

Table 2. Molecular non-hydrogen geometries (4). Paired values in each entry, correspond to molecules 1,2.

Atoms	Parameter	Atoms	Parameter
Distances (Å)			
O-C(1)	1.399(3), 1.402(3)	O-C(1')	1.379(3), 1.366(3)
C(1)-C(2)	1.390(3), 1.385(3)	C(1')-C(2')	1.416(4), 1.416(4)
C(2)-C(3)	1.403(4), 1.398(4)	C(2')-C(3')	1.418(4), 1.406(3)
C(3)-C(4)	1.376(5), 1.384(4)	C(3')-C(4')	1.381(4), 1.409(5)
C(4)-C(5)	1.393(3), 1.395(4)	C(4')-C(5')	1.385(4), 1.380(5)
C(5)-C(6)	1.387(4), 1.380(4)	C(5')-C(6')	1.391(3), 1.395(3)
C(1)-C(6)	1.397(4), 1.401(4)	C(1')-C(6')	1.379(4), 1.392(4)
C(2)-C(21)	1.490(4), 1.494(4)	C(2')-C(21')	1.474(4), 1.477(4)
C(21)-O(21)	1.200(4), 1.210(3)	C(21')-O(21')	1.226(3), 1.219(4)
C(21)-O(22)	1.330(3), 1.328(3)	C(21')-O(22')	1.328(3), 1.304(3)
O(22)-C(22)	1.452(5), 1.447(4)	O(22')-C(22')	1.453(4), 1.449(5)
C(4)-O(4)	1.368(4), 1.381(4)	C(3')-O(3')	1.357(4), 1.342(4)
C(6)-O(6)	1.365(3), 1.361(3)	C(5')-C(51')	1.504(4), 1.519(5)
O(6)-C(61)	1.425(4), 1.430(4)		
O...O(21)	2.758(3), 2.848(3)	O...O(22')	2.567(2), 2.521(3)
Angles (degrees)			
C(1)-O-C(1')	118.1(2), 118.2(2)	O-C(1')-C(2')	116.8(2), 117.5(2)
O-C(1)-C(2)	121.7(3), 120.4(2)	O-C(1')-C(6')	121.3(2), 121.7(2)
O-C(1)-C(6)	117.7(2), 118.8(2)	C(2')-C(1')-C(6')	121.9(2), 120.8(2)
C(2)-C(1)-C(6)	120.3(2), 120.3(2)	C(1')-C(2')-C(3')	116.0(2), 117.8(3)
C(1)-C(2)-C(3)	119.4(3), 119.4(2)	C(1')-C(2')-C(21')	125.7(2), 124.4(2)
C(1)-C(2)-C(21)	121.0(2), 120.5(2)	C(32')-C(2')-C(21')	118.3(2), 117.8(3)
C(3)-C(2)-C(21)	119.6(2), 119.9(2)	C(2')-C(21')-O(21')	122.7(3), 122.1(2)
C(2)-C(21)-O(21)	125.9(2), 125.9(2)	C(2')-C(21')-O(22')	115.7(2), 116.1(3)
C(2)-C(21)-O(22)	111.7(2), 110.5(2)	O(21')-C(21')-O(22')	121.6(2), 121.7(3)
O(21)-C(21)-O(22)	122.4(3), 123.5(3)	C(21')-O(22')-C(22')	115.9(2), 115.5(3)
C(21)-O(22)-C(22)	115.2(3), 116.5(2)	C(2')-C(3')-C(4')	121.6(3), 120.9(3)
C(2)-C(3)-C(4)	119.7(2), 119.7(2)	C(3')-C(4')-C(5')	120.8(3), 120.0(2)
C(3)-C(4)-C(5)	121.3(2), 119.2(3)	C(4')-C(5')-C(6')	119.2(2), 120.2(3)
C(4)-C(5)-C(6)	119.1(3), 119.2(3)	C(1')-C(6')-C(5')	120.5(2), 120.2(3)
C(1)-C(6)-C(5)	120.2(2), 120.1(2)	C(2')-C(3')-O(3')	121.6(2), 123.4(5)
C(3)-C(4)-O(4)	122.5(2), 117.7(2)	C(4')-C(3')-O(3')	116.8(3), 115.7(2)
C(5)-C(4)-O(4)	116.1(3), 121.3(3)	C(4')-C(5')-C(51')	120.7(2), 120.9(3)
C(5)-C(6)-O(6)	124.5(3), 123.9(2)		

C(1)-C(6)-O(6)	115.3(2), 116.0(2)	C(6')-C(5')-C(51')	120.1(3), 118.9(3)
C(6)-O(6)-C(61)	117.7(2), 117.7(4)		

Interplanar dihedral angles (degrees)

C ₆ /C ₂ O ₂	15.0(1), 36.5(1)	C ₆ '/C ₂ 'O ₂ '	10.6(1), 3.5(1)
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O, H(3')...O(21') (intramolecular) are 2.553(3), 1.73(3); 2.546(6), 1.74(5) Å.

Also: O,H(14)...O(221) (1-x, \bar{y} , 1-z) 2.807(3), 2.03(3); O,H(24)...H(121) (1-x, 1-y, 1-z) 2.960(3), 1.89(5) Å

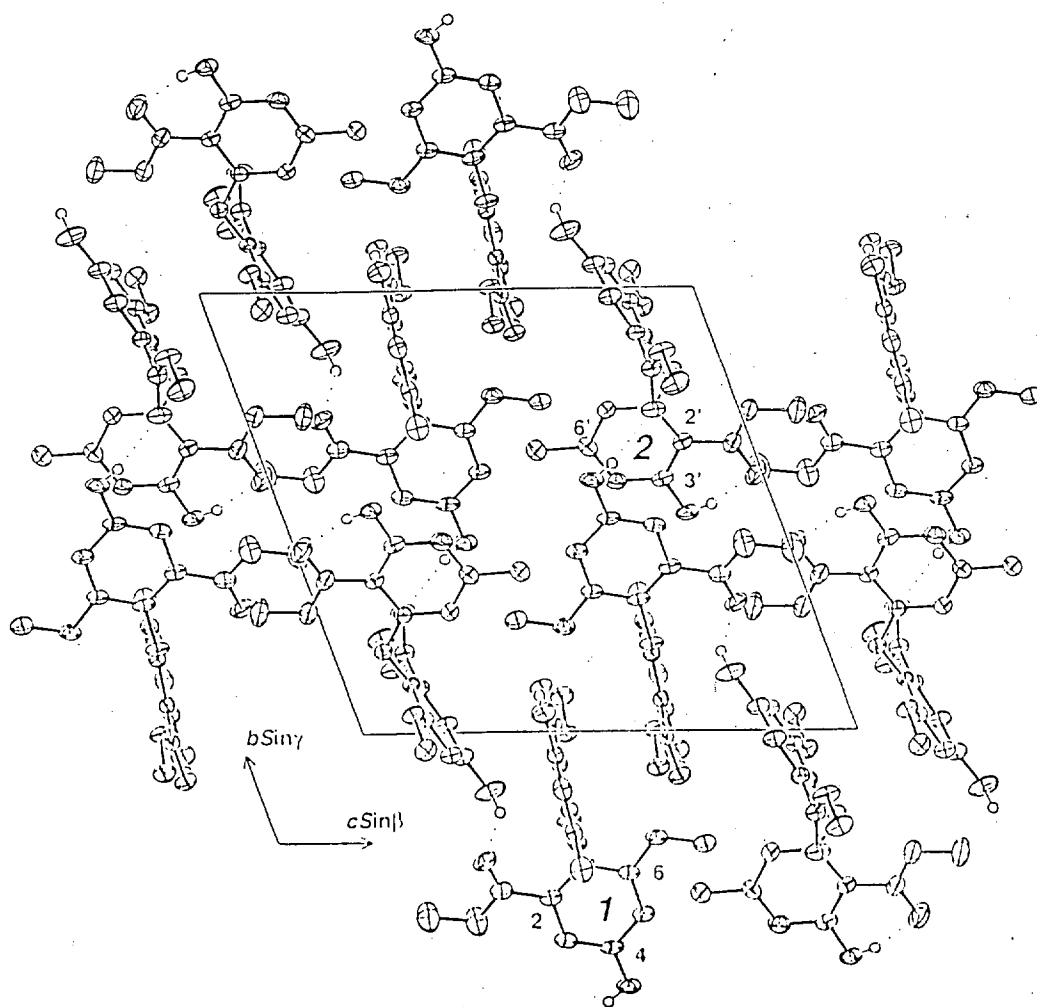


Figure 3. Unit cells contents of 4, projected down *a*.