

ORGANIC LETTERS

Anion-Orchestrated Formation in the Crystalline State of [2]Pseudorotaxane Arrays

Peter R. Ashton, Stuart J. Cantrill, Jon A. Preece, J. Fraser Stoddart, Zhen-He Wang,
Andrew J. P. White and David J. Williams

SUPPORTING INFORMATION (20 PAGES)

CRYSTAL DATA FOR [TB24C8/DBA][PF6]

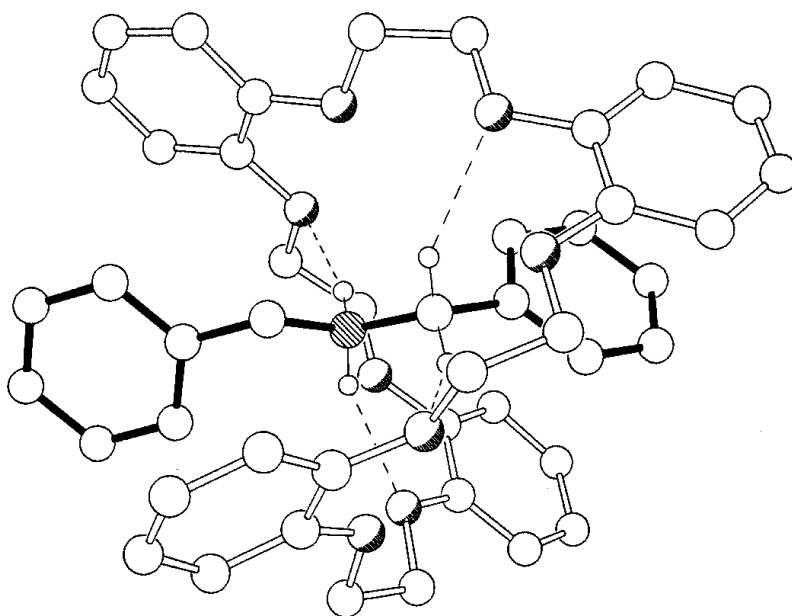


Table 1. Crystal data and structure refinement for 1.

Identification code	FS9812
Empirical formula	$[\text{C}_{46}\text{H}_{48}\text{NO}_8][\text{PF}_6] \cdot 1/2\text{MeCN} \cdot 1/8\text{CH}_2\text{Cl}_2$
Formula weight	918.97
Temperature	183(2) K
Diffractometer Used	Siemens P4/RA
Wavelength	1.54178 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	$a = 14.1821(10)$ Å $\alpha = 91.513(5)^\circ$ $b = 23.357(2)$ Å $\beta = 90.506(5)^\circ$ $c = 28.107(2)$ Å $\gamma = 104.367(6)^\circ$
Volume, Z	$9014.8(11)$ Å ³ , 8
Density (calculated)	1.354 Mg/m ³
Absorption coefficient	1.366 mm ⁻¹
F(000)	3842
Crystal colour/morphology	Clear platy prisms
Crystal size	0.43 x 0.20 x 0.07 mm
θ range for data collection	1.57 to 57.50°
Limiting indices	$0 \leq h \leq 14$, $-25 \leq k \leq 24$, $-30 \leq l \leq 30$
Scan type	ω -scans
Reflections collected	25394
Independent reflections	24143 ($R_{\text{int}} = 0.0864$)
Observed reflections [$F > 4\sigma(F)$]	12765
Absorption correction	None
Structure solution method	Direct
Refinement method	Full-matrix-block least-squares on F^2
Data / restraints / parameters	20485 / 457 / 2264
Goodness-of-fit on F^2	1.051
Final R indices [$F > 4\sigma(F)$]	$R1 = 0.0889$, $wR2 = 0.2158$
R indices (all data)	$R1 = 0.1744$, $wR2 = 0.2863$
Extinction coefficient	$0.00006(2)$
Largest diff. peak and hole	0.875 and -0.348 eÅ ⁻³
Mean and maximum shift/error	0.000 and 0.003

Table 2. Atomic coordinates [$\times 10^4$], equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] and site occupancy factors for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)	sof
O(1)	8186 (4)	6902 (2)	8803 (2)	46 (1)	1
C(2)	8556 (6)	6831 (4)	8339 (3)	44 (2)	1
C(3)	9120 (6)	7421 (4)	8198 (3)	51 (2)	1
O(4)	10044 (4)	7562 (2)	8438 (2)	42 (1)	1
C(5)	10644 (6)	8109 (3)	8385 (2)	37 (2)	1
C(6)	10422 (7)	8575 (4)	8138 (3)	49 (2)	1
C(7)	11087 (8)	9101 (4)	8102 (3)	57 (3)	1
C(8)	11995 (8)	9201 (4)	8311 (3)	57 (2)	1
C(9)	12246 (6)	8739 (4)	8562 (3)	43 (2)	1
C(10)	11581 (6)	8213 (3)	8600 (2)	38 (2)	1
O(11)	11719 (4)	7741 (2)	8856 (2)	41 (1)	1
C(12)	12685 (5)	7781 (3)	9024 (2)	35 (2)	1
C(13)	12657 (6)	7242 (3)	9305 (2)	34 (2)	1
O(14)	12202 (4)	7291 (2)	9749 (2)	34 (1)	1
C(15)	12177 (6)	6838 (3)	10054 (3)	35 (2)	1
C(16)	12492 (6)	6330 (3)	9935 (3)	45 (2)	1
C(17)	12411 (7)	5896 (4)	10262 (3)	54 (2)	1
C(18)	12034 (7)	5945 (4)	10708 (3)	54 (2)	1
C(19)	11697 (6)	6443 (3)	10833 (3)	41 (2)	1
C(20)	11789 (6)	6885 (3)	10507 (3)	33 (2)	1
O(21)	11501 (4)	7410 (2)	10594 (2)	33 (1)	1
C(22)	11131 (6)	7467 (3)	11061 (2)	37 (2)	1
C(23)	10881 (6)	8052 (4)	11116 (3)	40 (2)	1
O(24)	9996 (4)	8022 (2)	10852 (2)	35 (1)	1
C(25)	9593 (5)	8504 (3)	10900 (2)	31 (2)	1
C(26)	10001 (6)	9008 (3)	11168 (3)	41 (2)	1
C(27)	9540 (7)	9468 (3)	11178 (3)	47 (2)	1
C(28)	8707 (7)	9432 (3)	10933 (3)	47 (2)	1
C(29)	8277 (6)	8924 (3)	10660 (3)	40 (2)	1
C(30)	8734 (6)	8459 (3)	10646 (2)	33 (2)	1
O(31)	8370 (4)	7933 (2)	10390 (2)	35 (1)	1
C(32)	7390 (6)	7839 (3)	10202 (3)	37 (2)	1
C(33)	7021 (6)	7200 (3)	10050 (3)	39 (2)	1
O(34)	7452 (4)	7088 (2)	9610 (2)	38 (1)	1
C(35)	7209 (6)	6504 (3)	9444 (3)	37 (2)	1
C(36)	6638 (6)	6050 (4)	9672 (3)	48 (2)	1
C(37)	6443 (8)	5476 (4)	9475 (3)	59 (2)	1
C(38)	6849 (7)	5382 (4)	9049 (3)	56 (2)	1
C(39)	7422 (6)	5839 (4)	8803 (3)	47 (2)	1
C(40)	7616 (6)	6410 (3)	9000 (3)	37 (2)	1
N(41)	10418 (4)	7803 (2)	9861 (2)	37 (1)	1
C(42)	9740 (6)	7303 (2)	9597 (2)	41 (2)	1
C(43)	9766 (5)	6238 (2)	9603 (2)	58 (2)	1
C(44)	9574 (5)	5692 (2)	9815 (2)	72 (3)	1
C(45)	9199 (5)	5630 (2)	10271 (2)	69 (3)	1
C(46)	9017 (4)	6116 (2)	10516 (2)	54 (2)	1
C(47)	9209 (4)	6663 (2)	10303 (2)	34 (2)	1
C(48)	9583 (4)	6724 (2)	9847 (2)	44 (2)	1
C(49)	10405 (6)	8383 (2)	9660 (2)	46 (2)	1
C(50)	10848 (4)	9390 (2)	10047 (2)	60 (3)	1
C(51)	11524 (5)	9881 (2)	10237 (2)	74 (3)	1
C(52)	12499 (5)	9874 (2)	10275 (2)	70 (3)	1
C(53)	12798 (3)	9376 (3)	10124 (2)	68 (3)	1

C(54)	12122 (4)	8886 (2)	9934 (2)	50 (2)	1
C(55)	11147 (3)	8893 (2)	9895 (2)	43 (2)	1
O(1')	2564 (4)	7368 (2)	7237 (2)	37 (1)	1
C(2')	2048 (6)	7309 (3)	7672 (2)	38 (2)	1
C(3')	2079 (6)	6738 (4)	7895 (3)	43 (2)	1
O(4')	3061 (4)	6798 (2)	8071 (2)	35 (1)	1
C(5')	3201 (6)	6354 (3)	8366 (2)	31 (2)	1
C(6')	2490 (7)	5872 (3)	8487 (3)	44 (2)	1
C(7')	2695 (7)	5454 (3)	8782 (3)	53 (2)	1
C(8')	3639 (8)	5535 (4)	8949 (3)	56 (3)	1
C(9')	4367 (7)	6009 (3)	8836 (3)	47 (2)	1
C(10')	4157 (6)	6440 (3)	8549 (2)	33 (2)	1
O(11')	4814 (4)	6941 (2)	8418 (2)	35 (1)	1
C(12')	5743 (6)	7057 (3)	8667 (2)	39 (2)	1
C(13')	6307 (6)	7682 (3)	8602 (2)	35 (2)	1
O(14')	6739 (4)	7737 (2)	8147 (2)	35 (1)	1
C(15')	7325 (6)	8270 (3)	8047 (3)	35 (2)	1
C(16')	7544 (6)	8753 (3)	8362 (3)	39 (2)	1
C(17')	8176 (6)	9279 (3)	8234 (3)	46 (2)	1
C(18')	8583 (6)	9320 (3)	7790 (3)	42 (2)	1
C(19')	8370 (6)	8842 (3)	7465 (3)	42 (2)	1
C(20')	7760 (5)	8321 (3)	7603 (2)	31 (2)	1
O(21')	7531 (4)	7810 (2)	7324 (2)	37 (1)	1
C(22')	8051 (6)	7828 (3)	6879 (2)	38 (2)	1
C(23')	7766 (6)	7217 (3)	6641 (3)	37 (2)	1
O(24')	6813 (4)	7130 (2)	6444 (2)	35 (1)	1
C(25')	6460 (6)	6619 (3)	6179 (2)	35 (2)	1
C(26')	7008 (6)	6201 (3)	6085 (2)	39 (2)	1
C(27')	6583 (6)	5702 (3)	5791 (3)	43 (2)	1
C(28')	5679 (6)	5628 (3)	5611 (3)	39 (2)	1
C(29')	5122 (6)	6024 (3)	5711 (3)	41 (2)	1
C(30')	5544 (6)	6529 (3)	5991 (2)	33 (2)	1
O(31')	5055 (4)	6961 (2)	6108 (2)	36 (1)	1
C(32')	4204 (6)	6969 (3)	5837 (3)	37 (2)	1
C(33')	3894 (6)	7519 (3)	5959 (2)	34 (2)	1
O(34')	3461 (4)	7466 (2)	6421 (2)	34 (1)	1
C(35')	3089 (6)	7946 (3)	6567 (3)	35 (2)	1
C(36')	3199 (6)	8446 (3)	6315 (3)	43 (2)	1
C(37')	2811 (7)	8903 (4)	6495 (3)	51 (2)	1
C(38')	2350 (7)	8854 (4)	6920 (3)	49 (2)	1
C(39')	2241 (6)	8344 (3)	7176 (3)	40 (2)	1
C(40')	2634 (6)	7885 (3)	7006 (2)	33 (2)	1
N(41')	4317 (5)	6901 (3)	7224 (2)	36 (1)	1
C(42')	5302 (5)	7320 (3)	7278 (3)	37 (2)	1
C(43')	5659 (4)	8292 (2)	6886 (2)	54 (2)	1
C(44')	5613 (5)	8879 (2)	6865 (2)	78 (3)	1
C(45')	5155 (6)	9125 (2)	7223 (3)	97 (5)	1
C(46')	4743 (6)	8785 (3)	7602 (2)	89 (4)	1
C(47')	4788 (5)	8199 (2)	7623 (2)	59 (2)	1
C(48')	5246 (4)	7952 (2)	7265 (2)	41 (2)	1
C(49')	4403 (6)	6277 (3)	7165 (3)	45 (2)	1
C(50')	3354 (4)	5375 (2)	7505 (2)	53 (2)	1
C(51')	2491 (5)	4936 (2)	7520 (2)	61 (3)	1
C(52')	1728 (4)	4944 (2)	7208 (2)	63 (3)	1
C(53')	1828 (4)	5391 (3)	6882 (2)	67 (3)	1
C(54')	2691 (4)	5830 (2)	6867 (2)	53 (2)	1
C(55')	3454 (3)	5822 (2)	7178 (2)	41 (2)	1
O(1")	8140 (4)	7233 (2)	3748 (2)	42 (1)	1
C(2")	8589 (6)	7341 (4)	3291 (2)	41 (2)	1
C(3")	9214 (6)	7949 (3)	3297 (3)	38 (2)	1
O(4")	10105 (4)	7979 (2)	3557 (2)	38 (1)	1
C(5")	10816 (6)	8487 (3)	3515 (2)	34 (2)	1

C(6")	10705 (7)	8991 (3)	3309 (3)	42 (2)	1
C(7")	11479 (8)	9487 (4)	3280 (3)	54 (2)	1
C(8")	12377 (8)	9484 (4)	3460 (3)	62 (3)	1
C(9")	12489 (7)	8974 (4)	3689 (3)	49 (2)	1
C(10")	11728 (6)	8482 (3)	3717 (2)	35 (2)	1
O(11")	11798 (4)	7967 (2)	3927 (2)	39 (1)	1
C(12")	12745 (6)	7958 (4)	4094 (3)	44 (2)	1
C(13")	12705 (6)	7355 (4)	4284 (2)	41 (2)	1
O(14")	12184 (4)	7290 (2)	4720 (2)	39 (1)	1
C(15")	12146 (6)	6784 (3)	4960 (3)	38 (2)	1
C(16")	12546 (7)	6322 (4)	4807 (3)	49 (2)	1
C(17")	12455 (7)	5831 (4)	5076 (3)	55 (2)	1
C(18")	11992 (7)	5781 (4)	5500 (3)	53 (2)	1
C(19")	11578 (6)	6243 (3)	5658 (3)	45 (2)	1
C(20")	11665 (5)	6732 (3)	5392 (2)	33 (2)	1
O(21")	11283 (4)	7206 (2)	5520 (2)	41 (1)	1
C(22")	10870 (6)	7195 (3)	5987 (2)	38 (2)	1
C(23")	10623 (6)	7775 (4)	6088 (3)	42 (2)	1
O(24")	9771 (4)	7784 (2)	5812 (2)	42 (1)	1
C(25")	9384 (6)	8259 (3)	5895 (2)	37 (2)	1
C(26")	9858 (6)	8772 (4)	6141 (3)	45 (2)	1
C(27")	9393 (7)	9230 (4)	6193 (3)	51 (2)	1
C(28")	8485 (7)	9182 (3)	6007 (3)	46 (2)	1
C(29")	8005 (6)	8673 (3)	5749 (3)	40 (2)	1
C(30")	8466 (5)	8213 (3)	5697 (2)	33 (2)	1
O(31")	8051 (4)	7687 (2)	5452 (2)	34 (1)	1
C(32")	7092 (5)	7626 (3)	5262 (2)	31 (2)	1
C(33")	6792 (5)	7040 (3)	4996 (2)	30 (2)	1
O(34")	7305 (4)	7098 (2)	4556 (2)	35 (1)	1
C(35")	7139 (6)	6588 (3)	4264 (2)	34 (2)	1
C(36")	6592 (6)	6050 (3)	4392 (3)	47 (2)	1
C(37")	6470 (7)	5574 (4)	4060 (3)	59 (3)	1
C(38")	6898 (7)	5660 (4)	3623 (3)	62 (3)	1
C(39")	7457 (7)	6202 (4)	3501 (3)	53 (2)	1
C(40")	7599 (6)	6679 (3)	3828 (3)	37 (2)	1
N(41")	10383 (6)	7709 (3)	4717 (3)	47 (2)	0.70
C(42")	9481 (7)	7220 (4)	4630 (5)	54 (3)	0.70
C(43")	10092 (7)	6568 (4)	4051 (3)	58 (4)	0.70
C(44")	10250 (8)	6023 (5)	3914 (4)	89 (6)	0.70
C(45")	10039 (9)	5556 (3)	4223 (5)	102 (6)	0.70
C(46")	9670 (10)	5633 (4)	4670 (5)	113 (7)	0.70
C(47")	9511 (8)	6177 (4)	4808 (3)	96 (6)	0.70
C(48")	9722 (7)	6644 (3)	4498 (3)	50 (3)	0.70
C(49")	10126 (7)	8287 (4)	4740 (4)	41 (3)	0.70
C(50")	11842 (6)	8753 (3)	5042 (3)	51 (3)	0.70
C(51")	12570 (5)	9250 (4)	5176 (4)	58 (3)	0.70
C(52")	12396 (7)	9809 (3)	5154 (4)	80 (5)	0.70
C(53")	11494 (8)	9870 (3)	4999 (5)	108 (7)	0.70
C(54")	10766 (6)	9373 (4)	4865 (4)	89 (6)	0.70
C(55")	10940 (5)	8814 (3)	4887 (3)	44 (3)	0.70
N(41B)	10237 (17)	7423 (7)	4540 (9)	53 (7)	0.30
C(42B)	9554 (19)	6831 (7)	4606 (10)	51 (10)	0.30
C(43B)	10110 (19)	6379 (8)	3877 (6)	54 (10)	0.30
C(44B)	10346 (21)	5908 (10)	3635 (6)	76 (11)	0.30
C(45B)	10384 (21)	5402 (9)	3877 (8)	77 (10)	0.30
C(46B)	10186 (22)	5368 (8)	4361 (8)	69 (10)	0.30
C(47B)	9949 (21)	5840 (9)	4602 (6)	84 (12)	0.30
C(48B)	9911 (18)	6345 (7)	4360 (6)	49 (7)	0.30
C(49B)	9851 (15)	7895 (7)	4769 (10)	55 (8)	0.30
C(50B)	11467 (15)	8573 (8)	5005 (9)	60 (11)	0.30
C(51B)	12101 (14)	9132 (10)	5039 (10)	69 (11)	0.30
C(52B)	11816 (19)	9617 (8)	4867 (10)	84 (11)	0.30

C(53B)	10898 (20)	9543 (8)	4661 (11)	107 (16)	0.30
C(54B)	10263 (16)	8984 (9)	4627 (10)	102 (13)	0.30
C(55B)	10548 (14)	8499 (7)	4799 (9)	46 (10)	0.30
O(1*)	2795 (4)	7884 (3)	2234 (2)	47 (1)	1
C(2*)	2246 (7)	7775 (4)	2656 (3)	59 (2)	1
C(3*)	2264 (7)	7172 (4)	2838 (3)	53 (2)	1
O(4*)	3199 (4)	7244 (2)	3060 (2)	45 (1)	1
C(5*)	3372 (7)	6754 (3)	3271 (3)	45 (2)	1
C(6*)	2698 (8)	6205 (4)	3280 (3)	63 (3)	1
C(7*)	2931 (11)	5743 (4)	3520 (4)	80 (4)	1
C(8*)	3813 (9)	5830 (4)	3751 (4)	68 (3)	1
C(9*)	4487 (8)	6369 (4)	3740 (3)	59 (2)	1
C(10*)	4268 (7)	6839 (3)	3506 (3)	43 (2)	1
O(11*)	4873 (4)	7396 (2)	3494 (2)	40 (1)	1
C(12*)	5758 (6)	7485 (4)	3751 (3)	45 (2)	1
C(13*)	6329 (7)	8110 (4)	3717 (3)	51 (2)	1
O(14*)	6781 (4)	8191 (2)	3261 (2)	43 (1)	1
C(15*)	7387 (6)	8727 (3)	3177 (2)	36 (2)	1
C(16*)	7634 (6)	9198 (3)	3510 (3)	45 (2)	1
C(17*)	8291 (7)	9721 (3)	3391 (3)	49 (2)	1
C(18*)	8709 (6)	9787 (3)	2957 (3)	44 (2)	1
C(19*)	8469 (6)	9314 (3)	2614 (3)	41 (2)	1
C(20*)	7821 (6)	8799 (3)	2733 (2)	34 (2)	1
O(21*)	7543 (4)	8311 (2)	2420 (2)	38 (1)	1
C(22*)	8080 (6)	8325 (3)	1985 (2)	34 (2)	1
C(23*)	7759 (6)	7727 (3)	1747 (3)	36 (2)	1
O(24*)	6821 (4)	7656 (2)	1532 (2)	32 (1)	1
C(25*)	6436 (5)	7116 (3)	1296 (2)	32 (2)	1
C(26*)	6899 (6)	6651 (3)	1302 (3)	44 (2)	1
C(27*)	6434 (7)	6116 (4)	1072 (3)	50 (2)	1
C(28*)	5571 (7)	6050 (4)	848 (3)	54 (2)	1
C(29*)	5099 (6)	6514 (3)	839 (3)	42 (2)	1
C(30*)	5541 (6)	7044 (3)	1068 (2)	32 (2)	1
O(31*)	5150 (4)	7525 (2)	1084 (2)	36 (1)	1
C(32*)	4244 (6)	7466 (3)	834 (3)	39 (2)	1
C(33*)	3910 (6)	8018 (4)	916 (2)	40 (2)	1
O(34*)	3619 (4)	8014 (2)	1412 (2)	37 (1)	1
C(35*)	3205 (6)	8460 (4)	1564 (3)	43 (2)	1
C(36*)	3237 (7)	8965 (4)	1311 (3)	55 (2)	1
C(37*)	2819 (8)	9402 (4)	1517 (4)	65 (3)	1
C(38*)	2433 (8)	9339 (5)	1956 (3)	67 (3)	1
C(39*)	2419 (7)	8844 (4)	2205 (3)	57 (2)	1
C(40*)	2805 (7)	8397 (4)	2014 (3)	48 (2)	1
N(41*)	5332 (5)	8163 (3)	2029 (2)	37 (1)	1
C(42*)	5072 (7)	7778 (3)	2445 (2)	42 (2)	1
C(43*)	4186 (4)	6819 (3)	2057 (2)	61 (3)	1
C(44*)	4104 (6)	6227 (3)	1939 (2)	88 (4)	1
C(45*)	4819 (7)	5955 (2)	2087 (3)	105 (6)	1
C(46*)	5615 (6)	6274 (3)	2354 (3)	102 (5)	1
C(47*)	5697 (4)	6866 (3)	2472 (2)	60 (3)	1
C(48*)	4982 (4)	7139 (2)	2324 (2)	45 (2)	1
C(49*)	5557 (7)	8811 (3)	2177 (3)	41 (2)	1
C(50*)	6073 (4)	9113 (2)	1341 (2)	47 (2)	1
C(51*)	6129 (4)	9503 (2)	971 (1)	45 (2)	1
C(52*)	5745 (5)	9993 (2)	1024 (2)	57 (2)	1
C(53*)	5304 (5)	10094 (2)	1448 (2)	63 (3)	1
C(54*)	5248 (4)	9704 (2)	1818 (2)	55 (2)	1
C(55*)	5632 (4)	9214 (2)	1765 (1)	39 (2)	1
P(10)	5258 (2)	8529 (1)	9661 (1)	39 (1)	1
F(11)	6336 (4)	8686 (2)	9451 (2)	56 (1)	1
F(12)	4828 (4)	8571 (3)	9142 (2)	69 (2)	1
F(13)	5189 (5)	7843 (2)	9563 (2)	69 (2)	1

F(14)	5689(4)	8476(2)	10178(2)	52(1)	1
F(15)	5311(4)	9205(2)	9765(2)	66(2)	1
F(16)	4187(4)	8354(2)	9870(2)	58(1)	1
P(20)	-449(2)	6207(1)	7036(1)	60(1)	1
F(21)	634(4)	6316(3)	6853(2)	71(2)	1
F(22)	-842(5)	6171(3)	6499(2)	87(2)	1
F(23)	-556(5)	5509(3)	7021(2)	90(2)	1
F(24)	-67(5)	6247(3)	7568(2)	86(2)	1
F(25)	-338(5)	6908(3)	7041(3)	88(2)	1
F(26)	-1530(5)	6106(4)	7224(3)	100(2)	1
P(30)	5200(2)	8611(1)	4957(1)	44(1)	1
F(31)	4111(4)	8457(3)	5138(2)	68(2)	1
F(32)	5601(4)	8607(3)	5491(2)	63(1)	1
F(33)	5262(5)	9297(2)	5019(2)	74(2)	1
F(34)	4812(4)	8620(3)	4426(2)	65(2)	1
F(35)	5140(5)	7922(2)	4902(2)	74(2)	1
F(36)	6295(4)	8757(2)	4774(2)	60(1)	1
P(40)	-450(2)	6683(1)	2142(1)	45(1)	1
F(41)	643(4)	6771(3)	1972(2)	64(1)	1
F(42)	-755(4)	6884(3)	1637(2)	75(2)	1
F(43)	-704(5)	6027(3)	1942(3)	96(2)	1
F(44)	-160(5)	6489(3)	2643(2)	89(2)	1
F(45)	-224(5)	7354(3)	2323(3)	93(2)	1
F(46)	-1546(4)	6595(2)	2315(2)	60(1)	1
N(60)	5055(10)	9385(6)	3267(4)	115(4)	1
C(61)	5073(9)	9645(5)	3604(4)	67(3)	1
C(62)	5047(9)	9999(4)	4040(4)	76(3)	1
N(63)	6157(11)	5926(8)	7837(5)	59(5)	0.50
C(64)	6271(8)	5640(5)	7620(5)	75(3)	1
C(65)	6406(12)	5225(6)	7187(5)	103(4)	1
N(66)	5302(18)	5101(9)	6894(7)	91(7)	0.50
C(70)	638(17)	5116(9)	1964(6)	77(8)	0.50
Cl(1)	225(4)	4735(3)	1425(2)	75(2)	0.50
Cl(2)	1712(5)	5419(3)	2046(2)	81(2)	0.50

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

O(1)-C(40)	1.365(10)	O(1)-C(2)	1.431(9)
C(2)-C(3)	1.479(12)	C(3)-O(4)	1.427(10)
O(4)-C(5)	1.362(10)	C(5)-C(6)	1.404(10)
C(5)-C(10)	1.416(12)	C(6)-C(7)	1.357(13)
C(7)-C(8)	1.375(14)	C(8)-C(9)	1.420(11)
C(9)-C(10)	1.358(11)	C(10)-O(11)	1.385(8)
O(11)-C(12)	1.425(9)	C(12)-C(13)	1.496(10)
C(13)-O(14)	1.425(8)	O(14)-C(15)	1.373(8)
C(15)-C(16)	1.401(10)	C(15)-C(20)	1.402(10)
C(16)-C(17)	1.370(12)	C(17)-C(18)	1.379(13)
C(18)-C(19)	1.400(12)	C(19)-C(20)	1.380(10)
C(20)-O(21)	1.402(8)	O(21)-C(22)	1.432(8)
C(22)-C(23)	1.501(10)	C(23)-O(24)	1.437(9)
O(24)-C(25)	1.388(8)	C(25)-C(26)	1.376(10)
C(25)-C(30)	1.386(10)	C(26)-C(27)	1.391(11)
C(27)-C(28)	1.346(12)	C(28)-C(29)	1.397(11)
C(29)-C(30)	1.396(10)	C(30)-O(31)	1.389(8)
O(31)-C(32)	1.445(9)	C(32)-C(33)	1.504(10)
C(33)-O(34)	1.431(9)	O(34)-C(35)	1.389(9)
C(35)-C(36)	1.346(11)	C(35)-C(40)	1.413(11)
C(36)-C(37)	1.399(12)	C(37)-C(38)	1.367(14)
C(38)-C(39)	1.378(13)	C(39)-C(40)	1.391(11)
N(41)-C(49)	1.486(6)	N(41)-C(42)	1.491(6)
C(42)-C(48)	1.509(6)	C(49)-C(55)	1.510(6)
O(1')-C(40')	1.368(8)	O(1')-C(2')	1.422(8)
C(2')-C(3')	1.499(10)	C(3')-O(4')	1.446(10)
O(4')-C(5')	1.396(8)	C(5')-C(6')	1.366(11)
C(5')-C(10')	1.410(11)	C(6')-C(7')	1.379(11)
C(7')-C(8')	1.381(14)	C(8')-C(9')	1.361(13)
C(9')-C(10')	1.391(10)	C(10')-O(11')	1.366(9)
O(11')-C(12')	1.447(9)	C(12')-C(13')	1.498(11)
C(13')-O(14')	1.418(8)	O(14')-C(15')	1.352(9)
C(15')-C(16')	1.388(10)	C(15')-C(20')	1.390(10)
C(16')-C(17')	1.387(12)	C(17')-C(18')	1.375(12)
C(18')-C(19')	1.395(11)	C(19')-C(20')	1.375(11)
C(20')-O(21')	1.378(8)	O(21')-C(22')	1.455(9)
C(22')-C(23')	1.518(10)	C(23')-O(24')	1.420(9)
O(24')-C(25')	1.371(8)	C(25')-C(30')	1.363(11)
C(25')-C(26')	1.411(10)	C(26')-C(27')	1.413(11)
C(27')-C(28')	1.343(12)	C(28')-C(29')	1.383(11)
C(29')-C(30')	1.399(10)	C(30')-O(31')	1.394(8)
O(31')-C(32')	1.425(9)	C(32')-C(33')	1.490(10)
C(33')-O(34')	1.438(8)	O(34')-C(35')	1.404(8)
C(35')-C(36')	1.359(11)	C(35')-C(40')	1.394(10)
C(36')-C(37')	1.402(11)	C(37')-C(38')	1.361(12)
C(38')-C(39')	1.384(11)	C(39')-C(40')	1.400(10)
N(41')-C(49')	1.498(9)	N(41')-C(42')	1.499(10)
C(42')-C(48')	1.499(8)	C(49')-C(55')	1.495(9)
O(1'')-C(40'')	1.356(9)	O(1'')-C(2'')	1.440(9)
C(2'')-C(3'')	1.476(11)	C(3'')-O(4'')	1.440(9)
O(4'')-C(5'')	1.362(9)	C(5'')-C(6'')	1.368(10)
C(5'')-C(10'')	1.412(11)	C(6'')-C(7'')	1.389(12)
C(7'')-C(8'')	1.369(14)	C(8'')-C(9'')	1.410(13)
C(9'')-C(10'')	1.373(11)	C(10'')-O(11'')	1.378(9)
O(11'')-C(12'')	1.425(10)	C(12'')-C(13'')	1.506(11)
C(13'')-O(14'')	1.428(9)	O(14'')-C(15'')	1.366(9)
C(15'')-C(20'')	1.392(11)	C(15'')-C(16'')	1.397(11)
C(16'')-C(17'')	1.371(12)	C(17'')-C(18'')	1.358(13)
C(18'')-C(19'')	1.416(12)	C(19'')-C(20'')	1.364(11)

C(20")-O(21")	1.387(8)	O(21")-C(22")	1.440(9)
C(22")-C(23")	1.502(10)	C(23")-O(24")	1.434(9)
O(24")-C(25")	1.370(9)	C(25")-C(26")	1.383(11)
C(25")-C(30")	1.390(11)	C(26")-C(27")	1.394(12)
C(27")-C(28")	1.362(12)	C(28")-C(29")	1.396(11)
C(29")-C(30")	1.395(10)	C(30")-O(31")	1.384(8)
O(31")-C(32")	1.428(9)	C(32")-C(33")	1.506(9)
C(33")-O(34")	1.433(8)	O(34")-C(35")	1.399(8)
C(35")-C(36")	1.362(11)	C(35")-C(40")	1.388(10)
C(36")-C(37")	1.409(11)	C(37")-C(38")	1.372(12)
C(38")-C(39")	1.371(12)	C(39")-C(40")	1.401(10)
N(41")-C(49")	1.483(8)	N(41")-C(42")	1.502(8)
C(42")-C(48")	1.505(8)	C(49")-C(55")	1.509(8)
N(41B)-C(49B)	1.481(9)	N(41B)-C(42B)	1.496(10)
C(42B)-C(48B)	1.508(8)	C(49B)-C(55B)	1.509(8)
O(1*)-C(40*)	1.359(10)	O(1*)-C(2*)	1.420(10)
C(2*)-C(3*)	1.517(13)	C(3*)-O(4*)	1.431(11)
O(4*)-C(5*)	1.377(9)	C(5*)-C(10*)	1.393(13)
C(5*)-C(6*)	1.397(12)	C(6*)-C(7*)	1.39(2)
C(7*)-C(8*)	1.37(2)	C(8*)-C(9*)	1.381(14)
C(9*)-C(10*)	1.391(11)	C(10*)-O(11*)	1.371(10)
O(11*)-C(12*)	1.410(10)	C(12*)-C(13*)	1.490(12)
C(13*)-O(14*)	1.433(9)	O(14*)-C(15*)	1.359(9)
C(15*)-C(20*)	1.392(11)	C(15*)-C(16*)	1.399(10)
C(16*)-C(17*)	1.391(12)	C(17*)-C(18*)	1.357(12)
C(18*)-C(19*)	1.421(11)	C(19*)-C(20*)	1.373(11)
C(20*)-O(21*)	1.396(8)	O(21*)-C(22*)	1.442(9)
C(22*)-C(23*)	1.495(10)	C(23*)-O(24*)	1.425(9)
O(24*)-C(25*)	1.394(8)	C(25*)-C(30*)	1.387(11)
C(25*)-C(26*)	1.401(10)	C(26*)-C(27*)	1.397(11)
C(27*)-C(28*)	1.343(13)	C(28*)-C(29*)	1.408(12)
C(29*)-C(30*)	1.382(10)	C(30*)-O(31*)	1.371(8)
O(31*)-C(32*)	1.433(9)	C(32*)-C(33*)	1.491(11)
C(33*)-O(34*)	1.456(9)	O(34*)-C(35*)	1.379(9)
C(35*)-C(36*)	1.384(12)	C(35*)-C(40*)	1.388(12)
C(36*)-C(37*)	1.415(13)	C(37*)-C(38*)	1.351(14)
C(38*)-C(39*)	1.364(13)	C(39*)-C(40*)	1.391(11)
N(41*)-C(42*)	1.487(9)	N(41*)-C(49*)	1.514(9)
C(42*)-C(48*)	1.496(8)	C(49*)-C(55*)	1.498(8)
C(40)-O(1)-C(2)	117.0(6)	O(1)-C(2)-C(3)	107.0(7)
O(4)-C(3)-C(2)	109.3(6)	C(5)-O(4)-C(3)	118.4(6)
O(4)-C(5)-C(6)	126.2(8)	O(4)-C(5)-C(10)	116.3(6)
C(6)-C(5)-C(10)	117.5(8)	C(7)-C(6)-C(5)	121.0(9)
C(6)-C(7)-C(8)	121.5(8)	C(7)-C(8)-C(9)	119.0(9)
C(10)-C(9)-C(8)	119.6(9)	C(9)-C(10)-O(11)	125.0(8)
C(9)-C(10)-C(5)	121.4(7)	O(11)-C(10)-C(5)	113.5(7)
C(10)-O(11)-C(12)	116.4(6)	O(11)-C(12)-C(13)	107.3(6)
O(14)-C(13)-C(12)	109.5(5)	C(15)-O(14)-C(13)	115.5(5)
O(14)-C(15)-C(16)	124.0(7)	O(14)-C(15)-C(20)	117.4(6)
C(16)-C(15)-C(20)	118.6(7)	C(17)-C(16)-C(15)	119.2(8)
C(16)-C(17)-C(18)	122.0(7)	C(17)-C(18)-C(19)	119.9(7)
C(20)-C(19)-C(18)	118.2(8)	C(19)-C(20)-O(21)	123.5(7)
C(19)-C(20)-C(15)	122.0(7)	O(21)-C(20)-C(15)	114.5(6)
C(20)-O(21)-C(22)	114.6(5)	O(21)-C(22)-C(23)	109.5(6)
O(24)-C(23)-C(22)	108.4(6)	C(25)-O(24)-C(23)	116.8(5)
C(26)-C(25)-C(30)	120.2(7)	C(26)-C(25)-O(24)	124.3(7)
C(30)-C(25)-O(24)	115.5(6)	C(25)-C(26)-C(27)	119.0(8)
C(28)-C(27)-C(26)	121.6(7)	C(27)-C(28)-C(29)	120.4(7)
C(30)-C(29)-C(28)	118.6(8)	C(25)-C(30)-O(31)	116.3(6)
C(25)-C(30)-C(29)	120.3(7)	O(31)-C(30)-C(29)	123.4(7)
C(30)-O(31)-C(32)	116.1(5)	O(31)-C(32)-C(33)	108.9(6)

O(34)-C(33)-C(32)	110.1(6)	C(35)-O(34)-C(33)	115.6(6)
C(36)-C(35)-O(34)	124.9(7)	C(36)-C(35)-C(40)	120.6(7)
O(34)-C(35)-C(40)	114.4(7)	C(35)-C(36)-C(37)	120.4(9)
C(38)-C(37)-C(36)	119.0(9)	C(37)-C(38)-C(39)	121.9(8)
C(38)-C(39)-C(40)	118.9(8)	O(1)-C(40)-C(39)	125.5(7)
O(1)-C(40)-C(35)	115.5(6)	C(39)-C(40)-C(35)	119.1(8)
C(49)-N(41)-C(42)	111.8(5)	N(41)-C(42)-C(48)	113.2(5)
C(47)-C(48)-C(42)	121.0(4)	C(43)-C(48)-C(42)	118.9(4)
N(41)-C(49)-C(55)	112.9(5)	C(54)-C(55)-C(49)	121.3(4)
C(50)-C(55)-C(49)	118.6(4)	C(40')-O(1')-C(2')	116.2(5)
O(1')-C(2')-C(3')	110.0(6)	O(4')-C(3')-C(2')	107.5(7)
C(5')-O(4')-C(3')	116.2(6)	C(6')-C(5')-O(4')	124.8(7)
C(6')-C(5')-C(10')	120.4(6)	O(4')-C(5')-C(10')	114.9(6)
C(5')-C(6')-C(7')	120.9(8)	C(6')-C(7')-C(8')	118.2(8)
C(9')-C(8')-C(7')	122.6(8)	C(8')-C(9')-C(10')	119.3(9)
O(11')-C(10')-C(9')	125.1(7)	O(11')-C(10')-C(5')	116.3(6)
C(9')-C(10')-C(5')	118.6(7)	C(10')-O(11')-C(12')	114.5(5)
O(11')-C(12')-C(13')	110.5(6)	O(14')-C(13')-C(12')	109.9(5)
C(15')-O(14')-C(13')	116.9(5)	O(14')-C(15')-C(16')	124.3(7)
O(14')-C(15')-C(20')	116.9(6)	C(16')-C(15')-C(20')	118.7(7)
C(17')-C(16')-C(15')	120.5(7)	C(18')-C(17')-C(16')	119.5(7)
C(17')-C(18')-C(19')	121.2(8)	C(20')-C(19')-C(18')	118.3(7)
C(19')-C(20')-O(21')	123.9(7)	C(19')-C(20')-C(15')	121.8(7)
O(21')-C(20')-C(15')	114.3(7)	C(20')-O(21')-C(22')	116.0(6)
O(21')-C(22')-C(23')	108.5(6)	O(24')-C(23')-C(22')	108.2(6)
C(25')-O(24')-C(23')	116.7(5)	C(30')-C(25')-O(24')	117.2(6)
C(30')-C(25')-C(26')	119.7(7)	O(24')-C(25')-C(26')	123.1(7)
C(25')-C(26')-C(27')	118.2(8)	C(28')-C(27')-C(26')	120.5(7)
C(27')-C(28')-C(29')	122.0(7)	C(28')-C(29')-C(30')	118.0(8)
C(25')-C(30')-O(31')	115.6(6)	C(25')-C(30')-C(29')	121.6(7)
O(31')-C(30')-C(29')	122.9(7)	C(30')-O(31')-C(32')	117.9(5)
O(31')-C(32')-C(33')	109.5(6)	O(34')-C(33')-C(32')	109.1(6)
C(35')-O(34')-C(33')	114.7(5)	C(36')-C(35')-C(40')	121.6(7)
C(36')-C(35')-O(34')	123.5(7)	C(40')-C(35')-O(34')	114.8(6)
C(35')-C(36')-C(37')	119.0(8)	C(38')-C(37')-C(36')	120.7(7)
C(37')-C(38')-C(39')	120.1(7)	C(38')-C(39')-C(40')	120.2(7)
O(1')-C(40')-C(35')	117.8(6)	O(1')-C(40')-C(39')	123.9(7)
C(35')-C(40')-C(39')	118.3(7)	C(49')-N(41')-C(42')	110.7(6)
N(41')-C(42')-C(48')	111.7(6)	C(47')-C(48')-C(42')	121.1(4)
C(43')-C(48')-C(42')	118.9(4)	C(55')-C(49')-N(41')	114.2(6)
C(54')-C(55')-C(49')	121.6(5)	C(50')-C(55')-C(49')	118.4(5)
C(40'')-O(1'')-C(2'')	117.7(6)	O(1'')-C(2'')-C(3'')	108.6(6)
O(4'')-C(3'')-C(2'')	110.3(6)	C(5'')-O(4'')-C(3'')	115.7(6)
O(4'')-C(5'')-C(6'')	125.7(8)	O(4'')-C(5'')-C(10'')	115.3(6)
C(6'')-C(5'')-C(10'')	119.0(7)	C(5'')-C(6'')-C(7'')	121.4(9)
C(8'')-C(7'')-C(6'')	120.4(8)	C(7'')-C(8'')-C(9'')	118.5(8)
C(10'')-C(9'')-C(8'')	121.2(9)	C(9'')-C(10'')-O(11'')	123.9(8)
C(9'')-C(10'')-C(5'')	119.3(7)	O(11'')-C(10'')-C(5'')	116.8(6)
C(10'')-O(11'')-C(12'')	115.5(6)	O(11'')-C(12'')-C(13'')	108.6(7)
O(14'')-C(13'')-C(12'')	109.0(6)	C(15'')-O(14'')-C(13'')	116.6(6)
O(14'')-C(15'')-C(20'')	116.2(6)	O(14'')-C(15'')-C(16'')	125.6(7)
C(20'')-C(15'')-C(16'')	118.2(7)	C(17'')-C(16'')-C(15'')	120.5(8)
C(18'')-C(17'')-C(16'')	121.4(8)	C(17'')-C(18'')-C(19'')	118.8(8)
C(20'')-C(19'')-C(18'')	119.9(8)	C(19'')-C(20'')-O(21'')	123.8(7)
C(19'')-C(20'')-C(15'')	121.1(7)	O(21'')-C(20'')-C(15'')	115.1(6)
C(20'')-O(21'')-C(22'')	116.4(6)	O(21'')-C(22'')-C(23'')	108.8(6)
O(24'')-C(23'')-C(22'')	108.1(6)	C(25'')-O(24'')-C(23'')	116.0(6)
O(24'')-C(25'')-C(26'')	124.5(7)	O(24'')-C(25'')-C(30'')	115.7(6)
C(26'')-C(25'')-C(30'')	119.8(7)	C(25'')-C(26'')-C(27'')	119.0(8)
C(28'')-C(27'')-C(26'')	121.5(7)	C(27'')-C(28'')-C(29'')	120.3(8)
C(30'')-C(29'')-C(28'')	118.6(8)	O(31'')-C(30'')-C(25'')	115.9(6)
O(31'')-C(30'')-C(29'')	123.2(7)	C(25'')-C(30'')-C(29'')	120.9(7)

C(30")-O(31")-C(32")	116.4(5)	O(31")-C(32")-C(33")	108.1(6)
O(34")-C(33")-C(32")	107.5(6)	C(35")-O(34")-C(33")	115.7(5)
C(36")-C(35")-C(40")	122.8(7)	C(36")-C(35")-O(34")	123.8(6)
C(40")-C(35")-O(34")	113.4(6)	C(35")-C(36")-C(37")	117.9(7)
C(38")-C(37")-C(36")	120.0(8)	C(39")-C(38")-C(37")	121.4(7)
C(38")-C(39")-C(40")	119.5(8)	O(1")-C(40")-C(35")	117.0(6)
O(1")-C(40")-C(39")	124.7(7)	C(35")-C(40")-C(39")	118.3(7)
C(49")-N(41")-C(42")	109.9(7)	N(41")-C(42")-C(48")	111.7(7)
C(47")-C(48")-C(42")	120.2(7)	C(43")-C(48")-C(42")	119.7(7)
N(41")-C(49")-C(55")	115.9(7)	C(54")-C(55")-C(49")	118.1(5)
C(50")-C(55")-C(49")	121.9(5)	C(49B)-N(41B)-C(42B)	110.4(12)
N(41B)-C(42B)-C(48B)	111.5(12)	C(47B)-C(48B)-C(42B)	120.3(9)
C(43B)-C(48B)-C(42B)	119.4(10)	N(41B)-C(49B)-C(55B)	115.4(13)
C(54B)-C(55B)-C(49B)	119.8(9)	C(50B)-C(55B)-C(49B)	120.2(9)
C(40*)-O(1*)-C(2*)	116.6(6)	O(1*)-C(2*)-C(3*)	109.7(7)
O(4*)-C(3*)-C(2*)	105.8(7)	C(5*)-O(4*)-C(3*)	116.4(7)
O(4*)-C(5*)-C(10*)	115.7(7)	O(4*)-C(5*)-C(6*)	124.3(9)
C(10*)-C(5*)-C(6*)	119.9(8)	C(7*)-C(6*)-C(5*)	119.7(11)
C(8*)-C(7*)-C(6*)	120.0(10)	C(7*)-C(8*)-C(9*)	120.7(10)
C(8*)-C(9*)-C(10*)	120.3(10)	O(11*)-C(10*)-C(9*)	124.4(9)
O(11*)-C(10*)-C(5*)	116.3(7)	C(9*)-C(10*)-C(5*)	119.3(8)
C(10*)-O(11*)-C(12*)	115.9(6)	O(11*)-C(12*)-C(13*)	110.2(6)
O(14*)-C(13*)-C(12*)	109.4(7)	C(15*)-O(14*)-C(13*)	117.8(6)
O(14*)-C(15*)-C(20*)	117.1(6)	O(14*)-C(15*)-C(16*)	124.7(7)
C(20*)-C(15*)-C(16*)	118.2(7)	C(17*)-C(16*)-C(15*)	119.9(8)
C(18*)-C(17*)-C(16*)	121.5(7)	C(17*)-C(18*)-C(19*)	119.5(8)
C(20*)-C(19*)-C(18*)	118.7(8)	C(19*)-C(20*)-C(15*)	122.2(7)
C(19*)-C(20*)-O(21*)	122.8(7)	C(15*)-C(20*)-O(21*)	115.1(7)
C(20*)-O(21*)-C(22*)	117.3(6)	O(21*)-C(22*)-C(23*)	107.5(6)
O(24*)-C(23*)-C(22*)	109.9(6)	C(25*)-O(24*)-C(23*)	115.7(5)
C(30*)-C(25*)-O(24*)	116.9(6)	C(30*)-C(25*)-C(26*)	120.7(6)
O(24*)-C(25*)-C(26*)	122.4(7)	C(27*)-C(26*)-C(25*)	118.2(8)
C(28*)-C(27*)-C(26*)	121.1(8)	C(27*)-C(28*)-C(29*)	121.3(8)
C(30*)-C(29*)-C(28*)	118.5(8)	O(31*)-C(30*)-C(29*)	123.7(7)
O(31*)-C(30*)-C(25*)	116.1(6)	C(29*)-C(30*)-C(25*)	120.2(7)
C(30*)-O(31*)-C(32*)	116.8(5)	O(31*)-C(32*)-C(33*)	108.8(6)
O(34*)-C(33*)-C(32*)	106.0(6)	C(35*)-O(34*)-C(33*)	116.8(6)
O(34*)-C(35*)-C(36*)	123.9(8)	O(34*)-C(35*)-C(40*)	115.4(7)
C(36*)-C(35*)-C(40*)	120.6(8)	C(35*)-C(36*)-C(37*)	118.2(9)
C(38*)-C(37*)-C(36*)	120.9(9)	C(37*)-C(38*)-C(39*)	120.4(8)
C(38*)-C(39*)-C(40*)	120.8(9)	O(1*)-C(40*)-C(35*)	116.5(7)
O(1*)-C(40*)-C(39*)	124.4(8)	C(35*)-C(40*)-C(39*)	119.1(8)
C(42*)-N(41*)-C(49*)	111.5(5)	N(41*)-C(42*)-C(48*)	112.8(6)
C(47*)-C(48*)-C(42*)	120.2(5)	C(43*)-C(48*)-C(42*)	119.8(5)
C(55*)-C(49*)-N(41*)	113.5(5)	C(54*)-C(55*)-C(49*)	117.7(4)
C(50*)-C(55*)-C(49*)	122.3(4)		

Table 4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 1.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(h a^*)^2 U_{11} + \dots + 2h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
O(1)	48(4)	53(3)	37(3)	-10(2)	1(2)	17(3)
C(2)	36(5)	65(5)	32(4)	-11(4)	0(3)	14(4)
C(3)	43(5)	80(6)	32(4)	9(4)	-6(4)	23(5)
O(4)	39(3)	55(3)	39(3)	3(2)	-5(2)	21(3)
C(5)	52(5)	46(4)	21(3)	4(3)	8(3)	29(4)
C(6)	64(6)	61(6)	35(4)	8(4)	5(4)	40(5)
C(7)	84(8)	47(5)	52(5)	19(4)	14(5)	40(5)
C(8)	89(8)	46(5)	41(4)	4(4)	5(5)	26(5)
C(9)	46(5)	51(5)	34(4)	4(3)	3(3)	20(4)
C(10)	53(5)	41(4)	26(3)	10(3)	10(3)	24(4)
O(11)	41(3)	48(3)	39(3)	11(2)	-1(2)	19(3)
C(12)	27(4)	52(4)	28(3)	4(3)	-1(3)	12(3)
C(13)	39(5)	40(4)	32(4)	-2(3)	-6(3)	23(3)
O(14)	49(3)	35(3)	26(2)	4(2)	3(2)	25(2)
C(15)	38(5)	34(4)	36(4)	-2(3)	-1(3)	17(3)
C(16)	53(6)	44(4)	47(4)	4(3)	-9(4)	28(4)
C(17)	70(7)	36(4)	68(6)	-6(4)	-5(5)	38(4)
C(18)	66(6)	38(4)	65(6)	21(4)	-5(5)	24(4)
C(19)	36(5)	41(4)	48(4)	9(3)	-3(4)	11(3)
C(20)	40(5)	27(4)	39(4)	0(3)	-9(3)	19(3)
O(21)	41(3)	36(3)	28(2)	5(2)	1(2)	21(2)
C(22)	42(5)	49(4)	25(3)	8(3)	8(3)	21(4)
C(23)	33(5)	52(5)	40(4)	-12(3)	-6(3)	21(4)
O(24)	35(3)	40(3)	35(3)	-7(2)	-4(2)	17(2)
C(25)	31(4)	37(4)	28(3)	1(3)	-2(3)	14(3)
C(26)	43(5)	35(4)	42(4)	-5(3)	5(4)	2(3)
C(27)	51(6)	37(4)	53(5)	-16(4)	2(4)	15(4)
C(28)	52(6)	33(4)	59(5)	-8(4)	7(4)	15(4)
C(29)	33(5)	42(4)	49(4)	-3(3)	3(3)	17(3)
C(30)	43(5)	26(3)	32(4)	-2(3)	1(3)	12(3)
O(31)	39(3)	28(2)	42(3)	-11(2)	-7(2)	17(2)
C(32)	38(5)	36(4)	41(4)	-3(3)	-3(3)	18(3)
C(33)	38(5)	43(4)	35(4)	1(3)	7(3)	11(4)
O(34)	47(3)	34(3)	33(3)	-5(2)	1(2)	15(2)
C(35)	33(4)	39(4)	38(4)	-3(3)	-9(3)	9(3)
C(36)	47(5)	45(5)	50(5)	3(4)	-9(4)	10(4)
C(37)	72(7)	34(4)	66(6)	-6(4)	-10(5)	3(4)
C(38)	56(6)	40(5)	72(6)	-20(4)	-21(5)	13(4)
C(39)	49(5)	49(5)	45(4)	-17(4)	-15(4)	22(4)
C(40)	40(5)	36(4)	35(4)	-7(3)	-9(3)	13(3)
N(41)	40(4)	45(4)	30(3)	0(3)	-5(3)	20(3)
C(42)	46(5)	46(4)	33(4)	-7(3)	-5(3)	16(4)
C(43)	62(7)	65(6)	52(5)	-13(4)	2(4)	30(5)
C(44)	104(9)	53(6)	74(7)	-16(5)	-7(6)	50(6)
C(45)	99(9)	43(5)	73(7)	11(5)	12(6)	30(5)
C(46)	51(6)	47(5)	61(5)	-2(4)	1(4)	9(4)
C(47)	37(5)	36(4)	33(4)	-6(3)	1(3)	15(3)
C(48)	47(5)	42(4)	41(4)	-9(3)	-3(4)	11(4)
C(49)	62(6)	51(5)	33(4)	10(3)	-2(4)	26(4)
C(50)	84(8)	53(5)	53(5)	9(4)	21(5)	33(5)
C(51)	92(9)	36(5)	91(8)	-2(5)	14(7)	12(5)
C(52)	90(9)	43(5)	67(6)	13(4)	8(6)	-5(5)
C(53)	68(7)	81(7)	52(5)	-1(5)	6(5)	10(6)

C(54)	46(6)	61(5)	46(5)	-10(4)	4(4)	19(4)
C(55)	63(6)	42(4)	28(4)	10(3)	12(4)	20(4)
O(1')	46(3)	35(3)	38(3)	1(2)	9(2)	25(2)
C(2')	52(5)	44(4)	29(4)	1(3)	12(3)	31(4)
C(3')	47(5)	49(5)	35(4)	0(3)	6(4)	13(4)
O(4')	35(3)	39(3)	35(3)	4(2)	3(2)	14(2)
C(5')	50(5)	25(3)	22(3)	1(3)	4(3)	19(3)
C(6')	49(5)	41(4)	47(4)	4(3)	0(4)	16(4)
C(7')	70(7)	27(4)	60(5)	5(4)	-2(5)	4(4)
C(8')	93(8)	39(5)	47(5)	11(4)	10(5)	35(5)
C(9')	66(6)	30(4)	51(5)	4(3)	-2(4)	22(4)
C(10')	48(5)	25(3)	29(3)	-1(3)	3(3)	16(3)
O(11')	43(3)	32(3)	33(2)	8(2)	2(2)	12(2)
C(12')	48(5)	45(4)	30(4)	1(3)	1(3)	24(4)
C(13')	42(5)	44(4)	19(3)	-5(3)	0(3)	14(3)
O(14')	47(3)	37(3)	25(2)	-1(2)	3(2)	16(2)
C(15')	34(4)	41(4)	35(4)	-2(3)	-4(3)	20(3)
C(16')	46(5)	42(4)	33(4)	-6(3)	-6(3)	20(4)
C(17')	52(6)	36(4)	52(5)	-5(3)	-1(4)	18(4)
C(18')	49(5)	27(4)	52(5)	2(3)	-8(4)	12(3)
C(19')	38(5)	47(5)	41(4)	2(3)	-1(3)	11(4)
C(20')	30(4)	35(4)	35(4)	-7(3)	-2(3)	19(3)
O(21')	44(3)	37(3)	29(2)	-7(2)	-1(2)	11(2)
C(22')	38(5)	47(4)	31(4)	-5(3)	-1(3)	17(4)
C(23')	40(5)	44(4)	33(4)	-9(3)	-4(3)	22(4)
O(24')	39(3)	39(3)	33(3)	-9(2)	-3(2)	19(2)
C(25')	46(5)	37(4)	25(3)	-6(3)	0(3)	19(3)
C(26')	47(5)	45(4)	32(4)	4(3)	1(3)	25(4)
C(27')	56(6)	33(4)	44(4)	-4(3)	9(4)	21(4)
C(28')	57(6)	23(3)	37(4)	-6(3)	8(4)	8(3)
C(29')	48(5)	34(4)	36(4)	-9(3)	5(3)	4(4)
C(30')	36(5)	33(4)	33(4)	5(3)	12(3)	16(3)
O(31')	35(3)	45(3)	34(3)	-10(2)	-4(2)	21(2)
C(32')	35(5)	47(4)	33(4)	-8(3)	2(3)	18(3)
C(33')	32(4)	50(4)	26(3)	2(3)	9(3)	21(3)
O(34')	40(3)	35(3)	34(3)	3(2)	0(2)	20(2)
C(35')	31(4)	39(4)	37(4)	-6(3)	-4(3)	16(3)
C(36')	41(5)	48(5)	44(4)	5(3)	-2(4)	17(4)
C(37')	62(6)	37(4)	63(5)	14(4)	-3(5)	26(4)
C(38')	61(6)	48(5)	51(5)	-2(4)	1(4)	38(4)
C(39')	48(5)	39(4)	43(4)	0(3)	1(4)	27(4)
C(40')	39(5)	33(4)	33(4)	-4(3)	-3(3)	18(3)
N(41')	39(4)	35(3)	38(3)	0(3)	4(3)	17(3)
C(42')	28(4)	51(4)	34(4)	5(3)	2(3)	15(3)
C(43')	58(6)	41(5)	60(5)	14(4)	-12(5)	5(4)
C(44')	93(9)	36(5)	103(9)	12(5)	-27(7)	9(5)
C(45')	141(13)	39(6)	114(10)	-8(6)	-44(9)	27(7)
C(46')	128(11)	55(6)	92(8)	-38(6)	-32(8)	42(7)
C(47')	62(6)	49(5)	69(6)	-22(4)	-12(5)	23(5)
C(48')	42(5)	39(4)	44(4)	-3(3)	-7(4)	12(4)
C(49')	50(5)	31(4)	59(5)	1(3)	3(4)	17(4)
C(50')	78(7)	42(5)	42(4)	1(4)	15(4)	23(5)
C(51')	68(7)	55(6)	56(5)	-5(4)	21(5)	10(5)
C(52')	57(7)	47(5)	80(7)	-9(5)	34(5)	5(4)
C(53')	60(7)	56(6)	87(7)	-10(5)	-1(5)	20(5)
C(54')	48(6)	46(5)	70(6)	5(4)	-6(5)	17(4)
C(55')	54(5)	31(4)	43(4)	-3(3)	9(4)	18(4)
O(1")	45(3)	47(3)	32(3)	-2(2)	12(2)	10(3)
C(2")	41(5)	55(5)	28(4)	-2(3)	5(3)	17(4)
C(3")	37(5)	47(4)	35(4)	7(3)	2(3)	17(4)
O(4")	38(3)	41(3)	37(3)	8(2)	1(2)	14(2)
C(5")	42(5)	36(4)	26(3)	2(3)	14(3)	12(3)

C(6")	56(6)	38(4)	35(4)	8(3)	18(4)	16(4)
C(7")	79(7)	37(5)	49(5)	4(4)	4(5)	19(5)
C(8")	79(8)	37(5)	57(5)	2(4)	7(5)	-9(5)
C(9")	41(5)	42(5)	59(5)	-2(4)	-3(4)	-1(4)
C(10")	42(5)	36(4)	25(3)	-1(3)	8(3)	5(3)
O(11")	41(3)	39(3)	36(3)	2(2)	0(2)	9(2)
C(12")	30(5)	63(5)	41(4)	2(4)	6(3)	12(4)
C(13")	37(5)	59(5)	30(4)	-4(3)	6(3)	20(4)
O(14")	36(3)	52(3)	31(3)	-2(2)	3(2)	17(2)
C(15")	43(5)	39(4)	35(4)	-10(3)	-12(3)	17(3)
C(16")	56(6)	54(5)	43(4)	-12(4)	0(4)	28(4)
C(17")	70(7)	46(5)	57(5)	-19(4)	-14(5)	27(5)
C(18")	54(6)	41(5)	62(6)	2(4)	-21(5)	10(4)
C(19")	41(5)	42(4)	50(5)	-3(4)	-4(4)	8(4)
C(20")	28(4)	37(4)	36(4)	-6(3)	-4(3)	11(3)
O(21")	41(3)	52(3)	37(3)	0(2)	5(2)	26(3)
C(22")	38(5)	51(5)	29(4)	2(3)	-2(3)	21(4)
C(23")	30(5)	59(5)	41(4)	-9(4)	1(3)	22(4)
O(24")	37(3)	46(3)	48(3)	-16(2)	-8(2)	20(2)
C(25")	39(5)	48(4)	27(3)	-5(3)	5(3)	18(4)
C(26")	31(5)	47(5)	52(5)	-19(4)	-1(4)	2(4)
C(27")	54(6)	45(5)	54(5)	-22(4)	-18(4)	18(4)
C(28")	65(6)	35(4)	39(4)	-9(3)	-6(4)	17(4)
C(29")	43(5)	43(4)	40(4)	-7(3)	-4(3)	21(4)
C(30")	26(4)	37(4)	35(4)	-7(3)	-1(3)	9(3)
O(31")	29(3)	37(3)	38(3)	-12(2)	-6(2)	14(2)
C(32")	31(4)	33(4)	29(3)	-4(3)	6(3)	8(3)
C(33")	33(4)	36(4)	21(3)	-1(3)	6(3)	7(3)
O(34")	42(3)	37(3)	26(2)	-3(2)	6(2)	8(2)
C(35")	45(5)	32(4)	25(3)	-9(3)	0(3)	13(3)
C(36")	46(5)	42(4)	51(5)	-8(4)	19(4)	6(4)
C(37")	68(7)	33(4)	69(6)	-6(4)	31(5)	2(4)
C(38")	73(7)	33(4)	70(6)	-27(4)	22(5)	-4(4)
C(39")	70(6)	49(5)	36(4)	-20(4)	14(4)	11(4)
C(40")	36(5)	42(4)	32(4)	-7(3)	5(3)	11(3)
N(41")	50(7)	66(7)	31(5)	13(5)	10(4)	24(5)
C(42")	17(7)	75(9)	69(8)	-3(7)	-1(5)	10(6)
C(43")	48(9)	55(8)	79(10)	-2(8)	3(7)	26(7)
C(44")	56(10)	82(12)	130(16)	-36(11)	-15(10)	20(9)
C(45")	90(12)	60(9)	155(14)	12(10)	-31(11)	19(9)
C(46")	108(13)	78(11)	141(14)	30(11)	-56(11)	2(10)
C(47")	85(13)	81(11)	99(12)	34(10)	-42(10)	-23(10)
C(48")	23(7)	56(8)	69(9)	13(8)	-14(6)	4(6)
C(49")	44(8)	66(9)	22(5)	1(5)	10(5)	29(8)
C(50")	54(9)	44(8)	54(8)	0(6)	17(6)	11(8)
C(51")	65(10)	53(8)	60(8)	-2(6)	3(8)	20(7)
C(52")	84(12)	60(9)	91(11)	9(8)	6(9)	7(8)
C(53")	118(17)	79(12)	145(18)	40(12)	34(14)	54(12)
C(54")	86(13)	86(12)	117(14)	35(11)	12(11)	59(10)
C(55")	48(8)	62(8)	33(6)	14(5)	16(5)	37(7)
O(1*)	61(4)	61(4)	30(3)	-3(2)	4(3)	35(3)
C(2*)	54(6)	82(7)	45(5)	-5(4)	9(4)	24(5)
C(3*)	49(6)	76(6)	31(4)	1(4)	5(4)	8(5)
O(4*)	53(4)	50(3)	33(3)	-2(2)	8(2)	12(3)
C(5*)	73(7)	37(4)	30(4)	5(3)	24(4)	18(4)
C(6*)	66(7)	53(6)	57(5)	-15(4)	16(5)	-7(5)
C(7*)	113(11)	43(6)	76(7)	1(5)	27(7)	5(6)
C(8*)	103(10)	39(5)	65(6)	10(4)	31(6)	19(5)
C(9*)	75(7)	51(5)	61(6)	14(4)	10(5)	33(5)
C(10*)	56(6)	46(5)	31(4)	4(3)	17(4)	18(4)
O(11*)	46(3)	40(3)	37(3)	6(2)	5(2)	15(2)
C(12*)	56(6)	58(5)	33(4)	10(3)	3(4)	33(4)

C(13*)	50(6)	79(6)	28(4)	-3(4)	0(4)	26(5)
O(14*)	59(4)	43(3)	29(3)	2(2)	5(2)	21(3)
C(15*)	46(5)	34(4)	34(4)	2(3)	-7(3)	24(4)
C(16*)	50(5)	44(5)	46(4)	-13(3)	-12(4)	25(4)
C(17*)	56(6)	34(4)	58(5)	-19(4)	-19(4)	16(4)
C(18*)	51(5)	30(4)	52(5)	-5(3)	-12(4)	12(4)
C(19*)	44(5)	34(4)	48(4)	-1(3)	-6(4)	12(4)
C(20*)	40(5)	33(4)	34(4)	-1(3)	-11(3)	18(3)
O(21*)	45(3)	35(3)	33(3)	-8(2)	0(2)	11(2)
C(22*)	38(5)	33(4)	32(4)	5(3)	0(3)	12(3)
C(23*)	33(5)	45(4)	33(4)	-3(3)	-6(3)	16(3)
O(24*)	36(3)	31(2)	33(2)	-10(2)	-5(2)	15(2)
C(25*)	36(4)	24(3)	34(4)	-5(3)	4(3)	4(3)
C(26*)	46(5)	38(4)	50(5)	-6(3)	2(4)	17(4)
C(27*)	57(6)	38(4)	57(5)	-8(4)	8(4)	17(4)
C(28*)	60(6)	39(5)	60(5)	-20(4)	6(5)	9(4)
C(29*)	39(5)	39(4)	48(4)	-12(3)	-3(4)	10(4)
C(30*)	42(5)	29(4)	26(3)	-7(3)	2(3)	13(3)
O(31*)	35(3)	37(3)	37(3)	-9(2)	-4(2)	14(2)
C(32*)	37(5)	45(4)	31(4)	-5(3)	-4(3)	3(3)
C(33*)	44(5)	51(5)	29(4)	4(3)	1(3)	15(4)
O(34*)	44(3)	43(3)	32(3)	0(2)	4(2)	25(2)
C(35*)	35(5)	50(5)	50(5)	-7(4)	-4(4)	24(4)
C(36*)	57(6)	57(5)	56(5)	-2(4)	-8(4)	23(5)
C(37*)	73(7)	50(5)	84(7)	4(5)	-15(6)	41(5)
C(38*)	87(8)	70(6)	59(6)	-19(5)	-14(5)	49(6)
C(39*)	74(7)	70(6)	42(5)	-16(4)	-7(4)	47(5)
C(40*)	51(6)	62(5)	40(4)	-8(4)	-4(4)	33(4)
N(41*)	43(4)	40(3)	32(3)	-6(3)	0(3)	16(3)
C(42*)	58(6)	41(4)	27(4)	3(3)	6(3)	14(4)
C(43*)	68(7)	65(6)	48(5)	3(4)	15(5)	11(5)
C(44*)	135(12)	47(6)	61(6)	-9(5)	28(7)	-15(7)
C(45*)	205(18)	39(6)	80(8)	15(6)	61(10)	45(9)
C(46*)	168(15)	64(7)	91(9)	40(7)	56(10)	58(9)
C(47*)	76(7)	63(6)	52(5)	16(4)	16(5)	37(5)
C(48*)	57(6)	45(4)	32(4)	4(3)	12(4)	9(4)
C(49*)	56(5)	37(4)	34(4)	-5(3)	-4(4)	17(4)
C(50*)	57(6)	50(5)	39(4)	-9(4)	-7(4)	26(4)
C(51*)	57(6)	37(4)	41(4)	1(3)	0(4)	13(4)
C(52*)	75(7)	36(4)	62(6)	3(4)	-22(5)	18(4)
C(53*)	93(8)	34(4)	69(6)	0(4)	-1(5)	32(5)
C(54*)	75(7)	46(5)	53(5)	-8(4)	-4(5)	33(5)
C(55*)	40(5)	41(4)	41(4)	-11(3)	-10(3)	20(4)
P(10)	45(1)	42(1)	33(1)	-4(1)	2(1)	17(1)
F(11)	49(3)	63(3)	58(3)	-4(2)	14(2)	20(2)
F(12)	71(4)	100(4)	37(3)	1(3)	-8(3)	23(3)
F(13)	96(5)	41(3)	71(3)	-8(2)	12(3)	17(3)
F(14)	51(3)	75(3)	37(2)	1(2)	-5(2)	30(3)
F(15)	82(4)	52(3)	77(4)	-8(3)	-4(3)	42(3)
F(16)	46(3)	84(4)	45(3)	-1(2)	6(2)	19(3)
P(20)	46(2)	79(2)	63(2)	23(1)	3(1)	29(1)
F(21)	52(4)	103(4)	71(4)	26(3)	17(3)	39(3)
F(22)	70(4)	126(6)	67(4)	17(4)	-16(3)	28(4)
F(23)	102(5)	76(4)	98(5)	21(4)	5(4)	29(4)
F(24)	88(5)	129(6)	50(3)	22(3)	3(3)	44(4)
F(25)	93(5)	80(4)	104(5)	28(4)	9(4)	42(4)
F(26)	56(4)	144(7)	115(5)	47(5)	21(4)	46(4)
P(30)	48(1)	52(1)	39(1)	7(1)	1(1)	22(1)
F(31)	46(3)	107(5)	58(3)	20(3)	8(2)	28(3)
F(32)	64(4)	93(4)	35(2)	12(2)	-8(2)	24(3)
F(33)	104(5)	58(3)	71(4)	-1(3)	1(3)	43(3)
F(34)	56(3)	106(4)	37(3)	5(3)	-3(2)	29(3)

F(35)	82(4)	50(3)	95(4)	-2(3)	-8(3)	24(3)
F(36)	40(3)	71(3)	69(3)	4(3)	12(2)	13(2)
P(40)	54(1)	53(1)	33(1)	6(1)	9(1)	21(1)
F(41)	47(3)	104(4)	49(3)	21(3)	9(2)	32(3)
F(42)	54(4)	135(5)	42(3)	24(3)	8(2)	33(3)
F(43)	102(5)	56(4)	131(6)	-20(4)	32(5)	23(4)
F(44)	87(5)	148(6)	45(3)	37(3)	3(3)	52(4)
F(45)	83(5)	63(4)	121(5)	-27(4)	28(4)	-1(3)
F(46)	57(3)	73(3)	53(3)	10(2)	21(2)	21(3)
N(60)	137(12)	151(11)	71(7)	-18(7)	15(7)	65(9)
C(61)	82(8)	65(6)	58(6)	16(5)	9(5)	24(6)
C(62)	102(9)	54(6)	67(6)	3(5)	-19(6)	14(6)
N(63)	53(10)	89(12)	50(8)	-31(8)	-44(7)	52(9)
C(64)	48(7)	57(6)	127(11)	3(7)	-13(7)	30(5)
C(65)	134(13)	76(8)	96(9)	-9(7)	17(9)	25(8)
N(66)	134(20)	81(13)	68(11)	-19(10)	-6(12)	46(13)
C(70)	125(20)	84(14)	60(11)	55(11)	58(12)	92(15)
Cl(1)	55(3)	104(4)	52(3)	-9(2)	11(2)	-6(3)
Cl(2)	74(4)	96(4)	62(3)	-4(3)	-11(3)	0(3)

Table 5. Hydrogen coordinates ($\times 10^4$), isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) and site occupancy factors for 1.

	x	y	z	U(eq)	sof
H(2A)	8014 (6)	6673 (4)	8110 (3)	53	1
H(2B)	8980 (6)	6552 (4)	8346 (3)	53	1
H(3A)	9214 (6)	7422 (4)	7849 (3)	61	1
H(3B)	8761 (6)	7722 (4)	8282 (3)	61	1
H(6A)	9796 (7)	8521 (4)	7994 (3)	59	1
H(7A)	10921 (8)	9406 (4)	7928 (3)	68	1
H(8A)	12448 (8)	9575 (4)	8288 (3)	68	1
H(9A)	12875 (6)	8798 (4)	8703 (3)	51	1
H(12A)	12919 (5)	8142 (3)	9227 (2)	42	1
H(12B)	13130 (5)	7799 (3)	8753 (2)	42	1
H(13A)	12289 (6)	6886 (3)	9125 (2)	41	1
H(13B)	13328 (6)	7202 (3)	9361 (2)	41	1
H(16A)	12760 (6)	6287 (3)	9632 (3)	54	1
H(17A)	12620 (7)	5551 (4)	10179 (3)	65	1
H(18A)	12004 (7)	5642 (4)	10930 (3)	65	1
H(19A)	11413 (6)	6476 (3)	11134 (3)	49	1
H(22A)	11626 (6)	7438 (3)	11303 (2)	44	1
H(22B)	10543 (6)	7143 (3)	11109 (2)	44	1
H(23A)	10793 (6)	8142 (4)	11456 (3)	48	1
H(23B)	11414 (6)	8370 (4)	10993 (3)	48	1
H(26A)	10587 (6)	9040 (3)	11344 (3)	49	1
H(27A)	9820 (7)	9817 (3)	11362 (3)	56	1
H(28A)	8409 (7)	9754 (3)	10945 (3)	57	1
H(29A)	7687 (6)	8895 (3)	10488 (3)	48	1
H(32A)	7384 (6)	8094 (3)	9927 (3)	45	1
H(32B)	6963 (6)	7944 (3)	10449 (3)	45	1
H(33A)	7185 (6)	6946 (3)	10298 (3)	46	1
H(33B)	6304 (6)	7103 (3)	10011 (3)	46	1
H(36A)	6367 (6)	6119 (4)	9969 (3)	57	1
H(37A)	6034 (8)	5155 (4)	9633 (3)	71	1
H(38A)	6733 (7)	4991 (4)	8920 (3)	68	1
H(39A)	7681 (6)	5766 (4)	8503 (3)	56	1
H(41A)	10248 (4)	7801 (2)	10169 (2)	44	1
H(41B)	11027 (4)	7753 (2)	9848 (2)	44	1
H(42A)	10004 (6)	7258 (2)	9277 (2)	49	1
H(42B)	9105 (6)	7400 (2)	9554 (2)	49	1
H(43A)	10022 (5)	6280 (2)	9291 (2)	69	1
H(44A)	9698 (8)	5360 (2)	9648 (3)	86	1
H(45A)	9068 (8)	5257 (2)	10417 (3)	83	1
H(46A)	8761 (7)	6074 (3)	10828 (2)	64	1
H(47A)	9085 (6)	6995 (2)	10470 (2)	41	1
H(49A)	9748 (6)	8451 (2)	9699 (2)	56	1
H(49B)	10535 (6)	8372 (2)	9315 (2)	56	1
H(50A)	10182 (4)	9395 (2)	10020 (2)	72	1
H(51A)	11320 (7)	10221 (2)	10341 (3)	88	1
H(52A)	12962 (6)	10209 (3)	10405 (3)	84	1
H(53A)	13464 (3)	9372 (4)	10150 (3)	82	1
H(54A)	12326 (5)	8546 (3)	9830 (3)	60	1
H(2'A)	1363 (6)	7317 (3)	7611 (2)	46	1
H(2'B)	2345 (6)	7644 (3)	7893 (2)	46	1
H(3'A)	1614 (6)	6655 (4)	8161 (3)	52	1
H(3'B)	1899 (6)	6408 (4)	7657 (3)	52	1
H(6'A)	1846 (7)	5823 (3)	8367 (3)	53	1
H(7'A)	2200 (7)	5119 (3)	8867 (3)	64	1
H(8'A)	3785 (8)	5248 (4)	9152 (3)	67	1

H(9'A)	5012 (7)	6046 (3)	8951 (3)	57	1
H(12C)	6121 (6)	6783 (3)	8543 (2)	46	1
H(12D)	5636 (6)	6986 (3)	9010 (2)	46	1
H(13C)	5868 (6)	7950 (3)	8633 (2)	42	1
H(13D)	6820 (6)	7797 (3)	8852 (2)	42	1
H(16B)	7260 (6)	8724 (3)	8668 (3)	47	1
H(17B)	8326 (6)	9608 (3)	8452 (3)	55	1
H(18B)	9016 (6)	9680 (3)	7703 (3)	51	1
H(19B)	8640 (6)	8876 (3)	7156 (3)	50	1
H(22C)	8762 (6)	7945 (3)	6942 (2)	45	1
H(22D)	7879 (6)	8121 (3)	6668 (2)	45	1
H(23C)	8231 (6)	7186 (3)	6386 (3)	45	1
H(23D)	7779 (6)	6912 (3)	6877 (3)	45	1
H(26B)	7645 (6)	6254 (3)	6216 (2)	47	1
H(27B)	6939 (6)	5416 (3)	5720 (3)	51	1
H(28B)	5415 (6)	5294 (3)	5407 (3)	47	1
H(29B)	4472 (6)	5955 (3)	5594 (3)	49	1
H(32C)	3675 (6)	6619 (3)	5909 (3)	45	1
H(32D)	4343 (6)	6954 (3)	5493 (3)	45	1
H(33C)	4464 (6)	7864 (3)	5959 (2)	41	1
H(33D)	3417 (6)	7580 (3)	5718 (2)	41	1
H(36B)	3534 (6)	8486 (3)	6022 (3)	52	1
H(37B)	2870 (7)	9251 (4)	6318 (3)	62	1
H(38B)	2102 (7)	9170 (4)	7042 (3)	59	1
H(39B)	1900 (6)	8305 (3)	7467 (3)	49	1
H(41C)	3961 (5)	6933 (3)	7482 (2)	43	1
H(41D)	4007 (5)	6996 (3)	6968 (2)	43	1
H(42C)	5724 (5)	7241 (3)	7019 (3)	44	1
H(42D)	5602 (5)	7253 (3)	7584 (3)	44	1
H(43B)	5971 (4)	8124 (2)	6642 (2)	65	1
H(44B)	5895 (8)	9111 (3)	6606 (3)	94	1
H(45B)	5124 (9)	9526 (2)	7209 (4)	117	1
H(46B)	4430 (8)	8954 (4)	7847 (3)	107	1
H(47B)	4506 (7)	7967 (3)	7882 (2)	71	1
H(49C)	4716 (6)	6234 (3)	6857 (3)	54	1
H(49D)	4836 (6)	6199 (3)	7420 (3)	54	1
H(50B)	3875 (4)	5369 (2)	7718 (2)	63	1
H(51B)	2422 (6)	4630 (3)	7743 (3)	73	1
H(52B)	1138 (4)	4644 (3)	7218 (3)	76	1
H(53B)	1307 (5)	5396 (4)	6669 (3)	80	1
H(54B)	2760 (6)	6136 (3)	6644 (2)	64	1
H(2"A)	8083 (6)	7293 (4)	3038 (2)	49	1
H(2"B)	8985 (6)	7054 (4)	3224 (2)	49	1
H(3"A)	9366 (6)	8074 (3)	2967 (3)	46	1
H(3"B)	8865 (6)	8223 (3)	3448 (3)	46	1
H(6"A)	10086 (7)	9002 (3)	3184 (3)	50	1
H(7"A)	11384 (8)	9831 (4)	3133 (3)	65	1
H(8"A)	12914 (8)	9817 (4)	3431 (3)	74	1
H(9"A)	13102 (7)	8972 (4)	3827 (3)	59	1
H(12E)	12962 (6)	8264 (4)	4349 (3)	53	1
H(12F)	13214 (6)	8043 (4)	3831 (3)	53	1
H(13E)	12375 (6)	7045 (4)	4049 (2)	49	1
H(13F)	13374 (6)	7311 (4)	4340 (2)	49	1
H(16C)	12883 (7)	6349 (4)	4515 (3)	58	1
H(17C)	12722 (7)	5518 (4)	4964 (3)	67	1
H(18C)	11947 (7)	5442 (4)	5686 (3)	63	1
H(19C)	11239 (6)	6212 (3)	5950 (3)	53	1
H(22E)	11343 (6)	7131 (3)	6228 (2)	45	1
H(22F)	10276 (6)	6867 (3)	6001 (2)	45	1
H(23E)	10497 (6)	7818 (4)	6431 (3)	50	1
H(23F)	11172 (6)	8106 (4)	6000 (3)	50	1
H(26C)	10492 (6)	8813 (4)	6271 (3)	54	1

H(27C)	9715 (7)	9582 (4)	6363 (3)	61	1
H(28C)	8178 (7)	9497 (3)	6053 (3)	55	1
H(29C)	7378 (6)	8640 (3)	5613 (3)	48	1
H(32E)	7087 (5)	7952 (3)	5045 (2)	37	1
H(32F)	6634 (5)	7641 (3)	5523 (2)	37	1
H(33E)	6958 (5)	6726 (3)	5185 (2)	37	1
H(33F)	6081 (5)	6933 (3)	4934 (2)	37	1
H(36C)	6303 (6)	5998 (3)	4697 (3)	56	1
H(37C)	6092 (7)	5193 (4)	4139 (3)	70	1
H(38C)	6805 (7)	5337 (4)	3400 (3)	74	1
H(39C)	7747 (7)	6253 (4)	3196 (3)	63	1
H(41E)	10671 (6)	7653 (3)	4992 (3)	56	0.70
H(41F)	10806 (6)	7707 (3)	4480 (3)	56	0.70
H(42G)	9090 (7)	7329 (4)	4370 (5)	65	0.70
H(42H)	9084 (7)	7169 (4)	4921 (5)	65	0.70
H(43D)	10236 (7)	6887 (4)	3839 (3)	69	0.70
H(44D)	10503 (12)	5971 (7)	3608 (4)	107	0.70
H(45D)	10147 (13)	5184 (4)	4129 (7)	122	0.70
H(46D)	9526 (14)	5313 (5)	4882 (6)	135	0.70
H(47D)	9259 (12)	6229 (6)	5113 (3)	115	0.70
H(49G)	9589 (7)	8259 (4)	4968 (4)	49	0.70
H(49H)	9877 (7)	8359 (4)	4423 (4)	49	0.70
H(50D)	11961 (6)	8371 (3)	5057 (3)	61	0.70
H(51D)	13187 (6)	9208 (5)	5282 (5)	70	0.70
H(52D)	12894 (9)	10149 (4)	5246 (6)	96	0.70
H(53D)	11375 (11)	10252 (3)	4984 (7)	130	0.70
H(54D)	10150 (7)	9415 (5)	4759 (6)	107	0.70
H(41I)	10823 (17)	7429 (7)	4668 (9)	64	0.30
H(41J)	10314 (17)	7490 (7)	4227 (9)	64	0.30
H(42I)	8903 (19)	6832 (7)	4477 (10)	61	0.30
H(42J)	9489 (19)	6754 (7)	4950 (10)	61	0.30
H(43E)	10084 (19)	6725 (8)	3711 (6)	65	0.30
H(44E)	10482 (31)	5931 (14)	3305 (6)	92	0.30
H(45E)	10546 (29)	5080 (12)	3712 (10)	92	0.30
H(46E)	10212 (32)	5023 (10)	4526 (10)	83	0.30
H(47E)	9813 (31)	5816 (12)	4932 (6)	101	0.30
H(49I)	9650 (15)	7775 (7)	5095 (10)	66	0.30
H(49J)	9262 (15)	7924 (7)	4590 (10)	66	0.30
H(50E)	11662 (15)	8242 (8)	5122 (9)	72	0.30
H(51E)	12729 (17)	9183 (14)	5179 (14)	82	0.30
H(52E)	12250 (24)	10000 (9)	4890 (15)	101	0.30
H(53E)	10703 (27)	9875 (10)	4544 (17)	128	0.30
H(54E)	9635 (18)	8934 (13)	4487 (15)	122	0.30
H(2*A)	1565 (7)	7789 (4)	2590 (3)	71	1
H(2*B)	2524 (7)	8084 (4)	2902 (3)	71	1
H(3*A)	1740 (7)	7038 (4)	3070 (3)	64	1
H(3*B)	2174 (7)	6877 (4)	2572 (3)	64	1
H(6*A)	2084 (8)	6147 (4)	3124 (3)	75	1
H(7*A)	2479 (11)	5367 (4)	3524 (4)	96	1
H(8*A)	3962 (9)	5517 (4)	3921 (4)	82	1
H(9*A)	5103 (8)	6420 (4)	3893 (3)	71	1
H(12G)	6140 (6)	7216 (4)	3621 (3)	55	1
H(12H)	5623 (6)	7391 (4)	4089 (3)	55	1
H(13G)	5893 (7)	8379 (4)	3758 (3)	61	1
H(13H)	6833 (7)	8205 (4)	3973 (3)	61	1
H(16D)	7354 (6)	9161 (3)	3817 (3)	53	1
H(17D)	8451 (7)	10039 (3)	3619 (3)	59	1
H(18D)	9159 (6)	10147 (3)	2883 (3)	53	1
H(19D)	8752 (6)	9354 (3)	2307 (3)	50	1
H(22G)	8788 (6)	8420 (3)	2056 (2)	41	1
H(22H)	7947 (6)	8630 (3)	1775 (2)	41	1
H(23G)	8233 (6)	7682 (3)	1501 (3)	43	1

H(23H)	7733 (6)	7418 (3)	1984 (3)	43	1
H(26D)	7512 (6)	6698 (3)	1457 (3)	52	1
H(27D)	6733 (7)	5795 (4)	1075 (3)	60	1
H(28D)	5273 (7)	5682 (4)	693 (3)	65	1
H(29D)	4491 (6)	6463 (3)	678 (3)	51	1
H(32G)	3752 (6)	7122 (3)	950 (3)	47	1
H(32H)	4331 (6)	7402 (3)	489 (3)	47	1
H(33G)	4443 (6)	8371 (4)	857 (2)	48	1
H(33H)	3353 (6)	8021 (4)	702 (2)	48	1
H(36D)	3531 (7)	9017 (4)	1008 (3)	66	1
H(37D)	2811 (8)	9745 (4)	1344 (4)	78	1
H(38D)	2169 (8)	9641 (5)	2091 (3)	80	1
H(39D)	2142 (7)	8804 (4)	2513 (3)	68	1
H(41G)	4835 (5)	8081 (3)	1817 (2)	45	1
H(41H)	5855 (5)	8086 (3)	1887 (2)	45	1
H(42E)	4446 (7)	7824 (3)	2574 (2)	50	1
H(42F)	5577 (7)	7909 (3)	2698 (2)	50	1
H(43C)	3697 (4)	7005 (3)	1956 (2)	73	1
H(44C)	3560 (7)	6008 (4)	1756 (3)	105	1
H(45C)	4763 (10)	5550 (2)	2006 (4)	126	1
H(46C)	6104 (8)	6088 (4)	2455 (4)	122	1
H(47C)	6241 (5)	7085 (4)	2654 (3)	72	1
H(49E)	5039 (7)	8877 (3)	2390 (3)	50	1
H(49F)	6179 (7)	8916 (3)	2359 (3)	50	1
H(50C)	6335 (4)	8778 (2)	1305 (2)	56	1
H(51C)	6430 (6)	9434 (3)	682 (2)	54	1
H(52C)	5783 (7)	10259 (3)	771 (2)	68	1
H(53C)	5042 (7)	10429 (3)	1484 (3)	75	1
H(54C)	4947 (6)	9773 (3)	2107 (2)	66	1
H(62A)	5067 (9)	10407 (4)	3957 (4)	113	1
H(62B)	5611 (9)	9996 (4)	4243 (4)	113	1
H(62C)	4447 (9)	9832 (4)	4211 (4)	113	1
H(70A)	271 (17)	5422 (9)	2009 (6)	92	0.50
H(70B)	443 (17)	4832 (9)	2222 (6)	92	0.50