-H(61)	120.6
C(63)-C(62)-C(61)	122.0(10)
C(63)-C(62)-H(62)	119.0
C(61)-C(62)-H(62)	119.0
C(62)-C(63)-C(64)	121.3(11)
C(62)-C(63)-C(68)	119.5(10)
C(64)-C(63)-C(68)	119.2(11)
C(65)-C(64)-C(63)	119.9(12)
C(65)-C(64)-H(64)	120.1
C(63)-C(64)-H(64)	120.1
C(64)-C(65)-C(66)	120.0(12)
C(64)-C(65)-H(65)	120.0
C(66)-C(65)-H(65)	120.0
C(65)-C(66)-C(67)	124.9(13)
C(65)-C(66)-H(66)	117.5
C(67)-C(66)-H(66)	117.5
C(66)-C(67)-C(68)	116.6(11)
C(66)-C(67)-H(67)	121.7
C(68)-C(67)-H(67)	121.7
C(67)-C(68)-C(59)	121.5(9)
C(67)-C(68)-C(63)	119.4(11)
C(59)-C(68)-C(63)	119.1(9)
N(13)-C(69)-N(15)	120.6(10)
N(13)-C(69)-N(17)	119.5(10)
N(15)-C(69)-N(17)	119.7(10)
N(14)-C(70)-C(71)	119.1(10)

C(72)-C(71)-C(80)	120.5(11)
C(72)-C(71)-C(70)	121.9(11)
C(80)-C(71)-C(70)	117.6(10)
O(7)-C(72)-C(71)	124.3(11)
O(7)-C(72)-C(73)	115.1(10)
C(71)-C(72)-C(73)	120.6(12)
C(74)-C(73)-C(72)	120.8(11)
C(74)-C(73)-H(73)	119.6
C(72)-C(73)-H(73)	119.6
C(73)-C(74)-C(75)	119.8(12)
C(73)-C(74)-H(74)	120.1
C(75)-C(74)-H(74)	120.1
C(74)-C(75)-C(76)	120.2(12)
C(74)-C(75)-C(80)	120.8(11)
C(76)-C(75)-C(80)	119.0(12)
C(77)-C(76)-C(75)	121.9(13)
C(77)-C(76)-H(76)	119.0
C(75)-C(76)-H(76)	119.0
C(76)-C(77)-C(78)	119.8(12)
C(76)-C(77)-H(77)	120.1
C(78)-C(77)-H(77)	120.1
C(79)-C(78)-C(77)	121.8(12)
C(79)-C(78)-H(78)	119.1
C(77)-C(78)-H(78)	119.1
C(78)-C(79)-C(80)	117.2(13)
C(78)-C(79)-H(79)	121.4
C(80)-C(79)-H(79)	121.4
C(71)-C(80)-C(79)	122.3(11)
C(71)-C(80)-C(75)	117.5(10)
C(79)-C(80)-C(75)	120.2(11)
N(16)-C(81)-C(82)	118.2(10)
C(91)-C(82)-C(83)	119.6(11)
C(91)-C(82)-C(81)	118.5(10)
C(83)-C(82)-C(81)	121.9(10)
O(8)-C(83)-C(84)	114.4(11)
O(8)-C(83)-C(82)	124.7(11)
C(84)-C(83)-C(82)	120.9(11)

C(83)-C(84)-C(85)	120.3(13)
C(83)-C(84)-H(84)	119.9
C(85)-C(84)-H(84)	119.9
C(84)-C(85)-C(86)	120.7(12)
C(84)-C(85)-H(85)	119.7
C(86)-C(85)-H(85)	119.7
C(87)-C(86)-C(85)	121.2(12)
C(87)-C(86)-C(91)	120.0(12)
C(85)-C(86)-C(91)	118.8(11)
C(88)-C(87)-C(86)	123.1(13)
C(88)-C(87)-H(87)	118.4
C(86)-C(87)-H(87)	118.4
C(87)-C(88)-C(89)	119.2(12)
C(87)-C(88)-H(88)	120.4
C(89)-C(88)-H(88)	120.4
C(90)-C(89)-C(88)	121.9(13)
C(90)-C(89)-H(89)	119.0
C(88)-C(89)-H(89)	119.0
C(89)-C(90)-C(91)	118.1(12)
C(89)-C(90)-H(90)	120.9
C(91)-C(90)-H(90)	120.9
C(82)-C(91)-C(90)	122.9(11)
C(82)-C(91)-C(86)	119.5(11)
C(90)-C(91)-C(86)	117.5(10)
N(18)-C(92)-C(93)	119.1(10)
C(94)-C(93)-C(102)	119.1(10)
C(94)-C(93)-C(92)	121.6(10)
C(102)-C(93)-C(92)	119.3(10)
C(93)-C(94)-O(9)	122.4(11)
C(93)-C(94)-C(95)	120.8(11)
O(9)-C(94)-C(95)	116.8(11)
C(96)-C(95)-C(94)	120.1(11)
C(96)-C(95)-H(95)	120.0
C(94)-C(95)-H(95)	120.0
C(95)-C(96)-C(97)	120.5(11)
C(95)-C(96)-H(96)	119.8
C(97)-C(96)-H(96)	119.8

C(96)-C(97)-C(98)	119.3(11)
C(96)-C(97)-C(102)	120.3(10)
C(98)-C(97)-C(102)	120.3(11)
C(99)-C(98)-C(97)	120.9(12)
C(99)-C(98)-H(98)	119.6
C(97)-C(98)-H(98)	119.6
C(98)-C(99)-C(100)	119.1(12)
C(98)-C(99)-H(99)	120.4
C(100)-C(99)-H(99)	120.4
C(101)-C(100)-C(99)	123.8(13)
C(101)-C(100)-H(100)	118.1
C(99)-C(100)-H(100)	118.1
C(100)-C(101)-C(102)	115.7(12)
C(100)-C(101)-H(101)	122.2
C(102)-C(101)-H(101)	122.2
C(93)-C(102)-C(97)	119.0(10)
C(93)-C(102)-C(101)	120.8(11)
C(97)-C(102)-C(101)	120.1(10)
N(19)-C(103)-N(23)	120.8(10)
N(19)-C(103)-N(21)	119.7(10)
N(23)-C(103)-N(21)	119.5(10)
N(20)-C(104)-C(105)	119.0(11)
C(106)-C(105)-C(114)	119.3(11)
C(106)-C(105)-C(104)	123.6(11)
C(114)-C(105)-C(104)	117.0(11)
O(10)-C(106)-C(105)	123.3(11)
O(10)-C(106)-C(107)	114.5(12)
C(105)-C(106)-C(107)	122.1(13)
C(108)-C(107)-C(106)	117.6(13)
C(108)-C(107)-H(107)	121.2
C(106)-C(107)-H(107)	121.2
C(107)-C(108)-C(109)	123.6(12)
C(107)-C(108)-H(108)	118.2
C(109)-C(108)-H(108)	118.2
C(108)-C(109)-C(114)	118.9(12)
C(108)-C(109)-C(110)	124.1(14)
C(114)-C(109)-C(110)	116.9(15)

C(111)-C(110)-C(109)	121.9(15)
C(111)-C(110)-H(110)	119.1
C(109)-C(110)-H(110)	119.1
C(112)-C(111)-C(110)	121.5(15)
C(112)-C(111)-H(111)	119.3
C(110)-C(111)-H(111)	119.3
C(111)-C(112)-C(113)	117.2(16)
C(111)-C(112)-H(112)	121.4
C(113)-C(112)-H(112)	121.4
C(112)-C(113)-C(114)	125.3(14)
C(112)-C(113)-H(113)	117.3
C(114)-C(113)-H(113)	117.3
C(109)-C(114)-C(113)	116.9(12)
C(109)-C(114)-C(105)	118.4(11)
C(113)-C(114)-C(105)	124.5(11)
N(24)-C(115)-C(116)	120.6(11)
C(117)-C(116)-C(125)	119.3(10)
C(117)-C(116)-C(115)	122.9(10)
C(125)-C(116)-C(115)	117.6(11)
O(12)-C(117)-C(116)	122.0(11)
O(12)-C(117)-C(118)	116.8(12)
C(116)-C(117)-C(118)	121.2(12)
C(119)-C(118)-C(117)	116.2(13)
C(119)-C(118)-H(118)	121.9
C(117)-C(118)-H(118)	121.9
C(120)-C(119)-C(118)	124.7(12)
C(120)-C(119)-H(119)	117.6
C(118)-C(119)-H(119)	117.6
C(119)-C(120)-C(125)	118.4(12)
C(119)-C(120)-C(121)	120.8(14)
C(125)-C(120)-C(121)	120.6(15)
C(122)-C(121)-C(120)	124.1(15)
C(122)-C(121)-H(121)	118.0
C(120)-C(121)-H(121)	118.0
C(121)-C(122)-C(123)	115.7(14)
C(121)-C(122)-H(122)	122.2
C(123)-C(122)-H(122)	122.2

C(124)-C(123)-C(122)	117.6(16)
C(124)-C(123)-H(123)	121.2
C(122)-C(123)-H(123)	121.2
C(123)-C(124)-C(125)	128.0(14)
C(123)-C(124)-H(124)	116.0
C(125)-C(124)-H(124)	116.0
C(120)-C(125)-C(124)	113.9(12)
C(120)-C(125)-C(116)	119.8(11)
C(124)-C(125)-C(116)	126.3(11)
N(22)-C(126)-C(127)	121.3(11)
C(128)-C(127)-C(136)	120.1(11)
C(128)-C(127)-C(126)	122.8(10)
C(136)-C(127)-C(126)	116.9(11)
O(11)-C(128)-C(127)	122.4(11)
O(11)-C(128)-C(129)	117.3(11)
C(127)-C(128)-C(129)	120.3(11)
C(130)-C(129)-C(128)	120.0(13)
C(130)-C(129)-H(129)	120.0
C(128)-C(129)-H(129)	120.0
C(129)-C(130)-C(131)	121.6(12)
C(129)-C(130)-H(130)	119.2
C(131)-C(130)-H(130)	119.2
C(136)-C(131)-C(130)	121.6(12)
C(136)-C(131)-C(132)	117.3(15)
C(130)-C(131)-C(132)	121.2(14)
C(133)-C(132)-C(131)	122.2(15)
C(133)-C(132)-H(132)	118.9
C(131)-C(132)-H(132)	118.9
C(132)-C(133)-C(134)	120.6(13)
C(132)-C(133)-H(133)	119.7
C(134)-C(133)-H(133)	119.7
C(135)-C(134)-C(133)	114.8(15)
C(135)-C(134)-H(134)	122.6
C(133)-C(134)-H(134)	122.6
C(134)-C(135)-C(136)	125.7(13)
C(134)-C(135)-H(135)	117.2
C(136)-C(135)-H(135)	117.2

C(131)-C(136)-C(135)	119.4(12)
C(131)-C(136)-C(127)	116.5(12)
C(135)-C(136)-C(127)	124.0(12)
N(25)-C(137)-N(27)	120.7(9)
N(25)-C(137)-N(29)	119.6(10)
N(27)-C(137)-N(29)	119.6(9)
N(26)-C(138)-C(139)	126.5(10)
C(148)-C(139)-C(138)	123.3(10)
C(148)-C(139)-C(140)	115.4(10)
C(138)-C(139)-C(140)	120.8(11)
C(141)-C(140)-O(13)	118.0(11)
C(141)-C(140)-C(139)	120.6(13)
O(13)-C(140)-C(139)	121.3(10)
C(142)-C(141)-C(140)	123.5(14)
C(142)-C(141)-H(141)	118.3
C(140)-C(141)-H(141)	118.3
C(141)-C(142)-C(143)	120.4(14)
C(141)-C(142)-H(142)	119.8
C(143)-C(142)-H(142)	119.8
C(144)-C(143)-C(142)	120.8(13)
C(144)-C(143)-C(148)	120.6(14)
C(142)-C(143)-C(148)	118.6(12)
C(143)-C(144)-C(145)	123.3(13)
C(143)-C(144)-H(144)	118.4
C(145)-C(144)-H(144)	118.4
C(146)-C(145)-C(144)	114.7(13)
C(146)-C(145)-H(145)	122.7
C(144)-C(145)-H(145)	122.7
C(147)-C(146)-C(145)	123.8(14)
C(147)-C(146)-H(146)	118.1
C(145)-C(146)-H(146)	118.1
C(146)-C(147)-C(148)	120.3(13)
C(146)-C(147)-H(147)	119.9
C(148)-C(147)-H(147)	119.9
C(139)-C(148)-C(147)	121.2(11)
C(139)-C(148)-C(143)	121.5(12)
C(147)-C(148)-C(143)	117.2(13)

N(28)-C(149)-C(150)	126.3(11)
C(151)-C(150)-C(149)	120.7(11)
C(151)-C(150)-C(159)	117.4(11)
C(149)-C(150)-C(159)	121.6(10)
C(152)-C(151)-O(14)	115.5(12)
C(152)-C(151)-C(150)	121.6(13)
O(14)-C(151)-C(150)	122.9(11)
C(153)-C(152)-C(151)	123.3(14)
C(153)-C(152)-H(152)	118.3
C(151)-C(152)-H(152)	118.3
C(152)-C(153)-C(154)	119.4(13)
C(152)-C(153)-H(153)	120.3
C(154)-C(153)-H(153)	120.3
C(155)-C(154)-C(159)	119.2(13)
C(155)-C(154)-C(153)	122.1(13)
C(159)-C(154)-C(153)	118.6(12)
C(154)-C(155)-C(156)	123.2(14)
C(154)-C(155)-H(155)	118.4
C(156)-C(155)-H(155)	118.4
C(157)-C(156)-C(155)	116.6(13)
C(157)-C(156)-H(156)	121.7
C(155)-C(156)-H(156)	121.7
C(156)-C(157)-C(158)	124.4(14)
C(156)-C(157)-H(157)	117.8
C(158)-C(157)-H(157)	117.8
C(157)-C(158)-C(159)	118.6(13)
C(157)-C(158)-H(158)	120.7
C(159)-C(158)-H(158)	120.7
C(150)-C(159)-C(154)	119.5(11)
C(150)-C(159)-C(158)	122.5(11)
C(154)-C(159)-C(158)	117.9(12)
N(30)-C(160)-C(161)	124.3(10)
C(162)-C(161)-C(160)	122.7(11)
C(162)-C(161)-C(170)	115.0(11)
C(160)-C(161)-C(170)	122.1(10)
C(163)-C(162)-C(161)	123.0(12)
C(163)-C(162)-O(15)	115.2(10)

C(161)-C(162)-O(15)	121.8(10)
C(164)-C(163)-C(162)	122.6(13)
C(164)-C(163)-H(163)	118.7
C(162)-C(163)-H(163)	118.7
C(163)-C(164)-C(165)	119.7(13)
C(163)-C(164)-H(164)	120.2
C(165)-C(164)-H(164)	120.2
C(166)-C(165)-C(170)	120.4(13)
C(166)-C(165)-C(164)	121.3(12)
C(170)-C(165)-C(164)	118.3(12)
C(167)-C(166)-C(165)	124.2(14)
C(167)-C(166)-H(166)	117.9
C(165)-C(166)-H(166)	117.9
C(166)-C(167)-C(168)	118.4(12)
C(166)-C(167)-H(167)	120.8
C(168)-C(167)-H(167)	120.8
C(169)-C(168)-C(167)	119.8(13)
C(169)-C(168)-H(168)	120.1
C(167)-C(168)-H(168)	120.1
C(168)-C(169)-C(170)	117.2(12)
C(168)-C(169)-H(169)	121.4
C(170)-C(169)-H(169)	121.4
C(165)-C(170)-C(161)	121.2(11)
C(165)-C(170)-C(169)	119.9(12)
C(161)-C(170)-C(169)	118.8(11)
N(31)-C(171)-H(17H)	109.5
N(31)-C(171)-H(17I)	109.5
H(17H)-C(171)-H(17I)	109.5
N(31)-C(171)-H(17J)	109.5
H(17H)-C(171)-H(17J)	109.5
H(17I)-C(171)-H(17J)	109.5
N(31)-C(172)-H(17N)	109.5
N(31)-C(172)-H(17O)	109.5
H(17N)-C(172)-H(17O)	109.5
N(31)-C(172)-H(17P)	109.5
H(17N)-C(172)-H(17P)	109.5
H(17O)-C(172)-H(17P)	109.5

O(16)-C(173)-N(31)	130.9(19)
O(16)-C(173)-H(173)	114.6
N(31)-C(173)-H(173)	114.6
O(18)-C(174)-N(32)	130(2)
O(18)-C(174)-H(174)	114.9
N(32)-C(174)-H(174)	114.9
N(32)-C(175)-H(17B)	109.5
N(32)-C(175)-H(17C)	109.5
H(17B)-C(175)-H(17C)	109.5
N(32)-C(175)-H(17D)	109.5
H(17B)-C(175)-H(17D)	109.5
H(17C)-C(175)-H(17D)	109.5
N(32)-C(176)-H(17K)	109.5
N(32)-C(176)-H(17L)	109.5
H(17K)-C(176)-H(17L)	109.5
N(32)-C(176)-H(17M)	109.5
H(17K)-C(176)-H(17M)	109.5
H(17L)-C(176)-H(17M)	109.5
N(33)-C(177)-H(17E)	109.5
N(33)-C(177)-H(17F)	109.5
H(17E)-C(177)-H(17F)	109.5
N(33)-C(177)-H(17G)	109.5
H(17E)-C(177)-H(17G)	109.5
H(17F)-C(177)-H(17G)	109.5
N(33)-C(178)-H(17Q)	109.5
N(33)-C(178)-H(17R)	109.5
H(17Q)-C(178)-H(17R)	109.5
N(33)-C(178)-H(17S)	109.5
H(17Q)-C(178)-H(17S)	109.5
H(17R)-C(178)-H(17S)	109.5
O(17)-C(179)-N(33)	138(2)
O(17)-C(179)-H(179)	110.8
N(33)-C(179)-H(179)	110.8
C(1)-N(1)-N(2)	118.3(9)
C(1)-N(1)-H(1A)	120.8
N(2)-N(1)-H(1A)	120.8
C(2)-N(2)-N(1)	117.1(10)

C(1)-N(3)-N(4)	119.8(9)
C(1)-N(3)-H(3)	120.1
N(4)-N(3)-H(3)	120.1
C(13)-N(4)-N(3)	116.3(9)
C(1)-N(5)-N(6)	119.1(9)
C(1)-N(5)-H(5)	120.4
N(6)-N(5)-H(5)	120.4
C(24)-N(6)-N(5)	117.6(9)
C(35)-N(7)-N(8)	117.2(8)
C(35)-N(7)-H(7)	121.4
N(8)-N(7)-H(7)	121.4
C(36)-N(8)-N(7)	114.3(9)
N(10)-N(9)-C(35)	118.3(9)
N(10)-N(9)-H(9A)	120.8
C(35)-N(9)-H(9A)	120.8
C(47)-N(10)-N(9)	114.5(9)
C(35)-N(11)-N(12)	117.1(9)
C(35)-N(11)-H(11B)	121.5
N(12)-N(11)-H(11B)	121.5
C(58)-N(12)-N(11)	114.6(9)
C(69)-N(13)-N(14)	118.1(9)
C(69)-N(13)-H(13A)	120.9
N(14)-N(13)-H(13A)	120.9
C(70)-N(14)-N(13)	113.8(9)
C(69)-N(15)-N(16)	117.2(9)
C(69)-N(15)-H(15A)	121.4
N(16)-N(15)-H(15A)	121.4
C(81)-N(16)-N(15)	110.6(9)
C(69)-N(17)-N(18)	117.4(9)
C(69)-N(17)-H(17A)	121.3
N(18)-N(17)-H(17A)	121.3
C(92)-N(18)-N(17)	111.7(9)
C(103)-N(19)-N(20)	120.1(9)
C(103)-N(19)-H(19)	120.0
N(20)-N(19)-H(19)	120.0
C(104)-N(20)-N(19)	111.1(9)
N(22)-N(21)-C(103)	120.0(9)

N(22)-N(21)-H(21)	120.0
C(103)-N(21)-H(21)	120.0
C(126)-N(22)-N(21)	113.0(9)
N(24)-N(23)-C(103)	118.3(9)
N(24)-N(23)-H(23)	120.9
C(103)-N(23)-H(23)	120.9
C(115)-N(24)-N(23)	111.1(9)
C(137)-N(25)-N(26)	119.3(9)
C(137)-N(25)-H(25)	120.3
N(26)-N(25)-H(25)	120.3
C(138)-N(26)-N(25)	115.3(9)
C(137)-N(27)-N(28)	119.8(8)
C(137)-N(27)-H(27)	120.1
N(28)-N(27)-H(27)	120.1
C(149)-N(28)-N(27)	115.2(9)
C(137)-N(29)-N(30)	120.4(9)
C(137)-N(29)-H(29)	119.8
N(30)-N(29)-H(29)	119.8
C(160)-N(30)-N(29)	115.0(9)
C(172)-N(31)-C(173)	122.0(19)
C(172)-N(31)-C(171)	123(2)
C(173)-N(31)-C(171)	115(2)
C(176)-N(32)-C(174)	123.0(18)
C(176)-N(32)-C(175)	117(2)
C(174)-N(32)-C(175)	119(2)
C(178)-N(33)-C(179)	117.8(18)
C(178)-N(33)-C(177)	116(2)
C(179)-N(33)-C(177)	126(2)
C(4)-O(1)-H(1)	109.5
C(15)-O(2)-H(2)	109.5
C(26)-O(3)-H(3A)	109.5
C(38)-O(4)-H(4)	109.5
C(49)-O(5)-H(5B)	109.5
C(60)-O(6)-H(6A)	109.5
C(72)-O(7)-H(7A)	109.5
C(83)-O(8)-H(8A)	109.5
C(94)-O(9)-H(9B)	109.5

C(106)-O(10)-H(10)	109.5
C(128)-O(11)-H(11)	109.5
C(117)-O(12)-H(12)	109.5
C(140)-O(13)-H(13)	109.5
C(151)-O(14)-H(14)	109.5
C(162)-O(15)-H(15)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 1a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	26(6)	21(6)	41(5)	-3(4)	10(4)	-5(5)
C(2)	29(6)	44(7)	35(5)	-5(5)	20(4)	-1(6)
C(3)	42(7)	38(7)	36(5)	6(5)	14(5)	3(6)
C(4)	45(8)	32(7)	44(6)	-12(5)	11(5)	-3(6)
C(5)	58(9)	50(8)	44(6)	-18(5)	6(6)	10(7)
C(6)	64(9)	48(8)	47(6)	-9(5)	25(6)	4(7)
C(7)	52(8)	51(8)	36(6)	0(5)	17(5)	18(7)
C(8)	95(11)	46(8)	36(6)	-1(5)	4(6)	36(8)
C(9)	69(10)	73(10)	50(7)	13(7)	6(7)	27(9)
C(10)	57(9)	53(9)	45(6)	-12(6)	17(6)	-12(7)
C(11)	32(7)	44(7)	45(6)	2(5)	16(5)	5(6)
C(12)	51(8)	38(7)	37(5)	3(5)	31(5)	14(6)
C(13)	32(7)	38(7)	35(5)	-11(4)	11(5)	-7(5)
C(14)	28(6)	41(7)	44(5)	-3(5)	14(5)	-12(6)
C(15)	35(7)	37(7)	56(7)	11(5)	26(5)	14(6)
C(16)	38(8)	62(9)	59(7)	0(6)	-9(6)	8(7)
C(17)	28(6)	56(8)	57(7)	1(6)	20(5)	-2(6)
C(18)	23(6)	66(8)	33(5)	-7(5)	6(4)	4(6)
C(19)	41(7)	93(11)	42(6)	-2(6)	26(5)	-19(7)
C(20)	40(8)	102(12)	51(7)	10(7)	23(6)	-24(8)
C(21)	45(8)	55(9)	66(8)	2(6)	9(6)	-1(7)
C(22)	29(6)	48(7)	39(6)	-4(5)	7(5)	-10(6)
C(23)	26(6)	52(7)	23(4)	-14(4)	6(4)	-7(5)
C(24)	39(6)	26(6)	32(5)	1(4)	-2(4)	7(5)
C(25)	42(7)	25(6)	33(5)	-1(4)	5(5)	-5(5)
C(26)	45(7)	35(7)	44(6)	11(5)	21(5)	1(6)
C(27)	62(9)	41(7)	51(6)	13(5)	34(6)	-13(6)
C(28)	49(7)	24(6)	49(6)	0(5)	17(5)	-11(5)
C(29)	47(7)	41(7)	33(5)	9(5)	10(5)	-3(6)
C(30)	96(11)	46(8)	45(7)	2(6)	13(7)	-30(8)
C(31)	82(10)	49(9)	55(7)	-17(6)	28(7)	-4(8)
C(32)	65(9)	48(8)	53(7)	0(6)	23(6)	-6(7)

C(33)	48(7)	39(7)	43(6)	4(5)	9(5)	14(6)
C(34)	45(7)	36(7)	26(5)	5(4)	-1(5)	-4(6)
C(35)	35(6)	39(7)	38(5)	-2(5)	12(4)	5(5)
C(36)	30(6)	54(8)	38(5)	-12(5)	9(5)	-16(6)
C(37)	37(7)	49(7)	28(5)	-1(5)	9(4)	-10(6)
C(38)	53(8)	49(8)	27(5)	-5(5)	2(5)	3(7)
C(39)	46(7)	63(8)	40(6)	3(5)	12(5)	-28(6)
C(40)	38(7)	48(7)	45(6)	-3(5)	15(5)	-14(6)
C(41)	27(6)	70(9)	31(5)	-11(5)	5(4)	0(6)
C(42)	23(7)	113(13)	51(7)	-8(7)	17(5)	5(7)
C(43)	37(7)	112(13)	75(9)	13(9)	26(7)	32(8)
C(44)	56(9)	57(9)	62(8)	7(6)	27(7)	26(7)
C(45)	28(6)	55(8)	49(6)	-6(6)	5(5)	-12(6)
C(46)	25(6)	42(7)	36(5)	-12(5)	2(4)	4(5)
C(47)	49(7)	24(6)	42(6)	8(4)	9(5)	9(6)
C(48)	36(6)	30(6)	29(5)	0(4)	11(4)	-8(5)
C(49)	31(7)	53(8)	38(6)	9(5)	11(5)	-7(6)
C(50)	73(9)	36(7)	42(6)	-4(5)	23(6)	6(6)
C(51)	70(8)	27(6)	37(6)	4(4)	17(6)	2(6)
C(52)	54(7)	44(7)	25(5)	5(5)	10(5)	-30(6)
C(53)	63(9)	64(9)	39(6)	-6(6)	14(6)	-28(7)
C(54)	56(9)	79(10)	71(9)	-12(7)	16(7)	-44(8)
C(55)	48(8)	71(10)	80(9)	11(8)	26(7)	-11(8)
C(56)	67(10)	35(7)	49(7)	17(5)	3(6)	-14(7)
C(57)	36(6)	34(7)	34(5)	13(5)	11(5)	5(5)
C(58)	37(7)	59(8)	30(5)	3(5)	8(5)	3(6)
C(59)	33(6)	32(6)	33(5)	-2(4)	18(4)	5(5)
C(60)	80(10)	25(6)	34(5)	-1(5)	4(6)	5(7)
C(61)	39(7)	68(9)	50(7)	-1(6)	4(5)	9(6)
C(62)	38(6)	53(7)	43(6)	-2(5)	15(5)	10(6)
C(63)	52(8)	29(6)	39(5)	0(4)	25(5)	12(6)
C(64)	80(10)	42(8)	45(6)	10(5)	18(6)	25(7)
C(65)	98(12)	31(7)	83(10)	6(6)	5(9)	23(8)
C(66)	51(9)	44(9)	105(11)	-17(7)	39(8)	-18(7)
C(67)	40(7)	53(8)	45(6)	-5(5)	23(5)	3(6)
C(68)	56(8)	30(6)	39(6)	7(5)	17(5)	3(6)
C(69)	34(7)	44(7)	50(6)	4(5)	22(5)	4(6)

C(70)	25(6)	33(6)	48(6)	-4(5)	15(5)	-10(5)
C(71)	33(7)	35(7)	39(5)	-2(5)	1(5)	-7(6)
C(72)	49(8)	31(7)	43(6)	-11(5)	-2(5)	-14(6)
C(73)	32(7)	36(7)	58(7)	-2(5)	11(5)	11(6)
C(74)	44(7)	52(8)	43(6)	-10(6)	8(5)	-3(6)
C(75)	40(7)	56(8)	40(6)	-20(6)	20(5)	-15(6)
C(76)	49(8)	49(8)	48(6)	-11(6)	17(6)	-13(6)
C(77)	55(9)	104(13)	50(7)	-21(8)	35(6)	-34(9)
C(78)	75(10)	50(8)	50(7)	8(6)	24(7)	-24(7)
C(79)	63(9)	43(8)	46(6)	-5(5)	14(6)	-18(7)
C(80)	40(7)	36(7)	38(5)	-7(5)	8(5)	-12(6)
C(81)	42(7)	28(6)	44(6)	1(5)	15(5)	-8(5)
C(82)	43(7)	37(7)	38(5)	6(5)	17(5)	8(6)
C(83)	39(7)	55(8)	38(6)	3(5)	12(5)	3(6)
C(84)	51(8)	54(9)	58(7)	13(6)	25(6)	-10(7)
C(85)	60(9)	57(9)	34(6)	4(5)	5(6)	-8(7)
C(86)	53(8)	28(6)	45(6)	10(5)	1(6)	-6(6)
C(87)	62(8)	35(7)	44(6)	0(5)	5(6)	0(6)
C(88)	112(13)	15(6)	56(8)	-5(5)	-5(8)	-15(8)
C(89)	88(11)	42(8)	43(6)	-7(5)	20(6)	13(8)
C(90)	64(8)	38(7)	39(6)	3(5)	15(6)	5(6)
C(91)	45(7)	26(6)	32(5)	0(4)	10(5)	1(5)
C(92)	44(7)	30(6)	41(5)	4(4)	16(5)	9(6)
C(93)	41(7)	32(6)	37(5)	-3(4)	16(5)	4(6)
C(94)	41(7)	46(8)	44(6)	1(5)	21(5)	2(6)
C(95)	65(9)	35(7)	59(7)	-16(5)	32(7)	-15(7)
C(96)	69(9)	32(7)	37(6)	-3(5)	8(6)	17(7)
C(97)	46(7)	44(7)	26(5)	2(5)	13(5)	8(6)
C(98)	57(9)	56(8)	47(6)	3(6)	18(6)	17(7)
C(99)	60(9)	87(11)	43(7)	15(7)	27(6)	41(9)
C(100)	44(8)	89(12)	46(7)	-1(7)	0(6)	9(8)
C(101)	40(7)	67(9)	40(6)	-4(6)	13(5)	4(7)
C(102)	36(7)	49(8)	29(5)	2(5)	12(5)	6(6)
C(103)	44(7)	33(7)	32(5)	0(4)	10(5)	-3(6)
C(104)	32(7)	62(8)	35(5)	-3(5)	3(5)	13(6)
C(105)	28(6)	54(8)	35(5)	-17(5)	9(5)	1(6)
C(106)	36(7)	59(9)	47(6)	7(6)	7(5)	21(7)

C(107)	58(9)	33(7)	72(8)	-6(6)	-5(7)	5(7)
C(108)	41(8)	45(8)	73(8)	-19(6)	-3(6)	21(7)
C(109)	52(9)	90(11)	40(6)	-14(7)	14(6)	23(8)
C(110)	27(7)	130(15)	63(8)	-20(9)	13(6)	11(8)
C(111)	31(8)	154(18)	83(11)	3(11)	21(7)	-3(10)
C(112)	36(8)	115(13)	74(9)	-3(8)	38(7)	8(8)
C(113)	50(9)	95(12)	39(6)	-3(7)	-9(6)	17(8)
C(114)	32(6)	30(6)	33(5)	-1(4)	11(4)	-7(5)
C(115)	61(8)	44(8)	34(5)	-11(5)	17(5)	-9(7)
C(116)	55(8)	30(7)	44(6)	2(5)	30(6)	7(6)
C(117)	57(9)	27(7)	51(6)	2(5)	9(6)	2(6)
C(118)	69(10)	67(10)	74(9)	-19(7)	39(7)	-46(9)
C(119)	143(16)	15(6)	77(9)	-13(6)	55(10)	-16(9)
C(120)	94(11)	43(8)	38(6)	0(5)	27(7)	14(8)
C(121)	120(15)	21(7)	88(10)	10(6)	53(10)	19(8)
C(122)	102(13)	45(9)	68(9)	-3(6)	13(8)	14(9)
C(123)	93(12)	62(10)	65(8)	24(7)	13(8)	31(9)
C(124)	98(12)	50(9)	51(7)	-4(6)	37(8)	-2(9)
C(125)	50(7)	27(6)	36(5)	-10(4)	17(5)	3(6)
C(126)	45(7)	43(7)	37(5)	16(5)	14(5)	7(6)
C(127)	41(7)	38(7)	24(5)	16(4)	-4(4)	-14(6)
C(128)	44(8)	27(7)	60(7)	-10(5)	24(6)	-10(6)
C(129)	49(8)	77(11)	57(8)	20(7)	21(6)	18(8)
C(130)	35(7)	82(11)	69(8)	22(7)	29(6)	-7(8)
C(131)	50(8)	75(10)	34(6)	20(6)	-5(5)	-25(8)
C(132)	72(10)	62(10)	68(9)	0(7)	12(7)	-28(8)
C(133)	116(14)	80(12)	54(8)	24(8)	1(8)	-69(11)
C(134)	94(11)	58(9)	47(7)	-10(6)	7(7)	-24(8)
C(135)	60(9)	54(9)	46(6)	16(6)	15(6)	-15(7)
C(136)	51(8)	35(7)	37(6)	10(5)	8(5)	-2(6)
C(137)	32(6)	28(6)	35(5)	-1(4)	12(4)	7(5)
C(138)	27(6)	31(6)	36(5)	-8(4)	13(4)	3(5)
C(139)	30(6)	30(6)	28(5)	2(4)	-3(4)	2(5)
C(140)	51(8)	25(7)	51(6)	-10(5)	7(6)	6(6)
C(141)	60(9)	40(8)	58(7)	-2(6)	12(6)	6(7)
C(142)	46(9)	63(10)	76(9)	-6(7)	3(7)	1(7)
C(143)	35(7)	62(9)	52(7)	-19(6)	6(5)	2(7)

C(144)	52(9)	72(10)	72(9)	-20(7)	15(7)	23(8)
C(145)	42(8)	98(13)	81(10)	-5(9)	21(7)	13(9)
C(146)	51(8)	59(9)	60(7)	-9(6)	15(6)	-4(7)
C(147)	32(7)	87(10)	39(6)	-6(6)	18(5)	-5(7)
C(148)	57(9)	41(7)	31(5)	-8(5)	3(5)	5(6)
C(149)	35(6)	26(6)	33(5)	7(4)	5(4)	-14(5)
C(150)	36(7)	46(7)	28(5)	-3(4)	15(4)	-2(6)
C(151)	20(6)	83(11)	46(6)	13(6)	8(5)	9(7)
C(152)	37(7)	50(8)	68(8)	6(6)	19(6)	-5(6)
C(153)	54(9)	78(11)	78(9)	27(8)	24(7)	4(8)
C(154)	36(7)	52(8)	57(7)	22(6)	13(6)	-6(6)
C(155)	42(8)	85(11)	56(8)	26(7)	-2(6)	-23(8)
C(156)	74(11)	86(12)	46(7)	28(7)	-6(7)	-35(9)
C(157)	60(8)	27(7)	73(8)	8(5)	28(7)	-4(6)
C(158)	77(10)	53(9)	33(6)	-6(5)	-1(6)	-20(8)
C(159)	36(7)	56(8)	34(5)	14(5)	3(5)	3(6)
C(160)	52(7)	22(6)	29(5)	9(4)	23(5)	13(5)
C(161)	38(7)	47(8)	24(5)	-1(4)	11(4)	-4(6)
C(162)	41(7)	38(7)	44(6)	-5(5)	11(5)	-17(6)
C(163)	47(8)	50(8)	58(7)	-5(6)	18(6)	6(7)
C(164)	61(9)	53(9)	92(10)	-28(7)	34(8)	-2(8)
C(165)	65(9)	38(7)	56(7)	-1(5)	33(6)	-8(7)
C(166)	85(11)	47(9)	72(9)	13(6)	43(8)	7(8)
C(167)	121(15)	47(9)	77(9)	5(7)	48(10)	51(10)
C(168)	63(9)	58(9)	66(8)	4(6)	28(7)	27(7)
C(169)	64(9)	50(8)	36(6)	2(5)	12(5)	26(7)
C(170)	59(8)	45(8)	39(6)	1(5)	24(6)	3(7)
C(171)	250(30)	240(30)	290(40)	-100(30)	150(30)	-200(30)
C(172)	160(20)	170(20)	210(30)	130(20)	80(20)	19(18)
C(173)	119(16)	83(13)	86(11)	2(10)	43(11)	-4(12)
C(174)	56(11)	142(17)	122(15)	-67(12)	52(11)	-32(11)
C(176)	127(19)	210(30)	130(20)	65(19)	-27(15)	-19(18)
C(177)	400(50)	120(20)	190(30)	28(19)	-50(30)	-150(30)
C(178)	270(30)	116(19)	230(30)	31(19)	190(30)	50(20)
C(179)	94(12)	45(10)	130(15)	21(9)	0(11)	-18(9)
N(1)	33(6)	29(5)	61(6)	-2(4)	25(4)	-11(4)
N(2)	49(6)	29(5)	39(5)	1(4)	14(4)	-1(5)

N(3)	26(5)	20(5)	61(5)	3(4)	14(4)	6(4)
N(4)	26(5)	31(5)	47(5)	-2(4)	10(4)	-3(4)
N(5)	23(5)	39(6)	65(6)	3(4)	21(4)	2(4)
N(6)	35(5)	26(5)	48(5)	5(4)	14(4)	4(4)
N(7)	35(5)	23(4)	56(5)	2(4)	22(4)	-5(4)
N(8)	42(6)	36(6)	42(5)	4(4)	10(4)	4(5)
N(9)	34(5)	27(5)	60(5)	-3(4)	19(4)	0(4)
N(10)	38(6)	20(5)	55(5)	3(4)	24(4)	3(4)
N(11)	23(4)	27(5)	60(5)	1(4)	20(4)	5(4)
N(12)	40(6)	31(6)	44(5)	-9(4)	4(4)	-8(5)
N(13)	31(5)	26(5)	60(6)	0(4)	11(4)	-5(4)
N(14)	26(5)	50(6)	40(4)	-4(4)	5(4)	12(5)
N(15)	44(6)	21(5)	52(5)	6(4)	22(4)	4(4)
N(16)	28(5)	44(6)	41(5)	2(4)	12(4)	-18(4)
N(17)	31(5)	32(5)	51(5)	-3(4)	14(4)	-1(4)
N(18)	42(6)	19(5)	47(5)	-3(4)	24(4)	4(4)
N(19)	39(6)	28(5)	48(5)	1(4)	8(4)	-6(5)
N(20)	38(6)	28(5)	27(4)	-3(3)	10(4)	4(4)
N(21)	35(6)	37(6)	46(5)	9(4)	16(4)	12(5)
N(22)	27(5)	30(5)	40(5)	-3(4)	4(4)	-2(4)
N(23)	28(5)	24(5)	52(5)	-5(4)	15(4)	-3(4)
N(24)	37(5)	28(5)	29(4)	6(3)	11(4)	1(4)
N(25)	14(4)	31(5)	51(5)	-1(4)	14(3)	-3(4)
N(26)	36(5)	30(5)	40(5)	0(4)	9(4)	5(4)
N(27)	30(5)	19(5)	56(5)	4(4)	24(4)	3(4)
N(28)	37(5)	45(6)	30(4)	-1(4)	18(4)	0(5)
N(29)	34(5)	25(5)	48(5)	-3(4)	22(4)	-3(4)
N(30)	29(5)	36(6)	41(5)	-3(4)	20(4)	1(4)
N(31)	127(13)	87(10)	88(10)	14(8)	23(9)	10(10)
N(32)	80(11)	133(13)	106(11)	-3(10)	53(9)	-23(10)
N(33)	104(11)	76(10)	88(9)	-10(7)	22(8)	-20(8)
O(1)	39(5)	19(4)	88(6)	-14(4)	14(4)	-6(4)
O(2)	33(5)	46(5)	83(6)	15(4)	16(4)	7(4)
O(3)	52(5)	32(5)	86(6)	-3(4)	44(4)	-9(4)
O(4)	51(6)	47(5)	78(6)	12(4)	25(5)	2(5)
O(5)	60(6)	42(5)	65(5)	-16(4)	29(4)	-1(4)
O(6)	55(5)	51(6)	57(5)	9(4)	5(4)	5(4)

O(7)	57(5)	51(5)	66(5)	16(4)	35(4)	4(4)
O(8)	68(6)	37(5)	71(5)	-15(4)	35(5)	0(4)
O(9)	42(5)	77(6)	56(5)	0(4)	5(4)	16(5)
O(10)	45(5)	44(5)	103(7)	16(5)	21(5)	8(4)
O(11)	59(6)	57(6)	97(6)	-4(5)	59(5)	3(5)
O(12)	47(5)	45(5)	96(7)	-15(5)	9(5)	-7(5)
O(13)	47(5)	51(5)	75(5)	17(4)	33(4)	8(4)
O(14)	56(6)	29(5)	88(6)	-8(4)	31(4)	-11(4)
O(15)	37(5)	42(5)	85(6)	-5(4)	16(4)	2(4)
O(16)	55(6)	75(7)	89(7)	-14(5)	40(5)	-20(5)
O(17)	75(6)	46(6)	78(6)	8(4)	19(5)	-4(5)
O(18)	55(6)	74(6)	67(5)	-14(4)	17(4)	-20(5)