Supporting Information Section.

Synthesis of the Phenoxonium Cation of an α -Tocopherol Model Compound Crystallized With Non-Nucleophilic $[B(C_6F_5)_4]^-$ and $(CB_{11}H_6Br_6)^-$ Anions.

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Bond	Bond Length / Å					
	$(CH_3)\alpha$ -TOH ^b		(CH ₃)α-TO ⁺			
	Crystal	Theoretical	Cry	rstal	Theoretical	
		(EDF2/6-31+G*)	$(CB_{11}H_6Br_6)^-$	$[B(C_6F_5)]^-$	(EDF2/6-31+G*)	
$C_1 - C_2$	1.4055 (14)	1.404	1.468 (7)	1.455 (4)	1.454	
$C_2 - C_3$	1.3954 (14)	1.398	1.324 (7)	1.355 (4)	1.360	
$C_3 - C_4$	1.3974 (15)	1.399	1.511 (7)	1.488 (4)	1.498	
$C_4 - C_5$	1.3929 (15)	1.397	1.488 (7)	1.491 (4)	1.501	
$C_5 - C_6$	1.4012 (15)	1.406	1.339 (7)	1.355 (4)	1.359	
$C_6 - C_1$	1.3934 (14)	1.400	1.433 (7)	1.447 (4)	1.447	
$C_{6}-C_{7}$	1.5132 (14)	1.511	1.520 (7)	1.505 (4)	1.504	
$C_7 - C_8$	1.5202 (16)	1.526	1.512 (7)	1.518 (4)	1.525	
$C_8 - C_9$	1.5217 (16)	1.526	1.503 (7)	1.515 (4)	1.519	
$C_9 - C_{13}$	1.5159 (16)	1.521	1.516 (8)	1.518 (5)	1.516	
$C_9 - C_{14}$	1.5207 (16)	1.529	1.515 (7)	1.511 (5)	1.521	
$C_2 - C_{10}$	1.5084 (14)	1.504	1.474 (7)	1.499 (4)	1.498	
$C_3 - C_{11}$	1.5113 (15)	1.508	1.499 (7)	1.493 (4)	1.490	
$C_5 - C_{12}$	1.5097 (15)	1.508	1.473 (7)	1.495 (4)	1.487	
$C_4 - O_1$	1.3950 (13)	1.377	1.219 (6)	1.214 (3)	1.217	
$C_1 - O_2$	1.3827 (12)	1.374	1.296 (5)	1.282 (3)	1.289	
C ₉ –O ₂	1.4566 (12)	1.440	1.534 (6)	1.520 (4)	1.510	

Table S1. A selection of crystallographic bond lengths and angles compared with data from molecular orbital calculations using the EDF2/6-31+G* model.^{*a*}

Bond	Bond Angle / °					
	(CH ₃)	α-TOH	$(CH_3)\alpha$ -TO ⁺			
	Crystal	Theoretical	Cry	vstal	Theoretical	
		(EDF2/6-31+G*)	$(CB_{11}H_6Br_6)^-$	$[B(C_6F_5)]^-$	(EDF2/6-31+G*)	
$C_1 - C_2 - C_3$	118.91 (9)	119.3	117.6 (5)	117.7 (2)	118.3	
$C_2 - C_3 - C_4$	119.09 (9)	118.8	119.5 (5)	118.8 (3)	119.0	
$C_3 - C_4 - C_5$	122.08 (10)	122.2	119.9 (5)	120.6 (2)	120.4	
$C_4 - C_5 - C_6$	118.86 (9)	119.1	119.3 (5)	119.4 (2)	119.3	
$C_5 - C_6 - C_1$	119.19 (9)	118.8	118.4 (5)	117.2 (3)	118.1	
$C_6 - C_1 - C_2$	121.67 (9)	121.7	124.9 (5)	125.0 (2)	124.8	
$C_{5}-C_{6}-C_{7}$	120.66 (9)	121.4	122.7 (5)	123.7 (2)	123.0	
$C_{6}-C_{7}-C_{8}$	111.53 (9)	112.0	110.8 (5)	110.9 (2)	111.5	
$C_7 - C_8 - C_9$	111.31 (9)	111.6	112.1 (5)	111.4 (2)	112.5	
$C_8 - C_9 - O_2$	107.95 (9)	108.2	107.5 (4)	107.2 (2)	107.8	
$C_9 - O_2 - C_1$	117.42 (8)	118.8	122.8 (4)	123.5 (2)	124.8	
$O_2 - C_1 - C_2$	115.63 (9)	115.8	113.0 (5)	113.2 (2)	113.7	
$Q_2 - C_1 - C_2$	122.69 (9)	122.5	122.5 (5)	121.8 (2)	121.6	



^{*a*}The calculated Cartesian coordinates of α -TOH and α -TO⁺ (which were used to obtain the theoretical bond lengths and bond angles) are given in the Supporting Information section of reference 7c. ^{*b*}Values are given for one of the two molecules in the crystallographic asymmetric unit.

16 Feb 2006

${\rm Crystal\ structure\ of\ } ({\rm C}_{14}{\rm H}_{19}{\rm O}_2)^+ ({\rm CH}_6{\rm B}_{11}{\rm Br}_6)^-.{\rm C}_2{\rm H}_4{\rm Cl}_2 \ -{\rm web0601}$

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Abstract

The crystal structure of $(C_{14}H_{19}O_2)^+(CH_6B_{11}Br_6)^-.C_2H_4Cl_2$ is reported.

Comment

The crystallographic asymmetric unit consists of one $(C_{14}H_{19}O_2)^+$ cation, one $(CH_6B_{11}Br_6)^$ anion and one dichloroethane molecule of solvation. The observation of a peak in a difference electron density map just beyond the H atom on B7 suggests the presence of a low occupancy Br atom site. This could correspond to a small amount of $(CH_5B_{11}Br_7)^-$ impurity (*ca.* 2%). The Br7—B7 distance is shorter than the other Br—B distances, but this could arise from the dodecahedral core of $(CH_5B_{11}Br_7)^-$ being displaced by a small amount with respect to the core of the dominant $(CH_6B_{11}Br_6)^-$ species as a consequence of packing interactions.

The largest peaks in the final difference map are all of near-equal intensity and have no chemical significance.

Experimental

The compound was prepared by SBL and recrystallized from dichloroethane/acetonitrile. The sample ID is SBL-06.

Crystal data $C_{14}H_{19}O_2^+.CH_{5.98}B_{11}Br_{6.02}^-.C_2H_4Cl_2$ Cell parameters from 272638 reflections $M_r = 936.19$ $\theta = 3 - 25^{\circ}$ $\mu = 7.536 \text{ mm}^{-1}$ Orthorhombic T = 200 KPbcaa = 11.5677(2) Å Plate b = 20.2995(3) ÅOrange c = 27.9851(6) Å0.24 \times 0.19 \times 0.06 mm $V = 6571.4(2) \text{ Å}^3$ Crystal source: local Z = 8 $D_x = 1.892 \text{ Mg m}^{-3}$ D_m not measured Mo $K\alpha$ radiation $\lambda = 0.71073 \text{ Å}$ Data collection Nonius KappaCCD diffractometer 3223 reflections with φ and ω scans with CCD $I > 2.0\sigma(I)$ $R_{\rm int} = 0.076$ Absorption correction: $\theta_{\rm max} = 25.0^{\circ}$ by integration via Gaussian method (Cop $h = -13 \rightarrow 13$ pens, 1970) implemented in maXus (2000) $k = -24 \rightarrow 22$ $T_{\min} = 0.342, T_{\max} = 0.642$ $l = -33 \rightarrow 30$ 68824 measured reflections 5825 independent reflections Refinement Method= Modified Sheldrick $w=1/[\sigma^2(F^2) +$ Refinement on F^2 $(0.02P)^2 + 0.00P$, R(F) = 0.0321where $P = (\max(F_o^2, 0) + 2F_c^2)/3$ $wR(F^2) = 0.0716$ $(\Delta/\sigma)_{\rm max} = 0.006837$ S = 0.7283 $\Delta \rho_{\rm max} = 1.28 \ {\rm e} \ {\rm \AA}^{-3}$ 5806 reflections $\Delta \rho_{\rm min} = -1.13 \ {\rm e} \ {\rm \AA}^{-3}$ 410 parameters Extinction correction: none H atoms treated by a mixture of independent Scattering factors from International Tables and constrained refinement Vol C 4.2.6.8 and 6.1.1.4

	Table 1. Selected geom	etric parameters (Å, °)	
Br1—B1	1.942~(6)	C20—B10	1.709(8)
Br2—B2	1.942~(6)	C20—B11	1.692(8)
Br3—B3	1.949(6)	C51— $C52$	1.481(8)
Br4—B4	1.954(6)	B1—B2	1.797(8)
Br5—B5	1.953~(6)	B1—B3	1.785(8)
Br6—B6	1.955~(6)	B1—B4	1.788(9)
Cl1-C51	1.787~(6)	B1—B5	1.795(8)
Cl2— $C52$	1.783(5)	B1—B6	1.792(8)
O1—C4	1.219(6)	B2—B3	1.773(9)
O2—C1	1.296(5)	B2—B6	1.796(8)
O2—C9	1.534~(6)	B2—B7	1.753~(9)
C1— $C2$	1.468(7)	B2—B8	1.751 (9)
C1—C6	1.433(7)	B3—B4	1.786(8)
C2-C3	1.324(7)	B3—B8	1.763(8)
C2—C10	1.474(7)	B3—B9	1.773 (9)
C3—C4	1.511(7)	B4-B5	1.785(8)
C3—C11	1.499(7)	B4-B9	1.770(8)
C4-C5	1.488(7)	B4—B10	1.780(8)
C5-C6	1.339(7)	B5-B6	1.795(8)
C5—C12	1.473(7)	B5 - B10	1.779(8)
C6—C7	1.520(7)	B5—B11	1.772(8)
C7—C8	1.512(7)	B6-B7	1.768(8)
C8—C9	1.503(7)	B6—B11	1.780(8)
C9—C13	1.516(8)	B7—B8	1.738(9)
C9—C14	1.515(7)	B7—B11	1.768(9)
C20—B7	1.676(8)	B8—B9	1.782(9)
C20—B8	1.690(8)	B9—B10	1.774(8)
C20—B9	1.707(7)	B10—B11	1.773(8)
C1—O2—C9	122.8(4)	C3—C4—O1	119.4(5)
O2— $C1$ — $C2$	113.0(5)	C3— $C4$ — $C5$	119.9(5)
O2—C1—C6	122.2(5)	O1— $C4$ — $C5$	120.7(5)
C2-C1-C6	124.9(5)	C4— $C5$ — $C6$	119.3(5)
C1-C2-C3	117.6(5)	C4— $C5$ — $C12$	116.6(5)
C1-C2-C10	118.0(5)	C6-C5-C12	124.1(5)
C3—C2—C10	124.5(5)	C1— $C6$ — $C5$	118.4(5)
C2—C3—C4	119.5(5)	C1—C6—C7	118.9(5)
C2—C3—C11	125.2(5)	C5— $C6$ — $C7$	122.7(5)
C4—C3—C11	115.3(5)	C6—C7—C8	110.8(5)

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C7—C8—C9	112.1 (4)	B3—B2—B6	107.9(4)
O2—C9—C8	107.5(4)	B1—B2—B7	107.2~(4)
O2—C9—C13	101.6(5)	Br2-B2-B7	122.9(4)
C8—C9—C13	113.8(5)	B3—B2—B7	107.2(5)
O2—C9—C14	104.3(4)	B6 - B2 - B7	59.7(3)
C8—C9—C14	115.0(5)	B1—B2—B8	107.9(4)
C13—C9—C14	113.0(5)	Br2-B2-B8	122.5~(4)
B7—C20—B8	62.2~(4)	B3—B2—B8	60.0(3)
B7—C20—B9	114.7(4)	B6-B2-B8	107.7~(4)
B8—C20—B9	63.3~(3)	B7—B2—B8	59.5(4)
B7—C20—B10	115.2 (4)	B1—B3—B2	60.7(3)
B8—C20—B10	115.2 (4)	B1—B3—Br3	120.9(4)
B9—C20—B10	62.6(3)	B2—B3—Br3	121.8(4)
B7—C20—B11	63.3~(4)	B1—B3—B4	60.1(3)
B8—C20—B11	115.1 (4)	B2—B3—B4	108.6~(4)
B9—C20—B11	114.8(4)	Br3—B3—B4	121.0(4)
B10—C20—B11	62.8(3)	B1—B3—B8	107.8(4)
Cl1-C51-C52	111.7(4)	B2—B3—B8	59.4(3)
C51— $C52$ — $Cl2$	113.4(4)	Br3—B3—B8	122.8(4)
Br1 - B1 - B2	121.9(4)	B4—B3—B8	107.9(4)
Br1—B1—B3	121.7~(4)	B1—B3—B9	108.0(4)
B2—B1—B3	59.3(3)	B2—B3—B9	108.3~(4)
Br1—B1—B4	121.8(4)	Br3—B3—B9	121.8(4)
B2—B1—B4	107.5~(4)	B4—B3—B9	59.6~(3)
B3—B1—B4	60.0(3)	B8—B3—B9	60.5~(3)
Br1—B1—B5	122.2~(4)	B1—B4—B3	59.9(3)
B2—B1—B5	107.8(4)	B1 - B4 - Br4	122.9(4)
B3—B1—B5	107.6~(4)	B3—B4—Br4	121.9(4)
B4—B1—B5	59.8(3)	B1 - B4 - B5	60.3~(3)
Br1—B1—B6	122.1 (4)	B3—B4—B5	108.0(4)
B2—B1—B6	60.1~(3)	Br4-B4-B5	122.5~(4)
B3—B1—B6	107.5~(4)	B1—B4—B9	108.0(4)
B4—B1—B6	107.8(4)	B3—B4—B9	59.8(3)
B5—B1—B6	60.1(3)	Br4— $B4$ — $B9$	120.4(4)
B1 - B2 - Br2	121.2~(4)	B5 - B4 - B9	107.9(4)
B1—B2—B3	60.0(3)	B1—B4—B10	108.2~(4)
Br2—B2—B3	121.8(4)	B3—B4—B10	107.7~(4)
B1—B2—B6	59.8(3)	Br4—B4—B10	120.9(4)
Br2—B2—B6	121.4(4)	B5 - B4 - B10	59.9(3)

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B9—B4—B10	60.0(3)	B2—B7—B11	109.6~(4)
B1—B5—B4	59.9(3)	B8—B7—B11	108.9(5)
B1—B5—Br5	122.3~(4)	C20—B8—B3	104.9~(4)
B4—B5—Br5	122.0(4)	C20—B8—B2	105.4(4)
B1—B5—B6	59.9(3)	B3—B8—B2	60.6~(4)
B4—B5—B6	107.8(4)	C20—B8—B7	58.5(3)
Br5—B5—B6	121.9(4)	B3—B8—B7	108.3~(4)
B1—B5—B10	107.9(4)	B2—B8—B7	60.3~(4)
B4—B5—B10	59.9(3)	C20—B8—B9	58.8(3)
Br5—B5—B10	121.4(4)	B3—B8—B9	60.0(3)
B6—B5—B10	108.0(4)	B2—B8—B9	108.9(4)
B1—B5—B11	107.5~(4)	B7—B8—B9	108.0(5)
B4—B5—B11	107.6(4)	C20—B9—B8	57.9(3)
Br5—B5—B11	121.8(4)	C20—B9—B3	103.8~(4)
B6—B5—B11	59.9(3)	B8—B9—B3	59.5(4)
B10—B5—B11	59.9(3)	C20—B9—B4	104.6~(4)
B2—B6—B5	107.8(4)	B8—B9—B4	107.8~(4)
B2—B6—B1	60.1(3)	B3—B9—B4	60.6(3)
B5—B6—B1	60.1(3)	C20—B9—B10	58.8(3)
B2—B6—Br6	123.2~(4)	B8—B9—B10	107.7~(4)
B5—B6—Br6	121.5(4)	B3—B9—B10	108.6~(4)
B1—B6—Br6	122.9(4)	B4—B9—B10	60.3(3)
B2—B6—B7	58.9(3)	C20—B10—B4	104.0~(4)
B5—B6—B7	106.9(4)	C20—B10—B5	104.0(4)
B1—B6—B7	106.7(4)	B4—B10—B5	60.2(3)
Br6—B6—B7	122.5~(4)	C20—B10—B9	58.7(3)
B2—B6—B11	107.1 (4)	B4—B10—B9	59.7(3)
B5—B6—B11	59.4(3)	B5—B10—B9	108.0(4)
B1—B6—B11	107.3(4)	C20—B10—B11	58.1(3)
Br6—B6—B11	120.9(4)	B4—B10—B11	107.7~(4)
B7—B6—B11	59.8(3)	B5—B10—B11	59.9(3)
C20—B7—B6	105.8(4)	B9—B10—B11	107.7(5)
C20—B7—B2	105.9(4)	C20—B11—B6	104.6~(4)
B6—B7—B2	61.4(3)	C20—B11—B10	59.1(3)
C20—B7—B8	59.3(3)	B6—B11—B10	108.9(4)
B6—B7—B8	109.6~(4)	C20—B11—B5	105.0(4)
B2—B7—B8	60.2~(4)	B6—B11—B5	60.7(3)
C20—B7—B11	58.8(3)	B10—B11—B5	60.2(3)
B6—B7—B11	60.5~(3)	C20—B11—B7	57.9(3)

B6—B11—B7	59.8(3)	B5—B11—B7	107.9(4)
B10—B11—B7	107.7(4)		

H atoms were included at calculated positions with methyl H atoms oriented to best-match peaks in difference electron density maps. Restraints were imposed on distances and angles involving H atoms of the cation as they were refined positionally. Other H atoms ride on the atom to which they are attached.

Data collection: COLLECT (Nonius BV, 1997). Cell refinement: Denzo/Scalepack . Data reduction: Denzo/Scalepack (Otwinowski & Minor, 1996). Program(s) used to solve structure: SIR92 (Altomare *et al.* 1994). Program(s) used to refine structure: CRYSTALS (Watkin *et al.*2003). Molecular graphics: ORTEP–II (Johnson 1976) in teXsan (MSC, 1992–1997) . Software used to prepare material for publication: CRYSTALS .

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Supplementary data

		$U_{\rm eq} = (1/3)\Sigma_{\rm eq}$	$_{i}\Sigma_{j}U^{ij}a^{i}a^{j}\mathbf{a}_{i}.\mathbf{a}_{j}.$		X
	Occupancy	x	u	z	U_{eq}
Br1	1.0000	0.60711(5)	0.33738(3)	0.07643(2)	0.0481
Br2	1.0000	0.29738(5)	0.39726(3)	0.05529(2)	0.0621
Br3	1.0000	0.35642(5)	0.25449(3)	0.14091(2)	0.0560
Br4	1.0000	0.63405(5)	0.29075(3)	0.21013(2)	0.0491
Br5	1.0000	0.75277(5)	0.45788(3)	0.16527(2)	0.0429
Br6	1.0000	0.54366(5)	0.52517(3)	0.07012(2)	0.0492
Br7	0.0194(16)	0.266(2)	0.5476(13)	0.1320(11)	0.0449
Cl1	1.0000	0.81035(15)	0.34192(9)	-0.02580(7)	0.0842
Cl2	1.0000	0.98812(13)	0.43320(7)	0.03798(6)	0.0585
O1	1.0000	0.5768(3)	0.08948(18)	0.21772(14)	0.0528
O2	1.0000	0.8609(3)	0.20860(17)	0.09978(13)	0.0441
C1	1.0000	0.7998(4)	0.1751(2)	0.13004(19)	0.0344
C2	1.0000	0.6938(4)	0.1479(2)	0.10895(19)	0.0335
C3	1.0000	0.6209(4)	0.1174(2)	0.1379(2)	0.0406
C4	1.0000	0.6488(5)	0.1120(2)	0.1905(2)	0.0356
C5	1.0000	0.7627(4)	0.1353(2)	0.20859(19)	0.0343
C6	1.0000	0.8352(4)	0.1660(2)	0.17865(19)	0.0333
C7	1.0000	0.9526(4)	0.1917(2)	0.1943(2)	0.0442
C8	1.0000	1.0311(4)	0.2015(3)	0.1516(2)	0.0531
C9	1.0000	0.9749(4)	0.2424(3)	0.1134(2)	0.0500
C10	1.0000	0.6748(5)	0.1575(3)	0.0573(2)	0.0542
C11	1.0000	0.5088(5)	0.0865(3)	0.1229(2)	0.0579
C12	1.0000	0.7865(5)	0.1242(3)	0.2597(2)	0.0530
C13	1.0000	1.0392(5)	0.2417(3)	0.0662(2)	0.0787
C14	1.0000	0.9392(5)	0.3110(3)	0.1288(2)	0.0584
C20	1.0000	0.3738(5)	0.4579(2)	0.20776(19)	0.0424
C51	1.0000	0.7939(5)	0.4287(3)	-0.0176(2)	0.0588
C52	1.0000	0.8383(4)	0.4504(3)	0.0295(2)	0.0536
B1	1.0000	0.5202(5)	0.3829(3)	0.1258(2)	0.0332
B2	1.0000	0.3745(5)	0.4107(3)	0.1161(2)	0.0415
B3	1.0000	0.4020(5)	0.3446(3)	0.1559(2)	0.0392
B4	1.0000	0.5331(5)	0.3613(3)	0.1875(2)	0.0359
B5	1.0000	0.5874(5)	0.4386(3)	0.1671(2)	0.0345
B6	1.0000	0.4898(5)	0.4693(3)	0.1225(2)	0.0358
B7	1.0000	0.3550(5)	0.4816(3)	0.1509(2)	0.0453
B8	1.0000	0.3014(5)	0.4065(3)	0.1708(2)	0.0437
B9	1.0000	0.3978(5)	0.3755(3)	0.2151(2)	0.0437
B10	1.0000	0.5110(5)	0.4337(3)	0.2221(2)	0.0369
B11	1.0000	0.4841(5)	0.4997(3)	0.1821(2)	0.0414
H7	0.9810	0.3010(5)	0.5178(3)	0.1415(2)	0.0531
H8	1.0000	0.2164(5)	0.3983(3)	0.1734(2)	0.0525
H9	1.0000	0.3686(5)	0.3498(3)	0.2431(2)	0.0478
H10	1.0000	0.5476(5)	0.4419(3)	0.2540(2)	0.0470
H11	1.0000	0.5051(5)	0.5459(3)	0.1908(2)	0.0520
H20	1.0000	0.3281(5)	0.4813(2)	0.23288 (19)	0.0542
H71	1.0000	0.985(2)	0.1608(12)	0.2166(9)	0.0582
H72	1.0000	0.943(2)	0.2324(11)	0.2105(9)	0.0582
H81	1.0000	1.100 (2)	0.2229(13)	0.1623(9)	0.0630
H82	1.0000	1.052(2)	0.1593(11)	0.1378(9)	0.0630
H101	1.0000	0.607(2)	0.1367(16)	0.0478 (9)	0.0671
H102	1.0000	0.738(2)	0.1404 (17)	0.0397(9)	0.0671
H103	1.0000	0.668(3)	0.2021(10)	0.0503(9)	0.0671
H111	1.0000	0.458(2)	0.0848 (17)	0.1488 (8)	0.0695
H112	1.0000	0.521(2)	0.0434(11)	0.1117 (13)	0.0695
H113	1.0000	0.477(2)	0.1113 (14)	0.0977(10)	0.0695
H121	1.0000	0.7180(19)	0.1121(16)	0.2764(9)	0.0618
H122	1.0000	0.840(3)	0.0887(13)	0.2627(9)	0.0618

Table S1. Fractional atomic coordinates and equivalent isotropic displacement parameters (\mathring{A}^2

 $\overline{7}$

H123	1.0000	0.818(3)	0.1620(12)	0.2742(9)	0.0618
H131	1.0000	1.111(2)	0.2637(18)	0.0708(10)	0.0946
H132	1.0000	1.052(3)	0.1962(11)	0.0566(11)	0.0946
H133	1.0000	0.994(3)	0.2641(18)	0.0419(9)	0.0946
H141	1.0000	1.0051(19)	0.3372(12)	0.1337(13)	0.0707
H142	1.0000	0.896(3)	0.3096(13)	0.1576(10)	0.0707
H143	1.0000	0.893(3)	0.3316(13)	0.1041(10)	0.0707
H511	1.0000	0.8370(5)	0.4522(3)	-0.0435(2)	0.0717
H512	1.0000	0.7099(5)	0.4401(3)	-0.0196(2)	0.0717
H521	1.0000	0.8270(4)	0.4991(3)	0.0319(2)	0.0612
H522	1.0000	0.7932(4)	0.4279(3)	0.0552(2)	0.0612

Table S2. Anisotropic displacement parameters (\mathring{A}^2)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br1	0.0473 (3)	0.0452(3)	0.0518(4)	-0.0031(3)	0.0139 (3)	-0.0153(3)
Br2	0.0551(4)	0.0758(5)	0.0555(4)	-0.0056(4)	-0.0198(3)	-0.0021(4)
Br3	0.0482(3)	0.0395(3)	0.0804(5)	-0.0146(3)	0.0027(3)	-0.0058(3)
Br4	0.0431(3)	0.0362(3)	0.0681(4)	0.0033(3)	-0.0036(3)	0.0113(3)
Br5	0.0375(3)	0.0398(3)	0.0514(4)	-0.0091(3)	-0.0047(3)	-0.0002(3)
Br6	0.0565(4)	0.0462(3)	0.0450(4)	-0.0019(3)	0.0031(3)	0.0124(3)
Br7	0.047(14)	0.034(13)	0.054(15)	0.017(11)	-0.008(12)	0.016(12)
Cl1	0.0753(12)	0.0784(12)	0.0989(15)	-0.0216(10)	0.0263(11)	-0.0382(11)
Cl2	0.0517(9)	0.0527(9)	0.0712(12)	-0.0050(8)	0.0051(8)	0.0110(9)
O1	0.047(2)	0.050(2)	0.061(3)	0.001(2)	0.018(2)	0.002(2)
O2	0.041(2)	0.044(2)	0.047(3)	0.0008(19)	0.002(2)	0.006(2)
C1	0.037(3)	0.025(3)	0.041(4)	0.010(3)	0.010(3)	0.006(3)
C2	0.037(3)	0.027(3)	0.036(4)	0.005(3)	-0.001(3)	-0.004(3)
C3	0.039(3)	0.034(3)	0.049(4)	0.004(3)	-0.005(3)	-0.015(3)
C4	0.041(3)	0.024(3)	0.041(4)	0.003(3)	0.006(3)	-0.003(3)
C5	0.037(3)	0.032(3)	0.034(3)	0.008(3)	-0.006(3)	-0.003(3)
C6	0.032(3)	0.027(3)	0.041(4)	0.003(2)	-0.006(3)	-0.001(3)
C7	0.041(3)	0.031(3)	0.061(4)	-0.001(3)	-0.008(3)	-0.002(3)
C8	0.031(3)	0.043(3)	0.085(5)	-0.001(3)	-0.002(3)	0.004(4)
C9	0.037(3)	0.046(4)	0.066(5)	-0.005(3)	0.009(3)	0.016(3)
C10	0.066(4)	0.053(4)	0.043(4)	-0.005(3)	-0.012(3)	-0.002(3)
C11	0.037(3)	0.058(4)	0.079(5)	-0.001(3)	-0.007(3)	-0.009(4)
C12	0.051(4)	0.059(4)	0.049(5)	-0.003(3)	0.001(3)	0.006(3)
C13	0.061(4)	0.082(5)	0.093~(6)	-0.004(4)	0.028(4)	0.025(5)
C14	0.054(4)	0.035(3)	0.086(5)	-0.006(3)	-0.001(4)	0.013(3)
C20	0.049(3)	0.040(3)	0.039(4)	0.008(3)	0.007(3)	0.002(3)
C51	0.048(4)	0.066(4)	0.062(5)	-0.004(3)	0.008(4)	-0.002(4)
C52	0.045(3)	0.050(4)	0.066(5)	-0.006(3)	0.017(3)	0.002(3)
B1	0.029(3)	0.032(3)	0.039(4)	0.000(3)	0.005(3)	-0.006(3)
B2	0.034(4)	0.046(4)	0.045(4)	-0.002(3)	-0.010(3)	0.000(3)
B3	0.030(3)	0.039(4)	0.048(4)	0.002(3)	0.001(3)	-0.002(3)
B4	0.034(3)	0.029(3)	0.045(4)	0.003(3)	-0.001(3)	0.003(3)
B5	0.041(3)	0.029(3)	0.034(4)	-0.003(3)	0.000(3)	0.000(3)
B6	0.039(4)	0.039(4)	0.030(4)	-0.001(3)	0.001(3)	0.002(3)
B7	0.040(4)	0.039(4)	0.057(5)	0.014(3)	0.004(3)	0.006(3)
B8	0.034(3)	0.046(4)	0.051(5)	0.002(3)	0.006(3)	0.006(4)
B9	0.041(4)	0.042(4)	0.048(5)	0.004(3)	0.021(3)	0.009(3)
B10	0.048(4)	0.032(3)	0.031(4)	-0.002(3)	0.001(3)	0.000(3)
B11	0.048(4)	0.034(3)	0.043(4)	0.006(3)	0.003(3)	-0.009(3)

Table 53. Geometric parameters (A, γ)
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Br1—B1	1.942(6)	C14—H142	0.947(19)
Br2—B2	1.942(6)	C14—H143	0.970(19)
Br3—B3	1.949 (6)	C20—B7	1.676(8)
Br4—B4	1.954 (6)	C20—B8	1.690(8)
Br5—B5	1.953 (6)	C20—B9	1.707(7)
Br6-B6	1.955 (6)	C20—B10	1.709 (8)
Br7—B7	1.77 (2)	C20—B11	1.692 (8)
Cl1—C51	1.787 (6)	C20—H20	1.000
Cl2—C52	1.783 (5)	C51—C52	1.481 (8)
01-C4	1 219 (6)	C51—H511	1,000
$O^2 - C^1$	1.210(0) 1.296(5)	C51—H512	1.000
$O_2 = O_1$	1.230(6)	C52_H521	1.000
02-09	1.004(0)	C52_11521	1.000
C1 = C2	1.408(7)	C32—n322	1.000
C1 = C6	1.433(7)	BI-B2	1.797 (8)
02-03	1.324(7)	BI-B3	1.785 (8)
C2—C10	1.474 (7)	B1—B4	1.788 (9)
C3—C4	1.511 (7)	B1—B5	1.795(8)
C3—C11	1.499 (7)	B1—B6	1.792(8)
C4-C5	1.488(7)	B2—B3	1.773(9)
C5-C6	1.339(7)	B2-B6	1.796(8)
C5-C12	1.473(7)	B2—B7	1.753(9)
C6-C7	1.520(7)	B2—B8	1.751(9)
C7—C8	1.512(7)	B3—B4	1.786(8)
C7—H71	0.963(19)	B3—B8	1.763(8)
C7—H72	0.949 (18)	B3—B9	1.773(9)
C8—C9	1.503 (7)	B4—B5	1.785(8)
C8—H81	0.960 (19)	B4—B9	1.770 (8)
C8—H82	0.973 (19)	B4—B10	1.780 (8)
C9—C13	1.516 (8)	B5—B6	1.795(8)
C9-C14	1.515(7)	B5—B10	1.779(8)
C10_H101	0.930(19)	B5-B11	1.772(8)
C10—H102	0.947(19)	B6—B7	1.772(0) 1.768(8)
C10_H102	0.030(10)	B6_B11	1.780(8)
C11 H111	0.930(19)	D0-D11 D7 D0	1.730(0)
	0.934(19)	D7 D11	1.738(9) 1.768(0)
C11_H112	0.939(19)	D7-D11	1.708 (9)
C12_H113	0.942(19)	B/—H/	1.000
C12—H121	0.952 (19)	B8—B9	1.782 (9)
C12—H122	0.950 (19)	B8—H8	1.000
C12—H123	0.945 (19)	B9—B10	1.774(8)
C13—H131	0.950(19)	В9—Н9	1.000
C13—H132	0.974(19)	B10—B11	1.773(8)
C13—H133	0.968(19)	B10—H10	1.000
C14—H141	0.939(19)	B11—H11	1.000
C1—O2—C9	122.8 (4)	H71—C7—H72	107.6(17)
O2-C1-C2	113.0 (5)	C7—C8—C9	112.1 (4)
Q2-C1-C6	122.2(5)	C7—C8—H81	108.3(15)
$C_{2}^{-}C_{1}^{-}C_{6}^{-}$	124.9(5)	C9-C8-H81	109.5(15)
$C_1 - C_2 - C_3$	1176(5)	C7-C8-H82	110.4 (15)
C1 - C2 - C10	1180(5)	C9-C8-H82	108.1(15)
C_{3} C_{2} C_{10}	1245(5)	H81_C8_H82	108.1(10) 108.3(17)
$C_{2}^{-} C_{3}^{-} C_{4}^{-}$	124.0(0) 110.5(5)	$0^{2}-0^{2}-0^{8}$	107.5(11)
$C_2 = C_3 = C_4$	125.2(5)	$O_2 = O_3 = O_3$	107.5(4) 101.6(5)
$C_2 = C_3 = C_{11}$	125.2(5)	02-09-013	101.0(5)
	115.3(5)	02 02 014	113.8(3)
C3-C4-01	119.4(5)	02-09-014	104.3(4)
C3—C4—C5	119.9 (5)	C8—C9—C14	115.0(5)
01	120.7 (5)	C13—C9—C14	113.0(5)
C4-C5-C6	119.3 (5)	C2—C10—H101	110.4(16)
C4-C5-C12	116.6 (5)	C2-C10-H102	110.3(16)
C6-C5-C12	124.1(5)	H101—C10—H102	109.5(17)
C1-C6-C5	118.4(5)	C2-C10-H103	110.4(16)
C1-C6-C7	118.9(5)	H101—C10—H103	107.9(17)
C5-C6-C7	122.7(5)	H102—C10—H103	108.4(17)
C6—C7—C8	110.8(5)	C3—C11—H111	110.0(16)
C6—C7—H71	108.3 (15)	C3—C11—H112	110.8 (16)
C8—C7—H71	111.2 (15)	H111—C11—H112	108.4 (17)
C6—C7—H72	109.7 (15)	C3-C11-H113	108.9 (16)
C8—C7—H72	109.2 (15)	H111—C11—H113	110.9 (17)
			× · · /

H112—C11—H113

B2-B1-B5

B3-B1-B5

B4—B1—B5

Br1-B1-B6

B2—B1—B6

B3-B1-B6

B4-B1-B6

B5—B1—B6

B1 - B2 - Br2

B1—B2—B3

Br2-B2-B3

B1 - B2 - B6

Br2-B2-B6

B3—B2—B6

B1 - B2 - B7

Br2-B2-B7

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B3—B2—B7

B2-B6-B1

B5-B6-B1

B2—B6—Br6

B5 - B6 - Br6

B1 - B6 - Br6

B2-B6-B7

B5 - B6 - B7

B1—B6—B7

Br6—B6—B7

B2—B6—B11

B5 - B6 - B11

B1 - B6 - B11

Br6—B6—B11

B7—B6—B11

C20-B7-B6

 $\rm C20{--}B7{--}B2$

S12

107.2(5)

59.7(3)

107.9(4)

122.5(4)

60.0(3)

107.7(4)

59.5(4)

60.7(3)

120.9(4)

121.8(4)

60.1(3)108.6(4)

121.0 (4)

107.8(4)

59.4(3)122.8(4)

107.9(4)

108.0(4)

108.3(4)

121.8(4)59.6(3)

60.5(3)

59.9(3)

122.9 (4)

121.9(4)60.3(3)

108.0(4)

122.5(4)

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59.8(3)

120.4(4)107.9(4)

108.2(4)

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59.9(3)60.0(3)

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107.9(4)

59.9(3)

121.4(4)108.0(4)

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107.6(4)

121.8(4)59.9(3)

59.9(3)

107.8(4)

60.1(3)

60.1(3)

123.2(4)

121.5(4)

122.9(4)

58.9(3)

106.9(4)

106.7(4)

122.5(4)

107.1(4)

59.4(3)

107.3(4)

120.9(4)

59.8(3)

105.8(4)

105.9(4)

C5—C12—H121	111.1 (16)	B6—B2—B7
C5—C12—H122	108.8 (16)	B1—B2—B8
H121—C12—H122	107.5 (17)	Br2-B2-B8
C5—C12—H123	111.6 (16)	B3—B2—B8
H121—C12—H123	108.8 (17)	B6—B2—B8
H122—C12—H123	109.0 (17)	B7—B2—B8
C9—C13—H131	107.8 (17)	B1—B3—B2
C9—C13—H132	108.9 (16)	B1—B3—Br3
H131—C13—H132	110.3 (17)	B2—B3—Br3
C9—C13—H133	110.1 (16)	B1—B3—B4
H131—C13—H133	110.1 (17)	B2—B3—B4
H132—C13—H133	109.7 (17)	Br3—B3—B4
C9—C14—H141	109.9 (16)	B1—B3—B8
C9—C14—H142	111.0 (16)	B2—B3—B8
H141—C14—H142	108.6 (17)	Br3—B3—B8
C9-C14-H143	110.1 (16)	B4—B3—B8
H141—C14—H143	107.9 (17)	B1—B3—B9
H142—C14—H143	109.2 (17)	B2—B3—B9
B7—C20—B8	62.2 (4)	Br3—B3—B9
B7—C20—B9	114.7 (4)	B4—B3—B9
B8—C20—B9	63.3 (3)	B8—B3—B9
B7-C20-B10	115.2 (4)	B1—B4—B3
B8-C20-B10	115.2 (4)	B1—B4—Br4
B9—C20—B10	62.6 (3)	B3—B4—Br4
B7—C20—B11	63.3 (4)	B1—B4—B5
B8—C20—B11	115.1 (4)	B3—B4—B5
B9—C20—B11	114.8 (4)	Br4—B4—B5
B10-C20-B11	62.8 (3)	B1—B4—B9
B7—C20—H20	117.5	B3—B4—B9
B8—C20—H20	117.5	Br4—B4—B9
B9—C20—H20	117.8	B5—B4—B9
B10-C20-H20	117.5	B1—B4—B10
B11-C20-H20	117.3	B3—B4—B10
Cl1—C51—C52	111.7 (4)	Br4—B4—B10
Cl1—C51—H511	108.9	B5-B4-B10
C52—C51—H511	109.3	B9—B4—B10
Cl1—C51—H512	108.9	B1—B5—B4
C52—C51—H512	108.6	B1—B5—Br5
H511—C51—H512	109.5	B4—B5—Br5
C51—C52—Cl2	113.4 (4)	B1-B5-B6
C51—C52—H521	108.0	B4—B5—B6
Cl2—C52—H521	108.2	Br5—B5—B6
C51—C52—H522	108.9	B1-B5-B10
Cl2-C52-H522	108.8	B4—B5—B10
H521-C52-H522	109.5	Br5-B5-B10
Br1—B1—B2	121.9 (4)	B6-B5-B10
Br1—B1—B3	121.7(4)	B1-B5-B11
B2—B1—B3	59.3 (3)	B4—B5—B11
Br1—B1—B4	121 8 (4)	Br5-B5-B11
B2—B1—B4	107.5(4)	B6-B5-B11
B3—B1—B4	60.0 (3)	B10-B5-B11
Br1B5	122.2 (4)	B2B5B5
DIT DI _D0	144.4 (4)	D0_D0

107.8(4)

107.6(4)

59.8 (3)

122.1(4)

60.1(3)

107.5(4)

107.8(4)

60.1(3)

121.2(4)

60.0(3)

121.8(4)

59.8(3)

121.4(4)

107.9(4)

107.2(4)

122.9(4)

107.8 (17)

B6—B7—B2	61.4(3)	C20—I
C20— $B7$ — $Br7$	125.3(11)	B8—B
B6-B7-Br7	118.9(10)	B3—B9
B2—B7—Br7	122.0(11)	B4—B
C20—B7—B8	59.3 (3)	C20—1
B6-B7-B8	109.6(4)	B8—B
B2-B7-B8 D-7 D7 D8	60.2(4)	B3—B
$Br_{1} - B_{1} - B_{8}$	123.0(10)	B4—B
B6 B7 B11	50.0(3)	C20-1
B2_B7_B11	109.6(4)	C20—1
Br7—B7—B11	103.0(4) 118.8(10)	B4—B
B8—B7—B11	108.9(5)	C20—I
C20—B7—H7	122.9	B4—B
B6—B7—H7	122.4	B5—B
B2—B7—H7	122.4	C20—I
B8—B7—H7	120.4	B4—B
B11—B7—H7	120.5	B5—B
C20—B8—B3	104.9(4)	B9—B
C20— $B8$ — $B2$	105.4(4)	C20—H
B3—B8—B2	60.6(4)	B4—B
C20—B8—B7	58.5(3)	B5—B
B3—B8—B7	108.3(4)	B9—B
B2—B8—B7	60.3(4)	B11—I
C20—B8—B9	58.8(3)	C20—I
B3—B8—B9	60.0 (3)	C20—I
B2—B8—B9	108.9(4)	B6—B
B7—B8—B9	108.0 (5)	C20—1
C20—B8—H8	123.1	B6—B
B3—B8—H8	123.2	B10—1
B2—B8—H8 D7 D0 U0	123.0	C20—1
	121.5	D0-D
C20_B0_B8	57.0 (3)	B10—1 B5—B
C_{20} B_{9} B_{3}	103.8 (4)	C20-F
B8-B9-B3	59.5(4)	B6—B
C20—B9—B4	104.6(4)	B10—F
B8—B9—B4	107.8(4)	B5—B
B3—B9—B4	60.6 (3)	B7—B
$D_{n1} D_{1} D_{2} D_{n2}$	0.6.(6)	D., 9 D
Br1 - B1 - B2 - B12 Br1 - B1 - B2 - B3	-0.0(0)	Br2—E
Br1 = B1 = B2 = B6	-111.3(4)	Br2—F
Br1 - B1 - B2 - B7	-149.2(4)	Br2—F
Br1 - B1 - B2 - B8	148.2(4)	Br2—F
Br1—B1—B3—Br3	0.8 (6)	Br2—E
Br1—B1—B3—B2	-110.7 (4)	Br2—E
Br1-B1-B3-B4	111.1 (5)	Br2—E
Br1—B1—B3—B8	-148.1 (4)	Br2—E
Br1—B1—B3—B9	147.9 (4)	Br2—E
Br1 - B1 - B4 - Br4	-0.2(6)	Br2—E
Br1-B1-B4-B3	-110.9(5)	Br2—E
Br1 - B1 - B4 - B5	111.4 (4)	Br2—E
Br1 - B1 - B4 - B9	-147.7 (4)	Br2—E
Br1 - B1 - B4 - B10	148.8(4)	Br2—E
Br1 - B1 - B5 - Br5	0.3(6)	Br2—E
Br1 - B1 - B5 - B4	-110.7 (5)	Br2—E
Br1—B1—B5—B6	111.2(4)	Br2—E
Br1—B1—B5—B10	-148.0(4)	Br3—E
Br1—B1—B5—B11	148.7(4)	Br3—E
Br1 - B1 - B6 - Br6	-1.3(6)	Br3—E
Br1 - B1 - B6 - B2	110.9(4)	Br3—E
Br1 B1 B6 B7	-111.5(4)	Br3—E
$B_{1} = B_{1} = B_{0} = B_{1}$	148.3(4)	Br3—E
$B_{r^{2}} B_{2} B_{2} B_{1} D_{2} B_{1} D_{2}$	-140.9(4) -111.2(5)	Bro—E
$B_{12} - B_{2} - B_{1} - B_{3}$ Br $2 - B_{2} - B_{1} - B_{4}$	-111.2(0) -148.4(4)	Dro—E Bro_E
$Br_2 - B_2 - B_1 - B_4$ Br_2 - B_2 - B_1 - B_5	-140.4(4) 148.5(4)	Br3_F
$Br_2 = B_2 = B_1 = B_0$	110.7(4)	Br3_F
Br2 B2 B3 Br3	0.0 (6)	Br3—F
	0.0 (0)	210 1

	58.8(3)
D0 D10	107.7 (4)
-B9-B10	107.7(4)
-B9-B10	108.6(4)
-B9-B10	60.3(3)
-B9-H9	123.5
_B0H0	191.9
	121.2
—В9—Н9	123.7
-B9-H9	123.8
—B9—H9	120.7
-B10-B4	104.0(4)
D10 D5	101.0(1) 104.0(4)
-B10-B5	104.0(4)
-B10-B2	60.2(3)
-B10-B9	58.7(3)
-B10-B9	59.7(3)
-B10-B9	108.0(4)
-B10-B11	58 1 (3)
	107.7(4)
-B10-B11	107.7 (4)
-B10-B11	59.9(3)
-B10-B11	107.7(5)
-B10-H10	123.7
-B10-H10	124.3
-B10-H10	123.4
P10 H10	120.1
	121.0
-B10-H10	120.7
-B11-B6	104.6(4)
-B11-B10	59.1(3)
-B11-B10	108.9(4)
-B11-B5	105.0.(4)
D11 D5	60.7(2)
-B11-B3	00.7(3)
-B11-B5	60.2(3)
—B11—B7	57.9(3)
-B11-B7	59.8(3)
-B11-B7	107.7(4)
-B11-B7	107.9(4)
H11H11	193.4
	123.4
D11 U11	100.0
-B11-H11	122.9
-B11-H11 -B11-H11	$122.9 \\ 120.9$
-B11H11 B11H11 B11H11	$122.9 \\ 120.9 \\ 123.4$
-B11-H11 -B11-H11 -B11-H11 -B11-H11 -B11-H11	$122.9 \\ 120.9 \\ 123.4 \\ 121.3$
-B11-H11 -B11-H11 -B11-H11 -B11-H11 -B11-H11	122.9 120.9 123.4 121.3
-B11H11 B11H11 B11H11 B11H11 B2B3B1 B2B1	122.9 120.9 123.4 121.3 110.3 (4)
-B11-H11 -B11-H11 -B11-H11 -B11-H11 -B11-H11 -B2-B3-B1 -B2-B3-B4	122.9 120.9 123.4 121.3 110.3 (4) 147.9 (4)
-B11-H11 -B11-H11 -B11-H11 -B11-H11 -B2-B3-B1 -B2-B3-B4 -B2-B3-B8	$122.9 \\ 120.9 \\ 123.4 \\ 121.3 \\ 110.3 (4) \\ 147.9 (4) \\ -111.9 (5)$
$\begin{array}{c} -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B8 \\ -B2 - B3 - B9 \end{array}$	$122.9 \\ 120.9 \\ 123.4 \\ 121.3 \\ 110.3 (4) \\ 147.9 (4) \\ -111.9 (5) \\ -149.0 (4)$
$\begin{array}{c} -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B8 \\ -B2 - B3 - B9 \\ -B2 - B6 - Br6 \end{array}$	$122.9 \\ 120.9 \\ 123.4 \\ 121.3 \\ 110.3 (4) \\ 147.9 (4) \\ -111.9 (5) \\ -149.0 (4) \\ 1.6 (6) $
$\begin{array}{c} -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B8 \\ -B2 - B3 - B9 \\ -B2 - B6 - Br6 \\ -B2 - B6 - B1 \end{array}$	$122.9 \\ 120.9 \\ 123.4 \\ 121.3 \\ 110.3 (4) \\ 147.9 (4) \\ -111.9 (5) \\ -149.0 (4) \\ 1.6 (6) \\ -110.4 (4) \\ \end{array}$
$\begin{array}{c} -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B8 \\ -B2 - B3 - B9 \\ -B2 - B6 - B76 \\ -B2 - B6 - B1 \\ -B2 - B6 - B5 \end{array}$	$122.9 \\ 120.9 \\ 123.4 \\ 121.3 \\ 110.3 (4) \\ 147.9 (4) \\ -111.9 (5) \\ -149.0 (4) \\ 1.6 (6) \\ -110.4 (4) \\ -148.2 (4) \\ -110.4 (4) \\ -148.2 (4) \\ -1$
$\begin{array}{c} -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B8 \\ -B2 - B3 - B9 \\ -B2 - B6 - B7 \\ -B2 - B6 - B1 \\ -B2 - B6 - B5 \\ -B3 - B6 - B6 \\ -B3 - B6 - B6 \\ -B3 - B6 \\ -B5 - B6 \\ -B5 - B6 \\ -B5 - B6 \\ -B5 - B$	$122.9 \\ 120.9 \\ 123.4 \\ 121.3 \\ 110.3 (4) \\ 147.9 (4) \\ -111.9 (5) \\ -149.0 (4) \\ 1.6 (6) \\ -110.4 (4) \\ -148.2 (4) \\ 112.4 (5) \\ 112.4 $
$\begin{array}{c} -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B8 \\ -B2 - B3 - B9 \\ -B2 - B6 - B7 \\ -B2 - B6 - B1 \\ -B2 - B6 - B7 \\ -B3 - B2 - B6 - B7 \\ -B3 - B4 - B7 \\ -B3 - B$	$122.9 \\ 120.9 \\ 123.4 \\ 121.3 \\ 110.3 (4) \\ 147.9 (4) \\ -111.9 (5) \\ -149.0 (4) \\ 1.6 (6) \\ -110.4 (4) \\ -148.2 (4) \\ 112.4 (5) \\ 142.4 $
$\begin{array}{c} -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B8 \\ -B2 - B3 - B9 \\ -B2 - B6 - B7 \\ -B2 - B6 - B1 \\ -B2 - B6 - B7 \\ -B2 - B6 - B7 \\ -B2 - B6 - B11 \\ -B3 - B6 - B1 \\ -B3 - $	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 (4)\\ 147.9 (4)\\ -111.9 (5)\\ -149.0 (4)\\ 1.6 (6)\\ -110.4 (4)\\ -148.2 (4)\\ 112.4 (5)\\ 149.1 (4)\end{array}$
$\begin{array}{c} -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B8 \\ -B2 - B3 - B9 \\ -B2 - B6 - B1 \\ -B2 - B6 - B1 \\ -B2 - B6 - B1 \\ -B2 - B6 - B5 \\ -B2 - B6 - B7 \\ -B2 - B6 - B11 \\ -B2 - B6 - B11 \\ -B2 - B6 - B11 \\ -B2 - B7 - B7 \\ \end{array}$	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 \ (4)\\ 147.9 \ (4)\\ -111.9 \ (5)\\ -149.0 \ (4)\\ 1.6 \ (6)\\ -110.4 \ (4)\\ -148.2 \ (4)\\ 112.4 \ (5)\\ 149.1 \ (4)\\ -2 \ (1) \end{array}$
$\begin{array}{c} -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B8 \\ -B2 - B3 - B9 \\ -B2 - B6 - B7 \\ -B2 - B6 - B1 \\ -B2 - B6 - B7 \\ -B2 - B6 - B1 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - C20 \\ \end{array}$	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 \ (4)\\ 147.9 \ (4)\\ -111.9 \ (5)\\ -149.0 \ (4)\\ 1.6 \ (6)\\ -110.4 \ (4)\\ -148.2 \ (4)\\ 112.4 \ (5)\\ 149.1 \ (4)\\ -2 \ (1)\\ 150.5 \ (4)\\ \end{array}$
$\begin{array}{c} -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B9 \\ -B2 - B6 - B7 \\ -B2 - B6 - B1 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - C20 \\ -B2 - B7 - B6 \end{array}$	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 \ (4)\\ 147.9 \ (4)\\ -111.9 \ (5)\\ -149.0 \ (4)\\ 1.6 \ (6)\\ -110.4 \ (4)\\ -148.2 \ (4)\\ 112.4 \ (5)\\ 149.1 \ (4)\\ -2 \ (1)\\ 150.5 \ (4)\\ -110.0 \ (5)\end{array}$
$\begin{array}{c} -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B8 \\ -B2 - B3 - B9 \\ -B2 - B6 - B7 \\ -B2 - B6 - B1 \\ -B2 - B6 - B7 \\ -B2 - B6 - B1 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - B6 \\ -B2 - B7 - B8 \\ \end{array}$	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 (4)\\ 147.9 (4)\\ -111.9 (5)\\ -149.0 (4)\\ 1.6 (6)\\ -110.4 (4)\\ -148.2 (4)\\ 112.4 (5)\\ 149.1 (4)\\ -2 (1)\\ 150.5 (4)\\ -110.0 (5)\\ 111 2 (5)\end{array}$
$\begin{array}{c} -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B8 \\ -B2 - B6 - B1 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - B6 \\ -B2 - B7 - B8 \\ -B2 - B7 - B8 \\ -B2 - B7 - B1 \\ -B2 - B7 - B1 \\ -B2 - B7 - B8 \\ -B2 - B7 - B1 \\ -B2 - B7 - B1 \\ -B2 - B7 - B8 \\ -B2 - B7 - B8 \\ -B2 - B7 - B1 \\ -B2 - B7 - B8 \\ -B2 - B7 - B1 \\ -B2 - B7 - B1 \\ -B2 - B7 - B8 \\ -B2 - B7 - B8 \\ -B2 - B7 - B1 \\ -B2 - B7 - B1 \\ -B2 - B7 - B1 \\ -B2 - B7 - B8 \\ -B2 - B7 - B1 \\ -B2 - B7 - B8 \\ -B2 - B7 - B8 \\ -B2 - B7 - B1 \\ -B2 - B7 - B8 \\ -B2 - B7 - B1 \\ -B2 - B7 \\ -B2 \\ -B2 - B7 \\ -B2 \\ -B2 \\ -B2 \\ -B2 \\ -B1 \\ -B2 \\ -B2 \\ -B1 \\ -B2 \\ -B$	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 \ (4)\\ 147.9 \ (4)\\ -111.9 \ (5)\\ -149.0 \ (4)\\ 1.6 \ (6)\\ -110.4 \ (4)\\ 112.4 \ (5)\\ 149.1 \ (4)\\ -2 \ (1)\\ 150.5 \ (4)\\ -110.0 \ (5)\\ 111.2 \ (5)\\ 147.6 \ (4)\\ -110.2 \ (5)\\ 147.6 \ (4)\\ -110.2 \ (5)\\ 147.6 \ (4)\\ -110.4 \ (5)\\ 147.6 \ (4)\\ -110.4 \ (5)\\ 147.6 \ (4)\\ -110.4 \ (5)\\ 147.6 \ (4)\\ -110.4 \ (5)\\ 147.6 \ (4)\\ -110.4 \ (5)\\ 147.6 \ (5)\\ 147.6 \ (4)\\ -110.4 \ (5)\\ 147.6 \ (4)\\ -110.4 \ (5)\\ 147.6 \ (4)\\ -110.4 \ (5)\\ 147.6 \ (4)\\ -110.4 \ (5)\\ 147.6 \ (4)\\ -110.4 \ (5)\\ 147.6 \ (4)\\ -110.4 \ (5)\ -110.4 \ (5)\\ -110.4 \ (5)\ -110.4 \$
$\begin{array}{c} -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B8 \\ -B2 - B3 - B9 \\ -B2 - B6 - B7 \\ -B2 - B6 - B7 \\ -B2 - B6 - B1 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - B8 \\ -B2 - B7 - B1 \\ -B3 - B2 - B7 - B1 \\ -B3 - B3 - C2 \\ -B3 - $	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 \ (4)\\ 147.9 \ (4)\\ -111.9 \ (5)\\ -149.0 \ (4)\\ 1.6 \ (6)\\ -110.4 \ (4)\\ -148.2 \ (4)\\ 112.4 \ (5)\\ 149.1 \ (4)\\ -2 \ (1)\\ 150.5 \ (4)\\ -110.0 \ (5)\\ 111.2 \ (5)\\ -147.6 \ (4)\\ -247.6 \ (4)\\ -25.6 \ (4)\\ -5.6 \ (5)\\ -147.6 \ (4)\\ -5.6 \ (5)\\ -147.6 \ (4)\\ -5.6 \ (5)\\ -147.6 \ (4)\\ -5.6 \ (5)\\ -147.6 \ (4)\\ -5.6 \ (5)\\ -147.6 \ (4)\\ -5.6 \ (5)\\ -147.6 \ (4)\\ -5.6 \ (5)\\ -147.6 \ (4)\\ -5.6 \ (5)\\ -147.6 \ (4)\\ -5.6 \ (5)\\ -147.6 \ (4)\\ -5.6 \ (5)\\ -147.6 \ (4)\\ -5.6 \ (5)\\ -147.6 \ (4)\\ -5.6 \ (5)\ (5)\ (5)\ (5)\ (5)\ (5)\ (5)\ (5$
$\begin{array}{c} -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B9 \\ -B2 - B6 - B7 \\ -B2 - B6 - B7 \\ -B2 - B6 - B1 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - B6 \\ -B2 - B7 - B8 \\ -B2 - B7 - B1 \\ -B2 - B7 - B11 \\ -B2 - B8 - C20 \end{array}$	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 \ (4)\\ 147.9 \ (4)\\ -111.9 \ (5)\\ -149.0 \ (4)\\ 116.6 \ (6)\\ -110.4 \ (4)\\ -148.2 \ (4)\\ 112.4 \ (5)\\ 149.1 \ (4)\\ -2 \ (1)\\ 150.5 \ (4)\\ -110.0 \ (5)\\ 111.2 \ (5)\\ -147.6 \ (4)\\ -150.6 \ (4)\\ \end{array}$
$\begin{array}{c} -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B8 \\ -B2 - B6 - B7 \\ -B2 - B6 - B1 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - B6 \\ -B2 - B7 - B8 \\ -B2 - B7 - B11 \\ -B2 - B8 - C20 \\ -B2 - B8 - B3 \\ \end{array}$	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 (4)\\ 147.9 (4)\\ -111.9 (5)\\ -149.0 (4)\\ 1.6 (6)\\ -110.4 (4)\\ -148.2 (4)\\ 112.4 (5)\\ 149.1 (4)\\ -2 (1)\\ 150.5 (4)\\ -110.0 (5)\\ 111.2 (5)\\ -147.6 (4)\\ -150.6 (4)\\ 110.7 (5)\\ \end{array}$
$\begin{array}{c} -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B8 \\ -B2 - B3 - B9 \\ -B2 - B6 - B1 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - B1 \\ -B2 - B8 - C20 \\ -B2 - B8 - B3 \\ -B2 - B8 - B3 \\ -B2 - B8 - B7 \\ -B2 - B8 - B7 \\ -B1 \\ -B2 - B8 - B7 \\ -B1 \\ -B2 - B8 - B3 \\ -B2 - B8 - B7 \\ -B1 \\ -B2 - B8 - B3 \\ -B2 - B8 - B7 \\ -B1 \\ -B2 - B8 - B7 \\ -B1 \\ -B2 - B8 - B7 \\ -B1 \\ -B2 - B8 - B3 \\ -B2 - B8 - B7 \\ -B1 \\ -B2 - B8 - B7 \\ -B1 \\ -B2 - B8 - B7 \\ -B1 \\ -B2 - B8 - B3 \\ -B2 - B8 - B7 \\ -B1 \\ -B1 \\ -B1 \\ -B2 - B8 - B7 \\ -B1 \\ -B1 \\ -B1 \\ -B1 \\ -B2 - B8 - B3 \\ -B2 - B8 - B3 \\ -B2 - B8 - B7 \\ -B1 $	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 \ (4)\\ 147.9 \ (4)\\ -111.9 \ (5)\\ -149.0 \ (4)\\ 1.6 \ (6)\\ -110.4 \ (4)\\ 112.4 \ (5)\\ 149.1 \ (4)\\ -2 \ (1)\\ 150.5 \ (4)\\ -110.0 \ (5)\\ 111.2 \ (5)\\ -147.6 \ (4)\\ -150.6 \ (4)\\ 110.7 \ (5)\\ -111.9 \ (5)\\ \end{array}$
$\begin{array}{c} -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B8 \\ -B2 - B3 - B9 \\ -B2 - B6 - B7 \\ -B2 - B6 - B1 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - B6 \\ -B2 - B7 - B8 \\ -B2 - B7 - B1 \\ -B2 - B8 - B3 \\ -B2 - B8 - B7 \\ -B2 - B8 - B9 \\ -B1 \\ -B1 - B1 \\ -B2 - B8 - B9 \\ -B1 \\ -B1 - B1 \\ -B1 -$	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 \ (4)\\ 147.9 \ (4)\\ -111.9 \ (5)\\ -149.0 \ (4)\\ 1.6 \ (6)\\ -110.4 \ (4)\\ -148.2 \ (4)\\ 112.4 \ (5)\\ 149.1 \ (4)\\ -2 \ (1)\\ 150.5 \ (4)\\ -110.0 \ (5)\\ 111.2 \ (5)\\ -147.6 \ (4)\\ 110.7 \ (5)\\ -111.9 \ (5)\\ 147.7 \ (4)\\ 147.7 \ (4)\\ \end{array}$
$\begin{array}{c} -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B9 \\ -B3 - B6 - B7 \\ -B2 - B6 - B7 \\ -B2 - B6 - B1 \\ -B2 - B6 - B1 \\ -B2 - B6 - B1 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - B6 \\ -B2 - B7 - B6 \\ -B2 - B7 - B1 \\ -B2 - B8 - C20 \\ -B2 - B7 - B1 \\ -B2 - B8 - B3 \\ -B2 - B8 - B3 \\ -B2 - B8 - B7 \\ -B2 - B8 - B1 \\ -B2 - B1 - B2 \\ -B3 - B1 - B2 \\ -B$	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 \ (4)\\ 147.9 \ (4)\\ -111.9 \ (5)\\ -149.0 \ (4)\\ 111.9 \ (5)\\ -149.0 \ (4)\\ -148.2 \ (4)\\ 112.4 \ (5)\\ 149.1 \ (4)\\ -2 \ (1)\\ 150.5 \ (4)\\ -110.0 \ (5)\\ 111.2 \ (5)\\ -147.6 \ (4)\\ -150.6 \ (4)\\ 110.7 \ (5)\\ -111.9 \ (5)\\ 147.7 \ (4)\\ 111.6 \ (4)\\ \end{array}$
$\begin{array}{c} -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B8 \\ -B2 - B6 - B7 \\ -B2 - B6 - B1 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - B8 \\ -B2 - B7 - B1 \\ -B2 - B7 - B1 \\ -B2 - B8 - B3 \\ -B2 - B8 - B7 \\ -B2 - B8 - B9 \\ -B3 - B1 - B2 \\ -B3 - B1 - B4 \\ \end{array}$	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 (4)\\ 147.9 (4)\\ -111.9 (5)\\ -149.0 (4)\\ 1.6 (6)\\ -110.4 (4)\\ -148.2 (4)\\ 112.4 (5)\\ 149.1 (4)\\ -2 (1)\\ 150.5 (4)\\ -110.0 (5)\\ 111.2 (5)\\ -111.0 (5)\\ 111.2 (5)\\ -147.6 (4)\\ 110.7 (5)\\ -111.9 (5)\\ 147.7 (4)\\ 111.6 (4)\\ -110.2 (1)\\ -10.2 (1)$
$\begin{array}{c} -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B8 \\ -B2 - B3 - B9 \\ -B2 - B6 - B1 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - B8 \\ -B2 - B7 - B8 \\ -B2 - B7 - B1 \\ -B2 - B8 - C20 \\ -B2 - B8 - B3 \\ -B2 - B8 - B1 \\ -B2 - B1 - B2 \\ -B3 - B1 - B2 \\ -B3 - B1 - B2 \\ -B3 - B1 - B1 \\ -B4 \\ -B2 - B1 - B4 \\ -B2 - B1 - B1 \\ -B1 - B4 \\ -B1 - B1 \\ -B1 - B1$	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 (4)\\ 147.9 (4)\\ -111.9 (5)\\ -149.0 (4)\\ 1.6 (6)\\ -110.4 (4)\\ -148.2 (4)\\ 112.4 (5)\\ 149.1 (4)\\ -2 (1)\\ 150.5 (4)\\ -110.0 (5)\\ 111.2 (5)\\ -147.6 (4)\\ -150.6 (4)\\ 110.7 (5)\\ -111.9 (5)\\ 147.7 (4)\\ 111.6 (4)\\ -110.2 (4)\\ 147.7 (4)\\ 111.2 (4)\\ -110.2 (4)\\ 147.7 (4)\\ -110.2 (4)\\ -110.2 (4)\\ -110.2 (4)\\ -110.2 (4)\\ -10.2 (4)\\ $
$\begin{array}{c} -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B6 - B1 \\ -B2 - B7 - B7 \\ -B2 - B7 - C20 \\ -B2 - B7 - B6 \\ -B2 - B7 - B6 \\ -B2 - B7 - B1 \\ -B2 - B7 - B1 \\ -B2 - B8 - C20 \\ -B2 - B8 - B3 \\ -B2 - B8 - B3 \\ -B2 - B8 - B1 \\ -B2 - B8 - B1 \\ -B3 - B1 - B2 \\ -B3 - B1 - B4 \\ -B3 - B1 - B5 \\ -B2 - B1 - B1 \\ -B2 - B1 \\ -B2 - B1 \\ -B2 - B1 \\ -B2 - B1 \\ -B1 -$	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 \ (4)\\ 147.9 \ (4)\\ -111.9 \ (5)\\ -149.0 \ (4)\\ -149.0 \ (4)\\ -148.2 \ (4)\\ 112.4 \ (5)\\ 149.1 \ (4)\\ -2 \ (1)\\ 150.5 \ (4)\\ -110.0 \ (5)\\ 111.2 \ (5)\\ -147.6 \ (4)\\ -150.6 \ (4)\\ 110.7 \ (5)\\ -111.9 \ (5)\\ 147.7 \ (4)\\ -110.2 \ (4)\\ -110.2 \ (4)\\ -147.8 $
$\begin{array}{c} -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B9 \\ -B2 - B6 - B7 \\ -B2 - B6 - B1 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - B6 \\ -B2 - B7 - B8 \\ -B2 - B7 - B1 \\ -B2 - B8 - C20 \\ -B2 - B7 - B1 \\ -B2 - B8 - B3 \\ -B2 - B8 - B3 \\ -B2 - B8 - B1 \\ -B2 - B8 - B1 \\ -B2 - B8 - B1 \\ -B3 - B1 - B2 \\ -B3 - B1 - B1 \\ -B3 - B1 - B5 \\ -B3 - B1 - B6 \end{array}$	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 \ (4)\\ 147.9 \ (4)\\ -111.9 \ (5)\\ -149.0 \ (4)\\ -149.0 \ (4)\\ -148.2 \ (4)\\ 112.4 \ (5)\\ 149.1 \ (4)\\ -2 \ (1)\\ 150.5 \ (4)\\ -110.0 \ (5)\\ 111.2 \ (5)\\ -147.6 \ (4)\\ -150.6 \ (4)\\ 110.7 \ (5)\\ -111.9 \ (5)\\ 147.7 \ (4)\\ 111.6 \ (4)\\ -110.2 \ (4)\\ -147.8 \ (4)\\ 148.9 \ (4)\\ \end{array}$
$\begin{array}{c} -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B8 \\ -B2 - B6 - B7 \\ -B2 - B6 - B1 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - B1 \\ -B2 - B7 - B1 \\ -B2 - B7 - B1 \\ -B2 - B8 - B3 \\ -B2 - B8 - B3 \\ -B2 - B8 - B1 \\ -B3 - B1 - B4 \\ -B3 - B1 - B5 \\ -B3 - B1 - B6 \\ -B3 - B2 - B1 \\ -B1 - B1 - B1 \\ -B1 - B2 - B1 \\ -B1 - B2 - B1 \\ -B1 - B2 - B1 \\ -B1 - B1 - B5 \\ -B3 - B1 - B6 \\ -B3 - B2 - B1 \\ -B1 - B1 - B1 \\ -B1 - B1 - B1 \\ -B1 - B1 - $	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 (4)\\ 147.9 (4)\\ -111.9 (5)\\ -149.0 (4)\\ 1.6 (6)\\ -110.4 (4)\\ -148.2 (4)\\ 112.4 (5)\\ 149.1 (4)\\ -2 (1)\\ 150.5 (4)\\ -110.0 (5)\\ 111.2 (5)\\ -111.0 (5)\\ 111.2 (5)\\ -147.6 (4)\\ 110.7 (5)\\ -111.9 (5)\\ 147.7 (4)\\ 111.6 (4)\\ -110.2 (4)\\ -147.8 (4)\\ 148.9 (4)\\ -110.3 (4)\\ \end{array}$
$\begin{array}{c} -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B6 - B1 \\ -B2 - B7 - B7 \\ -B2 - B7 - B8 \\ -B2 - B7 - B8 \\ -B2 - B7 - B1 \\ -B2 - B8 - C20 \\ -B2 - B8 - B1 \\ -B3 - B1 - B2 \\ -B3 - B1 - B5 \\ -B3 - B1 - B6 \\ -B3 - B2 - B6 \\ -B1 - B6 \\ -B3 - B2 - B6 \\ -B1 - B6 \\ -B3 - B2 - B6 \\ -B1 - B1 \\ -B3 - B2 - B6 \\ -B1 - B1 \\ -B3 - B2 - B6 \\ -B1 - B1 \\ -B3 - B2 - B6 \\ -B1 - B1 \\ -B1 - B2 \\ -B1 - B1 \\ -B3 - B2 - B6 \\ -B1 - B1 \\ -B1 - B2 \\ -B1 - B1 \\ -B1 \\ -B1 - B1 \\ -B1 \\ -B1 - B1 \\ -B1 \\ -B$	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 (4)\\ 147.9 (4)\\ -111.9 (5)\\ -149.0 (4)\\ 1.6 (6)\\ -110.4 (4)\\ -148.2 (4)\\ 112.4 (5)\\ 149.1 (4)\\ -2 (1)\\ 150.5 (4)\\ -110.0 (5)\\ 111.2 (5)\\ -147.6 (4)\\ -150.6 (4)\\ 110.7 (5)\\ -111.9 (5)\\ 147.7 (4)\\ 111.6 (4)\\ -110.2 (4)\\ -147.8 (4)\\ 148.9 (4)\\ -110.3 (4)\\ -147.5 (4)\\ \end{array}$
$\begin{array}{c} -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B6 - B1 \\ -B2 - B7 - B7 \\ -B2 - B7 - C20 \\ -B2 - B7 - B6 \\ -B2 - B7 - B6 \\ -B2 - B7 - B1 \\ -B2 - B8 - C20 \\ -B2 - B8 - B3 \\ -B2 - B8 - B1 \\ -B2 - B8 - B1 \\ -B3 - B1 - B4 \\ -B3 - B1 - B6 \\ -B3 - B2 - B7 \\ -B1 - B6 \\ -B3 - B2 - B7 \\ -B1 - B6 \\ -B3 - B2 - B7 \\ -B1 - B6 \\ -B3 - B2 - B7 \\ -B1 - B6 \\ -B3 - B2 - B7 \\ -B1 - B6 \\ -B3 - B2 - B7 \\ -B1 - B6 \\ -B3 - B2 - B7 \\ -B1 - B6 \\ -B3 - B2 - B7 \\ -B1 - B6 \\ -B3 - B2 - B7 \\ -B1 - B6 \\ -B3 - B2 - B6 \\ -B3 - B2 - B7 \\ -B1 - B5 \\ -B3 - B2 - B7 \\ -B1 - B5 \\ -B3 - B2 - B6 \\ -B3 - B2 - B7 \\ -B1 - B1 \\ -B3 - B2 - B6 \\ -B3 - B2 - B7 \\ -B1 - B1 \\ -B3 - B2 - B6 \\ -B3 - B2 - B7 \\ -B1 - B1 \\ -B3 - B2 - B6 \\ -B3 - B2 - B7 \\ -B1 - B1 \\ -B1 - B2 - B6 \\ -B3 - B2 - B7 \\ -B1 - B1 \\ -B1 - B2 - B6 \\ -B3 - B2 - B7 \\ -B1 - B1 \\ -B1 - B2 - B6 \\ -B3 - B2 - B7 \\ -B1 - B1 \\ -B1 - B1 \\ -B1 - B2 - B6 \\ -B3 - B2 - B7 \\ -B1 - B1 \\ -B1 - B1 \\ -B1 - B2 - B6 \\ -B3 - B2 - B7 \\ -B1 - B1 \\ -B1 - B1 \\ -B1 - B2 - B6 \\ -B3 - B2 - B7 \\ -B1 - B1 \\ -B1 \\ -B1 - B1 \\ -B1 \\ -B1 - B1 \\ -B1 \\ -$	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 \ (4)\\ 147.9 \ (4)\\ -111.9 \ (5)\\ -149.0 \ (4)\\ -149.0 \ (4)\\ -148.2 \ (4)\\ -148.2 \ (4)\\ 112.4 \ (5)\\ 149.1 \ (4)\\ -2 \ (1)\\ 150.5 \ (4)\\ -110.0 \ (5)\\ 111.2 \ (5)\\ -147.6 \ (4)\\ -150.6 \ (4)\\ 110.7 \ (5)\\ -111.9 \ (5)\\ 147.7 \ (4)\\ -110.2 \ (4)\\ -147.8 \ (4)\\ -147.8 \ (4)\\ -147.5 \ (4)\\ -147.5 \ (4)\\ -149.5 $
$\begin{array}{c} -B11 - H11 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B9 \\ -B2 - B6 - B7 \\ -B2 - B6 - B1 \\ -B2 - B7 - B7 \\ -B2 - B7 - C20 \\ -B2 - B7 - B7 \\ -B2 - B7 - B8 \\ -B2 - B7 - B8 \\ -B2 - B7 - B1 \\ -B2 - B8 - C20 \\ -B2 - B8 - B3 \\ -B2 - B8 - B1 \\ -B3 - B1 - B2 \\ -B3 - B1 - B4 \\ -B3 - B2 - B1 \\ -B3 - B2 - B7 \\ -B3 - B2 - B7 \\ -B2 - B7 \\ -B3 - B2 - B7 \\ -B3 - B3 - B1 \\ -B3 - B1 - B1 \\ -B3 - B1 \\ -$	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 (4)\\ 147.9 (4)\\ -111.9 (5)\\ -149.0 (4)\\ 116.6 (6)\\ -110.4 (4)\\ -148.2 (4)\\ 112.4 (5)\\ 149.1 (4)\\ -2 (1)\\ 150.5 (4)\\ -110.0 (5)\\ 111.2 (5)\\ -147.6 (4)\\ -150.6 (4)\\ 110.7 (5)\\ -147.6 (4)\\ -150.6 (4)\\ 110.7 (5)\\ -111.9 (5)\\ 147.7 (4)\\ 111.6 (4)\\ -110.2 (4)\\ -147.8 (4)\\ 148.9 (4)\\ -110.3 (4)\\ -147.5 (4)\\ 149.5 (4)\\ 111 (9.6)$
$\begin{array}{c} -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B8 \\ -B2 - B6 - B7 \\ -B2 - B6 - B1 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - B1 \\ -B2 - B7 - B1 \\ -B2 - B7 - B1 \\ -B2 - B8 - B3 \\ -B2 - B8 - B3 \\ -B2 - B8 - B1 \\ -B3 - B1 - B2 \\ -B3 - B1 - B5 \\ -B3 - B2 - B7 \\ -B3 - B1 - B1 \\ -B3 - B1 \\$	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 (4)\\ 147.9 (4)\\ -111.9 (5)\\ -149.0 (4)\\ 1.6 (6)\\ -110.4 (4)\\ -148.2 (4)\\ 112.4 (5)\\ 149.1 (4)\\ -2 (1)\\ 150.5 (4)\\ -110.0 (5)\\ 111.2 (5)\\ -147.6 (4)\\ 110.7 (5)\\ -111.9 (5)\\ 147.7 (4)\\ 111.6 (4)\\ -110.2 (4)\\ -147.8 (4)\\ 148.9 (4)\\ -147.8 (4)\\ 149.5 (4)\\ 111.9 (4)\\ 129.5 (4)\\ 111.9 (4)\\ 149.5 (4)\\ 111.9 (4)\\ 149.5 (4)\\ 111.9 (4)\\ 149.5 (4)\\ 111.9 (4)\\ 149.5 (4)\\ 111.9 (4)\\ 149.5 (4)\\ 111.9 (4)\\ 149.5 (4)\\ 111.9 (4)\\ 149.5 (4)\\ 111.9 (4)\\ 149.5 (4)\\ 111.9 (4)\\ 149.5 (4)\\ 111.9 (4)\\ 149.5 (4)\\ 111.9 (4)\\ 140.5 (4)\\ 140.$
$\begin{array}{c} -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B6 - B1 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - B7 \\ -B2 - B7 - B8 \\ -B2 - B7 - B8 \\ -B2 - B7 - B8 \\ -B2 - B7 - B1 \\ -B2 - B8 - C20 \\ -B2 - B8 - B1 \\ -B2 - B8 - B1 \\ -B3 - B1 - B2 \\ -B3 - B1 - B4 \\ -B3 - B2 - B7 \\ -B2 - B7 \\ -B2 - B7 \\ -B2 - B8 \\ -B3 - B2 - B7 \\ -B3 - B2 - B7 \\ -B3 - B2 - B8 \\ -B3 - B2 - B7 \\ -B3 - B2 - B8 \\ -B3 - B2 - B7 \\ -B3 - B2 - B8 \\ -B3 - B2 - B7 \\ -B3 - B2 - B8 \\ -B3 - B2 - B7 \\ -B3 - B2 - B8 \\ -B3 - B2 - B7 \\ -B3 - B2 - B8 \\ -B3 - B2 - B7 \\ -B3 - B2 - B8 \\ -B3 - B4 - B7 \\ -B4 -$	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 (4)\\ 147.9 (4)\\ -111.9 (5)\\ -149.0 (4)\\ 1.6 (6)\\ -110.4 (4)\\ -148.2 (4)\\ 112.4 (5)\\ 149.1 (4)\\ -2 (1)\\ 150.5 (4)\\ -110.0 (5)\\ 111.2 (5)\\ -147.6 (4)\\ -150.6 (4)\\ 110.7 (5)\\ -111.9 (5)\\ 147.7 (4)\\ 111.6 (4)\\ -110.2 (4)\\ -147.8 (4)\\ 148.9 (4)\\ -147.5 (4)\\ 149.5 (4)\\ 111.9 (6)\\ 111.9 (6)\\ 112.4 (5)\\ -1.9 (6)\\ 112.4 (5)\\ -1.9 (6)\\ 112.4 (5)\\ -1.9 (6)\\ 112.4 (5)\\ -1.9 (6)\\ 112.4 (5)\\ -1.9 (6)\\ 112.4 (5)\\ -1.9 (6)\\ 112.4 (5)\\ -1.9 (6)\\ 112.4 (5)\\ -1.9 (6)\\ 112.4 (5)\\ -1.9 (6)\\ 112.4 (5)\\ -1.9 (6)\\ 112.4 (5)\\ -1.9 (6)\\ 112.4 (5)\\ -1.9 (6)\\ 112.4 (5)\\ -1.9 (6)\\ 112.4 (5)\\ -1.9 (6)\\ 122.4 (5)\\ -1.9 (6)\\$
$\begin{array}{c} -B11 - H11 \\ -B2 - B3 - B1 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B9 \\ -B2 - B6 - B1 \\ -B2 - B7 - B7 \\ -B2 - B7 - C20 \\ -B2 - B7 - B6 \\ -B2 - B7 - B6 \\ -B2 - B7 - B6 \\ -B2 - B7 - B1 \\ -B2 - B8 - C20 \\ -B2 - B8 - B3 \\ -B2 - B8 - B1 \\ -B3 - B1 - B4 \\ -B3 - B1 - B6 \\ -B3 - B2 - B7 \\ -B3 - B2 - B7 \\ -B3 - B2 - B8 \\ -B3 - B1 - B4 \\ -B3 - B2 - B7 \\ -B3 - B2 - B8 \\ -B3 - B1 - B6 \\ -B3 - B2 - B7 \\ -B3 - B2 - B7 \\ -B3 - B2 - B8 \\ -B3 - B1 - B4 \\ -B3 - B2 - B7 \\ -B3 - B2 - B8 \\ -B3 - B1 - B4 \\ -B3 - B2 - B7 \\ -B3 - B2 - B8 \\ -B3 - B1 - B4 \\ -B3 - B2 - B7 \\ -B3 - B2 - B8 \\ -B3 - B4 - B1 \\ -B4 $	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 (4)\\ 147.9 (4)\\ -111.9 (5)\\ -149.0 (4)\\ 1.6 (6)\\ -110.4 (4)\\ -148.2 (4)\\ 112.4 (5)\\ 149.1 (4)\\ -2 (1)\\ 150.5 (4)\\ -110.0 (5)\\ 111.2 (5)\\ -147.6 (4)\\ -150.6 (4)\\ 110.7 (5)\\ -111.9 (5)\\ 147.7 (4)\\ 111.6 (4)\\ -110.2 (4)\\ -147.8 (4)\\ 148.9 (4)\\ -147.8 (4)\\ 148.9 (4)\\ -147.5 (4)\\ 149.5 (4)\\ 111.9 (6)\\ 111.9 (6)\\ 110.3 (4)\\ \end{array}$
$\begin{array}{c} -B11 - H11 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B4 \\ -B2 - B3 - B9 \\ -B2 - B6 - B7 \\ -B2 - B6 - B1 \\ -B2 - B6 - B1 \\ -B2 - B6 - B1 \\ -B2 - B7 - B7 \\ -B2 - B7 - C20 \\ -B2 - B7 - B7 \\ -B2 - B7 - B8 \\ -B2 - B7 - B8 \\ -B2 - B7 - B8 \\ -B2 - B7 - B1 \\ -B2 - B8 - B3 \\ -B2 - B8 - B3 \\ -B2 - B8 - B1 \\ -B3 - B1 - B4 \\ -B3 - B2 - B7 \\ -B3 - B4 - B1 \\ -B3 - B4 - B1 \\ -B3 - B4 - B5 \\ -B3 -$	$\begin{array}{c} 122.9\\ 120.9\\ 123.4\\ 121.3\\ 110.3 (4)\\ 147.9 (4)\\ -111.9 (5)\\ -149.0 (4)\\ 116.6 (6)\\ -110.4 (4)\\ -148.2 (4)\\ 112.4 (5)\\ 149.1 (4)\\ -2 (1)\\ 150.5 (4)\\ -110.0 (5)\\ 111.2 (5)\\ -147.6 (4)\\ -150.6 (4)\\ 110.7 (5)\\ -147.6 (4)\\ -150.6 (4)\\ 110.7 (5)\\ -147.7 (4)\\ 111.6 (4)\\ -110.2 (4)\\ -147.8 (4)\\ 148.9 (4)\\ -147.8 (4)\\ 149.5 (4)\\ 111.9 (4)\\ -1.9 (6)\\ 110.3 (4)\\ -19.9 (6)\\ 110.3 (4)\\ -148.2 (4)\\ \end{array}$

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Br3-	-B3-	-B4—B10	-148.6(4)
Br3-	-B3-	-B8-C20	150.2(4)
Br3_	_B3_	_B8B2	-110.3(4)
D10 D12	D0 D0	D0 D2 D0 D7	1485(4)
Бгэ-	-дэ-	-Do-D/	-146.0(4)
Br3–	-B3-	-B8B9	110.8(4)
Br3-	-B3-	-B9-C20	-151.2(4)
Br3-	-B3-	-B9—B4	109.7(5)
Br3-	-B3-	-B9—B8	-112.4(5)
Br3–	-B3-	-B9-B10	147.6(4)
Br4_	_B4_	B1B2	147.6(4)
Dr4 Dr4		D1 D2 D1 D2	1106 (5)
Dr4-	-D4-	-D1D3	110.0(3)
Br4–	-B4-	-B1B5	-111.7(5)
Br4-	-B4-	-B1-B6	-149.1 (4)
Br4-	-B4-	-B3-B1	-112.2 (4)
Br4-	-B4-	-B3—B2	-150.1(4)
Br4-	-B4-	-B3—B8	147.1(4)
Br4-	-B4-	-B3-B9	109.2(4)
Br4–	-B4-	-B5-Br5	0.7 (6)
Br4_	_B/_	_B5B1	112.2(4)
Dr4 Dr4			112.2(4)
D14-	-D4-	-B3-B0	149.3(4)
Br4–	-B4-	-B5-B10	-109.7(4)
Br4–	-B4-	-B5-B11	-147.4(4)
Br4-	-B4-	-B9-C20	150.6(4)
Br4-	-B4-	-B9—B3	-111.5(4)
Br4-	-B4-	-B9—B8	-148.9(4)
Br4-	-B4-	-B9—B10	110.5(4)
Br4-	-B4-	-B10-C20	-149.6(4)
Br4–	-B4-	-B10-B5	112.1 (4)
Br4	_B4_	-B10-B9	-109.6(4)
Dr1		D10 D11	140.0(1)
D14	-D4-	-B10-B11	149.9(4)
Dro-	-БЭ-	-B1B2	-146.7(4)
Br5-	-B2-	-B1B3	148.7(4)
Br5-	-B5-	-B1B4	111.0(5)
Br5-	-B5-	-B1-B6	-110.9(4)
Br5-	-B5-	-B4-B1	-111.5(4)
Br5-	-B5-	-B4—B3	-149.1(4)
Br5-	-B5-	-B4—B9	147.7(4)
Br5-	-B5-	-B4-B10	110.4 (4)
Br5-	-B5-	-B6-Br6	-11(6)
Br5	_B5_	B6B1	1115(4)
DIU-	-D0-	-D0D1 D6 D0	111.0(4)
Dro-	-D0-		149.4(4)
Bro-	-вэ-	-B0-B7	-148.0(4)
Br5-	-B2-	-B6-B11	-110.8(5)
Br5-	-B5-	-B10-C20	150.3(4)
Br5-	-B5-	-B10—B4	-111.3(5)
Br5-	-B5-	-B10-B9	-148.5(4)
Br5-	-B5-	-B10-B11	111.0(5)
Br5-	-B5-	-B11-C20	-150.4(4)
Br5-	-B5-	-B11-B6	1110(4)
D.F			111.0(4)
D(0) =	-B5-	-B11-B7	111.0(4) 149.1(4)
Br5-	-B5- -B5-	-B11-B7 -B11-B10	111.0(4) 149.1(4) -110.5(4)
Br5– Br5–	-B5- -B5-	-B11-B7 -B11-B10 -B1-B2	111.0(4) 149.1(4) -110.5(4) -112.2(4)
Br5– Br5– Br6–	-B5- -B5- -B6-	-B11-B7 -B11-B10 -B1-B2 B1-B2	$\begin{array}{c} 111.0 (4) \\ 149.1 (4) \\ -110.5 (4) \\ -112.2 (4) \\ 140.2 (4) \end{array}$
Br5– Br5– Br6– Br6–	-B5- -B5- -B6- -B6-	-B11-B7 -B11-B10 -B1-B2 -B1-B3	$\begin{array}{c} 111.0 (4) \\ 149.1 (4) \\ -110.5 (4) \\ -112.2 (4) \\ -149.2 (4) \end{array}$
Br5- Br6- Br6- Br6-	-B5- -B5- -B6- -B6- -B6-	-B11-B7 -B11-B10 -B1-B2 -B1-B3 -B1-B4	$\begin{array}{c} 111.0 (4) \\ 149.1 (4) \\ -110.5 (4) \\ -112.2 (4) \\ -149.2 (4) \\ 147.4 (4) \\ 147.4 (4) \end{array}$
Br5- Br5- Br6- Br6- Br6- Br6-	-B5- -B5- -B6- -B6- -B6- -B6-	-B11—B7 -B11—B10 -B1—B2 -B1—B3 -B1—B4 -B1—B5	$\begin{array}{c} 111.0 (4) \\ 149.1 (4) \\ -110.5 (4) \\ -112.2 (4) \\ -149.2 (4) \\ 147.4 (4) \\ 110.2 (4) \end{array}$
Br5- Br5- Br6- Br6- Br6- Br6- Br6-	-B5- -B5- -B6- -B6- -B6- -B6- -B6-	-B11—B7 -B11—B10 -B1—B2 -B1—B3 -B1—B4 -B1—B5 -B2—B1	$\begin{array}{c} 111.0 (4) \\ 149.1 (4) \\ -110.5 (4) \\ -112.2 (4) \\ -149.2 (4) \\ 147.4 (4) \\ 110.2 (4) \\ 112.0 (5) \end{array}$
Br5- Br6- Br6- Br6- Br6- Br6- Br6- Br6-	-B5- -B5- -B6- -B6- -B6- -B6- -B6- -B6-	-B11-B7 -B11-B10 -B1-B2 -B1-B3 -B1-B4 -B1-B5 -B2-B1 -B2-B3	$\begin{array}{c} 111.0 (4) \\ 149.1 (4) \\ -110.5 (4) \\ -112.2 (4) \\ -149.2 (4) \\ 147.4 (4) \\ 110.2 (4) \\ 112.0 (5) \\ 149.3 (4) \end{array}$
Br5- Br5- Br6- Br6- Br6- Br6- Br6- Br6- Br6-	-B5- -B5- -B6- -B6- -B6- -B6- -B6- -B6-	-B11-B7 -B11-B10 -B1-B2 -B1-B3 -B1-B4 -B1-B5 -B2-B1 -B2-B3 -B2-B7	$\begin{array}{c} 111.0 (4) \\ 149.1 (4) \\ -110.5 (4) \\ -112.2 (4) \\ 149.2 (4) \\ 147.4 (4) \\ 110.2 (4) \\ 112.0 (5) \\ 149.3 (4) \\ -110.7 (5) \end{array}$
Br5- Br6- Br6- Br6- Br6- Br6- Br6- Br6- Br6	-B5- -B5- -B6- -B6- -B6- -B6- -B6- -B6-	-B11-B7 -B11-B10 -B1-B2 -B1-B3 -B1-B4 -B1-B5 -B2-B1 -B2-B3 -B2-B7 -B2-B8	$\begin{array}{c} 111.0 \ (4) \\ 149.1 \ (4) \\ -110.5 \ (4) \\ -112.2 \ (4) \\ 147.4 \ (4) \\ 110.2 \ (4) \\ 112.0 \ (5) \\ 149.3 \ (4) \\ -110.7 \ (5) \\ -147.3 \ (4) \end{array}$
Br5- Br6- Br6- Br6- Br6- Br6- Br6- Br6- Br6	-B5- -B5- -B6- -B6- -B6- -B6- -B6- -B6-	-B11-B7 -B11-B10 -B1-B2 -B1-B3 -B1-B4 -B1-B5 -B2-B1 -B2-B3 -B2-B7 -B2-B8 -B5-B1	$\begin{array}{c} 111.0 & (4) \\ 149.1 & (4) \\ -110.5 & (4) \\ -112.2 & (4) \\ 147.4 & (4) \\ 110.2 & (4) \\ 112.0 & (5) \\ 149.3 & (4) \\ -110.7 & (5) \\ -147.3 & (4) \\ -112.5 & (4) \end{array}$
Br5- Br6- Br6- Br6- Br6- Br6- Br6- Br6- Br6	-B5 -B5 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6B6	$\begin{array}{c} -B11 \\ -B11 \\ -B10 \\ -B1 \\ -B2 \\ -B1 \\ -B3 \\ -B1 \\ -B3 \\ -B1 \\ -B4 \\ -B1 \\ -B5 \\ -B2 \\ -B1 \\ -B2 \\ -B3 \\ -B2 \\ -B7 \\ -B2 \\ -B8 \\ -B5 \\ -B1 \\ -B5 \\ -B4 \end{array}$	$\begin{array}{c} 111.0 \ (4) \\ -110.5 \ (4) \\ -110.5 \ (4) \\ -112.2 \ (4) \\ 147.4 \ (4) \\ 110.2 \ (4) \\ 112.0 \ (5) \\ 149.3 \ (4) \\ -110.7 \ (5) \\ -147.3 \ (4) \\ -112.5 \ (4) \\ -112.5 \ (4) \\ -149.9 \ (4) \end{array}$
Br5- Br6- Br6- Br6- Br6- Br6- Br6- Br6- Br6	-B5 -B5 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6	-B11-B7 -B11-B10 -B1-B2 -B1-B3 -B1-B4 -B1-B5 -B2-B1 -B2-B7 -B2-B8 -B5-B1 -B5-B4 -B5-B10	$\begin{array}{c} 111.0 \ (4) \\ -110.5 \ (4) \\ -110.5 \ (4) \\ -112.2 \ (4) \\ 147.4 \ (4) \\ 110.2 \ (4) \\ 112.0 \ (5) \\ 149.3 \ (4) \\ -110.7 \ (5) \\ -147.3 \ (4) \\ -112.5 \ (4) \\ -149.9 \ (4) \\ 146.8 \ (4) \end{array}$
Br5- Br6- Br6- Br6- Br6- Br6- Br6- Br6- Br6	-B5 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6	-B11-B7 -B11-B10 -B1-B2 -B1-B3 -B1-B4 -B1-B5 -B2-B1 -B2-B3 -B2-B7 -B2-B8 -B5-B1 -B5-B1 -B5-B10 -B5-B11	$\begin{array}{c} 111.0 \ (4) \\ 149.1 \ (4) \\ -110.5 \ (4) \\ -112.2 \ (4) \\ 147.4 \ (4) \\ 110.2 \ (4) \\ 110.2 \ (4) \\ 112.0 \ (5) \\ 149.3 \ (4) \\ -110.7 \ (5) \\ -147.3 \ (4) \\ -112.5 \ (4) \\ -149.9 \ (4) \\ 146.8 \ (4) \\ 100 \ 7 \ (5) \end{array}$
Br5- Br6- Br6- Br6- Br6- Br6- Br6- Br6- Br6	-B5- -B6- -B6- -B6- -B6- -B6- -B6- -B6-	-B11-B7 -B11-B10 -B1-B2 -B1-B3 -B1-B4 -B1-B5 -B2-B1 -B2-B3 -B2-B7 -B2-B8 -B5-B1 -B5-B4 -B5-B10 -B5-B11 -B7-Br7	$\begin{array}{c} 111.0 (4) \\ 149.1 (4) \\ -110.5 (4) \\ -112.2 (4) \\ 147.4 (4) \\ 110.2 (4) \\ 112.0 (5) \\ 149.3 (4) \\ -110.7 (5) \\ -147.3 (4) \\ -112.5 (4) \\ -112.5 (4) \\ -149.9 (4) \\ 146.8 (4) \\ 109.7 (5) \\ -1 (1) \end{array}$
Br5- Br5- Br6- Br6- Br6- Br6- Br6- Br6- Br6- Br6	-B5 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6	$\begin{array}{c} -B11 \\ -B11 \\ -B10 \\ -B1 \\ -B2 \\ -B1 \\ -B2 \\ -B1 \\ -B3 \\ -B1 \\ -B4 \\ -B1 \\ -B5 \\ -B2 \\ -B1 \\ -B2 \\ -B3 \\ -B2 \\ -B3 \\ -B5 \\ -B1 \\ -B5 \\ -B1 \\ -B5 \\ -B1 \\ -B5 \\ -B11 \\ -B7 \\ -B7 \\ -B7 \\ -C20 \end{array}$	$\begin{array}{c} 111.0 & (4) \\ 149.1 & (4) \\ -110.5 & (4) \\ -112.2 & (4) \\ 147.4 & (4) \\ 110.2 & (4) \\ 112.0 & (5) \\ 149.3 & (4) \\ -110.7 & (5) \\ -147.3 & (4) \\ -112.5 & (4) \\ -149.9 & (4) \\ 146.8 & (4) \\ 109.7 & (5) \\ -1 & (1) \\ 148.2 & (4) \end{array}$
Br5- Br6- Br6- Br6- Br6- Br6- Br6- Br6- Br6	-B5 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6	$\begin{array}{c} -B11 \\ -B11 \\ -B10 \\ -B1 \\ -B2 \\ -B1 \\ -B2 \\ -B1 \\ -B3 \\ -B1 \\ -B4 \\ -B1 \\ -B5 \\ -B2 \\ -B1 \\ -B2 \\ -B3 \\ -B2 \\ -B7 \\ -B2 \\ -B7 \\ -B5 \\ -B1 \\ -B5 \\ -B1 \\ -B5 \\ -B11 \\ -B7 \\ -$	$\begin{array}{c} 111.0 \ (4) \\ 149.1 \ (4) \\ -110.5 \ (4) \\ -112.2 \ (4) \\ 149.2 \ (4) \\ 147.4 \ (4) \\ 110.2 \ (4) \\ 112.0 \ (5) \\ 149.3 \ (4) \\ -112.5 \ (4) \\ -112.5 \ (4) \\ -112.5 \ (4) \\ 149.9 \ (4) \\ 146.8 \ (4) \\ 109.7 \ (5) \\ -1 \ (1) \\ -148.3 \ (4) \\ 109.7 \ (5) \\ -1 \ (1) \\ -148.3 \ (4) \\ 109.7 \ (5) \\ -1 \ (1) \\ -148.3 \ (4) \\ 109.7 \ (5) \\ -1 \ (1) \\ -148.3 \ (4) \\ 109.7 \ (5) \\ -1 \ (1) \\ -148.3 \ (4) \\ 109.7 \ (5) \\ -1 \ (1) \\ -148.3 \ (4) \\ 109.7 \ (5) \\ -1 \ (1) \\ -148.3 \ (4) \\ 109.7 \ (5) \\ -1 \ (1) \\ -148.3 \ (4) \\ 109.7 \ (5) \\ -1 \ (1) \\ -148.3 \ (4) \\ 109.7 \ (5) \\ -1 \ (1) \\ -148.3 \ (4) \\ 109.7 \ (5) \\ -1 \ (1) \\ -148.3 \ (4) \\ 100.7 \ (5) \\ -1 \ (1) \\ -148.3 \ (4) \\ 100.7 \ (5) \\ -1 \ (1) \\ -148.3 \ (4) \\ 100.7 \ (5) \\ -1 \ (1) \\ -148.3 \ (4) \\ 100.7 \ (5) \\ -1 \ (1) \\ -148.3 \ (4) \\ 100.7 \ (5) \\ -1 \ (1) \\ -148.3 \ (4) \\ 100.7 \ (5) \\ -1 \ (1) \\ -148.3 \ (4) \\ -110.7 \ (5) \\ -1 \ (1) \\ -148.3 \ (4) \\ -110.7 \ (5) \\ -1 \ (5) \ (5) \\ -1 \ (5) \ (5) \\ -1 \ (5) \ $
Br5- Br5- Br6- Br6- Br6- Br6- Br6- Br6- Br6- Br6	-B5- -B5- -B6- -B6- -B6- -B6- -B6- -B6-	$\begin{array}{c} -B11 \\ -B11 \\ -B10 \\ -B1 \\ -B2 \\ -B1 \\ -B2 \\ -B1 \\ -B3 \\ -B1 \\ -B5 \\ -B2 \\ -B1 \\ -B5 \\ -B$	$\begin{array}{c} 111.0 \ (4) \\ 149.1 \ (4) \\ -110.5 \ (4) \\ -112.2 \ (4) \\ 147.4 \ (4) \\ 110.2 \ (4) \\ 112.0 \ (5) \\ 149.3 \ (4) \\ -110.7 \ (5) \\ -147.3 \ (4) \\ -112.5 \ (4) \\ -149.9 \ (4) \\ 146.8 \ (4) \\ 109.7 \ (5) \\ -1 \ (1) \\ -148.3 \ (4) \\ 111.9 \ (4) \\ 111.9 \ (4) \\ -112.9 \ (4) \\ -112.9 \ (4) \\ -112.9 \ (4) \\ -112.9 \ (4) \\ -112.5 \ (4) \ ($
Br5- Br5- Br6- Br6- Br6- Br6- Br6- Br6- Br6- Br6	-B5 -B5 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6 -B6	$\begin{array}{c} -B11 \\ -B11 \\ -B10 \\ -B1 \\ -B2 \\ -B1 \\ -B3 \\ -B1 \\ -B5 \\ -B2 \\ -B1 \\ -B5 \\ -B2 \\ -B1 \\ -B5 \\ -B11 \\ -B7 \\ -B7 \\ -B7 \\ -C20 \\ -B7 \\ -B2 \\ -B7 \\ $	$\begin{array}{c} 111.0 \ (4) \\ 149.1 \ (4) \\ -110.5 \ (4) \\ -112.2 \ (4) \\ 149.2 \ (4) \\ 147.4 \ (4) \\ 110.2 \ (4) \\ 112.0 \ (5) \\ 149.3 \ (4) \\ -110.7 \ (5) \\ -147.3 \ (4) \\ -112.5 \ (4) \\ -149.9 \ (4) \\ 146.8 \ (4) \\ 109.7 \ (5) \\ -1 \ (1) \\ -148.3 \ (4) \\ 111.9 \ (4) \\ 149.2 \ (4) \\ 149.2 \ (4) \\ \end{array}$
Br5- Br5- Br6- Br6- Br6- Br6- Br6- Br6- Br6- Br6	-B5- -B5- -B6- -B6- -B6- -B6- -B6- -B6-	$\begin{array}{c} -B11 - B7 \\ -B11 - B10 \\ -B1 - B2 \\ -B1 - B3 \\ -B1 - B4 \\ -B1 - B5 \\ -B2 - B1 \\ -B2 - B3 \\ -B2 - B7 \\ -B2 - B8 \\ -B5 - B1 \\ -B5 - B1 \\ -B5 - B1 \\ -B5 - B11 \\ -B7 - Br7 \\ -B7 - C20 \\ -B7 - B2 \\ -B7 - B11 \\ -B7 - B1 \\ -B7 - B11 \\ -B7 - B1 \\ -B7 - B$	$\begin{array}{c} 111.0 \ (4) \\ 149.1 \ (4) \\ -110.5 \ (4) \\ -112.2 \ (4) \\ 149.2 \ (4) \\ 147.4 \ (4) \\ 110.2 \ (4) \\ 112.0 \ (5) \\ 149.3 \ (4) \\ -110.7 \ (5) \\ -147.3 \ (4) \\ -112.5 \ (4) \\ -149.9 \ (4) \\ 146.8 \ (4) \\ 109.7 \ (5) \\ -1 \ (1) \\ -148.3 \ (4) \\ 111.9 \ (4) \\ 149.2 \ (4) \\ -109.5 \ (5) \end{array}$

Br6—B6—B11—B5	-110.7(4)
Br6—B6—B11—B7	112.0(5)
Br6—B6—B11—B10	-148.1(4)
Br7—B7—C20—B8	112 (1)
Br7_B7_C20_B9	1/2 (1)
P_{r7} $P7$ $C20$ $P10$	140(1) 149(1)
Br7 = B7 = C20 = B10	-142(1)
Br7—B7—C20—B11	-105(1)
Br7—B7—B2—B1	146(1)
Br7—B7—B2—B3	-151(1)
Br7—B7—B2—B6	108(1)
Br7—B7—B2—B8	-113(1)
Br7—B7—B6—B1	-151(1)
Br7—B7—B6—B2	-113 (1)
Br7 B7 B6 B5	146(1)
$D_{1}^{-} D_{1}^{-} D_{0}^{-} D_{0}^{-} D_{0}^{-}$	140(1)
$B_1 - B_1 - B_0 - B_1 $	109(1)
Br7—B7—B8—C20	-114(1)
Br7—B7—B8—B2	111(1)
Br7—B7—B8—B3	149(1)
Br7-B7-B8-B9	-147(1)
Br7—B7—B11—C20	116(1)
Br7—B7—B11—B5	-147(1)
Br7—B7—B11—B6	-109(1)
Br7 - B7 - B11 - B10	149(1)
$C_{11} - C_{51} - C_{52} - C_{12}$	60.0 (5)
01 - 031 - 032 - 012	179.1(4)
01-04-03-02	175.1 (4)
01	-6.8(6)
O1-C4-C5-C6	-173.1(4)
O1-C4-C5-C12	5.2(6)
O2-C1-C2-C3	-174.7(4)
O2— $C1$ — $C2$ — $C10$	4.2(6)
O2-C1-C6-C5	174.7(4)
O2-C1-C6-C7	-5.0(6)
02 - C9 - C8 - C7	-56.2(6)
$C_1 - C_2 - C_0 - C_8$	31.7 (6)
C1 - O2 - C9 - C8	151.7(0)
C1 = 02 = C9 = C13	151.4 (4)
C1—O2—C9—C14	-91.0(5)
C1-C2-C3-C4	0.2(6)
C1-C2-C3-C11	-179.9(4)
C1— $C6$ — $C5$ — $C4$	-0.1(6)
C1-C6-C5-C12	-178.3(4)
C1-C6-C7-C8	-20.4(6)
C2-C1-O2-C9	179.4(4)
$C_{2}-C_{1}-C_{6}-C_{5}$	-6.0(7)
$C_{2}^{2} - C_{1}^{2} - C_{6}^{2} - C_{7}^{2}$	174.4.(4)
C^2 C^2 C^4 C^5	E 9 (C)
$C_2 = C_3 = C_4 = C_5$	-5.8 (0)
C3-C2-C1-C6	5.9 (7)
C3-C4-C5-C6	5.7(6)
C3-C4-C5-C12	-175.9(4)
C4-C3-C2-C10	-178.6(4)
C4-C5-C6-C7	179.6(4)
C5-C4-C3-C11	174.3(4)
C5-C6-C7-C8	159.9 (4)
C6-C1-O2-C9	-1.1(7)
C6-C1-C2-C10	-175.2(4)
$C_{0} = C_{1} = C_{2} = C_{10}$	-175.2(4) 51.0(6)
$C_{0} - C_{1} - C_{0} - C_{9}$	51.9 (0) 1 4 (7)
07-06-05-012	1.4 (7)
C7—C8—C9—C13	-167.9(5)
C7—C8—C9—C14	59.5(6)
C10-C2-C3-C11	1.4(8)
C20—B7—B2—B1	-61.7(5)
C20—B7—B2—B3	1.4(5)
C20—B7—B2—B6	. ,
	-99.5(4)
C20 - B7 - B2 - B8	-99.5(4) 39.2(4)
C20—B7—B2—B8 C20—B7—B6—B1	-99.5 (4) 39.2 (4) 61.9 (5)
C20—B7—B2—B8 C20—B7—B6—B1 C20—B7—B6—B2	$ \begin{array}{c} -99.5 (4) \\ 39.2 (4) \\ 61.9 (5) \\ 00.0 (4) \end{array} $
$\begin{array}{c} C20 - B7 - B2 - B8\\ C20 - B7 - B6 - B1\\ C20 - B7 - B6 - B2\\ C20 - B7 - B6 - B2\\ C20 - B7 - B6 - B2\\ \end{array}$	$ \begin{array}{c} -99.5 (4) \\ 39.2 (4) \\ 61.9 (5) \\ 99.9 (4) \\ 11 (5) \end{array} $
$\begin{array}{c} C20 - B7 - B2 - B8\\ C20 - B7 - B6 - B1\\ C20 - B7 - B6 - B2\\ C20 - B7 - B6 - B2\\ C20 - B7 - B6 - B5\\ C20 - B7 - B6 - B1\\ \end{array}$	$\begin{array}{c} -99.5 (4) \\ 39.2 (4) \\ 61.9 (5) \\ 99.9 (4) \\ -1.1 (5) \\ 28.2 (4) \end{array}$
$\begin{array}{c} C20 - B7 - B2 - B8 \\ C20 - B7 - B6 - B1 \\ C20 - B7 - B6 - B2 \\ C20 - B7 - B6 - B5 \\ C20 - B7 - B6 - B11 \\ C20 - B7 - B7 - B6 - B11 \\ C20 - B7 - B7 - B7 - B7 \\ C20 - B7 - B7 - B7 \\ C20 - B7 \\ C2$	$\begin{array}{c} -99.5 (4) \\ 39.2 (4) \\ 61.9 (5) \\ 99.9 (4) \\ -1.1 (5) \\ -38.8 (4) \end{array}$
$\begin{array}{c} C20 - B7 - B2 - B8\\ C20 - B7 - B6 - B1\\ C20 - B7 - B6 - B2\\ C20 - B7 - B6 - B5\\ C20 - B7 - B6 - B11\\ C20 - B7 - B8 - B2\\ \end{array}$	$\begin{array}{c} -99.5 \ (4) \\ 39.2 \ (4) \\ 61.9 \ (5) \\ 99.9 \ (4) \\ -1.1 \ (5) \\ -38.8 \ (4) \\ -135.0 \ (4) \end{array}$

(6)

12

C20—B7—B8—B9

C20—B7—B11—B6

C20 - B7 - B11 - B10

C20 - B11 - B7 - B2

C20—B11—B7—B6

C20—B11—B7—B8

C20—B11—B10—B4

C20 - B11 - B10 - B5

C20 - B11 - B10 - B9

B1—B2—B3—B4

B1—B2—B3—B8

B1—B2—B3—B9

B1 - B2 - B6 - B5

B1 - B2 - B6 - B7

B1—B2—B6—B11

B1—B2—B7—B6

B1 - B2 - B7 - B8

B1 - B2 - B7 - B11

C20—B7—B11—B5

C20-	-B8—B2—B1	61.1(5)
C20-	-B8—B2—B3	98.7 (4)
C20-	-B8-B2-B6	-2.0(5)
C20-	-B8—B2—B7	-38.7(4)
C20-	-B8-B3-B1	-61.5(5)
C20-	-B8—B3—B2	-99.5(4)
C20-	-B8-B3-B4	2.0(5)
C20-	-B8—B3—B9	39.4 (4)
C20-	-B8—B7—B2	135.0 (4)
C20-	-B8-B7-B6	97.2 (4)
C20-	-B8-B7-B11	32.7 (4)
C20-	-B8—B9—B3	-134.2(4)
C20-	-B8-B9-B4	-96.2(4)
C20-	-B8—B9—B10	-32.6(4)
C20-	-B9—B3—B1	62.1(5)
C20-	-B9—B3—B2	-2.2(5)
C20-	-B9—B3—B4	99.1 (4)
C20-	-B9—B3—B8	-38.7(4)
C20-	-B9—B4—B1	-61.0(5)
C20-	-B9—B4—B3	-97.9(4)
C20-	-B9—B4—B5	2.8(5)
C20-	-B9—B4—B10	40.1 (4)
C20-	-B9—B8—B2	97.0 (5)
C20-	-B9—B8—B3	134.2 (4)
C20-	–B9—B8—B7	33.0(4)
C20-	-B9—B10—B4	-133.2 (4)
C20-	-B9—B10—B5	-95.8(4)
C20-	-B9-B10-B11	-32.5 (4)
C20-	-B10—B4—B1	60.7(5)
C20-	-B10—B4—B3	-2.5(5)
C20-	-B10—B4—B5	98.3(4)
C20-	-B10—B4—B9	-39.9(4)
C20-	-B10—B5—B1	-61.1(5)
C20-	-B10—B5—B4	-98.4(4)
C20-	-B10—B5—B6	2.2(5)
C20-	-B10—B5—B11	39.3(4)
C20-	-B10—B9—B3	95.2(4)
C20-	-B10—B9—B4	133.2 (4)
C20-	-B10—B9—B8	32.3(4)
C20-	-B10—B11—B5	-133.7 (4)
C20-	-B10—B11—B6	-96.1 (4)
C20-	-B10—B11—B7	-32.8 (4)
C20-	-B11—B5—B1	61.0(5)
C20-	-B11—B5—B4	-2.2(5)
C20-	-B11—B5—B6	98.6(4)
C20-	-B11—B5—B10	-39.9(4)
C20-	-B11—B6—B1	-61.6(5)
C20-	-B11—B6—B2	1.8(5)
C20-	-B11—B6—B5	-99.2 (4)
C20-	-B11—B6—B7	38.1(4)

-97.2(4)

-135.2(4)

-33.0 (4)95.8 (4)

 $\begin{array}{c}
133.7 (4) \\
32.8 (4) \\
37.6 (4)
\end{array}$

137.8 (4)100.7 (4)

-37.9(4)

-137.2(4)

37.9(4)

0.3(5)

S15

-100.9 (4)

-100.5 (4)

-33.2 (4)

135.2(4)

33.2(4)

B1—B2 B1—B2			
B1—B2	2—B8—	-B3 -37.6	(4)
	2—B8—	·B7 99.8	(4)
B1—B2	2—B8—	-B9 -0.7	(6)
B1—B3	3—B2—	-B6 -37.2	(4)
B1—B3	3—B2—	·B7 -100.2	(4)
B1—B3	3—B2—	B8 -137.8	(4)
B1—B3	B—B4—	B5 37.9	(4)
B1—B	, D1 3—B4—	-B9 138.6	(1) (4)
B1_B3	, D4 8	B10 101.1	(-1)
B1_B1		B10 101.1	(-1)
D1 D2	р—100— р ро	D7 0.2	(4)
D1 D	о—во— о во	-0.3 P0 100.0	(3)
D1 D1	р р р р р р	-B9 -100.9	(4)
BI-Ba	ы—В9—	-B4 -37.0	(4)
BI-Ba	ы—В9—	-B8 100.8	(4)
BI-Ba	з—В9—	B10 0.8	(5)
BI-B4	I-B3-	-B2 -37.8	(4)
BI-B4	I—B3—	-100.7	(4)
B1—B4	I—B3—	-138.6	(4)
B1—B4	I—B5—	·B6 37.3	(4)
B1—B4	1—B5—	·B10 138.2	(4)
B1 - B4	1—B5—	B11 100.5	(4)
B1 - B4	4—B9—	-B3 36.9	(4)
B1—B4	1—B9—	·B8 -0.5	(5)
B1—B4	4—B9—	B10 -101.0	(4)
B1—B4	4—B10-	-B5 -37.5	(4)
B1—B4	4—B10-	-B9 100.7	(4)
B1—B4	4—B10-	-B11 0.2	(5)
B1—B5	5—B4—	-B3 -37.7	(4)
B1—B5	б—В4—	-B9 -100.8	(4)
B1—B5	5—B4—	B10 -138.2	(4)
B1—B5	5—B6—	·B2 37.9	(4)
B1—B5	5—B6—	·B7 99.9	(4)
B1—B3	5—B6—	·B11 137.7	(4)
B1—B	5—B10-	-B4 37.3	(4)
B1—B	5—B10-	-B9 0.1	(5)
B1—B	5-B10-	-B11 -100.3	(4)
B1—B	5—B11-	-B6 -37.6	(4)
B1—B	5-B11-	-B7 04	(1) (5)
DI Di	, DII	D1 0.4	(0)
B1_B	-B11_	_B10 100.9	$\dot{(A)}$
B1—B5	5—B11- 3—B2	-B10 100.9 B3 37.3	(4)
B1—B3 B1—B6 B1—B6	5—B11- 5—B2— 3—B2	-B10 100.9 B3 37.3 B7 137.2	(4) (4) (4)
B1—B3 B1—B6 B1—B6 B1—B6	5—B11– 5—B2— 5—B2— 5—B2—	-B10 100.9 B3 37.3 B7 137.2 B8 100.7	(4) (4) (4) (4)
B1—B3 B1—B6 B1—B6 B1—B6	5—B11- 5—B2— 5—B2— 5—B2—	-B10 100.9 B3 37.3 B7 137.2 B8 100.7 B4 27.4	(4) (4) (4) (4) (4)
B1—B3 B1—B6 B1—B6 B1—B6 B1—B6	5—B11- 5—B2— 5—B2— 5—B2— 5—B5—	-B10 100.9 B3 37.3 B7 137.2 B8 100.7 B4 -37.4 P10 100.7	(4) (4) (4) (4) (4) (4)
B1—B3 B1—B6 B1—B6 B1—B6 B1—B6 B1—B6 B1—B6	5—B11- 5—B2— 5—B2— 5—B2— 5—B5— 5—B5—	-B10 100.9 B3 37.3 B7 137.2 B8 100.7 B4 -37.4 B10 -100.7	(4) (4) (4) (4) (4) (4) (4)
B1—B3 B1—B6 B1—B6 B1—B6 B1—B6 B1—B6 B1—B6 B1—B6	5 - B11 - 5 - B2 - 5 - B2 - 5 - B2 - 5 - B5 - 5 - B5 - 5 - B5 - 5 - B5 - 5 -	$\begin{array}{ccc} -B10 & 100.9 \\ B3 & 37.3 \\ B7 & 137.2 \\ B8 & 100.7 \\ B4 & -37.4 \\ B10 & -100.7 \\ B11 & -137.7 \\ B12 & 28.0 \\ B2 & 28.0 \\ B3 & 28.0 \\ B4 & -37.4 \\ B10 & -37.4 \\ B$	(4) (4) (4) (4) (4) (4) (4) (4)
B1B3 B1B6 B1B6 B1	5 - B11 - 5 - B2 - 5 - B2 - 5 - B2 - 5 - B5 - 5 - B5 - 5 - B5 - 5 - B5 - 5 -	$\begin{array}{cccc} -B10 & 100.9 \\ B3 & 37.3 \\ B7 & 137.2 \\ B8 & 100.7 \\ B4 & -37.4 \\ B10 & -100.7 \\ B11 & -137.7 \\ B2 & -38.0 \\ B2 & 0.6 \\ B2 & 0.6 \\ B3 & 0.6 \\ B4 & 0.6 \\ B4 & 0.6 \\ B5 & 0.6 \\ B5$	(4) (4) (4) (4) (4) (4) (4) (4) (4)
B1—B3 B1—B6 B1—B6 B1—B6 B1—B6 B1—B6 B1—B6 B1—B6 B1—B6	5 - B11 - 5 - B2 - 5 - B2 - 5 - B2 - 5 - B5 - 5 - B5 - 5 - B5 - 5 - B5 - 5 -	-B10 100.9 B3 37.3 B7 137.2 B8 100.7 B4 -37.4 B10 -100.7 B11 -137.7 B2 -38.0 B8 -0.6	(4) (4) (4) (4) (4) (4) (4) (4) (5)
B1B3 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6	5 - B11 - 5 - B2 - 5 - B2 - 5 - B2 - 5 - B5 - 5 - B5 - 5 - B5 - 5 - B7 - 5 - 5 - B7 - 5 - 5 - 5 - 5 - 5 - 5 - 5 - 5 - 5 -	$\begin{array}{cccc} -B10 & 100.9 \\ B3 & 37.3 \\ B7 & 137.2 \\ B8 & 100.7 \\ B4 & -37.4 \\ B10 & -100.7 \\ B11 & -137.7 \\ B2 & -38.0 \\ B8 & -0.6 \\ B11 & 100.7 \\ Dr & 27.6 \\ B11 & 27.7 \\ Dr & 27.6 \\ B7.6 & 27.6 \\ Dr & 27.6 \\ Dr$	(4) (4) (4) (4) (4) (4) (4) (4) (5) (4)
B1B3 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6	5 - B11 - 5 - B2 - 5 - B2 - 5 - B2 - 5 - B5 - 5 - B5 - 5 - B7 - 5 - B11 - 5 - B	$\begin{array}{cccc} -B10 & 100.9 \\ B3 & 37.3 \\ B7 & 137.2 \\ B8 & 100.7 \\ B4 & -37.4 \\ B10 & -100.7 \\ B11 & -137.7 \\ B2 & -38.0 \\ B8 & -0.6 \\ B11 & 100.7 \\ -B5 & 37.6 \\ B7 & 09.2 \\ \end{array}$	(4) (4) (4) (4) (4) (4) (4) (4) (5) (4) (4) (4)
B1B3 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6	5 - B11 - 5 - B11 - 5 - B2 - 5 - B2 - 5 - B5 - 5 - B5 - 5 - B7 - 5 - B7 - 5 - B7 - 5 - B7 - 5 - B11 - 5 - 5 - B11 - 5 - 5 - 5 - 5 - 5 - 5 - 5 - 5 - 5 -	$\begin{array}{cccc} -B10 & 100.9 \\ B3 & 37.3 \\ B7 & 137.2 \\ B8 & 100.7 \\ B4 & -37.4 \\ B10 & -100.7 \\ B11 & -137.7 \\ B2 & -38.0 \\ B8 & -0.6 \\ B11 & 100.7 \\ -B5 & 37.6 \\ -B7 & -99.6 \\ B10 & 0.2 \\ \end{array}$	(4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (5) (4) (4) (5) (4) (5) (4) (5) (4) (5) (4) (5) (4) (5) (4) (5) (5) (4) (5) (5) (4) (5) (5) (4) (5) (5) (4) (5)
B1B3 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6	5 - B11 - 5 - B11 - 5 - B2 - 5 - B2 - 5 - B5 - 5 - B5 - 5 - B5 - 5 - B7 - 5 - B7 - 5 - B7 - 5 - B11 - 5	$\begin{array}{cccc} -B10 & 100.9 \\ B3 & 37.3 \\ B7 & 137.2 \\ B8 & 100.7 \\ B4 & -37.4 \\ B10 & -100.7 \\ B11 & -137.7 \\ B2 & -38.0 \\ B8 & -0.6 \\ B11 & 100.7 \\ -B5 & 37.6 \\ -B7 & -99.6 \\ -B10 & 0.2 \\ D1 & 0.2 \\ D2 & 0.2 \\ D1 & 0.2 \\ D1 & 0.2 \\ D2 & 0.2 \\ D2$	(4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (5) (4) (4) (5)
B1B3 B1B6 B1	5 - B11 - 5 - B11 - 5 - B2 - 5 - B2 - 5 - B5 - 5 - B5 - 5 - B5 - 5 - B7 - 5 - B11 - 5 - 5 - 5 - 5 - 5 - 5 - 5 - 5 - 5 -	$\begin{array}{cccc} -B10 & 100.9 \\ B3 & 37.3 \\ B7 & 137.2 \\ B8 & 100.7 \\ B4 & -37.4 \\ B10 & -100.7 \\ B11 & -137.7 \\ B2 & -38.0 \\ B8 & -0.6 \\ B11 & 100.7 \\ -B5 & 37.6 \\ -B7 & -99.6 \\ -B10 & 0.2 \\ B4 & -138.2 \\ \end{array}$	(4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (5) (4) (5) (4) (5) (4) (5) (4) (5) (5) (4) (4) (5) (5) (4) (4) (5) (4) (4) (5) (4) (4) (5) (4) (4) (4) (5) (4)
B1B3 B1B6 B1	5 - B11 - B2 - B1 - B2 - B2 - B2 - B5 - B5 - B5 - B5 - B7 - B7 - B7 - B7	$\begin{array}{cccc} -B10 & 100.9 \\ B3 & 37.3 \\ B7 & 137.2 \\ B8 & 100.7 \\ B4 & -37.4 \\ B10 & -100.7 \\ B11 & -137.7 \\ B2 & -38.0 \\ B8 & -0.6 \\ B11 & 100.7 \\ -B5 & 37.6 \\ -B7 & -99.6 \\ -B10 & 0.2 \\ B4 & -138.2 \\ B8 & -37.4 \\ \end{array}$	(4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (5) (4) (4) (5) (4) (5) (4)
B1B3 B1B6 B2B3 B2B3 B2B3 B2B3	5 - B11 - B2 - B1 - B2 - B1 - B2 - B1 - B1	$\begin{array}{cccc} -B10 & 100.9 \\ B3 & 37.3 \\ B7 & 137.2 \\ B8 & 100.7 \\ B4 & -37.4 \\ B10 & -100.7 \\ B11 & -137.7 \\ B2 & -38.0 \\ B8 & -0.6 \\ B11 & 100.7 \\ -B5 & 37.6 \\ -B7 & -99.6 \\ -B10 & 0.2 \\ B4 & -138.2 \\ B8 & -37.4 \\ B9 & -101.4 \\ \end{array}$	(4) (4)
B1B3 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B2-B3 B2-B3 B2-B3	5 - B11 - B2 - B1 - B2 - B1 - B2 - B1 - B1	$\begin{array}{cccc} -B10 & 100.9 \\ B3 & 37.3 \\ B7 & 137.2 \\ B8 & 100.7 \\ B4 & -37.4 \\ B10 & -100.7 \\ B11 & -137.7 \\ B2 & -38.0 \\ B8 & -0.6 \\ B11 & 100.7 \\ -B5 & 37.6 \\ -B7 & -99.6 \\ -B10 & 0.2 \\ B4 & -138.2 \\ B8 & -37.4 \\ B9 & -101.4 \\ B3 & 36.9 \\ \end{array}$	(4) (4)
B1B3 B1B6 B2B3 B2B3 B2B3	5 - B11 - B2 - B1 - B2 - B1 - B1 - B1 - B	$\begin{array}{cccc} -B10 & 100.9 \\ B3 & 37.3 \\ B7 & 137.2 \\ B8 & 100.7 \\ B4 & -37.4 \\ B10 & -100.7 \\ B11 & -137.7 \\ B2 & -38.0 \\ B8 & -0.6 \\ B11 & 100.7 \\ -B5 & 37.6 \\ -B7 & -99.6 \\ -B10 & 0.2 \\ B4 & -138.2 \\ B8 & -37.4 \\ B9 & -101.4 \\ B3 & 36.9 \\ B5 & -100.8 \end{array}$	(4) (4)
B1B3 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6 B1B6 B1B3 B2B3 B2B3 B2B3 B2B3 B2B3	5 - B11 - B2 - B1 - B2 - B1 - B1 - B1 - B	$\begin{array}{cccc} -B10 & 100.9 \\ B3 & 37.3 \\ B7 & 137.2 \\ B8 & 100.7 \\ B4 & -37.4 \\ B10 & -100.7 \\ B11 & -137.7 \\ B2 & -38.0 \\ B8 & -0.6 \\ B11 & 100.7 \\ -B5 & 37.6 \\ -B7 & -99.6 \\ -B7 & 0.2 \\ B4 & -138.2 \\ B8 & -37.4 \\ B9 & -101.4 \\ B3 & 36.9 \\ B5 & -100.8 \\ B9 & 0.1 \\ \end{array}$	(4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (5) (4) (4) (4) (4) (5) (4) (5) (4) (4) (4) (5) (5) (4) (4) (5) (5) (4) (4) (5) (5) (4) (5)
B1B3 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B2B3 B2-B3	5 - B11 - B2 - B1 - B2 - B1 - B1 - B1 - B	$\begin{array}{cccc} -B10 & 100.9 \\ B3 & 37.3 \\ B7 & 137.2 \\ B8 & 100.7 \\ B4 & -37.4 \\ B10 & -100.7 \\ B11 & -137.7 \\ B2 & -38.0 \\ B8 & -0.6 \\ B11 & 100.7 \\ -B5 & 37.6 \\ -B7 & -99.6 \\ -B7 & -99.6 \\ -B10 & 0.2 \\ B4 & -138.2 \\ B8 & -37.4 \\ B9 & -101.4 \\ B3 & 36.9 \\ B5 & -100.8 \\ B9 & 0.1 \\ B10 & -63.4 \\ \end{array}$	(4) (5) (4) (5)
B1B3 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B2B3 B2-B3	5 - B11 - B2 - B1 - B2 - B2 - B1 - B1 - B	$\begin{array}{c cccc} -B10 & 100.9 \\ B3 & 37.3 \\ B7 & 137.2 \\ B8 & 100.7 \\ B4 & -37.4 \\ B10 & -100.7 \\ B11 & -137.7 \\ B2 & -38.0 \\ B8 & -0.6 \\ B11 & 100.7 \\ -B5 & 37.6 \\ -B7 & -99.6 \\ -B10 & 0.2 \\ B4 & -138.2 \\ B8 & -37.4 \\ B9 & -101.4 \\ B3 & 36.9 \\ B5 & -100.8 \\ B9 & 0.1 \\ B10 & -63.4 \\ B4 & 100.3 \\ -B10 & -63.4 \\ B4 & 100.3 \\ -200.3 $	(4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (5) (4) (4) (4) (5) (5) (4) (4) (5)
B1B3 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B2B3 B2B3 B2B3 B2B3 B2B3 B2B3 B2B3 B2B3 B2B3 B2B3 B2B3 B2-B	5 - B11 - B2 - B1 - B2 - B1 - B2 - B1 - B1	$\begin{array}{cccc} -B10 & 100.9 \\ B3 & 37.3 \\ B7 & 137.2 \\ B8 & 100.7 \\ B4 & -37.4 \\ B10 & -100.7 \\ B11 & -137.7 \\ B2 & -38.0 \\ B8 & -0.6 \\ B11 & 100.7 \\ -B5 & 37.6 \\ -B7 & -99.6 \\ -B7 & -99.6 \\ -B7 & -09.6 \\ -B10 & 0.2 \\ B4 & -138.2 \\ B8 & -37.4 \\ B9 & -101.4 \\ B3 & 36.9 \\ B5 & -100.8 \\ B9 & 0.1 \\ B10 & -63.4 \\ B4 & 100.3 \\ B6 & -37.9 \\ \end{array}$	(4) (5) (5) (5) (4) (4) (4) (4) (5) (5) (4) (4) (4) (4) (5) (5) (4) (4) (4) (5) (5) (4) (4) (4) (4) (5) (4)
B1B3 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B1B4 B2B3 B2B3 B2B3 B2-B3 B2	5 - B11 - B2 - B1 - B2 - B1 - B2 - B1 - B1	$\begin{array}{cccc} -B10 & 100.9 \\ B3 & 37.3 \\ B7 & 137.2 \\ B8 & 100.7 \\ B4 & -37.4 \\ B10 & -100.7 \\ B11 & -137.7 \\ B2 & -38.0 \\ B8 & -0.6 \\ B11 & 100.7 \\ -B5 & 37.6 \\ -B7 & -99.6 \\ -B7 & -99.6 \\ -B10 & 0.2 \\ B4 & -138.2 \\ B8 & -37.4 \\ B9 & -101.4 \\ B3 & 36.9 \\ B5 & -100.8 \\ B9 & 0.1 \\ B10 & -63.4 \\ B4 & 100.3 \\ B6 & -37.9 \\ B10 & 63.0 \\ \end{array}$	(4) (5) (4) (4) (4) (5) (4) (4) (4) (5) (4) (4) (4) (5) (4) (4) (4) (5) (4) (4) (4) (5) (4) (4) (4) (4) (4) (4) (4) (5) (4) (5) (5) (4) (4) (4) (5) (5) (4) (4) (5) (5) (4) (4) (5) (5) (4) (4) (5)
$\begin{array}{c} B1 Bi \\ B2 - $	5 - B11 - B2 - B1 - B2 - B1 - B2 - B1 - B1	$\begin{array}{cccc} -B10 & 100.9 \\ B3 & 37.3 \\ B7 & 137.2 \\ B8 & 100.7 \\ B4 & -37.4 \\ B10 & -100.7 \\ B11 & -137.7 \\ B2 & -38.0 \\ B8 & -0.6 \\ B11 & 100.7 \\ -B5 & 37.6 \\ -B7 & -99.6 \\ -B7 & -99.6 \\ -B10 & 0.2 \\ B4 & -138.2 \\ B8 & -37.4 \\ B9 & -101.4 \\ B3 & 36.9 \\ B5 & -100.8 \\ B9 & 0.1 \\ B10 & -63.4 \\ B4 & 100.3 \\ B6 & -37.9 \\ B10 & 63.0 \\ B11 & -0.3 \\ \end{array}$	(4) (5) (5) (4) (4) (4) (4) (4) (4) (5) (5) (4) (4) (4) (5) (5) (4) (4) (5)
$\begin{array}{c} B1 Bi \\ B2 - Bi \\ B$	5 - B11 - B2 - B1 - B2 - B1 - B2 - B1 - B1	$\begin{array}{cccc} -B10 & 100.9 \\ B3 & 37.3 \\ B7 & 137.2 \\ B8 & 100.7 \\ B4 & -37.4 \\ B10 & -100.7 \\ B11 & -137.7 \\ B2 & -38.0 \\ B8 & -0.6 \\ B11 & 100.7 \\ -B5 & 37.6 \\ -B7 & -99.6 \\ -B7 & -99.6 \\ -B10 & 0.2 \\ B4 & -138.2 \\ B8 & -37.4 \\ B9 & -101.4 \\ B3 & 36.9 \\ B5 & -100.8 \\ B9 & 0.1 \\ B10 & -63.4 \\ B4 & 100.3 \\ B6 & -37.9 \\ B10 & 63.0 \\ B11 & -0.3 \\ B5 & 137.6 \\ \end{array}$	(4) (5) (5) (4) (4) (4) (4) (4) (4) (5) (5) (4) (4) (4) (5) (5) (4) (4) (4) (5) (5) (4) (4) (5) (5) (4) (4) (5) (5) (4) (4) (5) (5) (4) (4) (5) (5) (5) (5) (5) (5) (5) (4) (5) (5) (5) (5) (4) (5) (5) (5) (4) (5) (5) (5) (4) (5)
$\begin{array}{c} B1 Bi \\ B2 - Bi \\ B$	5 - B11 - B2 - B11 - B2 - B11 - B2 - B11 - B1	$\begin{array}{cccc} -B10 & 100.9 \\ B3 & 37.3 \\ B7 & 137.2 \\ B8 & 100.7 \\ B4 & -37.4 \\ B10 & -100.7 \\ B11 & -137.7 \\ B2 & -38.0 \\ B8 & -0.6 \\ B11 & 100.7 \\ -B5 & 37.6 \\ -B7 & -99.6 \\ -B10 & 0.2 \\ B4 & -138.2 \\ B8 & -37.4 \\ B9 & -101.4 \\ B3 & 36.9 \\ B5 & -100.8 \\ B9 & 0.1 \\ B10 & -63.4 \\ B4 & 100.3 \\ B6 & -37.9 \\ B10 & 63.0 \\ B11 & -0.3 \\ B5 & 137.6 \\ B7 & 37.4 \\ \end{array}$	(4) (5) (5) (4) (4) (5) (5) (4) (4) (5) (5) (5) (4) (4) (5) (5) (4) (4) (5) (5) (5) (4) (4) (5) (5) (5) (4) (4) (5) (5) (5) (4) (4) (5) (5) (5) (4) (4) (5) (5) (5) (4) (4) (5) (5) (5) (4) (5) (5) (5) (4) (4) (5) (5) (4) (4) (5) (5) (4) (4) (4) (5) (5) (4) (4) (4) (4) (4) (5) (5) (4) (4) (4) (4) (4) (4) (5) (5) (4)
$\begin{array}{c} B1 Bi \\ B2 Bi \\ B2 - Bi \\$	5 - B11 - B2 - B1 - B2 - B1 - B2 - B1 - B1	$\begin{array}{cccc} -B10 & 100.9 \\ B3 & 37.3 \\ B7 & 137.2 \\ B8 & 100.7 \\ B4 & -37.4 \\ B10 & -100.7 \\ B11 & -137.7 \\ B2 & -38.0 \\ B8 & -0.6 \\ B11 & 100.7 \\ -B5 & 37.6 \\ -B7 & -99.6 \\ -B7 & 0.2 \\ B4 & -138.2 \\ B8 & -37.4 \\ B9 & -101.4 \\ B3 & 36.9 \\ B5 & -100.8 \\ B9 & 0.1 \\ B10 & -63.4 \\ B4 & 100.3 \\ B6 & -37.9 \\ B10 & 63.0 \\ B11 & -0.3 \\ B5 & 137.6 \\ B7 & 37.4 \\ B11 & 100.2 \\ \end{array}$	(4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (5) (5) (4) (4) (5) (5) (4) (4) (4) (5) (5) (5) (4) (4) (4) (4) (5) (5) (5) (4) (4) (4) (5) (5) (5) (4) (5) (5) (5) (4) (4) (4) (4) (4) (4) (5) (5) (4) (4) (4) (4) (4) (4) (4) (5) (5) (4)
$\begin{array}{c} B1 Bi \\ B1 Bi \\ B1 Bi \\ B1 Bi \\ B1 - Bi \\ B2 - Bi \\ B$	5 - B11 - B2 - B1 - B2 - B1 - B2 - B1 - B1	$\begin{array}{cccc} -B10 & 100.9 \\ B3 & 37.3 \\ B7 & 137.2 \\ B8 & 100.7 \\ B4 & -37.4 \\ B10 & -100.7 \\ B11 & -137.7 \\ B2 & -38.0 \\ B8 & -0.6 \\ B11 & 100.7 \\ -B5 & 37.6 \\ -B7 & -99.6 \\ -B7 & -99.6 \\ -B7 & -99.6 \\ -B10 & 0.2 \\ B4 & -138.2 \\ B8 & -37.4 \\ B9 & -101.4 \\ B3 & 36.9 \\ B5 & -100.8 \\ B9 & 0.1 \\ B10 & -63.4 \\ B4 & 100.3 \\ B6 & -37.9 \\ B10 & 63.0 \\ B11 & -0.3 \\ B5 & 137.6 \\ B7 & 37.4 \\ B11 & 100.2 \\ B4 & 138.2 \\ B7 & 37.4 \\ B10 & 20.2 \\ B4 & 138.2 \\ B4 & 20.2 \\ B4 & 20.2 \\ B4 & 20.2 \\ B4 & 20.2 \\ B7 & 20.2 \\ B10.2 \\ B4 & 20.2 \\ B10.2 \\ B4 & 20.2 \\ B4$	(4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (5) (4) (4) (4) (5) (4) (4) (5) (4) (5) (4) (4) (4) (5) (5) (4) (4) (5) (5) (4) (4) (5) (5) (4) (4) (5) (5) (4) (4) (5) (5) (4) (4) (4) (5) (5) (4) (4) (4) (5) (5) (4) (4) (4) (4) (5) (5) (4)
$\begin{array}{c} B1 Bi \\ B2 - Bi \\$	5 - B11 - B2 - B1 - B2 - B1 - B2 - B1 - B1	$\begin{array}{cccc} -B10 & 100.9 \\ B3 & 37.3 \\ B7 & 137.2 \\ B8 & 100.7 \\ B4 & -37.4 \\ B10 & -100.7 \\ B11 & -137.7 \\ B2 & -38.0 \\ B8 & -0.6 \\ B11 & 100.7 \\ -B5 & 37.6 \\ -B7 & -99.6 \\ -B7 & -99.6 \\ -B10 & 0.2 \\ B4 & -138.2 \\ B8 & -37.4 \\ B9 & -101.4 \\ B3 & 36.9 \\ B5 & -100.8 \\ B9 & 0.1 \\ B10 & -63.4 \\ B4 & 100.3 \\ B6 & -37.9 \\ B10 & 63.0 \\ B11 & -0.3 \\ B5 & 137.6 \\ B7 & 37.4 \\ B11 & 100.2 \\ B4 & 138.2 \\ B5 & 100.6 \\ \end{array}$	(4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (5) (4) (4) (4) (5) (4) (4) (5) (4) (5) (4) (4) (4) (5) (5) (4) (4) (5) (5) (4) (4) (5) (5) (4) (4) (5) (5) (4) (4) (4) (5) (5) (4) (4) (4) (5) (5) (4) (4) (4) (5) (5) (4) (4) (4) (4) (5) (5) (4)
$\begin{array}{c} B1 - Bi\\ B2 - $	5 - B11 - B2 - B1 - B2 - B1 - B2 - B1 - B1	$\begin{array}{cccc} -B10 & 100.9 \\ B3 & 37.3 \\ B7 & 137.2 \\ B8 & 100.7 \\ B4 & -37.4 \\ B10 & -100.7 \\ B11 & -137.7 \\ B2 & -38.0 \\ B8 & -0.6 \\ B11 & 100.7 \\ -B5 & 37.6 \\ -B7 & -99.6 \\ -B7 & -99.6 \\ -B10 & 0.2 \\ B4 & -138.2 \\ B8 & -37.4 \\ B9 & -101.4 \\ B3 & 36.9 \\ B5 & -100.8 \\ B9 & 0.1 \\ B10 & -63.4 \\ B4 & 100.3 \\ B6 & -37.9 \\ B10 & 63.0 \\ B11 & -0.3 \\ B5 & 137.6 \\ B7 & 37.4 \\ B11 & 100.2 \\ B4 & 138.2 \\ B4 & 138.2 \\ B5 & 100.6 \\ B6 & 37.3 \\ \end{array}$	(4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4) (5) (5) (4) (4) (4) (5) (5) (5) (4) (4) (4) (5) (5) (4) (4) (4) (5) (5) (4) (4) (4) (5) (5) (4) (4) (4) (4) (5) (5) (4) (4) (4) (4) (5) (5) (4) (4) (4) (5) (5) (4) (4) (4) (4) (5) (5) (4) (4) (4) (4) (5) (5) (5) (4) (4) (4) (5) (5) (5) (5) (4) (4) (4) (4) (5) (5) (5) (4)

B2-	-B3-	-B4—B9	100.8(4)
B2_	_B3_	_B4B10	63.2 (5)
D2	D0 D2	D4 D10	28.2(0)
D2-	-до-	-Во-Ві	-38.3(4)
B2-	-B3-	-B8—B9	-138.9(4)
B2-	-B3-	-B9-B4	-101.3 (4)
B2-	-B3-	-B9-B8	36.5(4)
B2-	-B3-	-B9-B10	-63.4(5)
B2-	-B6-	-B1-B3	-370(4)
D2	DG	D1 D0	100.2 (4)
D2-	-D0-	-B1-B4	-100.3 (4)
B2–	-B6-	-B1-B2	-137.6(4)
B2-	-B6-	-B5-B4	0.6(5)
B2-	-B6-	-B5 - B10	-62.7(5)
B2-	-B6-	-B5-B11	-99.8(4)
B2_	_B6_	_B7B8	37.4(4)
D2	DC	D7 D11	199.6 (4)
D2-	-D0-		138.0 (4)
B2-	-B6-	-B11—B5	101.0 (4)
B2-	-B6-	-B11-B7	-36.3(4)
B2-	-B6-	-B11-B10	63.6(5)
B2-	-B7-	-C20-B8	-39.7(4)
B2-	-B7-	-C20-B9	-3.0(6)
B2_	_B7_	-C20-B10	66.8 (5)
D2-	-D7-	-C20	100.6 (3)
B2-	-B7-	-C20-B11	103.6 (4)
B2-	-B7-	-B6-B5	-101.0(4)
B2-	-B7-	-B6B11	-138.6(4)
B2-	-B7-	-B8-B3	38.4(4)
B2-	-B7-	-B8-B9	101.9 (4)
B2_	_B7_	_B11B5	-0.4 (5)
D2-	-D7-	-D11 DC	-0.4(0)
B2-	-B7-	-BII-B6	38.0 (4)
B2-	-B7-	-B11—B10	-64.0(5)
B2-	-B8-	-C20-B7	39.6(4)
B2-	-B8-	-C20-B9	-103.0(4)
B2-	-B8-	-C20-B10	-66.9(5)
B2-	-B8-	-C20-B11	34(6)
B2_	-B8-	-B3-B4	101.5(4)
D2-	-D0-	-D3-D4	101.5 (4)
B2-	-B8-	-B3-B9	138.9(4)
B2-	-B8-	-B7-B6	-37.9(4)
B2-	-B8-	-B7 - B11	-102.3 (4)
B2-	-B8-	–B9—B3	-37.2(4)
B2-	-B8-	-B9—B4	0.7(6)
B2-	-B8-	_B9B10	64.3 (5)
D2	D1	DO DIO	128.9(4)
- со Бо	-DI-	-B2-B0	138.2(4)
B3-	-BI-	-B2-B7	100.3(4)
B3–	-B1-	-B2-B8	37.7(4)
B3–	-B1-	-B4-B5	-137.7(4)
B3-	-B1-	-B4-B9	-36.9(4)
В3-	-B1-	-B4-B10	-100.4(4)
B3-	_B1_	-B5-B4	37 7 (4)
B3_	_B1_	_B5B6	-100.4 (4)
-с- ро	-D1-		-100.4(4)
<u>ы</u> з–	-DI-	-D0-B10	0.4(5)
В3–	–В1–	–въ—в11	-62.9(5)
B3–	-B1-	-B6-B5	100.6 (4)
B3-	-B1-	-B6-B7	0.4(5)
В3-	-B1-	-B6-B11	63.3 (5)
R3_	_B2_	_B1B4	-373(4)
D9	D2	DI DI	100.2(4)
D0-	-D2-	-D1 - D0	-100.3(4)
B3-	-B2-	-BI-B0	-138.2(4)
B3–	-B2-	-B6-B5	-0.5(5)
B3–	-B2-	-B6-B7	-99.9(4)
В3-	-B2-	-B6 - B11	-63.2(5)
В3-	-B2-	–B7—B6	100.9 (4)
B3-	-B2-	-B7B8	-37.8(4)
-00-	D2-	D7 D11	
D3-		-DI-BII	03.3 (5)
В3–	–B2–	–B8—B7	137.4(4)
B3–	-B2-	-B8-B9	36.9(4)
В3-	-B4-	-B1-B5	137.7 (4)
В3-	-B4-	-B1-B6	100.3 (4)
B3-	-B4-	-B5-B6	-0.4(5)
B3	_B4	_B5B10	100 5 (4)
-00 -	D4-	D5 - D10	100.3(4)
В 3-	-ы4-	-B9-B11	62.8 (5)

B3—B4-	—B9—B8	-37.4	(4)
B3—B4-	-B9-B10	-137.9	(4)
B3—B4-	-B10-B5	-100.8	(4)
B3—B4-	-B10-B9	37.4	(4)
B3—B4-	-B10-B11	-63.1	(5)
B3_B8	-C20-B7	-40.0	(4)
B3—B8-	-C20 B3	-3.9	$(\frac{1}{5})$
B3—B8-	-C20-B11	66.5	(5)
B3—B8-	-B2-B6	-100.7	(4)
B3—B8-	-B2-B7	-137.4	(4)
B3—B8-	-B7-B6	0.5	(5)
B3—B8-	-B7-B11	-63.9	(5)
B3—B8-	-B9-B4	37.9	(4)
B3—B8- B3—B0	-B9-B10 -C20-B7	101.0	(4)
B3—B9-	-C20-B7 -C20-B8	39.5	(0) (4)
B3—B9-	-C20-B10	-103.6	(4)
B3—B9-	-C20-B11	-67.3	(5)
B3—B9-	-B4-B5	100.7	(4)
B3—B9-	-B4-B10	137.9	(4)
B3—B9-	—B8—B7	-101.2	(4)
B3—B9-	-B10-B4	-38.0	(4)
B3—B9-	-BI0-B5 B10 B11	-0.6	(5)
B4—B1-	-B10-B11 -B2-B6	100.9	(3)
B4—B1-	-B2-B0 -B2-B7	63.0	(4) (5)
B4—B1-	-B2-B8	0.4	(5)
B4—B1-	—B3—B8	100.8	(4)
B4—B1-	—B3—B9	36.8	(4)
B4—B1-	-B5-B6	-138.2	(4)
B4—B1-	-B5-B10	-37.3	(4)
B4—B1-	-B5-B11 D6 D5	-100.6	(4)
B4—B1- B4—B1-	-B6-B7	-63 0	(4) (5)
B4—B1-	-B6-B11	-0.1	(5) (5)
B4—B3-	-B1-B5	-37.6	(4)
B4—B3-	-B1-B6	-100.9	(4)
B4—B3-	-B2-B6	0.3	(5)
B4—B3-	-B2-B7	-62.7	(5)
B4—B3-	-B2-B8	-100.2	(4)
B4—B3-	-B8-B7	63.2	(5)
B4—B3-	—Бо—Б9 —В0—В8	-37.3	(4)
B4—B3-	-B9-B10	37.9	(4)
B4—B5-	-B1-B6	138.2	(4)
B4—B5-	-B6-B7	62.6	(5)
B4—B5-	-B6-B11	100.4	(4)
B4—B5-	-B10-B9	-37.2	(4)
B4—B5-	-B10-B11	-137.7	(4)
B4—B5-	-BII-B6 D11 D7	-100.8	(4)
B4—B5-	-B11-B7 -B11-B10	-02.8	(3)
B4 B9	-C20-B7	66.0	$(\frac{1}{5})$
B4—B9-	-C20-B8	102.3	(4)
B4—B9-	-C20-B10	-40.8	(4)
B4—B9-	-C20-B11	-4.5	(5)
B4—B9-	B3B8	-137.8	(4)
B4—B9-	-B8-B7	-63.2	(5)
B4 D0	-B10-B11	37.4	(4)
Б4—В9- В4—В10	-B10-B11 -C20-B7	100.7	(4) (5)
B4—B10	-C20-B8	-05.5	(5)
B4—B10	0—C20—B9	40.4	(4)
B4—B10	0—C20—B11	-102.4	(4)
B4—B10	0—B5—B6	100.6	(4)
B4—B10	0—B5—B11	137.7	(4)
B4—B10	D—B9—B8	-100.9	(4)
в4—В10	J—В11—В2	-37.9	(4)

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62.8(5)

B4-		
	-B10—B11—B6	-0.3(5)
B4-	-B10—B11—B7	63.0(5)
B5-	-B1—B2—B6	37.9(4)
B5-	-B1—B2—B7	0.0(5)
B5-	-B1—B2—B8	-62.6(5)
B5_	-B1-B3-B8	63.2(5)
DE	D1 D3 D0 D1 D2 D0	0.8 (5)
DJ-	-B1-B3-B9	-0.8(3)
B9-	-B1-B4-B9	100.8(4)
B2-	-B1—B4—B10	37.4(4)
B5—	-B1—B6—B7	-100.2(4)
B5-	-B1—B6—B11	-37.4(4)
B5-	-B4—B1—B6	-37.4(4)
B5-	-B4—B3—B8	-62.8(5)
B5-	-B4—B3—B9	-100.7(4)
B5-	-B4—B9—B8	63.2(5)
B5-	-B4—B9—B10	-37.3(4)
В5—	-B4—B10—B9	138.2(4)
B5-	-B4-B10-B11	377(4)
B5_	-B6-B2-B7	99.4 (4)
B5_	-B6-B2-B8	62.8 (5)
DJ-	-D0 - D2 - D8	62.6(5)
- БЭ-	$-D_0 - D_1 - D_0$	-03.0(3)
B5-	-B0-B1-B11	37.7 (4)
B2-	-B6—B11—B7	-137.3(4)
B5—	-B6—B11—B10	-37.4(4)
B5-	-B10—C20—B7	-3.2(5)
B5-	-B10-C20-B8	66.4(5)
B5-	-B10—C20—B9	102.7(4)
B5-	-B10—C20—B11	-40.2(4)
B5-	-B10—B4—B9	-138.2(4)
B5-	-B10—B9—B8	-63.5(5)
B5-	-B10—B11—B6	37.6(4)
B5-	-B10—B11—B7	100.9(4)
B5-	-B11—C20—B7	-102.0(4)
B5—	-B11-C20-B8	-66.3(5)
B5_	-B11-C20-B9	43(5)
B5_	-B11 - C20 - B10	40.5(0)
D0-	D11 = 0.20 = D10 D11 = D6 = D7	127.2(4)
DJ-	-B11 - B0 - B7	137.3(4)
- БЭ-	-B11 - B7 - B0	
B0-	-B11—B(—B8	-36.4(4)
- B 5	D11 D10 D0	-38.4(4) 63.8(5)
D0-	-B11—B10—B9	-38.4 (4) 63.8 (5) -100.9 (4)
B6-	-B11—B10—B9 -B1—B2—B7	-38.4 (4) 63.8 (5) -100.9 (4) -37.9 (4)
В6— В6—	-B11—B10—B9 -B1—B2—B7 -B1—B2—B8	$\begin{array}{c} -38.4 \ (4) \\ 63.8 \ (5) \\ -100.9 \ (4) \\ -37.9 \ (4) \\ -100.5 \ (4) \end{array}$
B6- B6- B6-	-B11—B10—B9 -B1—B2—B7 -B1—B2—B8 -B1—B3—B8	$\begin{array}{r} -38.4 (4) \\ 63.8 (5) \\ -100.9 (4) \\ -37.9 (4) \\ -100.5 (4) \\ -0.1 (5) \end{array}$
B6- B6- B6- B6-	-B11—B10—B9 -B1—B2—B7 -B1—B2—B8 -B1—B3—B8 -B1—B3—B9	$\begin{array}{c} -38.4 & (4) \\ 63.8 & (5) \\ -100.9 & (4) \\ -37.9 & (4) \\ -100.5 & (4) \\ -0.1 & (5) \\ -64.1 & (5) \end{array}$
B6- B6- B6- B6- B6-	-B11—B10—B9 -B1—B2—B7 -B1—B2—B8 -B1—B3—B8 -B1—B3—B9 -B1—B4—B9	$\begin{array}{c} -36.4 (4) \\ 63.8 (5) \\ -100.9 (4) \\ -37.9 (4) \\ -100.5 (4) \\ -0.1 (5) \\ -64.1 (5) \\ 63.4 (5) \end{array}$
B6- B6- B6- B6- B6- B6- B6-	-B11—B10—B9 -B1—B2—B7 -B1—B2—B8 -B1—B3—B8 -B1—B3—B9 -B1—B4—B9 -B1—B4—B10	$\begin{array}{c} -36.4 & (4) \\ 63.8 & (5) \\ -100.9 & (4) \\ -37.9 & (4) \\ -100.5 & (4) \\ -0.1 & (5) \\ -64.1 & (5) \\ 63.4 & (5) \\ -0.0 & (5) \end{array}$
B6- B6- B6- B6- B6- B6- B6- B6-	$\begin{array}{c} -B11 &B10 &B9 \\ -B1 &B2 &B7 \\ -B1 &B3 &B8 \\ -B1 &B3 &B9 \\ -B1 &B4 &B9 \\ -B1 &B4 &B10 \\ -B1 &B5 &B10 \end{array}$	$\begin{array}{c} -33.4 (4) \\ 63.8 (5) \\ -100.9 (4) \\ -37.9 (4) \\ -100.5 (4) \\ -0.1 (5) \\ -64.1 (5) \\ 63.4 (5) \\ -0.0 (5) \\ 100.8 (4) \end{array}$
B6	$\begin{array}{c} -B11 &B10 &B9 \\ -B1 &B2 &B7 \\ -B1 &B3 &B8 \\ -B1 &B3 &B8 \\ -B1 &B3 &B9 \\ -B1 &B4 &B9 \\ -B1 &B5 &B10 \\ -B1 &B5 &B11 \end{array}$	$\begin{array}{c} -36.4 & (4) \\ 63.8 & (5) \\ -100.9 & (4) \\ -37.9 & (4) \\ -100.5 & (4) \\ -0.1 & (5) \\ -64.1 & (5) \\ 63.4 & (5) \\ -0.0 & (5) \\ 100.8 & (4) \\ 37.6 & (4) \end{array}$
B6	$\begin{array}{c} -B11 &B10 &B9 \\ -B1 &B2 &B7 \\ -B1 &B3 &B8 \\ -B1 &B3 &B9 \\ -B1 &B4 &B9 \\ -B1 &B4 &B10 \\ -B1 &B5 &B10 \\ -B1 &B5 &B11 \\ -B2 &B3 &B8 \end{array}$	$\begin{array}{c} -36.4 & (4) \\ 63.8 & (5) \\ -100.9 & (4) \\ -37.9 & (4) \\ -100.5 & (4) \\ -0.1 & (5) \\ -64.1 & (5) \\ 63.4 & (5) \\ -0.0 & (5) \\ 100.8 & (4) \\ 37.6 & (4) \\ 100.6 & (4) \end{array}$
B6	$\begin{array}{c} -B11 \\ -B10 \\ -B2 \\ -B2 \\ -B3 \\ -B1 \\ -B3 \\ -B1 \\ -B3 \\ -B1 \\ -B5 \\ -B11 \\ -B2 \\ -B3 \\ -B$	$\begin{array}{c} -36.4 & (4) \\ 63.8 & (5) \\ -100.9 & (4) \\ -37.9 & (4) \\ -100.5 & (4) \\ -0.1 & (5) \\ -64.1 & (5) \\ 63.4 & (5) \\ -0.0 & (5) \\ 100.8 & (4) \\ 37.6 & (4) \\ 100.6 & (4) \\ 63.5 & (5) \end{array}$
B6	$\begin{array}{c} -B11 \\ -B10 \\ -B2 \\ -B1 \\ -B2 \\ -B3 \\ -B4 \\ -B1 \\ -B1 \\ -B4 \\ -B1 \\ -B1 \\ -B5 \\ -B1 \\ -B1 \\ -B5 \\ -B1 \\ -B1 \\ -B5 \\ -B1 \\ -B1 \\ -B3 \\ -B3$	$\begin{array}{c} -36.4 & (4) \\ 63.8 & (5) \\ -100.9 & (4) \\ -37.9 & (4) \\ -100.5 & (4) \\ -0.1 & (5) \\ -64.1 & (5) \\ 63.4 & (5) \\ -0.0 & (5) \\ 100.8 & (4) \\ 37.6 & (4) \\ 100.6 & (4) \\ 63.5 & (5) \\ -138.8 & (4) \end{array}$
B6	$\begin{array}{c} -B11 &B10 &B9 \\ -B1 &B2 &B7 \\ -B1 &B3 &B8 \\ -B1 &B3 &B9 \\ -B1 &B4 &B9 \\ -B1 &B4 &B10 \\ -B1 &B5 &B11 \\ -B2 &B3 &B8 \\ -B2 &B7 &B8 \\ -B2 &B7 &B11 \\ \end{array}$	$\begin{array}{c} -33.4 (4) \\ -33.4 (5) \\ -100.9 (4) \\ -37.9 (4) \\ -100.5 (4) \\ -0.1 (5) \\ -64.1 (5) \\ 63.4 (5) \\ -0.0 (5) \\ 100.8 (4) \\ 37.6 (4) \\ 100.6 (4) \\ 63.5 (5) \\ -138.8 (4) \\ -37.6 (4) \end{array}$
B6	$\begin{array}{c} -B11 \\ -B10 \\ -B2 \\ -B1 \\ -B2 \\ -B3 \\ -B4 \\ -B3 \\ -B1 \\ -B4 \\ -B1 \\ -B5 \\ -B5 \\ -B7 \\ -B1 \\ -B5 \\ -B7 \\ -B7$	$\begin{array}{c} -36.4 & (4) \\ 63.8 & (5) \\ -100.9 & (4) \\ -37.9 & (4) \\ -100.5 & (4) \\ -0.1 & (5) \\ 63.4 & (5) \\ -0.0 & (5) \\ 100.8 & (4) \\ 37.6 & (4) \\ 100.6 & (4) \\ 63.5 & (5) \\ -138.8 & (4) \\ -37.6 & (4) \\ 36.7 & (4) \end{array}$
B6	$\begin{array}{c} -B11 \\ -B10 \\ -B2 \\ -B1 \\ -B2 \\ -B3 \\ -B1 \\ -B3 \\ -B3$	$\begin{array}{c} -36.4 & (4) \\ 63.8 & (5) \\ -100.9 & (4) \\ -37.9 & (4) \\ -010.5 & (4) \\ -0.1 & (5) \\ -64.1 & (5) \\ 63.4 & (5) \\ -0.0 & (5) \\ 100.8 & (4) \\ 37.6 & (4) \\ 100.6 & (4) \\ 63.5 & (5) \\ -138.8 & (4) \\ -37.6 & (4) \\ 36.7 & (4) \\ 36.7 & (4) \\ 36.7 & (5) \\ -63.8 & (5) \\ \end{array}$
B6	$\begin{array}{c} -B11 \\ -B10 \\ -B2 \\ -B1 \\ -B2 \\ -B3 \\ -B1 \\ -B3 \\ -B1 \\ -B5 \\ -B1 \\ -B3 \\ -B3$	$\begin{array}{c} -36.4 & (4) \\ 63.8 & (5) \\ -100.9 & (4) \\ -37.9 & (4) \\ -100.5 & (4) \\ -0.1 & (5) \\ -64.1 & (5) \\ 63.4 & (5) \\ -0.0 & (5) \\ 100.8 & (4) \\ 37.6 & (4) \\ 100.6 & (4) \\ 63.5 & (5) \\ -138.8 & (4) \\ -37.6 & (4) \\ 36.7 & (4) \\ -63.8 & (5) \\ 62.5 & (5) \end{array}$
B6 =	$\begin{array}{c} -B11 \\ -B10 \\ -B2 \\ -B1 \\ -B2 \\ -B3 \\ -B1 \\ -B3 \\ -B4 \\ -B10 \\ -B1 \\ -B5 \\ -B10 \\ -B1 \\ -B5 \\ -B10 \\ -B1 \\ -B5 \\ -B11 \\ -B2 \\ -B3 \\ -B4 \\ -B9 \\ -B5 \\ -B4 \\ -B10 \\ -B10 \\ -B1 \\ -B2 \\ -B3 \\ -B4 \\ -B10 \\ -B1 \\ -B1 \\ -B2 \\ -B3 \\ -B4 \\ -B10 \\ -B1 \\ -B1 \\ -B1 \\ -B2 \\ -B3 \\ -B4 \\ -B10 \\ -B1 \\ $	$\begin{array}{c} -36.4 & (4) \\ 63.8 & (5) \\ -100.9 & (4) \\ -37.9 & (4) \\ -100.5 & (4) \\ -0.1 & (5) \\ -64.1 & (5) \\ 63.4 & (5) \\ -0.0 & (5) \\ 100.8 & (4) \\ 37.6 & (4) \\ 100.6 & (4) \\ 63.5 & (5) \\ -138.8 & (4) \\ -37.6 & (4) \\ 36.7 & (4) \\ -63.8 & (5) \\ -63.5 & (5) \\ -63.5 & (5) \\ -0.0 & (4) \\ -63.8 & (5) \\ -63.5 & (5) \\ -0.0 & (4) \\ -63.8 & (5) \\ -0.0 & (4) \\ -63.8 & (5) \\ -0.0 & (4) \\ -0.0 & (5) \\ -0.0 $
B6 -	$\begin{array}{c} -B11 \\ -B10 \\ -B2 \\ -B1 \\ -B2 \\ -B3 \\ -B1 \\ -B3 \\ -B1 \\ -B5 \\ -B10 \\ -B1 \\ -B5 \\ -B10 \\ -B1 \\ -B5 \\ -B11 \\ -B2 \\ -B3 \\ -B10 \\ -B3 \\ -B3 \\ -B10 \\ -B3 \\ -B10 \\ -B3 \\ $	$\begin{array}{c} -33.4 & (4) \\ 63.8 & (5) \\ -100.9 & (4) \\ -37.9 & (4) \\ -100.5 & (4) \\ -0.1 & (5) \\ -64.1 & (5) \\ 63.4 & (5) \\ -0.0 & (5) \\ 100.8 & (4) \\ 37.6 & (4) \\ 100.6 & (4) \\ 63.5 & (5) \\ -138.8 & (4) \\ -37.6 & (4) \\ 36.7 & (4) \\ -63.8 & (5) \\ -63.5 & (5) \\ -100.9 & (4) \\ 24.5 & (5) \\ -100.9 & (4) \\ -63.5 & (5) \\ -100.9 & (5) \\ -1$
B3-B6-B6-B6-B6-B6-B6-B6-B6-B6-B6-B6-B6-B6-	$\begin{array}{c} -B11 \\ -B10 \\ -B2 \\ -B1 \\ -B2 \\ -B3 \\ -B4 \\ -B1 \\ -B3 \\ -B3$	$\begin{array}{c} -33.4 & (4) \\ 63.8 & (5) \\ -100.9 & (4) \\ -37.9 & (4) \\ -100.5 & (4) \\ -0.1 & (5) \\ 63.4 & (5) \\ -64.1 & (5) \\ 63.4 & (5) \\ -0.0 & (5) \\ 100.8 & (4) \\ 37.6 & (4) \\ 100.6 & (4) \\ 63.5 & (5) \\ -138.8 & (4) \\ -37.6 & (4) \\ 36.7 & (4) \\ -63.8 & (5) \\ -63.8 & (5) \\ -63.5 & (5) \\ -100.9 & (4) \\ 63.4 & (5) \\ -25.6 & (2) \\ $
B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B	$\begin{array}{c} -B11 \\ -B10 \\ -B2 \\ -B1 \\ -B2 \\ -B3 \\ -B1 \\ -B1 \\ -B1 \\ -B3 \\ -B1 \\ -B1 \\ -B1 \\ -B3 \\ -B1 \\ -B1$	$\begin{array}{c} -33.4 & (4) \\ 63.8 & (5) \\ -100.9 & (4) \\ -37.9 & (4) \\ -100.5 & (4) \\ -0.1 & (5) \\ 63.4 & (5) \\ -0.0 & (5) \\ 100.8 & (4) \\ 37.6 & (4) \\ 100.6 & (4) \\ 63.5 & (5) \\ -138.8 & (4) \\ -37.6 & (4) \\ 36.7 & (4) \\ -63.8 & (5) \\ -63.5 & (5) \\ -100.9 & (4) \\ 63.4 & (5) \\ -37.0 & (4) \\ 63.4 & (5) \\ -37.0 & (4) \\ \end{array}$
B6 B6	$\begin{array}{c} -B11 &B10 &B9 \\ -B1 &B2 &B7 \\ -B1 &B3 &B8 \\ -B1 &B3 &B9 \\ -B1 &B4 &B9 \\ -B1 &B4 &B10 \\ -B1 &B5 &B10 \\ -B1 &B5 &B10 \\ -B1 &B5 &B11 \\ -B2 &B3 &B8 \\ -B2 &B7 &B8 \\ -B2 &B7 &B11 \\ -B2 &B8 &B7 \\ -B2 &B8 &B9 \\ -B5 &B4 &B9 \\ -B5 &B4 &B10 \\ -B5 &B10 &B11 \\ -B5 &B11 &B7 \\ -B1 &B11 \\ -B1 &B1 \\ -B1 &B1 \\ -B1 &B1 \\ -B1 &B1 \\ -B1 & $	$\begin{array}{c} -33.4 & (4) \\ 63.8 & (5) \\ -100.9 & (4) \\ -37.9 & (4) \\ -100.5 & (4) \\ -0.1 & (5) \\ 63.4 & (5) \\ 100.8 & (4) \\ 37.6 & (4) \\ 100.6 & (4) \\ 63.5 & (5) \\ -138.8 & (4) \\ -37.6 & (4) \\ 36.7 & (4) \\ 36.7 & (4) \\ 36.7 & (4) \\ -63.8 & (5) \\ -63.5 & (5) \\ -100.9 & (4) \\ 63.4 & (5) \\ -37.0 & (4) \\ 38.0 & (4) \\ \end{array}$
B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B	$\begin{array}{c} -B11 \\ -B10 \\ -B2 \\ -B1 \\ -B2 \\ -B3 \\ -B1 \\ -B3 \\ -B4 \\ -B3 \\ -B3 \\ -B4 \\ -B3 \\ -B10 \\ -B5 \\ -B10 \\ -B1 \\ -B5 \\ -B11 \\ -B7 \\ -B5 \\ -B11 \\ -B10 \\ -B1 $	$\begin{array}{c} -36.4 \ (4) \\ 63.8 \ (5) \\ -100.9 \ (4) \\ -37.9 \ (4) \\ -100.5 \ (4) \\ -0.1 \ (5) \\ -64.1 \ (5) \\ 63.4 \ (5) \\ 100.8 \ (4) \\ 37.6 \ (4) \\ 37.6 \ (4) \\ 36.7 \ (4) \\ 36.7 \ (4) \\ -63.8 \ (5) \\ -63.5 \ (5) \\ -100.9 \ (4) \\ 63.4 \ (5) \\ -37.0 \ (4) \\ 38.0 \ (4) \\ 138.5 \ (4) \end{array}$
B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B	$\begin{array}{c} -B11 &B10 &B9 \\ -B1 &B2 &B7 \\ -B1 &B3 &B8 \\ -B1 &B3 &B9 \\ -B1 &B4 &B9 \\ -B1 &B5 &B10 \\ -B1 &B5 &B10 \\ -B1 &B5 &B11 \\ -B2 &B3 &B8 \\ -B2 &B3 &B8 \\ -B2 &B7 &B8 \\ -B2 &B7 &B8 \\ -B2 &B7 &B8 \\ -B2 &B7 &B11 \\ -B2 &B8 &B9 \\ -B5 &B4 &B9 \\ -B5 &B10 &B9 \\ -B5 &B10 &B9 \\ -B5 &B10 &B11 \\ -B5 &B11 &B7 \\ -B5 &B11 &B7 \\ -B5 &B11 &B10 \\ -B7 &C20 &B8 \end{array}$	$\begin{array}{c} -36.4 & (4) \\ 63.8 & (5) \\ -100.9 & (4) \\ -37.9 & (4) \\ -100.5 & (4) \\ -0.1 & (5) \\ -64.1 & (5) \\ 63.4 & (5) \\ -0.0 & (5) \\ 100.8 & (4) \\ 37.6 & (4) \\ 100.6 & (4) \\ 63.5 & (5) \\ -138.8 & (4) \\ -37.6 & (4) \\ 36.7 & (4) \\ 36.7 & (4) \\ -63.8 & (5) \\ -100.9 & (4) \\ 63.4 & (5) \\ -37.0 & (4) \\ 38.0 & (4) \\ 138.5 & (4) \\ -103.7 & (4) \end{array}$
B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B	$\begin{array}{c} -B11 &B10 &B9 \\ -B1 &B2 &B7 \\ -B1 &B3 &B8 \\ -B1 &B3 &B9 \\ -B1 &B4 &B10 \\ -B1 &B5 &B11 \\ -B2 &B3 &B8 \\ -B2 &B3 &B8 \\ -B2 &B7 &B8 \\ -B2 &B7 &B8 \\ -B3 &B7 \\ -B2 &B8 &B7 \\ -B2 &B8 &B7 \\ -B3 &B11 \\ -B5 &B10 &B11 \\ -B5 &B11 &B7 \\ -B5 &B11 &B10 \\ -B7 &C20 &B8 \\ -B7 &C20 &B9 \\ \end{array}$	$\begin{array}{c} -33.4 \ (4) \\ 63.8 \ (5) \\ -100.9 \ (4) \\ -37.9 \ (4) \\ -100.5 \ (4) \\ -0.1 \ (5) \\ -64.1 \ (5) \\ 63.4 \ (5) \\ 100.8 \ (4) \\ 37.6 \ (4) \\ 100.6 \ (4) \\ 100.6 \ (4) \\ 63.5 \ (5) \\ -138.8 \ (4) \\ -37.6 \ (4) \\ 36.7 \ (4) \\ -63.8 \ (5) \\ -100.9 \ (4) \\ 63.4 \ (5) \\ -37.0 \ (4) \\ 38.0 \ (4) \\ 138.5 \ (4) \\ -103.7 \ (4) \\ -67.1 \ (5) \end{array}$
B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B	$\begin{array}{c} -B11 \\ -B10 \\ -B2 \\ -B1 \\ -B2 \\ -B3 \\ -B4 \\ -B5 \\ -B1 \\ -B4 \\ -B1 \\ -B5 \\ -B1 \\ -B4 \\ -B1 \\ -B5 \\ -B1 \\ -B5 \\ -B1 \\ -B3 \\ -B3$	$\begin{array}{c} -33.4 & (4) \\ 63.8 & (5) \\ -100.9 & (4) \\ -37.9 & (4) \\ -100.5 & (4) \\ -0.1 & (5) \\ 63.4 & (5) \\ -0.0 & (5) \\ 100.8 & (4) \\ 37.6 & (4) \\ 100.6 & (4) \\ 63.5 & (5) \\ -138.8 & (4) \\ -37.6 & (4) \\ 36.7 & (4) \\ 36.7 & (4) \\ 36.7 & (4) \\ -63.8 & (5) \\ -63.8 & (5) \\ -100.9 & (4) \\ 63.4 & (5) \\ -37.0 & (4) \\ 38.0 & (4) \\ 138.5 & (4) \\ -103.7 & (4) \\ -67.1 & (5) \\ 2.8 & (5) \end{array}$
B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B	$\begin{array}{c} -B11 &B10 &B9 \\ -B1 &B2 &B7 \\ -B1 &B3 &B8 \\ -B1 &B3 &B9 \\ -B1 &B4 &B9 \\ -B1 &B5 &B10 \\ -B1 &B5 &B10 \\ -B1 &B5 &B10 \\ -B1 &B5 &B11 \\ -B2 &B3 &B8 \\ -B2 &B7 &B8 \\ -B2 &B7 &B8 \\ -B2 &B8 &B9 \\ -B5 &B4 &B9 \\ -B5 &B4 &B9 \\ -B5 &B10 &B11 \\ -B5 &B11 &B7 \\ -B5 &B11 &B10 \\ -B7 &C20 &B8 \\ -B7 &C20 &B10 \\ -B7 &C20 &B11 \\ -B7 &B1 \\ -B7 &$	$\begin{array}{c} -33.4 & (4) \\ 63.8 & (5) \\ -100.9 & (4) \\ -37.9 & (4) \\ -100.5 & (4) \\ -0.1 & (5) \\ 63.4 & (5) \\ 100.8 & (4) \\ 37.6 & (4) \\ 100.6 & (4) \\ 63.5 & (5) \\ -138.8 & (4) \\ -37.6 & (4) \\ 36.7 & (4) \\ 36.7 & (4) \\ 36.7 & (4) \\ 36.7 & (4) \\ 36.7 & (4) \\ 36.7 & (4) \\ 36.7 & (4) \\ 36.7 & (4) \\ 36.7 & (4) \\ 36.7 & (4) \\ 38.0 & (4) \\ 138.5 & (4) \\ -103.7 & (4) \\ -67.1 & (5) \\ 2.8 & (5) \\ 39.6 & (4) \end{array}$
B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B6 B	$\begin{array}{c} -B11 &B10 &B9 \\ -B1 &B2 &B7 \\ -B1 &B3 &B8 \\ -B1 &B3 &B8 \\ -B1 &B3 &B9 \\ -B1 &B4 &B9 \\ -B1 &B5 &B10 \\ -B1 &B5 &B10 \\ -B1 &B5 &B11 \\ -B2 &B3 &B8 \\ -B2 &B7 &B8 \\ -B2 &B7 &B11 \\ -B2 &B8 &B9 \\ -B5 &B4 &B9 \\ -B5 &B10 &B11 \\ -B5 &B11 &B7 \\ -B5 &B11 &B7 \\ -B5 &B11 &B10 \\ -B7 &C20 &B8 \\ -B7 &C20 &B10 \\ -B7 &C20 &B11 \\ -B7 &B2 &B8 \end{array}$	$\begin{array}{c} -36.4 & (4) \\ 63.8 & (5) \\ -100.9 & (4) \\ -37.9 & (4) \\ -100.5 & (4) \\ -0.1 & (5) \\ 63.4 & (5) \\ 100.8 & (4) \\ 37.6 & (4) \\ 100.6 & (4) \\ 63.5 & (5) \\ -138.8 & (4) \\ -37.6 & (4) \\ 36.7 & (4) \\ 36.7 & (4) \\ 36.7 & (4) \\ -63.8 & (5) \\ -63.5 & (5) \\ -100.9 & (4) \\ 38.0 & (4) \\ 138.5 & (4) \\ -103.7 & (4) \\ 38.0 & (4) \\ 138.5 & (4) \\ -103.7 & (4) \\ 38.0 & (4) \\ 138.8 & (4) \\ \end{array}$
B6	$\begin{array}{c} -B11 &B10 &B9 \\ -B1 &B2 &B7 \\ -B1 &B3 &B8 \\ -B1 &B3 &B9 \\ -B1 &B4 &B9 \\ -B1 &B4 &B10 \\ -B1 &B5 &B10 \\ -B1 &B5 &B10 \\ -B1 &B5 &B11 \\ -B2 &B3 &B8 \\ -B2 &B7 &B8 \\ -B2 &B7 &B8 \\ -B2 &B8 &B9 \\ -B5 &B4 &B10 \\ -B5 &B10 &B11 \\ -B5 &B11 &B7 \\ -B5 &B11 &B7 \\ -B5 &B11 &B7 \\ -B5 &B11 &B10 \\ -B7 &C20 &B11 \\ -B7 &B2 &B8 \\ -B7 &B8 &B9 \\ -B5 &B8 &B9 \\ -B7 &B8 &B8 \\ -B7$	$\begin{array}{c} -36.4 & (4) \\ 63.8 & (5) \\ -100.9 & (4) \\ -37.9 & (4) \\ -100.5 & (4) \\ -0.1 & (5) \\ -64.1 & (5) \\ 63.4 & (5) \\ 100.8 & (4) \\ 37.6 & (4) \\ 100.6 & (4) \\ 63.5 & (5) \\ -138.8 & (4) \\ -37.6 & (4) \\ 36.7 & (4) \\ 36.7 & (4) \\ 36.7 & (4) \\ -37.6 & (4) \\ 36.7 & (4) \\ -63.8 & (5) \\ -100.9 & (4) \\ 63.4 & (5) \\ -37.0 & (4) \\ 38.0 & (4) \\ 138.5 & (4) \\ -103.7 & (4) \\ 38.0 & (4) \\ 138.5 & (4) \\ -67.1 & (5) \\ 2.8 & (5) \\ 39.6 & (4) \\ 138.8 & (4) \\ 64.0 & (5) \end{array}$

B6—B11—C20—B7
B6-B11-C20-B8
B6—B11—C20—B9
B6—B11—C20—B10
B6 - B11 - B5 - B10
B6—B11—B7—B8
B6—B11—B10—B9
B7—C20—B8—B9
B7—C20—B9—B8
B7-C20-B9-B10
B7-C20-B10-B9
B7-C20-B10-B11
B7-C20-B11-B10
B7—B2—B3—B8
B7—B2—B3—B9
B7 - B2 - B6 - B11
B7-B2-B8-B9
B7—B6—B2—B8
B7 - B6 - B5 - B10
B7—B6—B5—B11
B7—B6—B11—B10
B7—B8—C20—B9
B7—B8—C20—B10
B7—B8—C20—B11
B7—B8—B3—B9
B7—B8—B9—B10
B7—B11—C20—B8
B7—B11—C20—B9
B7-B11-C20-B10
B7-B11-B5-B10
B7-B11-B10-B9
B8-C20-B7-B11
B8-C20-B9-B10 B8-C20-B10 B0
B8-C20-B10-B9 B8-C20-B10-B11
B8-C20-B10-B11 B8-C20-B11-B10
$B_{0} = C_{20} = B_{11} = B_{10}$
$B_{0} = B_{2} = B_{0} = B_{0}$
$B_{0} = B_{2} = B_{0} = B_{11}$ $B_{0} = B_{11} = B_{11}$
B8-B3-B4-B9
B8-B3-B4-B10
B8 = B3 = B9 = B10
B8 - B7 - C20 - B9
B8 - B7 - C20 - B10
B8—B7—C20—B11
B8—B7—B6—B11
B8—B7—B11—B10
B8—B9—C20—B10
B8—B9—C20—B11
B8—B9—B4—B10
B8—B9—B10—B11
B9—C20—B7—B11
B9—C20—B10—B11
B9—C20—B11—B10
B9—B3—B4—B10
B9 - B4 - B5 - B10
B9 - B4 - B5 - B11
B9 - B4 - B10 - B11
B9 - B8 - C20 - B10
B9 - B8 - C20 - B11
B9—B8—B7—B11
B9 - B10 - C20 - B11
B9 - B10 - B5 - B11
B10-C20-B7-B11
B10—B4—B5—B11
B10—B5—B6—B11
B10—B9—C20—B11

-39.0(4)

-3.3(5)

67.3(5)

103.5(4)

-138.5(4)

102.2(5)

-63.3(5)

142.6(4)

-36.2(4)

106.9(5)

37.0(4)

37.6(4)

0.5(5)

36.7(4)

-100.5(4)

-36.6(4)

-0.7(5)-37.8 (4)

99.9 (4)

-142.6(4)

-106.5(5)

-36.1(4)

100.7(4)

0.4(5)

35.7(4)

106.3(5)

142.5(4)

-100.5(4)

-143.3(4)

143.1(4)

-36.4(4)

106.5(5)

-106.8(4)

-37.1(4)

101.2(4)

37.9 (4)

0.4(5)

36.6(4)

106.5(4)

143.3(4)-101.3(4)

0.3(5)

-143.1 (4)

-106.8(5)

100.5(4)

-0.2(5)

-106.6(5)

142.9(4)

-36.2(4)

-37.5(4)

37.3 (4)

-0.4(5)-100.5(4)

36.1(4)

106.4(5)

-0.4(5)

-142.9(4)

100.4(4)

-36.8(4)

-37.7(4)

37.1(4)

36.3(4)

-100.0(4)

0.2(5)

-0.0(5)

-105.9(4)

-142.5(4)

PREVIEW (FM)

Table S4. Contact distances (\mathring{A})						
$Br4 \cdots C5$	3.489(4)	$Cl2 \cdot \cdot \cdot Cl2^V$	3.457(3)			
$Br4 \cdot \cdot \cdot C6$	3.550(4)	$Cl2 \cdot \cdot \cdot C14$	3.596(6)			
$Br5 \cdots C4^{i}$	3.403(4)	$O1 \cdot \cdot \cdot B11^{vi}$	3.417(7)			
Br7···C11 ⁱⁱ	3.29 (2)	$O1 \cdots C20^{vi}$	3.437 (6)			
$Br7 \cdot \cdot \cdot C51^{iii}$	3.31 (3)	$O1 \cdots C12^{vii}$	3.489 (7)			
$Br7 \cdot \cdot \cdot C12^{iv}$	3.46(3)	$O1 \cdot \cdot \cdot C7^{vii}$	3.526~(6)			
Symmetry codes: (i) $\frac{3}{2} - x, \frac{1}{2} + y, z$; (ii) $\frac{1}{2} - x, \frac{1}{2} + y, z$; (iii) $1 - x, 1 - y, -z$; (iv) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$; (v) $2 - x, 1 - y, -z$; (vi) $1 - x, y - \frac{1}{2}, \frac{1}{2} - z$; (vii) $x - \frac{1}{2}, y, \frac{1}{2} - z$.						



Figure 1. Molecular structure of the cation of $(C_{14}H_{19}O_2)^+(CH_6B_{11}Br_6)^- \bullet C_2H_4Cl_2$ with labelling of selected atoms. Anisotropic displacement ellipsoids show 30% probability levels. Hydrogen atoms are drawn as circles with small radii.



Figure 2. Molecular structure of the anion of $(C_{14}H_{19}O_2)^+(CH_6B_{11}Br_6)^- \bullet C_2H_4Cl_2$ with labelling of selected atoms. Anisotropic displacement ellipsoids show 30% probability levels. Hydrogen atoms are drawn as circles with small radii. The low-ocupancy site Br7 is not shown.



Figure 3. Unit cell packing diagram of $(C_{14}H_{19}O_2)^+(CH_6B_{11}Br_6)^- \bullet C_2H_4Cl_2$ projected down the *a* axis. Hydrogen atoms and the low-ocupancy site Br7 are not shown.

 $31~{\rm Mar}$ 2006

Crystal structure of $(C_{14}H_{19}O_2)^+(B(C_6F_5)_4)^-$ -web0602

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Abstract

The crystal structure of $(C_{14}H_{19}O_2)^+(B(C_6F_5)_4)^-$ is reported.

Comment

The space group is noncentrosymmetric but the anomolous dispersion terms are very small for all elements in the structure, so the absolute structure of the crystal can not be determined in this experiment. Consequently Friedel-pair reflections have been averaged and the Flack parameter has not been refined. The space group is not enantiomorphic so the compound is present as a racemate within the crystal structure.

The crystallographic asymmetric unit consists of one $(C_{14}H_{19}O_2)^+$ cation and one $(B(C_6F_5)_4)^-$ anion.

The largest peaks in the final difference map are all of near-equal intensity and have no chemical significance.

Experimental

The compound was prepared by SBL and recrystallized from dichloroethane. The sample ID is RDW02.

Crystal data $C_{14}H_{19}O_2^+.C_{24}BF_{20}^-$ Cell parameters from 29935 reflections $M_r = 898.34$ $\theta = 3 - 27^{\circ}$ $\mu = 0.173 \text{ mm}^{-1}$ Monoclinic T = 200 KCca = 11.9549(2) ÅPlate b = 17.4980(4) Å Red c = 17.3301(3) Å 0.31 \times 0.20 \times 0.07 mm $\beta = 98.7693 \, (13)^{\circ}$ Crystal source: local $V = 3582.85 (12) \text{ Å}^3$ Z = 4 $D_x = 1.665 \text{ Mg m}^{-3}$ D_m not measured Mo $K\alpha$ radiation $\lambda = 0.71073 \text{ Å}$ Data collection Nonius KappaCCD diffractometer 3377 reflections with $I > 2.0\sigma(I)$ φ and ω scans with CCD $R_{\rm int} = 0.032$ Absorption correction: multi-scan Denzo/Scalepack (Otwinowski $\theta_{\rm max} = 27.5^{\circ}$ & Minor, 1997) $h = -15 \rightarrow 15$ $k=-22\rightarrow 22$ $T_{\rm min} = 0.87, T_{\rm max} = 0.99$ $l = -22 \rightarrow 22$ 38073 measured reflections 4113 independent reflections Refinement Method= Modified Sheldrick $w=1/[\sigma^2(F^2) +$ Refinement on ${\cal F}^2$ $(0.05P)^2 + 1.28P$], R(F) = 0.0316where $P = (\max(F_o^2, 0) + 2F_c^2)/3$ $wR(F^2) = 0.0733$ $(\Delta/\sigma)_{\rm max} = 0.038298$ S = 0.8816 $\Delta \rho_{\rm max} = 0.24 \ {\rm e} \ {\rm \AA}^{-3}$ 4104 reflections $\Delta \rho_{\rm min} = -0.23 \ {\rm e} \ {\rm \AA}^{-3}$ 607 parameters Only coordinates of H atoms refined Extinction correction: none Scattering factors from International Tables

Vol C 4.2.6.8 and 6.1.1.4

	Table 1. Selected geom	etric parameters (Å, °)	
F102—C102	1.354(3)	C7—C8	1.518(4)
F103—C103	1.356(3)	C8—C9	1.515(4)
F104—C104	1.352(3)	C9—C13	1.518(5)
F105— $C105$	1.346(3)	C9—C14	1.511(5)
F106—C106	1.356(3)	C101—C102	1.390(4)
F202—C202	1.360(3)	C101—C106	1.383(4)
F203—C203	1.345(3)	C101—B1	1.656(4)
F204— $C204$	1.343(3)	C102—C103	1.382(4)
F205 - C205	1.349(3)	C103—C104	1.363(4)
F206—C206	1.355(3)	C104 - C105	1.373(4)
F302—C302	1.358(3)	C105—C106	1.373(3)
F303—C303	1.353(3)	C201 - C202	1.387(4)
F304—C304	1.345(4)	C201 - C206	1.394(3)
F305—C305	1.347(3)	C201—B1	1.662(4)
F306—C306	1.365(3)	C202 - C203	1.380(4)
F402—C402	1.353(3)	C203 - C204	1.375(4)
F403—C403	1.342(3)	C204 - C205	1.374(4)
F404—C404	1.343(3)	C205 - C206	1.379(4)
F405 - C405	1.354(3)	C301—C302	1.388(4)
F406—C406	1.358(3)	C301—C306	1.391(4)
O1—C4	1.214(3)	C301—B1	1.659(4)
O2—C1	1.282(3)	C302—C303	1.374(4)
O2—C9	1.520(4)	C303—C304	1.371(4)
C1-C2	1.455(4)	C304 - C305	1.378(4)
C1—C6	1.447(4)	C305 - C306	1.374(4)
C2—C3	1.355(4)	C401 - C402	1.388(3)
C2—C10	1.499(4)	C401—C406	1.386(4)
C3—C4	1.488(4)	C401—B1	1.653(4)
C3—C11	1.493(4)	C402—C403	1.388(4)
C4-C5	1.491(4)	C403—C404	1.370(4)
C5-C6	1.355(4)	C404-C405	1.365(4)
C5—C12	1.495(4)	C405 - C406	1.379(4)
C6-C7	1.505(4)		
C1—O2—C9	123.5(2)	C1— $C2$ — $C10$	117.4(2)
O2— $C1$ — $C2$	113.2(2)	C3—C2—C10	124.9(3)
O2—C1—C6	121.8(2)	C2—C3—C4	118.8(3)
C2— $C1$ — $C6$	125.0(2)	C2—C3—C11	124.1 (3)
C1— $C2$ — $C3$	117.7(2)	C4—C3—C11	117.1(2)

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C3—C4—O1	119.9(3)	F202-C202-C203	114.3(2)
C3-C4-C5	120.6(2)	C201 - C202 - C203	125.0(2)
O1—C4—C5	119.5(3)	F203—C203—C202	120.7(2)
C4— $C5$ — $C6$	119.4(2)	F203—C203—C204	119.6(3)
C4— $C5$ — $C12$	117.7(3)	C202—C203—C204	119.7(3)
C6-C5-C12	122.9(3)	F204-C204-C203	120.7(3)
C1-C6-C5	117.2(3)	F204-C204-C205	120.8(3)
C1—C6—C7	119.0(2)	C203 - C204 - C205	118.5(3)
C5-C6-C7	123.7(2)	F205-C205-C204	119.7(3)
C6—C7—C8	110.9(2)	F205-C205-C206	120.6(3)
C7—C8—C9	111.4(2)	C204-C205-C206	119.7(3)
O2—C9—C8	107.2(2)	F206-C206-C201	119.2(2)
O2—C9—C13	102.3~(3)	F206-C206-C205	115.9(2)
C8—C9—C13	112.8(3)	C201 - C206 - C205	124.9(3)
O2—C9—C14	106.0(2)	C302 - C301 - C306	112.4(2)
C8—C9—C14	114.0(3)	C302—C301—B1	127.9(2)
C13—C9—C14	113.3(3)	C306—C301—B1	119.3(2)
C102-C101-C106	112.9(2)	F302—C302—C301	120.3(2)
C102—C101—B1	127.9(2)	F302—C302—C303	115.3(2)
C106—C101—B1	118.9(2)	C301 - C302 - C303	124.4(2)
F102—C102—C101	121.1(2)	F303—C303—C302	120.7(2)
F102-C102-C103	115.3(2)	F303—C303—C304	118.9(3)
C101-C102-C103	123.6(2)	C302 - C303 - C304	120.4(2)
F103—C103—C102	120.3(2)	F304-C304-C303	121.0(3)
F103—C103—C104	119.4(2)	F304-C304-C305	120.7(3)
C102—C103—C104	120.3(2)	C303 - C304 - C305	118.3(3)
F104-C104-C103	120.8(2)	F305—C305—C304	119.9(3)
F104-C104-C105	120.4(2)	F305—C305—C306	120.9(3)
C103-C104-C105	118.8(2)	C304 - C305 - C306	119.2~(2)
F105-C105-C104	120.0(2)	F306—C306—C301	119.0(2)
F105-C105-C106	120.9(2)	F306—C306—C305	115.6(2)
C104-C105-C106	119.0(2)	C301 - C306 - C305	125.3(2)
F106—C106—C101	119.2(2)	C402-C401-C406	113.4(2)
F106-C106-C105	115.5(2)	C402 - C401 - B1	126.3(2)
C101-C106-C105	125.3(2)	C406 - C401 - B1	119.9(2)
C202—C201—C206	112.3(2)	F402-C402-C401	121.2~(2)
C202—C201—B1	127.3(2)	F402-C402-C403	114.7(2)
C206—C201—B1	119.8(2)	C401-C402-C403	124.0(2)
F202—C202—C201	120.7(2)	C402-C403-F403	120.5(2)

PREVIEW (FO)

C402-C403-C404	119.5(2)	F406 - C406 - C405	116.3(2)
F403—C403—C404	120.0(2)	C401 - C406 - C405	124.2(2)
F404—C404—C403	120.4(3)	C201—B1—C301	115.6(2)
F404-C404-C405	120.7(3)	C201—B1—C101	112.1 (2)
C403 - C404 - C405	118.9(2)	C301—B1—C101	100.54 (19)
F405-C405-C404	120.1(3)	C201—B1—C401	$101.34\ (19)$
F405-C405-C406	120.0(3)	C301 - B1 - C401	112.8(2)
C404-C405-C406	120.0(3)	C101—B1—C401	115.0(2)
F406—C406—C401	119.5(2)		

H atoms were included at calculated positions with methyl H atoms oriented to best-match peaks in difference electron density maps. Restraints were imposed on distances and angles involving H atoms as they were refined positionally.

Data collection: *COLLECT* (Nonius BV, 1997). Cell refinement: Denzo/Scalepack . Data reduction: Denzo/Scalepack (Otwinowski & Minor, 1997). Program(s) used to solve structure: *SIR*92 (Altomare *et al.* 1994). Program(s) used to refine structure: *CRYSTALS* (Watkin *et al.*2003). Molecular graphics: *ORTEP*–II (Johnson 1976) in teXsan (MSC, 1992–1997) . Software used to prepare material for publication: *CRYSTALS*.

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Supplementary data

$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Table S1. Fractional atomic coordinates and equivalent isotropic displacement parameters (\mathring{A}^2)					
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		$U_{ m ed}$	$_{\mathbf{q}} = (1/3)\Sigma_i \Sigma_j U^{ij} a^i a^j$	$\mathbf{a}_i.\mathbf{a}_j.$		
F102 0.0921 (14) 0.64485 ($\hat{9}$) 0.3427 ($\hat{9}$) 0.0489 \mathbf{x} F103 -0.0144 (16) 0.16820 (10) 0.16726 ($\hat{9}$) 0.0660 F104 0.07215 (15) 0.24883 (11) 0.10736 ($\hat{9}$) 0.0617 F106 0.34485 (13) 0.43622 ($\hat{9}$) 0.31330 ($\hat{9}$) 0.0513 F202 0.15873 (14) 0.42113 ($\hat{9}$) 0.3293 (10) 0.0613 F203 0.16846 (17) 0.30442 (12) 0.67722 (12) 0.0711 F204 0.3120 (13) 0.49623 ($\hat{8}$) 0.43871 ($\hat{10}$) 0.0466 F303 0.7107 (15) 0.55768 (11) 0.38970 (12) 0.0666 F304 0.71018 (17) 0.69944 (12) 0.3283 (13) 0.0717 F304 0.7018 (17) 0.69944 (12) 0.32871 (10) 0.0611 F403 0.29747 (15) 0.7788 ($\hat{9}$ 0.62940 ($\hat{9}$) 0.0511 F404 0.7666 (17) 0.7288 (13) 0.49071 (12) 0.0687 F404 0.7667 (2) 0.86385 (11) 0.3712 (16)		x	y	z	$U_{ m eq}$	
F103 -0.0144 (16) 0.04105 (11) 0.18820 (10) 0.0660 F104 0.0721 (15) 0.52683 (11) 0.1073 (8) 0.0652 F105 0.24729 (15) 0.4592 (9) 0.31330 (9) 0.0645 F202 0.15873 (14) 0.44916 (13) 0.0665 F204 0.31250 (18) 0.30448 (12) 0.62722 (12) 0.06191 F205 0.44988 (16) 0.42782 (12) 0.66491 (10) 0.0191 F206 0.44446 (13) 0.46628 (8) 0.35700 (12) 0.0673 F302 0.53120 (13) 0.57786 (11) 0.38030 (12) 0.06661 F303 0.71075 (15) 0.57786 (11) 0.38031 (12) 0.06661 F304 0.71076 (15) 0.77786 (11) 0.38031 (12) 0.066161 F305 0.22747 (15) 0.77788 (9) 0.44940 (10) 0.0411 F403 0.22747 (15) 0.77788 (9) 0.44904 (10) 0.0487 F404 0.07662 (2) 0.86864 (15) 0.273514 (1) 0.0372 C2 0.16612 (16) 0.37242 (1	F102	0.09321(14)	0.66485 (9)	0.33427(9)	0.0489	
F1040.07215 (15)0.26893 (11)0.10173 (0)0.0662F1050.24729 (15)0.43652 (10)0.16726 (0)0.0517F1060.34485 (13)0.43522 (9)0.31330 (9)0.0513F2020.15873 (14)0.30442 (10)0.48916 (13)0.0665F2030.16846 (17)0.30442 (10)0.46916 (13)0.0613F2040.31250 (18)0.34488 (16)0.42722 (12)0.0711F2050.44488 (16)0.42782 (12)0.66491 (10)0.019F3030.7107 (15)0.54968 (0)0.56820 (0)0.0449F3030.70118 (17)0.69944 (12)0.3283 (13)0.0717F3040.70118 (17)0.69944 (12)0.3283 (13)0.0666F3060.32947 (15)0.77285 (11)0.36933 (12)0.0666F3060.32947 (15)0.77285 (12)0.63935 (11)0.0671F4040.07666 (17)0.7528 (12)0.63935 (11)0.0671F405-0.40463 (15)0.45131 (13)0.54679 (11)0.0648C10.1733 (2)0.86285 (13)0.49917 (12)0.0582C20.3664 (15)0.42978 (15)0.23541 (15)0.3374C40.4766 (2)0.8985 (15)0.27354 (14)0.3374C40.4766 (2)0.8987 (15)0.42978 (15)0.0430C50.2819 (2)0.8636 (15)0.42978 (15)0.0430C60.2816 (2)0.9897 (15)0.42978 (15)0.930C10.1765 (3)0.8536 (15)0.2397 (17)<	F103	-0.00144(16)	0.64108 (11)	0.18820 (10)	0.0600	
F1060.24729 (15)0.43652 (10)0.16726 (9)0.0617F1060.34845 (13)0.45022 (9)0.31330 (9)0.0613F2030.15873 (14)0.42113 (9)0.39233 (10)0.0613F2040.31250 (18)0.30448 (12)0.42816 (13)0.4691 (10)0.06119F2050.4498 (16)0.42782 (12)0.66491 (10)0.0619F2060.44446 (13)0.4668 (9)0.56820 (9)0.0442F3030.71073 (15)0.55768 (11)0.32787 (12)0.0073F3040.70173 (15)0.55768 (11)0.32787 (12)0.0666F3030.71073 (15)0.5766 (11)0.32883 (13)0.0717F3050.50263 (18)0.77665 (11)0.32878 (10)0.0661F4020.39924 (13)0.70260 (9)0.55719 (10)0.04151F4030.29747 (15)0.44931 (13)0.54799 (11)0.0670F405-0.04063 (15)0.44931 (13)0.54679 (11)0.0670F4060.01736 (2)0.46258 (13)0.49917 (12)0.0682C20.16612 (16)0.30865 (15)0.2333 (14)0.3085C30.0756 (2)0.451510.2333 (14)0.3072C40.1756 (3)0.46491 (12)0.3288 (15)0.4141C50.2819 (2)0.866150.42747 (16)0.4432C10.1780 (2)0.3645 (15)0.42747 (16)0.4432C20.0768 (2)0.45150.42874 (16)0.4432C30.0776 (2)0.3724 (2)0.46274 (1	F104	0.07215(15)	0.52693(11)	0.10173(9)	0.0562	
F1060.34485 (13)0.45922 (9)0.31330 (9)0.0615F2030.10846 (17)0.30442 (10)0.43928 (10)0.0665F2040.31250 (18)0.30443 (12)0.62722 (12)0.0711F2050.44988 (16)0.42782 (12)0.06491 (10)0.0019F2060.4446 (13)0.45680 (9)0.56820 (9)0.0449F3020.51120 (13)0.46923 (8)0.438770 (12)0.0573F3040.70118 (17)0.69944 (12)0.32283 (13)0.0717F3050.5263 (18)0.77865 (11)0.30803 (12)0.0666F4020.33924 (13)0.70786 (11)0.36830 (12)0.0666F4030.29747 (15)0.77856 (12)0.62940 (9)0.6511F4040.07569 (17)0.75258 (12)0.63933 (11)0.0671F405-0.04065 (15)0.46931 (13)0.54679 (11)0.0648F4060.06188 (13)0.6186 (9)0.44901 (10)0.0487C20.16612 (16)0.90667 (12)0.20353 (15)0.0385C30.0756 (2)0.85155 (15)0.29733 (14)0.0372C20.1780 (2)0.8528 (15)0.42971 (15)0.0430C50.2816 (2)0.90412 (14)0.32846 (15)0.0412C40.1756 (3)0.86386 (15)0.42971 (15)0.0403C50.2816 (2)0.90412 (2)0.37242 (16)0.0412C60.2816 (2)0.93042 (12)0.42926 (15)0.0309C70.3313 (2)0.3645 (15)0.42971 (15) <td>F105</td> <td>0.24729(15)</td> <td>0.43652(10)</td> <td>0.16726(9)</td> <td>0.0517</td>	F105	0.24729(15)	0.43652(10)	0.16726(9)	0.0517	
F2020.15873 (14)0.42113 (9)0.39293 (10)0.0513F2030.16846 (17)0.30448 (12)0.48916 (13)0.04891 (10)0.0011F2050.4498 (16)0.42782 (12)0.6491 (10)0.0019F2060.44446 (13)0.45608 (9)0.56520 (9)0.0449F3020.51120 (13)0.49623 (8)0.43591 (9)0.0426F3030.71073 (15)0.55768 (11)0.38870 (12)0.0666F3060.52240 (14)0.72661 (19)0.35751 (10)0.0511F3050.50263 (18)0.77686 (11)0.38935 (11)0.0677F4040.0759 (17)0.77258 (12)0.63335 (11)0.0670F405-0.04063 (15)0.44391 (13)0.54679 (11)0.0648F4060.0618 (13)0.56186 (9)0.44904 (9)0.0457C10.1703 (2)0.88258 (13)0.49917 (12)0.0682C20.1686 (12)0.30851 (15)0.33736 (14)0.0372C30.0756 (2)0.8499 (15)0.3734 (16)0.0411C40.1756 (3)0.86286 (15)0.29338 (15)0.0385C30.0756 (2)0.8499 (15)0.3724 (16)0.0411C40.1756 (3)0.8638 (15)0.4274 (16)0.0412C60.2816 (2)0.9041 (2)0.16338 (13)0.0552C10.0756 (2)0.9219 (2)0.2066 (18)0.0552C20.786 (2)0.9349 (15)0.4274 (16)0.0412C50.2816 (2)0.9345 (12)0.1638 (16)<	F106	0.34485(13)	0.45922(9)	0.31330(9)	0.0459	
F2030.16846 (17)0.30442 (10)0.48916 (13)0.0665F2040.31250 (18)0.30448 (12)0.62722 (12)0.0711F2050.44988 (16)0.42782 (12)0.66491 (10)0.0619F3030.71073 (15)0.45626 (8)0.45826 (9)0.0442F3030.70118 (17)0.69044 (12)0.32870 (12)0.0673F3040.70118 (17)0.69044 (12)0.3283 (13)0.0707F3050.50263 (18)0.77665 (11)0.30803 (12)0.0666F3060.32140 (14)0.72061 (9)0.35751 (10)0.0511F4020.39924 (13)0.70280 (8)0.62940 (9)0.0511F4030.077569 (17)0.75288 (12)0.63935 (11)0.0670F4040.077590 (17)0.75288 (12)0.63935 (11)0.0671F405-0.04063 (15)0.6493 (13)0.54679 (11)0.0648F4060.06188 (13)0.6186 (9)0.44904 (10)0.0487C20.16612 (16)0.00667 (12)0.20085 (10)0.0466C10.1736 (2)0.82545 (15)0.29735 (15)0.0385C30.0756 (2)0.84969 (15)0.32742 (16)0.0411C40.1756 (3)0.86386 (15)0.42978 (15)0.0430C50.2816 (2)0.90412 (14)0.32586 (15)0.0407C60.2816 (2)0.93042 (12)0.29278 (15)0.0432C50.2816 (2)0.93042 (12)0.46325 (19)0.6632C60.2816 (2)0.93042 (12)0.29278 (1	F202	0.15873(14)	0.42113(9)	0.39293(10)	0.0513	
F2040.31250 (18)0.30448 (12)0.62722 (12)0.0711F2050.4488 (16)0.24728 (12)0.66491 (10)0.6619F3020.53120 (13)0.49022 (8)0.43510 (9)0.0426F3030.71073 (15)0.55768 (11)0.38770 (12)0.0573F3040.70118 (17)0.69944 (12)0.32283 (13)0.0717F3050.50263 (18)0.77965 (11)0.38803 (12)0.0666F3060.32140 (14)0.72061 (9)0.35751 (10)0.0453F4020.39294 (13)0.70280 (9)0.52790 (10)0.0453F4030.29747 (15)0.77788 (9)0.62240 (9)0.0451F4040.0766 (917)0.75258 (12)0.436479 (11)0.06670F405-0.04063 (15)0.64391 (13)0.44679 (11)0.0648F4060.06188 (13)0.66186 (9)0.44004 (10)0.0487C10.1703 (2)0.88258 (13)0.49917 (12)0.0582C20.0766 (2)0.85155 (15)0.27335 (14)0.0372C30.0756 (2)0.84090 (15)0.37242 (16)0.0411C40.1766 (3)0.88897 (15)0.40274 (16)0.0429C50.2819 (2)0.93412 (2)0.20285 (15)0.0407C70.3813 (2)0.9349 (12)0.32357 (13)0.0447C80.3702 (2)0.9219 (2)0.20664 (18)0.0452C90.2563 (2)0.9414 (2)0.32357 (13)0.0427C140.2329 (3)0.9224 (2)0.16335 (14)0	F203	0.16846 (17)	0.30442 (10)	0.48916(13)	0.0665	
F205 0.4498 (6) 0.42782 (2) 0.66491 (10) 0.0619 F206 0.4444 (13) 0.49623 0.3591 0.56220 0.0426 F303 0.7107 (15) 0.5576 $11)$ 0.38770 0.0273 F304 0.7018 0.7776 0.39283 0.312 0.0666 F306 0.32140 0.72061 0.35751 0.05671 F402 0.39924 0.77280 0.32790 0.0511 F403 0.29747 0.7788 0.62240 0.906511 F404 0.07560 0.7788 0.62240 0.906511 F405 -0.04063 0.5785 0.44991 0.0648 F406 0.06188 0.33 0.56186 0.44904 0.0552 C1 0.1703 0.8665613 0.44904 0.0552 0.64391 C2 0.16612 0.80667 0.2008510 0.0466 C1 0.1703 0.86386151 0.27351 0.0385 C3 0.0756 0.84990 0.511 0.0430 C4 0.1756 0.86386151 0.42977151 0.04430 C5 0.2819 0.86386151 0.42977151 0.0430 C5 0.2819 0.93645 0.42977151 0.0437 C6 0.2816 0.90412 0.3835101 0.04575 C7 0.3813 0.904121241 0.32582 0.904717 0.0559 C1 -0.02393 0.9253310 0.9025310 0.90472 <t< td=""><td>F204</td><td>0.31250 (18)</td><td>0.30448 (12)</td><td>0.62722(12)</td><td>0.0711</td></t<>	F204	0.31250 (18)	0.30448 (12)	0.62722(12)	0.0711	
P206 0.4446 (13) 0.54608 (9) 0.66820 (9) 0.0449 F302 0.53120 (13) 0.49628 (8) 0.43591 (9) 0.0426 F303 0.71073 (15) 0.55768 (11) 0.38770 (12) 0.0573 F304 0.70173 (15) 0.55768 (11) 0.38870 (12) 0.0666 F306 0.32140 (14) 0.77965 (11) 0.33803 (12) 0.0666 F402 0.32940 (14) 0.77206 (9) 0.52790 (10) 0.0443 F403 0.29747 (15) 0.77788 (9) 0.62240 (9) 0.0670 F405 -0.04063 (15) 0.64391 (13) 0.54679 (11) 0.0667 F406 0.06188 (13) 0.56186 (9) 0.44940 (10) 0.0447 O1 0.1703 (2) 0.86258 (13) 0.49917 (12) 0.0582 O2 0.1612 (16) 0.90667 (12) 0.20854 (15) 0.07335 (14) 0.0372 C2 0.0786 (2) 0.84515 (15) 0.27335 (14) 0.0472 C3 0.0756 (2) 0.84509 (15) 0.42974 (16) 0.0439 C4 0.1756 (3) 0.86286 (15) 0.42974 (16) 0.0439 C5 0.2819 (2) 0.84617 (12) 0.3385 (13) 0.0497 C6 0.2816 (2) 0.9341 (2) 0.36351 0.42974 (16) 0.0439 C7 0.3813 (2) 0.9342 (2) 0.4064 (18) 0.0525 C9 0.2563 (2) 0.94814 (2) 0.33256 (15) 0.04074 C7 0.3813 (2) 0.93454 (12) 0.33851 (19) 0.0603 </td <td>F205</td> <td>0.44988 (16)</td> <td>0.42782(12)</td> <td>0.66491 (10)</td> <td>0.0619</td>	F205	0.44988 (16)	0.42782(12)	0.66491 (10)	0.0619	
F3020.53120 (13)0.49623 (8)0.43591 (9)0.0426F3030.71073 (15)0.55768 (11)0.38770 (12)0.0573F3040.70118 (17)0.69944 (12)0.32283 (13)0.0717F3050.50263 (18)0.77066 (19)0.35751 (10)0.0666F3060.32140 (14)0.72061 (9)0.35751 (10)0.0666F4020.39924 (13)0.70280 (9)0.5270 (10)0.04453F4030.29747 (15)0.7788 (9)0.62940 (9)0.0511F4040.07569 (17)0.75256 (12)0.63935 (11)0.06648F4060.06188 (13)0.56186 (9)0.44904 (10)0.0487C10.1703 (2)0.86258 (13)0.49917 (12)0.0552C20.16612 (16)0.90667 (12)0.20085 (10)0.0466C10.1703 (2)0.88464 (15)0.27335 (14)0.0372C20.0766 (2)0.84896 (15)0.42978 (15)0.0430C30.0756 (2)0.84909 (15)0.42978 (15)0.04407C40.1756 (3)0.86386 (15)0.42978 (15)0.04407C50.2819 (2)0.93445 (12)0.16383 (18)0.0525C90.2563 (2)0.9414 (2)0.16383 (18)0.0525C90.2563 (2)0.9414 (2)0.16383 (14)0.0367C1 $-0.0147 (3)$ 0.8304 (2)0.23029 (15)0.0400C1 $-0.0147 (3)$ 0.8304 (2)0.23025 (19)0.0663C30.2283 (3)0.9025 (3)0.07888 (19)0.0572 </td <td>F206</td> <td>0.44446(13)</td> <td>0.54608(9)</td> <td>0.56820(9)</td> <td>0.0449</td>	F206	0.44446(13)	0.54608(9)	0.56820(9)	0.0449	
F3030.71073 (15)0.55768 (11)0.38770 (12)0.06773F3040.70118 (17)0.69944 (12)0.32823 (13)0.0717F3050.50263 (18)0.77965 (11)0.30803 (12)0.0666F3060.32140 (14)0.70261 (9)0.52750 (10)0.0453F4030.29747 (15)0.77528 (12)0.63935 (11)0.0670F4040.075569 (17)0.75258 (12)0.63935 (11)0.0670F405-0.04063 (15)0.64391 (13)0.54679 (11)0.0448C10.1703 (2)0.86258 (13)0.49917 (12)0.0582C20.16612 (16)0.90667 (12)0.20953 (10)0.0466C10.1780 (2)0.88545 (15)0.29335 (14)0.0372C20.0786 (2)0.85155 (15)0.29534 (15)0.0430C30.0756 (2)0.84090 (15)0.37242 (16)0.0411C40.1756 (3)0.86386 (15)0.42978 (15)0.0430C50.2816 (2)0.9414 (2)0.3256 (15)0.0407C70.8313 (2)0.93045 (18)0.0525C90.2563 (2)0.9414 (2)0.23097 (17)0.0509C11-0.0239 (3)0.80941 (19)0.40453 (19)0.0529C120.3335 (3)0.9024 (2)0.43385 (14)0.0337C130.2328 (3)0.9205 (3)0.07988 (19)0.0772C100.2260 (2)0.50581 (14)0.23355 (14)0.0330C130.2328 (3)0.9205 (15)0.04900.0443C14	F302	0.53120(13)	0.49623(8)	0.43591(9)	0.0426	
F3040.70118 (17)0.68944 (12)0.32283 (13)0.0717F3050.50263 (18)0.77056 (11)0.30303 (12)0.0666F3060.32140 (14)0.72061 (9)0.35751 (10)0.0453F4020.39924 (13)0.70280 (9)0.52790 (10)0.0453F4030.29747 (15)0.77588 (12)0.63935 (11)0.0670F4040.07569 (17)0.75288 (12)0.63935 (11)0.0670F405-0.04063 (15)0.64391 (13)0.54679 (11)0.0648F4060.06188 (13)0.56186 (9)0.44904 (10)0.04487O10.1703 (2)0.88258 (13)0.49917 (12)0.0582C20.0766 (2)0.88155 (15)0.29335 (14)0.0372C20.07766 (2)0.88155 (15)0.29334 (15)0.0437C30.0756 (2)0.84090 (15)0.37242 (16)0.0411C40.1756 (3)0.86386 (15)0.42978 (15)0.0407C60.2816 (2)0.93045 (18)0.29320 (18)0.0487C80.3702 (2)0.9219 (2)0.20604 (18)0.0525C90.2563 (2)0.9418 (2)0.16333 (18)0.0525C90.2563 (2)0.9418 (2)0.16333 (18)0.0525C90.2563 (2)0.9414 (2)0.46325 (19)0.0603C11 $-0.0239 (3)$ 0.8094 (19)0.46333 (19)0.0529C120.3353 (3)0.9024 (2)0.1725 (2)0.0722C140.23393 (3)1.0324 (2)0.1725 (2)0.0722 <td>F303</td> <td>0.71073(15)</td> <td>0.55768(11)</td> <td>0.38770(12)</td> <td>0.0573</td>	F303	0.71073(15)	0.55768(11)	0.38770(12)	0.0573	
F3050.50263 (18)0.77965 (11)0.30803 (12)0.06666F3060.32140 (14)0.70280 (9)0.52750 (10)0.0511F4020.39924 (13)0.70280 (9)0.52790 (10)0.04513F4040.07559 (17)0.75258 (12)0.63935 (11)0.0670F405-0.04063 (15)0.64391 (13)0.54679 (11)0.06648F4060.06188 (13)0.56186 (9)0.44904 (10)0.0487O10.1703 (2)0.86258 (13)0.49917 (12)0.0582O20.16612 (16)0.90667 (12)0.20055 (10)0.0466C10.1780 (2)0.85155 (15)0.29534 (15)0.0385C30.0756 (2)0.85155 (15)0.29534 (15)0.0430C40.1756 (3)0.86386 (15)0.42978 (15)0.0440C50.2819 (2)0.86386 (15)0.42978 (15)0.0447C60.2816 (2)0.9141 (14)0.32566 (15)0.0447C70.813 (2)0.9219 (2)0.26064 (18)0.0525C90.2563 (2)0.9414 (2)0.1633 (18)0.0522C11-0.0239 (3)0.80941 (19)0.40453 (19)0.0529C120.3835 (3)0.9205 (3)0.07988 (19)0.0772C1010.2226 (2)0.56081 (14)0.3335 (14)0.0330C1340.2328 (3)0.9205 (15)0.20934 (15)0.0400C140.2339 (3)1.0324 (2)0.1758 (14)0.0366C110.2226 (2)0.56081 (15)0.20934 (15)0.0400 <td>F304</td> <td>0.70118(17)</td> <td>0.69944(12)</td> <td>0.32283(13)</td> <td>0.0717</td>	F304	0.70118(17)	0.69944(12)	0.32283(13)	0.0717	
F306 0.32140 (14) 0.72061 (9) 0.35751 (10) 0.0611 F402 0.39924 (13) 0.77280 (9) 0.62940 (9) 0.0511 F403 0.29747 (15) 0.77788 (9) 0.62940 (9) 0.0511 F404 0.07569 (17) 0.75288 (12) 0.63935 (11) 0.0648 F406 0.06188 (13) 0.56186 (9) 0.44904 (10) 0.0447 C1 0.1703 (2) 0.86288 (13) 0.49917 (12) 0.0682 C2 0.16612 (16) 0.90667 (12) 0.20085 (10) 0.0466 C1 0.1786 (2) 0.88464 (15) 0.27335 (14) 0.0372 C3 0.0756 (2) 0.86196 (15) 0.29534 (15) 0.0385 C3 0.0756 (2) 0.86196 (15) 0.42978 (15) 0.0430 C4 0.1756 (3) 0.86386 (15) 0.42978 (15) 0.0430 C5 0.2819 (2) 0.99645 (18) 0.29320 (18) 0.0487 C6 0.2816 (2) 0.99412 (14) 0.32586 (15) 0.0407 C7 0.3813 (2) 0.9944 (2) 0.16383 (18) 0.6532 C9 0.2563 (2) 0.9941 (2) 0.16383 (18) 0.0532 C10 -0.0147 (3) 0.8904 (12) 0.16383 (18) 0.0532 C11 -0.0239 (3) 0.9924 (2) 0.46325 (19) 0.0603 C12 0.3835 (3) 0.9924 (2) 0.7722 0.7722 C13 0.2328 (3) 0.9925 (3) 0.7928 (19) 0.06529 C14 0.2339 (3) 0.9925 (3) <td>F305</td> <td>0.50263(18)</td> <td>0.77965(11)</td> <td>0.30803(12)</td> <td>0.0666</td>	F305	0.50263(18)	0.77965(11)	0.30803(12)	0.0666	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	F306	0.32140(14)	0.72061 (9)	0.35751 (10)	0.0511	
F403 0.29747 (15) 0.77788 (9) 0.62940 (9) 0.0511 F404 0.07569 (17) 0.75258 (12) 0.63935 (11) 0.06648 F406 0.06188 (13) 0.56186 (9) 0.44904 (10) 0.04487 O1 0.1703 (2) 0.86258 (13) 0.449917 (12) 0.0582 O2 0.16612 (16) 0.90667 (12) 0.20085 (10) 0.0466 C1 0.1786 (2) 0.8846 (15) 0.27335 (14) 0.0372 C2 0.0786 (2) 0.85155 (15) 0.29534 (15) 0.0430 C4 0.1756 (3) 0.86386 (15) 0.42278 (16) 0.0411 C5 0.2819 (2) 0.93645 (18) 0.29320 (18) 0.0487 C6 0.2816 (2) 0.9441 (2) 0.16383 (18) 0.0525 C9 0.2663 (2) 0.9441 (2) 0.16383 (18) 0.0525 C11 -0.039 (3) 0.89041 (19) 0.04635 (19) 0.0672 C12 0.3335 (3) 0.9924 (2) 0.46325 (19) 0.6632 C14 0.2328 (3) 0.9205 (3) 0.07988 (19) 0.0772 C102 0.137 (2) 0.60581 (15) 0.2907 (15) 0.3390 C13 0.2328 (3) 0.9924 (2) 0.46325 (19) 0.6632 C14 0.2329 (3) 0.9205 (3) 0.07988 (19) 0.0772 C101 0.2262 (2) 0.56081 (14) 0.33385 (14) 0.365 C12 0.3336 (3) 0.9924 (2) 0.1725 (2) 0.0722 C104 0.1214 (2) 0.5847 (16) </td <td>F402</td> <td>0.39924(13)</td> <td>0.70280 (9)</td> <td>0.52790(10)</td> <td>0.0453</td>	F402	0.39924(13)	0.70280 (9)	0.52790(10)	0.0453	
F404 $0.07609 (1)$ $0.7328 (12)$ $0.6333 (11)$ 0.0670 F405 $-0.04063 (15)$ $0.6331 (13)$ $0.54679 (11)$ 0.0648 F406 $0.06188 (13)$ $0.56186 (9)$ $0.44004 (10)$ 0.0487 O1 $0.1703 (2)$ $0.86258 (13)$ $0.449017 (12)$ 0.0582 O2 $0.16612 (16)$ $0.90667 (12)$ $0.20085 (10)$ 0.0466 C1 $0.1780 (2)$ $0.8884 (15)$ $0.27335 (14)$ 0.0372 C2 $0.0786 (2)$ $0.88155 (15)$ $0.29534 (15)$ 0.0430 C3 $0.0756 (2)$ $0.84090 (15)$ $0.37242 (16)$ 0.0411 C4 $0.1756 (3)$ $0.86386 (15)$ $0.42978 (15)$ 0.0430 C5 $0.2816 (2)$ $0.9412 (14)$ $0.3286 (15)$ 0.0407 C7 $0.3813 (2)$ $0.9345 (18)$ $0.29320 (18)$ 0.0487 C6 $0.2816 (2)$ $0.9919 (2)$ $0.26064 (18)$ 0.0552 C9 $0.2563 (2)$ $0.9914 (2)$ $0.66383 (18)$ 0.0552 C10 $-0.0147 (3)$ $0.8094 (19)$ $0.40452 (19)$ 0.0603 C11 $-0.2239 (3)$ $0.8094 (19)$ $0.40452 (19)$ 0.0603 C12 $0.3385 (3)$ $0.9025 (3)$ $0.0788 (19)$ $0.0772 (10) ($	F403	0.29747(15)	0.77788(9)	0.62940(9)	0.0511	
P405 $-0.04063 (13)$ $0.6439 (13)$ $0.54679 (11)$ 0.0648 F406 $0.06188 (13)$ $0.56186 (9)$ $0.44904 (10)$ 0.0487 O1 $0.1703 (2)$ $0.86258 (13)$ $0.49017 (12)$ 0.0582 O2 $0.16612 (16)$ $0.96667 (12)$ $0.2085 (10)$ 0.0466 C1 $0.1780 (2)$ $0.8895 (15)$ $0.27335 (14)$ 0.0372 C2 $0.0756 (2)$ $0.84090 (15)$ $0.37242 (16)$ 0.0441 C4 $0.1756 (3)$ $0.86386 (15)$ $0.42978 (15)$ 0.0430 C5 $0.2819 (2)$ $0.99412 (14)$ $0.32286 (15)$ 0.0447 C6 $0.2816 (2)$ $0.9412 (14)$ $0.32286 (15)$ 0.0447 C7 $0.3813 (2)$ $0.93645 (18)$ $0.292307 (17)$ 0.059 C8 $0.3702 (2)$ $0.9414 (2)$ $0.16383 (18)$ 0.0532 C9 $0.2563 (2)$ $0.9481 (2)$ $0.16383 (18)$ 0.0525 C9 $0.2563 (2)$ $0.9481 (2)$ $0.16383 (18)$ 0.0529 C11 $-0.0239 (3)$ $0.8994 (19)$ $0.40453 (19)$ 0.0572 C11 $-0.223 (3)$ $0.925 (3)$ $0.7988 (19)$ 0.0772 C11 $0.2226 (2)$ $0.5651 (14)$ $0.3385 (14)$ 0.337 C12 $0.3347 (2)$ $0.5654 (16)$ $0.29679 (15)$ 0.390 C13 $0.2328 (3)$ $0.9254 (16)$ $0.29679 (15)$ 0.390 C14 $0.2339 (3)$ $1.0324 (2)$ $0.1725 (2)$ 0.7722 C101 $0.2362 (2)$ $0.5654 (16)$ 0.276	F404	0.07569(17)	0.75258(12)	0.63935(11)	0.0670	
P4060.06.188 (13)0.50186 (9)0.444061 (10)0.1487O10.1703 (2)0.86258 (13)0.49917 (12)0.0552O20.16612 (16)0.90667 (12)0.20085 (10)0.0466C10.1780 (2)0.88155 (15)0.29334 (15)0.0385C20.0786 (2)0.84090 (15)0.37242 (16)0.0411C40.1756 (3)0.86386 (15)0.42978 (15)0.0430C50.2819 (2)0.86386 (15)0.42978 (15)0.0407C60.2816 (2)0.9914 (2)0.20300 (18)0.0429C60.2816 (2)0.9914 (2)0.20300 (18)0.0452C70.3813 (2)0.93645 (18)0.29320 (18)0.0467C80.3702 (2)0.9219 (2)0.20604 (18)0.0522C90.2563 (2)0.9481 (2)0.16383 (18)0.0529C11-0.0239 (3)0.8944 (19)0.40453 (19)0.0772C140.3335 (3)0.9024 (2)0.1725 (2)0.0722C1010.2226 (2)0.60581 (15)0.29679 (15)0.0390C1140.2339 (3)1.0324 (2)0.17635 (14)0.0437C1020.1347 (2)0.6551 (14)0.23385 (14)0.0365C1030.0848 (2)0.55524 (16)0.29679 (15)0.0390C1040.1214 (2)0.5847 (16)0.2763 (14)0.0365C1050.2093 (2)0.49258 (15)0.20938 (15)0.4040C1040.2124 (2)0.5571 (14)0.28538 (14)0.0366C105 <td>F405</td> <td>-0.04063(15)</td> <td>0.64391(13)</td> <td>0.54679(11)</td> <td>0.0648</td>	F405	-0.04063(15)	0.64391(13)	0.54679(11)	0.0648	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	F 400	0.06188(13)	0.36186(9)	0.44904(10)	0.0487	
O2 0.10012 (10) 0.50007 (12) 0.27335 (14) 0.0372 C1 0.1780 (2) 0.88864 (15) 0.27335 (14) 0.0372 C2 0.0756 (2) 0.8100 (15) 0.37242 (16) 0.0411 C4 0.1756 (2) 0.86386 (15) 0.42978 (15) 0.0430 C5 0.2816 (2) 0.99912 (14) 0.32586 (15) 0.0407 C7 0.3813 (2) 0.93645 (18) 0.29320 (18) 0.0487 C8 0.3702 (2) 0.9481 (2) 0.16383 (18) 0.0525 C9 0.2563 (2) 0.9481 (2) 0.16383 (19) 0.0529 C11 -0.0239 (3) 0.80941 (19) 0.44325 (19) 0.0603 C12 0.3335 (3) 0.9024 (2) 0.4325 (19) 0.0603 C13 0.2328 (3) 0.9024 (2) 0.4325 (19) 0.0603 C14 0.2339 (3) 1.0324 (2) 0.1725 (2) 0.0722 C14 0.2339 (2) 0.59524 (16) 0.22024 (16) 0.03	01	0.1703(2) 0.16612(16)	0.80258(13)	0.49917(12)	0.0582	
C10.1180 (2)0.05056 (13)0.2153 (14)0.0512C20.0756 (2)0.85155 (15)0.29534 (15)0.0385C30.0756 (2)0.84090 (15)0.37242 (16)0.0411C40.1756 (3)0.86386 (15)0.42978 (15)0.0430C50.2819 (2)0.93645 (18)0.29320 (18)0.0467C60.2816 (2)0.90141 (14)0.32586 (15)0.0407C70.3813 (2)0.93645 (18)0.29320 (18)0.0652C90.2563 (2)0.9414 (2)0.16383 (18)0.0522C10-0.0147 (3)0.80941 (2)0.23097 (17)0.5009C11-0.0239 (3)0.80941 (19)0.40453 (19)0.0529C120.3835 (3)0.9024 (2)0.43325 (19)0.0603C130.2328 (3)0.9025 (3)0.07988 (19)0.0772C140.2339 (3)1.0324 (2)0.1725 (2)0.0722C1010.2226 (2)0.56581 (15)0.2967 (15)0.3900C130.0848 (2)0.59524 (16)0.22024 (16)0.0430C1040.1214 (2)0.53847 (16)0.17635 (14)0.0365C2020.2361 (2)0.40551 (14)0.28583 (15)0.0400C1050.2093 (2)0.42634 (15)0.4883 (15)0.4041C2040.3106 (3)0.3377 (17)0.57779 (18)0.0365C2040.3106 (3)0.36377 (17)0.57779 (18)0.0375C3010.4158 (2)0.65672 (14)0.4153 (14)0.0345C302 <td>02 C1</td> <td>0.10012(10) 0.1780(2)</td> <td>0.90007 (12)</td> <td>0.20085(10) 0.27225(14)</td> <td>0.0400</td>	02 C1	0.10012(10) 0.1780(2)	0.90007 (12)	0.20085(10) 0.27225(14)	0.0400	
C2 $0.0165(2)$ $0.03195(13)$ $0.0214(16)$ 0.0411 C3 $0.0756(2)$ $0.84090(15)$ $0.37242(16)$ 0.0411 C4 $0.1756(3)$ $0.88997(15)$ $0.40274(16)$ 0.0429 C5 $0.2819(2)$ $0.88997(15)$ $0.40274(16)$ 0.0429 C6 $0.2816(2)$ $0.90412(14)$ $0.32586(15)$ 0.0407 C7 $0.3813(2)$ $0.93645(18)$ $0.22320(18)$ 0.06525 C9 $0.2563(2)$ $0.9418(2)$ $0.2664(18)$ 0.0525 C10 $-0.0147(3)$ $0.80941(19)$ $0.40453(19)$ 0.0529 C11 $-0.0239(3)$ $0.9024(2)$ $0.46325(19)$ 0.0603 C12 $0.3835(3)$ $0.9024(2)$ $0.46325(19)$ 0.0603 C13 $0.2238(3)$ $0.9024(2)$ $0.1725(2)$ 0.7722 C101 $0.2226(2)$ $0.56081(14)$ $0.3385(14)$ 0.0357 C102 $0.1347(2)$ $0.56581(15)$ $0.2904(16)$ 0.04430 C104 $0.1214(2)$ $0.53847(16)$ $0.17635(14)$ 0.0417 C105 $0.2093(2)$ $0.49059(14)$ $0.47334(14)$ 0.0366 C201 $0.3040(2)$ $0.49059(14)$ $0.47334(14)$ 0.0366 C201 $0.34040(2)$ $0.42569(18)$ $0.59590(16)$ 0.0404 C204 $0.3106(3)$ $0.36377(17)$ $0.57779(18)$ 0.0673 C301 $0.4158(2)$ $0.6652(14)$ $0.4153(14)$ 0.0345 C302 $0.3803(2)$ $0.56774(14)$ $0.4053(15)$ 0.0372 <td< td=""><td>C1 C2</td><td>0.1780(2) 0.0786(2)</td><td>0.85155(15)</td><td>0.27535(14) 0.20534(15)</td><td>0.0372</td></td<>	C1 C2	0.1780(2) 0.0786(2)	0.85155(15)	0.27535(14) 0.20534(15)	0.0372	
C5 $0.0130(2)$ $0.034300(15)$ $0.42978(15)$ 0.0411 C4 $0.1756(3)$ $0.86386(15)$ $0.42978(15)$ 0.0429 C5 $0.2819(2)$ $0.90412(14)$ $0.32586(15)$ 0.0407 C7 $0.3813(2)$ $0.93645(18)$ $0.29320(18)$ 0.0487 C8 $0.3702(2)$ $0.9219(2)$ $0.26604(18)$ 0.0525 C9 $0.2563(2)$ $0.9481(2)$ $0.16383(18)$ 0.0525 C10 $-0.0147(3)$ $0.8304(2)$ $0.23097(17)$ 0.0559 C11 $-0.239(3)$ $0.80941(19)$ $0.40453(19)$ 0.0603 C13 $0.3228(3)$ $0.9024(2)$ $0.46325(19)$ 0.0603 C14 $0.2339(3)$ $1.0324(2)$ $0.1725(2)$ 0.0772 C14 $0.2339(3)$ $1.0324(2)$ $0.1725(2)$ 0.0772 C101 $0.2226(2)$ $0.66081(14)$ $0.3385(14)$ 0.0357 C102 $0.1347(2)$ $0.6552(15)$ $0.2997(15)$ 0.0390 C103 $0.0848(2)$ $0.59524(16)$ $0.22024(16)$ 0.4430 C104 $0.1214(2)$ $0.53847(16)$ $0.17635(14)$ 0.4430 C105 $0.2093(2)$ $0.49285(15)$ $0.2093(15)$ 0.0400 C106 $0.2572(2)$ $0.50571(14)$ $0.28538(14)$ 0.0366 C201 $0.3040(2)$ $0.49265(15)$ $0.47334(14)$ 0.0365 C202 $0.2361(2)$ $0.42669(18)$ $0.59590(16)$ 0.0404 C203 $0.2382(2)$ $0.36406(16)$ $0.59803(18)$ 0.0470 C204	C2 C3	0.0756(2)	0.83133(13)	0.23534(10) 0.37242(16)	0.0335	
C10.1100 (0)0.00005 (10)0.1001 (10)0.0100 (10)C50.2816 (2)0.90412 (14)0.32586 (15)0.0407C70.3813 (2)0.93645 (18)0.2920 (18)0.0487C80.3702 (2)0.9219 (2)0.20604 (18)0.0525C90.2563 (2)0.9481 (2)0.16383 (18)0.0532C10 -0.0147 (3)0.8394 (2)0.23097 (17)0.0509C11 -0.0239 (3)0.80941 (19)0.40453 (19)0.0729C120.3835 (3)0.9024 (2)0.46325 (19)0.0603C130.2328 (3)0.9205 (3)0.07988 (19)0.0772C140.2339 (3)1.0324 (2)0.1725 (2)0.0772C1010.2226 (2)0.56081 (14)0.33385 (14)0.0357C1020.1347 (2)0.60581 (15)0.29679 (15)0.0390C1030.0848 (2)0.59524 (16)0.2024 (16)0.0440C1040.1214 (2)0.53847 (16)0.17635 (14)0.0417C1050.2993 (2)0.49285 (15)0.20934 (15)0.0400C1060.2572 (2)0.50571 (14)0.28538 (14)0.0365C2020.2361 (2)0.42634 (15)0.45893 (15)0.0404C2030.2382 (2)0.36406 (16)0.50803 (18)0.0470C2040.3106 (3)0.36377 (17)0.57779 (18)0.0503C3010.4158 (2)0.6652 (14)0.40153 (14)0.0345C3020.5186 (2)0.56774 (14)0.40533 (15)0.0372<	C4	0.0756(2)	0.86386 (15)	0.42978(15)	0.0411	
C60.2816 (2)0.904012 (14)0.32586 (15)0.0407C70.3813 (2)0.93645 (18)0.29320 (18)0.0487C80.3702 (2)0.9219 (2)0.20604 (18)0.0525C90.2563 (2)0.9481 (2)0.16383 (18)0.0522C10 -0.0147 (3)0.8304 (2)0.23097 (17)0.0509C11 $-0.0239 (3)$ 0.80941 (19)0.40453 (19)0.0622C120.3835 (3)0.9025 (3)0.07988 (19)0.0772C140.2328 (3)0.9205 (3)0.07988 (19)0.0772C140.2339 (3)1.0324 (2)0.1725 (2)0.0722C1010.2226 (2)0.56081 (14)0.33385 (14)0.0357C1020.1347 (2)0.60581 (15)0.29679 (15)0.0390C1030.0848 (2)0.59524 (16)0.21765 (14)0.0440C1040.1214 (2)0.53847 (16)0.17635 (14)0.0366C2010.3040 (2)0.49285 (15)0.20934 (15)0.0400C1060.2572 (2)0.50571 (14)0.28583 (14)0.0366C2020.2361 (2)0.42634 (15)0.45893 (15)0.0404C2030.2382 (2)0.36406 (16)0.59803 (18)0.0470C2040.3106 (3)0.36377 (17)0.57779 (18)0.0375C3010.4158 (2)0.60562 (14)0.4053 (14)0.0345C3020.5186 (2)0.56774 (14)0.40533 (15)0.0372C3030.6129 (2)0.59783 (17)0.38037 (16)0.0438	C5	0.2819(2)	0.88997 (15)	0.40274(16)	0.0429	
C70.3813 (2)0.93044 (14)0.4263 (18)0.0487C80.3702 (2)0.9219 (2)0.20604 (18)0.0525C90.2563 (2)0.9481 (2)0.16383 (18)0.0532C10 -0.0147 (3)0.8304 (2)0.23097 (17)0.0509C11 -0.0239 (3)0.80941 (19)0.40453 (19)0.0529C120.3835 (3)0.9024 (2)0.46325 (19)0.0603C130.2328 (3)0.9205 (3)0.07888 (19)0.0772C140.2339 (3)1.0324 (2)0.1725 (2)0.0722C1010.2226 (2)0.56081 (14)0.33385 (14)0.0337C1020.1347 (2)0.60581 (15)0.29079 (15)0.0390C1330.0848 (2)0.59524 (16)0.22024 (16)0.0430C1040.1214 (2)0.53847 (16)0.17635 (14)0.0417C1050.2093 (2)0.49285 (15)0.20934 (15)0.0400C1060.2572 (2)0.50571 (14)0.28588 (14)0.0365C2010.3040 (2)0.49059 (14)0.47334 (14)0.0365C2020.2361 (2)0.46364 (15)0.45893 (15)0.0404C2040.3106 (3)0.36437 (17)0.57779 (18)0.0503C2050.3803 (2)0.42569 (18)0.59590 (16)0.0463C2060.3752 (2)0.46866 (15)0.5484 (15)0.0375C3010.4158 (2)0.66652 (14)0.40153 (14)0.0345C3020.5186 (2)0.56774 (14)0.40533 (15)0.0372	C6	0.2816(2)	0.90412(14)	0.32586(15)	0.0407	
C8 $0.3702(2)$ $0.9219(2)$ $0.20604(18)$ 0.0525 C9 $0.2563(2)$ $0.9481(2)$ $0.16383(18)$ 0.0532 C10 $-0.0147(3)$ $0.8304(2)$ $0.23097(17)$ 0.0509 C11 $-0.0239(3)$ $0.80941(19)$ $0.40453(19)$ 0.0529 C12 $0.3835(3)$ $0.9024(2)$ $0.46325(19)$ 0.0603 C13 $0.2328(3)$ $0.9205(3)$ $0.07988(19)$ 0.0772 C14 $0.2339(3)$ $1.0324(2)$ $0.1725(2)$ 0.0722 C101 $0.2226(2)$ $0.56081(14)$ $0.33385(14)$ 0.0357 C102 $0.1347(2)$ $0.60581(15)$ $0.29679(15)$ 0.0390 C103 $0.0848(2)$ $0.59524(16)$ $0.22024(16)$ 0.0440 C104 $0.1214(2)$ $0.53847(16)$ $0.17635(14)$ 0.0417 C105 $0.2093(2)$ $0.49285(15)$ $0.20934(15)$ 0.4040 C202 $0.2361(2)$ $0.49285(15)$ $0.2934(15)$ 0.0400 C106 $0.2572(2)$ $0.50571(14)$ $0.28538(14)$ 0.0366 C201 $0.3040(2)$ $0.49285(18)$ $0.5950(16)$ 0.4044 C203 $0.2382(2)$ $0.36377(17)$ $0.57779(18)$ 0.0503 C204 $0.3106(3)$ $0.36377(17)$ $0.57779(18)$ 0.0372 C301 $0.4158(2)$ $0.66562(14)$ $0.40153(14)$ 0.0345 C302 $0.5186(2)$ $0.56774(14)$ $0.40543(15)$ 0.0372 C303 $0.6129(2)$ $0.567730(15)$ $0.36700(15)$ 0.0397 <td>C7</td> <td>0.3813 (2)</td> <td>0.93645 (18)</td> <td>0.29320 (18)</td> <td>0.0487</td>	C7	0.3813 (2)	0.93645 (18)	0.29320 (18)	0.0487	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C8	0.3702(2)	0.9219(2)	0.20604 (18)	0.0525	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C9	0.2563(2)	0.9481 (2)	0.16383 (18)	0.0532	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C10	-0.0147(3)	0.8304 (2)	0.23097 (17)	0.0509	
C12 $0.3835 (3)$ $0.9024 (2)$ $0.46325 (19)$ 0.0603 C13 $0.2328 (3)$ $0.9205 (3)$ $0.07988 (19)$ 0.0772 C14 $0.2339 (3)$ $1.0324 (2)$ $0.1725 (2)$ 0.0722 C101 $0.2226 (2)$ $0.56081 (14)$ $0.33385 (14)$ 0.0357 C102 $0.1347 (2)$ $0.60581 (15)$ $0.29679 (15)$ 0.0390 C103 $0.0848 (2)$ $0.59524 (16)$ $0.22024 (16)$ 0.0440 C104 $0.1214 (2)$ $0.53847 (16)$ $0.2093 (15)$ 0.0400 C105 $0.2093 (2)$ $0.49285 (15)$ $0.2093 (15)$ 0.0400 C106 $0.2572 (2)$ $0.50571 (14)$ $0.28538 (14)$ 0.0366 C201 $0.3040 (2)$ $0.49059 (14)$ $0.47334 (14)$ 0.0365 C202 $0.2361 (2)$ $0.42634 (15)$ $0.45803 (18)$ 0.0470 C204 $0.3106 (3)$ $0.36377 (17)$ $0.5779 (18)$ 0.0503 C205 $0.3803 (2)$ $0.42569 (18)$ $0.59590 (16)$ 0.0463 C206 $0.3752 (2)$ $0.48646 (15)$ $0.5484 (15)$ 0.375 C301 $0.4158 (2)$ $0.66520 (14)$ $0.4053 (15)$ 0.0372 C302 $0.5186 (2)$ $0.59783 (17)$ $0.38037 (16)$ 0.0438 C304 $0.6095 (3)$ $0.66930 (18)$ $0.34761 (18)$ 0.0495 C305 $0.5993 (3)$ $0.70947 (16)$ $0.34036 (17)$ 0.0473 C306 $0.4175 (2)$ $0.67730 (15)$ $0.36700 (15)$ 0.0397 C401 $0.2351 (2)$ <t< td=""><td>C11</td><td>-0.0239(3)</td><td>0.80941 (19)</td><td>0.40453 (19)</td><td>0.0529</td></t<>	C11	-0.0239(3)	0.80941 (19)	0.40453 (19)	0.0529	
C13 0.2328 (3) 0.9205 (3) 0.07988 (19) 0.0772 C14 0.2339 (3) 1.0324 (2) 0.1725 (2) 0.0722 C101 0.2262 (2) 0.56081 (14) 0.3385 (14) 0.0357 C102 0.1347 (2) 0.60581 (15) 0.29679 (15) 0.0390 C103 0.0848 (2) 0.59524 (16) 0.20224 (16) 0.0430 C104 0.1214 (2) 0.53847 (16) 0.17635 (14) 0.0417 C105 0.2093 (2) 0.49285 (15) 0.2934 (15) 0.0400 C106 0.2572 (2) 0.50571 (14) 0.28538 (14) 0.0366 C201 0.3040 (2) 0.49059 (14) 0.47334 (14) 0.0366 C202 0.2361 (2) 0.42634 (15) 0.45893 (15) 0.0404 C203 0.2382 (2) 0.36406 (16) 0.50803 (18) 0.0470 C204 0.3106 (3) 0.36377 (17) 0.57779 (18) 0.0375 C301 0.4158 (2) 0.42569 (18) 0.59590 (16) 0.0463 C205 0.3803 (2) 0.42569 (18) 0.59590 (16) 0.0463 C304 0.6095 (3) 0.66930 (18) 0.34761 (18) 0.0495 C303 0.6129 (2) 0.59783 (17) 0.38037 (16) 0.0438 C304 0.6095 (3) 0.66930 (18) 0.34761 (18) 0.0495 C305 0.5093 (3) 0.70947 (16) 0.34066 (17) 0.0473 C306 0.4175 (2) 0.62884 (14) 0.48065 (14) 0.0348 C402 0.2896 (2)	C12	0.3835(3)	0.9024 (2)	0.46325(19)	0.0603	
C14 0.2339 (3) 1.0324 (2) 0.1725 (2) 0.0722 C101 0.2226 (2) 0.56081 (14) 0.33385 (14) 0.0357 C102 0.1347 (2) 0.60581 (15) 0.29679 (15) 0.0430 C103 0.0848 (2) 0.59524 (16) 0.22024 (16) 0.0430 C104 0.1214 (2) 0.53847 (16) 0.17635 (14) 0.0417 C105 0.2093 (2) 0.49285 (15) 0.20934 (15) 0.0400 C106 0.2572 (2) 0.50571 (14) 0.28538 (14) 0.0366 C201 0.3040 (2) 0.49059 (14) 0.47334 (14) 0.0366 C202 0.2361 (2) 0.36406 (16) 0.50803 (18) 0.0470 C203 0.2382 (2) 0.36406 (16) 0.50803 (18) 0.0470 C204 0.3106 (3) 0.36377 (17) 0.57779 (18) 0.0503 C205 0.3803 (2) 0.42569 (18) 0.59590 (16) 0.0463 C206 0.3752 (2) 0.4846 (15) 0.54484 (15) 0.0375 C301 0.4158 (2) 0.6672 (14) 0.40153 (14) 0.0345 C302 0.5186 (2) 0.59783 (17) 0.38037 (16) 0.438 C304 0.6095 (3) 0.66930 (18) 0.34761 (18) 0.0495 C305 0.5093 (3) 0.70947 (16) 0.34036 (17) 0.0473 C306 0.4175 (2) 0.67730 (15) 0.36700 (15) 0.0397 C401 0.2351 (2) 0.68460 (14) 0.52952 (14) 0.0368 C402 0.2866 (C13	0.2328(3)	0.9205(3)	0.07988 (19)	0.0772	
C101 0.2226 (2) 0.56081 (14) 0.33385 (14) 0.0357 C102 0.1347 (2) 0.60581 (15) 0.29679 (15) 0.0390 C103 0.0848 (2) 0.59524 (16) 0.22024 (16) 0.0430 C104 0.1214 (2) 0.53847 (16) 0.17635 (14) 0.0417 C105 0.2993 (2) 0.49285 (15) 0.20934 (15) 0.0400 C106 0.2572 (2) 0.50571 (14) 0.28538 (14) 0.0366 C201 0.3040 (2) 0.49059 (14) 0.47334 (14) 0.0365 C202 0.2361 (2) 0.42634 (15) 0.45893 (15) 0.0404 C203 0.2382 (2) 0.36406 (16) 0.50803 (18) 0.0470 C204 0.3106 (3) 0.36377 (17) 0.57779 (18) 0.0503 C205 0.3803 (2) 0.42569 (18) 0.59590 (16) 0.0463 C206 0.3752 (2) 0.48646 (15) 0.54484 (15) 0.0375 C301 0.4158 (2) 0.60562 (14) 0.40153 (14) 0.0345 C302 0.5186 (2) 0.59783 (17) 0.38037 (16) 0.0443 C304 0.6095 (3) 0.66930 (18) 0.34761 (18) 0.0473 C305 0.5093 (3) 0.70947 (16) 0.34036 (17) 0.0473 C306 0.4175 (2) 0.66730 (15) 0.36700 (15) 0.3977 C401 0.2351 (2) 0.68460 (14) 0.52952 (14) 0.0348 C402 0.2896 (2) 0.68460 (14) 0.52952 (14) 0.0368	C14	0.2339(3)	1.0324(2)	0.1725(2)	0.0722	
C102 0.1347 (2) 0.60581 (15) 0.29679 (15) 0.0390 C103 0.0848 (2) 0.59524 (16) 0.22024 (16) 0.0430 C104 0.1214 (2) 0.53847 (16) 0.17635 (14) 0.0417 C105 0.2093 (2) 0.49285 (15) 0.20934 (15) 0.0400 C106 0.2572 (2) 0.50571 (14) 0.28538 (14) 0.0366 C201 0.3040 (2) 0.49059 (14) 0.47334 (14) 0.0365 C202 0.2361 (2) 0.42634 (15) 0.45893 (15) 0.0404 C203 0.2382 (2) 0.36406 (16) 0.50803 (18) 0.0470 C204 0.3106 (3) 0.36377 (17) 0.5779 (18) 0.0503 C205 0.3803 (2) 0.42569 (18) 0.59590 (16) 0.0463 C206 0.3752 (2) 0.48646 (15) 0.54484 (15) 0.0375 C301 0.4158 (2) 0.60562 (14) 0.40153 (14) 0.0345 C302 0.5186 (2) 0.56774 (14) 0.40543 (15) 0.0372 C303 0.6129 (2) 0.59783 (17) 0.38037 (16) 0.0408 C304 0.6095 (3) 0.66930 (18) 0.34761 (18) 0.0473 C305 0.5093 (3) 0.70947 (16) 0.34036 (17) 0.0473 C306 0.4175 (2) 0.687730 (15) 0.36700 (15) 0.0397 C401 0.2351 (2) 0.68460 (14) 0.52952 (14) 0.0368 C402 0.2896 (2) 0.68460 (14) 0.52952 (14) 0.0368	C101	0.2226(2)	0.56081 (14)	0.33385(14)	0.0357	
C103 0.0848 (2) 0.59524 (16) 0.22024 (16) 0.0430 C104 0.1214 (2) 0.53847 (16) 0.17635 (14) 0.0417 C105 0.2093 (2) 0.49285 (15) 0.20934 (15) 0.0400 C106 0.2572 (2) 0.50571 (14) 0.28538 (14) 0.0366 C201 0.3040 (2) 0.49059 (14) 0.47334 (14) 0.0365 C202 0.2361 (2) 0.42634 (15) 0.45893 (15) 0.0404 C203 0.2382 (2) 0.36406 (16) 0.50803 (18) 0.0470 C204 0.3106 (3) 0.36377 (17) 0.57779 (18) 0.0503 C205 0.3803 (2) 0.42569 (18) 0.59590 (16) 0.0463 C206 0.3752 (2) 0.48646 (15) 0.54484 (15) 0.0375 C301 0.4158 (2) 0.60562 (14) 0.40153 (14) 0.0345 C302 0.5186 (2) 0.56774 (14) 0.40153 (14) 0.0345 C303 0.6129 (2) 0.59783 (17) 0.38037 (16) 0.0495 C304 0.6095 (3) 0.66930 (18) 0.34761 (18) 0.0495 C305 0.5093 (3) 0.70947 (16) 0.34066 (17) 0.0473 C306 0.4175 (2) 0.67730 (15) 0.36700 (15) 0.0397 C401 0.2351 (2) 0.6884 (14) 0.48065 (14) 0.0348 C402 0.2896 (2) 0.68460 (14) 0.52952 (14) 0.0368 C403 0.2388 (2) 0.72523 (15) 0.58359 (15) 0.0400	C102	0.1347(2)	0.60581 (15)	0.29679(15)	0.0390	
C104 0.1214 (2) 0.53847 (16) 0.17635 (14) 0.0417 C105 0.2093 (2) 0.49285 (15) 0.20934 (15) 0.0400 C106 0.2572 (2) 0.50571 (14) 0.28538 (14) 0.0366 C201 0.3040 (2) 0.49059 (14) 0.47334 (14) 0.0365 C202 0.2361 (2) 0.42634 (15) 0.45893 (15) 0.0404 C203 0.2382 (2) 0.36406 (16) 0.50803 (18) 0.0470 C204 0.3106 (3) 0.36377 (17) 0.57779 (18) 0.0503 C205 0.3803 (2) 0.42569 (18) 0.59590 (16) 0.0463 C206 0.3752 (2) 0.48646 (15) 0.54484 (15) 0.0375 C301 0.4158 (2) 0.60562 (14) 0.40153 (14) 0.0345 C302 0.5186 (2) 0.56774 (14) 0.40153 (14) 0.0345 C303 0.6129 (2) 0.59783 (17) 0.38037 (16) 0.0438 C304 0.6095 (3) 0.66930 (18) 0.34761 (18) 0.0495 C305 0.5093 (3) 0.70947 (16) 0.34036 (17) 0.0473 C306 0.4175 (2) 0.67730 (15) 0.36700 (15) 0.0397 C401 0.2351 (2) 0.6884 (14) 0.48065 (14) 0.0348 C402 0.2896 (2) 0.68460 (14) 0.52952 (14) 0.0368 C403 0.2388 (2) 0.72523 (15) 0.58359 (15) 0.0400	C103	0.0848(2)	0.59524(16)	0.22024(16)	0.0430	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C104	0.1214(2)	0.53847(16)	0.17635(14)	0.0417	
C106 0.2572 (2) 0.50571 (14) 0.28538 (14) 0.0366 C201 0.3040 (2) 0.49059 (14) 0.47334 (14) 0.0365 C202 0.2361 (2) 0.42634 (15) 0.45893 (15) 0.0404 C203 0.2382 (2) 0.36406 (16) 0.50803 (18) 0.0470 C204 0.3106 (3) 0.36377 (17) 0.57779 (18) 0.0503 C205 0.3803 (2) 0.42569 (18) 0.59590 (16) 0.0463 C206 0.3752 (2) 0.48646 (15) 0.54484 (15) 0.0375 C301 0.4158 (2) 0.60562 (14) 0.40153 (14) 0.0345 C302 0.5186 (2) 0.56774 (14) 0.40543 (15) 0.0372 C303 0.6129 (2) 0.59783 (17) 0.38037 (16) 0.0495 C304 0.6095 (3) 0.66930 (18) 0.34761 (18) 0.0495 C305 0.5093 (3) 0.70947 (16) 0.34036 (17) 0.0473 C306 0.4175 (2) 0.67730 (15) 0.36700 (15) 0.0397 C401 0.2351 (2) 0.6884 (14) 0.48065 (14) 0.0348 C402 0.2896 (2) 0.68460 (14) 0.52952 (14) 0.0368 C403 0.2388 (2) 0.72523 (15) 0.58359 (15) 0.0400	C105	0.2093 (2)	0.49285 (15)	0.20934 (15)	0.0400	
C201 $0.3040(2)$ $0.49059(14)$ $0.47334(14)$ 0.0365 C202 $0.2361(2)$ $0.42634(15)$ $0.47893(15)$ 0.0404 C203 $0.2382(2)$ $0.36406(16)$ $0.50803(18)$ 0.0470 C204 $0.3106(3)$ $0.36377(17)$ $0.57779(18)$ 0.0503 C205 $0.3803(2)$ $0.42569(18)$ $0.59590(16)$ 0.0463 C206 $0.3752(2)$ $0.48646(15)$ $0.54484(15)$ 0.0375 C301 $0.4158(2)$ $0.60562(14)$ $0.4053(15)$ 0.0372 C303 $0.6129(2)$ $0.59783(17)$ $0.38037(16)$ 0.0438 C304 $0.6095(3)$ $0.66930(18)$ $0.34761(18)$ 0.0473 C305 $0.5093(3)$ $0.70947(16)$ $0.34036(17)$ 0.0473 C306 $0.4175(2)$ $0.62884(14)$ $0.48065(14)$ 0.0348 C401 $0.2351(2)$ $0.68460(14)$ $0.52952(14)$ 0.0368 C403 $0.2388(2)$ $0.72523(15)$ $0.58359(15)$ 0.0400	C106	0.2572(2)	0.50571 (14)	0.28538 (14)	0.0366	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C201	0.3040(2)	0.49059(14)	0.47334(14)	0.0365	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C202	0.2361(2)	0.42634(15)	0.45893(15)	0.0404	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C203	0.2382(2)	0.36406(10)	0.50803(18)	0.0470	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C204 C205	0.3106(3)	0.30377(17)	0.57779(18)	0.0503	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C205	0.3803(2) 0.3752(2)	0.42509(18) 0.48646(15)	0.59590(10) 0.54484(15)	0.0405	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C301	0.4158(2)	0.60562(14)	0.40153(14)	0.0345	
C302 0.105 (2) 0.5011 (1) 0.4045 (10) 0.0012 C303 0.6129 (2) 0.59783 (17) 0.38037 (16) 0.0438 C304 0.6095 (3) 0.66930 (18) 0.34761 (18) 0.0495 C305 0.5093 (3) 0.70947 (16) 0.34036 (17) 0.0473 C306 0.4175 (2) 0.67730 (15) 0.36700 (15) 0.0397 C401 0.2351 (2) 0.62884 (14) 0.48065 (14) 0.0348 C402 0.2896 (2) 0.68460 (14) 0.52952 (14) 0.0368 C403 0.2388 (2) 0.72523 (15) 0.58359 (15) 0.0400	C302	0.5186(2)	0.56774(14)	0.40543(15)	0.0372	
C304 0.6095 (3) 0.66930 (18) 0.34761 (18) 0.0495 C305 0.5093 (3) 0.70947 (16) 0.34036 (17) 0.0473 C306 0.4175 (2) 0.67730 (15) 0.36700 (15) 0.0397 C401 0.2351 (2) 0.68846 (14) 0.48065 (14) 0.0348 C402 0.2896 (2) 0.68460 (14) 0.52952 (14) 0.0368 C403 0.2388 (2) 0.72523 (15) 0.58359 (15) 0.0400	C303	0.6129(2)	0.59783(17)	0.38037(16)	0.0438	
C305 0.5093 (3) 0.70947 (16) 0.34036 (17) 0.0473 C306 0.4175 (2) 0.67730 (15) 0.36700 (15) 0.0397 C401 0.2351 (2) 0.62884 (14) 0.48065 (14) 0.0348 C402 0.2896 (2) 0.68460 (14) 0.52952 (14) 0.0368 C403 0.2388 (2) 0.72523 (15) 0.58359 (15) 0.0400	C304	0.6095(3)	0.66930(18)	0.34761 (18)	0.0495	
C306 0.4175 (2) 0.67730 (15) 0.36700 (15) 0.0397 C401 0.2351 (2) 0.62884 (14) 0.48065 (14) 0.0348 C402 0.2896 (2) 0.68460 (14) 0.52952 (14) 0.0368 C403 0.2388 (2) 0.72523 (15) 0.58359 (15) 0.0400	C305	0.5093 (3)	0.70947 (16)	0.34036(17)	0.0473	
C401 0.2351 (2) 0.62884 (14) 0.48065 (14) 0.0348 C402 0.2896 (2) 0.68460 (14) 0.52952 (14) 0.0368 C403 0.2388 (2) 0.72523 (15) 0.58359 (15) 0.0400	C306	0.4175(2)	0.67730(15)	0.36700 (15)	0.0397	
C402 0.2896 (2) 0.68460 (14) 0.52952 (14) 0.0368 C403 0.2388 (2) 0.72523 (15) 0.58359 (15) 0.0400	C401	0.2351 (2)	0.62884(14)	0.48065(14)	0.0348	
C403 0.2388 (2) 0.72523 (15) 0.58359 (15) 0.0400	C402	0.2896 (2)	0.68460 (14)	0.52952(14)	0.0368	
	C403	0.2388(2)	0.72523 (15)	0.58359(15)	0.0400	

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C404	0.1274(3)	0.71208(17)	0.58922(15)	0.0450
C405	0.0698(2)	0.65762(18)	0.54272(16)	0.0446
C406	0.1238(2)	0.61703(15)	0.49099(15)	0.0391
B1	0.2946(2)	0.57163(16)	0.42271 (16)	0.0343
H71	0.383(2)	0.9919(11)	0.3035(13)	0.0557
H72	0.4504(16)	0.9130(13)	0.3192(12)	0.0557
H81	0.4287(17)	0.9500(13)	0.1851(12)	0.0600
H82	0.380(2)	0.8668(11)	0.1971(13)	0.0600
H101	-0.0728(18)	0.8018 (14)	0.2500(13)	0.0585
H102	-0.0467(19)	0.8758(11)	0.2062(13)	0.0585
H103	0.0166(19)	0.8011(13)	0.1922(13)	0.0585
H111	-0.031(2)	0.8322(14)	0.4528(12)	0.0622
H112	-0.0905(17)	0.8168(15)	0.3693(12)	0.0622
H113	-0.017(2)	0.7558(11)	0.4121(15)	0.0622
H121	0.368(2)	0.8933(15)	0.5146(11)	0.0671
H122	0.411(2)	0.9543(11)	0.4606(14)	0.0671
H123	0.4423(18)	0.8693(14)	0.4537(14)	0.0671
H131	0.285(2)	0.9460(16)	0.0499(14)	0.0909
H132	0.1565(18)	0.9322(17)	0.0577(14)	0.0909
H133	0.243(3)	0.8653(11)	0.0775(15)	0.0909
H141	0.294(2)	1.0609(13)	0.1535(17)	0.0857
H142	0.233(3)	1.0452(14)	0.2262(12)	0.0857
H143	0.1621(19)	1.0467(14)	0.1412(15)	0.0857

Table S2. Anisotropic displacement parameters $(Å^2)$

$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		F102	0.0559 (9)	0.0415(8)	0.0452(8)	0.0186(7)	-0.0051(7)	-0.0065(7)
		F103	0.0590(10)	0.0620(11)	0.0510(9)	0.0230(9)	-0.0171(8)	0.0016 (8)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	F104	0.0618(10)	0.0662(11)	0.0344(8)	0.0031(9)	-0.0130(7)	-0.0045(7)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	F105	0.0615(10)	0.0514(10)	0.0400(8)	0.0082(8)	-0.0001(7)	-0.0151(7)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	F106	0.0491(9)	0.0423(8)	0.0422(8)	0.0161(7)	-0.0063(7)	-0.0068(6)
	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	F202	0.0520(9)	0.0427(9)	0.0531(9)	-0.0095(7)	-0.0111(7)	-0.0015(7)
	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	F203	0.0691(12)	0.0438(10)	0.0834(13)	-0.0174(9)	0.0015(10)	0.0075(9)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	F204	0.0753(13)	0.0606(12)	0.0765(12)	0.0012(10)	0.0088(10)	0.0347(10)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	F205	0.0578(10)	0.0787(13)	0.0442(9)	0.0039(9)	-0.0081(8)	0.0190(9)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	F206	0.0444(8)	0.0471(9)	0.0389(8)	-0.0035(7)	-0.0067(6)	-0.0030(7)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	F302	0.0458(8)	0.0326(7)	0.0484(8)	0.0090~(6)	0.0033~(6)	0.0025~(6)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	F303	0.0452(9)	0.0589(11)	0.0701~(11)	0.0138(8)	0.0158 (8)	0.0029 (9)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	F304	0.0622(12)	0.0694(13)	0.0904(14)	-0.0034(10)	0.0341(10)	0.0152(10)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	F305	0.0789(13)	0.0448(10)	0.0794(13)	0.0045(9)	0.0228(10)	0.0213 (9)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	F306	0.0530(9)	0.0375(8)	0.0620(10)	0.0120(7)	0.0063~(8)	0.0084(7)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	F402	0.0405(8)	0.0457(9)	0.0478(8)	-0.0027(7)	0.0009~(6)	-0.0111(7)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	F403	0.0672(11)	0.0430(9)	0.0386(8)	0.0064(8)	-0.0065(7)	-0.0115(7)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	F404	0.0744(12)	0.0795(13)	0.0506(10)	0.0173(10)	0.0210 (9)	-0.0137(9)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	F405	0.0459(9)	0.0855(14)	0.0664(11)	-0.0035(9)	0.0199(8)	-0.0003(10)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	F406	0.0426(8)	0.0473(9)	0.0538(9)	-0.0088(7)	-0.0001(7)	-0.0050(7)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O1	0.0840(15)	0.0538(12)	0.0355(10)	0.0130(11)	0.0046(10)	0.0055 (9)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	O2	0.0397(10)	0.0619(12)	0.0367(10)	0.0092(9)	0.0010 (8)	0.0083~(9)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C1	0.0430(13)	0.0344~(13)	0.0336~(12)	0.0097(11)	0.0034(10)	0.0011(10)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C2	0.0417(13)	0.0340(13)	0.0383~(13)	0.0045(11)	0.0017(10)	-0.0015(10)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C3	0.0498(15)	0.0298(12)	0.0438(14)	0.0089(11)	0.0075(11)	0.0020(11)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C4	0.0598(17)	0.0316(13)	0.0359(13)	0.0118(12)	0.0018(11)	0.0013(10)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C5	0.0523(15)	0.0336~(13)	0.0395~(13)	0.0060(12)	-0.0042(11)	-0.0043(11)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C6	0.0462(14)	0.0325~(13)	0.0400(13)	0.0068 (11)	-0.0039(11)	-0.0011(10)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C7	0.0408(14)	0.0499(17)	0.0526 (16)	0.0021 (12)	-0.0022(12)	0.0007(13)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C8	0.0391~(15)	0.066(2)	0.0511 (16)	0.0083(14)	0.0040(12)	0.0077(14)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C9	0.0389(14)	0.078(2)	0.0445~(15)	0.0075(14)	0.0114(12)	0.0190(14)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C10	0.0467(16)	0.0561~(18)	0.0466~(15)	-0.0039(13)	-0.0032(12)	-0.0037(13)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C11	0.0590(18)	0.0485(17)	0.0536(16)	0.0095(14)	0.0158(14)	0.0081 (13)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C12	0.067(2)	0.064(2)	0.0438(15)	-0.0006(17)	-0.0124(14)	-0.0023(15)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C13	0.0493(18)	0.143(4)	0.0392~(16)	0.020(2)	0.0047(13)	0.014(2)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C14	0.063(2)	0.072(2)	0.085(2)	0.0172(18)	0.0208 (19)	0.038(2)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C101	0.0379(13)	0.0328(12)	0.0344~(12)	0.0009(10)	-0.0009(10)	-0.0009(10)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C102	0.0446(14)	0.0339(13)	0.0361~(12)	0.0073(11)	-0.0013(10)	-0.0012(10)
C104 0.0465 (15) 0.0456 (15) 0.0297 (12) -0.0016 (12) -0.0046 (10) -0.0008 (10) C105 0.0464 (14) 0.0375 (13) 0.0352 (12) -0.0013 (11) 0.0035 (10) -0.0071 (11) C106 0.0266 (12) 0.0272 (12) -0.0013 (11) 0.0047 (10) 0.0006 (10)	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C103	0.0417(14)	0.0408(14)	0.0425~(14)	0.0062~(11)	-0.0068(11)	0.0035(11)
C105 0.0464 (14) 0.0375 (13) 0.0352 (12) -0.0013 (11) 0.0035 (10) -0.0071 (11) C106 0.0260 (12) 0.0225 (12) 0.0272 (12) 0.0060 (10) 0.0047 (10) 0.0000 (10)	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C104	0.0465~(15)	0.0456(15)	0.0297~(12)	-0.0016(12)	-0.0046(10)	-0.0008(10)
$C_{106} = 0.0260(12) = 0.0295(12) = 0.0272(12) = 0.0060(10) = 0.0047(10) = 0.0000(10)$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C105	0.0464(14)	0.0375(13)	0.0352 (12)	-0.0013(11)	0.0035~(10)	-0.0071(11)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C201 0.0376 (13) 0.0329 (12) 0.0377 (13) 0.0033 (10) 0.0012 (10) -0.0020 (12) C202 0.0396 (13) 0.0382 (14) 0.0410 (13) 0.0020 (11) -0.0013 (11) -0.0025 (12) C203 0.0453 (15) 0.0355 (14) 0.0601 (17) -0.0019 (12) 0.0022 (12) 0.0026 (13)	C106	0.0369(13)	0.0325(12)	0.0373(12)	0.0069(10)	-0.0047(10)	0.0000(10)
C201 $0.0376(13)$ $0.0329(12)$ $0.0377(13)$ $0.0033(10)$ $0.0012(10)$ $-0.0020(10)$	C202 0.0396 (13) 0.0382 (14) 0.0410 (13) 0.0020 (11) -0.0013 (11) -0.0025 (12) C203 0.0453 (15) 0.0355 (14) 0.0601 (17) -0.0019 (12) 0.0022 (13) 0.0026 (13)	C201	0.0376~(13)	0.0329(12)	0.0377~(13)	0.0033~(10)	0.0012(10)	-0.0020(10)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C203 0.0453 (15) 0.0355 (14) 0.0601 (17) -0.0010 (12) 0.0092 (12) 0.0026 (1	C202	0.0396~(13)	0.0382(14)	0.0410(13)	0.0020 (11)	-0.0013(11)	-0.0025(11)
$C_{203} = 0.0453(15) = 0.0355(14) = 0.0601(17) = 0.0019(12) = 0.0082(13) = 0.0036(13)$	(253 0.0455 (15) 0.0555 (14) 0.0001 (17) -0.0013 (12) 0.0022 (15) 0.0050 (15)	C203	0.0453 (15)	0.0355(14)	0.0601(17)	-0.0019(12)	0.0082 (13)	0.0036(13)

C204	0.0508(16)	0.0451(16)	0.0556(17)	0.0057(13)	0.0096(13)	0.0178(13)
C205	0.0417(14)	0.0557(17)	0.0403(14)	0.0087(13)	0.0024(11)	0.0075(12)
C206	0.0366(12)	0.0349(13)	0.0397(13)	0.0024(10)	0.0012(10)	-0.0010(10)
C301	0.0394(13)	0.0298(12)	0.0325(11)	0.0033(10)	0.0000(10)	-0.0033(9)
C302	0.0461(14)	0.0308(13)	0.0331(12)	0.0024(11)	0.0015(10)	-0.0010(9)
C303	0.0429(15)	0.0446(15)	0.0445(14)	0.0085(12)	0.0081(12)	-0.0036(12)
C304	0.0507(16)	0.0484(17)	0.0521(16)	-0.0038(13)	0.0161(13)	-0.0001(13)
C305	0.0606(17)	0.0341(14)	0.0477(15)	0.0039(13)	0.0104(13)	0.0061(12)
C306	0.0422(14)	0.0358(14)	0.0399(13)	0.0071(11)	0.0026(11)	-0.0009(10)
C401	0.0373(13)	0.0309(12)	0.0341(11)	0.0044(10)	-0.0012(10)	-0.0003(10)
C402	0.0377(13)	0.0356(13)	0.0352(12)	0.0025(11)	-0.0007(10)	0.0016(10)
C403	0.0519(15)	0.0350(13)	0.0306(11)	0.0022(11)	-0.0018(10)	-0.0003(10)
C404	0.0553(16)	0.0480(16)	0.0327(12)	0.0127(13)	0.0096(11)	0.0011 (11)
C405	0.0400(14)	0.0548(16)	0.0397(14)	0.0036(12)	0.0082(11)	0.0083(12)
C406	0.0426(14)	0.0370(13)	0.0356(12)	-0.0003(11)	-0.0003(10)	-0.0005(10)
B1	0.0364(14)	0.0311(14)	0.0329(13)	0.0036(11)	-0.0029(11)	-0.0020(11)
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Table S3. Geometric parameters (Å, $^\circ)$

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F102—C102	1.354(3)	C10—H102	0.954(18)
F103—C103	1.356(3)	C10—H103	0.965(18)
F104—C104	1.352(3)	C11—H111	0.943(18)
F105—C105	1.346(3)	C11—H112	0.936(18)
F106—C106	1.356(3)	C11—H113	0.950(18)
F202—C202	1.360(3)	C12—H121	0.951(18)
F203—C203	1.345(3)	C12—H122	0.970(18)
F204—C204	1.343(3)	C12—H123	0.944(18)
F205—C205	1.349(3)	C13—H131	0.980(18)
F206—C206	1.355(3)	C13—H132	0.957(18)
F302—C302	1.358(3)	C13—H133	0.975(18)
F303—C303	1.353 (3)	C14—H141	0.969(18)
F304—C304	1.345 (4)	C14—H142	0.960(18)
F305—C305	1.347 (3)	C14—H143	0.975(18)
F306—C306	1.365 (3)	C101—C102	1.390 (4)
F402—C402	1.353 (3)	C101—C106	1.383 (4)
F403—C403	1.342 (3)	C101—B1	1.656(4)
F404—C404	1.343 (3)	C102—C103	1.382 (4)
F405—C405	1.354 (3)	C103—C104	1.363 (4)
F406—C406	1.358 (3)	C104—C105	1.373(4)
O1—C4	1.214 (3)	C105—C106	1.373 (3)
O2—C1	1.282 (3)	C201-C202	1.387(4)
O2—C9	1.520 (4)	C201-C206	1.394(3)
C1—C2	1.455 (4)	C201—B1	1.662(4)
C1—C6	1.447 (4)	C202—C203	1.380(4)
C2—C3	1.355 (4)	C203—C204	1.375(4)
C_{2}^{2} = C10	1 499 (4)	$C_{204} - C_{205}$	1.374(4)
C3—C4	1 488 (4)	C205—C206	1.379(4)
C_{3} — C_{11}	1.493(4)	C301—C302	1.375(1) 1.388(4)
C4-C5	1 491 (4)	C301—C306	1.300(1) 1.391(4)
C5—C6	1.355(4)	C301—B1	1.659(4)
$C_{5}^{-}-C_{12}^{-}$	1.000(4) 1.495(4)	C302—C303	1.005(4) 1.374(4)
C6-C7	1.505(4)	C302 C303	1.374(4) 1.371(4)
C7-C8	1.505(4) 1.518(4)	$C_{304} - C_{305}$	1.371(4) 1.378(4)
C7—H71	0.086(18)	C_{305} C_{306}	1.376(4) 1.374(4)
C7—H72	0.971(17)	C401—C402	1.374(4) 1.388(3)
$C_{1} = 11/2$	1515(4)	C401 - C402	1.386(3)
C8-H81	0.068(18)	C401_B1	1.653(4)
C8_H82	0.966(18)	C402 - C403	1.003(4) 1.388(4)
$C_0 = C_{12}$	1 519 (5)	$C_{402} = C_{403}$	1.333(4)
$C_{9} = C_{13}$	1.518(5)	C403 - C404	1.370(4) 1.265(4)
C10 II101	1.511(5)	C404 - C403	1.303(4) 1.270(4)
C10—H101	0.955 (18)	0405-0406	1.379 (4)
C1 - O2 - C9	123.5(2)	C2-C3-C4	118.8(3)
O2-C1-C2	113.2(2)	C2-C3-C11	124.1(3)
O2-C1-C6	121.8(2)	C4—C3—C11	117.1(2)
C2-C1-C6	125.0(2)	C3—C4—O1	119.9(3)
C1-C2-C3	117.7(2)	C3-C4-C5	120.6(2)
C1— $C2$ — $C10$	117.4(2)	O1-C4-C5	119.5(3)
C3-C2-C10	124.9(3)	C4-C5-C6	119.4(2)

C4-C5-C12	117.7(3)	F105-C105-C106	120.9(2)
C6-C5-C12	122.9(3)	C104-C105-C106	119.0(2)
C1-C6-C5	117.2(3)	F106—C106—C101	119.2(2)
C1 - C6 - C7	119.0(2)	F106-C106-C105	115.5(2)
$C_{5} - C_{6} - C_{7}$	123.7(2) 110.0(2)	C101 - C106 - C105 C202 - C201 - C206	125.3(2) 112.2(2)
C6 - C7 - C8	110.9(2) 107.2(13)	$C_{202} - C_{201} - C_{200}$	112.3(2) 127.3(2)
C8-C7-H71	110.0(13)	C206—C201—B1	127.5(2) 119.8(2)
C6—C7—H72	109.4(13)	F202—C202—C201	120.7(2)
C8—C7—H72	109.3 (13)	F202—C202—C203	114.3 (2)
H71—C7—H72	110.0(15)	C201-C202-C203	125.0(2)
C7—C8—C9	111.4(2)	F203—C203—C202	120.7(2)
C7—C8—H81	109.2(13)	F203—C203—C204	119.6(3)
C7 C8 H82	108.2(13) 100.0(12)	C202 - C203 - C204	119.7(3) 120.7(2)
С1—С8—Н82	109.0(13) 109.7(13)	F204-C204-C205	120.7(3) 120.8(3)
H81—C8—H82	109.3 (15)	C203 - C204 - C205	120.0(3) 118.5(3)
O2—C9—C8	107.2 (2)	F205-C205-C204	119.7 (3)
O2—C9—C13	102.3 (3)	F205—C205—C206	120.6(3)
C8-C9-C13	112.8(3)	C204-C205-C206	119.7(3)
O2—C9—C14	106.0(2)	F206—C206—C201	119.2(2)
C8—C9—C14	114.0(3)	F206—C206—C205	115.9(2)
C13 - C9 - C14 C2 - C10 - H101	113.3(3)	C201 - C206 - C205	124.9(3) 1124(2)
$C_2 = C_{10} = H_{101}$	111.8(14) 109.4(14)	C302—C301—C306	112.4(2) 127.9(2)
H_{101} $-C_{10}$ $-H_{102}$	109.2(14) 109.2(15)	C306—C301—B1	127.3(2) 119.3(2)
C2-C10-H103	109.0(14)	F302—C302—C301	120.3(2)
H101—C10—H103	109.9 (16)	F302—C302—C303	115.3(2)
H102-C10-H103	107.5(16)	C301 - C302 - C303	124.4(2)
C3—C11—H111	111.1 (14)	F303—C303—C302	120.7(2)
C3—C11—H112	110.6(14)	F303—C303—C304	118.9(3)
$H_{111} - C_{11} - H_{112}$ $C_{3} - C_{11} - H_{113}$	109.8 (16) 110.8 (14)	C302 - C303 - C304 F304 - C304 - C303	120.4(2) 121.0(3)
H111-C11-H113	10.8 (14) 108 3 (16)	F304-C304-C305	121.0(3) 120.7(3)
H112—C11—H113	106.1 (16)	C303—C304—C305	118.3(3)
C5—C12—H121	112.1 (14)	F305-C305-C304	119.9 (3)
C5— $C12$ — $H122$	110.5(14)	F305—C305—C306	120.9(3)
H121 - C12 - H122	108.5(16)	C304 - C305 - C306	119.2(2)
C5—C12—H123	109.6(14)	F306—C306—C301	119.0(2)
H121—C12—H123	108.6(16) 107.4(16)	F306—C306—C305	115.6(2) 125.2(2)
C9-C13-H131	107.4(10) 108.9(15)	C402—C401—C406	123.3(2) 113.4(2)
C9—C13—H132	110.0(15)	C402—C401—B1	126.3(2)
H131—C13—H132	109.7 (16)	C406—C401—B1	119.9(2)
C9—C13—H133	110.4(15)	F402—C402—C401	121.2(2)
H131—C13—H133	109.7(16)	F402-C402-C403	114.7(2)
H132—C13—H133	108.0 (17)	C401—C402—C403	124.0(2)
C9—C14—H141	108.5(15)	C402 - C403 - F403	120.5(2)
$H_{141} - C_{14} - H_{142}$	110.6 (15) 109.1 (16)	C402 - C403 - C404 F403 - C403 - C404	119.5(2) 120.0(2)
C9-C14-H143	110.4(15)	F404—C404—C403	120.0(2) 120.4(3)
H141—C14—H143	108.2(16)	F404-C404-C405	120.7(3)
H142-C14-H143	109.9 (16)	C403 - C404 - C405	118.9 (2)
C102-C101-C106	112.9 (2)	F405-C405-C404	120.1(3)
C102—C101—B1	127.9(2)	F405—C405—C406	120.0(3)
C106—C101—B1	118.9(2)	C404-C405-C406	120.0(3)
F102 - C102 - C101	121.1(2) 115.2(2)	F406—C406—C401 F406 C406 C405	119.5(2) 116.2(2)
C102 - C102 - C103	123.6(2)	C401 - C406 - C405	124.2(2)
F103—C103—C102	120.3(2)	C201 - B1 - C301	115.6(2)
F103—C103—C104	119.4 (2)	C201—B1—C101	112.1(2)
C102-C103-C104	120.3 (2)	C301—B1—C101	100.54 (19)
F104-C104-C103	120.8(2)	C201— $B1$ — $C401$	101.34(19)
F104—C104—C105	120.4 (2)	C301—B1—C401	112.8 (2)
C103 - C104 - C105	118.8(2)	C101—B1—C401	115.0(2)
F105-C105-C104	120.0 (2)		
F102—C102—C101—C106	-177.1(2)	F102—C102—C103—F103	-1.6(4)
г 102—С102—С101—В1	-3.5(4)	F102—C102—C103—C104	1(8.7(2))

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F103—C103—	-C102-	-C101	179.4(2)
F103-C103-	-C104-	-F104	-0.6(4)
F103—C103—	-C104-	-C105	179.5(2)
F104-C104-	-C103-	-C102	179.1(2)
F104-C104-	-C105-	-F105	0.3(4)
F104-C104-	-C105-	-C106	-179.7(2)
F105-C105-	-C104-	-C103	-179.8(2)
F105-C105-	-C106-	-F106	1.2(4)
F105-C105-	-C106-	-C101	-178.4(2)
F106—C106—	-C101-	-C102	178.0(2)
F106-C106-	-C101-	-B1	3.7 (3)
F106-C106-	-C105-	-C104	-178.8(2)
F202-C202-	-C201-	-C206	178.1(2)
F202-C202-	-C201-	-B1	7.5(4)
F202-C202-	-C203-	-F203	0.5(4)
F202-C202-	-C203-	-C204	-178.0(3)
F203-C203-	-C202-	-C201	179.6(3)
F203-C203-	-C204-	-F204	0.1(5)
F203-C203-	-C204-	-C205	-179.5(3)
F204—C204—	-C203-	-C202	178.6(3)
F204—C204—	-C205-	-F205	-14(5)
F204—C204—	-C205-	-C206	-178.8(3)
F205-C205-	-C204-	-C203	178.2(3)
F205-C205-	-C206-	-F206	0.9(4)
F205-C205-	-C206-	-C201	-178.2(2)
F206—C206—	-C200	-C201	-178.1(2)
F206—C206—	-C201	-B1	-68(4)
F206—C206—	-C201	-C204	178.2(3)
F302—C302—	-C301-	-C306	-178.6(2)
F302 C302	-C301	-B1	-63(4)
F302—C302—	-C303-	-F303	-10(4)
F302 C302	-C303-	-C304	1.0(4) 179.1(2)
F303_C303_	-C302-	-C301	173.1(2) 178.7(2)
F303-C303-	-C304-	-F304	0.2(4)
F303—C303—	-C304-	-C305	179.9(3)
F304—C304—	-C303-	-C302	-180.0(3)
F304—C304—	-C305-	-F305	0.1(4)
F304—C304—	-C305-	-C306	-1794(3)
F305-C305-	-C304-	-C303	-179.6(3)
F305-C305-	-C306-	-F306	0.7(4)
F305—C305—	-C306-	-C301	-179.7(2)
F306-C306-	-C301-	-C302	178.5(2)
F306-C306-	-C301-	-B1	5.5(3)
F306-C306-	-C305-	-C304	-179.8(2)
F402-C402-	-C401-	-C406	179.2(2)
F402-C402-	-C401-	-B1	7.0 (4)
F402-C402-	-C403-	-F403	-0.0(3)
F402-C402-	-C403-	-C404	179.0(2)
F403-C403-	-C402-	-C401	179.4(2)
F403-C403-	-C404-	-F404	1.2(4)
F403-C403-	-C404-	-C405	-179.2(2)
F404—C404—	-C403-	-C402	-177.8(2)
F404—C404—	-C405-	-F405	0.0(4)
F404—C404—	-C405-	-C406	179.4(2)
F405-C405-	-C404-	-C403	-179.5(2)
F405-C405-	-C406-	-F406	-3.1(4)
F405-C405-	-C406-	-C401	177.6(2)
F406-C406-	-C401-	-C402	-177.4(2)
F406—C406—	-C401-	-B1	-4.7(3)
F406—C406—	-C405-	-C404	177.5(2)
01-C4-C3-	-C2		172.1(3)
01—C4—C3-	-C11		-6.1(4)
01-C4-C5-	-C6		-168.6(3)
01-C4-C5-	-C12		9.0 (4)
02-C1-C2-	-C3		-170.0(2)
02-C1-C2-	-C10		7.9(4)
02-C1-C6-	-C5		173.5(2)
O2-C1-C6-	-C7		-5.0(4)
00			FC 7 (9)
O2-C9-C8-	-C7		-30.7 (3)

C1 - C2 - C9 - C8	33 2 (4)
C1 = 02 = C9 = C8	150.2(4)
C1 = O2 = C9 = C13	152.0(3)
C1 - O2 - C9 - C14	-89.0(3)
C1-C2-C3-C4	-3.0(4)
C1—C2—C3—C11	175.0(3)
C1 - C6 - C5 - C4	-34(4)
	170.0 (9)
C1 - C6 - C5 - C12	179.2(3)
C1 - C6 - C7 - C8	-20.1(3)
C2-C1-O2-C9	178.1(2)
$C_{2}-C_{1}-C_{6}-C_{5}$	-70(4)
02-01-00-05	-1.0 (4)
C2-C1-C6-C7	174.5(3)
C2-C3-C4-C5	-6.7(4)
C3-C2-C1-C6	10.4(4)
$C_{3}-C_{4}-C_{5}-C_{6}$	10.2(4)
$C_{3} - C_{4} - C_{5} - C_{0}$	10.2 (4)
C3 - C4 - C5 - C12	-172.2(3)
C4-C3-C2-C10	179.2(3)
C4-C5-C6-C7	175.1(2)
C5 - C4 - C3 - C11	175 1 (3)
	101 5 (0)
$C_{0} = C_{0} = C_{1} = C_{8}$	101.0(3)
C6-C1-O2-C9	-2.3(4)
C6-C1-C2-C10	-171.6(3)
C6-C7-C8-C9	51 6 (3)
	01.0 (0)
$C_1 - C_0 - C_2 - C_{12}$	-2.3(4)
C7—C8—C9—C13	-168.6(3)
C7—C8—C9—C14	60.3(4)
C10—C2—C3—C11	-2.8(4)
C_{101} C_{102} C_{102} C_{104}	0.2 (4)
0101-0102-0103-0104	-0.3 (4)
C101 - C106 - C105 - C104	1.6(4)
C101—B1—C201—C202	-19.3(4)
C101—B1—C201—C206	170.7(2)
C101—B1—C301—C302	-105.6(3)
C101 B1 C201 C206	66 Q (2)
С101—В1—С301—С306	00.2(3)
C101—B1—C401—C402	-136.1(2)
C101—B1—C401—C406	52.2(3)
C102—C101—C106—C105	-2.5(4)
C_{102} C_{101} B_{1} C_{201}	131.9(3)
C102-C101-B1-C201	101.2 (0)
C102—C101—B1—C301	-105.5(3)
C102—C101—B1—C401	16.1(4)
C102—C103—C104—C105	-0.8(4)
C103—C102—C101—C106	1 8 (4)
C102 C102 C101 C100	175.4(2)
C103—C102—C101—B1	175.4(2)
C103 - C104 - C105 - C106	0.2(4)
C105—C106—C101—B1	-176.7(2)
C106—C101—B1—C201	-55.6(3)
C106 C101 P1 C201	67 9 (2)
C100-C101-B1-C301	07.8(3)
C106—C101—B1—C401	-170.7(2)
C201—C202—C203—C204	1.1(4)
C201—C206—C205—C204	-0.8(4)
C201_B1_C301_C302	15 3 (1)
C201 B1 C001 C002	170.0 (1)
C201—B1—C301—C306	-172.9(2)
C201—B1—C401—C402	102.7(3)
C201—B1—C401—C406	-69.0(3)
C202—C201—C206—C205	0.9(4)
C202 C201 C200 C200	122.9(2)
C202—C201—B1—C301	-133.8 (3)
C202—C201—B1—C401	103.9(3)
C202-C203-C204-C205	-0.9(5)
C203—C202—C201—C206	-1.0(4)
C203—C202—C201—B1	-171.6(3)
C202 C202 C201-D1	111.0 (3)
C203-C204-C205-C206	0.8 (5)
C205—C206—C201—B1	172.2(2)
C206—C201—B1—C301	56.3(3)
C206—C201—B1—C401	-66.1 (3)
C201 C202 C202 C204	1 0 (4)
	-1.2(4)
C301 - C306 - C305 - C304	-0.2(4)
C301 - B1 - C401 - C402	-21.5(3)
C301—B1—C401—C406	166.8(2)
C302—C301—C306—C305	-11(4)
C202 C201 P1 C401	191.9 (9)
C302—C301—D1—C401	131.3 (3)
C302 - C303 - C304 - C305	-0.3(4)

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C303—C302—C301—C306	1.8 (4)	C402— $C401$ — $C406$ — $C405$	1.9(4)
C303—C302—C301—B1	174.0 (2)	C402— $C403$ — $C404$ — $C405$	1.7(4)
C303 - C304 - C305 - C306	0.9(4)	C403— $C402$ — $C401$ — $C406$	-0.2(4)
C305—C306—C301—B1	-174.1 (2)	C403 - C402 - C401 - B1	-172.3(2)
C306—C301—B1—C401	-56.9(3)	C403 - C404 - C405 - C406	-0.2(4)
C401—C402—C403—C404	-1.6(4)	C405 - C406 - C401 - B1	174.5(2)
C401—C406—C405—C404	-1.8(4)		
	Table S4. Conte	act distances (\AA)	
$F102 \cdot \cdot \cdot C3$	3.164(3)	$F206 \cdots O2^{vi}$	3.337(2)
$F102 \cdot \cdot \cdot C11$	3.219 (4)	$F206 \cdot \cdot \cdot C13^{vi}$	3.472 (4)
$F102 \cdot \cdot \cdot C2$	3.335 (3)	$F_{206} \cdot \cdot \cdot C_{10}^{vi}$	3.528(4)
$F102 \cdot \cdot \cdot C10$	3.543(4)	$F_{302} \dots C_{4}^{iii}$	2,900,(3)
$F103 \cdot \cdot \cdot F403^{i}$	2.843(2)	$F_{202} = 01^{iii}$	2.500(3)
$F103 \cdot \cdot \cdot C10$	3.404(4)		2.980(3)
$F104 \cdot \cdot \cdot F406^{ii}$	3.055(2)		3.010 (3)
$F104 \cdot \cdot \cdot C12^{i}$	3.275(4)	$F302 \cdot \cdot \cdot C11^{111}$	3.362(4)
$F104 \cdot \cdot \cdot C406^{ii}$	3.282 (3)	$F302 \cdots C13^{v_1}$	3.510(4)
$F104 \cdots C203^{ii}$	3.346 (3)	$F303 \cdot \cdot \cdot C5$	3.056(3)
$F104 \cdots F405^{ii}$	3357(3)	$F303 \cdot \cdot \cdot C6^{111}$	3.060(3)
$F104 \dots C405^{ii}$	3 386 (4)	$F303 \cdot \cdot \cdot C13^{V1}$	3.323(4)
F104 C202 ⁱⁱ	3.380(4)	$F303 \cdot \cdot \cdot C4^{iii}$	3.508(3)
$F_{104} \cdots C_{202}$	3.460 (3)	$F303 \cdot \cdot \cdot C7^{iii}$	3.515(4)
	3.510(4)	$F303 \cdot \cdot \cdot C12^{iii}$	3.541(4)
F105···C206**	3.106 (3)	$F303 \cdot \cdot \cdot C1^{iii}$	3.549(3)
$F105 \cdots F206$	3.135 (2)	$F304 \cdots F404^{vii}$	3.408 (3)
$F105 \cdots C404^{11}$	3.171(3)	$F305 \cdot \cdot \cdot C7$	3.096(4)
$F105 \cdots C403^{II}$	3.175(3)	$F305 \cdots F404^{vii}$	3.226 (3)
$F105 \cdots C205^{11}$	3.236(4)	$F305 \cdots C8$	3.312(4)
$F105 \cdot \cdot \cdot C405^{11}$	3.237(3)	$F305 \cdot \cdot \cdot C6$	3.474 (3)
$F105 \cdot \cdot \cdot C402^{ii}$	3.288(3)	$F306 \cdot \cdot \cdot C5$	3.120 (3)
$F105 \cdots C406^{ii}$	3.319(3)	$F306 \cdot \cdot \cdot C6$	3.280(3)
$F105 \cdot \cdot \cdot F205^{ii}$	3.396(3)	$F306 \cdot \cdot \cdot C4$	3.399(4)
$F105 \cdot \cdot \cdot C401^{ii}$	3.412(3)	$F306 \cdots C1$	3.598(3)
$F105 \cdot \cdot \cdot C10^{iii}$	3.436(4)	$F402 \cdot \cdot \cdot C10^{V1}$	3.560(3)
F106···C10 ⁱⁱⁱ	3.266 (4)	$F403 \cdots O1$	2.925(3)
$F106 \cdots C11^{iii}$	3 328 (4)	$F403 \cdot \cdot \cdot C10^{V1}$	3.244(4)
$F106 \dots C2^{iii}$	3.424(3)	$F403 \cdot \cdot \cdot C14^{V111}$	3.511(4)
Flog C2 ⁱⁱⁱ	3.424(3)	$F404 \cdots O1$	3.424(3)
	3.470(3)	$F405 \cdots C13^{1X}$	3.068(4)
F 202F 305	3.307(2)	$F405 \cdot \cdot \cdot C8^{1X}$	3.313(4)
	3.509 (3)	$F406 \cdot \cdot \cdot C12^{1V}$	3.543(4)
$F203 \cdots C305$	3.396 (4)	$O1 \cdot \cdot \cdot C403$	2.867(3)
$F203 \cdot \cdot \cdot C304^{1v}$	3.402(4)	$O1 \cdots C404$	3.143 (4)
$F203 \cdots F305^{1v}$	3.475(3)	$O1 \cdots C402$	3.432(3)
$F203 \cdots F304^{1V}$	3.490(3)	$O1 \cdots C14^{v_{111}}$	3.504(4)
$F204 \cdots F404^{111}$	3.251(3)	$C4 \cdots C403$	3.598(4)
$F205 \cdots C105^{\vee}$	3.386(3)	$C13 \cdot \cdot \cdot C303^{1}$	3.550(4)
$F205 \cdot \cdot \cdot C14^{V1}$	3.449(4)	$C104 \cdots C204^{11}$	3.484(4)
$F205 \cdot \cdot \cdot F404^{iii}$	3.473(3)	$C105 \cdots C205^{11}$	3.362(4)
$F205 \cdots C106^{V}$	3.533(3)		
Symmetry codes: (i) $x - \frac{1}{2}$, $\frac{3}{2}$	$-u_{1}z - \frac{1}{2}$; (ii) $x_{1}1 - u_{2}$	x = 1; (iii) $1 + x, y = 1, z$; (iv) $x = 1$	$\frac{1}{2}$, $y = \frac{1}{2}$, z ; (v)

Symmetry codes: (i) $x - \frac{1}{2}, \frac{3}{2} - y, z - \frac{1}{2}$; (ii) $x, 1 - y, z - \frac{1}{2}$; (iii) $\frac{1}{2} + x, y - \frac{1}{2}, z$; (iv) $x - \frac{1}{2}, y - \frac{1}{2}, z$; (v) $x, 1 - y, \frac{1}{2} + z$; (vi) $\frac{1}{2} + x, \frac{3}{2} - y, \frac{1}{2} + z$; (vii) $\frac{1}{2} + x, \frac{3}{2} - y, z - \frac{1}{2}$; (viii) $x, 2 - y, \frac{1}{2} + z$; (ix) $x - \frac{1}{2}, \frac{3}{2} - y, \frac{1}{2} + z$.

Table of Least-Squares Planes

		Plane	numbe	er 1	
Atoms De	efining	Plane		Distance	esd
	C1	(1)	-0.0608	0.0026
	C2	(1)	0.0475	0.0026
	C3	(1)	0.0118	0.0026
	C4	(1)	-0.0656	0.0028
	C5	(1)	0.0470	0.0026
	C6	(1)	0.0109	0.0025
Addition	al Ator	ns		Distance	
	01	(1)	-0.2436	
	02	ì	1)	-0.2217	
	C7	ì	1)	0.0081	
	C8	ì	1)	0.4153	
	C9	ì	1)	-0.4028	
	C10	ì	-, 1)	0.1428	
	C11	ì	1)	0.0034	
	C12	$\tilde{\mathbf{c}}$	1)	0 1392	
	C12		1)	0.1532	
	C14		1)	1 0001	
	C14	(1)	-1.0004	
Mean dev	viation	from p	plane	is 0.0406	angstroms
Chi-squ	lared:	1'	791.2		
		Plane	numbe	er 2	
Atoms De	fining	Plane		Distance	esd
	02	(1)	0.0037	0.0021
	C1	ì	-, 1)	0.0854	0.0026
	C6	ì	1)	-0.0352	0.0025
	C7	(1)	-0 1484	0 0031
	C8	(1)	0 3663	0 0034
	CO		1)	0.2752	0.0034
	09	(1)	-0.2752	0.0034
Addition	al Ator	ns		Distance	
	01	(1)	-0.3001	
	C2	(1)	0.3164	
	C3	(1)	0.2129	
	C4	(1)	-0.0605	
	C5	(1)	-0.0695	
	C10	ĺ	1)	0.6052	
	C11	(1)	0.3147	
	C12	ì	1)	-0.1738	
	C13	ì	1)	0.4069	
		,	,		
Mean dev	viation	from p	plane	is 0.1524	angstroms
Chi-squ	lared:	212	205.3		
Dibodral	anglo	a hotu	oon 1		og planag
DIHEULAI				agt_gauger	
	. anyre:	lanc '	lanc	east-squar	es planes
	p.	lane p	plane	angle	es planes

Table	of	Least-Squares	Planes	(continued)

		Plane	numbe	er 3		
		_ 7				
Atoms	Defining	Plane	:	Dist	ance	esd
	02	(1)	0.	0204	0.0021
	C1	(1)	0.	0056	0.0026
	C6	(1)	-0.	0367	0.0025
	C7	(1)	0.	0510	0.0031
	C9	(1)	-0.	0563	0.0034
Additi	ional Ator	ns		Dist	ance	
	C8	(1)	0.	6543	
	01	ì	1)	-0.	7123	
	C2	ì	1)	0.	0461	
	C3	ì	1)	-0.	1729	
	C4	ì	$\frac{-}{1}$	-0.	3726	
	C5	ì	1)	-0.	1850	
	C10	ì	-, 1)	0.	2807	
	C11	ì	1)	-0.	2703	
	C12	ì	-, 1)	-0.	2268	
	C13	ì	1)	0	6826	
	C14		1)	_1	5271	
	014	(I)	-1.	5271	
Mean d	deviation	from	plane	is O	.0340	angstroms
Chi-s	squared:		865.2			
Dihedı	cal angles	s betw	veen le	east-	squares	s planes
	- g	lane	plane	an	qle	-
	-	3	- 1	7	.88	
		3	2	7	.68	

Figure Captions for (C₁₄H₁₉O₂)⁺(B(C₆F₅)₄)⁻



Figure 1. Molecular structure of the cation of $(C_{14}H_{19}O_2)^+(B(C_6F_5)_4)^-$ with labelling of selected atoms. Anisotropic displacement ellipsoids show 30% probability levels. Hydrogen atoms are drawn as circles with small radii.



Figure 2. Unit cell packing diagram of $(C_{14}H_{19}O_2)^+(B(C_6F_5)_4)^-$ projected down the *a* axis. Hydrogen atoms are not shown.

9 May 2006

Crystal structure of $C_{14}H_{20}O_2$ -web0603

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Abstract

The crystal structure of $C_{14}H_{20}O_2$ is reported.

Comment

The crystallographic asymmetric unit consists of two $C_{14}H_{20}O_2$ molecules.

The structure was solved by direct methods in space group P1, revealing 4 molecules in the unit cell. A centre of inversion was identified [*PLATON*]. Appropriate translations were applied and 2 molecules discarded as redundant. All further refinement was performed in space group $P\bar{1}$.

H atoms bonded to carbon were included at calculated positions with methyl H atoms oriented to best-match peaks in difference electron density maps. They were then refined positionally with restraints being imposed on distances and angles involving them. A difference electron density map at this stage revealed two alternative positions for each alcohol H atom. These were included in refinement with occupancies of 0.5 and refined positionally. A subsequent difference map revealed peaks in the methyl groups attached to sp^2 C atoms. Alternative H sites were therefore added between the original ones and the relative populations refined. These minor sites have not been refined positionally but simply ride on their respective C atoms.

There is hydrogen bonding between the alcohol groups of adjacent molecules giving rise to a chain extending in the a direction. There are two possible connectivities: O1[-x,1-y,1-z]...H11[x,y,z]—O1[x,y,z]... H1012[1-x,1-y,1-z]—O101[1-x,1-y,1-z]...H1011[x,y,z]—O101[x,y,z]... H12[1-x,1-y,1-z]—O101[1-x,1-y,1-z] or O1[-x,1-y,1-z]—H11[-x,1-y,1-z]...O1[x,y,z]—H12[x,y,z]... O101[1-x,1-y,1-z]—H1011[1-x,1-y,1-z]...O1[1-x,1-y,1-z]....O1[1-x,1-y,1-z]...O1[1-x,1-y,1-z]...O1[1-x,1-y,1-z]

The largest peaks in the final difference map are all of near-equal intensity and have no chemical significance.

Experimental

The compound was prepared by SBL and recrystallized from methanol/water. The sample ID is SBL-06–4–26.

Crystal data	
$\mathrm{C}_{14}\mathrm{H}_{20}\mathrm{O}_{2}$	Cell parameters from 12916 reflections
$M_r = 220.31$	$ heta=3 ext{}27^\circ$
Triclinic	$\mu = 0.076 \text{ mm}^{-1}$
$P\overline{1}$	T = 200 K
a = 9.0787(2) Å	Block
$b = 10.7742 (3) \text{\AA}$	Colourless
c = 13.2895(3) Å	$0.48 \times 0.22 \times 0.21 \ \mathrm{mm}$
$\alpha = 91.1222 (16)^{\circ}$	Crystal source: local
$\beta = 103.4637(14)^{\circ}$	
$\gamma = 97.1591 \ (16)^{\circ}$	
$V = 1252.75(5) \text{ Å}^3$	
Z = 4	
$D_x = 1.168 \text{ Mg m}^{-3}$	
D_m not measured	
Mo $K\alpha$ radiation	
$\lambda = 0.71073 \text{ \AA}$	
Data collection	
Nonius KappaCCD diffractometer	4234 reflections with
φ and ω scans with CCD	$I > 2.0\sigma(I)$
Absorption correction:	$R_{\rm int} = 0.034$
by integration via Gaussian method (Cop-	$\theta_{\rm max} = 27.553^{\circ}$
pens, 1970) implemented in maXus (2000) $$	$h = -11 \to 10$
$T_{\rm min} = 0.973, T_{\rm max} = 0.989$	$k = -14 \to 13$
20668 measured reflections	$l = -17 \rightarrow 17$
5745 independent reflections	
Refinement	
Refinement on F^2	Method= Modified Sheldrick $w=1/[\sigma^2(F^2) +$
R(F) = 0.0382	$(0.05P)^2 + 0.09P]$,
$wR(F^2) = 0.0982$	where $P = (\max(F_o^2, 0) + 2F_c^2)/3$
S = 0.9001	$(\Delta/\sigma)_{\rm max} = 0.007584$
5732 reflections	$\Delta \rho_{\rm max} = 0.23 \ {\rm e} \ {\rm \AA}^{-3}$
421 parameters	$\Delta \rho_{\rm min} = -0.27 \ {\rm e} \ {\rm \AA}^{-3}$
H atoms treated by a mixture of independent	Extinction correction: none
and constrained refinement	Scattering factors from International Tables Vol C 4.2.6.8 and 6.1.1.4

	Table 1. Selected geometric	ric parameters (Å, °)	
O1—C4	1.3950(13)	C8—C9	1.5217 (16)
O2—C1	1.3827 (12)	C9—C13	1.5159(16)
O2—C9	1.4566 (12)	C9—C14	1.5207(16)
O101—C104	$1.3923\ (13)$	C101 - C102	1.4012(14)
O102—C101	1.3851 (12)	C101—C106	1.3926(14)
O102—C109	1.4532(12)	C102-C103	1.3963(14)
C1-C2	1.4055~(14)	C102—C110	1.5019(15)
C1—C6	1.3934(14)	C103—C104	1.3979(14)
C2—C3	1.3954(14)	C103—C111	1.5074(15)
C2—C10	1.5084(14)	C104— $C105$	1.3884(15)
C3—C4	$1.3974\ (15)$	C105—C106	1.4023(14)
C3—C11	1.5113(15)	C105—C112	1.5086(15)
C4-C5	$1.3929\ (15)$	C106—C107	1.5112(14)
C5-C6	1.4012 (15)	C107—C108	1.5212(16)
C5—C12	1.5097 (15)	C108—C109	1.5233 (16)
C6—C7	1.5132(14)	C109—C113	1.5172(16)
C7—C8	$1.5202 \ (16)$	C109—C114	1.5200(16)

C1—O2—C9	117.42(8)	C13 - C9 - C14	110.49(10)
C101—O102—C109	116.67(8)	O102—C101—C102	115.28(9)
O2— $C1$ — $C2$	115.63 (9)	O102—C101—C106	122.66 (9)
O2—C1—C6	122.69 (9)	C102—C101—C106	122.06 (9)
C2-C1-C6	121.67(9)	C101 - C102 - C103	118.98(9)
C1— $C2$ — $C3$	118.91 (9)	C101—C102—C110	119.91 (9)
C1—C2—C10	119.96 (9)	C103—C102—C110	121.11 (9)
C3—C2—C10	121.13(9)	C102—C103—C104	118.67 (9)
C2—C3—C4	119.09(9)	C102—C103—C111	121.23(10)
C2—C3—C11	120.68(10)	C104—C103—C111	120.10(10)
C4—C3—C11	120.23(10)	C103—C104—O101	118.70(9)
C3—C4—O1	118.57 (9)	C103 - C104 - C105	122.47(9)
C3-C4-C5	122.08(10)	O101—C104—C105	118.83(10)
O1— $C4$ — $C5$	119.35 (9)	C104-C105-C106	118.91 (9)
C4— $C5$ — $C6$	118.86(9)	C104-C105-C112	120.74(10)
C4— $C5$ — $C12$	121.11(10)	C106-C105-C112	120.35(10)
C6-C5-C12	120.03(10)	C105—C106—C101	118.85 (9)
C5—C6—C1	119.19 (9)	C105 - C106 - C107	120.80(9)
C5-C6-C7	120.66 (9)	C101—C106—C107	120.35(9)
C1—C6—C7	120.15(9)	C106—C107—C108	111.43 (9)
C6—C7—C8	111.53 (9)	C107—C108—C109	111.27 (9)
C7—C8—C9	111.31 (9)	C108—C109—O102	107.72(8)
C8—C9—O2	107.95 (9)	C108—C109—C113	111.45(10)
C8—C9—C13	111.68(10)	O102—C109—C113	104.83(9)
O2—C9—C13	104.50 (9)	C108—C109—C114	113.33(10)
C8—C9—C14	112.69 (9)	O102—C109—C114	108.67~(9)
O2—C9—C14	109.15 (9)	C113—C109—C114	110.42(10)
	Table 2. Hydrogen-bond	ling geometry (\AA, \circ)	

4

D—H···A	D—H	$\mathrm{H}{\cdots}A$	$D \cdots A$	D—H···A
$01 - H11 \cdots O1^i$	0.82(2)	1.90(2)	2.713(2)	171(3)
$O1 - H12 \cdots O101^{ii}$	0.82(2)	1.86(2)	2.683(1)	178(3)
$O101 - H1012 \cdots O1^{ii}$	0.81(2)	1.89(2)	2.683(1)	171(3)
$O101 - H1011 \cdots O101^{ii}$	0.81(2)	1.83(3)	2.634(2)	178(3)

Symmetry codes: (i) -x, 1-y, 1-z; (ii) 1-x, 1-y, 1-z.

PREVIEW (FO)

H atoms were were refined positionally or ride on their respective C atom.

Data collection: *COLLECT* (Nonius BV, 1997). Cell refinement: Denzo/Scalepack . Data reduction: Denzo/Scalepack (Otwinowski & Minor, 1997). Program(s) used to solve structure: *SIR*92 (Altomare *et al.* 1994). Program(s) used to refine structure: *CRYSTALS* (Watkin *et al.*2003). Molecular graphics: *ORTEP*–II (Johnson 1976) in teXsan (MSC, 1992–1997) . Software used to prepare material for publication: *CRYSTALS*.

5

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Supplementary data

		$U = (1/2) \Sigma$	S Uijaiaj-	1 1	(
	2	$U_{\rm eq} = (1/3)\Sigma_i$	$\Sigma_j U^{*j} u^* u^j \mathbf{a}_i . \mathbf{a}_j.$		17
	Occupancy	<i>x</i>	y	<i>Z</i>	$U_{\rm eq}$
01	1.0000	0.12791(10)	0.54457(8)	0.46899(7)	0.0441
02	1.0000	0.08699(9)	0.90889(7)	0.18008(6)	0.0348
0101	1.0000	0.60224(11) 0.46750(0)	0.53152(9)	0.44595(7)	0.0401
0102 C1	1.0000	0.40750(9) 0.10484(11)	0.81200(7)	0.10154(5)	0.0338
Cl	1.0000	0.10464(11) 0.00222(11)	0.82043(9)	0.23443(8)	0.0287
C2	1.0000	0.00232(11) 0.01265(12)	0.70908(10) 0.61527(10)	0.23093(8)	0.0287
C3	1.0000	0.01303(12) 0.12226(12)	0.01527 (10) 0.63680 (10)	0.30218(8) 0.30648(8)	0.0300
C5	1.0000	0.12220(12) 0.22402(12)	0.03030(10) 0.74707(10)	0.39048(8) 0.42001(8)	0.0307
C6	1.0000	0.22402(12) 0.21838(11)	0.83851(10)	0.34617(8)	0.0297
C7	1.0000	0.33517(13)	0.95479(11)	0.36466(9)	0.0362
C8	1.0000	0.32783(13)	1.02695(11)	0.26684(10)	0.0383
C9	1.0000	0.16336(13)	1.03566(10)	0.21056(9)	0.0345
C10	1.0000	-0.11654(13)	0.69213(11)	0.12962(9)	0.0352
C11	1.0000	-0.09070(14)	0.49229(11)	0.27848 (10)	0.0394
C12	1.0000	0.33926 (15)	0.76876(13)	0.52289(9)	0.0429
C13	1.0000	0.15451(17)	1.09984(12)	0.10924 (10)	0.0466
C14	1.0000	0.07666 (14)	1.09927(11)	0.27733(10)	0.0396
C101	1.0000	0.49406(11)	0.73868(9)	0.18630(7)	0.0272
C102	1.0000	0.61672(11)	0.78680(9)	0.26820 (8)	0.0286
C103	1.0000	0.65170(11)	0.71786(10)	0.35652 (8)	0.0298
C104	1.0000	0.56504(12)	0.60172(10)	0.35896(8)	0.0306
C105	1.0000	0.44292(12)	0.55410(10)	0.27816(8)	0.0301
C106	1.0000	0.40484(11)	0.62492(9)	0.19069(8)	0.0281
C107	1.0000	0.26957(13)	0.57898(11)	0.10245(9)	0.0341
C108	1.0000	0.23195(13)	0.68080(12)	0.02654(9)	0.0361
C109	1.0000	0.37633(12)	0.75150(10)	0.00465(8)	0.0332
C110	1.0000	0.70892(13)	0.91026(11)	0.25963(10)	0.0370
CIII	1.0000	0.78058(14) 0.25084(15)	0.76620(12)	0.44772(9)	0.0403
C112 C112	1.0000	0.35284(15) 0.22008(17)	0.42800(11)	0.28378(10)	0.0404
C115 C114	1.0000	0.33998(17) 0.47998(15)	0.65701(13) 0.66722(12)	-0.00055(10)	0.0471
H11	0.5000	0.47228(13) 0.050(2)	0.00733(12) 0.511(3)	-0.03800(10)	0.0390
H19	0.5000	0.030(2) 0.210(2)	0.511(3) 0.520(3)	0.483(2) 0.494(2)	0.0520
H71	1,0000	0.210(2) 0.3178(13)	1.0099(10)	0.434(2) 0.4206(9)	0.0422
H72	1.0000	0.4380 (13)	0.9291(10)	0.3890(9)	0.0422
H81	1.0000	0.3844(13)	1.1124(10)	0.2833(9)	0.0443
H82	1.0000	0.3768 (13)	0.9848 (11)	0.2176(9)	0.0443
H101	0.804(12)	-0.1251(15)	0.7707(12)	0.0974 (10)	0.0417
H102	0.804(12)	-0.2175(15)	0.6618(13)	0.1418 (10)	0.0417
H103	0.804(12)	-0.0933(15)	0.6299(12)	0.0807(10)	0.0417
H111	0.779(13)	-0.0539(16)	0.4286(13)	0.3275(11)	0.0465
H112	0.779(13)	-0.1969(15)	0.5028(13)	0.2824(11)	0.0465
H113	0.779(13)	-0.0923(16)	0.4574(13)	0.2086(11)	0.0465
H121	0.819(13)	0.3093~(16)	0.7147(13)	0.5742(11)	0.0509
H122	0.819(13)	0.3470(16)	0.8578(13)	0.5495(11)	0.0509
H123	0.819(13)	0.4443(16)	0.7531(13)	0.5149(11)	0.0509
H131	1.0000	0.1970(14)	1.1898 (11)	0.1228(9)	0.0538
H132	1.0000	0.0458(14)	1.0959(11)	0.0691(9)	0.0538
H133	1.0000	0.2163(14)	1.0601(11)	0.0674(9)	0.0538
H141	1.0000	0.1308(13)	1.1834(11) 1.0590(11)	0.2986(9)	0.0458
H142	1.0000	0.0080 (13)	1.0520(11) 1.1000(11)	0.3404(9)	0.0458
H143 H1011	1.0000	-0.0261(13)	1.1069(11)	0.2379(9)	0.0458
П1011 П1019	0.5000	0.341(3) 0.687(2)	0.311(3) 0.516(2)	0.480(2)	0.0540
H1012	1.0000	0.007 (2) 0.2030 (12)	0.510(3) 0.5041(10)	0.409(2)	0.0340
H1072	1.0000	0.2939 (13)	0.5041 (10) 0.5515 (10)	0.0004(8)	0.0391
111072	1.0000	0.1797 (12)	0.3313 (10)	0.1300 (8)	0.0391

Table S1. Fractional atomic coordinates and equivalent isotropic displacement parameters (\mathring{A}	2)
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H1081	1.0000	0.1796(13)	0.7415(10)	0.0552 (9)	0.0416
H1082	1.0000	0.1632(12)	0.6444(10)	-0.0402(9)	0.0416
H1101	0.698(12)	0.6951(18)	0.9330(14)	0.1868(11)	0.0443
H1102	0.698(12)	0.8178(16)	0.9054(14)	0.2861(12)	0.0443
H1103	0.698(12)	0.6811(18)	0.9800(14)	0.2985(12)	0.0443
H1111	0.721(13)	0.7777(17)	0.7187(14)	0.5090(11)	0.0482
H1112	0.721(13)	0.8832(16)	0.7642(15)	0.4329(12)	0.0482
H1113	0.721(13)	0.7767(18)	0.8544(13)	0.4675(12)	0.0482
H1121	0.713(13)	0.4055(17)	0.3786(14)	0.3384(12)	0.0476
H1122	0.713(13)	0.3295(18)	0.3782(14)	0.2180(11)	0.0476
H1123	0.713(13)	0.2535(17)	0.4367(14)	0.2999(12)	0.0476
H1131	1.0000	0.2842(14)	0.8226(11)	-0.1357(10)	0.0565
H1132	1.0000	0.4349(14)	0.9085(12)	-0.0738(10)	0.0565
H1133	1.0000	0.2736(14)	0.9103(12)	-0.0409(10)	0.0565
H1141	1.0000	0.4112(13)	0.6204(11)	-0.1010(9)	0.0465
H1142	1.0000	0.5579(13)	0.7170(11)	-0.0555(9)	0.0465
H1143	1.0000	0.5097(13)	0.6050(11)	0.0126(9)	0.0465
H104	0.196(12)	-0.16176(13)	0.60207(11)	0.11744(9)	0.0403
H105	0.196(12)	-0.19888(13)	0.74482(11)	0.13239(9)	0.0403
H106	0.196(12)	-0.06778(13)	0.71829(11)	0.07187(9)	0.0403
H114	0.221(13)	-0.17694(14)	0.50054(11)	0.21764(10)	0.0460
H115	0.221(13)	-0.13240(14)	0.46978(11)	0.34002(10)	0.0460
H116	0.221(13)	-0.03181(14)	0.42521 (11)	0.26210(10)	0.0460
H124	0.181(13)	0.42375(15)	0.83518(13)	0.51700(9)	0.0486
H125	0.181(13)	0.28821 (15)	0.79623 (13)	0.57698 (9)	0.0486
H126	0.181(13)	0.38215(15)	0.68923(13)	0.54284(9)	0.0486
H1104	0.302(12)	0.76604(13)	0.94452(11)	0.33033(10)	0.0429
H1105	0.302(12)	0.78306(13)	0.89804(11)	0.21637(10)	0.0429
H1106	0.302(12)	0.63904(13)	0.97040(11)	0.22646(10)	0.0429
H1114	0.279(13)	0.84494(14)	0.83901(12)	0.42716(9)	0.0467
H1115	0.279(13)	0.84470(14)	0.69819(12)	0.47045(9)	0.0467
H1116	0.279(13)	0.73759(14)	0.79345(12)	0.50605 (9)	0.0467
H1124	0.287(13)	0.25466 (15)	0.41919(11)	0.22955 (10)	0.0482
H1125	0.287(13)	0.33044~(15)	0.42093(11)	0.35380(10)	0.0482
H1126	0.287(13)	0.41371(15)	0.36032(11)	0.27173(10)	0.0482

Table S2. Anisotropic displacement parameters (\mathring{A}^2)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O1	0.0431(5)	0.0463(5)	0.0437(5)	0.0066(4)	0.0103(4)	0.0177(4)
O2	0.0398(4)	0.0283(4)	0.0303(4)	-0.0023(3)	-0.0001(3)	0.0012(3)
O101	0.0488(5)	0.0549(6)	0.0368(5)	0.0133(5)	0.0093(4)	0.0223(4)
O102	0.0404(4)	0.0302(4)	0.0270(4)	0.0034(3)	0.0005(3)	0.0056(3)
C1	0.0287(5)	0.0287(5)	0.0281(5)	0.0045(4)	0.0055(4)	0.0005(4)
C2	0.0255(5)	0.0321(5)	0.0277(5)	0.0030(4)	0.0056(4)	-0.0027(4)
C3	0.0278(5)	0.0309(5)	0.0316(5)	0.0028(4)	0.0089(4)	-0.0008(4)
C4	0.0283(5)	0.0343(6)	0.0307(5)	0.0068(4)	0.0079(4)	0.0055(4)
C5	0.0274(5)	0.0354~(6)	0.0302(5)	0.0071(4)	0.0031(4)	-0.0009(4)
C6	0.0265(5)	0.0305(5)	0.0306(5)	0.0041(4)	0.0037(4)	-0.0028(4)
C7	0.0293(5)	0.0334(6)	0.0402~(6)	0.0009(5)	-0.0007(5)	-0.0032(5)
C8	0.0331~(6)	0.0331~(6)	0.0451(7)	-0.0030(5)	0.0061(5)	-0.0004(5)
C9	0.0366~(6)	0.0269(5)	0.0352~(6)	-0.0026(4)	0.0029(5)	-0.0003(4)
C10	0.0329(6)	0.0369(6)	0.0310(6)	-0.0014(5)	0.0013(5)	-0.0022(5)
C11	0.0404~(6)	0.0351~(6)	0.0395~(6)	-0.0043(5)	0.0077(5)	0.0011(5)
C12	0.0425(7)	0.0431(7)	0.0357~(6)	0.0035(5)	-0.0041(5)	0.0026~(5)
C13	0.0573(8)	0.0364(7)	0.0398(7)	-0.0059(6)	0.0051~(6)	0.0049(5)
C14	0.0374~(6)	0.0342~(6)	0.0429(7)	0.0039(5)	0.0016(5)	-0.0019(5)
C101	0.0294(5)	0.0277(5)	0.0254(5)	0.0068(4)	0.0063(4)	0.0037(4)
C102	0.0283(5)	0.0280(5)	0.0297(5)	0.0046(4)	0.0070(4)	0.0015(4)
C103	0.0282(5)	0.0348(6)	0.0268(5)	0.0074(4)	0.0059(4)	0.0005(4)
C104	0.0323(5)	0.0354~(6)	0.0274(5)	0.0105(4)	0.0099(4)	0.0084(4)
C105	0.0321(5)	0.0294(5)	0.0313(5)	0.0053(4)	0.0115(4)	0.0036(4)
C106	0.0280(5)	0.0295(5)	0.0274(5)	0.0049(4)	0.0073(4)	0.0003(4)
C107	0.0313(6)	0.0365~(6)	0.0322~(6)	-0.0004(5)	0.0059(5)	-0.0015(5)
C108	0.0310(6)	0.0447(7)	0.0299(6)	0.0070(5)	0.0011(4)	-0.0010(5)
C109	0.0361~(6)	0.0356~(6)	0.0252(5)	0.0060(5)	0.0009(4)	0.0026~(4)
C110	0.0346(6)	0.0328~(6)	0.0398~(6)	-0.0003(5)	0.0033(5)	0.0031(5)
C111	0.0379(6)	0.0468(7)	0.0321~(6)	0.0062(5)	0.0000(5)	-0.0006(5)
C112	0.0458(7)	0.0333~(6)	0.0413(7)	-0.0003(5)	0.0115(5)	0.0073(5)
C113	0.0556(8)	0.0471(7)	0.0345(6)	0.0111(6)	-0.0006(6)	0.0114(6)
C114	0.0415(7)	0.0433(7)	0.0352(6)	0.0048(5)	0.0120(5)	0.0013(5)

O1—C4	1.3950(13)	C13—H132	1.002(12)
O1—H11	0.814(15)	C13—H133	1.001(12)
O1—H12	0.818(17)	C14—H141	0.978 (11)
01 1112	1 2027 (12)		1.000(11)
02-01	1.3827 (12)	C14—n142	1.002 (11)
O2—C9	1.4566(12)	C14—H143	0.972(11)
O101—C104	1.3923(13)	C101—C102	1.4012(14)
O101—H1011	0.813(15)	C101—C106	1.3926(14)
O101—H1012	0.802(17)	C102—C103	1.3963 (14)
0102 C101	1.2851(12)	C102 C110	1.5000 (11) 1.5010 (15)
0102-0101	1.3651(12)	C102-C110	1.0019(10)
0102—C109	1.4532(12)	C103—C104	1.3979 (14)
C1-C2	1.4055(14)	C103—C111	1.5074(15)
C1—C6	1.3934(14)	C104—C105	1.3884(15)
C2-C3	1.3954 (14)	C105—C106	1.4023 (14)
C_{2} C_{10}	15084(14)	C105 - C112	15086(15)
	1.0054 (15)	C100 C112	1.50000(10)
03-04	1.3974 (15)	0106-0107	1.5112(14)
C3—C11	1.5113(15)	C107—C108	1.5212(16)
C4-C5	1.3929(15)	C107—H1071	1.004(10)
C5-C6	1.4012(15)	C107—H1072	0.990(10)
C5-C12	1 5097 (15)	C108—C109	1 5233 (16)
C6 C7	1.5057(10)	C108 U1081	1.0255(10)
00-01	1.5152(14)	C108—111081	0.975(11)
07-08	1.5202(16)	C108—H1082	0.998 (11)
C7—H71	0.995(11)	C109—C113	1.5172(16)
C7—H72	0.990 (11)	C109—C114	1.5200(16)
C8—C9	1.5217(16)	C110—H1101	0.986(14)
C8_H81	0.000(11)	C110_H1102	0.077(14)
Co	1.000 (11)	C110-111102	0.377(14)
C8—H82	1.002 (11)	C110—H1103	0.994(14)
C9—C13	1.5159(16)	C110—H1104	1.000
C9—C14	1.5207(16)	C110—H1105	1.000
C10—H101	0.959(13)	C110—H1106	1.000
C10—H102	0.985 (13)	С111—Н1111	0.974(14)
C10 H102	0.000(10)	C111 H1112	0.000(14)
C10—11103	0.999 (12)	C111—III112	0.999(14)
C10—H104	1.000	С111—Н1113	0.988(14)
C10—H105	1.000	C111—H1114	1.000
C10—H106	1.000	C111—H1115	1.000
C11—H111	0.990(13)	C111—H1116	1.000
C11_H112	0.998 (13)	C112_H1121	0.978(14)
C11 II112	0.001 (12)	C112 III121	0.070(11)
	0.991 (13)	C112—H1122	0.982(14)
C11—H114	1.000	C112—H1123	0.988(14)
C11—H115	1.000	C112—H1124	1.000
C11—H116	1.000	C112—H1125	1.000
C12—H121	0.970(13)	C112—H1126	1.000
C12H122	1.004 (13)	C113_H1131	0.083(12)
C12—11122	1.004 (13)	C113—11131 C119—11199	0.963(12)
C12—H123	1.018 (13)	C113—H1132	0.988(12)
C12—H124	1.000	C113—H1133	0.987(12)
C12—H125	1.000	C114—H1141	0.980(11)
C12—H126	1.000	C114—H1142	0.964(11)
C13—H131	0.994(12)	C114—H1143	0.994(11)
010 11101	01001 (12)	0111 11110	01001 (11)
C4—O1—H11	121(2)	C4-C5-C6	118.86(9)
C4—O1—H12	119 (2)	C4-C5-C12	121.11(10)
H11-01-H12	120 (3)	C6-C5-C12	120.03 (10)
$C_{1} = C_{2} = C_{0}$	117 42 (8)	$C_{5} - C_{6} - C_{1}$	110 10 (0)
C1-02-09	101 (0)	05-00-01	119.19(9)
C104—O101—H1011	121 (2)	05-06-07	120.66(9)
C104—O101—H1012	122 (2)	C1-C6-C7	120.15(9)
H1011—O101—H1012	116 (3)	C6-C7-C8	111.53(9)
C101-O102-C109	116.67 (8)	C6—C7—H71	109.8(7)
02 - C1 - C2	115.63 (9)	C8—C7—H71	109.6 (6)
$O_2 C_1 C_6$	122.60(0)	C6 C7 H79	108.4(7)
	122.09 (9)	C0-C7-H72	108.4(7)
02-01-06	121.07 (9)	U8-U7-H72	110.0 (7)
C1-C2-C3	118.91 (9)	H71—C7—H72	107.4(9)
C1— $C2$ — $C10$	119.96 (9)	C7—C8—C9	111.31(9)
C3-C2-C10	121.13 (9)	C7—C8—H81	110.8 (7)
C2—C3—C4	119.09 (9)	C9—C8—H81	109.4(7)
C_{2} C_{3} C_{11}	120.68(10)	C7_C8_H82	110.0 (7)
	120.00 (10)		10.9(1)
C4—C3—C11	120.23(10)	C9—C8—H82	107.6(7)
C3-C4-O1	118.57(9)	H81—C8—H82	106.7(9)
C3-C4-C5	122.08 (10)	C8—C9—O2	107.95 (9)
O1—C4—C5	119.35 (9)	C8—C9—C13	111.68 (10)

Table S3. Geometric parameters (\mathring{A}, \circ)

O2—C9—C13

C8---C9---C14

 ${\rm O2-C9-C14}$

O102 - C101 - C102

O102-C101-C106

C102—C101—C106

C101 - C102 - C103

 ${\rm C101}{--}{\rm C102}{--}{\rm C110}$

		4
	t	4
	÷	2

C103—C102—C110

C102-C103-C104

 ${\rm C102}{--}{\rm C103}{--}{\rm C111}$

C105-C112-H1126

H1124—C112—H1126

H1125—C112—H1126

C109—C113—H1131

 ${\rm C109}{--}{\rm C113}{--}{\rm H1132}$

S45

121.11(9)

118.67 (9)

121.23(10)

120.10 (10) 118.70 (9) 122.47 (9) 118.83 (10) 118.91 (9)120.74 (10) 120.35 (10) 118.85 (9) 120.80 (9) 120.35(9)111.43 (9) 108.5(6)110.4 (6) 109.3(6)109.4(6)107.7 (8) 111.27 (9) 110.2(7)107.6(7)110.8(6)109.1 (6) 107.8 (9) 107.72 (8) 111.45 (10) 104.83(9)113.33 (10) 108.67 (9) 110.42 (10) 111.3(9)110.2(9)106.7 (12) 112.6 (9) 107.5 (11) 108.3(11)109.5109.5109.5109.5109.5109.5112.2(9)112.5(9)107.5 (11) 111.6(9)106.6 (11) 105.9(11)109.5109.5109.5109.5109.5109.5112.5(9)112.3 (9) 108.3(12)111.4(9)105.7 (11) 106.3 (11) 109.5109.5

109.5

109.5

109.5

109.5

109.3(7)

110.6(7)

104.50(9)

112.69(9)

109.15(9)

C13—C9—C14	110.49 (10)	C104—C103—C111
C2-C10-H101	110.5 (8)	C103—C104—O101
C2-C10-H102	110.1 (8)	C103—C104—C105
H101—C10—H102	107.0 (10)	O101-C104-C105
C2-C10-H103	112.1 (8)	C104—C105—C106
H101-C10-H103	109.5 (10)	C104—C105—C112
H102—C10—H103	107.5 (10)	C106-C105-C112
C2-C10-H104	109.5	C105-C106-C101
C2-C10-H105	109.5	C105—C106—C107
H104—C10—H105	109.5	C101—C106—C107
C2-C10-H106	109.5	C106—C107—C108
H104—C10—H106	109.5	C106—C107—H1071
H105-C10-H106	109.5	C108—C107—H1071
C3—C11—H111	111.3 (8)	C106—C107—H1072
C3-C11-H112	111.2 (8)	C108-C107-H1072
H111—C11—H112	108.4 (11)	H1071-C107-H1072
C3—C11—H113	110.5 (8)	C107—C108—C109
H111—C11—H113	106.0(11)	C107—C108—H1081
H112—C11—H113	109.4 (11)	C109—C108—H1081
C3-C11-H114	109.5	C107—C108—H1082
H111—C11—H114	139.3	C109 - C108 - H1082
H112-C11-H114	54.9	H1081 - C108 - H1082
H113—C11—H114	58 7	C108 - C109 - O102
C3—C11—H115	109.5	C108 - C109 - C113
H114—C11—H115	109.5	0102 - C109 - C113
C3-C11-H116	109.5	C102 = C109 = C114
H114—C11—H116	109.5	0102 - C109 - C114
H115—C11—H116	109.5	C113 - C109 - C114
C5-C12-H121	111.2 (8)	C102 - C110 - H1101
C5-C12-H122	110.0(8)	C102 - C110 - H1102
H121_C12_H122	107.8(11)	H1101_C110_H1102
C5-C12-H123	110 4 (8)	C102—C110—H1103
H121_C12_H123	109.3(11)	H1101_C110_H1103
H122 C12 H123	108.1(10)	H1102-C110-H1103
C_{5} C_{12} H_{123}	100.5	C102_C110_H1104
H121_C12_H124	139.4	C102 - C110 - H1104
H122 C12 H124	56.8	H1104-C110-H1105
H122 C12 H124	54.7	C102—C110—H1106
C5_C12_H125	109.5	H1104 - C110 - H1106
H121-C12-H125	55.9	H1105-C110-H1106
H122 - C12 - H125	55.5	C103—C111—H1111
H123 - C12 - H125	140.1	C103—C111—H1112
H124 - C12 - H125	109.5	H1111—C111—H1112
C5-C12-H126	109.5	C103—C111—H1113
H121-C12-H126	56.0	H1111—C111—H1113
H122 - C12 - H126	140.5	H1112-C111-H1113
H122 C12 H126	57 /	C103—C111—H1114
H124-C12-H126	109.5	C103—C111—H1115
H124 - C12 - H120 H125 - C12 - H126	109.5	H_{1114} C_{111} H_{1115}
C0_C13_H131	109.3 110.2 (7)	C_{103} C_{111} H_{1116}
C_{9} C_{13} H_{132}	110.2(7)	H_{1114} C_{111} H_{1116}
H131-C13-H132	107.4(10)	H1115_C111_H1116
C9-C13-H133	109.9(7)	C105-C112-H1121
H131—C13—H133	108.0(1)	C105—C112—H1121
H132_C13_H133	110.5 (10)	H1121_C112_H1122
C_{0} C14 H141	108 1 (7)	C105_C112_H1122
C_{0} C_{14} H_{142}	112.2(7)	H1121_C112_H1123
H141_C14_H142	1094(9)	H1122-C112-H1123
C0_C14_H142	110.4(7)	$C_{105} - C_{112} - H_{1124}$
H141_C14_H143	1085(9)	C105 - C112 - H1124 C105 - C112 - H1125
Ш149 C14 Ш149	108.9 (0)	U1104 C112 U1125
11174 -014-11140	100.4 (3)	111124 0112 111120

115.28(9)

122.66 (9)

122.06 (9)

118.98 (9)

119.91 (9)

H1131—C113—H1132	107.8(10)	C109—C114—H1142	110.1(7)
C109—C113—H1133	110.8 (7)	H1141—C114—H1142	108.1(9)
H1131—C113—H1133	107.5 (10)	C109—C114—H1143	111.2 (7)
H1132—C113—H1133	110.8 (10)	H1141—C114—H1143	107.2 (9)
C109-C114-H1141	110.4 (7)	H1142—C114—H1143	109.7(9)
O1-C4-C3-C2	177.2 (1)	C5-C4-C3-C11	177.8(1)
O1-C4-C3-C11	-2.3(2)	C5-C6-C7-C8	168.3(1)
O1-C4-C5-C6	179.3 (1)	C6-C1-O2-C9	-15.8(2)
O1-C4-C5-C12	-0.5(2)	C6— $C1$ — $C2$ — $C10$	-178.6(1)
O2— $C1$ — $C2$ — $C3$	179.8(1)	C6-C7-C8-C9	43.5(1)
O2— $C1$ — $C2$ — $C10$	0.3(2)	C7-C6-C5-C12	5.0(2)
O2-C1-C6-C5	176.8(1)	C7-C8-C9-C13	-176.2(1)
O2-C1-C6-C7	-4.1(2)	C7-C8-C9-C14	58.8(1)
O2-C9-C8-C7	-61.8(1)	C10-C2-C3-C11	1.6(2)
O101 - C104 - C103 - C102	178.4(1)	C101—O102—C109—C108	50.3(1)
O101—C104—C103—C111	-1.2(2)	C101—O102—C109—C113	169.1(1)
O101 - C104 - C105 - C106	179.7(1)	C101—O102—C109—C114	-72.9(1)
O101 - C104 - C105 - C112	-0.6(2)	C101 - C102 - C103 - C104	1.5(2)
O102 - C101 - C102 - C103	-179.8(1)	C101—C102—C103—C111	-178.9(1)
O102—C101—C102—C110	-0.3(2)	C101 - C106 - C105 - C104	2.2(2)
O102—C101—C106—C105	177.9(1)	C101-C106-C105-C112	-177.5(1)
O102—C101—C106—C107	-2.0(2)	C101-C106-C107-C108	-11.0(2)
O102—C109—C108—C107	-62.5(1)	C102-C101-O102-C109	161.4(1)
C1 - O2 - C9 - C8	47.8 (1)	C102 - C101 - C106 - C105	-2.6(2)
C1 - O2 - C9 - C13	166.8(1)	C102-C101-C106-C107	177.5(1)
C1—O2—C9—C14	-75.0(1)	C102 - C103 - C104 - C105	-1.9(2)
C1—C2—C3—C4	2.6(2)	C103 - C102 - C101 - C106	0.7(2)
C1-C2-C3-C11	-177.9(1)	C103 - C104 - C105 - C106	0.0(2)
C1—C6—C5—C4	4.3 (2)	C103 - C104 - C105 - C112	179.7(1)
C1 - C6 - C5 - C12	-175.8(1)	C104 - C103 - C102 - C110	-178.0(1)
C1_C6_C7_C8	-10.9(2)	C104-C105-C106-C107	-177.9(1)
$C_2 - C_1 - O_2 - C_9$	165.3(1)	C105-C104-C103-C111	178.5(1)
$C_2 = C_1 = C_6 = C_5$	-4.4(2)	C105 - C106 - C107 - C108	169.1(1)
$C_2 = C_1 = C_6 = C_7$	174.7(1)	C106 - C101 - O102 - C109	-19.2(2)
$C_2 = C_3 = C_4 = C_5$	-2.7(2)	C106 - C101 - C102 - C110	-179.8(1)
$C_3 = C_2 = C_1 = C_6$	0.9(2)	C106 - C107 - C108 - C109	42.8(1)
C_{3} C_{4} C_{5} C_{6}	-0.8(2)	C107 - C106 - C105 - C112	2.4(2)
C_{3} C_{4} C_{5} C_{12}	179.3(1)	C107 - C108 - C109 - C113	-177.0(1)
C4 - C5 - C2 - C10	-177.9(1)	C107 - C108 - C109 - C114	$\frac{37.7}{1.6}$
04-05-06-07	-174.8(1)	0110-0102-0103-0111	1.0 (2)
	Table S4. Conte	$act\ distances\ (\AA)$	
$O1 \cdot \cdot \cdot O101^{i}$	2.683(1)	$O101 \cdots C112^{i}$	3.531(2)
$O1 \cdots O1^{ii}$	2.713 (2)	$O101 \cdots C104^{i}$	3.539(2)
$O1 \cdot \cdot \cdot C11^{ii}$	3.476(2)	$O101 \cdots C4^{i}$	3.573 (1)
$O101 \cdot \cdot \cdot O101^{i}$	2.634(2)	$C10 \cdots C102^{iii}$	3.594(2)
$O101 \dots C12^{i}$	3361(2)	010 010-	5.001 (2)
0101012	3.301 (2)		

Symmetry codes: (i) 1 - x, 1 - y, 1 - z; (ii) -x, 1 - y, 1 - z; (iii) x - 1, y, z.

Table of Least-Squares Planes

		Plane	numbe	er 1	
Atoms	Defining	Plane		Distance	esd
	C1	(1)	-0.0151	0.0011
	C2	(1)	-0.0083	0.0012
	C3	(1)	0.0226	0.0012
	C4	(1)	-0.0097	0.0012
	C5	(1)	-0.0165	0.0012
	C6	(1)	0.0274	0.0012
Additi	ional Ator	ns		Distance	
	01	(1)	-0.0391	
	02	(1)	-0.0421	
	C7	(1)	0.1395	
	C8	(1)	0.4572	
	C9	(1)	-0.3783	
	C10	(1)	-0.0224	
	C11	(1)	0.0785	
	C12	(1)	-0.0664	
	C13	(1)	-0.0027	
	C14	(1)	-1.8729	
Mean d Chi-s	deviation squared:	from 1	plane 400.1	is 0.0166	angstroms
		Plane	numbe	er 2	
Atoms	Defining	Plane		Distance	esd
	02	(1)	0.0793	0.0009
	C1	(1)	0.0387	0.0011
	C6	(1)	-0.0770	0.0012
	C7	(1)	-0.0709	0.0013
	C8	(1)	0.3331	0.0014
	C9	(1)	-0.3518	0.0013
Additi	ional Ator	ns		Distance	
	01	(1)	-0.1600	
	C2	(1)	0.1470	
	C3	(1)	0.1180	
	C4	(1)	-0.0727	
	C5	(1)	-0.1802	
	C10	(1)	0.3033	
	C11	ì	1)	0.2785	
	C12	(1)	-0.4007	
	C13	(1)	0.1156	
	C14	(1)	-1.8687	
Mean d	deviation	from	plane	is 0.1585	angstroms
Chi-s	squared:	147	967.0		
Dihedı	cal angles	s betw	een le	east-square	es planes
	p.	lane	plane	angle	
		2	1	6.57	

		Plane	e numbe	er 3	
Ntoma Do	finina	Dlanc		Dictore	ogd
ACOMS De			1)		
	02	(1) 1)	-0.0034	0.0009
		(1) 1)	0.0175	0.0011
	07	(1)	-0.01/3	0.0012
	C7	(1)	0.0106	0.0013
Addition	al Ator	ns		Distance	
	01	(1)	-0.0017	
	C2	ì	1)	0.1037	
	C3	ì	1)	0.1356	
	C4	ì	1)	0.0256	
	C5	ì	1)	-0.0599	
	C8	ì	1)	0.3420	
	C9		1)	_0 4191	
	C10		1)	0 1718	
	C10 C11	(1)	0.2752	
		(1) 1)	0.2755	
		(1)	-0.1928	
	C13	(1)	-0.0255	
	C14	(1)	-1.9270	
Mean dev Chi-squ	iation ared:	from	plane 565.0	is 0.0127	angstroms
Dibodral	angla	- hote	roon 1	ant aguar	
Dinedial	angres	s Detw lana	veen Ie	east-square	es planes
	р.	Lane	prane	angre	
		3	1	3.08	
		3	Z	3.47	
		Plane	e numbe	er 4	
Atoms De	fining	Plane	9	Distance	esd
	C101	(1)	0.0098	0.0011
	C102	ì	1)	0.0036	0.0011
	C103	ì	1)	-0.0131	0.0012
	C104	ì	$\frac{-}{1}$	0.0085	0.0012
	C105	ì	-)	0.0075	0.0012
	C106	ì	1)	-0.0155	0.0011
		`	,		
Addition	al Ator	ns		Distance	
	0101	(1)	0.0252	
	0102	(1)	0.0316	
	C107	(1)	-0.0653	
	C108	(1)	-0.3503	
	C109	(1)	0.4539	
	C110	(1)	0.0262	
	C111	Ì	1)	-0.0457	
	C112				
		(1)	0.0376	
	C112	(1) 1)	0.0376 0.1178	
	C113 C114	((1) 1) 1)	0.0376 0.1178 1.9546	
Mean dev Chi-squ	C113 C114 iation ared:	(((from	1) 1) 1) plane 499.0	0.0376 0.1178 1.9546 is 0.0097	angstroms
Mean dev Chi-squ	C113 C114 iation ared:	(((from	1) 1) 1) plane 499.0	0.0376 0.1178 1.9546 is 0.0097	angstroms
Mean dev Chi-squ Dihedral	C112 C113 C114 iation ared: angles	((from s betw	1) 1) 1) plane 499.0	0.0376 0.1178 1.9546 is 0.0097	angstroms es planes
Mean dev Chi-squ Dihedral	C113 C114 iation ared: angles	((from s betw lane	1) 1) 1) plane 499.0 ween le plane	0.0376 0.1178 1.9546 is 0.0097 east-square angle	angstroms es planes
Mean dev Chi-squ Dihedral	C113 C114 iation ared: angles pi	((from s betw lane 4	1) 1) 1) plane 499.0 veen le plane 1	0.0376 0.1178 1.9546 is 0.0097 east-square angle 2.94	angstroms es planes
Mean dev Chi-squ Dihedral	C113 C114 iation ared: angles	((from s betw lane 4 4	1) 1) 1) plane 499.0 veen lo plane 1 2	0.0376 0.1178 1.9546 is 0.0097 east-square angle 2.94 6.19	angstroms es planes

Table of Least-Squares Planes (continued)

	Plane	numbe	er	5	
Atoms Defining	Plane		Die	tance	esd
0102	(1)	-0	0.0974	0.0009
C101	ì	1)	-0	0.0184	0.0011
C106		1)	-0	0788	0 0011
C100		1)	0	0571	0.0011
C108		1)	0	1 3/32	0.0013
C100		1)	-0	3432	0.0014
0109	(I)	U	.3472	0.0012
Additional Ator	ns		Dis	stance	
0101	(1)	0	.2818	
C102	Ì	1)	-0	.0543	
C103	ì	1)	0	.0252	
C104	ì	1)	0	.1694	
C105	ì	1)	0	.1981	
C110	ì	1)	_0	1654	
C110 C111		1)	-0	0330	
C112		1)	-0	2619	
C112 0112	(1) 1)	0	1052	
C113	(1)	-0	0.1053	
C114	(1)	T	.8639	
Mean deviation Chi-squared:	from 168	plane 641.9	is	0.1570	angstroms
Dihedral angles	s hetw	een le	aat	-square	s planes
n'	lane	nlane	aust	nale	5 prunes
Р.	5	1	0	Q 21	
	5	2		0.47	
	J	2		9.47	
	5	3 1		5 33	
	5	-		5.55	
	Plane	numbe	er	6	
Atoms Defining	Plane		Dis	stance	esd
0102	(1)	0	.0025	0.0009
C101	ì	$1\hat{)}$	-0	.0083	0.0011
C106	ì	$\frac{-}{1}$	0	.0084	0.0011
C107	(1)	-0	.0054	0.0013
Additional Ator	ns	.	Dis	stance	
0101	(1)	0	0.0317	
C102	(1)	-0	0.0487	
C103	(1)	-0	0.0571	
C104	(1)	0	.0068	
C105	(1)	0	.0397	
C108	(1)	-0	.3066	
C109	(1)	0	.4573	
C110	(1)	-0	.0708	
C111	(1)	-0	.1252	
C112	ì	1)	0	.1149	
C113	ì	1)	0	.1038	
C114	ì	1)	1	.9635	
	-	_			
Mean deviation Chi-squared:	from	plane 140.5	is	0.0062	angstroms

Table of Least-Squares Planes (continued)

Dihedral angles between least-squares planes

plane	plane	angle
6	1	4.68
6	2	5.93
6	3	2.90
6	4	1.82
6	5	4.03

Figure Captions for C₁₄H₂₀O₂



Figure 1. Structure of molecule one of $C_{14}H_{20}O_2$ with labelling of selected atoms. Anisotropic displacement ellipsoids show 30% probability levels. Hydrogen atoms are drawn as circles with small radii; only the major sites are shown for methyl groups, but both half-occupancy sites are displayed for alcohol hydrogens.



Figure 2. Structure of molecule two of $C_{14}H_{20}O_2$ with labelling of selected atoms. Anisotropic displacement ellipsoids show 30% probability levels. Hydrogen atoms are drawn as circles with small radii; only the major sites are shown for methyl groups, but both half-occupancy sites are displayed for alcohol hydrogens.



Figure 3. Unit cell packing diagram of $C_{14}H_{20}O_2$ projected down the *a* axis. Hydrogen atoms are drawn as circles with small radii; only the major sites are shown for methyl groups, but both half-occupancy sites are displayed for alcohol hydrogens.



Figure 4. Unit cell packing diagram of $C_{14}H_{20}O_2$ projected down the *b* axis, showing hydrogenbonding. Hydrogen atoms are drawn as circles with small radii; only the major sites are shown for methyl groups, but both half-occupancy sites are displayed for alcohol hydrogens.