2,8'-Disubstituted-1,1'-Binaphthyls

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Supporting Information:

2,8'-Disubstituted-1,1'-Binaphthyls: A New Pattern in Chiral Ligands

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1. Quantum Chemistry Calculations

Optimized structures of **18** (DFT-B3LYP with 6-31G** basis set; Cartesian coordinates in Ångströms)

Ground State

C	-1.781039	-0.482796	-1.005993
C	-1.720281	0.457067	0.073744
C	-0.568011	0.792728	0.869914
C	0.781018	0.149143	0.757714
C	1.849891	0.792252	0.066154
C	1.678627	2.022196	-0.632080
C	2.727990	2.613261	-1.297416
C	4.010470	2.012132	-1.307606
C	4.210330	0.821235	-0.650548
C	3.148272	0.181628	0.043965
C	3.333205	-1.047998	0.720128
C	2.298998	-1.654920	1.394871
C	1.017367	-1.053236	1.416785
C	-0.681667	1.761893	1.853150
C	-1.891463	2.430870	2.126817
C	-3.011976	2.111830	1.404827
C	-2.962935	1.133808	0.376911
C	-4.148809	0.838524	-0.344819
C	-4.149150	-0.090367	-1.353751
C	-2.949408	-0.749328	-1.687682
Br	-0.256102	-1.447942	-1.662715

O	-0.053325	-1.605396	2.061315
H	0.701680	2.492672	-0.634098
H	2.571523	3.550696	-1.823551
H	4.828872	2.491800	-1.836134
H	5.188303	0.346266	-0.653012
H	4.315038	-1.513857	0.705741
H	2.470857	-2.593763	1.906827
H	0.200378	1.998978	2.439792
H	-1.929239	3.181552	2.910360
H	-3.961180	2.602178	1.602571
H	-5.058669	1.368834	-0.078469
H	-5.056460	-0.317827	-1.904571
H	-2.933556	-1.470769	-2.496009
C	0.095476	-2.873480	2.678857
H	0.382709	-3.646569	1.955350
H	0.831872	-2.849146	3.492480
H	-0.883401	-3.118563	3.093584

Transition State

C	-2.338362	0.121466	0.388809
C	-1.239036	0.983946	0.073394
C	0.061021	0.681105	-0.532700
C	1.094770	-0.344188	-0.126867
C	2.472668	0.121781	0.018632
C	2.836836	1.493559	0.190662
C	4.147250	1.897120	0.316934
C	5.205910	0.962197	0.273351
C	4.902985	-0.373257	0.183091
C	3.555810	-0.820994	0.102517
C	3.261688	-2.200703	0.168182
C	1.962698	-2.622126	0.263826
C	0.888735	-1.700092	0.173741
C	0.531538	1.654891	-1.410778
C	0.034871	2.978801	-1.445454
C	-0.866779	3.368280	-0.489429
C	-1.533052	2.380125	0.291239
C	-2.568300	2.762288	1.186824
C	-3.407849	1.823428	1.736925
C	-3.352954	0.503899	1.242590
Br	-2.812448	-1.338948	-0.784423
O	-0.381117	-2.113185	0.379724
H	2.061772	2.243553	0.256874
H	4.364325	2.951011	0.466178
H	6.236746	1.294671	0.348364
H	5.689456	-1.123403	0.204008
H	4.075983	-2.919135	0.203505
H	1.749414	-3.675356	0.390910
H	1.419985	1.433878	-1.991366
H	0.466158	3.695845	-2.136979

H	-1.148633	4.409585	-0.362260
H	-2.707366	3.820250	1.390412
H	-4.192229	2.109635	2.430405
H	-4.166484	-0.185608	1.438025
C	-0.663534	-3.475743	0.659132
H	-0.365524	-4.131929	-0.167740
H	-0.174515	-3.806639	1.582890
H	-1.745949	-3.522376	0.776043

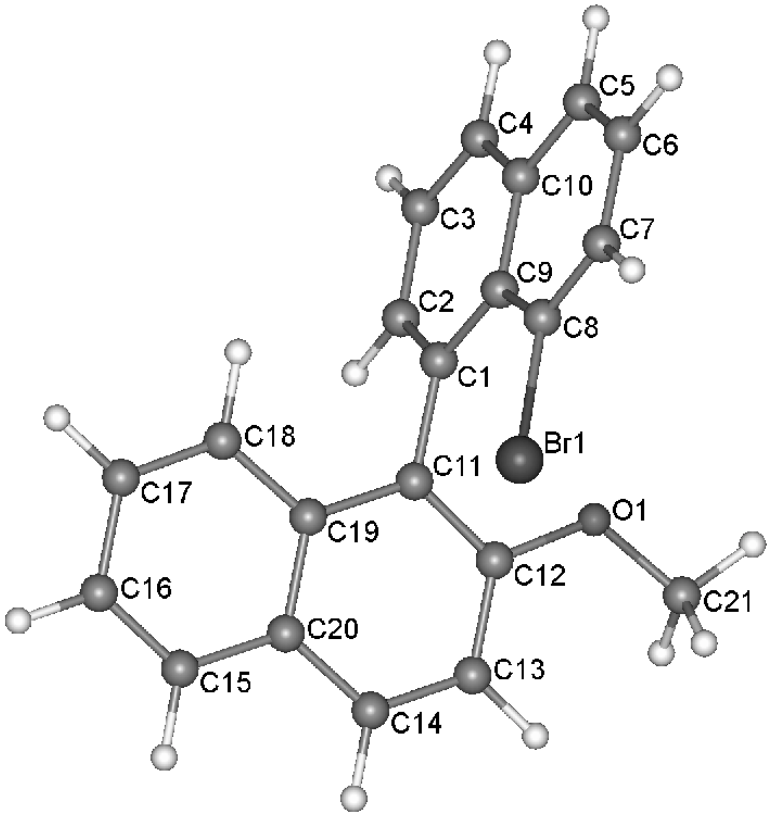

Figure 6. Optimized geometry of **18**. Important atom distances and angles are as follows: C1-C11 (1.50 Å), Br1-C8 (1.92 Å), Br1-O1 (3.73 Å), Br1-C8-C9 (123.6^{o}), C9-C1-C11 (125.3^{o}), dihedral C9-C1-C11-C19 (101.4^{o}), dihedral C21-O1-C12-C11 (175.9^{o}).

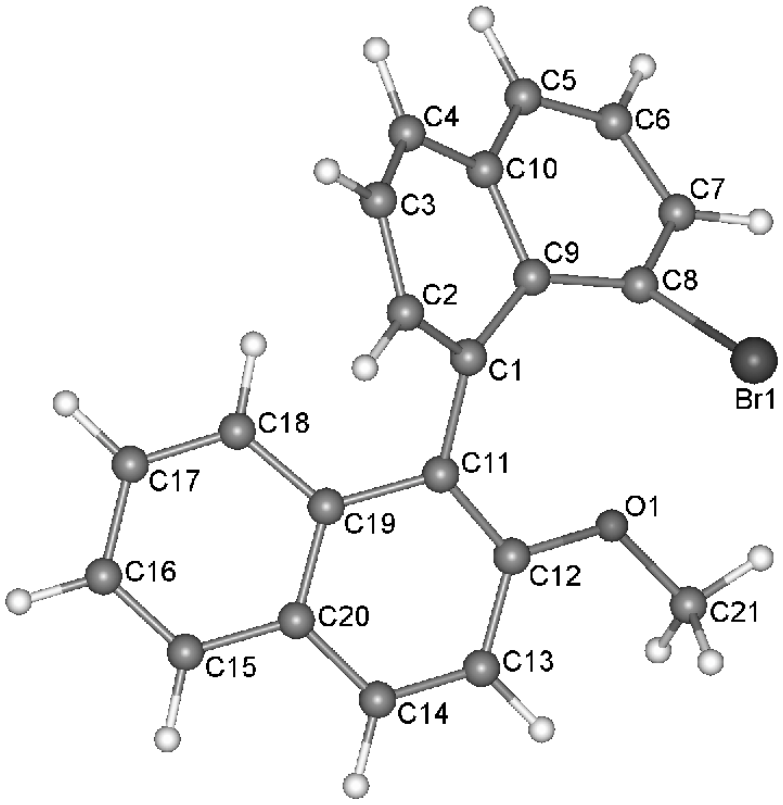

Figure 7. Transition structure geometry of **18**. Important atom distances and angles are as follows: C1-C11 (1.51 Å), Br1-C8 (1.93 Å), Br1-O1 (2.80 Å), Br1-C8-C9 (120.6^{o}), C9-C1-C11 (129.5^{o}), dihedral C9-C1-C11-C19 (-129.7^{o}), dihedral C21-O1-C12-C11 (178.6).

2. X-Ray Crystallography

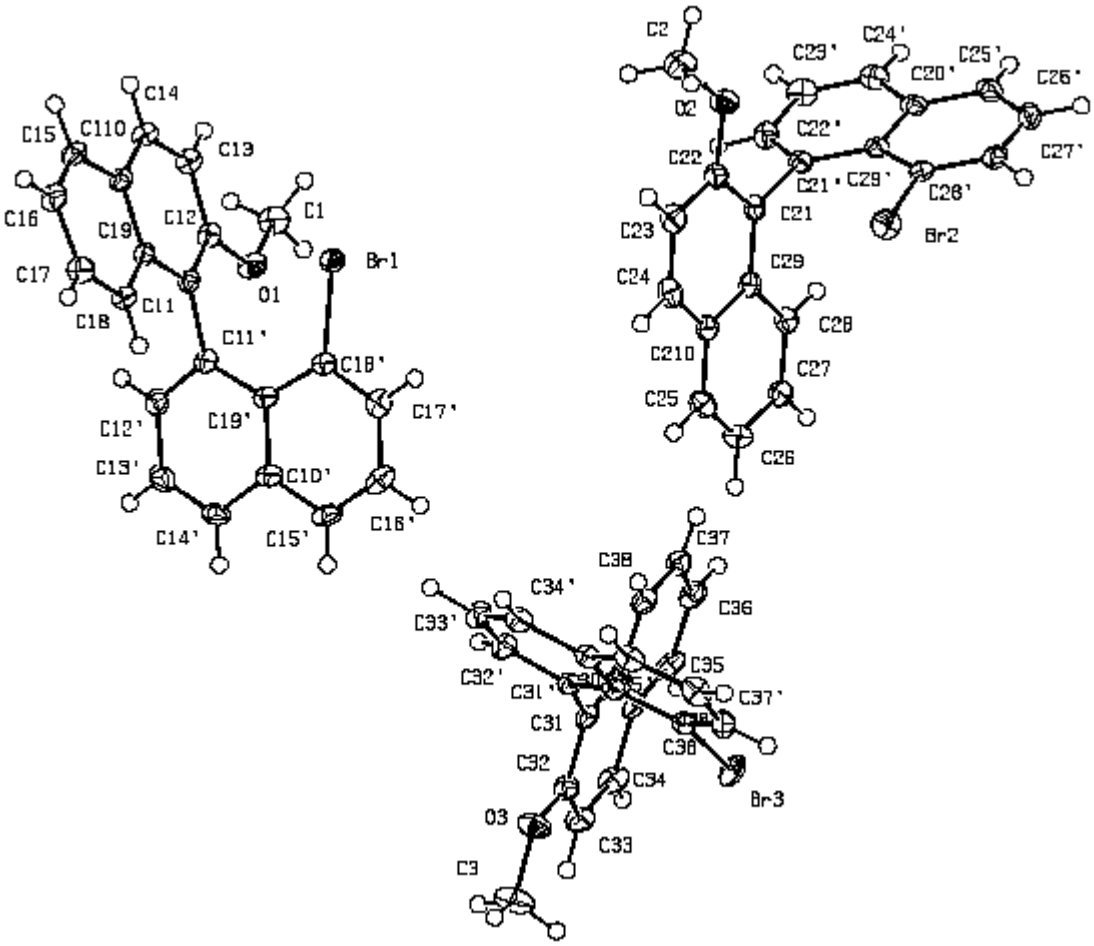

Figure 8. ORTEP diagram of (±)-**18** showing the atom labeling scheme. Displacement parameters are shown at the 50% probability level.

Table 1. Crystal data and structure refinement for (±)-**18**.

Identification code	(±)-**18**
Empirical formula	C21 H15 Br O
Formula weight	363.24
Temperature	105(2) K
Wavelength	0.71070 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 9.8350(2) A alpha = 108.0840(12) deg. b = 15.2530(2) A beta = 91.3530(10) deg. c = 17.0760(3) A gamma = 99.3550(11) deg.
Volume	2395.20(7) A^3
Z, Calculated density	6, 1.511 Mg/m^3
Absorption coefficient	2.576 mm^-1
F(000)	1104
Crystal size	0.5 x 0.4 x 0.2 mm
Theta range for data collection	3.19 to 25.07 deg.
Limiting indices	-11<=h<=11, -18<=k<=18, -19<=l<=20
Reflections collected / unique	34246 / 8418 [R(int) = 0.0594]
Completeness to theta = 25.07	99.0 %
Absorption correction	Multiscan
Max. and min. transmission	0.598 and 0.415
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8418 / 0 / 802
Goodness-of-fit on F^2	0.993
Final R indices [I>2sigma(I)]	R1 = 0.0335, wR2 = 0.0850
R indices (all data)	R1 = 0.0397, wR2 = 0.0900
Largest diff. peak and hole	0.561 and -0.753 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for (±)-**18**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Br(1)	6521(1)	5165(1)	13721(1)	22(1)
C(11)	8994(3)	6579(2)	13547(1)	17(1)
C(12)	9943(3)	6031(2)	13626(2)	19(1)
C(13)	10421(3)	5424(2)	12925(2)	21(1)
C(14)	9985(3)	5405(2)	12151(2)	20(1)
C(15)	8611(3)	5971(2)	11237(2)	21(1)
C(16)	7655(3)	6490(2)	11139(2)	24(1)
C(17)	7069(3)	7026(2)	11834(2)	23(1)
C(18)	7493(3)	7062(2)	12613(2)	20(1)
C(19)	8509(3)	6548(2)	12743(2)	17(1)
C(110)	9044(3)	5964(2)	12035(2)	18(1)
C(11')	8594(3)	7279(2)	14296(1)	18(1)
C(12')	9502(3)	8126(2)	14568(2)	23(1)
C(13')	9239(3)	8881(2)	15234(2)	28(1)
C(14')	8049(3)	8797(2)	15614(2)	26(1)
C(15')	5904(3)	7859(2)	15823(2)	25(1)
C(16')	4996(3)	7044(2)	15639(2)	25(1)
C(17')	5225(3)	6256(2)	14994(2)	21(1)
C(18')	6366(3)	6311(2)	14556(1)	16(1)
C(19')	7366(3)	7149(2)	14713(1)	18(1)
C(10')	7105(3)	7938(2)	15382(2)	21(1)
O(1)	10351(2)	6101(1)	14421(1)	24(1)
C(1)	11338(3)	5553(2)	14531(2)	27(1)
Br(2)	5464(1)	9170(1)	12557(1)	27(1)
C(21)	2624(3)	8206(2)	12841(2)	18(1)
C(22)	3104(3)	8320(2)	13641(2)	21(1)
C(23)	3719(3)	7631(2)	13825(2)	24(1)
C(24)	3844(3)	6827(2)	13208(2)	23(1)
C(25)	3427(3)	5826(2)	11747(2)	23(1)
C(26)	2898(3)	5675(2)	10959(2)	24(1)
C(27)	2278(3)	6366(2)	10773(2)	21(1)
C(28)	2191(3)	7183(2)	11372(2)	19(1)
C(29)	2707(3)	7361(2)	12202(2)	18(1)
C(210)	3337(3)	6662(2)	12387(2)	19(1)
C(21')	1983(3)	8949(2)	12652(2)	18(1)
C(22')	578(3)	8877(2)	12703(2)	22(1)
C(23')	-168(3)	9514(2)	12532(2)	26(1)
C(24')	507(3)	10224(2)	12286(2)	24(1)
C(25')	2605(3)	11056(2)	11911(2)	25(1)
C(26')	3981(3)	11172(2)	11809(2)	28(1)
C(27')	4774(3)	10569(2)	12002(2)	24(1)
C(28')	4172(3)	9868(2)	12293(2)	19(1)
C(29')	2725(3)	9685(2)	12386(1)	17(1)
C(20')	1944(3)	10321(2)	12193(2)	20(1)
O(2)	2990(2)	9158(1)	14220(1)	26(1)
C(2)	3358(4)	9283(2)	15068(2)	34(1)
Br(3)	10125(1)	2704(1)	10427(1)	26(1)
C(31)	7670(3)	2072(2)	11320(2)	18(1)
C(32)	7547(3)	1165(2)	10788(2)	21(1)
C(33)	6643(3)	841(2)	10062(2)	24(1)
C(34)	5880(3)	1429(2)	9880(2)	24(1)
C(35)	5177(3)	2984(2)	10212(2)	23(1)
C(36)	5297(3)	3888(2)	10712(2)	24(1)
C(37)	6194(3)	4212(2)	11440(2)	22(1)
C(38)	6949(3)	3630(2)	11649(2)	21(1)
C(39)	6858(3)	2686(2)	11139(2)	17(1)
C(310)	5943(3)	2358(2)	10403(2)	19(1)

C(31')	8599(3)	2383(2)	12101(2)	17(1)
C(32')	7976(3)	2282(2)	12792(2)	21(1)
C(33')	8721(3)	2510(2)	13564(2)	24(1)
C(34')	10092(3)	2851(2)	13644(2)	22(1)
C(35')	12226(3)	3381(2)	13086(2)	23(1)
C(36')	12931(3)	3545(2)	12456(2)	26(1)
C(37')	12230(3)	3320(2)	11672(2)	24(1)
C(38')	10855(3)	2945(2)	11539(2)	19(1)
C(39')	10040(3)	2759(2)	12171(2)	17(1)
C(30')	10790(3)	2994(2)	12964(2)	19(1)
O(3)	8364(2)	613(1)	10998(1)	27(1)
C(3)	8301(4)	-322(2)	10452(2)	37(1)

Table 3. Bond lengths [A] and angles [deg] for (±)-**18**.

Br(1)-C(18')	1.913(2)
C(11)-C(12)	1.380(4)
C(11)-C(19)	1.426(3)
C(11)-C(11')	1.499(3)
C(12)-O(1)	1.374(3)
C(12)-C(13)	1.411(4)
C(13)-C(14)	1.370(4)
C(13)-H(13)	0.94(3)
C(14)-C(110)	1.405(4)
C(14)-H(14)	0.96(3)
C(15)-C(16)	1.362(4)
C(15)-C(110)	1.422(4)
C(15)-H(15)	0.97(3)
C(16)-C(17)	1.411(4)
C(16)-H(16)	0.94(3)
C(17)-C(18)	1.366(4)
C(17)-H(17)	0.90(3)
C(18)-C(19)	1.421(4)
C(18)-H(18)	0.93(3)
C(19)-C(110)	1.430(3)
C(11')-C(12')	1.384(4)
C(11')-C(19')	1.433(4)
C(12')-C(13')	1.407(4)
C(12')-H(12')	0.88(3)
C(13')-C(14')	1.360(4)
C(13')-H(13')	0.88(3)
C(14')-C(10')	1.414(4)
C(14')-H(14')	0.92(3)
C(15')-C(16')	1.351(4)
C(15')-C(10')	1.425(4)
C(15')-H(15')	0.91(3)
C(16')-C(17')	1.409(4)
C(16')-H(16')	0.97(3)
C(17')-C(18')	1.369(4)
C(17')-H(17')	0.94(3)
C(18')-C(19')	1.428(4)
C(19')-C(10')	1.444(3)
O(1)-C(1)	1.425(3)
C(1)-H(1A)	0.97(3)
C(1)-H(1B)	0.97(4)
C(1)-H(1C)	0.93(3)
Br(2)-C(28')	1.914(3)
C(21)-C(22)	1.383(4)
C(21)-C(29)	1.422(4)
C(21)-C(21')	1.496(4)
C(22)-O(2)	1.376(3)
C(22)-C(23)	1.404(4)
C(23)-C(24)	1.372(4)
C(23)-H(23)	0.93(3)
C(24)-C(210)	1.409(4)
C(24)-H(24)	0.99(3)
C(25)-C(26)	1.367(4)
C(25)-C(210)	1.415(4)
C(25)-H(25)	0.95(3)
C(26)-C(27)	1.411(4)
C(26)-H(26)	0.93(3)
C(27)-C(28)	1.362(4)
C(27)-H(27)	0.95(3)
C(28)-C(29)	1.422(4)
C(28)-H(28)	0.96(3)
C(29)-C(210)	1.425(4)
C(21')-C(22')	1.375(4)
C(21')-C(29')	1.436(4)
C(22')-C(23')	1.402(4)
C(22')-H(22')	0.92(3)

C(23')-C(24')	1.361(4)
C(23')-H(23')	0.93(3)
C(24')-C(20')	1.415(4)
C(24')-H(24')	0.93(3)
C(25')-C(26')	1.358(4)
C(25')-C(20')	1.422(4)
C(25')-H(25')	0.91(3)
C(26')-C(27')	1.405(4)
C(26')-H(26')	0.97(4)
C(27')-C(28')	1.370(4)
C(27')-H(27')	0.98(3)
C(28')-C(29')	1.428(4)
C(29')-C(20')	1.438(4)
O(2)-C(2)	1.431(3)
C(2)-H(2A)	0.98(3)
C(2)-H(2B)	0.94(4)
C(2)-H(2C)	1.07(4)
Br(3)-C(38')	1.915(3)
C(31)-C(32)	1.384(4)
C(31)-C(39)	1.421(4)
C(31)-C(31')	1.500(3)
C(32)-O(3)	1.370(3)
C(32)-C(33)	1.412(4)
C(33)-C(34)	1.359(4)
C(33)-H(33)	0.96(4)
C(34)-C(310)	1.412(4)
C(34)-H(34)	0.95(3)
C(35)-C(36)	1.362(4)
C(35)-C(310)	1.414(4)
C(35)-H(35)	0.97(3)
C(36)-C(37)	1.412(4)
C(36)-H(36)	0.98(3)
C(37)-C(38)	1.366(4)
C(37)-H(37)	0.93(3)
C(38)-C(39)	1.420(4)
C(38)-H(38)	0.98(4)
C(39)-C(310)	1.432(4)
C(31')-C(32')	1.382(4)
C(31')-C(39')	1.427(4)
C(32')-C(33')	1.408(4)
C(32')-H(32')	0.85(3)
C(33')-C(34')	1.351(4)
C(33')-H(33')	1.01(3)
C(34')-C(30')	1.419(4)
C(34')-H(34')	0.95(3)
C(35')-C(36')	1.359(4)
C(35')-C(30')	1.423(4)
C(35')-H(35')	0.97(3)
C(36')-C(37')	1.407(4)
C(36')-H(36')	0.93(3)
C(37')-C(38')	1.365(4)
C(37')-H(37')	0.90(3)
C(38')-C(39')	1.430(4)
C(39')-C(30')	1.440(3)
O(3)-C(3)	1.432(4)
C(3)-H(3A)	0.99(4)
C(3)-H(3B)	0.98(3)
C(3)-H(3C)	0.96(4)

C(12)-C(11)-C(19)	119.5(2)
C(12)-C(11)-C(11')	120.3(2)
C(19)-C(11)-C(11')	119.8(2)
O(1)-C(12)-C(11)	115.7(2)
O(1)-C(12)-C(13)	123.0(2)
C(11)-C(12)-C(13)	121.2(2)
C(14)-C(13)-C(12)	119.6(2)
C(14)-C(13)-H(13)	120.6(17)
C(12)-C(13)-H(13)	119.7(17)

C(13)-C(14)-C(110)	121.6(2)
C(13)-C(14)-H(14)	120(2)
C(110)-C(14)-H(14)	119(2)
C(16)-C(15)-C(110)	121.0(2)
C(16)-C(15)-H(15)	119.9(17)
C(110)-C(15)-H(15)	119.2(17)
C(15)-C(16)-C(17)	120.1(3)
C(15)-C(16)-H(16)	120(2)
C(17)-C(16)-H(16)	120(2)
C(18)-C(17)-C(16)	120.6(3)
C(18)-C(17)-H(17)	120.9(18)
C(16)-C(17)-H(17)	118.5(18)
C(17)-C(18)-C(19)	121.0(2)
C(17)-C(18)-H(18)	118.3(19)
C(19)-C(18)-H(18)	120.7(19)
C(18)-C(19)-C(11)	122.7(2)
C(18)-C(19)-C(110)	118.2(2)
C(11)-C(19)-C(110)	119.1(2)
C(14)-C(110)-C(15)	122.2(2)
C(14)-C(110)-C(19)	118.9(2)
C(15)-C(110)-C(19)	119.0(2)
C(12')-C(11')-C(19')	119.6(2)
C(12')-C(11')-C(11)	114.6(2)
C(19')-C(11')-C(11)	125.8(2)
C(11')-C(12')-C(13')	121.9(3)
C(11')-C(12')-H(12')	117.7(16)
C(13')-C(12')-H(12')	120.5(16)
C(14')-C(13')-C(12')	120.0(3)
C(14')-C(13')-H(13')	120(2)
C(12')-C(13')-H(13')	120(2)
C(13')-C(14')-C(10')	120.7(3)
C(13')-C(14')-H(14')	122(2)
C(10')-C(14')-H(14')	117(2)
C(16')-C(15')-C(10')	121.2(3)
C(16')-C(15')-H(15')	119.9(19)
C(10')-C(15')-H(15')	118.9(19)
C(15')-C(16')-C(17')	119.9(3)
C(15')-C(16')-H(16')	123.0(19)
C(17')-C(16')-H(16')	117.1(19)
C(18')-C(17')-C(16')	120.4(3)
C(18')-C(17')-H(17')	118.8(18)
C(16')-C(17')-H(17')	120.8(18)
C(17')-C(18')-C(19')	123.0(2)
C(17')-C(18')-Br(1)	114.4(2)
C(19')-C(18')-Br(1)	122.68(18)
C(18')-C(19')-C(11')	127.4(2)
C(18')-C(19')-C(10')	115.1(2)
C(11')-C(19')-C(10')	117.4(2)
C(14')-C(10')-C(15')	119.3(2)
C(14')-C(10')-C(19')	120.3(2)
C(15')-C(10')-C(19')	120.5(2)
C(12)-O(1)-C(1)	117.6(2)
O(1)-C(1)-H(1A)	109.3(19)
O(1)-C(1)-H(1B)	112(2)
H(1A)-C(1)-H(1B)	110(3)
O(1)-C(1)-H(1C)	105.6(19)
H(1A)-C(1)-H(1C)	114(3)
H(1B)-C(1)-H(1C)	106(3)
C(22)-C(21)-C(29)	119.3(2)
C(22)-C(21)-C(21')	120.5(2)
C(29)-C(21)-C(21')	120.1(2)
O(2)-C(22)-C(21)	115.6(2)
O(2)-C(22)-C(23)	123.3(2)
C(21)-C(22)-C(23)	121.1(2)
C(24)-C(23)-C(22)	120.0(3)
C(24)-C(23)-H(23)	119(2)
C(22)-C(23)-H(23)	121(2)
C(23)-C(24)-C(210)	121.4(2)

C(23)-C(24)-H(24)	121.0(17)
C(210)-C(24)-H(24)	117.6(17)
C(26)-C(25)-C(210)	120.9(2)
C(26)-C(25)-H(25)	120.1(19)
C(210)-C(25)-H(25)	119.0(19)
C(25)-C(26)-C(27)	119.9(3)
C(25)-C(26)-H(26)	121.4(19)
C(27)-C(26)-H(26)	118.7(19)
C(28)-C(27)-C(26)	120.7(3)
C(28)-C(27)-H(27)	119.8(18)
C(26)-C(27)-H(27)	119.5(18)
C(27)-C(28)-C(29)	121.2(2)
C(27)-C(28)-H(28)	121.0(16)
C(29)-C(28)-H(28)	117.8(16)
C(28)-C(29)-C(21)	122.3(2)
C(28)-C(29)-C(210)	117.9(2)
C(21)-C(29)-C(210)	119.7(2)
C(24)-C(210)-C(25)	122.1(2)
C(24)-C(210)-C(29)	118.5(2)
C(25)-C(210)-C(29)	119.4(2)
C(22')-C(21')-C(29')	119.4(2)
C(22')-C(21')-C(21)	116.2(2)
C(29')-C(21')-C(21)	124.3(2)
C(21')-C(22')-C(23')	122.7(3)
C(21')-C(22')-H(22')	117.6(19)
C(23')-C(22')-H(22')	119.6(19)
C(24')-C(23')-C(22')	119.3(3)
C(24')-C(23')-H(23')	124(2)
C(22')-C(23')-H(23')	117(2)
C(23')-C(24')-C(20')	121.0(3)
C(23')-C(24')-H(24')	120.7(19)
C(20')-C(24')-H(24')	118.1(19)
C(26')-C(25')-C(20')	121.3(3)
C(26')-C(25')-H(25')	122.8(18)
C(20')-C(25')-H(25')	115.8(19)
C(25')-C(26')-C(27')	119.4(3)
C(25')-C(26')-H(26')	122(2)
C(27')-C(26')-H(26')	119(2)
C(28')-C(27')-C(26')	120.6(3)
C(28')-C(27')-H(27')	119.3(17)
C(26')-C(27')-H(27')	120.1(17)
C(27')-C(28')-C(29')	122.8(3)
C(27')-C(28')-Br(2)	113.3(2)
C(29')-C(28')-Br(2)	123.89(19)
C(28')-C(29')-C(21')	127.4(2)
C(28')-C(29')-C(20')	115.2(2)
C(21')-C(29')-C(20')	117.4(2)
C(24')-C(20')-C(25')	119.3(3)
C(24')-C(20')-C(29')	120.2(2)
C(25')-C(20')-C(29')	120.6(3)
C(22)-O(2)-C(2)	118.0(2)
O(2)-C(2)-H(2A)	111(2)
O(2)-C(2)-H(2B)	107(2)
H(2A)-C(2)-H(2B)	112(3)
O(2)-C(2)-H(2C)	112(2)
H(2A)-C(2)-H(2C)	107(3)
H(2B)-C(2)-H(2C)	109(3)
C(32)-C(31)-C(39)	119.4(2)
C(32)-C(31)-C(31')	119.9(2)
C(39)-C(31)-C(31')	120.6(2)
O(3)-C(32)-C(31)	116.3(2)
O(3)-C(32)-C(33)	122.5(2)
C(31)-C(32)-C(33)	121.2(2)
C(34)-C(33)-C(32)	119.6(3)
C(34)-C(33)-H(33)	121(2)
C(32)-C(33)-H(33)	119(2)
C(33)-C(34)-C(310)	121.9(3)
C(33)-C(34)-H(34)	121.1(18)

C(310)-C(34)-H(34)	117.0(18)
C(36)-C(35)-C(310)	121.4(2)
C(36)-C(35)-H(35)	122(2)
C(310)-C(35)-H(35)	116(2)
C(35)-C(36)-C(37)	119.8(3)
C(35)-C(36)-H(36)	121.1(18)
C(37)-C(36)-H(36)	119.1(18)
C(38)-C(37)-C(36)	120.7(3)
C(38)-C(37)-H(37)	118.2(19)
C(36)-C(37)-H(37)	121.0(19)
C(37)-C(38)-C(39)	121.0(3)
C(37)-C(38)-H(38)	122(2)
C(39)-C(38)-H(38)	117(2)
C(38)-C(39)-C(31)	122.5(2)
C(38)-C(39)-C(310)	118.1(2)
C(31)-C(39)-C(310)	119.4(2)
C(34)-C(310)-C(35)	122.5(2)
C(34)-C(310)-C(39)	118.4(2)
C(35)-C(310)-C(39)	119.0(2)
C(32')-C(31')-C(39')	119.3(2)
C(32')-C(31')-C(31)	115.6(2)
C(39')-C(31')-C(31)	125.1(2)
C(31')-C(32')-C(33')	122.3(3)
C(31')-C(32')-H(32')	117.7(19)
C(33')-C(32')-H(32')	119.9(19)
C(34')-C(33')-C(32')	119.5(2)
C(34')-C(33')-H(33')	120.5(17)
C(32')-C(33')-H(33')	119.9(17)
C(33')-C(34')-C(30')	121.0(2)
C(33')-C(34')-H(34')	120.6(18)
C(30')-C(34')-H(34')	118.4(18)
C(36')-C(35')-C(30')	120.8(3)
C(36')-C(35')-H(35')	123.1(19)
C(30')-C(35')-H(35')	116.1(19)
C(35')-C(36')-C(37')	119.4(3)
C(35')-C(36')-H(36')	121.5(19)
C(37')-C(36')-H(36')	119.1(19)
C(38')-C(37')-C(36')	120.9(3)
C(38')-C(37')-H(37')	122(2)
C(36')-C(37')-H(37')	117(2)
C(37')-C(38')-C(39')	123.1(2)
C(37')-C(38')-Br(3)	113.44(19)
C(39')-C(38')-Br(3)	123.50(19)
C(31')-C(39')-C(38')	127.6(2)
C(31')-C(39')-C(30')	117.8(2)
C(38')-C(39')-C(30')	114.6(2)
C(34')-C(30')-C(35')	118.8(2)
C(34')-C(30')-C(39')	119.9(2)
C(35')-C(30')-C(39')	121.2(2)
C(32)-O(3)-C(3)	118.2(2)
O(3)-C(3)-H(3A)	105(2)
O(3)-C(3)-H(3B)	112(2)
H(3A)-C(3)-H(3B)	108(3)
O(3)-C(3)-H(3C)	111(2)
H(3A)-C(3)-H(3C)	111(3)
H(3B)-C(3)-H(3C)	110(3)

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for (±)-**18**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Br(1)	25(1)	19(1)	17(1)	2(1)	3(1)	1(1)
C(11)	17(1)	18(1)	12(1)	4(1)	1(1)	0(1)
C(12)	18(1)	24(1)	14(1)	6(1)	-3(1)	1(1)
C(13)	18(1)	24(1)	20(1)	6(1)	1(1)	6(1)
C(14)	18(1)	24(1)	16(1)	4(1)	2(1)	5(1)
C(15)	24(1)	25(1)	13(1)	4(1)	3(1)	3(1)
C(16)	28(2)	29(2)	13(1)	7(1)	-3(1)	3(1)
C(17)	25(1)	25(1)	22(1)	9(1)	-2(1)	9(1)
C(18)	21(1)	22(1)	16(1)	4(1)	2(1)	5(1)
C(19)	17(1)	17(1)	15(1)	5(1)	2(1)	0(1)
C(110)	17(1)	20(1)	14(1)	4(1)	1(1)	1(1)
C(11')	23(1)	22(1)	11(1)	7(1)	-2(1)	5(1)
C(12')	30(2)	23(1)	15(1)	7(1)	-1(1)	1(1)
C(13')	43(2)	18(1)	19(1)	4(1)	-3(1)	-2(1)
C(14')	45(2)	18(1)	14(1)	2(1)	-1(1)	11(1)
C(15')	34(2)	30(2)	12(1)	4(1)	1(1)	18(1)
C(16')	22(1)	41(2)	17(1)	12(1)	3(1)	16(1)
C(17')	19(1)	29(2)	19(1)	11(1)	-2(1)	6(1)
C(18')	20(1)	21(1)	11(1)	5(1)	-3(1)	8(1)
C(19')	24(1)	20(1)	10(1)	4(1)	-2(1)	9(1)
C(10')	29(2)	22(1)	12(1)	5(1)	-2(1)	12(1)
O(1)	30(1)	31(1)	14(1)	6(1)	-2(1)	13(1)
C(1)	31(2)	32(2)	21(2)	9(1)	-3(1)	12(1)
Br(2)	18(1)	30(1)	33(1)	9(1)	0(1)	4(1)
C(21)	18(1)	19(1)	18(1)	8(1)	-1(1)	1(1)
C(22)	23(1)	21(1)	18(1)	6(1)	0(1)	1(1)
C(23)	29(2)	27(2)	18(1)	11(1)	-5(1)	5(1)
C(24)	24(1)	24(1)	24(1)	13(1)	-4(1)	4(1)
C(25)	22(1)	21(1)	28(2)	10(1)	0(1)	7(1)
C(26)	24(1)	21(1)	24(1)	2(1)	1(1)	6(1)
C(27)	21(1)	25(1)	17(1)	7(1)	0(1)	4(1)
C(28)	19(1)	21(1)	19(1)	9(1)	-1(1)	4(1)
C(29)	15(1)	20(1)	18(1)	8(1)	1(1)	2(1)
C(210)	18(1)	20(1)	20(1)	9(1)	1(1)	3(1)
C(21')	23(1)	16(1)	13(1)	4(1)	-2(1)	3(1)
C(22')	22(1)	23(1)	22(1)	9(1)	1(1)	1(1)
C(23')	20(2)	29(2)	28(2)	7(1)	-1(1)	7(1)
C(24')	30(2)	23(1)	19(1)	5(1)	-4(1)	10(1)
C(25')	44(2)	16(1)	15(1)	4(1)	-2(1)	7(1)
C(26')	44(2)	19(1)	16(1)	4(1)	4(1)	-4(1)
C(27')	30(2)	20(1)	15(1)	0(1)	4(1)	-2(1)
C(28')	23(1)	17(1)	14(1)	1(1)	2(1)	3(1)
C(29')	23(1)	15(1)	11(1)	1(1)	-2(1)	2(1)
C(20')	31(2)	17(1)	11(1)	1(1)	-2(1)	7(1)
O(2)	40(1)	24(1)	14(1)	4(1)	-3(1)	10(1)
C(2)	49(2)	32(2)	17(1)	4(1)	-4(1)	7(2)
Br(3)	25(1)	41(1)	16(1)	13(1)	2(1)	6(1)
C(31)	16(1)	23(1)	11(1)	4(1)	-1(1)	-1(1)
C(32)	22(1)	22(1)	16(1)	5(1)	-1(1)	2(1)
C(33)	26(1)	26(2)	14(1)	-1(1)	-4(1)	1(1)
C(34)	21(1)	33(2)	14(1)	2(1)	-5(1)	2(1)
C(35)	18(1)	37(2)	13(1)	5(1)	-1(1)	7(1)
C(36)	21(1)	32(2)	22(1)	11(1)	5(1)	10(1)
C(37)	21(1)	22(1)	22(1)	6(1)	4(1)	4(1)
C(38)	18(1)	26(1)	16(1)	4(1)	1(1)	1(1)
C(39)	14(1)	24(1)	12(1)	6(1)	0(1)	1(1)
C(310)	16(1)	27(1)	12(1)	4(1)	2(1)	1(1)
C(31')	22(1)	17(1)	12(1)	3(1)	-3(1)	3(1)

C(32')	19(2)	24(1)	15(1)	3(1)	-1(1)	-1(1)
C(33')	31(2)	28(2)	13(1)	6(1)	-1(1)	2(1)
C(34')	30(2)	21(1)	13(1)	4(1)	-6(1)	4(1)
C(35')	23(1)	21(1)	22(1)	4(1)	-8(1)	4(1)
C(36')	18(1)	24(1)	33(2)	8(1)	-6(1)	0(1)
C(37')	23(1)	25(1)	28(2)	13(1)	5(1)	5(1)
C(38')	25(1)	18(1)	15(1)	5(1)	-1(1)	7(1)
C(39')	20(1)	15(1)	14(1)	4(1)	-2(1)	3(1)
C(30')	24(1)	16(1)	17(1)	4(1)	-4(1)	4(1)
O(3)	38(1)	21(1)	19(1)	0(1)	-10(1)	9(1)
C(3)	46(2)	24(2)	34(2)	-3(1)	-12(2)	13(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for (±)-**18**.

	x	y	z	U(eq)
H(13)	11060(30)	5050(20)	12993(17)	17(7)
H(14)	10320(30)	5000(20)	11670(20)	33(8)
H(15)	9020(30)	5610(20)	10756(18)	20(7)
H(16)	7370(30)	6480(20)	10610(20)	32(8)
H(17)	6420(30)	7340(20)	11753(17)	18(7)
H(18)	7110(30)	7440(20)	13060(20)	27(8)
H(12')	10260(30)	8181(17)	14309(15)	5(6)
H(15')	5750(30)	8370(20)	16231(19)	21(7)
H(16')	4160(30)	6970(20)	15930(20)	32(8)
H(17')	4590(30)	5690(20)	14848(18)	24(7)
H(13')	9830(30)	9420(20)	15386(18)	26(8)
H(14')	7820(30)	9290(20)	16030(20)	29(8)
H(1A)	12180(40)	5720(20)	14280(20)	32(8)
H(1B)	10980(30)	4890(30)	14300(20)	35(9)
H(1C)	11470(30)	5680(20)	15100(20)	27(8)
H(23)	4060(30)	7710(20)	14360(20)	31(8)
H(24)	4280(30)	6340(20)	13325(18)	24(7)
H(25)	3840(30)	5360(20)	11875(19)	30(8)
H(26)	2950(30)	5120(20)	10530(20)	28(8)
H(27)	1950(30)	6270(20)	10220(19)	21(7)
H(28)	1790(30)	7662(18)	11247(16)	11(6)
H(22')	120(30)	8390(20)	12856(18)	22(7)
H(23')	-1100(40)	9430(20)	12621(19)	32(8)
H(24')	20(30)	10620(20)	12129(19)	27(8)
H(25')	2040(30)	11420(20)	11783(18)	22(7)
H(26')	4440(40)	11680(20)	11620(20)	42(9)
H(27')	5770(30)	10630(20)	11913(18)	24(7)
H(2A)	2820(30)	8790(20)	15242(19)	30(8)
H(2B)	3200(30)	9880(30)	15370(20)	37(9)
H(2C)	4420(40)	9250(30)	15170(20)	52(11)
H(33)	6600(40)	210(30)	9690(20)	48(10)
H(34)	5270(30)	1230(20)	9400(20)	25(8)
H(35)	4550(30)	2730(20)	9720(20)	33(8)
H(36)	4760(30)	4320(20)	10579(18)	26(8)
H(37)	6330(30)	4840(20)	11770(18)	23(7)
H(38)	7640(40)	3850(20)	12120(20)	37(9)
H(32')	7110(30)	2085(19)	12742(17)	15(7)
H(33')	8220(30)	2430(20)	14057(18)	22(7)
H(34')	10610(30)	3010(20)	14159(19)	23(7)
H(35')	12650(30)	3530(20)	13640(20)	30(8)
H(36')	13870(30)	3800(20)	12530(18)	26(8)
H(37')	12720(30)	3430(20)	11270(20)	37(9)
H(3A)	8990(40)	-580(30)	10710(20)	48(10)
H(3B)	8580(30)	-340(20)	9900(20)	35(9)
H(3C)	7390(40)	-690(30)	10410(20)	46(10)

Table 6. Torsion angles [deg] for (±)-**18**.

C(19)-C(11)-C(12)-O(1)	-179.7(2)
C(11')-C(11)-C(12)-O(1)	7.0(3)
C(19)-C(11)-C(12)-C(13)	-1.4(4)
C(11')-C(11)-C(12)-C(13)	-174.6(2)
O(1)-C(12)-C(13)-C(14)	-178.9(2)
C(11)-C(12)-C(13)-C(14)	2.9(4)
C(12)-C(13)-C(14)-C(110)	-1.4(4)
C(110)-C(15)-C(16)-C(17)	-0.6(4)
C(15)-C(16)-C(17)-C(18)	2.8(4)
C(16)-C(17)-C(18)-C(19)	-1.4(4)
C(17)-C(18)-C(19)-C(11)	179.0(2)
C(17)-C(18)-C(19)-C(110)	-2.1(4)
C(12)-C(11)-C(19)-C(18)	177.4(2)
C(11')-C(11)-C(19)-C(18)	-9.4(4)
C(12)-C(11)-C(19)-C(110)	-1.5(4)
C(11')-C(11)-C(19)-C(110)	171.8(2)
C(13)-C(14)-C(110)-C(15)	178.3(3)
C(13)-C(14)-C(110)-C(19)	-1.5(4)
C(16)-C(15)-C(110)-C(14)	177.3(3)
C(16)-C(15)-C(110)-C(19)	-2.9(4)
C(18)-C(19)-C(110)-C(14)	-176.0(2)
C(11)-C(19)-C(110)-C(14)	2.9(4)
C(18)-C(19)-C(110)-C(15)	4.3(4)
C(11)-C(19)-C(110)-C(15)	-176.8(2)
C(12)-C(11)-C(11')-C(12')	82.5(3)
C(19)-C(11)-C(11')-C(12')	-90.7(3)
C(12)-C(11)-C(11')-C(19')	-99.7(3)
C(19)-C(11)-C(11')-C(19')	87.1(3)
C(19')-C(11')-C(12')-C(13')	-1.8(4)
C(11)-C(11')-C(12')-C(13')	176.1(2)
C(11')-C(12')-C(13')-C(14')	-1.7(4)
C(12')-C(13')-C(14')-C(10')	3.9(4)
C(10')-C(15')-C(16')-C(17')	-0.6(4)
C(15')-C(16')-C(17')-C(18')	0.3(4)
C(16')-C(17')-C(18')-C(19')	-0.6(4)
C(16')-C(17')-C(18')-Br(1)	178.79(19)
C(17')-C(18')-C(19')-C(11')	179.6(2)
Br(1)-C(18')-C(19')-C(11')	0.3(4)
C(17')-C(18')-C(19')-C(10')	1.1(4)
Br(1)-C(18')-C(19')-C(10')	-178.18(17)
C(12')-C(11')-C(19')-C(18')	-175.5(2)
C(11)-C(11')-C(19')-C(18')	6.8(4)
C(12')-C(11')-C(19')-C(10')	2.9(4)
C(11)-C(11')-C(19')-C(10')	-174.7(2)
C(13')-C(14')-C(10')-C(15')	176.6(3)
C(13')-C(14')-C(10')-C(19')	-2.6(4)
C(16')-C(15')-C(10')-C(14')	-178.0(3)
C(16')-C(15')-C(10')-C(19')	1.2(4)
C(18')-C(19')-C(10')-C(14')	177.8(2)
C(11')-C(19')-C(10')-C(14')	-0.8(4)
C(18')-C(19')-C(10')-C(15')	-1.4(3)
C(11')-C(19')-C(10')-C(15')	179.9(2)
C(11)-C(12)-O(1)-C(1)	-179.5(2)
C(13)-C(12)-O(1)-C(1)	2.2(4)
C(29)-C(21)-C(22)-O(2)	179.8(2)
C(21')-C(21)-C(22)-O(2)	-2.1(4)
C(29)-C(21)-C(22)-C(23)	2.5(4)
C(21')-C(21)-C(22)-C(23)	-179.4(2)
O(2)-C(22)-C(23)-C(24)	-177.4(2)
C(21)-C(22)-C(23)-C(24)	-0.3(4)
C(22)-C(23)-C(24)-C(210)	-1.6(4)
C(210)-C(25)-C(26)-C(27)	1.3(4)
C(25)-C(26)-C(27)-C(28)	-0.5(4)
C(26)-C(27)-C(28)-C(29)	-0.5(4)

C(27)-C(28)-C(29)-C(21)	-179.8(2)
C(27)-C(28)-C(29)-C(210)	0.8(4)
C(22)-C(21)-C(29)-C(28)	177.8(2)
C(21')-C(21)-C(29)-C(28)	-0.3(4)
C(22)-C(21)-C(29)-C(210)	-2.8(4)
C(21')-C(21)-C(29)-C(210)	179.1(2)
C(23)-C(24)-C(210)-C(25)	-178.4(3)
C(23)-C(24)-C(210)-C(29)	1.2(4)
C(26)-C(25)-C(210)-C(24)	178.5(3)
C(26)-C(25)-C(210)-C(29)	-1.1(4)
C(28)-C(29)-C(210)-C(24)	-179.6(2)
C(21)-C(29)-C(210)-C(24)	0.9(4)
C(28)-C(29)-C(210)-C(25)	0.0(4)
C(21)-C(29)-C(210)-C(25)	-179.4(2)
C(22)-C(21)-C(21')-C(22')	-89.7(3)
C(29)-C(21)-C(21')-C(22')	88.4(3)
C(22)-C(21)-C(21')-C(29')	93.5(3)
C(29)-C(21)-C(21')-C(29')	-88.4(3)
C(29')-C(21')-C(22')-C(23')	-2.1(4)
C(21)-C(21')-C(22')-C(23')	-179.1(2)
C(21')-C(22')-C(23')-C(24')	1.6(4)
C(22')-C(23')-C(24')-C(20')	0.6(4)
C(20')-C(25')-C(26')-C(27')	-1.4(4)
C(25')-C(26')-C(27')-C(28')	-0.1(4)
C(26')-C(27')-C(28')-C(29')	2.5(4)
C(26')-C(27')-C(28')-Br(2)	-177.5(2)
C(27')-C(28')-C(29')-C(21')	177.2(2)
Br(2)-C(28')-C(29')-C(21')	-2.8(4)
C(27')-C(28')-C(29')-C(20')	-3.0(4)
Br(2)-C(28')-C(29')-C(20')	176.92(17)
C(22')-C(21')-C(29')-C(28')	-179.8(2)
C(21)-C(21')-C(29')-C(28')	-3.0(4)
C(22')-C(21')-C(29')-C(20')	0.5(3)
C(21)-C(21')-C(29')-C(20')	177.2(2)
C(23')-C(24')-C(20')-C(25')	178.2(3)
C(23')-C(24')-C(20')-C(29')	-2.2(4)
C(26')-C(25')-C(20')-C(24')	-179.6(2)
C(26')-C(25')-C(20')-C(29')	0.7(4)
C(28')-C(29')-C(20')-C(24')	-178.2(2)
C(21')-C(29')-C(20')-C(24')	1.6(3)
C(28')-C(29')-C(20')-C(25')	1.5(3)
C(21')-C(29')-C(20')-C(25')	-178.8(2)
C(21)-C(22)-O(2)-C(2)	174.7(3)
C(23)-C(22)-O(2)-C(2)	-8.1(4)
C(39)-C(31)-C(32)-O(3)	179.8(2)
C(31')-C(31)-C(32)-O(3)	-3.4(3)
C(39)-C(31)-C(32)-C(33)	0.9(4)
C(31')-C(31)-C(32)-C(33)	177.7(2)
O(3)-C(32)-C(33)-C(34)	-178.7(2)
C(31)-C(32)-C(33)-C(34)	0.1(4)
C(32)-C(33)-C(34)-C(310)	-1.1(4)
C(310)-C(35)-C(36)-C(37)	-0.5(4)
C(35)-C(36)-C(37)-C(38)	0.2(4)
C(36)-C(37)-C(38)-C(39)	0.3(4)
C(37)-C(38)-C(39)-C(31)	177.4(2)
C(37)-C(38)-C(39)-C(310)	-0.6(4)
C(32)-C(31)-C(39)-C(38)	-178.9(2)
C(31')-C(31)-C(39)-C(38)	4.3(4)
C(32)-C(31)-C(39)-C(310)	-0.9(4)
C(31')-C(31)-C(39)-C(310)	-177.7(2)
C(33)-C(34)-C(310)-C(35)	178.6(3)
C(33)-C(34)-C(310)-C(39)	1.1(4)
C(36)-C(35)-C(310)-C(34)	-177.4(3)
C(36)-C(35)-C(310)-C(39)	0.1(4)
C(38)-C(39)-C(310)-C(34)	178.0(2)
C(31)-C(39)-C(310)-C(34)	0.0(3)
C(38)-C(39)-C(310)-C(35)	0.4(3)
C(31)-C(39)-C(310)-C(35)	-177.7(2)

C(32)-C(31)-C(31')-C(32')	-92.3(3)
C(39)-C(31)-C(31')-C(32')	84.5(3)
C(32)-C(31)-C(31')-C(39')	87.3(3)
C(39)-C(31)-C(31')-C(39')	-95.9(3)
C(39')-C(31')-C(32')-C(33')	-2.0(4)
C(31)-C(31')-C(32')-C(33')	177.6(2)
C(31')-C(32')-C(33')-C(34')	0.9(4)
C(32')-C(33')-C(34')-C(30')	0.7(4)
C(30')-C(35')-C(36')-C(37')	-0.6(4)
C(35')-C(36')-C(37')-C(38')	0.3(4)
C(36')-C(37')-C(38')-C(39')	0.2(4)
C(36')-C(37')-C(38')-Br(3)	179.7(2)
C(32')-C(31')-C(39')-C(38')	-177.7(2)
C(31)-C(31')-C(39')-C(38')	2.7(4)
C(32')-C(31')-C(39')-C(30')	1.6(4)
C(31)-C(31')-C(39')-C(30')	-178.0(2)
C(37')-C(38')-C(39')-C(31')	179.0(3)
Br(3)-C(38')-C(39')-C(31')	-0.5(4)
C(37')-C(38')-C(39')-C(30')	-0.4(4)
Br(3)-C(38')-C(39')-C(30')	-179.82(18)
C(33')-C(34')-C(30')-C(35')	178.2(3)
C(33')-C(34')-C(30')-C(39')	-1.1(4)
C(36')-C(35')-C(30')-C(34')	-178.8(3)
C(36')-C(35')-C(30')-C(39')	0.4(4)
C(31')-C(39')-C(30')-C(34')	-0.1(4)
C(38')-C(39')-C(30')-C(34')	179.3(2)
C(31')-C(39')-C(30')-C(35')	-179.4(2)
C(38')-C(39')-C(30')-C(35')	0.1(3)
C(31)-C(32)-O(3)-C(3)	-178.1(3)
C(33)-C(32)-O(3)-C(3)	0.7(4)

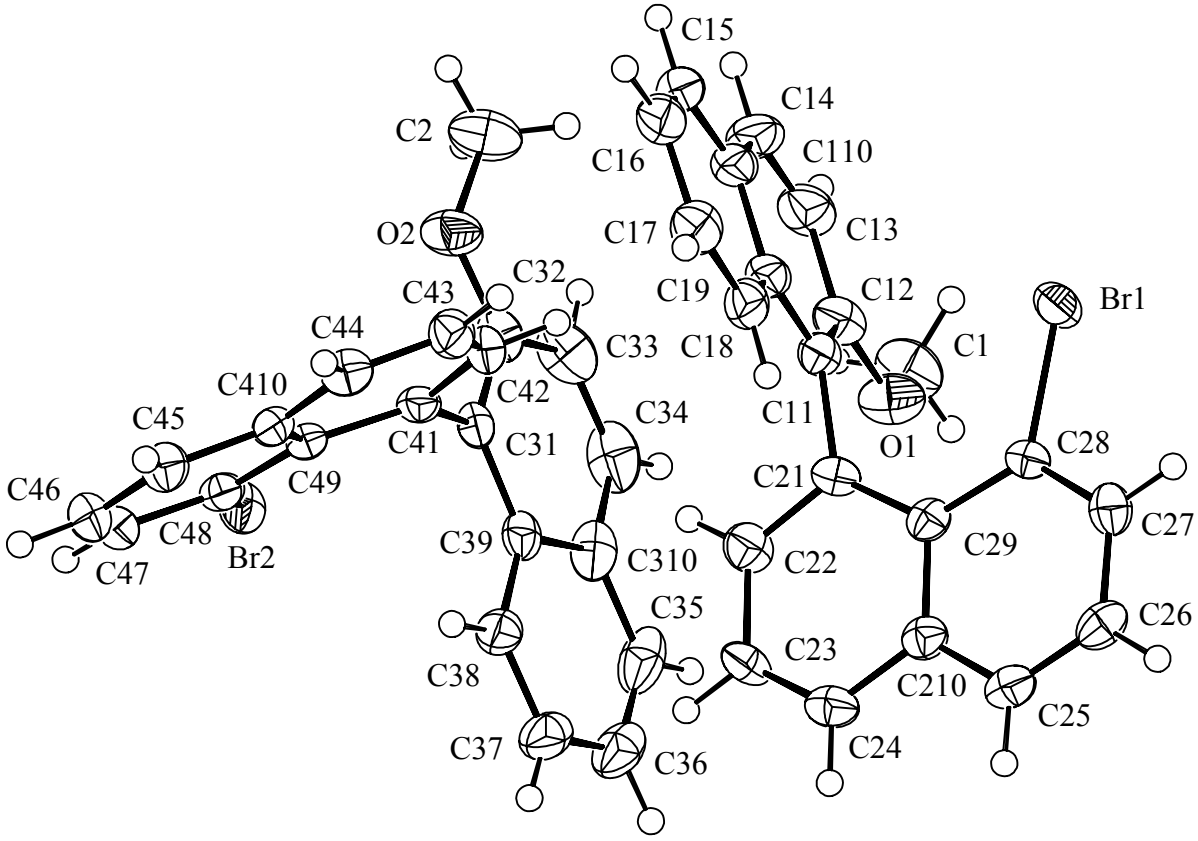

Figure 9. ORTEP diagram of (*S*)-(+)-**18** showing the atom labeling scheme. Displacement parameters are shown at the 50% probability level.

Table 7. Crystal data and structure refinement for (*S*)-(+)-**18**.

Identification code	(*S*)-(+)-**18**
Empirical formula	C21 H15 Br O
Formula weight	363.24
Temperature	150(2) K
Wavelength	0.71070 A
Crystal system, space group	Orthorhombic, P 212121
Unit cell dimensions	a = 14.6360(4) A alpha = 90 deg. b = 14.6340(3) A beta = 90 deg. c = 14.9980(3) A gamma = 90 deg.
Volume	3212.32(13) A^3
Z, Calculated density	8, 1.502 Mg/m^3
Absorption coefficient	2.561 mm^-1
F(000)	1472
Crystal size	0.29 x 0.13 x 0.12 mm
Theta range for data collection	3.05 to 26.07 deg.
Limiting indices	-18<=h<=16, -18<=k<=14, -18<=l<=18
Reflections collected / unique	47446 / 6311 [R(int) = 0.0711]
Completeness to theta = 26.07	99.2 %
Absorption correction	Gaussian
Max. and min. transmission	0.753 and 0.558
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6311 / 0 / 418
Goodness-of-fit on F^2	0.925
Final R indices [I>2sigma(I)]	R1 = 0.0296, wR2 = 0.0735
R indices (all data)	R1 = 0.0324, wR2 = 0.0765
Absolute structure parameter	0.000(9)
Largest diff. peak and hole	0.658 and -0.926 e.A^-3

Table 8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for (*S*)-(+)-**18**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Br(1)	4219(1)	6481(1)	2301(1)	35(1)
O(1)	2708(2)	6451(2)	89(2)	44(1)
C(1)	1882(3)	5975(4)	-124(4)	53(1)
C(11)	4296(3)	6460(3)	243(2)	28(1)
C(12)	3504(3)	5967(3)	72(3)	35(1)
C(13)	3553(3)	5015(3)	-100(3)	44(1)
C(14)	4378(4)	4582(3)	-100(3)	45(1)
C(15)	6056(4)	4596(3)	79(3)	45(1)
C(16)	6841(4)	5056(3)	254(3)	45(1)
C(17)	6799(4)	6000(3)	452(3)	42(1)
C(18)	5984(3)	6455(3)	444(3)	36(1)
C(19)	5149(3)	5998(3)	261(3)	33(1)
C(110)	5190(3)	5038(3)	77(3)	36(1)
C(21)	4275(3)	7485(2)	278(3)	28(1)
C(22)	4249(3)	7899(3)	-548(3)	35(1)
C(23)	4287(3)	8858(3)	-640(3)	33(1)
C(24)	4352(3)	9394(3)	96(3)	34(1)
C(25)	4458(3)	9601(3)	1700(3)	33(1)
C(26)	4484(3)	9276(3)	2549(3)	35(1)
C(27)	4421(3)	8321(3)	2689(3)	31(1)
C(28)	4339(3)	7730(2)	1977(3)	25(1)
C(29)	4328(3)	8035(3)	1067(3)	25(1)
C(210)	4375(3)	9011(3)	962(3)	28(1)
Br(2)	4053(1)	6554(1)	-4973(1)	33(1)
O(2)	4065(2)	4699(2)	-2940(2)	42(1)
C(2)	3660(4)	3829(3)	-2762(4)	52(1)
C(31)	3956(3)	6288(3)	-2937(2)	26(1)
C(32)	3520(3)	5459(3)	-2861(3)	35(1)
C(33)	2567(3)	5415(3)	-2741(3)	45(1)
C(34)	2065(3)	6197(4)	-2658(3)	48(1)
C(35)	1973(3)	7889(4)	-2618(3)	48(1)
C(36)	2390(4)	8716(3)	-2695(3)	47(1)
C(37)	3336(4)	8769(3)	-2870(3)	43(1)
C(38)	3848(3)	7993(3)	-2950(3)	34(1)
C(39)	3441(3)	7114(3)	-2868(2)	28(1)
C(310)	2475(3)	7062(3)	-2712(3)	38(1)
C(41)	4984(3)	6342(2)	-2931(3)	26(1)
C(42)	5386(3)	6150(3)	-2122(3)	30(1)
C(43)	6325(3)	6257(3)	-1966(3)	34(1)
C(44)	6878(3)	6556(3)	-2641(3)	31(1)
C(45)	7105(3)	7064(3)	-4180(3)	33(1)
C(46)	6783(3)	7230(3)	-5021(3)	36(1)
C(47)	5862(3)	7072(3)	-5217(3)	33(1)
C(48)	5273(3)	6782(2)	-4564(3)	26(1)
C(49)	5549(3)	6618(2)	-3664(2)	24(1)
C(410)	6508(3)	6740(2)	-3495(3)	27(1)

Table 9. Bond lengths [A] and angles [deg] for (*S*)-(+)-**18**.

Br(1)-C(28)	1.899(4)
O(1)-C(12)	1.364(5)
O(1)-C(1)	1.431(5)
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(11)-C(12)	1.389(6)
C(11)-C(19)	1.420(6)
C(11)-C(21)	1.501(5)
C(12)-C(13)	1.419(6)
C(13)-C(14)	1.363(7)
C(13)-H(13)	0.9300
C(14)-C(110)	1.389(7)
C(14)-H(14)	0.9300
C(15)-C(16)	1.357(7)
C(15)-C(110)	1.423(6)
C(15)-H(15)	0.9300
C(16)-C(17)	1.414(7)
C(16)-H(16)	0.9300
C(17)-C(18)	1.366(7)
C(17)-H(17)	0.9300
C(18)-C(19)	1.420(6)
C(18)-H(18)	0.9300
C(19)-C(110)	1.433(6)
C(21)-C(22)	1.379(6)
C(21)-C(29)	1.432(5)
C(22)-C(23)	1.411(6)
C(22)-H(22)	0.9300
C(23)-C(24)	1.358(6)
C(23)-H(23)	0.9300
C(24)-C(210)	1.416(6)
C(24)-H(24)	0.9300
C(25)-C(26)	1.361(6)
C(25)-C(210)	1.408(6)
C(25)-H(25)	0.9300
C(26)-C(27)	1.416(6)
C(26)-H(26)	0.9300
C(27)-C(28)	1.379(6)
C(27)-H(27)	0.9300
C(28)-C(29)	1.437(5)
C(29)-C(210)	1.439(5)
Br(2)-C(48)	1.917(4)
O(2)-C(32)	1.375(6)
O(2)-C(2)	1.430(5)
C(2)-H(2A)	0.9600
C(2)-H(2B)	0.9600
C(2)-H(2C)	0.9600
C(31)-C(32)	1.375(6)
C(31)-C(39)	1.428(5)
C(31)-C(41)	1.507(5)
C(32)-C(33)	1.407(7)
C(33)-C(34)	1.366(8)
C(33)-H(33)	0.9300
C(34)-C(310)	1.402(7)
C(34)-H(34)	0.9300
C(35)-C(36)	1.360(8)
C(35)-C(310)	1.424(7)
C(35)-H(35)	0.9300
C(36)-C(37)	1.410(8)
C(36)-H(36)	0.9300
C(37)-C(38)	1.366(6)
C(37)-H(37)	0.9300
C(38)-C(39)	1.422(6)
C(38)-H(38)	0.9300

C(39)-C(310)	1.435(6)
C(41)-C(42)	1.377(6)
C(41)-C(49)	1.434(5)
C(42)-C(43)	1.403(6)
C(42)-H(42)	0.9300
C(43)-C(44)	1.368(6)
C(43)-H(43)	0.9300
C(44)-C(410)	1.416(6)
C(44)-H(44)	0.9300
C(45)-C(46)	1.368(7)
C(45)-C(410)	1.430(6)
C(45)-H(45)	0.9300
C(46)-C(47)	1.399(6)
C(46)-H(46)	0.9300
C(47)-C(48)	1.372(6)
C(47)-H(47)	0.9300
C(48)-C(49)	1.429(6)
C(49)-C(410)	1.439(6)

C(12)-O(1)-C(1)	117.7(3)
O(1)-C(1)-H(1A)	109.5
O(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
O(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(12)-C(11)-C(19)	119.3(4)
C(12)-C(11)-C(21)	120.5(4)
C(19)-C(11)-C(21)	119.6(4)
O(1)-C(12)-C(11)	116.1(4)
O(1)-C(12)-C(13)	123.8(4)
C(11)-C(12)-C(13)	120.1(4)
C(14)-C(13)-C(12)	120.0(4)
C(14)-C(13)-H(13)	120.0
C(12)-C(13)-H(13)	120.0
C(13)-C(14)-C(110)	122.3(4)
C(13)-C(14)-H(14)	118.8
C(110)-C(14)-H(14)	118.8
C(16)-C(15)-C(110)	121.9(4)
C(16)-C(15)-H(15)	119.0
C(110)-C(15)-H(15)	119.0
C(15)-C(16)-C(17)	119.2(5)
C(15)-C(16)-H(16)	120.4
C(17)-C(16)-H(16)	120.4
C(18)-C(17)-C(16)	120.8(5)
C(18)-C(17)-H(17)	119.6
C(16)-C(17)-H(17)	119.6
C(17)-C(18)-C(19)	121.6(4)
C(17)-C(18)-H(18)	119.2
C(19)-C(18)-H(18)	119.2
C(18)-C(19)-C(11)	122.4(4)
C(18)-C(19)-C(110)	117.6(4)
C(11)-C(19)-C(110)	120.0(4)
C(14)-C(110)-C(15)	123.0(4)
C(14)-C(110)-C(19)	118.1(4)
C(15)-C(110)-C(19)	118.9(4)
C(22)-C(21)-C(29)	119.8(3)
C(22)-C(21)-C(11)	114.0(3)
C(29)-C(21)-C(11)	126.1(3)
C(21)-C(22)-C(23)	121.6(4)
C(21)-C(22)-H(22)	119.2
C(23)-C(22)-H(22)	119.2
C(24)-C(23)-C(22)	119.9(4)
C(24)-C(23)-H(23)	120.1
C(22)-C(23)-H(23)	120.1
C(23)-C(24)-C(210)	121.2(4)
C(23)-C(24)-H(24)	119.4
C(210)-C(24)-H(24)	119.4

C(26)-C(25)-C(210)	121.6(4)
C(26)-C(25)-H(25)	119.2
C(210)-C(25)-H(25)	119.2
C(25)-C(26)-C(27)	118.8(4)
C(25)-C(26)-H(26)	120.6
C(27)-C(26)-H(26)	120.6
C(28)-C(27)-C(26)	120.7(4)
C(28)-C(27)-H(27)	119.6
C(26)-C(27)-H(27)	119.6
C(27)-C(28)-C(29)	122.8(3)
C(27)-C(28)-Br(1)	114.5(3)
C(29)-C(28)-Br(1)	122.7(3)
C(21)-C(29)-C(28)	127.7(3)
C(21)-C(29)-C(210)	118.0(3)
C(28)-C(29)-C(210)	114.3(4)
C(25)-C(210)-C(24)	118.7(4)
C(25)-C(210)-C(29)	121.8(4)
C(24)-C(210)-C(29)	119.5(4)
C(32)-O(2)-C(2)	117.6(4)
O(2)-C(2)-H(2A)	109.5
O(2)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
O(2)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(32)-C(31)-C(39)	119.7(4)
C(32)-C(31)-C(41)	120.6(4)
C(39)-C(31)-C(41)	118.8(3)
O(2)-C(32)-C(31)	115.9(4)
O(2)-C(32)-C(33)	123.3(4)
C(31)-C(32)-C(33)	120.7(4)
C(34)-C(33)-C(32)	120.4(4)
C(34)-C(33)-H(33)	119.8
C(32)-C(33)-H(33)	119.8
C(33)-C(34)-C(310)	121.4(4)
C(33)-C(34)-H(34)	119.3
C(310)-C(34)-H(34)	119.3
C(36)-C(35)-C(310)	121.1(5)
C(36)-C(35)-H(35)	119.5
C(310)-C(35)-H(35)	119.5
C(35)-C(36)-C(37)	120.4(4)
C(35)-C(36)-H(36)	119.8
C(37)-C(36)-H(36)	119.8
C(38)-C(37)-C(36)	120.6(5)
C(38)-C(37)-H(37)	119.7
C(36)-C(37)-H(37)	119.7
C(37)-C(38)-C(39)	120.9(4)
C(37)-C(38)-H(38)	119.5
C(39)-C(38)-H(38)	119.5
C(38)-C(39)-C(31)	122.6(4)
C(38)-C(39)-C(310)	118.4(4)
C(31)-C(39)-C(310)	119.1(4)
C(34)-C(310)-C(35)	122.7(4)
C(34)-C(310)-C(39)	118.6(4)
C(35)-C(310)-C(39)	118.6(5)
C(42)-C(41)-C(49)	119.1(4)
C(42)-C(41)-C(31)	114.9(3)
C(49)-C(41)-C(31)	125.9(3)
C(41)-C(42)-C(43)	122.9(4)
C(41)-C(42)-H(42)	118.6
C(43)-C(42)-H(42)	118.6
C(44)-C(43)-C(42)	119.5(4)
C(44)-C(43)-H(43)	120.2
C(42)-C(43)-H(43)	120.2
C(43)-C(44)-C(410)	120.2(4)
C(43)-C(44)-H(44)	119.9
C(410)-C(44)-H(44)	119.9
C(46)-C(45)-C(410)	120.7(4)

C(46)-C(45)-H(45)	119.6
C(410)-C(45)-H(45)	119.6
C(45)-C(46)-C(47)	119.8(4)
C(45)-C(46)-H(46)	120.1
C(47)-C(46)-H(46)	120.1
C(48)-C(47)-C(46)	120.4(4)
C(48)-C(47)-H(47)	119.8
C(46)-C(47)-H(47)	119.8
C(47)-C(48)-C(49)	123.3(4)
C(47)-C(48)-Br(2)	114.3(3)
C(49)-C(48)-Br(2)	122.4(3)
C(48)-C(49)-C(41)	127.5(4)
C(48)-C(49)-C(410)	115.0(3)
C(41)-C(49)-C(410)	117.5(3)
C(44)-C(410)-C(45)	118.6(4)
C(44)-C(410)-C(49)	120.7(3)
C(45)-C(410)-C(49)	120.7(4)

Table 10. Anisotropic displacement parameters (A^2 x 10^3) for (*S*)-(+)-**18**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Br(1)	45(1)	30(1)	28(1)	6(1)	0(1)	-4(1)
O(1)	36(2)	34(1)	63(2)	0(2)	-8(2)	-7(1)
C(1)	41(3)	54(3)	63(3)	10(3)	-5(3)	-13(2)
C(11)	38(2)	24(2)	21(2)	-3(1)	-3(1)	-4(2)
C(12)	41(2)	33(2)	30(2)	2(2)	-10(2)	-6(2)
C(13)	57(3)	32(2)	42(3)	0(2)	-3(2)	-14(2)
C(14)	66(3)	25(2)	42(3)	-6(2)	-4(2)	2(2)
C(15)	69(3)	32(2)	33(2)	1(2)	7(2)	12(2)
C(16)	52(3)	47(3)	34(2)	9(2)	3(2)	17(2)
C(17)	46(3)	48(3)	33(2)	2(2)	-5(2)	8(2)
C(18)	42(2)	40(2)	24(2)	1(2)	-1(2)	6(2)
C(19)	46(3)	27(2)	25(2)	2(2)	-1(2)	1(2)
C(110)	54(3)	29(2)	26(2)	2(2)	-1(2)	7(2)
C(21)	28(2)	24(2)	32(2)	4(2)	-4(2)	0(2)
C(22)	41(2)	34(2)	31(2)	0(2)	-4(2)	-5(2)
C(23)	41(2)	29(2)	29(2)	10(2)	-4(2)	-4(2)
C(24)	33(2)	25(2)	43(2)	5(2)	-1(2)	-2(2)
C(25)	32(2)	26(2)	41(2)	-4(2)	1(2)	2(2)
C(26)	38(3)	30(2)	37(3)	-12(2)	-3(2)	1(2)
C(27)	28(2)	40(2)	26(2)	-1(2)	0(2)	-2(2)
C(28)	25(2)	22(2)	28(2)	3(1)	-1(2)	-1(1)
C(29)	19(2)	29(2)	28(2)	-1(1)	-3(2)	4(2)
C(210)	22(2)	28(2)	33(2)	0(2)	0(2)	2(2)
Br(2)	32(1)	42(1)	26(1)	1(1)	-5(1)	3(1)
O(2)	42(2)	27(1)	58(2)	4(1)	0(2)	-7(1)
C(2)	52(3)	35(2)	69(3)	9(2)	-12(3)	-11(2)
C(31)	24(2)	32(2)	20(2)	3(1)	3(1)	0(1)
C(32)	33(2)	42(2)	31(2)	3(2)	-1(2)	-3(2)
C(33)	35(3)	51(3)	50(3)	7(2)	-4(2)	-20(2)
C(34)	21(2)	79(4)	44(3)	6(3)	1(2)	-4(2)
C(35)	38(3)	75(3)	32(2)	-9(2)	-3(2)	23(3)
C(36)	52(3)	54(3)	33(2)	-8(2)	-9(2)	27(2)
C(37)	62(3)	38(2)	31(2)	-4(2)	-8(2)	17(2)
C(38)	37(2)	36(2)	28(2)	1(2)	-2(2)	10(2)
C(39)	29(2)	37(2)	18(2)	0(2)	-2(2)	1(2)
C(310)	26(2)	60(3)	28(2)	0(2)	-4(2)	9(2)
C(41)	30(2)	18(2)	28(2)	1(2)	0(2)	0(1)
C(42)	33(2)	33(2)	23(2)	0(2)	3(2)	0(2)
C(43)	36(2)	38(2)	28(2)	1(2)	-2(2)	4(2)
C(44)	21(2)	33(2)	38(2)	0(2)	-5(2)	2(2)
C(45)	24(2)	35(2)	40(2)	1(2)	6(2)	-1(2)
C(46)	41(2)	34(2)	32(2)	4(2)	10(2)	-2(2)
C(47)	43(2)	29(2)	27(2)	4(2)	4(2)	5(2)
C(48)	27(2)	21(2)	31(2)	-1(2)	1(2)	4(1)
C(49)	30(2)	18(2)	25(2)	-2(1)	2(1)	1(1)
C(410)	29(2)	22(2)	30(2)	-1(1)	5(2)	2(1)

Table 11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for (*S*)-(+)-**18**.

	x	y	z	U(eq)
H(1A)	1906	5770	-731	79
H(1B)	1370	6378	-48	79
H(1C)	1816	5458	265	79
H(13)	3021	4686	-213	52
H(14)	4397	3959	-222	53
H(15)	6085	3973	-43	54
H(16)	7400	4754	244	54
H(17)	7332	6315	590	51
H(18)	5976	7079	560	43
H(22)	4206	7537	-1056	42
H(23)	4268	9121	-1204	40
H(24)	4383	10025	29	40
H(25)	4495	10228	1604	39
H(26)	4542	9674	3029	42
H(27)	4435	8090	3266	37
H(2A)	3413	3826	-2169	78
H(2B)	4115	3360	-2814	78
H(2C)	3179	3717	-3183	78
H(33)	2278	4850	-2719	55
H(34)	1438	6156	-2565	57
H(35)	1349	7865	-2503	58
H(36)	2051	9249	-2632	56
H(37)	3613	9337	-2932	52
H(38)	4472	8040	-3060	40
H(42)	5019	5940	-1659	35
H(43)	6570	6126	-1408	41
H(44)	7500	6638	-2539	37
H(45)	7720	7162	-4054	40
H(46)	7175	7447	-5461	43
H(47)	5647	7164	-5794	40

Table 12. Torsion angles [deg] for (*S*)-(+)-**18**.

C(1)-O(1)-C(12)-C(11)	177.2(4)
C(1)-O(1)-C(12)-C(13)	-3.3(7)
C(19)-C(11)-C(12)-O(1)	178.3(4)
C(21)-C(11)-C(12)-O(1)	-10.5(5)
C(19)-C(11)-C(12)-C(13)	-1.2(6)
C(21)-C(11)-C(12)-C(13)	170.0(4)
O(1)-C(12)-C(13)-C(14)	-179.6(4)
C(11)-C(12)-C(13)-C(14)	-0.2(7)
C(12)-C(13)-C(14)-C(110)	0.9(8)
C(110)-C(15)-C(16)-C(17)	0.9(7)
C(15)-C(16)-C(17)-C(18)	-1.9(7)
C(16)-C(17)-C(18)-C(19)	1.7(7)
C(17)-C(18)-C(19)-C(11)	-179.6(4)
C(17)-C(18)-C(19)-C(110)	-0.5(6)
C(12)-C(11)-C(19)-C(18)	-179.1(4)
C(21)-C(11)-C(19)-C(18)	9.6(6)
C(12)-C(11)-C(19)-C(110)	1.9(6)
C(21)-C(11)-C(19)-C(110)	-169.5(4)
C(13)-C(14)-C(110)-C(15)	-179.9(5)
C(13)-C(14)-C(110)-C(19)	-0.3(7)
C(16)-C(15)-C(110)-C(14)	180.0(5)
C(16)-C(15)-C(110)-C(19)	0.4(7)
C(18)-C(19)-C(110)-C(14)	179.8(4)
C(11)-C(19)-C(110)-C(14)	-1.1(6)
C(18)-C(19)-C(110)-C(15)	-0.6(6)
C(11)-C(19)-C(110)-C(15)	178.5(4)
C(12)-C(11)-C(21)-C(22)	-77.7(5)
C(19)-C(11)-C(21)-C(22)	93.5(5)
C(12)-C(11)-C(21)-C(29)	105.9(5)
C(19)-C(11)-C(21)-C(29)	-82.9(5)
C(29)-C(21)-C(22)-C(23)	0.9(7)
C(11)-C(21)-C(22)-C(23)	-175.8(4)
C(21)-C(22)-C(23)-C(24)	0.1(8)
C(22)-C(23)-C(24)-C(210)	-0.6(7)
C(210)-C(25)-C(26)-C(27)	-0.3(7)
C(25)-C(26)-C(27)-C(28)	0.3(6)
C(26)-C(27)-C(28)-C(29)	1.0(6)
C(26)-C(27)-C(28)-Br(1)	-177.8(3)
C(22)-C(21)-C(29)-C(28)	178.4(4)
C(11)-C(21)-C(29)-C(28)	-5.3(7)
C(22)-C(21)-C(29)-C(210)	-1.4(6)
C(11)-C(21)-C(29)-C(210)	174.8(4)
C(27)-C(28)-C(29)-C(21)	178.0(4)
Br(1)-C(28)-C(29)-C(21)	-3.3(6)
C(27)-C(28)-C(29)-C(210)	-2.2(6)
Br(1)-C(28)-C(29)-C(210)	176.6(3)
C(26)-C(25)-C(210)-C(24)	-180.0(4)
C(26)-C(25)-C(210)-C(29)	-1.0(7)
C(23)-C(24)-C(210)-C(25)	179.0(4)
C(23)-C(24)-C(210)-C(29)	0.0(6)
C(21)-C(29)-C(210)-C(25)	-178.0(4)
C(28)-C(29)-C(210)-C(25)	2.1(6)
C(21)-C(29)-C(210)-C(24)	1.0(6)
C(28)-C(29)-C(210)-C(24)	-178.9(4)
C(2)-O(2)-C(32)-C(31)	172.8(4)
C(2)-O(2)-C(32)-C(33)	-9.4(6)
C(39)-C(31)-C(32)-O(2)	179.7(4)
C(41)-C(31)-C(32)-O(2)	-11.1(5)
C(39)-C(31)-C(32)-C(33)	1.8(6)
C(41)-C(31)-C(32)-C(33)	171.1(4)
O(2)-C(32)-C(33)-C(34)	179.4(4)
C(31)-C(32)-C(33)-C(34)	-3.0(7)
C(32)-C(33)-C(34)-C(310)	1.6(8)
C(310)-C(35)-C(36)-C(37)	0.0(7)

C(35)-C(36)-C(37)-C(38)	-1.1(7)
C(36)-C(37)-C(38)-C(39)	0.7(6)
C(37)-C(38)-C(39)-C(31)	-179.2(4)
C(37)-C(38)-C(39)-C(310)	0.8(6)
C(32)-C(31)-C(39)-C(38)	-179.3(4)
C(41)-C(31)-C(39)-C(38)	11.2(5)
C(32)-C(31)-C(39)-C(310)	0.6(5)
C(41)-C(31)-C(39)-C(310)	-168.8(3)
C(33)-C(34)-C(310)-C(35)	-179.3(5)
C(33)-C(34)-C(310)-C(39)	0.8(7)
C(36)-C(35)-C(310)-C(34)	-178.4(5)
C(36)-C(35)-C(310)-C(39)	1.5(7)
C(38)-C(39)-C(310)-C(34)	178.0(4)
C(31)-C(39)-C(310)-C(34)	-1.9(6)
C(38)-C(39)-C(310)-C(35)	-1.9(6)
C(31)-C(39)-C(310)-C(35)	178.2(4)
C(32)-C(31)-C(41)-C(42)	-69.8(5)
C(39)-C(31)-C(41)-C(42)	99.5(4)
C(32)-C(31)-C(41)-C(49)	113.7(4)
C(39)-C(31)-C(41)-C(49)	-76.9(5)
C(49)-C(41)-C(42)-C(43)	3.4(6)
C(31)-C(41)-C(42)-C(43)	-173.3(4)
C(41)-C(42)-C(43)-C(44)	-0.7(6)
C(42)-C(43)-C(44)-C(410)	-1.1(6)
C(410)-C(45)-C(46)-C(47)	-0.8(6)
C(45)-C(46)-C(47)-C(48)	2.3(6)
C(46)-C(47)-C(48)-C(49)	-0.5(6)
C(46)-C(47)-C(48)-Br(2)	-177.5(3)
C(47)-C(48)-C(49)-C(41)	178.0(4)
Br(2)-C(48)-C(49)-C(41)	-5.3(5)
C(47)-C(48)-C(49)-C(410)	-2.6(5)
Br(2)-C(48)-C(49)-C(410)	174.2(3)
C(42)-C(41)-C(49)-C(48)	175.2(3)
C(31)-C(41)-C(49)-C(48)	-8.5(6)
C(42)-C(41)-C(49)-C(410)	-4.3(5)
C(31)-C(41)-C(49)-C(410)	172.1(3)
C(43)-C(44)-C(410)-C(45)	179.2(4)
C(43)-C(44)-C(410)-C(49)	0.1(6)
C(46)-C(45)-C(410)-C(44)	178.4(4)
C(46)-C(45)-C(410)-C(49)	-2.5(6)
C(48)-C(49)-C(410)-C(44)	-176.9(3)
C(41)-C(49)-C(410)-C(44)	2.6(5)
C(48)-C(49)-C(410)-C(45)	4.0(5)
C(41)-C(49)-C(410)-C(45)	-176.5(3)

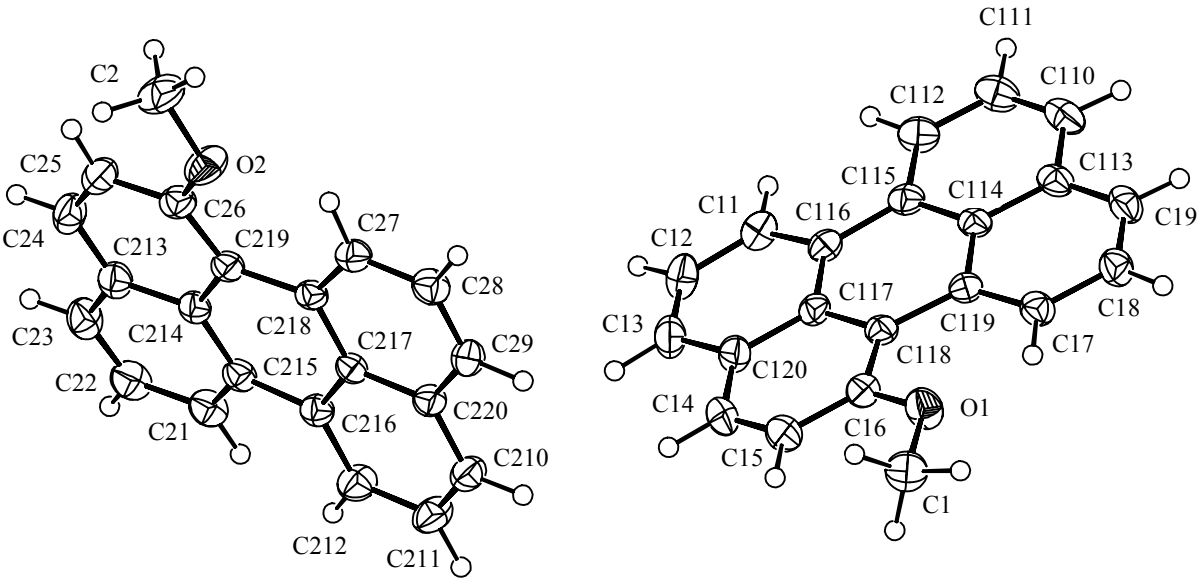

Figure 10. ORTEP diagram of **21** showing the atom labeling scheme. Displacement parameters are shown at the 50% probability level.

Table 13. Crystal data and structure refinement for **21**.

Identification code	**21**
Empirical formula	C21 H14 O
Formula weight	282.32
Temperature	150(2) K
Wavelength	0.71070 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 18.2280(2) A alpha = 90 deg. b = 15.2280(3) A beta = 104.4240(12) deg. c = 10.2160(4) A gamma = 90 deg.
Volume	2746.33(12) A^3
Z, Calculated density	8, 1.366 Mg/m^3
Absorption coefficient	0.082 mm^-1
F(000)	1184
Crystal size	0.5 x 0.4 x 0.3 mm
Theta range for data collection	1.15 to 27.50 deg.
Limiting indices	-23<=h<=23, -19<=k<=19, -13<=l<=12
Reflections collected / unique	43800 / 6287 [R(int) = 0.0300]
Completeness to theta = 27.50	99.8 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6287 / 0 / 509
Goodness-of-fit on F^2	1.051
Final R indices [I>2sigma(I)]	R1 = 0.0496, wR2 = 0.1170
R indices (all data)	R1 = 0.0753, wR2 = 0.1347
Largest diff. peak and hole	0.240 and -0.212 e.A^-3

Table 14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **21**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	11112(1)	5812(1)	14476(2)	42(1)
O(1)	10718(1)	5253(1)	13400(1)	39(1)
C(11)	7531(1)	4401(1)	10090(2)	35(1)
C(12)	7161(1)	5037(1)	10684(2)	42(1)
C(13)	7570(1)	5558(1)	11683(2)	40(1)
C(14)	8794(1)	6011(1)	13150(2)	38(1)
C(15)	9557(1)	5934(1)	13571(2)	38(1)
C(16)	9948(1)	5324(1)	12959(2)	31(1)
C(17)	10730(1)	4135(1)	11330(2)	31(1)
C(18)	11075(1)	3554(1)	10592(2)	35(1)
C(19)	10653(1)	3008(1)	9645(2)	34(1)
C(110)	9411(1)	2476(1)	8381(2)	38(1)
C(111)	8637(1)	2498(1)	8112(2)	40(1)
C(112)	8278(1)	3080(1)	8802(2)	36(1)
C(113)	9855(1)	3028(1)	9375(2)	31(1)
C(114)	9493(1)	3621(1)	10107(1)	26(1)
C(115)	8688(1)	3649(1)	9780(2)	28(1)
C(116)	8310(1)	4295(1)	10456(2)	28(1)
C(117)	8757(1)	4842(1)	11493(1)	27(1)
C(118)	9566(1)	4786(1)	11888(1)	26(1)
C(119)	9950(1)	4181(1)	11129(1)	26(1)
C(120)	8366(1)	5470(1)	12117(2)	33(1)
C(2)	4940(1)	-1011(1)	6316(2)	50(1)
O(2)	4661(1)	-362(1)	7081(1)	43(1)
C(21)	5697(1)	2518(1)	11253(2)	35(1)
C(22)	6465(1)	2492(1)	11247(2)	39(1)
C(23)	6701(1)	1931(1)	10399(2)	39(1)
C(24)	6428(1)	744(1)	8712(2)	38(1)
C(25)	5931(1)	183(1)	7919(2)	36(1)
C(26)	5159(1)	191(1)	7919(2)	32(1)
C(27)	3527(1)	183(1)	8170(2)	31(1)
C(28)	2765(1)	246(1)	8209(2)	34(1)
C(29)	2523(1)	912(1)	8882(2)	32(1)
C(210)	2808(1)	2224(1)	10310(2)	34(1)
C(211)	3309(1)	2824(1)	11004(2)	40(1)
C(212)	4078(1)	2754(1)	11024(2)	36(1)
C(213)	6183(1)	1354(1)	9553(2)	33(1)
C(214)	5397(1)	1368(1)	9560(1)	27(1)
C(215)	5160(1)	1996(1)	10410(2)	28(1)
C(216)	4349(1)	2086(1)	10346(2)	27(1)
C(217)	3830(1)	1469(1)	9577(1)	25(1)
C(218)	4069(1)	782(1)	8810(1)	25(1)
C(219)	4874(1)	761(1)	8741(1)	26(1)
C(220)	3051(1)	1538(1)	9591(1)	28(1)

Table 15. Bond lengths [A] and angles [deg] for **21**.

C(1)-O(1)	1.433(2)
C(1)-H(1A)	1.01(2)
C(1)-H(1B)	1.04(2)
C(1)-H(1C)	1.02(2)
O(1)-C(16)	1.3680(19)
C(11)-C(116)	1.386(2)
C(11)-C(12)	1.402(2)
C(11)-H(11)	1.008(18)
C(12)-C(13)	1.359(3)
C(12)-H(12)	0.984(19)
C(13)-C(120)	1.414(2)
C(13)-H(13)	1.02(2)
C(14)-C(15)	1.355(2)
C(14)-C(120)	1.411(2)
C(14)-H(14)	0.97(2)
C(15)-C(16)	1.409(2)
C(15)-H(15)	0.991(19)
C(16)-C(118)	1.405(2)
C(17)-C(119)	1.386(2)
C(17)-C(18)	1.408(2)
C(17)-H(17)	1.018(18)
C(18)-C(19)	1.359(2)
C(18)-H(18)	0.962(18)
C(19)-C(113)	1.412(2)
C(19)-H(19)	0.945(18)
C(110)-C(111)	1.368(2)
C(110)-C(113)	1.408(2)
C(110)-H(110)	0.97(2)
C(111)-C(112)	1.393(2)
C(111)-H(111)	0.99(2)
C(112)-C(115)	1.392(2)
C(112)-H(112)	0.989(17)
C(113)-C(114)	1.434(2)
C(114)-C(115)	1.422(2)
C(114)-C(119)	1.441(2)
C(115)-C(116)	1.468(2)
C(116)-C(117)	1.432(2)
C(117)-C(118)	1.432(2)
C(117)-C(120)	1.433(2)
C(118)-C(119)	1.487(2)
C(2)-O(2)	1.429(2)
C(2)-H(2A)	1.00(2)
C(2)-H(2B)	1.00(2)
C(2)-H(2C)	0.98(2)
O(2)-C(26)	1.3704(19)
C(21)-C(215)	1.382(2)
C(21)-C(22)	1.403(2)
C(21)-H(21)	0.989(19)
C(22)-C(23)	1.361(3)
C(22)-H(22)	0.99(2)
C(23)-C(213)	1.416(2)
C(23)-H(23)	0.978(18)
C(24)-C(25)	1.358(3)
C(24)-C(213)	1.410(2)
C(24)-H(24)	0.963(19)
C(25)-C(26)	1.407(2)
C(25)-H(25)	0.962(19)
C(26)-C(219)	1.396(2)
C(27)-C(218)	1.384(2)
C(27)-C(28)	1.403(2)
C(27)-H(27)	1.014(18)
C(28)-C(29)	1.359(2)
C(28)-H(28)	0.991(19)
C(29)-C(220)	1.418(2)

C(29)-H(29)	1.009(17)
C(210)-C(211)	1.360(2)
C(210)-C(220)	1.410(2)
C(210)-H(210)	1.012(19)
C(211)-C(212)	1.401(2)
C(211)-H(211)	1.02(2)
C(212)-C(216)	1.390(2)
C(212)-H(212)	0.968(19)
C(213)-C(214)	1.435(2)
C(214)-C(215)	1.428(2)
C(214)-C(219)	1.437(2)
C(215)-C(216)	1.471(2)
C(216)-C(217)	1.423(2)
C(217)-C(220)	1.428(2)
C(217)-C(218)	1.437(2)
C(218)-C(219)	1.486(2)

O(1)-C(1)-H(1A)	102.6(12)
O(1)-C(1)-H(1B)	110.6(11)
H(1A)-C(1)-H(1B)	112.9(16)
O(1)-C(1)-H(1C)	111.0(11)
H(1A)-C(1)-H(1C)	110.9(16)
H(1B)-C(1)-H(1C)	108.8(16)
C(16)-O(1)-C(1)	118.86(13)
C(116)-C(11)-C(12)	122.38(16)
C(116)-C(11)-H(11)	117.9(10)
C(12)-C(11)-H(11)	119.8(10)
C(13)-C(12)-C(11)	119.64(16)
C(13)-C(12)-H(12)	120.6(11)
C(11)-C(12)-H(12)	119.7(11)
C(12)-C(13)-C(120)	120.61(16)
C(12)-C(13)-H(13)	121.9(11)
C(120)-C(13)-H(13)	117.4(11)
C(15)-C(14)-C(120)	121.28(15)
C(15)-C(14)-H(14)	121.1(11)
C(120)-C(14)-H(14)	117.6(11)
C(14)-C(15)-C(16)	120.60(16)
C(14)-C(15)-H(15)	120.9(11)
C(16)-C(15)-H(15)	118.5(11)
O(1)-C(16)-C(118)	118.68(13)
O(1)-C(16)-C(15)	119.78(14)
C(118)-C(16)-C(15)	121.54(14)
C(119)-C(17)-C(18)	121.99(15)
C(119)-C(17)-H(17)	119.2(10)
C(18)-C(17)-H(17)	118.8(10)
C(19)-C(18)-C(17)	121.11(15)
C(19)-C(18)-H(18)	122.2(11)
C(17)-C(18)-H(18)	116.7(11)
C(18)-C(19)-C(113)	119.91(15)
C(18)-C(19)-H(19)	120.8(10)
C(113)-C(19)-H(19)	119.2(10)
C(111)-C(110)-C(113)	120.58(15)
C(111)-C(110)-H(110)	123.3(11)
C(113)-C(110)-H(110)	116.1(11)
C(110)-C(111)-C(112)	120.34(16)
C(110)-C(111)-H(111)	118.3(11)
C(112)-C(111)-H(111)	121.4(11)
C(115)-C(112)-C(111)	121.53(16)
C(115)-C(112)-H(112)	119.1(10)
C(111)-C(112)-H(112)	119.3(10)
C(110)-C(113)-C(19)	120.49(15)
C(110)-C(113)-C(114)	119.69(14)
C(19)-C(113)-C(114)	119.82(14)
C(115)-C(114)-C(113)	118.57(13)
C(115)-C(114)-C(119)	122.00(13)
C(113)-C(114)-C(119)	119.42(13)
C(112)-C(115)-C(114)	119.23(14)
C(112)-C(115)-C(116)	121.63(14)

C(114)-C(115)-C(116)	119.11(13)
C(11)-C(116)-C(117)	119.16(14)
C(11)-C(116)-C(115)	121.37(14)
C(117)-C(116)-C(115)	119.45(13)
C(118)-C(117)-C(116)	121.95(13)
C(118)-C(117)-C(120)	120.40(14)
C(116)-C(117)-C(120)	117.64(13)
C(16)-C(118)-C(117)	117.40(13)
C(16)-C(118)-C(119)	124.12(13)
C(117)-C(118)-C(119)	118.47(13)
C(17)-C(119)-C(114)	117.72(13)
C(17)-C(119)-C(118)	123.53(14)
C(114)-C(119)-C(118)	118.74(13)
C(14)-C(120)-C(13)	120.80(15)
C(14)-C(120)-C(117)	118.65(14)
C(13)-C(120)-C(117)	120.53(15)
O(2)-C(2)-H(2A)	110.2(12)
O(2)-C(2)-H(2B)	109.0(12)
H(2A)-C(2)-H(2B)	107.3(16)
O(2)-C(2)-H(2C)	104.7(13)
H(2A)-C(2)-H(2C)	109.6(18)
H(2B)-C(2)-H(2C)	116.0(18)
C(26)-O(2)-C(2)	119.78(14)
C(215)-C(21)-C(22)	122.18(16)
C(215)-C(21)-H(21)	119.4(11)
C(22)-C(21)-H(21)	118.4(11)
C(23)-C(22)-C(21)	119.69(16)
C(23)-C(22)-H(22)	120.1(11)
C(21)-C(22)-H(22)	120.2(11)
C(22)-C(23)-C(213)	120.66(15)
C(22)-C(23)-H(23)	121.5(11)
C(213)-C(23)-H(23)	117.8(11)
C(25)-C(24)-C(213)	120.80(15)
C(25)-C(24)-H(24)	120.3(11)
C(213)-C(24)-H(24)	118.9(11)
C(24)-C(25)-C(26)	120.89(16)
C(24)-C(25)-H(25)	123.1(11)
C(26)-C(25)-H(25)	115.9(11)
O(2)-C(26)-C(219)	118.06(13)
O(2)-C(26)-C(25)	120.07(14)
C(219)-C(26)-C(25)	121.86(15)
C(218)-C(27)-C(28)	122.43(15)
C(218)-C(27)-H(27)	120.9(10)
C(28)-C(27)-H(27)	116.7(10)
C(29)-C(28)-C(27)	120.96(15)
C(29)-C(28)-H(28)	120.7(11)
C(27)-C(28)-H(28)	118.3(11)
C(28)-C(29)-C(220)	119.67(14)
C(28)-C(29)-H(29)	120.9(10)
C(220)-C(29)-H(29)	119.4(10)
C(211)-C(210)-C(220)	120.79(15)
C(211)-C(210)-H(210)	121.5(11)
C(220)-C(210)-H(210)	117.7(11)
C(210)-C(211)-C(212)	119.77(15)
C(210)-C(211)-H(211)	120.9(11)
C(212)-C(211)-H(211)	119.3(11)
C(216)-C(212)-C(211)	121.76(15)
C(216)-C(212)-H(212)	119.8(11)
C(211)-C(212)-H(212)	118.5(11)
C(24)-C(213)-C(23)	121.05(15)
C(24)-C(213)-C(214)	118.79(15)
C(23)-C(213)-C(214)	120.15(15)
C(215)-C(214)-C(213)	117.80(14)
C(215)-C(214)-C(219)	121.81(13)
C(213)-C(214)-C(219)	120.39(14)
C(21)-C(215)-C(214)	119.36(14)
C(21)-C(215)-C(216)	121.44(14)
C(214)-C(215)-C(216)	119.18(13)

C(212)-C(216)-C(217)	119.31(14)
C(212)-C(216)-C(215)	121.59(14)
C(217)-C(216)-C(215)	119.10(13)
C(216)-C(217)-C(220)	118.15(13)
C(216)-C(217)-C(218)	122.10(13)
C(220)-C(217)-C(218)	119.75(13)
C(27)-C(218)-C(217)	117.39(13)
C(27)-C(218)-C(219)	124.07(13)
C(217)-C(218)-C(219)	118.53(13)
C(26)-C(219)-C(214)	117.23(13)
C(26)-C(219)-C(218)	124.17(14)
C(214)-C(219)-C(218)	118.59(13)
C(210)-C(220)-C(29)	120.15(14)
C(210)-C(220)-C(217)	120.15(14)
C(29)-C(220)-C(217)	119.69(13)

Symmetry transformations used to generate equivalent atoms:

Table 16. Anisotropic displacement parameters (A^2 x 10^3) for **21**. The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	39(1)	46(1)	39(1)	-11(1)	5(1)	-8(1)
O(1)	33(1)	44(1)	38(1)	-13(1)	4(1)	-1(1)
C(11)	31(1)	42(1)	32(1)	2(1)	9(1)	-3(1)
C(12)	29(1)	55(1)	44(1)	-2(1)	15(1)	1(1)
C(13)	35(1)	45(1)	44(1)	-1(1)	19(1)	5(1)
C(14)	42(1)	36(1)	43(1)	-10(1)	20(1)	1(1)
C(15)	42(1)	36(1)	37(1)	-11(1)	14(1)	-5(1)
C(16)	31(1)	31(1)	32(1)	-1(1)	10(1)	-2(1)
C(17)	32(1)	29(1)	33(1)	2(1)	8(1)	4(1)
C(18)	33(1)	33(1)	41(1)	4(1)	12(1)	8(1)
C(19)	42(1)	29(1)	35(1)	3(1)	15(1)	11(1)
C(110)	55(1)	27(1)	31(1)	-3(1)	12(1)	6(1)
C(111)	49(1)	33(1)	33(1)	-6(1)	3(1)	-2(1)
C(112)	39(1)	34(1)	33(1)	0(1)	4(1)	-2(1)
C(113)	42(1)	23(1)	28(1)	4(1)	10(1)	4(1)
C(114)	35(1)	20(1)	22(1)	5(1)	9(1)	1(1)
C(115)	34(1)	24(1)	26(1)	6(1)	7(1)	-1(1)
C(116)	31(1)	28(1)	26(1)	6(1)	9(1)	-2(1)
C(117)	29(1)	27(1)	26(1)	4(1)	11(1)	0(1)
C(118)	32(1)	22(1)	24(1)	4(1)	9(1)	0(1)
C(119)	31(1)	22(1)	26(1)	6(1)	9(1)	1(1)
C(120)	34(1)	34(1)	35(1)	2(1)	16(1)	2(1)
C(2)	61(1)	45(1)	48(1)	-13(1)	21(1)	10(1)
O(2)	44(1)	43(1)	44(1)	-17(1)	14(1)	4(1)
C(21)	32(1)	33(1)	36(1)	2(1)	2(1)	-4(1)
C(22)	31(1)	37(1)	44(1)	3(1)	0(1)	-4(1)
C(23)	25(1)	45(1)	45(1)	10(1)	4(1)	-1(1)
C(24)	28(1)	49(1)	40(1)	12(1)	12(1)	9(1)
C(25)	37(1)	42(1)	33(1)	6(1)	14(1)	12(1)
C(26)	36(1)	30(1)	28(1)	3(1)	9(1)	6(1)
C(27)	34(1)	27(1)	31(1)	-2(1)	8(1)	1(1)
C(28)	33(1)	31(1)	36(1)	-4(1)	5(1)	-5(1)
C(29)	24(1)	34(1)	36(1)	0(1)	6(1)	-1(1)
C(210)	29(1)	34(1)	41(1)	-2(1)	10(1)	4(1)
C(211)	38(1)	37(1)	45(1)	-11(1)	13(1)	4(1)
C(212)	35(1)	32(1)	39(1)	-10(1)	8(1)	-3(1)
C(213)	30(1)	37(1)	32(1)	11(1)	8(1)	4(1)
C(214)	26(1)	29(1)	25(1)	8(1)	5(1)	3(1)
C(215)	28(1)	27(1)	27(1)	5(1)	4(1)	0(1)
C(216)	29(1)	27(1)	25(1)	2(1)	5(1)	1(1)
C(217)	27(1)	23(1)	23(1)	4(1)	5(1)	0(1)
C(218)	28(1)	23(1)	23(1)	4(1)	5(1)	3(1)
C(219)	30(1)	26(1)	24(1)	6(1)	7(1)	4(1)
C(220)	29(1)	27(1)	28(1)	2(1)	8(1)	2(1)

Table 17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **21**.

	x	y	z	U(eq)
H(1A)	11657(12)	5615(13)	14610(20)	55(6)
H(1B)	11031(11)	6467(14)	14200(20)	55(6)
H(1C)	10927(11)	5712(13)	15330(20)	50(5)
H(11)	7227(10)	4011(12)	9355(18)	39(5)
H(12)	6608(11)	5110(13)	10363(19)	48(5)
H(13)	7320(11)	6020(14)	12150(20)	55(6)
H(14)	8522(11)	6446(13)	13542(19)	48(5)
H(15)	9854(10)	6318(12)	14295(19)	46(5)
H(17)	11065(10)	4528(12)	12039(18)	38(5)
H(18)	11619(11)	3564(12)	10793(18)	41(5)
H(19)	10886(9)	2638(11)	9124(17)	34(4)
H(110)	9685(10)	2090(13)	7920(19)	47(5)
H(111)	8343(11)	2101(13)	7400(20)	49(5)
H(112)	7718(10)	3079(11)	8609(16)	30(4)
H(2A)	5174(11)	-722(14)	5630(20)	56(6)
H(2B)	5347(12)	-1358(14)	6940(20)	55(6)
H(2C)	4488(13)	-1343(15)	5850(20)	68(7)
H(21)	5535(10)	2941(13)	11861(19)	46(5)
H(22)	6832(10)	2887(13)	11843(19)	48(5)
H(23)	7231(10)	1909(12)	10354(18)	40(5)
H(24)	6957(11)	728(12)	8715(19)	47(5)
H(25)	6080(10)	-256(12)	7358(18)	40(5)
H(27)	3668(9)	-330(12)	7646(17)	38(5)
H(28)	2406(11)	-204(13)	7724(19)	46(5)
H(29)	1973(10)	964(11)	8894(17)	36(4)
H(210)	2250(11)	2257(12)	10281(18)	46(5)
H(211)	3137(11)	3313(14)	11540(20)	57(6)
H(212)	4426(10)	3188(13)	11525(19)	45(5)

Table 18. Torsion angles [deg] for **21**.

C(116)-C(11)-C(12)-C(13)	-1.9(3)
C(11)-C(12)-C(13)-C(120)	0.8(3)
C(120)-C(14)-C(15)-C(16)	1.6(3)
C(1)-O(1)-C(16)-C(118)	178.84(15)
C(1)-O(1)-C(16)-C(15)	-0.5(2)
C(14)-C(15)-C(16)-O(1)	-179.75(16)
C(14)-C(15)-C(16)-C(118)	0.9(3)
C(119)-C(17)-C(18)-C(19)	-0.1(2)
C(17)-C(18)-C(19)-C(113)	1.0(2)
C(113)-C(110)-C(111)-C(112)	1.2(3)
C(110)-C(111)-C(112)-C(115)	-0.3(3)
C(111)-C(110)-C(113)-C(19)	-179.64(15)
C(111)-C(110)-C(113)-C(114)	-0.2(2)
C(18)-C(19)-C(113)-C(110)	178.98(15)
C(18)-C(19)-C(113)-C(114)	-0.4(2)
C(110)-C(113)-C(114)-C(115)	-1.6(2)
C(19)-C(113)-C(114)-C(115)	177.81(13)
C(110)-C(113)-C(114)-C(119)	179.63(13)
C(19)-C(113)-C(114)-C(119)	-1.0(2)
C(111)-C(112)-C(115)-C(114)	-1.6(2)
C(111)-C(112)-C(115)-C(116)	176.68(15)
C(113)-C(114)-C(115)-C(112)	2.5(2)
C(119)-C(114)-C(115)-C(112)	-178.79(13)
C(113)-C(114)-C(115)-C(116)	-175.83(13)
C(119)-C(114)-C(115)-C(116)	2.9(2)
C(12)-C(11)-C(116)-C(117)	1.0(2)
C(12)-C(11)-C(116)-C(115)	-177.42(15)
C(112)-C(115)-C(116)-C(11)	-4.0(2)
C(114)-C(115)-C(116)-C(11)	174.29(14)
C(112)-C(115)-C(116)-C(117)	177.58(14)
C(114)-C(115)-C(116)-C(117)	-4.2(2)
C(11)-C(116)-C(117)-C(118)	-177.91(14)
C(115)-C(116)-C(117)-C(118)	0.6(2)
C(11)-C(116)-C(117)-C(120)	0.9(2)
C(115)-C(116)-C(117)-C(120)	179.36(13)
O(1)-C(16)-C(118)-C(117)	176.92(13)
C(15)-C(16)-C(118)-C(117)	-3.7(2)
O(1)-C(16)-C(118)-C(119)	-4.4(2)
C(15)-C(16)-C(118)-C(119)	174.94(14)
C(116)-C(117)-C(118)-C(16)	-177.10(13)
C(120)-C(117)-C(118)-C(16)	4.1(2)
C(116)-C(117)-C(118)-C(119)	4.2(2)
C(120)-C(117)-C(118)-C(119)	-174.61(13)
C(18)-C(17)-C(119)-C(114)	-1.3(2)
C(18)-C(17)-C(119)-C(118)	179.99(14)
C(115)-C(114)-C(119)-C(17)	-176.93(13)
C(113)-C(114)-C(119)-C(17)	1.8(2)
C(115)-C(114)-C(119)-C(118)	1.8(2)
C(113)-C(114)-C(119)-C(118)	-179.44(12)
C(16)-C(118)-C(119)-C(17)	-5.3(2)
C(117)-C(118)-C(119)-C(17)	173.37(13)
C(16)-C(118)-C(119)-C(114)	176.02(13)
C(117)-C(118)-C(119)-C(114)	-5.32(19)
C(15)-C(14)-C(120)-C(13)	-179.80(17)
C(15)-C(14)-C(120)-C(117)	-1.1(3)
C(12)-C(13)-C(120)-C(14)	179.79(17)
C(12)-C(13)-C(120)-C(117)	1.2(3)
C(118)-C(117)-C(120)-C(14)	-1.8(2)
C(116)-C(117)-C(120)-C(14)	179.38(14)
C(118)-C(117)-C(120)-C(13)	176.85(14)
C(116)-C(117)-C(120)-C(13)	-2.0(2)
C(215)-C(21)-C(22)-C(23)	-0.7(3)
C(21)-C(22)-C(23)-C(213)	-2.0(3)
C(213)-C(24)-C(25)-C(26)	-0.4(2)

C(2)-O(2)-C(26)-C(219)	-174.29(16)
C(2)-O(2)-C(26)-C(25)	6.8(2)
C(24)-C(25)-C(26)-O(2)	177.96(15)
C(24)-C(25)-C(26)-C(219)	-0.9(2)
C(218)-C(27)-C(28)-C(29)	0.4(2)
C(27)-C(28)-C(29)-C(220)	-2.0(2)
C(220)-C(210)-C(211)-C(212)	-1.0(3)
C(210)-C(211)-C(212)-C(216)	0.3(3)
C(25)-C(24)-C(213)-C(23)	178.96(15)
C(25)-C(24)-C(213)-C(214)	0.3(2)
C(22)-C(23)-C(213)-C(24)	-177.31(16)
C(22)-C(23)-C(213)-C(214)	1.4(2)
C(24)-C(213)-C(214)-C(215)	-179.46(14)
C(23)-C(213)-C(214)-C(215)	1.8(2)
C(24)-C(213)-C(214)-C(219)	1.1(2)
C(23)-C(213)-C(214)-C(219)	-177.65(14)
C(22)-C(21)-C(215)-C(214)	4.0(2)
C(22)-C(21)-C(215)-C(216)	-174.71(15)
C(213)-C(214)-C(215)-C(21)	-4.4(2)
C(219)-C(214)-C(215)-C(21)	175.07(14)
C(213)-C(214)-C(215)-C(216)	174.31(13)
C(219)-C(214)-C(215)-C(216)	-6.2(2)
C(211)-C(212)-C(216)-C(217)	1.8(2)
C(211)-C(212)-C(216)-C(215)	-177.80(15)
C(21)-C(215)-C(216)-C(212)	6.6(2)
C(214)-C(215)-C(216)-C(212)	-172.11(14)
C(21)-C(215)-C(216)-C(217)	-173.07(14)
C(214)-C(215)-C(216)-C(217)	8.3(2)
C(212)-C(216)-C(217)-C(220)	-3.1(2)
C(215)-C(216)-C(217)-C(220)	176.51(13)
C(212)-C(216)-C(217)-C(218)	177.54(14)
C(215)-C(216)-C(217)-C(218)	-2.8(2)
C(28)-C(27)-C(218)-C(217)	2.4(2)
C(28)-C(27)-C(218)-C(219)	-177.18(14)
C(216)-C(217)-C(218)-C(27)	175.85(13)
C(220)-C(217)-C(218)-C(27)	-3.5(2)
C(216)-C(217)-C(218)-C(219)	-4.6(2)
C(220)-C(217)-C(218)-C(219)	176.09(12)
O(2)-C(26)-C(219)-C(214)	-176.73(13)
C(25)-C(26)-C(219)-C(214)	2.1(2)
O(2)-C(26)-C(219)-C(218)	2.8(2)
C(25)-C(26)-C(219)-C(218)	-178.35(14)
C(215)-C(214)-C(219)-C(26)	178.33(13)
C(213)-C(214)-C(219)-C(26)	-2.2(2)
C(215)-C(214)-C(219)-C(218)	-1.2(2)
C(213)-C(214)-C(219)-C(218)	178.25(13)
C(27)-C(218)-C(219)-C(26)	6.6(2)
C(217)-C(218)-C(219)-C(26)	-172.90(13)
C(27)-C(218)-C(219)-C(214)	-173.87(14)
C(217)-C(218)-C(219)-C(214)	6.60(19)
C(211)-C(210)-C(220)-C(29)	179.44(16)
C(211)-C(210)-C(220)-C(217)	-0.4(2)
C(28)-C(29)-C(220)-C(210)	-179.03(15)
C(28)-C(29)-C(220)-C(217)	0.8(2)
C(216)-C(217)-C(220)-C(210)	2.4(2)
C(218)-C(217)-C(220)-C(210)	-178.21(14)
C(216)-C(217)-C(220)-C(29)	-177.36(13)
C(218)-C(217)-C(220)-C(29)	2.0(2)

Table 19. Crystal data and structure refinement for (*S*)-**22**.

Identification code	(*S*)-**22**
Empirical formula	C20 H13 Br O
Formula weight	349.21
Temperature	150(2) K
Wavelength	0.71070 A
Crystal system, space group	Tetragonal, P 41
Unit cell dimensions	a = 8.74500(10) A alpha = 90 deg. b = 8.74500(10) A beta = 90 deg. c = 40.0620(6) A gamma = 90 deg.
Volume	3063.74(7) A^3
Z, Calculated density	8, 1.514 Mg/m^3
Absorption coefficient	2.682 mm^-1
F(000)	1408
Crystal size	0.5 x 0.5 x 0.35 mm
Theta range for data collection	3.09 to 27.47 deg.
Limiting indices	-11<=h<=11, -6<=k<=11, -51<=l<=46
Reflections collected / unique	15309 / 6463 [R(int) = 0.0290]
Completeness to theta = 27.47	98.9 %
Absorption correction	Multiscans
Max. and min. transmission	0.518 and 0.447
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6463 / 0 / 398
Goodness-of-fit on F^2	1.050
Final R indices [I>2sigma(I)]	R1 = 0.0303, wR2 = 0.0630
R indices (all data)	R1 = 0.0370, wR2 = 0.0657
Absolute structure parameter	-0.009(6)
Largest diff. peak and hole	0.285 and -0.466 e.A^-3

Table 20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for (*S*)-**22**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Br(1)	423(1)	8347(1)	722	46(1)
O(1)	3116(2)	7739(2)	-91(1)	39(1)
C(11)	2279(3)	5957(3)	330(1)	30(1)
C(12)	2184(3)	6579(3)	14(1)	32(1)
C(13)	1111(4)	6061(3)	-220(1)	39(1)
C(14)	103(4)	4959(4)	-136(1)	42(1)
C(15)	-946(4)	3133(4)	284(1)	49(1)
C(16)	-915(5)	2537(4)	596(1)	56(1)
C(17)	168(5)	3057(4)	829(1)	55(1)
C(18)	1202(4)	4150(3)	745(1)	44(1)
C(19)	1205(3)	4813(3)	421(1)	34(1)
C(110)	99(4)	4303(3)	187(1)	37(1)
C(11')	3598(3)	6348(3)	552(1)	30(1)
C(12')	4949(4)	5647(4)	469(1)	53(1)
C(13')	6274(4)	5774(5)	654(1)	68(1)
C(14')	6242(4)	6598(5)	942(1)	55(1)
C(15')	4939(4)	8246(4)	1336(1)	51(1)
C(16')	3719(5)	9034(5)	1434(1)	62(1)
C(17')	2367(4)	9031(4)	1242(1)	48(1)
C(18')	2295(3)	8179(3)	959(1)	33(1)
C(19')	3539(3)	7288(3)	844(1)	28(1)
C(20')	4912(4)	7372(4)	1045(1)	38(1)
Br(2)	9407(1)	6016(1)	1581(1)	45(1)
O(2)	10297(2)	1713(2)	1899(1)	41(1)
C(21)	8054(3)	3298(3)	1967(1)	31(1)
C(22)	8854(3)	2163(3)	1809(1)	34(1)
C(23)	8230(4)	1387(4)	1530(1)	43(1)
C(24)	6823(4)	1779(4)	1413(1)	44(1)
C(25)	4463(4)	3349(5)	1453(1)	51(1)
C(26)	3645(4)	4428(5)	1609(1)	57(1)
C(27)	4251(4)	5206(4)	1891(1)	51(1)
C(28)	5671(3)	4851(4)	2004(1)	39(1)
C(29)	6567(3)	3696(3)	1849(1)	33(1)
C(210)	5948(3)	2941(4)	1568(1)	40(1)
C(21')	8675(3)	3992(3)	2280(1)	28(1)
C(22')	8446(4)	3147(3)	2565(1)	38(1)
C(23')	8926(4)	3631(4)	2881(1)	45(1)
C(24')	9634(4)	4997(4)	2912(1)	41(1)
C(25')	10661(4)	7354(4)	2671(1)	52(1)
C(26')	10906(5)	8303(4)	2410(1)	63(1)
C(27')	10459(4)	7858(4)	2093(1)	51(1)
C(28')	9780(3)	6471(3)	2038(1)	34(1)
C(29')	9430(3)	5442(3)	2304(1)	28(1)
C(30')	9908(3)	5930(3)	2629(1)	37(1)

Table 21. Bond lengths [A] and angles [deg] for (*S*)-**22**.

Br(1)-C(18')	1.899(3)
O(1)-C(12)	1.368(3)
O(1)-H(1)	0.9752
C(11)-C(12)	1.383(4)
C(11)-C(19)	1.419(4)
C(11)-C(11')	1.494(4)
C(12)-C(13)	1.401(4)
C(13)-C(14)	1.348(5)
C(13)-H(13)	0.9300
C(14)-C(110)	1.417(5)
C(14)-H(14)	0.9300
C(15)-C(16)	1.357(5)
C(15)-C(110)	1.426(4)
C(15)-H(15)	0.9300
C(16)-C(17)	1.405(5)
C(16)-H(16)	0.9300
C(17)-C(18)	1.358(5)
C(17)-H(17)	0.9300
C(18)-C(19)	1.422(4)
C(18)-H(18)	0.9300
C(19)-C(110)	1.418(4)
C(11')-C(12')	1.372(4)
C(11')-C(19')	1.433(4)
C(12')-C(13')	1.381(5)
C(12')-H(12')	0.9300
C(13')-C(14')	1.358(6)
C(13')-H(13')	0.9300
C(14')-C(20')	1.408(5)
C(14')-H(14')	0.9300
C(15')-C(16')	1.329(6)
C(15')-C(20')	1.397(5)
C(15')-H(15')	0.9300
C(16')-C(17')	1.410(5)
C(16')-H(16')	0.9300
C(17')-C(18')	1.357(4)
C(17')-H(17')	0.9300
C(18')-C(19')	1.415(4)
C(19')-C(20')	1.445(4)
Br(2)-C(28')	1.901(3)
O(2)-C(22)	1.371(3)
O(2)-H(2)	0.9316
C(21)-C(22)	1.369(4)
C(21)-C(29)	1.426(4)
C(21)-C(21')	1.497(4)
C(22)-C(23)	1.415(4)
C(23)-C(24)	1.361(5)
C(23)-H(23)	0.9300
C(24)-C(210)	1.417(5)
C(24)-H(24)	0.9300
C(25)-C(26)	1.338(5)
C(25)-C(210)	1.422(4)
C(25)-H(25)	0.9300
C(26)-C(27)	1.423(6)
C(26)-H(26)	0.9300
C(27)-C(28)	1.358(4)
C(27)-H(27)	0.9300
C(28)-C(29)	1.421(4)
C(28)-H(28)	0.9300
C(29)-C(210)	1.414(4)
C(21')-C(22')	1.374(4)
C(21')-C(29')	1.433(4)
C(22')-C(23')	1.400(4)
C(22')-H(22')	0.9300
C(23')-C(24')	1.351(5)

C(23')-H(23')	0.9300
C(24')-C(30')	1.419(4)
C(24')-H(24')	0.9300
C(25')-C(26')	1.352(6)
C(25')-C(30')	1.418(4)
C(25')-H(25')	0.9300
C(26')-C(27')	1.384(6)
C(26')-H(26')	0.9300
C(27')-C(28')	1.369(4)
C(27')-H(27')	0.9300
C(28')-C(29')	1.430(4)
C(29')-C(30')	1.432(4)

C(12)-O(1)-H(1)	107.1
C(12)-C(11)-C(19)	118.2(3)
C(12)-C(11)-C(11')	120.0(3)
C(19)-C(11)-C(11')	121.4(2)
O(1)-C(12)-C(11)	122.6(3)
O(1)-C(12)-C(13)	115.7(3)
C(11)-C(12)-C(13)	121.7(3)
C(14)-C(13)-C(12)	120.2(3)
C(14)-C(13)-H(13)	119.9
C(12)-C(13)-H(13)	119.9
C(13)-C(14)-C(110)	121.2(3)
C(13)-C(14)-H(14)	119.4
C(110)-C(14)-H(14)	119.4
C(16)-C(15)-C(110)	120.9(3)
C(16)-C(15)-H(15)	119.6
C(110)-C(15)-H(15)	119.6
C(15)-C(16)-C(17)	120.1(3)
C(15)-C(16)-H(16)	119.9
C(17)-C(16)-H(16)	119.9
C(18)-C(17)-C(16)	120.8(3)
C(18)-C(17)-H(17)	119.6
C(16)-C(17)-H(17)	119.6
C(17)-C(18)-C(19)	121.0(3)
C(17)-C(18)-H(18)	119.5
C(19)-C(18)-H(18)	119.5
C(110)-C(19)-C(11)	120.3(3)
C(110)-C(19)-C(18)	118.3(3)
C(11)-C(19)-C(18)	121.5(3)
C(14)-C(110)-C(19)	118.4(3)
C(14)-C(110)-C(15)	122.7(3)
C(19)-C(110)-C(15)	118.9(3)
C(12')-C(11')-C(19')	119.1(3)
C(12')-C(11')-C(11)	114.7(3)
C(19')-C(11')-C(11)	126.1(2)
C(11')-C(12')-C(13')	123.8(3)
C(11')-C(12')-H(12')	118.1
C(13')-C(12')-H(12')	118.1
C(14')-C(13')-C(12')	118.8(3)
C(14')-C(13')-H(13')	120.6
C(12')-C(13')-H(13')	120.6
C(13')-C(14')-C(20')	121.3(3)
C(13')-C(14')-H(14')	119.4
C(20')-C(14')-H(14')	119.4
C(16')-C(15')-C(20')	121.1(3)
C(16')-C(15')-H(15')	119.5
C(20')-C(15')-H(15')	119.5
C(15')-C(16')-C(17')	120.8(3)
C(15')-C(16')-H(16')	119.6
C(17')-C(16')-H(16')	119.6
C(18')-C(17')-C(16')	119.7(3)
C(18')-C(17')-H(17')	120.2
C(16')-C(17')-H(17')	120.2
C(17')-C(18')-C(19')	122.5(3)
C(17')-C(18')-Br(1)	114.5(2)
C(19')-C(18')-Br(1)	122.9(2)

C(18')-C(19')-C(11')	127.5(3)
C(18')-C(19')-C(20')	115.5(3)
C(11')-C(19')-C(20')	117.0(3)
C(15')-C(20')-C(14')	119.6(3)
C(15')-C(20')-C(19')	120.4(3)
C(14')-C(20')-C(19')	120.0(3)
C(22)-O(2)-H(2)	111.0
C(22)-C(21)-C(29)	119.4(3)
C(22)-C(21)-C(21')	119.8(2)
C(29)-C(21)-C(21')	120.5(3)
C(21)-C(22)-O(2)	123.8(3)
C(21)-C(22)-C(23)	121.0(3)
O(2)-C(22)-C(23)	115.2(3)
C(24)-C(23)-C(22)	120.1(3)
C(24)-C(23)-H(23)	120.0
C(22)-C(23)-H(23)	120.0
C(23)-C(24)-C(210)	121.1(3)
C(23)-C(24)-H(24)	119.4
C(210)-C(24)-H(24)	119.4
C(26)-C(25)-C(210)	121.0(3)
C(26)-C(25)-H(25)	119.5
C(210)-C(25)-H(25)	119.5
C(25)-C(26)-C(27)	120.5(3)
C(25)-C(26)-H(26)	119.7
C(27)-C(26)-H(26)	119.7
C(28)-C(27)-C(26)	119.8(3)
C(28)-C(27)-H(27)	120.1
C(26)-C(27)-H(27)	120.1
C(27)-C(28)-C(29)	121.4(3)
C(27)-C(28)-H(28)	119.3
C(29)-C(28)-H(28)	119.3
C(210)-C(29)-C(28)	118.0(3)
C(210)-C(29)-C(21)	119.8(3)
C(28)-C(29)-C(21)	122.2(3)
C(29)-C(210)-C(24)	118.6(3)
C(29)-C(210)-C(25)	119.3(3)
C(24)-C(210)-C(25)	122.1(3)
C(22')-C(21')-C(29')	119.1(3)
C(22')-C(21')-C(21)	115.2(2)
C(29')-C(21')-C(21)	125.6(2)
C(21')-C(22')-C(23')	123.0(3)
C(21')-C(22')-H(22')	118.5
C(23')-C(22')-H(22')	118.5
C(24')-C(23')-C(22')	119.3(3)
C(24')-C(23')-H(23')	120.4
C(22')-C(23')-H(23')	120.4
C(23')-C(24')-C(30')	120.7(3)
C(23')-C(24')-H(24')	119.6
C(30')-C(24')-H(24')	119.6
C(26')-C(25')-C(30')	121.4(3)
C(26')-C(25')-H(25')	119.3
C(30')-C(25')-H(25')	119.3
C(25')-C(26')-C(27')	119.4(3)
C(25')-C(26')-H(26')	120.3
C(27')-C(26')-H(26')	120.3
C(28')-C(27')-C(26')	121.4(3)
C(28')-C(27')-H(27')	119.3
C(26')-C(27')-H(27')	119.3
C(27')-C(28')-C(29')	122.0(3)
C(27')-C(28')-Br(2)	114.6(2)
C(29')-C(28')-Br(2)	123.4(2)
C(28')-C(29')-C(30')	115.4(2)
C(28')-C(29')-C(21')	127.2(3)
C(30')-C(29')-C(21')	117.4(2)
C(25')-C(30')-C(24')	119.3(3)
C(25')-C(30')-C(29')	120.3(3)
C(24')-C(30')-C(29')	120.4(3)

Table 22. Anisotropic displacement parameters (A^2 x 10^3) for (*S*)-**22**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Br(1)	35(1)	52(1)	51(1)	-11(1)	-5(1)	15(1)
O(1)	51(1)	37(1)	29(1)	4(1)	-6(1)	-5(1)
C(11)	36(2)	30(1)	25(2)	-5(1)	-3(1)	6(1)
C(12)	40(2)	30(1)	25(2)	-4(1)	-3(1)	4(1)
C(13)	54(2)	38(2)	24(2)	-3(1)	-10(1)	3(1)
C(14)	50(2)	41(2)	33(2)	-12(1)	-10(1)	-2(1)
C(15)	52(2)	35(2)	61(2)	-9(2)	1(2)	-4(1)
C(16)	63(2)	34(2)	70(3)	0(2)	17(2)	-7(2)
C(17)	78(3)	44(2)	43(2)	10(2)	9(2)	-2(2)
C(18)	57(2)	38(2)	37(2)	0(1)	-2(2)	0(1)
C(19)	46(2)	26(1)	29(2)	-6(1)	0(1)	5(1)
C(110)	44(2)	26(1)	41(2)	-5(1)	2(1)	3(1)
C(11')	35(2)	31(1)	24(1)	1(1)	-4(1)	7(1)
C(12')	50(2)	70(2)	38(2)	-8(2)	-3(2)	28(2)
C(13')	40(2)	94(3)	71(3)	-1(2)	-4(2)	32(2)
C(14')	29(2)	84(3)	50(2)	17(2)	-14(2)	6(2)
C(15')	58(2)	64(2)	32(2)	1(2)	-18(2)	-17(2)
C(16')	82(3)	69(2)	33(2)	-22(2)	-8(2)	-13(2)
C(17')	54(2)	50(2)	39(2)	-16(2)	7(2)	-1(2)
C(18')	34(2)	35(2)	30(2)	1(1)	1(1)	-3(1)
C(19')	25(1)	32(1)	25(1)	5(1)	-2(1)	-1(1)
C(20')	42(2)	45(2)	27(2)	8(1)	-8(1)	-10(1)
Br(2)	38(1)	59(1)	38(1)	21(1)	-5(1)	-10(1)
O(2)	32(1)	41(1)	51(1)	-11(1)	-9(1)	3(1)
C(21)	28(1)	31(1)	32(2)	7(1)	-2(1)	-8(1)
C(22)	31(1)	34(2)	38(2)	2(1)	-2(1)	-6(1)
C(23)	41(2)	44(2)	45(2)	-9(2)	-2(2)	-8(1)
C(24)	42(2)	57(2)	32(2)	-6(2)	-7(1)	-20(2)
C(25)	33(2)	76(2)	43(2)	18(2)	-11(2)	-13(2)
C(26)	26(2)	86(3)	59(2)	32(2)	-11(2)	-1(2)
C(27)	38(2)	62(2)	54(2)	26(2)	6(2)	7(2)
C(28)	30(2)	46(2)	41(2)	14(1)	3(1)	-2(1)
C(29)	27(1)	38(2)	34(2)	11(1)	2(1)	-6(1)
C(210)	30(1)	54(2)	37(2)	11(2)	-6(1)	-15(1)
C(21')	22(1)	28(1)	33(2)	2(1)	-2(1)	0(1)
C(22')	44(2)	32(2)	36(2)	10(1)	2(1)	-4(1)
C(23')	56(2)	48(2)	30(2)	7(1)	-3(2)	5(2)
C(24')	42(2)	50(2)	31(2)	-5(1)	-7(1)	12(1)
C(25')	50(2)	49(2)	57(2)	-23(2)	-2(2)	-8(2)
C(26')	70(3)	37(2)	83(3)	-13(2)	14(2)	-23(2)
C(27')	57(2)	36(2)	59(2)	9(2)	11(2)	-10(2)
C(28')	28(1)	34(2)	42(2)	7(1)	2(1)	0(1)
C(29')	23(1)	27(1)	33(2)	2(1)	0(1)	2(1)
C(30')	30(1)	38(2)	42(2)	-6(1)	2(1)	3(1)

Table 23. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for (*S*)-**22**.

	x	y	z	U(eq)
H(13)	1093	6478	-433	47
H(14)	-602	4623	-294	50
H(15)	-1659	2774	130	59
H(16)	-1612	1782	656	67
H(17)	177	2648	1043	66
H(18)	1919	4469	902	53
H(12')	4974	5051	276	63
H(13')	7171	5304	584	82
H(14')	7117	6651	1073	66
H(15')	5826	8278	1464	62
H(16')	3757	9594	1631	74
H(17')	1529	9610	1309	57
H(23)	8781	609	1427	52
H(24)	6430	1275	1227	52
H(25)	4056	2857	1268	61
H(26)	2672	4672	1531	69
H(27)	3677	5956	1998	61
H(28)	6065	5374	2187	46
H(22')	7950	2210	2547	45
H(23')	8760	3019	3067	54
H(24')	9946	5329	3122	49
H(25')	10995	7640	2882	62
H(26')	11370	9248	2443	76
H(27')	10623	8515	1914	61
H(1)	3661	8116	104	85(14)
H(2)	10630	2242	2087	69(12)

Table 24. Torsion angles [deg] for (*S*)-**22**.

C(19)-C(11)-C(12)-O(1)	176.6(3)
C(11')-C(11)-C(12)-O(1)	-10.8(4)
C(19)-C(11)-C(12)-C(13)	-2.9(4)
C(11')-C(11)-C(12)-C(13)	169.6(3)
O(1)-C(12)-C(13)-C(14)	-177.6(3)
C(11)-C(12)-C(13)-C(14)	2.0(4)
C(12)-C(13)-C(14)-C(110)	0.2(5)
C(110)-C(15)-C(16)-C(17)	-0.8(5)
C(15)-C(16)-C(17)-C(18)	-0.5(6)
C(16)-C(17)-C(18)-C(19)	0.9(5)
C(12)-C(11)-C(19)-C(110)	1.8(4)
C(11')-C(11)-C(19)-C(110)	-170.7(2)
C(12)-C(11)-C(19)-C(18)	-178.2(3)
C(11')-C(11)-C(19)-C(18)	9.3(4)
C(17)-C(18)-C(19)-C(110)	-0.1(4)
C(17)-C(18)-C(19)-C(11)	179.9(3)
C(13)-C(14)-C(110)-C(19)	-1.2(4)
C(13)-C(14)-C(110)-C(15)	-179.8(3)
C(11)-C(19)-C(110)-C(14)	0.2(4)
C(18)-C(19)-C(110)-C(14)	-179.8(3)
C(11)-C(19)-C(110)-C(15)	178.9(3)
C(18)-C(19)-C(110)-C(15)	-1.1(4)
C(16)-C(15)-C(110)-C(14)	-179.9(3)
C(16)-C(15)-C(110)-C(19)	1.6(5)
C(12)-C(11)-C(11')-C(12')	-75.0(4)
C(19)-C(11)-C(11')-C(12')	97.3(3)
C(12)-C(11)-C(11')-C(19')	109.0(3)
C(19)-C(11)-C(11')-C(19')	-78.7(4)
C(19')-C(11')-C(12')-C(13')	0.9(6)
C(11)-C(11')-C(12')-C(13')	-175.5(4)
C(11')-C(12')-C(13')-C(14')	2.2(7)
C(12')-C(13')-C(14')-C(20')	-2.8(6)
C(20')-C(15')-C(16')-C(17')	-1.2(6)
C(15')-C(16')-C(17')-C(18')	1.9(6)
C(16')-C(17')-C(18')-C(19')	-0.5(5)
C(16')-C(17')-C(18')-Br(1)	-178.1(3)
C(17')-C(18')-C(19')-C(11')	180.0(3)
Br(1)-C(18')-C(19')-C(11')	-2.6(4)
C(17')-C(18')-C(19')-C(20')	-1.4(4)
Br(1)-C(18')-C(19')-C(20')	176.0(2)
C(12')-C(11')-C(19')-C(18')	175.5(3)
C(11)-C(11')-C(19')-C(18')	-8.6(4)
C(12')-C(11')-C(19')-C(20')	-3.0(4)
C(11)-C(11')-C(19')-C(20')	172.8(3)
C(16')-C(15')-C(20')-C(14')	177.6(4)
C(16')-C(15')-C(20')-C(19')	-0.9(5)
C(13')-C(14')-C(20')-C(15')	-178.0(4)
C(13')-C(14')-C(20')-C(19')	0.6(5)
C(18')-C(19')-C(20')-C(15')	2.2(4)
C(11')-C(19')-C(20')-C(15')	-179.1(3)
C(18')-C(19')-C(20')-C(14')	-176.4(3)
C(11')-C(19')-C(20')-C(14')	2.4(4)
C(29)-C(21)-C(22)-O(2)	179.0(3)
C(21')-C(21)-C(22)-O(2)	-7.3(4)
C(29)-C(21)-C(22)-C(23)	0.4(4)
C(21')-C(21)-C(22)-C(23)	174.0(3)
C(21)-C(22)-C(23)-C(24)	0.9(5)
O(2)-C(22)-C(23)-C(24)	-177.9(3)
C(22)-C(23)-C(24)-C(210)	-1.1(5)
C(210)-C(25)-C(26)-C(27)	0.6(5)
C(25)-C(26)-C(27)-C(28)	-0.1(5)
C(26)-C(27)-C(28)-C(29)	-0.8(5)
C(27)-C(28)-C(29)-C(210)	1.1(4)
C(27)-C(28)-C(29)-C(21)	-179.4(3)

C(22)-C(21)-C(29)-C(210)	-1.3(4)
C(21')-C(21)-C(29)-C(210)	-174.9(2)
C(22)-C(21)-C(29)-C(28)	179.2(3)
C(21')-C(21)-C(29)-C(28)	5.6(4)
C(28)-C(29)-C(210)-C(24)	-179.5(3)
C(21)-C(29)-C(210)-C(24)	1.1(4)
C(28)-C(29)-C(210)-C(25)	-0.5(4)
C(21)-C(29)-C(210)-C(25)	180.0(3)
C(23)-C(24)-C(210)-C(29)	0.2(5)
C(23)-C(24)-C(210)-C(25)	-178.8(3)
C(26)-C(25)-C(210)-C(29)	-0.3(5)
C(26)-C(25)-C(210)-C(24)	178.6(3)
C(22)-C(21)-C(21')-C(22')	-79.4(3)
C(29)-C(21)-C(21')-C(22')	94.2(3)
C(22)-C(21)-C(21')-C(29')	102.1(3)
C(29)-C(21)-C(21')-C(29')	-84.3(3)
C(29')-C(21')-C(22')-C(23')	-0.3(4)
C(21)-C(21')-C(22')-C(23')	-178.9(3)
C(21')-C(22')-C(23')-C(24')	0.7(5)
C(22')-C(23')-C(24')-C(30')	-0.7(5)
C(30')-C(25')-C(26')-C(27')	-2.2(6)
C(25')-C(26')-C(27')-C(28')	-0.3(6)
C(26')-C(27')-C(28')-C(29')	3.0(5)
C(26')-C(27')-C(28')-Br(2)	-175.1(3)
C(27')-C(28')-C(29')-C(30')	-3.0(4)
Br(2)-C(28')-C(29')-C(30')	175.0(2)
C(27')-C(28')-C(29')-C(21')	177.5(3)
Br(2)-C(28')-C(29')-C(21')	-4.5(4)
C(22')-C(21')-C(29')-C(28')	179.4(3)
C(21)-C(21')-C(29')-C(28')	-2.1(4)
C(22')-C(21')-C(29')-C(30')	-0.1(4)
C(21)-C(21')-C(29')-C(30')	178.4(2)
C(26')-C(25')-C(30')-C(24')	-178.0(3)
C(26')-C(25')-C(30')-C(29')	2.1(5)
C(23')-C(24')-C(30')-C(25')	-179.7(3)
C(23')-C(24')-C(30')-C(29')	0.3(4)
C(28')-C(29')-C(30')-C(25')	0.5(4)
C(21')-C(29')-C(30')-C(25')	-180.0(3)
C(28')-C(29')-C(30')-C(24')	-179.5(3)
C(21')-C(29')-C(30')-C(24')	0.1(4)

Table 25. Hydrogen bonds for (*S*)-**22** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2)...O(1)#1	0.93	2.07	2.936(3)	154.6

Symmetry transformations used to generate equivalent atoms:
#1 -y+2,x,z+1/4

Table 26. Crystal data and structure refinement for (±)-**24**.

Identification code	(±)-**24**
Empirical formula	C33 H23 N O
Formula weight	449.52
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 11.1055(1) A alpha = 90 deg. b = 11.6712(1) A beta = 102.6753(3) deg. c = 18.0627(1) A gamma = 90 deg.
Volume	2284.13(3) A^3
Z, Calculated density	4, 1.307 Mg/m^3
Absorption coefficient	0.078 mm^-1
F(000)	944
Crystal size	0.53 x 0.5 x 0.37 mm
Theta range for data collection	2.09 to 50 deg.
Limiting indices	-16<=h<=23, -26<=k<=26, -41<=l<=38
Reflections collected / unique	358895 / 23242 [R(int) = 0.0355]
Completeness to theta = 44	100 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.01 and 0.954
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	23242 / 0 / 408
Goodness-of-fit on F^2	1.043
Final R indices [I>2sigma(I)]	R1 = 0.0421, wR2 = 0.1247
R indices (all data)	R1 = 0.0547, wR2 = 0.1317
Largest diff. peak and hole	0.686 and -0.236 e.A^-3

Table 27. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for (±)-**24**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	3365(1)	1312(1)	571(1)	13(1)
C(2)	3654(1)	1389(1)	-136(1)	15(1)
C(3)	3250(1)	2314(1)	-632(1)	16(1)
C(4)	2535(1)	3155(1)	-417(1)	16(1)
C(5)	1515(1)	4033(1)	513(1)	18(1)
C(6)	1257(1)	4056(1)	1222(1)	20(1)
C(7)	1692(1)	3171(1)	1744(1)	17(1)
C(8)	2363(1)	2254(1)	1560(1)	13(1)
C(9)	2659(1)	2206(1)	822(1)	12(1)
C(10)	2227(1)	3126(1)	305(1)	14(1)
C(11)	3768(1)	255(1)	1023(1)	14(1)
C(12)	4851(1)	240(1)	1573(1)	16(1)
C(13)	5240(1)	-756(1)	2008(1)	21(1)
C(14)	4531(1)	-1728(1)	1892(1)	22(1)
C(15)	2656(1)	-2755(1)	1203(1)	26(1)
C(16)	1577(1)	-2764(1)	656(1)	28(1)
C(17)	1217(1)	-1786(1)	199(1)	24(1)
C(18)	1930(1)	-809(1)	309(1)	18(1)
C(19)	3041(1)	-764(1)	878(1)	15(1)
C(20)	3417(1)	-1762(1)	1327(1)	19(1)
C(21)	2267(1)	788(1)	2457(1)	12(1)
C(22)	2939(1)	59(1)	3091(1)	13(1)
C(23)	4193(1)	263(1)	3405(1)	17(1)
C(24)	4825(1)	-395(1)	4007(1)	22(1)
C(25)	4221(1)	-1274(1)	4302(1)	24(1)
C(26)	2982(1)	-1495(1)	3990(1)	23(1)
C(27)	2340(1)	-828(1)	3390(1)	17(1)
C(28)	902(1)	614(1)	2208(1)	13(1)
C(29)	484(1)	-325(1)	1742(1)	16(1)
C(30)	-776(1)	-522(1)	1486(1)	19(1)
C(31)	-1628(1)	211(1)	1699(1)	21(1)
C(32)	-1219(1)	1132(1)	2181(1)	21(1)
C(33)	45(1)	1331(1)	2440(1)	18(1)
N(1)	2902(1)	1476(1)	2136(1)	13(1)
O(1)	5600(1)	1179(1)	1745(1)	20(1)

Table 28. Bond lengths [A] and angles [deg] for (±)-**24**.

C(1)-C(2)	1.3866(5)
C(1)-C(9)	1.4375(4)
C(1)-C(11)	1.4926(4)
C(2)-C(3)	1.4116(5)
C(2)-H(2)	1.000(10)
C(3)-C(4)	1.3711(5)
C(3)-H(3)	0.981(9)
C(4)-C(10)	1.4197(5)
C(4)-H(4)	1.000(9)
C(5)-C(6)	1.3720(6)
C(5)-C(10)	1.4204(5)
C(5)-H(5)	1.006(9)
C(6)-C(7)	1.4106(5)
C(6)-H(6)	0.987(10)
C(7)-C(8)	1.3860(5)
C(7)-H(7)	1.011(10)
C(8)-N(1)	1.4104(4)
C(8)-C(9)	1.4432(4)
C(9)-C(10)	1.4337(4)
C(11)-C(12)	1.3813(5)
C(11)-C(19)	1.4294(5)
C(12)-O(1)	1.3692(5)
C(12)-C(13)	1.4171(5)
C(13)-C(14)	1.3699(7)
C(13)-H(13)	1.002(10)
C(14)-C(20)	1.4215(7)
C(14)-H(14)	0.983(10)
C(15)-C(16)	1.3751(9)
C(15)-C(20)	1.4227(7)
C(15)-H(15)	1.021(11)
C(16)-C(17)	1.4148(7)
C(16)-H(16)	1.004(11)
C(17)-C(18)	1.3777(6)
C(17)-H(17)	1.032(11)
C(18)-C(19)	1.4225(6)
C(18)-H(18)	0.996(10)
C(19)-C(20)	1.4285(5)
C(21)-N(1)	1.2883(4)
C(21)-C(22)	1.4887(4)
C(21)-C(28)	1.4969(5)
C(22)-C(27)	1.4007(5)
C(22)-C(23)	1.4039(5)
C(23)-C(24)	1.3885(5)
C(23)-H(23)	0.949(10)
C(24)-C(25)	1.3942(7)
C(24)-H(24)	1.020(11)
C(25)-C(26)	1.3919(7)
C(25)-H(25)	0.978(11)
C(26)-C(27)	1.3971(5)
C(26)-H(26)	0.959(11)
C(27)-H(27)	0.969(9)
C(28)-C(29)	1.3982(5)
C(28)-C(33)	1.3987(5)
C(29)-C(30)	1.3927(5)
C(29)-H(29)	0.983(10)
C(30)-C(31)	1.3916(6)
C(30)-H(30)	0.983(9)
C(31)-C(32)	1.3944(7)
C(31)-H(31)	0.981(10)
C(32)-C(33)	1.3980(6)
C(32)-H(32)	0.971(10)
C(33)-H(33)	0.976(9)
O(1)-H(1)	0.936(13)

C(2)-C(1)-C(9)	119.71(3)
C(2)-C(1)-C(11)	117.09(3)
C(9)-C(1)-C(11)	123.15(3)
C(1)-C(2)-C(3)	121.94(3)
C(1)-C(2)-H(2)	118.2(6)
C(3)-C(2)-H(2)	119.7(6)
C(4)-C(3)-C(2)	119.36(3)
C(4)-C(3)-H(3)	120.7(6)
C(2)-C(3)-H(3)	119.9(6)
C(3)-C(4)-C(10)	120.99(3)
C(3)-C(4)-H(4)	120.3(5)
C(10)-C(4)-H(4)	118.7(5)
C(6)-C(5)-C(10)	120.25(3)
C(6)-C(5)-H(5)	120.3(5)
C(10)-C(5)-H(5)	119.4(5)
C(5)-C(6)-C(7)	119.89(3)
C(5)-C(6)-H(6)	122.2(6)
C(7)-C(6)-H(6)	117.9(6)
C(8)-C(7)-C(6)	121.95(3)
C(8)-C(7)-H(7)	117.8(6)
C(6)-C(7)-H(7)	120.1(6)
C(7)-C(8)-N(1)	118.98(3)
C(7)-C(8)-C(9)	119.60(3)
N(1)-C(8)-C(9)	120.73(3)
C(10)-C(9)-C(1)	117.78(3)
C(10)-C(9)-C(8)	117.50(3)
C(1)-C(9)-C(8)	124.72(3)
C(4)-C(10)-C(5)	119.04(3)
C(4)-C(10)-C(9)	120.15(3)
C(5)-C(10)-C(9)	120.79(3)
C(12)-C(11)-C(19)	119.30(3)
C(12)-C(11)-C(1)	120.85(3)
C(19)-C(11)-C(1)	119.84(3)
O(1)-C(12)-C(11)	122.89(3)
O(1)-C(12)-C(13)	115.79(4)
C(11)-C(12)-C(13)	121.30(4)
C(14)-C(13)-C(12)	120.03(4)
C(14)-C(13)-H(13)	121.6(6)
C(12)-C(13)-H(13)	118.3(6)
C(13)-C(14)-C(20)	120.87(3)
C(13)-C(14)-H(14)	119.8(6)
C(20)-C(14)-H(14)	119.3(6)
C(16)-C(15)-C(20)	120.89(4)
C(16)-C(15)-H(15)	119.3(6)
C(20)-C(15)-H(15)	119.9(6)
C(15)-C(16)-C(17)	120.19(4)
C(15)-C(16)-H(16)	117.5(6)
C(17)-C(16)-H(16)	122.3(6)
C(18)-C(17)-C(16)	120.24(5)
C(18)-C(17)-H(17)	119.2(6)
C(16)-C(17)-H(17)	120.6(6)
C(17)-C(18)-C(19)	121.01(4)
C(17)-C(18)-H(18)	121.0(6)
C(19)-C(18)-H(18)	118.0(6)
C(18)-C(19)-C(20)	118.60(4)
C(18)-C(19)-C(11)	121.93(3)
C(20)-C(19)-C(11)	119.45(4)
C(14)-C(20)-C(15)	121.96(4)
C(14)-C(20)-C(19)	118.99(4)
C(15)-C(20)-C(19)	119.04(4)
N(1)-C(21)-C(22)	118.10(3)
N(1)-C(21)-C(28)	124.60(3)
C(22)-C(21)-C(28)	117.20(3)
C(27)-C(22)-C(23)	118.85(3)
C(27)-C(22)-C(21)	121.18(3)
C(23)-C(22)-C(21)	119.96(3)
C(24)-C(23)-C(22)	120.58(4)
C(24)-C(23)-H(23)	120.3(6)

C(22)-C(23)-H(23)	119.0(6)
C(23)-C(24)-C(25)	120.21(4)
C(23)-C(24)-H(24)	118.5(6)
C(25)-C(24)-H(24)	121.2(6)
C(26)-C(25)-C(24)	119.84(4)
C(26)-C(25)-H(25)	120.2(6)
C(24)-C(25)-H(25)	120.0(6)
C(25)-C(26)-C(27)	120.11(4)
C(25)-C(26)-H(26)	120.4(7)
C(27)-C(26)-H(26)	119.5(7)
C(26)-C(27)-C(22)	120.40(4)
C(26)-C(27)-H(27)	117.8(5)
C(22)-C(27)-H(27)	121.8(5)
C(29)-C(28)-C(33)	119.39(3)
C(29)-C(28)-C(21)	117.89(3)
C(33)-C(28)-C(21)	122.69(3)
C(30)-C(29)-C(28)	120.43(3)
C(30)-C(29)-H(29)	121.2(6)
C(28)-C(29)-H(29)	118.3(6)
C(31)-C(30)-C(29)	120.07(4)
C(31)-C(30)-H(30)	121.2(6)
C(29)-C(30)-H(30)	118.7(6)
C(30)-C(31)-C(32)	119.88(4)
C(30)-C(31)-H(31)	120.5(6)
C(32)-C(31)-H(31)	119.6(6)
C(31)-C(32)-C(33)	120.17(4)
C(31)-C(32)-H(32)	120.6(6)
C(33)-C(32)-H(32)	119.2(6)
C(32)-C(33)-C(28)	119.99(4)
C(32)-C(33)-H(33)	120.1(6)
C(28)-C(33)-H(33)	119.9(6)
C(21)-N(1)-C(8)	123.20(3)
C(12)-O(1)-H(1)	109.2(8)

Table 29. Anisotropic displacement parameters (A^2 x 10^3) for (±)-**24**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	14(1)	11(1)	13(1)	1(1)	3(1)	1(1)
C(2)	17(1)	15(1)	14(1)	0(1)	5(1)	1(1)
C(3)	20(1)	17(1)	13(1)	2(1)	5(1)	0(1)
C(4)	20(1)	14(1)	14(1)	3(1)	4(1)	0(1)
C(5)	22(1)	12(1)	20(1)	3(1)	6(1)	4(1)
C(6)	25(1)	14(1)	23(1)	1(1)	9(1)	6(1)
C(7)	22(1)	14(1)	18(1)	0(1)	8(1)	3(1)
C(8)	15(1)	11(1)	13(1)	1(1)	4(1)	1(1)
C(9)	13(1)	10(1)	13(1)	1(1)	3(1)	0(1)
C(10)	16(1)	11(1)	15(1)	2(1)	3(1)	1(1)
C(11)	16(1)	12(1)	14(1)	1(1)	4(1)	3(1)
C(12)	15(1)	18(1)	16(1)	1(1)	4(1)	5(1)
C(13)	22(1)	23(1)	18(1)	4(1)	6(1)	11(1)
C(14)	30(1)	18(1)	20(1)	6(1)	11(1)	12(1)
C(15)	41(1)	12(1)	29(1)	2(1)	17(1)	2(1)
C(16)	42(1)	14(1)	31(1)	-4(1)	16(1)	-7(1)
C(17)	33(1)	18(1)	22(1)	-5(1)	9(1)	-8(1)
C(18)	25(1)	15(1)	16(1)	-1(1)	5(1)	-3(1)
C(19)	21(1)	11(1)	15(1)	0(1)	7(1)	2(1)
C(20)	29(1)	12(1)	20(1)	3(1)	12(1)	5(1)
C(21)	13(1)	12(1)	11(1)	0(1)	3(1)	1(1)
C(22)	15(1)	13(1)	11(1)	0(1)	3(1)	1(1)
C(23)	15(1)	18(1)	16(1)	0(1)	1(1)	2(1)
C(24)	20(1)	23(1)	19(1)	0(1)	-3(1)	5(1)
C(25)	32(1)	21(1)	17(1)	4(1)	-2(1)	6(1)
C(26)	31(1)	18(1)	17(1)	5(1)	3(1)	1(1)
C(27)	21(1)	16(1)	15(1)	3(1)	3(1)	-1(1)
C(28)	12(1)	14(1)	13(1)	1(1)	3(1)	1(1)
C(29)	14(1)	18(1)	16(1)	-2(1)	3(1)	-1(1)
C(30)	15(1)	23(1)	18(1)	0(1)	2(1)	-3(1)
C(31)	13(1)	28(1)	21(1)	4(1)	3(1)	0(1)
C(32)	15(1)	24(1)	25(1)	3(1)	8(1)	4(1)
C(33)	16(1)	18(1)	21(1)	0(1)	7(1)	2(1)
N(1)	14(1)	13(1)	12(1)	1(1)	3(1)	0(1)
O(1)	15(1)	23(1)	22(1)	0(1)	1(1)	2(1)

Table 30. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for (±)-**24**.

	x	y	z	U(eq)
H(2)	4121(9)	744(8)	-305(6)	29(2)
H(3)	3473(9)	2345(8)	-1128(5)	26(2)
H(4)	2235(8)	3811(7)	-765(5)	22(2)
H(5)	1236(8)	4677(8)	145(5)	26(2)
H(6)	771(9)	4678(9)	1385(6)	31(2)
H(7)	1564(9)	3218(8)	2280(6)	29(2)
H(13)	6020(10)	-718(8)	2409(6)	31(2)
H(14)	4782(10)	-2405(9)	2212(6)	37(3)
H(15)	2911(10)	-3473(9)	1522(6)	36(3)
H(16)	1066(10)	-3482(10)	602(6)	37(3)
H(17)	422(10)	-1796(9)	-223(6)	37(3)
H(18)	1690(10)	-117(9)	-12(6)	35(2)
H(23)	4587(9)	893(8)	3226(6)	28(2)
H(24)	5724(10)	-199(9)	4238(6)	38(3)
H(25)	4663(10)	-1721(9)	4735(6)	36(3)
H(26)	2556(11)	-2091(10)	4194(6)	38(3)
H(27)	1478(9)	-1005(8)	3188(5)	25(2)
H(29)	1099(9)	-850(8)	1614(6)	30(2)
H(30)	-1045(9)	-1198(8)	1168(5)	25(2)
H(31)	-2516(9)	71(9)	1527(6)	33(2)
H(32)	-1805(10)	1639(9)	2343(6)	34(2)
H(33)	331(9)	1967(8)	2785(5)	28(2)
H(1)	5305(13)	1767(11)	1400(8)	55(3)