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Crystal Structure of 4-Isothiocyanato Phenyl 4-Pentylbicyclo[2,2,2] Octane-1-Carboxylate

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Crystal Structure of 4-isothiocyanato phenyl 4-pentylbicyclo[2,2,2] octane-1-carboxylate

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Abstract 4-isothiocyanato phenyl 4-pentylbicyclo[2,2,2]octane-1-carboxylate, $C_{21}H_{27}O_2NS$ is a nematogen containing an unusual eight membered ring in the rigid core. The compound crystallizes into the triclinic system $P\bar{1}$ with $a = 9.8969(1)$ Å, $b = 42.911(8)$ Å, $c = 9.877(2)$ Å, $\alpha = 92.86(2)°$, $\beta = 103.79(1)°$, $\gamma = 94.43(1)°$, $V = 4051.3(1)$ Å^3, $Z = 2$. The data were collected using MoK_α radiation ($\lambda = 0.71073$ Å) at $T = 300$K. The structure was solved by direct methods using SHELXS-86 and refined to a final R and wR of 0.0688 and 0.1814 respectively using 2452 observed reflections with $I > 2\sigma(I)$. The structure shows a layered packing down a-axis and imbrication along the other two axes. The crystal structure throws light on the liquid crystalline behaviour of the compound.

Introduction

The study of molecular and crystal structure of mesogens gives insight into the liquid crystalline phase. It has been established that the bulk properties of liquid crystals depend on the type of rigid core. So it is interesting to study structures of mesogens with different rigid cores. In view of this, we have under taken the crystal and molecular structure study of 4-isothiocyanato phenyl 4-pentylbicyclo[2,2,2] octane-1-carboxylate, which has an unusual eight membered ring. The title compound was obtained from Aldrich Chemicals and was recrystallized before mounting it on a diffractometer. The compound forms a nematic phase at 74.5°C and goes into the isotropic liquid phase at 113.5°C. The structural formula is given in Figure 1.

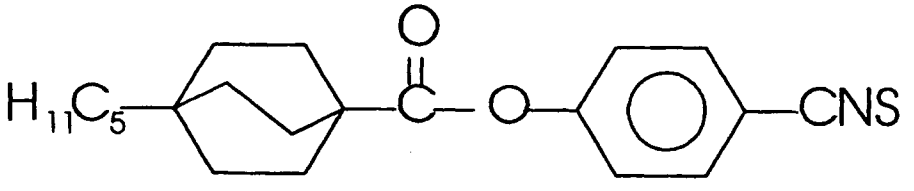

Figure 1: Structure of the molecule.

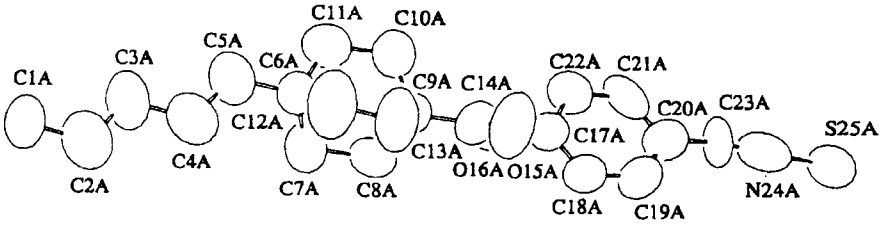

Figure 2: Projection of the molecule on the best plane.

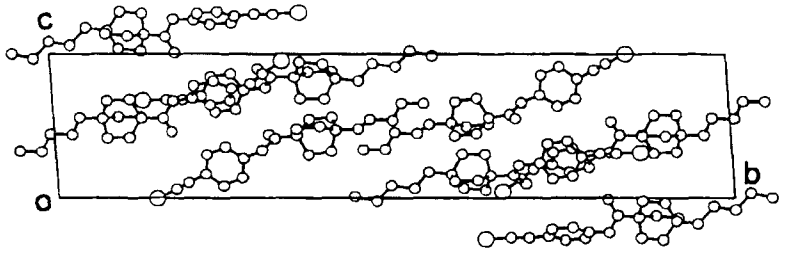

Figure 3: Packing of the molecules down *a*.

Experimental

The colourless crystals were obtained from a solution in acetone. A crystal of dimensions $0.3 \times 0.25 \times 0.2$ mm was used for data collection. The accurate cell dimensions and orientation matrix were obtained by a least-squares fit to the setting angles of 25 reflections on Rigaku AFC7S diffractometer with the use of graphite-monochromated MoK_α radiation. A total of 10884 unique reflections were measured in the range $4 \leq 2\theta \leq 25$, $-10 \leq h \leq 10$, $0 \leq k \leq 50$, $-11 \leq l \leq 11$, of which 2452 were with $I > 2\sigma(I)$. Three standard reflections monitored for every 150 reflections did not show any significant variation in intensity and indicating no deterioration of the crystal. Intensities were collected by ω-2θ scan. Lorentz, polarization and absorption corrections were applied. The structure was solved by SHELXS-86[1] and was refined by full matrix least-squares using SHELXL-93[1]. All the non-hydrogen atoms were located in the initial electron density map. The intramolecular bond distances and angles are within the expected range. Hydrogen atoms were placed in calculated positions (C-H 0.95 Å) in the structure. The hydrogen atoms were constrained to ride on the parent atom. 962 parameters were refined to $R1 = 0.0688$, $wR2 = 0.1814$, where $w = k/(\sigma(F^2) + P * F^2)$ with $k = 1.000$, $P = 0.04$. In the final difference map residual electron densities were $(\triangle\rho)_{\min} = -0.191$ and $(\triangle\rho)_{\max} = 0.235$ eÅ^{-3}.

Discussion

The projection of the thermal ellipsoids(ORTEP)[3] on the best plane for one of the molecules of the asymmetric unit and packing down *a*-axis are given in figures 2 and 3 respectively. The final positional parameters of the non-hydrogen atoms with their estimated standard deviations are given in Table 1. The bond distances and angles are given in tables 2 and 3. The values of the bond lengths

and angles are in good agreement with those of similar compounds. The bond distance C_{14}–O_{15} indicates strong double bond character while that of C_{23}–N_{24} indicates triple bond character. The asymmetric unit has four molecules which is quite rare among mesogens. The structure shows a layered packing when viewed along *a*-axis and imbrication is seen along the other two axes. Disorder is observed in few terminal atoms, which can be expected for any flexible end chain attached to a rigid core. The phenyl rings of all the molecules are planar whereas the bicyclo octane rings are not planar. The bicyclo rings of all the molecules when considered as two cyclohexane rings exhibit the boat conformation. The crystalline cohesion is mainly due to dispersion forces. The detailed tables of anisotropic thermal parameters, torsion angles and structure factor tables can be obtained from the authors.

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3. C.K.Johnson, ORTEP-II, A FORTRAN Thermal Eliipsoid plot diagram for structure illustrations, *ORNL-5138* (1976).

Table 1: Atomic coordinates and equivalent isotropic displacement parameters (A^2)

Atom	x	y	z	U_{eq}
C1A	0.8193(13)	0.5643(2)	0.9869(12)	0.169(5)
C2A	0.7917(12)	0.5320(3)	1.0208(11)	0.194(5)
C3A	0.7719(11)	0.5088(2)	0.9123(11)	0.177(4)
C4A	0.7220(10)	0.4750(2)	0.9328(10)	0.162(3)
C5A	0.6925(10)	0.4525(2)	0.8164(10)	0.148(3)
C6A	0.6486(10)	0.4188(2)	0.8314(9)	0.104(2)
C7A	0.5126(9)	0.4149(2)	0.8820(9)	0.133(3)
C8A	0.4562(8)	0.3801(2)	0.8773(8)	0.116(3)
C9A	0.5649(9)	0.3599(2)	0.8422(8)	0.093(2)
C10A	0.5715(9)	0.3662(2)	0.6920(9)	0.137(3)
C11A	0.6104(9)	0.4011(2)	0.6896(9)	0.136(3)
C12A	0.7544(9)	0.4020(2)	0.9318(10)	0.158(4)
C13A	0.7022(10)	0.3685(2)	0.9440(10)	0.148(3)
C14A	0.5195(14)	0.3253(2)	0.8415(9)	0.114(3)
O15A	0.5941(7)	0.30711(15)	0.8994(7)	0.164(3)
O16A	0.3896(7)	0.31706(14)	0.7697(5)	0.110(2)
C17A	0.3386(8)	0.2855(2)	0.7533(10)	0.096(2)
C18A	0.3401(8)	0.2679(2)	0.8661(9)	0.118(3)
C19A	0.2858(8)	0.2380(2)	0.8465(10)	0.113(3)
C20A	0.2227(10)	0.2227(3)	0.7122(12)	0.120(3)
C21A	0.2244(9)	0.2419(3)	0.6008(11)	0.120(3)
C22A	0.2802(9)	0.2721(2)	0.6190(9)	0.106(3)
C23A	0.1672(10)	0.1948(2)	0.6877(11)	0.132(4)
N24A	0.1210(7)	0.1706(2)	0.6871(7)	0.133(2)
S25A	0.0461(3)	0.13497(6)	0.6826(3)	0.1433(10)
C1B	0.0333(11)	-0.0525(2)	0.3301(11)	0.136(4)
C2B	0.0939(9)	-0.0205(2)	0.3286(9)	0.127(3)
C3B	0.2047(8)	-0.0061(2)	0.4470(8)	0.106(2)
C4B	0.2588(8)	0.0264(2)	0.4436(8)	0.111(2)
C5B	0.3804(7)	0.0391(2)	0.5601(7)	0.098(2)
C6B	0.4381(8)	0.0730(2)	0.5563(7)	0.086(2)
C7B	0.4852(8)	0.0783(2)	0.4208(7)	0.112(2)
C8B	0.5570(8)	0.1111(2)	0.4233(7)	0.112(3)
C9B	0.5492(8)	0.1303(2)	0.5577(7)	0.085(2)
C10B	0.4000(8)	0.13031(14)	0.5657(7)	0.104(2)
C11B	0.3347(7)	0.0963(2)	0.5675(8)	0.105(2)
C12B	0.5613(8)	0.0811(2)	0.6760(8)	0.115(2)
C13B	0.6277(7)	0.11480(15)	0.6854(7)	0.104(2)
C14B	0.6132(8)	0.1630(2)	0.5580(9)	0.102(2)
O15B	0.6520(7)	0.17473(13)	0.4655(7)	0.174(3)
O16B	0.6241(5)	0.18011(13)	0.6763(6)	0.113(2)
C17B	0.6978(12)	0.2091(2)	0.6962(9)	0.096(2)
C18B	0.8323(13)	0.2119(2)	0.7811(9)	0.110(3)
C19B	0.9036(9)	0.2414(2)	0.8135(7)	0.108(3)
C20B	0.8419(12)	0.2672(2)	0.7615(9)	0.088(2)
C21B	0.7091(13)	0.2642(2)	0.6765(10)	0.116(3)
C22B	0.6399(9)	0.2351(3)	0.6489(8)	0.107(3)
C23B	0.9120(10)	0.2954(2)	0.7953(10)	0.122(4)
N24B	0.9888(10)	0.3139(2)	0.8627(8)	0.153(3)
S25B	1.1050(3)	0.34276(5)	0.9528(3)	0.1526(10)

Table 1 continued

Atom	x	y	z	U_{eq}
C1C	1.4069(15)	0.5461(3)	0.6554(14)	0.203(6)
C2C	1.3355(20)	0.5135(3)	0.6548(15)	0.255(7)
C3C	1.2635(15)	0.4983(3)	0.5380(15)	0.245(7)
C4C	1.1860(22)	0.4649(4)	0.5450(19)	0.315(10)
C5C	1.1625(20)	0.4468(4)	0.4824(19)	0.270(9)
C6C	1.0827(11)	0.4139(3)	0.4727(14)	0.140(3)
C7C	0.9835(13)	0.4100(2)	0.5617(12)	0.200(5)
C8C	0.9116(11)	0.3769(2)	0.5471(10)	0.185(4)
C9C	0.9595(9)	0.3571(2)	0.4386(9)	0.099(2)
C11C	0.9988(14)	0.4056(3)	0.3281(13)	0.237(7)
C10C	0.9266(11)	0.3726(2)	0.3033(10)	0.184(4)
C12C	1.1136(10)	0.3574(2)	0.4800(11)	0.173(4)
C13C	1.1828(12)	0.3914(2)	0.4976(15)	0.237(7)
C14C	0.8835(11)	0.3251(2)	0.4152(11)	0.124(3)
O15C	0.7764(8)	0.31706(13)	0.4444(8)	0.167(3)
O16C	0.9370(5)	0.30576(15)	0.3337(6)	0.122(2)
C17C	0.8612(9)	0.2778(2)	0.2792(11)	0.089(2)
C18C	0.8615(9)	0.2528(3)	0.3579(9)	0.105(2)
C19C	0.7899(11)	0.2248(3)	0.3050(13)	0.124(4)
C20C	0.7145(12)	0.2213(2)	0.1677(18)	0.123(4)
C21C	0.7142(10)	0.2466(3)	0.0842(10)	0.119(3)
C22C	0.7872(10)	0.2745(2)	0.1429(12)	0.112(3)
C23C	0.6455(10)	0.1951(2)	0.1085(12)	0.140(4)
N24C	0.5607(9)	0.1765(2)	0.0645(9)	0.153(3)
S25C	0.4438(3)	0.14662(7)	-0.0020(3)	0.1692(12)
C1D	-0.3680(11)	-0.0537(2)	1.0004(10)	0.126(3)
C2D	-0.2996(9)	-0.0228(2)	0.9688(8)	0.130(3)
C3D	-0.2714(7)	0.0017(2)	1.0860(7)	0.108(2)
C4D	-0.1971(7)	0.0328(2)	1.0615(8)	0.105(2)
C5D	-0.1724(7)	0.05804(15)	1.1821(7)	0.092(2)
C6D	-0.0978(7)	0.08928(15)	1.1613(7)	0.077(2)
C7D	-0.0821(9)	0.1107(2)	1.2916(8)	0.136(3)
C8D	-0.0089(8)	0.1429(2)	1.2793(7)	0.110(2)
C9D	0.0230(8)	0.14419(15)	1.1353(7)	0.078(2)
C10D	-0.1106(7)	0.1373(2)	1.0243(7)	0.108(2)
C11D	-0.1800(8)	0.1043(2)	1.0397(8)	0.116(3)
C12D	0.0489(7)	0.0863(2)	1.1399(8)	0.112(2)
C13D	0.1214(7)	0.1187(2)	1.1250(7)	0.093(2)
C14D	0.1017(9)	0.1754(2)	1.1222(10)	0.094(2)
O15D	0.0859(6)	0.18764(11)	1.0125(6)	0.118(2)
O16D	0.1849(6)	0.18914(13)	1.2407(5)	0.0983(15)
C17D	0.2382(11)	0.2194(2)	1.2345(7)	0.084(2)
C18D	0.3795(11)	0.2254(2)	1.2781(7)	0.096(2)
C19D	0.4433(9)	0.2554(2)	1.2893(7)	0.104(3)
C20D	0.3592(12)	0.2799(2)	1.2615(8)	0.091(2)
C21D	0.2175(12)	0.2746(2)	1.2148(8)	0.090(2)
C22D	0.1590(9)	0.2430(2)	1.2036(7)	0.092(2)
C23D	0.4220(9)	0.3089(2)	1.2733(9)	0.100(3)
N24D	0.4334(8)	0.3359(2)	1.2724(7)	0.149(3)
S25D	0.4690(3)	0.37382(6)	1.2833(3)	0.1572(10)

Table 2: Bond lengths of non-hydrogens.

Atoms	d (Å)	Atoms	d (Å)	Atoms	d (Å)	Atoms	d (Å)
C1A-C2A	1.463(12)	C1B-C2B	1.455(11)	C1C-C2C	1.52(2)	C1D-C2D	1.523(10)
C2A-C3A	1.391(10)	C2B-C3B	1.470(9)	C2C-C3C	1.315(14)	C2D-C3D	1.483(8)
C3A-C4A	1.536(10)	C3B-C4B	1.463(8)	C3C-C4C	1.58(2)	C3D-C4D	1.531(8)
C4A-C5A	1.424(9)	C4B-C5B	1.498(8)	C4C-C5C	0.947(11)	C4D-C5D	1.531(8)
C5A-C6A	1.502(9)	C5B-C6B	1.527(8)	C5C-C6C	1.55(2)	C5D-C6D	1.527(8)
C6A-C11A	1.509(9)	C6B-C12B	1.487(8)	C6C-C13C	1.426(12)	C6D-C11D	1.488(8)
C6A-C12A	1.514(10)	C6B-C11B	1.503(8)	C6C-C11C	1.481(13)	C6D-C7D	1.513(8)
C6A-C7A	1.543(9)	C6B-C7B	1.539(8)	C6C-C7C	1.472(12)	C6D-C12D	1.531(8)
C7A-C8A	1.546(8)	C7B-C8B	1.524(7)	C7C-C8C	1.521(10)	C7D-C8D	1.533(8)
C8A-C9A	1.526(9)	C8B-C9B	1.548(8)	C8C-C9C	1.521(10)	C8D-C9D	1.531(8)
C9A-C13A	1.493(9)	C9B-C14B	1.494(9)	C9C-C12C	1.481(9)	C9D-C10D	1.502(8)
C9A-C14A	1.517(10)	C9B-C10B	1.498(8)	C9C-C14C	1.493(10)	C9D-C14D	1.523(9)
C9A-C10A	1.537(9)	C9B-C13B	1.527(8)	C9C-C10C	1.499(10)	C9D-C13D	1.534(8)
C10A-C11A	1.519(9)	C10B-C11B	1.552(8)	C11C-C10C	1.520(11)	C10D-C11D	1.556(8)
C12A-C13A	1.508(9)	C12B-C13B	1.529(7)	C12C-C13C	1.545(10)	C12D-C13D	1.547(7)
C14A-O15A	1.188(9)	C14B-O15B	1.192(8)	C14C-O15C	1.193(9)	C14D-O15D	1.209(7)
C14A-O16A	1.323(10)	C14B-O16B	1.326(8)	C14C-O16C	1.349(9)	C14D-O16D	1.338(8)
O16A-C17A	1.395(8)	O16B-C17B	1.372(8)	O16C-C17C	1.378(8)	O16D-C17D	1.372(8)
C17A-C18A	1.375(9)	C17B-C22B	1.347(9)	C17C-C22C	1.365(10)	C17D-C22D	1.333(9)
C17A-C22A	1.389(9)	C17B-C18B	1.386(10)	C17C-C18C	1.357(9)	C17D-C18D	1.362(9)
C18A-C19A	1.340(8)	C18B-C19B	1.385(9)	C18C-C19C	1.359(10)	C18D-C19D	1.378(9)
C19A-C20A	1.426(10)	C19B-C20B	1.368(9)	C19C-C20C	1.378(12)	C19D-C20D	1.385(9)
C20A-C23A	1.264(10)	C20B-C23B	1.331(9)	C20C-C23C	1.300(11)	C20D-C23D	1.334(10)
C20A-C21A	1.412(11)	C20B-C21B	1.372(10)	C20C-C21C	1.395(13)	C20D-C21D	1.365(9)
C21A-C22A	1.355(10)	C21B-C22B	1.361(11)	C21C-C22C	1.375(12)	C21D-C22D	1.419(10)
C23A-N24A	1.101(8)	C23B-N24B	1.125(9)	C23C-N24C	1.104(10)	C23D-N24D	1.158(9)
N24A-S25A	1.640(9)	N24B-S25B	1.682(10)	N24C-S25C	1.655(10)	N24D-S25D	1.630(10)

Table 3: Bond angles of non-hydrogens.

Atoms	Angle(°)	Atoms	Angle(°)	Atoms	Angle(°)
C3A-C2A-C1A	116.8(10)	C14B-C9B-C13B	109.7(6)	C22C-C17C-C18C	118.6(8)
C2A-C3A-C4A	120.3(9)	C10B-C9B-C13B	107.6(6)	C22C-C17C-O16C	120.3(9)
C5A-C4A-C3A	118.7(9)	C14B-C9B-C8B	109.8(6)	C18C-C17C-O16C	121.0(10)
C4A-C5A-C6A	121.0(8)	C10B-C9B-C8B	109.6(6)	C17C-C18C-C19C	121.8(9)
C5A-C6A-C11A	109.5(8)	C13B-C9B-C8B	109.4(6)	C20C-C19C-C18C	119.9(11)
C5A-C6A-C12A	115.2(8)	C9B-C10B-C11B	110.4(6)	C23C-C20C-C19C	123.6(14)
C11A-C6A-C12A	109.7(7)	C6B-C11B-C10B	110.9(6)	C23C-C20C-C21C	117.1(15)
C5A-C6A-C7A	112.4(7)	C6B-C12B-C13B	115.0(6)	C19C-C20C-C21C	119.3(10)
C11A-C6A-C7A	103.5(7)	C9B-C13B-C12B	107.1(6)	C22C-C21C-C20C	118.7(9)
C12A-C6A-C7A	105.8(7)	O15B-C14B-O16B	118.8(8)	C17C-C22C-C21C	121.7(9)
C6A-C7A-C8A	112.3(6)	O15B-C14B-C9B	127.5(8)	N24C-C23C-C20C	162.9(10)
C9A-C8A-C7A	108.2(6)	O16B-C14B-C9B	113.7(8)	C23C-N24C-S25C	175.2(9)
C13A-C9A-C14A	111.1(8)	C14B-O16B-C17B	119.0(6)	C3D-C2D-C1D	113.8(7)
C13A-C9A-C8A	109.3(7)	C22B-C17B-O16B	122.5(11)	C2D-C3D-C4D	115.8(6)
C14A-C9A-C8A	111.4(7)	C22B-C17B-C18B	119.1(8)	C3D-C4D-C5D	115.0(6)
C13A-C9A-C10A	111.8(7)	O16B-C17B-C18B	118.0(10)	C6D-C5D-C4D	116.3(5)
C14A-C9A-C10A	106.9(7)	C19B-C18B-C17B	118.9(8)	C11D-C6D-C7D	108.7(6)
C8A-C9A-C10A	106.2(6)	C20B-C19B-C18B	120.2(8)	C11D-C6D-C5D	111.1(6)
C11A-C10A-C9A	107.5(6)	C23B-C20B-C19B	119.0(11)	C7D-C6D-C5D	108.1(6)
C6A-C11A-C10A	114.5(7)	C23B-C20B-C21B	120.4(11)	C11D-C6D-C12D	108.4(6)
C13A-C12A-C6A	112.3(6)	C19B-C20B-C21B	120.6(8)	C7D-C6D-C12D	107.3(6)
C9A-C13A-C12A	110.7(7)	C22B-C21B-C20B	118.1(9)	C5D-C6D-C12D	113.2(6)
O15A-C14A-O16A	123.0(9)	C17B-C22B-C21B	123.0(9)	C6D-C7D-C8D	111.6(6)
O15A-C14A-C9A	123.1(11)	N24B-C23B-C20B	156.5(12)	C9D-C8D-C7D	109.9(5)
O16A-C14A-C9A	113.9(9)	C23B-N24B-S25B	175.9(9)	C10D-C9D-C14D	113.0(7)
C14A-O16A-C17A	119.4(7)	C3C-C2C-C1C	121.3(14)	C10D-C9D-C8D	109.1(6)
C18A-C17A-C22A	119.7(8)	C2C-C3C-C4C	118.9(15)	C14D-C9D-C8D	111.1(6)
C18A-C17A-O16A	121.8(8)	C5C-C4C-C3C	133.1(25)	C10D-C9D-C13D	109.8(5)
C22A-C17A-O16A	118.5(9)	C4C-C5C-C6C	138.4(26)	C14D-C9D-C13D	106.9(6)
C19A-C18A-C17A	120.1(8)	C13C-C6C-C11C	104.9(10)	C8D-C9D-C13D	106.7(5)
C18A-C19A-C20A	123.6(9)	C13C-C6C-C7C	111.2(12)	C9D-C10D-C11D	109.9(6)
C23A-C20A-C21A	120.1(11)	C11C-C6C-C7C	105.3(9)	C6D-C11D-C10D	111.5(6)
C23A-C20A-C19A	126.3(10)	C13C-C6C-C5C	108.2(11)	C6D-C12D-C13D	110.9(6)
C21A-C20A-C19A	113.6(9)	C11C-C6C-C5C	110.2(12)	C9D-C13D-C12D	109.7(6)
C22A-C21A-C20A	123.4(9)	C7C-C6C-C5C	116.5(10)	O15D-C14D-O16D	121.9(7)
C21A-C22A-C17A	119.6(8)	C6C-C7C-C8C	112.9(8)	O15D-C14D-C9D	122.1(8)
N24A-C23A-C20A	169.6(12)	C9C-C8C-C7C	109.8(7)	O16D-C14D-C9D	116.0(7)
C23A-N24A-S25A	177.7(9)	C12C-C9C-C14C	114.4(8)	C14D-O16D-C17D	116.3(6)
C1B-C2B-C3B	120.9(8)	C12C-C9C-C10C	105.9(8)	C22D-C17D-C18D	119.5(8)
C4B-C3B-C2B	119.1(7)	C14C-C9C-C10C	108.1(8)	C22D-C17D-O16D	123.5(9)
C3B-C4B-C5B	117.1(6)	C12C-C9C-C8C	109.0(8)	C18D-C17D-O16D	116.5(10)
C4B-C5B-C6B	117.3(6)	C14C-C9C-C8C	111.0(8)	C17D-C18D-C19D	121.5(8)
C12B-C6B-C11B	106.7(6)	C10C-C9C-C8C	108.2(8)	C18D-C19D-C20D	118.2(8)
C12B-C6B-C5B	109.8(6)	C6C-C11C-C10C	114.7(9)	C23D-C20D-C21D	120.4(11)
C11B-C6B-C5B	113.3(6)	C9C-C10C-C11C	108.3(8)	C23D-C20D-C19D	117.7(11)
C12B-C6B-C7B	107.9(6)	C9C-C12C-C13C	110.6(8)	C21D-C20D-C19D	121.7(8)
C11B-C6B-C7B	107.4(6)	C6C-C13C-C12C	112.4(9)	C20D-C21D-C22D	116.9(8)
C5B-C6B-C7B	111.6(6)	O15C-C14C-O16C	119.9(9)	C17D-C22D-C21D	122.0(9)
C8B-C7B-C6B	111.8(5)	O15C-C14C-C9C	127.3(10)	N24D-C23D-C20D	158.7(12)
C7B-C8B-C9B	109.3(5)	O16C-C14C-C9C	112.0(9)	C23D-N24D-S25D	172.9(9)
C14B-C9B-C10B	110.7(6)	C14C-O16C-C17C	118.5(6)		