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Bond angles involving hydrogen atoms (deg) with estimated standard deviations in parentheses for **1g**.

Bonds	Angle(deg)	Bonds	Angle(deg)
C(1)-C(2)-H(1)	105(2)	C(12)-C(13)-H(21)	108(1)
C(1)-C(2)-H(2)	108(1)	C(12)-C(13)-H(22)	108(2)
C(3)-C(2)-H(1)	109(2)	C(14)-C(13)-H(21)	107(2)
C(3)-C(2)-H(2)	107(1)	C(14)-C(13)-H(22)	108(2)
H(1)-C(2)-H(2)	109(2)	H(21)-C(13)-H(22)	111(2)
C(2)-C(3)-H(3)	109(1)	C(13)-C(14)-H(23)	109(1)
C(2)-C(3)-H(4)	107(1)	C(13)-C(14)-H(24)	110(1)
C(4)-C(3)-H(3)	110(1)	C(15)-C(14)-H(23)	108(1)
C(4)-C(3)-H(4)	105(1)	C(15)-C(14)-H(24)	108(1)
H(3)-C(3)-H(4)	111(2)	H(23)-C(14)-H(24)	109(2)
C(3)-C(4)-H(5)	112(2)	C(14)-C(15)-H(25)	108(1)
C(3)-C(4)-H(6)	108(1)	C(14)-C(15)-H(26)	109(1)
C(5)-C(4)-H(5)	104(2)	C(16)-C(15)-H(25)	111(1)
C(5)-C(4)-H(6)	108(1)	C(16)-C(15)-H(26)	108(1)
H(5)-C(4)-H(6)	110(2)	H(25)-C(15)-H(26)	108(2)
C(4)-C(5)-H(7)	108(1)	C(15)-C(16)-H(27)	110(2)
C(4)-C(5)-H(8)	108(1)	C(15)-C(16)-H(28)	107(2)
C(6)-C(5)-H(7)	110(1)	C(17)-C(16)-H(27)	108(2)
C(6)-C(5)-H(8)	110(1)	C(17)-C(16)-H(28)	111(2)
H(7)-C(5)-H(8)	105(2)	H(27)-C(16)-H(28)	106(2)
C(5)-C(6)-H(9)	109(1)	C(16)-C(17)-H(29)	109(1)
C(5)-C(6)-H(10)	110(1)	C(16)-C(17)-H(30)	108(1)
C(7)-C(6)-H(9)	112(1)	C(18)-C(17)-H(29)	104(1)
C(7)-C(6)-H(10)	108(1)	C(18)-C(17)-H(30)	110(1)

H(9)-C(6)-H(10)	106(2)	H(29)-C(17)-H(30)	110(2)
C(6)-C(7)-H(11)	109(1)	C(17)-C(18)-H(31)	108(1)
C(6)-C(7)-H(12)	108(2)	C(17)-C(18)-H(32)	116(1)
C(8)-C(7)-H(11)	110(1)	C(19)-C(18)-H(31)	110(1)
C(8)-C(7)-H(12)	113(2)	C(19)-C(18)-H(32)	108(1)
H(11)-C(7)-H(12)	101(2)	H(31)-C(18)-H(32)	101(2)
C(7)-C(8)-H(13)	111(1)	C(18)-C(19)-H(33)	110(2)
C(7)-C(8)-H(14)	112(1)	C(18)-C(19)-H(34)	108(1)
C(9)-C(8)-H(13)	108(1)	C(20)-C(19)-H(33)	105(1)
C(9)-C(8)-H(14)	106(1)	C(20)-C(19)-H(34)	110(1)
H(13)-C(8)-H(14)	108(2)	H(33)-C(19)-H(34)	109(2)
C(8)-C(9)-H(15)	107(1)	C(19)-C(20)-H(35)	106(1)
C(8)-C(9)-H(16)	108(2)	C(19)-C(20)-H(36)	109(1)
C(10)-C(9)-H(15)	111(1)	C(21)-C(20)-H(35)	110(1)
C(10)-C(9)-H(16)	113(2)	C(21)-C(20)-H(36)	108(1)
H(15)-C(9)-H(16)	101(2)	H(35)-C(20)-H(36)	109(2)
C(9)-C(10)-H(17)	113(1)	C(20)-C(21)-H(37)	107(2)
C(9)-C(10)-H(18)	111(2)	C(20)-C(21)-H(38)	109(1)
C(11)-C(10)-H(17)	108(1)	C(22)-C(21)-H(37)	109(1)
C(11)-C(10)-H(18)	108(1)	C(22)-C(21)-H(38)	110(1)
H(17)-C(10)-H(18)	103(2)	H(37)-C(21)-H(38)	107(2)
C(10)-C(11)-H(19)	110(1)	C(1)-C(22)-H(39)	104(1)
C(10)-C(11)-H(20)	109(1)	C(1)-C(22)-H(40)	107(1)
C(12)-C(11)-H(19)	107(1)	C(21)-C(22)-H(39)	113(1)
C(12)-C(11)-H(20)	107(1)	C(21)-C(22)-H(40)	112(1)
H(19)-C(11)-H(20)	109(2)	H(39)-C(22)-H(40)	105(2)

Torsion angles (deg) with estimated standard deviations in parentheses for **1g**

Atoms	Value(deg)	Atoms	Value(deg)
O(1)-C(1)-C(22)-H(39)	109(1)	C(3)-C(4)-C(5)-C(6)	174.9(2)
O(1)-C(1)-C(22)-H(40)	-139(1)	C(3)-C(2)-C(1)-C(22)	-52.0(3)
O(1)-C(1)-C(22)-C(21)	-14.1(3)	C(4)-C(5)-C(6)-H(9)	-61(1)
O(1)-C(1)-C(2)-H(1)	-106(2)	C(4)-C(5)-C(6)-H(10)	55(1)
O(1)-C(1)-C(2)-H(2)	10(2)	C(4)-C(5)-C(6)-C(7)	175.3(2)
O(1)-C(1)-C(2)-C(3)	132.6(2)	C(4)-C(3)-C(2)-H(1)	169(2)
O(2)-C(12)-C(13)-H(21)	-2(2)	C(4)-C(3)-C(2)-H(2)	52(2)
O(2)-C(12)-C(13)-H(22)	118(2)	C(5)-C(4)-C(3)-H(3)	-54(1)
O(2)-C(12)-C(13)-C(14)	-121.2(3)	C(5)-C(4)-C(3)-H(4)	-174(1)
O(2)-C(12)-C(11)-H(19)	-99(2)	C(5)-C(6)-C(7)-H(11)	-56(1)
O(2)-C(12)-C(11)-H(20)	144(1)	C(5)-C(6)-C(7)-H(12)	53(2)
O(2)-C(12)-C(11)-C(10)	23.3(3)	C(5)-C(6)-C(7)-C(8)	179.7(5)
C(1)-C(22)-C(21)-H(37)	171(2)	C(6)-C(7)-C(8)-H(13)	-61(2)
C(1)-C(22)-C(21)-H(38)	54(2)	C(6)-C(7)-C(8)-H(14)	60(1)
C(1)-C(22)-C(21)-C(20)	-69.4(3)	C(6)-C(7)-C(8)-C(9)	178.5(2)
C(1)-C(2)-C(3)-H(3)	52(1)	C(6)-C(5)-C(4)-H(5)	53(2)
C(1)-C(2)-C(3)-H(4)	172(1)	C(6)-C(5)-C(4)-H(6)	-64(1)
C(1)-C(2)-C(3)-C(4)	-71.5(3)	C(7)-C(8)-C(9)-H(15)	-59(2)
C(2)-C(1)-C(22)-H(39)	-66(1)	C(7)-C(8)-C(9)-H(16)	49(2)
C(2)-C(1)-C(22)-H(40)	45(1)	C(7)-C(8)-C(9)-C(10)	176.7(2)
C(2)-C(1)-C(22)-C(21)	170.6(2)	C(7)-C(6)-C(5)-H(7)	53(1)
C(2)-C(3)-C(4)-H(5)	-174(2)	C(7)-C(6)-C(5)-H(8)	-62(2)
C(2)-C(3)-C(4)-H(6)	-53(1)	C(8)-C(7)-C(6)-H(9)	58(2)
C(2)-C(3)-C(4)-C(5)	68.4(3)	C(8)-C(7)-C(6)-H(10)	-59(1)
C(3)-C(4)-C(5)-H(7)	-62(1)	C(8)-C(9)-C(10)-H(17)	-61(2)
C(3)-C(4)-C(5)-H(8)	51(1)	C(8)-C(9)-C(10)-H(18)	55(2)

Torsion angles (deg) with estimated standard deviations in parentheses for **1g** (continued)

Atoms	Value(deg)	Atoms	Value(deg)
C(8)-C(9)-C(10)-C(11)	175.6(2)	C(14)-C(15)-C(16)-C(17)	-177.2(2)
C(9)-C(10)-C(11)-H(19)	-172(2)	C(15)-C(16)-C(17)-H(29)	48(2)
C(9)-C(10)-C(11)-H(20)	-52(1)	C(15)-C(16)-C(17)-H(30)	168(2)
C(9)-C(10)-C(11)-C(12)	67.8(3)	C(15)-C(16)-C(17)-C(18)	-68.4(3)
C(9)-C(8)-C(7)-H(11)	55(1)	C(15)-C(14)-C(13)-H(21)	-60(2)
C(9)-C(8)-C(7)-H(12)	-57(2)	C(15)-C(14)-C(13)-H(22)	180(2)
C(10)-C(9)-C(8)-H(13)	54(2)	C(16)-C(17)-C(18)-H(31)	-50(2)
C(10)-C(9)-C(8)-H(14)	-61(1)	C(16)-C(17)-C(18)-H(32)	62(2)
C(10)-C(11)-C(12)-C(13)	-158.7(2)	C(16)-C(17)-C(18)-C(19)	-172.8(2)
C(11)-C(12)-C(13)-H(21)	-180(2)	C(16)-C(15)-C(14)-H(23)	67(2)
C(11)-C(12)-C(13)-H(22)	-60(2)	C(16)-C(15)-C(14)-H(24)	-50(1)
C(11)-C(12)-C(13)-C(14)	60.8(3)	C(17)-C(18)-C(19)-H(33)	-67(2)
C(11)-C(10)-C(9)-H(15)	54(2)	C(17)-C(18)-C(19)-H(34)	52(2)
C(11)-C(10)-C(9)-H(16)	-59(2)	C(17)-C(18)-C(19)-C(20)	174.5(2)
C(12)-C(13)-C(14)-H(23)	180(2)	C(17)-C(16)-C(15)-H(25)	-56(1)
C(12)-C(13)-C(14)-H(24)	-61(1)	C(17)-C(16)-C(15)-H(26)	62(1)
C(12)-C(13)-C(14)-C(15)	59.8(3)	C(18)-C(17)-C(16)-H(27)	169(2)
C(12)-C(11)-C(10)-H(17)	-58(2)	C(18)-C(17)-C(16)-H(28)	52(2)
C(12)-C(11)-C(10)-H(18)	-170(2)	C(18)-C(19)-C(20)-H(35)	-53(1)
C(13)-C(12)-C(11)-H(19)	79(2)	C(18)-C(19)-C(20)-H(36)	64(1)
C(13)-C(12)-C(11)-H(20)	-38(1)	C(18)-C(19)-C(20)-C(21)	-174.7(2)
C(13)-C(14)-C(15)-H(25)	65(1)	C(19)-C(20)-C(21)-H(37)	-57(2)
C(13)-C(14)-C(15)-H(26)	-52(1)	C(19)-C(20)-C(21)-H(38)	59(2)
C(13)-C(14)-C(15)-C(16)	-172.3(2)	C(19)-C(20)-C(21)-C(22)	-177.0(2)
C(14)-C(15)-C(16)-H(27)	-55(2)	C(19)-C(18)-C(17)-H(29)	68(1)
C(14)-C(15)-C(16)-H(28)	60(2)	C(19)-C(18)-C(17)-H(30)	-50(2)

Torsion angles (deg) with estimated standard deviations in parentheses for **1g** (continued)

Atoms	Value(deg)	Atoms	Value(deg)
C(20)-C(19)-C(18)-H(31)	53(1)	H(9)-C(6)-C(7)-H(11)	-178(2)
C(20)-C(19)-C(18)-H(32)	-56(1)	H(9)-C(6)-C(7)-H(12)	-69(2)
C(20)-C(21)-C(22)-H(39)	172(2)	H(10)-C(6)-C(7)-H(11)	65(2)
C(20)-C(21)-C(22)-H(40)	53(1)	H(10)-C(6)-C(7)-H(12)	174(2)
C(21)-C(20)-C(19)-H(33)	64(2)	H(11)-C(7)-C(8)-H(13)	176(2)
C(21)-C(20)-C(19)-H(34)	-53(2)	H(11)-C(7)-C(8)-H(14)	-64(2)
C(22)-C(1)-C(2)-H(1)	70(2)	H(12)-C(7)-C(8)-H(13)	63(2)
C(22)-C(1)-C(2)-H(2)	-175(1)	H(12)-C(7)-C(8)-H(14)	-176(2)
C(22)-C(21)-C(20)-H(35)	64(1)	H(13)-C(8)-C(9)-H(15)	179(2)
C(22)-C(21)-C(20)-H(36)	-55(1)	H(13)-C(8)-C(9)-H(16)	-73(2)
H(1)-C(2)-C(3)-H(3)	-68(2)	H(14)-C(8)-C(9)-H(15)	63(2)
H(1)-C(2)-C(3)-H(4)	52(2)	H(14)-C(8)-C(9)-H(16)	171(2)
H(2)-C(2)-C(3)-H(3)	175(2)	H(15)-C(9)-C(10)-H(17)	177(2)
H(2)-C(2)-C(3)-H(4)	-65(2)	H(15)-C(9)-C(10)-H(18)	-67(2)
H(3)-C(3)-C(4)-H(5)	63(2)	H(16)-C(9)-C(10)-H(17)	64(2)
H(3)-C(3)-C(4)-H(6)	-175(2)	H(16)-C(9)-C(10)-H(18)	180(2)
H(4)-C(3)-C(4)-H(5)	-56(2)	H(17)-C(10)-C(11)-H(19)	62(2)
H(4)-C(3)-C(4)-H(6)	65(2)	H(17)-C(10)-C(11)-H(20)	-178(2)
H(5)-C(4)-C(5)-H(7)	176(2)	H(18)-C(10)-C(11)-H(19)	-49(2)
H(5)-C(4)-C(5)-H(8)	-71(2)	H(18)-C(10)-C(11)-H(20)	71(2)
H(6)-C(4)-C(5)-H(7)	59(2)	H(21)-C(13)-C(14)-H(23)	60(2)
H(6)-C(4)-C(5)-H(8)	172(2)	H(21)-C(13)-C(14)-H(24)	179(2)
H(7)-C(5)-C(6)-H(9)	176(2)	H(22)-C(13)-C(14)-H(23)	-60(2)
H(7)-C(5)-C(6)-H(10)	-68(2)	H(22)-C(13)-C(14)-H(24)	59(2)
H(8)-C(5)-C(6)-H(9)	61(2)	H(23)-C(14)-C(15)-H(25)	-56(2)
H(8)-C(5)-C(6)-H(10)	177(2)	H(23)-C(14)-C(15)-H(26)	-173(2)

Torsion angles (deg) with estimated standard deviations in parentheses for **1g** (continued)

Atoms	Value(deg)	Atoms	Value(deg)
H(24)-C(14)-C(15)-H(25)	-173(2)	H(37)-C(21)-C(22)-H(39)	53(2)
H(24)-C(14)-C(15)-H(26)	70(2)	H(37)-C(21)-C(22)-H(40)	-66(2)
H(25)-C(15)-C(16)-H(27)	66(2)	H(38)-C(21)-C(22)-H(39)	-65(2)
H(25)-C(15)-C(16)-H(28)	-179(2)	H(38)-C(21)-C(22)-H(40)	177(2)
H(26)-C(15)-C(16)-H(27)	-176(2)		
H(26)-C(15)-C(16)-H(28)	-62(2)		
H(27)-C(16)-C(17)-H(29)	-75(2)		
H(27)-C(16)-C(17)-H(30)	45(2)		
H(28)-C(16)-C(17)-H(29)	168(2)		
H(28)-C(16)-C(17)-H(30)	-72(2)		
H(29)-C(17)-C(18)-H(31)	-169(2)		
H(29)-C(17)-C(18)-H(32)	-57(2)		
H(30)-C(17)-C(18)-H(31)	73(2)		
H(30)-C(17)-C(18)-H(32)	-175(2)		
H(31)-C(18)-C(19)-H(33)	171(2)		
H(31)-C(18)-C(19)-H(34)	-70(2)		
H(32)-C(18)-C(19)-H(33)	62(2)		
H(32)-C(18)-C(19)-H(34)	-179(2)		
H(33)-C(19)-C(20)-H(35)	-174(2)		
H(33)-C(19)-C(20)-H(36)	-57(2)		
H(34)-C(19)-C(20)-H(35)	68(2)		
H(34)-C(19)-C(20)-H(36)	-175(2)		
H(35)-C(20)-C(21)-H(37)	-176(2)		
H(35)-C(20)-C(21)-H(38)	-60(2)		
H(36)-C(20)-C(21)-H(37)	65(2)		
H(36)-C(20)-C(21)-H(38)	-179(2)		

Intermolecular Distances Involving the Nonhydrogen Atoms

atom	atom	distance	ADC(*)	atom	atom	distance	ADC(*)
O(1)	C(12)	3.313(3)	55404	O(2)	C(2)	3.454(3)	56504
O(1)	C(13)	3.382(3)	55404	O(2)	C(1)	3.484(3)	56504
O(1)	C(11)	3.561(3)	55404				

Contacts out to 3.60 angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

(*)footnote

The ADC (atom designator code) specifies the position of an atom in a crystal. The 5-digit number shown in the table is a composite of three one digit numbers and one two digit number: TA(1st digit) + TB(2nd digit) + TC(3rd digit) + SN(4th and 5th digit). TA, TB, & TC are the crystal lattice translation digits along cell edges a, b, and c. A translation digit of 5 indicates the origin unit cell. If TA=4, this indicates a translation of one unit cell length along the a axis in the negative direction. Each translation digit can range in value from 1 to 9 and thus (+/-)4 lattice translations from the origin (TA=5,TB=5,TC=5) can be represented.

The SN or symmetry operator number refers to the number of the symmetry operator used to generate the coordinates of the target atom. A list of the symmetry operators relevant to this structure are given below.

For a given intermolecular contact, the first atom (origin atom) is located in the origin unit cell (TA=5,TB=5,TC=5) and its position can be generated using the identity operator (SN=1). Thus, the ADC for an origin atom is always ADC=55501. The position of the second atom (target atom) can be generated using the ADC and the coordinates of that atom in the parameter table. For example, an ADC of 47502 refers to the target atom moved through operator two, then translated -1 cell translations along the a axis, +2 cell translations along the b axis, and 0 cell translations along the c axis.

An ADC of 1 indicates an intermolecular contact between two fragments (i.e.cation and anion) that reside in the same asymmetric unit.

Symmetry Operators

(1)	+X	,	+Y	,	+Z	(2)	-X	,1/2+Y ,1/2-Z
(3)	-X	,	-Y	,	-Z	(4)	+X	,1/2-Y ,1/2+Z

Table of Least-Squares Planes

---------- Plane number 1 ----------

Atoms Defining Plane	Distance	esd
C(1)	-0.0256	0.0023
O(1)	0.0054	0.0017
C(2)	0.0120	0.0028
C(22)	0.0064	0.0023

Mean deviation from plane is 0.0123 angstroms
Chi-squared: 177.2

---------- Plane number 2 ----------

Atoms Defining Plane	Distance	esd
C(12)	0.0107	0.0023
O(2)	-0.0022	0.0017
C(11)	-0.0027	0.0024
C(13)	-0.0056	0.0031

Mean deviation from plane is 0.0053 angstroms
Chi-squared: 49.6

Dihedral angles between least-squares planes

plane	plane	angle
2	1	5.61

Crystallographic data

for 1,13-Cyclotetracosanedione, **1h**

Hydrogen atom coordinates (fractional) and B_{iso}

atom	x	y	z	B_{iso}
H(1)	0.4582	0.7250	0.0585	6.3
H(2)	0.3385	0.6587	0.0243	6.3
H(3)	0.2487	0.7793	0.0892	6.2
H(4)	0.2152	0.5866	0.0889	6.2
H(5)	0.3974	0.5479	0.1444	5.5
H(6)	0.4136	0.7436	0.1472	5.5
H(7)	0.1956	0.7625	0.1753	5.7
H(8)	0.1849	0.5660	0.1744	5.7
H(9)	0.3573	0.5528	0.2324	5.5
H(10)	0.3589	0.7496	0.2345	5.5
H(11)	0.1364	0.7446	0.2598	5.6
H(12)	0.1422	0.5478	0.2604	5.6
H(13)	0.3092	0.5594	0.3202	5.6
H(14)	0.2968	0.7557	0.3204	5.6
H(15)	0.0759	0.7326	0.3451	5.5
H(16)	0.0918	0.5366	0.3462	5.5
H(17)	0.2598	0.5638	0.4059	5.7
H(18)	0.2346	0.7583	0.4059	5.7
H(19)	0.1291	0.6474	0.4687	5.7
H(20)	0.0151	0.7119	0.4320	5.7
H(21)	-0.0558	0.4631	0.4582	5.6
H(22)	-0.0135	0.4368	0.4054	5.6
H(23)	0.1377	0.0721	0.4536	6.2
H(24)	-0.0167	0.1266	0.4568	6.2
H(25)	0.0160	0.0009	0.3847	5.9

Hydrogen atom coordinates (fractional) and B_{iso} (cont.)

atom	x	y	z	B_{iso}
H(26)	-0.0262	0.1892	0.3769	5.9
H(27)	0.2060	0.2513	0.3676	5.4
H(28)	0.2362	0.0579	0.3691	5.4
H(29)	0.0963	0.0259	0.3010	5.5
H(30)	0.0787	0.2215	0.2988	5.5
H(31)	0.3106	0.2466	0.2865	5.5
H(32)	0.3221	0.0502	0.2857	5.5
H(33)	0.1785	0.0460	0.2183	5.5
H(34)	0.1782	0.2429	0.2184	5.5
H(35)	0.4099	0.2399	0.2052	5.5
H(36)	0.4047	0.0433	0.2025	5.5
H(37)	0.2640	0.0621	0.1351	5.2
H(38)	0.2750	0.2584	0.1375	5.2
H(39)	0.5064	0.2396	0.1244	5.8
H(40)	0.4927	0.0437	0.1207	5.8
H(41)	0.5054	0.1480	0.0465	6.0
H(42)	0.3567	0.0759	0.0520	6.0
H(43)	0.2774	0.3447	0.0635	5.6
H(44)	0.3377	0.3206	0.0129	5.6

Anisotropic thermal parameters

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	0.0501(9)	0.086(1)	0.064(1)	-0.0020(9)	0.0018(7)	0.0043(9)
O(2)	0.078(1)	0.089(1)	0.085(1)	-0.003(1)	-0.028(1)	0.006(1)
C(1)	0.057(1)	0.069(2)	0.028(1)	0.003(1)	0.006(1)	0.005(1)
C(2)	0.076(2)	0.076(2)	0.047(1)	0.010(1)	0.005(1)	0.010(1)
C(3)	0.072(1)	0.075(2)	0.050(1)	0.016(1)	0.007(1)	0.005(1)
C(4)	0.065(1)	0.064(2)	0.046(1)	0.002(1)	0.005(1)	0.000(1)
C(5)	0.066(1)	0.067(2)	0.048(1)	-0.001(1)	0.004(1)	-0.002(1)
C(6)	0.061(1)	0.064(2)	0.049(1)	0.001(1)	0.006(1)	-0.001(1)
C(7)	0.064(1)	0.065(2)	0.047(1)	0.001(1)	0.005(1)	0.001(1)
C(8)	0.061(1)	0.065(2)	0.053(1)	0.003(1)	0.006(1)	0.003(1)
C(9)	0.060(1)	0.064(2)	0.050(1)	0.002(1)	0.003(1)	0.003(1)
C(10)	0.062(1)	0.063(2)	0.054(1)	-0.004(1)	0.002(1)	-0.001(1)
C(11)	0.067(1)	0.069(2)	0.047(1)	0.006(1)	0.004(1)	-0.003(1)
C(12)	0.056(1)	0.076(2)	0.045(1)	0.001(1)	0.006(1)	-0.000(1)
C(13)	0.061(1)	0.071(2)	0.042(1)	-0.003(1)	0.006(1)	0.002(1)
C(14)	0.069(1)	0.068(2)	0.060(1)	-0.006(1)	0.014(1)	0.003(1)
C(15)	0.059(1)	0.064(2)	0.063(1)	-0.011(1)	0.008(1)	-0.008(1)

Anisotropic thermal parameters (continued)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(16)	0.051(1)	0.063(2)	0.058(1)	-0.003(1)	0.003(1)	-0.002(1)
C(17)	0.055(1)	0.065(2)	0.055(1)	-0.001(1)	0.002(1)	-0.004(1)
C(18)	0.052(1)	0.065(2)	0.058(1)	-0.002(1)	0.003(1)	0.001(1)
C(19)	0.054(1)	0.063(2)	0.055(1)	-0.000(1)	0.002(1)	0.001(1)
C(20)	0.050(1)	0.066(2)	0.060(1)	0.001(1)	0.003(1)	0.006(1)
C(21)	0.050(1)	0.063(2)	0.053(1)	-0.002(1)	0.002(1)	0.005(1)
C(22)	0.051(1)	0.067(2)	0.065(1)	0.009(1)	0.010(1)	0.016(1)
C(23)	0.059(1)	0.072(2)	0.059(1)	-0.002(1)	0.011(1)	0.000(1)
C(24)	0.052(1)	0.074(2)	0.050(1)	-0.002(1)	-0.001(1)	0.005(1)

Table . Bond lengths (Å) with estimated standard deviations.

atom	atom	distance	atom	atom	distance
O(1)	C(1)	1.208(2)	C(11)	C(12)	1.522(3)
O(2)	C(13)	1.210(2)	C(12)	C(13)	1.510(3)
C(1)	C(2)	1.505(3)	C(13)	C(14)	1.502(3)
C(1)	C(24)	1.510(3)	C(14)	C(15)	1.534(3)
C(2)	C(3)	1.513(3)	C(15)	C(16)	1.518(3)
C(3)	C(4)	1.520(3)	C(16)	C(17)	1.520(3)
C(4)	C(5)	1.509(3)	C(17)	C(18)	1.514(3)
C(5)	C(6)	1.503(3)	C(18)	C(19)	1.516(3)
C(6)	C(7)	1.514(3)	C(19)	C(20)	1.511(3)
C(7)	C(8)	1.507(3)	C(20)	C(21)	1.511(3)
C(8)	C(9)	1.509(3)	C(21)	C(22)	1.522(3)
C(9)	C(10)	1.516(3)	C(22)	C(23)	1.525(3)
C(10)	C(11)	1.527(3)	C(23)	C(24)	1.516(3)

Intramolecular Distances Involving the Hydrogen Atoms

atom	atom	distance	atom	atom	distance
C(2)	H(1)	0.980	C(14)	H(23)	0.980
C(2)	H(2)	0.980	C(14)	H(24)	0.980
C(3)	H(3)	0.980	C(15)	H(25)	0.980
C(3)	H(4)	0.980	C(15)	H(26)	0.980
C(4)	H(5)	0.980	C(16)	H(27)	0.980
C(4)	H(6)	0.980	C(16)	H(28)	0.980
C(5)	H(7)	0.980	C(17)	H(29)	0.980
C(5)	H(8)	0.980	C(17)	H(30)	0.980
C(6)	H(9)	0.980	C(18)	H(31)	0.980
C(6)	H(10)	0.980	C(18)	H(32)	0.980
C(7)	H(11)	0.980	C(19)	H(33)	0.980
C(7)	H(12)	0.980	C(19)	H(34)	0.980
C(8)	H(13)	0.980	C(20)	H(35)	0.980
C(8)	H(14)	0.980	C(20)	H(36)	0.980
C(9)	H(15)	0.980	C(21)	H(37)	0.980
C(9)	H(16)	0.980	C(21)	H(38)	0.980
C(10)	H(17)	0.980	C(22)	H(39)	0.980
C(10)	H(18)	0.980	C(22)	H(40)	0.980
C(11)	H(19)	0.980	C(23)	H(41)	0.980
C(11)	H(20)	0.980	C(23)	H(42)	0.980
C(12)	H(21)	0.980	C(24)	H(43)	0.980
C(12)	H(22)	0.980	C(24)	H(44)	0.980

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table . Bond angles (deg) with estimated standard deviations.

atom	atom	atom	angle	atom	atom	atom	angle
O(1)	C(1)	C(2)	120.7(2)	O(2)	C(13)	C(12)	120.7(2)
O(1)	C(1)	C(24)	121.0(2)	O(2)	C(13)	C(14)	121.3(2)
C(2)	C(1)	C(24)	118.2(2)	C(12)	C(13)	C(14)	117.9(2)
C(1)	C(2)	C(3)	114.2(2)	C(13)	C(14)	C(15)	114.0(2)
C(2)	C(3)	C(4)	113.9(2)	C(14)	C(15)	C(16)	114.4(2)
C(3)	C(4)	C(5)	113.0(2)	C(15)	C(16)	C(17)	113.6(2)
C(4)	C(5)	C(6)	115.6(2)	C(16)	C(17)	C(18)	115.1(2)
C(5)	C(6)	C(7)	113.9(2)	C(17)	C(18)	C(19)	114.4(2)
C(6)	C(7)	C(8)	115.3(2)	C(18)	C(19)	C(20)	114.9(2)
C(7)	C(8)	C(9)	114.4(2)	C(19)	C(20)	C(21)	114.9(2)
C(8)	C(9)	C(10)	114.3(2)	C(20)	C(21)	C(22)	114.1(2)
C(9)	C(10)	C(11)	115.4(2)	C(21)	C(22)	C(23)	115.7(2)
C(10)	C(11)	C(12)	113.8(2)	C(22)	C(23)	C(24)	113.9(2)
C(11)	C(12)	C(13)	115.0(2)	C(1)	C(24)	C(23)	115.5(2)

Intramolecular Bond Angles Involving the Hydrogen Atoms

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	C(2)	H(1)	108.29	C(6)	C(7)	H(12)	107.99
C(1)	C(2)	H(2)	108.29	C(8)	C(7)	H(11)	107.99
C(3)	C(2)	H(1)	108.29	C(8)	C(7)	H(12)	107.98
C(3)	C(2)	H(2)	108.29	H(11)	C(7)	H(12)	109.46
H(1)	C(2)	H(2)	109.46	C(7)	C(8)	H(13)	108.23
C(2)	C(3)	H(3)	108.35	C(7)	C(8)	H(14)	108.22
C(2)	C(3)	H(4)	108.36	C(9)	C(8)	H(13)	108.23
C(4)	C(3)	H(3)	108.35	C(9)	C(8)	H(14)	108.22
C(4)	C(3)	H(4)	108.35	H(13)	C(8)	H(14)	109.46
H(3)	C(3)	H(4)	109.46	C(8)	C(9)	H(15)	108.26
C(3)	C(4)	H(5)	108.58	C(8)	C(9)	H(16)	108.26
C(3)	C(4)	H(6)	108.58	C(10)	C(9)	H(15)	108.26
C(5)	C(4)	H(5)	108.58	C(10)	C(9)	H(16)	108.26
C(5)	C(4)	H(6)	108.58	H(15)	C(9)	H(16)	109.46
H(5)	C(4)	H(6)	109.46	C(9)	C(10)	H(17)	107.98
C(4)	C(5)	H(7)	107.92	C(9)	C(10)	H(18)	107.98
C(4)	C(5)	H(8)	107.92	C(11)	C(10)	H(17)	107.98
C(6)	C(5)	H(7)	107.93	C(11)	C(10)	H(18)	107.98
C(6)	C(5)	H(8)	107.93	H(17)	C(10)	H(18)	109.46
H(7)	C(5)	H(8)	109.46	C(10)	C(11)	H(19)	108.38
C(5)	C(6)	H(9)	108.35	C(10)	C(11)	H(20)	108.38
C(5)	C(6)	H(10)	108.35	C(12)	C(11)	H(19)	108.38
C(7)	C(6)	H(9)	108.35	C(12)	C(11)	H(20)	108.38
C(7)	C(6)	H(10)	108.34	H(19)	C(11)	H(20)	109.46
H(9)	C(6)	H(10)	109.46	C(11)	C(12)	H(21)	108.08
C(6)	C(7)	H(11)	107.99	C(11)	C(12)	H(22)	108.08

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Hydrogen Atoms (cont)

atom	atom	atom	angle	atom	atom	atom	angle
C(13)	C(12)	H(21)	108.08	C(19)	C(18)	H(32)	108.23
C(13)	C(12)	H(22)	108.08	H(31)	C(18)	H(32)	109.46
H(21)	C(12)	H(22)	109.46	C(18)	C(19)	H(33)	108.09
C(13)	C(14)	H(23)	108.33	C(18)	C(19)	H(34)	108.10
C(13)	C(14)	H(24)	108.33	C(20)	C(19)	H(33)	108.09
C(15)	C(14)	H(23)	108.33	C(20)	C(19)	H(34)	108.10
C(15)	C(14)	H(24)	108.33	H(33)	C(19)	H(34)	109.46
H(23)	C(14)	H(24)	109.46	C(19)	C(20)	H(35)	108.10
C(14)	C(15)	H(25)	108.23	C(19)	C(20)	H(36)	108.11
C(14)	C(15)	H(26)	108.24	C(21)	C(20)	H(35)	108.10
C(16)	C(15)	H(25)	108.23	C(21)	C(20)	H(36)	108.11
C(16)	C(15)	H(26)	108.24	H(35)	C(20)	H(36)	109.46
H(25)	C(15)	H(26)	109.46	C(20)	C(21)	H(37)	108.31
C(15)	C(16)	H(27)	108.44	C(20)	C(21)	H(38)	108.32
C(15)	C(16)	H(28)	108.44	C(22)	C(21)	H(37)	108.31
C(17)	C(16)	H(27)	108.44	C(22)	C(21)	H(38)	108.31
C(17)	C(16)	H(28)	108.44	H(37)	C(21)	H(38)	109.46
H(27)	C(16)	H(28)	109.46	C(21)	C(22)	H(39)	107.90
C(16)	C(17)	H(29)	108.05	C(21)	C(22)	H(40)	107.90
C(16)	C(17)	H(30)	108.05	C(23)	C(22)	H(39)	107.90
C(18)	C(17)	H(29)	108.05	C(23)	C(22)	H(40)	107.90
C(18)	C(17)	H(30)	108.05	H(39)	C(22)	H(40)	109.46
H(29)	C(17)	H(30)	109.46	C(22)	C(23)	H(41)	108.34
C(17)	C(18)	H(31)	108.23	C(22)	C(23)	H(42)	108.35
C(17)	C(18)	H(32)	108.23	C(24)	C(23)	H(41)	108.35
C(19)	C(18)	H(31)	108.23	C(24)	C(23)	H(42)	108.35

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Hydrogen Atoms (cont)

atom	atom	atom	angle	atom	atom	atom	angle
H(41)	C(23)	H(42)	109.46				
C(1)	C(24)	H(43)	107.95				
C(1)	C(24)	H(44)	107.95				
C(23)	C(24)	H(43)	107.95				
C(23)	C(24)	H(44)	107.95				
H(43)	C(24)	H(44)	109.46				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Torsion or Conformation Angles

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
O(1)	C(1)	C(2)	C(3)	-120.3(2)	C(3)	C(4)	C(5)	H(7)	-56
O(1)	C(1)	C(2)	H(1)	0	C(3)	C(4)	C(5)	H(8)	62
O(1)	C(1)	C(2)	H(2)	119	C(4)	C(3)	C(2)	H(1)	-59
O(1)	C(1)	C(24)	C(23)	21.6(3)	C(4)	C(3)	C(2)	H(2)	-178
O(1)	C(1)	C(24)	H(43)	143	C(4)	C(5)	C(6)	C(7)	-176.5(2)
O(1)	C(1)	C(24)	H(44)	-99	C(4)	C(5)	C(6)	H(9)	-56
O(2)	C(13)	C(12)	C(11)	18.0(3)	C(4)	C(5)	C(6)	H(10)	63
O(2)	C(13)	C(12)	H(21)	-103	C(5)	C(4)	C(3)	H(3)	66
O(2)	C(13)	C(12)	H(22)	139	C(5)	C(4)	C(3)	H(4)	-53
O(2)	C(13)	C(14)	C(15)	-122.5(2)	C(5)	C(6)	C(7)	C(8)	-176.3(2)
O(2)	C(13)	C(14)	H(23)	-2	C(5)	C(6)	C(7)	H(11)	-55
O(2)	C(13)	C(14)	H(24)	117	C(5)	C(6)	C(7)	H(12)	63
C(1)	C(2)	C(3)	C(4)	61.2(2)	C(6)	C(5)	C(4)	H(5)	62
C(1)	C(2)	C(3)	H(3)	-178	C(6)	C(5)	C(4)	H(6)	-57
C(1)	C(2)	C(3)	H(4)	-59	C(6)	C(7)	C(8)	C(9)	-177.5(2)
C(1)	C(24)	C(23)	C(22)	64.9(2)	C(6)	C(7)	C(8)	H(13)	-57
C(1)	C(24)	C(23)	H(41)	-56	C(6)	C(7)	C(8)	H(14)	62
C(1)	C(24)	C(23)	H(42)	-174	C(7)	C(6)	C(5)	H(7)	63
C(2)	C(1)	C(24)	C(23)	-161.6(2)	C(7)	C(6)	C(5)	H(8)	-56
C(2)	C(1)	C(24)	H(43)	-41	C(7)	C(8)	C(9)	C(10)	-178.2(2)
C(2)	C(1)	C(24)	H(44)	78	C(7)	C(8)	C(9)	H(15)	-57
C(2)	C(3)	C(4)	C(5)	-173.2(2)	C(7)	C(8)	C(9)	H(16)	61
C(2)	C(3)	C(4)	H(5)	-53	C(8)	C(7)	C(6)	H(9)	63
C(2)	C(3)	C(4)	H(6)	66	C(8)	C(7)	C(6)	H(10)	-56
C(3)	C(2)	C(1)	C(24)	62.9(2)	C(8)	C(9)	C(10)	C(11)	-176.4(2)
C(3)	C(4)	C(5)	C(6)	-177.4(2)	C(8)	C(9)	C(10)	H(17)	-56

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Torsion or Conformation Angles (cont)

(1)	(2)	(3)	(4)	angle
C(8)	C(9)	C(10)	H(18)	63
C(9)	C(8)	C(7)	H(11)	62
C(9)	C(8)	C(7)	H(12)	-57
C(9)	C(10)	C(11)	C(12)	64.6(2)
C(9)	C(10)	C(11)	H(19)	-175
C(9)	C(10)	C(11)	H(20)	-56
C(10)	C(9)	C(8)	H(13)	61
C(10)	C(9)	C(8)	H(14)	-57
C(10)	C(11)	C(12)	C(13)	68.2(2)
C(10)	C(11)	C(12)	H(21)	-171
C(10)	C(11)	C(12)	H(22)	-53
C(11)	C(10)	C(9)	H(15)	63
C(11)	C(10)	C(9)	H(16)	-56
C(11)	C(12)	C(13)	C(14)	-163.8(2)
C(12)	C(11)	C(10)	H(17)	-56
C(12)	C(11)	C(10)	H(18)	-175
C(12)	C(13)	C(14)	C(15)	59.2(2)
C(12)	C(13)	C(14)	H(23)	180
C(12)	C(13)	C(14)	H(24)	-61
C(13)	C(12)	C(11)	H(19)	-52
C(13)	C(12)	C(11)	H(20)	-171
C(13)	C(14)	C(15)	C(16)	59.9(2)
C(13)	C(14)	C(15)	H(25)	-179
C(13)	C(14)	C(15)	H(26)	-61
C(14)	C(13)	C(12)	H(21)	75
C(14)	C(13)	C(12)	H(22)	-43
C(14)	C(15)	C(16)	C(17)	-172.2(2)
C(14)	C(15)	C(16)	H(27)	-52
C(14)	C(15)	C(16)	H(28)	67
C(15)	C(16)	C(17)	C(18)	-175.4(2)
C(15)	C(16)	C(17)	H(29)	-55
C(15)	C(16)	C(17)	H(30)	64
C(16)	C(15)	C(14)	H(23)	-61
C(16)	C(15)	C(14)	H(24)	-179
C(16)	C(17)	C(18)	C(19)	-176.3(2)
C(16)	C(17)	C(18)	H(31)	-56
C(16)	C(17)	C(18)	H(32)	63
C(17)	C(16)	C(15)	H(25)	67
C(17)	C(16)	C(15)	H(26)	-51
C(17)	C(18)	C(19)	C(20)	-175.9(2)
C(17)	C(18)	C(19)	H(33)	-55
C(17)	C(18)	C(19)	H(34)	63
C(18)	C(17)	C(16)	H(27)	64
C(18)	C(17)	C(16)	H(28)	-55
C(18)	C(19)	C(20)	C(21)	-176.8(2)
C(18)	C(19)	C(20)	H(35)	-56
C(18)	C(19)	C(20)	H(36)	62
C(19)	C(18)	C(17)	H(29)	63
C(19)	C(18)	C(17)	H(30)	-55
C(19)	C(20)	C(21)	C(22)	-177.9(2)
C(19)	C(20)	C(21)	H(37)	-57
C(19)	C(20)	C(21)	H(38)	61

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Torsion or Conformation Angles (cont)

(1)	(2)	(3)	(4)	angle
C(20)	C(19)	C(18)	H(31)	63
C(20)	C(19)	C(18)	H(32)	-55
C(20)	C(21)	C(22)	C(23)	-178.4(2)
C(20)	C(21)	C(22)	H(39)	-57
C(20)	C(21)	C(22)	H(40)	61
C(21)	C(20)	C(19)	H(33)	62
C(21)	C(20)	C(19)	H(34)	-56
C(21)	C(22)	C(23)	C(24)	64.3(2)
C(21)	C(22)	C(23)	H(41)	-175
C(21)	C(22)	C(23)	H(42)	-56
C(22)	C(21)	C(20)	H(35)	61
C(22)	C(21)	C(20)	H(36)	-57
C(22)	C(23)	C(24)	H(43)	-56
C(22)	C(23)	C(24)	H(44)	-174
C(23)	C(22)	C(21)	H(37)	61
C(23)	C(22)	C(21)	H(38)	-58
C(24)	C(1)	C(2)	H(1)	-176
C(24)	C(1)	C(2)	H(2)	-58
C(24)	C(23)	C(22)	H(39)	-57
C(24)	C(23)	C(22)	H(40)	-175
H(1)	C(2)	C(3)	H(3)	61
H(1)	C(2)	C(3)	H(4)	180
H(2)	C(2)	C(3)	H(3)	-57
H(2)	C(2)	C(3)	H(4)	61
H(3)	C(3)	C(4)	H(5)	-173
H(3)	C(3)	C(4)	H(6)	-54
H(4)	C(3)	C(4)	H(5)	68
H(4)	C(3)	C(4)	H(6)	-173
H(5)	C(4)	C(5)	H(7)	-177
H(5)	C(4)	C(5)	H(8)	-59
H(6)	C(4)	C(5)	H(7)	64
H(6)	C(4)	C(5)	H(8)	-178
H(7)	C(5)	C(6)	H(9)	-177
H(7)	C(5)	C(6)	H(10)	-58
H(8)	C(5)	C(6)	H(9)	65
H(8)	C(5)	C(6)	H(10)	-176
H(9)	C(6)	C(7)	H(11)	-176
H(9)	C(6)	C(7)	H(12)	-58
H(10)	C(6)	C(7)	H(11)	65
H(10)	C(6)	C(7)	H(12)	-176
H(11)	C(7)	C(8)	H(13)	-178
H(11)	C(7)	C(8)	H(14)	-59
H(12)	C(7)	C(8)	H(13)	64
H(12)	C(7)	C(8)	H(14)	-177
H(13)	C(8)	C(9)	H(15)	-178
H(13)	C(8)	C(9)	H(16)	-60
H(14)	C(8)	C(9)	H(15)	63
H(14)	C(8)	C(9)	H(16)	-178
H(15)	C(9)	C(10)	H(17)	-176
H(15)	C(9)	C(10)	H(18)	-58
H(16)	C(9)	C(10)	H(17)	65
H(16)	C(9)	C(10)	H(18)	-177

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Torsion or Conformation Angles (cont)

(1) (2) (3) (4)	angle	(1) (2) (3) (4)	angle
H(17)C(10)C(11)H(19)	64	H(32)C(18)C(19)H(33)	66
H(17)C(10)C(11)H(20)	-177	H(32)C(18)C(19)H(34)	-176
H(18)C(10)C(11)H(19)	-54	H(33)C(19)C(20)H(35)	-177
H(18)C(10)C(11)H(20)	65	H(33)C(19)C(20)H(36)	-58
H(19)C(11)C(12)H(21)	68	H(34)C(19)C(20)H(35)	65
H(19)C(11)C(12)H(22)	-173	H(34)C(19)C(20)H(36)	-177
H(20)C(11)C(12)H(21)	-50	H(35)C(20)C(21)H(37)	-178
H(20)C(11)C(12)H(22)	68	H(35)C(20)C(21)H(38)	-59
H(23)C(14)C(15)H(25)	60	H(36)C(20)C(21)H(37)	64
H(23)C(14)C(15)H(26)	178	H(36)C(20)C(21)H(38)	-178
H(24)C(14)C(15)H(25)	-59	H(37)C(21)C(22)H(39)	-178
H(24)C(14)C(15)H(26)	60	H(37)C(21)C(22)H(40)	-60
H(25)C(15)C(16)H(27)	-172	H(38)C(21)C(22)H(39)	63
H(25)C(15)C(16)H(28)	-54	H(38)C(21)C(22)H(40)	-179
H(26)C(15)C(16)H(27)	69	H(39)C(22)C(23)H(41)	64
H(26)C(15)C(16)H(28)	-172	H(39)C(22)C(23)H(42)	-177
H(27)C(16)C(17)H(29)	-175	H(40)C(22)C(23)H(41)	-54
H(27)C(16)C(17)H(30)	-57	H(40)C(22)C(23)H(42)	65
H(28)C(16)C(17)H(29)	66	H(41)C(23)C(24)H(43)	-177
H(28)C(16)C(17)H(30)	-176	H(41)C(23)C(24)H(44)	65
H(29)C(17)C(18)H(31)	-176	H(42)C(23)C(24)H(43)	65
H(29)C(17)C(18)H(32)	-58	H(42)C(23)C(24)H(44)	-54
H(30)C(17)C(18)H(31)	65		
H(30)C(17)C(18)H(32)	-176		
H(31)C(18)C(19)H(33)	-176		
H(31)C(18)C(19)H(34)	-57		

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Table

Intra-annular torsion angles

Atoms	Value
C(24)-C(1)-C(2)-C(3)	62.9(2)
C(1)-C(2)-C(3)-C(4)	61.2(2)
C(2)-C(3)-C(4)-C(5)	-173.2(2)
C(3)-C(4)-C(5)-C(6)	-177.4(2)
C(4)-C(5)-C(6)-C(7)	-176.5(2)
C(5)-C(6)-C(7)-C(8)	-176.3(2)
C(6)-C(7)-C(8)-C(9)	-177.5(2)
C(7)-C(8)-C(9)-C(10)	-178.2(2)
C(8)-C(9)-C(10)-C(11)	-176.4(2)
C(9)-C(10)-C(11)-C(12)	64.6(2)
C(10)-C(11)-C(12)-C(13)	68.2(2)
C(11)-C(12)-C(13)-C(14)	-163.8(2)
C(12)-C(13)-C(14)-C(15)	59.2(2)
C(13)-C(14)-C(15)-C(16)	59.9(2)
C(14)-C(15)-C(16)-C(17)	-172.2(2)
C(15)-C(16)-C(17)-C(18)	-175.4(2)
C(16)-C(17)-C(18)-C(19)	-176.3(2)
C(17)-C(18)-C(19)-C(20)	-175.9(2)
C(18)-C(19)-C(20)-C(21)	-176.8(2)
C(19)-C(20)-C(21)-C(22)	-177.9(2)
C(20)-C(21)-C(22)-C(23)	-178.4(2)
C(21)-C(22)-C(23)-C(24)	64.3(2)
C(22)-C(23)-C(24)-C(1)	64.9(2)
C(23)-C(24)-C(1)-C(2)	-161.6(2)

Intermolecular Distances Involving the Nonhydrogen Atoms

atom	atom	distance	ADC(*)	atom	atom	distance	ADC(*)
O(1)	C(1)	3.318(2)	66503	O(1)	C(23)	3.594(3)	4
O(1)	C(2)	3.415(3)	66503	O(2)	C(11)	3.587(3)	54602
O(1)	C(21)	3.528(3)	4	C(1)	C(1)	3.354(4)	66503
O(1)	C(24)	3.586(3)	66503				

Non-bonded Distances Involving Hydrogen

atom	atom	distance	ADC(*)	atom	atom	distance	ADC(*)
O(1)	H(2)	2.77	66503	H(8)	H(40)	2.56	45504
O(1)	H(37)	2.83	4	H(10)	H(36)	2.60	56501
O(1)	H(42)	2.86	4	H(11)	H(29)	2.61	56501
O(1)	H(3)	2.86	56504	H(14)	H(32)	2.61	56501
O(1)	H(44)	2.91	66503	H(15)	H(25)	2.54	56501
O(2)	H(19)	2.72	54602	H(19)	H(21)	2.42	56603
O(2)	H(24)	2.72	4	H(1)	O(1)	2.43	1
O(2)	H(21)	2.97	56603	H(17)	O(2)	2.69	1
H(2)	H(44)	2.40	2	H(19)	O(2)	2.59	1
H(3)	H(37)	2.65	56501	H(23)	O(2)	2.44	1
H(4)	H(40)	2.64	45504	H(39)	O(1)	2.67	1
H(7)	H(33)	2.62	56501	H(41)	O(1)	2.64	1

Contacts out to 3.60 angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

(*)footnote

The ADC (atom designator code) specifies the position of an atom in a crystal. The 5-digit number shown in the table is a composite of three one digit numbers and one two digit number: TA(1st digit) + TB(2nd digit) + TC(3rd digit) + SN(4th and 5th digit). TA, TB, & TC are the crystal lattice translation digits along cell edges a, b, and c. A translation digit of 5 indicates the origin unit cell. If TA=4, this indicates a translation of one unit cell length along the a axis in the negative direction. Each translation digit can range in value from 1 to 9 and thus (+/-)4 lattice translations from the origin (TA=5,TB=5,TC=5) can be represented.

The SN or symmetry operator number refers to the number of the symmetry operator used to generate the coordinates of the target atom. A list of the symmetry operators relevant to this structure are given below.

For a given intermolecular contact, the first atom (origin atom) is located in the origin unit cell (TA=5,TB=5,TC=5) and its position can be generated using the identity operator (SN=1). Thus, the ADC for an origin atom is always ADC=55501. The position of the second atom (target atom) can be generated using the ADC and the coordinates of that atom in the parameter table. For example, an ADC of 47502 refers to the target atom moved through operator two, then translated -1 cell translations along the a axis, +2 cell translations along the b axis, and 0 cell translations along the c axis.

An ADC of 1 indicates an intermolecular contact between two fragments (i.e.cation and anion) that reside in the same asymmetric unit.

Symmetry Operators:

(1)	+X	,	+Y	,	+Z	(2)	1/2-X	,1/2+Y	,	-Z
(3)	-X	,	-Y	,	-Z	(4)	1/2+X	,1/2-Y	,	+Z

Table of Least-Squares Planes

---------- Plane number 1 ----------

Atoms Defining Plane	Distance	esd
O(1)	0.0051	0.0013
C(1)	-0.0166	0.0017
C(2)	0.0072	0.0020
C(24)	0.0059	0.0019

Additional Atoms	Distance
H(41)	0.0953
H(5)	-2.5880
H(6)	-2.5243
H(39)	-2.0607
H(40)	-2.0959

Mean deviation from plane is 0.0087 angstroms
Chi-squared: 117.6

---------- Plane number 2 ----------

Atoms Defining Plane	Distance	esd
O(2)	-0.0030	0.0016
C(12)	-0.0028	0.0019
C(13)	0.0090	0.0018
C(14)	-0.0036	0.0020

Additional Atoms	Distance
H(19)	-0.1537
H(17)	2.0472
H(18)	2.0083
H(27)	2.5942
H(28)	2.6211

Mean deviation from plane is 0.0046 angstroms
Chi-squared: 30.1

Dihedral angles between least-squares planes

plane	plane	angle
2	1	22.78

Table of Least-Squares Planes (continued)

---------- Plane number 3 ----------

Atoms Defining Plane	Distance	esd
C(2)	0.1337	0.0024
C(3)	-0.0955	0.0023
C(4)	0.0151	0.0022
C(5)	-0.0540	0.0022
C(6)	-0.0124	0.0022
C(7)	-0.0003	0.0022
C(8)	-0.0467	0.0022
C(9)	0.0255	0.0022
C(10)	-0.0643	0.0022
C(11)	0.0913	0.0023

Mean deviation from plane is 0.0539 angstroms
Chi-squared: 9931.5

Dihedral angles between least-squares planes

plane	plane	angle
3	1	93.62
3	2	92.48

---------- Plane number 4 ----------

Atoms Defining Plane	Distance	esd
C(14)	-0.1238	0.0023
C(15)	0.1195	0.0022
C(16)	-0.0204	0.0021
C(17)	0.0380	0.0022
C(18)	0.0117	0.0022
C(19)	-0.0177	0.0022
C(20)	0.0539	0.0022
C(21)	-0.0530	0.0021
C(22)	0.0720	0.0022
C(23)	-0.0691	0.0023

Mean deviation from plane is 0.0579 angstroms
Chi-squared: 10555.8

Dihedral angles between least-squares planes

plane	plane	angle
4	1	94.25
4	2	91.66
4	3	3.69

Crystallographic data

for 1,14-Cyclohexacosanedione, **1i** (n)

Hydrogen atom coordinates (fractional) and B_{iso}

atom	x	y	z	B_{iso}
H(1)	-0.0449	0.7494	0.3060	5.0
H(2)	-0.1628	0.6310	0.3406	5.0
H(3)	0.1862	0.5666	0.3537	5.1
H(4)	0.0959	0.7710	0.3809	5.1
H(5)	-0.0426	0.4651	0.4181	5.2
H(6)	0.0585	0.2661	0.3927	5.2
H(7)	0.3074	0.4145	0.4359	5.0
H(8)	0.1997	0.5968	0.4632	5.0
H(9)	0.0870	0.2758	0.5004	5.1
H(10)	0.1833	0.0870	0.4711	5.1
H(11)	0.4377	0.2310	0.5111	5.2
H(12)	0.3374	0.4081	0.5417	5.2
H(13)	0.2367	0.0795	0.5798	5.2
H(14)	0.3273	-0.1029	0.5478	5.2
H(15)	0.5873	0.0511	0.5838	5.5
H(16)	0.4910	0.2137	0.6180	5.5
H(17)	0.4948	-0.2973	0.6201	5.4
H(18)	0.6133	-0.1316	0.6568	5.4
H(19)	0.3783	0.0200	0.6865	4.9
H(20)	0.2628	-0.1542	0.6508	4.9
H(21)	0.4010	-0.4909	0.6922	5.1
H(22)	0.4906	-0.3034	0.7306	5.1
H(23)	0.2586	-0.4795	0.7584	5.5
H(24)	0.2339	-0.1933	0.7524	5.5

Anisotropic thermal parameters

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	0.0716(9)	0.077(1)	0.0671(9)	0.0238(9)	0.0064(7)	-0.0140(8)
C(1)	0.056(1)	0.057(1)	0.039(1)	0.004(1)	0.0112(8)	0.006(1)
C(2)	0.057(1)	0.048(1)	0.052(1)	0.004(1)	0.0049(9)	0.004(1)
C(3)	0.059(1)	0.049(1)	0.051(1)	-0.002(1)	0.0021(9)	0.002(1)
C(4)	0.056(1)	0.059(1)	0.048(1)	-0.003(1)	0.0045(8)	0.000(1)
C(5)	0.059(1)	0.055(1)	0.045(1)	-0.004(1)	0.0048(9)	0.000(1)
C(6)	0.059(1)	0.057(1)	0.046(1)	-0.005(1)	0.0080(9)	0.001(1)
C(7)	0.063(1)	0.056(1)	0.047(1)	-0.007(1)	0.0071(9)	0.003(1)
C(8)	0.061(1)	0.055(1)	0.047(1)	-0.006(1)	0.0082(9)	0.003(1)
C(9)	0.060(1)	0.062(1)	0.051(1)	-0.006(1)	0.007(1)	0.008(1)
C(10)	0.055(1)	0.062(1)	0.053(1)	0.002(1)	0.0043(9)	0.005(1)
C(11)	0.057(1)	0.051(1)	0.047(1)	0.0024(9)	0.0052(8)	0.004(1)
C(12)	0.054(1)	0.057(1)	0.048(1)	-0.0020(9)	-0.0022(8)	0.008(1)
C(13)	0.063(1)	0.070(1)	0.040(1)	-0.004(1)	0.0030(9)	0.006(1)

Table . Bond lengths (Å) with estimated standard deviations.

atom	atom	distance	atom	atom	distance
O(1)	C(1)	1.209(2)	C(6)	C(7)	1.515(2)
C(1)	C(2)	1.502(2)	C(7)	C(8)	1.519(2)
C(1)	C(13)*	1.503(2)	C(8)	C(9)	1.524(2)
C(2)	C(3)	1.516(2)	C(9)	C(10)	1.515(2)
C(3)	C(4)	1.518(2)	C(10)	C(11)	1.512(2)
C(4)	C(5)	1.514(2)	C(11)	C(12)	1.520(2)
C(5)	C(6)	1.517(2)	C(12)	C(13)	1.528(2)

* Refers, here and elsewhere, to symmetry operation: -x,-y,1-z.

Intramolecular Distances

atom	atom	distance	atom	atom	distance
C(2)	H(1)	0.98	C(8)	H(13)	0.98
C(2)	H(2)	0.98	C(8)	H(14)	0.98
C(3)	H(3)	0.98	C(9)	H(15)	0.98
C(3)	H(4)	0.98	C(9)	H(16)	0.98
C(4)	H(5)	0.98	C(10)	H(17)	0.98
C(4)	H(6)	0.98	C(10)	H(18)	0.98
C(5)	H(7)	0.98	C(11)	H(19)	0.98
C(5)	H(8)	0.98	C(11)	H(20)	0.98
C(6)	H(9)	0.98	C(12)	H(21)	0.98
C(6)	H(10)	0.98	C(12)	H(22)	0.98
C(7)	H(11)	0.98	C(13)	H(23)	0.98
C(7)	H(12)	0.98	C(13)	H(24)	0.98

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table . Bond angles (deg) with estimated standard deviations.

atom	atom	atom	angle	atom	atom	atom	angle
O(1)	C(1)	C(2)	121.2(2)	C(6)	C(7)	C(8)	115.4(1)
O(1)	C(1)	C(13)*	120.8(2)	C(7)	C(8)	C(9)	112.9(1)
C(2)	C(1)	C(13)*	118.0(2)	C(8)	C(9)	C(10)	115.7(1)
C(1)	C(2)	C(3)	115.5(1)	C(9)	C(10)	C(11)	114.3(2)
C(2)	C(3)	C(4)	113.7(1)	C(10)	C(11)	C(12)	114.2(1)
C(3)	C(4)	C(5)	114.0(1)	C(11)	C(12)	C(13)	112.4(1)
C(4)	C(5)	C(6)	114.9(1)	C(1)*	C(13)	C(12)	113.7(1)
C(5)	C(6)	C(7)	113.1(1)				

Intramolecular Bond Angles

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	C(2)	H(1)	107.96	C(6)	C(7)	H(12)	107.97
C(1)	C(2)	H(2)	107.96	C(8)	C(7)	H(11)	107.97
C(3)	C(2)	H(1)	107.95	C(8)	C(7)	H(12)	107.96
C(3)	C(2)	H(2)	107.95	H(11)	C(7)	H(12)	109.46
H(1)	C(2)	H(2)	109.46	C(7)	C(8)	H(13)	108.61
C(2)	C(3)	H(3)	108.41	C(7)	C(8)	H(14)	108.61
C(2)	C(3)	H(4)	108.40	C(9)	C(8)	H(13)	108.61
C(4)	C(3)	H(3)	108.41	C(9)	C(8)	H(14)	108.60
C(4)	C(3)	H(4)	108.41	H(13)	C(8)	H(14)	109.46
H(3)	C(3)	H(4)	109.46	C(8)	C(9)	H(15)	107.89
C(3)	C(4)	H(5)	108.32	C(8)	C(9)	H(16)	107.88
C(3)	C(4)	H(6)	108.33	C(10)	C(9)	H(15)	107.88
C(5)	C(4)	H(5)	108.33	C(10)	C(9)	H(16)	107.88
C(5)	C(4)	H(6)	108.33	H(15)	C(9)	H(16)	109.46
H(5)	C(4)	H(6)	109.46	C(9)	C(10)	H(17)	108.25
C(4)	C(5)	H(7)	108.10	C(9)	C(10)	H(18)	108.25
C(4)	C(5)	H(8)	108.10	C(11)	C(10)	H(17)	108.26
C(6)	C(5)	H(7)	108.11	C(11)	C(10)	H(18)	108.26
C(6)	C(5)	H(8)	108.10	H(17)	C(10)	H(18)	109.47
H(7)	C(5)	H(8)	109.46	C(10)	C(11)	H(19)	108.28
C(5)	C(6)	H(9)	108.56	C(10)	C(11)	H(20)	108.28
C(5)	C(6)	H(10)	108.56	C(12)	C(11)	H(19)	108.29
C(7)	C(6)	H(9)	108.56	C(12)	C(11)	H(20)	108.28
C(7)	C(6)	H(10)	108.56	H(19)	C(11)	H(20)	109.47
H(9)	C(6)	H(10)	109.47	C(11)	C(12)	H(21)	108.74
C(6)	C(7)	H(11)	107.98	C(11)	C(12)	H(22)	108.73

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles (cont.)

atom	atom	atom	angle	atom	atom	atom	angle
C(13)	C(12)	H(21)	108.74				
C(13)	C(12)	H(22)	108.73				
H(21)	C(12)	H(22)	109.46				
C(1)*	C(13)	H(23)	108.39				
C(1)*	C(13)	H(24)	108.39				
C(12)	C(13)	H(23)	108.40				
C(12)	C(13)	H(24)	108.41				
H(23)	C(13)	H(24)	109.46				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intra-annular torsion angles

Atoms	Value
C(13)*-C(1)-C(2)-C(3)	163.3(1)
C(1)-C(2)-C(3)-C(4)	-69.0(2)
C(2)-C(3)-C(4)-C(5)	-176.4(1)
C(3)-C(4)-C(5)-C(6)	-175.6(1)
C(4)-C(5)-C(6)-C(7)	176.2(1)
C(5)-C(6)-C(7)-C(8)	-177.0(1)
C(6)-C(7)-C(8)-C(9)	176.8(1)
C(7)-C(8)-C(9)-C(10)	-175.1(1)
C(8)-C(9)-C(10)-C(11)	-65.6(2)
C(9)-C(10)-C(11)-C(12)	-177.9(1)
C(10)-C(11)-C(12)-C(13)	-171.2(1)
C(11)-C(12)-C(13)-C(1)*	58.1(2)
C(12)-C(13)-C(1)*-C(2)*	58.0(2)

Symmetry-related values have the opposite sign.

Torsion or Conformation Angles

(1)	(2)	(3)	(4)	angle
O(1)	C(1)	C(2)	C(3)	-18.5(2)
O(1)	C(1)	C(2)	H(1)	102.34
O(1)	C(1)	C(2)	H(2)	-139.41
O(1)	C(1)	C(13)	C(12)	123.8(2)
O(1)	C(1)	C(13)	H(23)	-115.56
O(1)	C(1)	C(13)	H(24)	3.15
C(1)	C(2)	C(3)	C(4)	-69.0(2)
C(1)	C(2)	C(3)	H(3)	51.60
C(1)	C(2)	C(3)	H(4)	170.34
C(1)*	C(13)	C(12)	C(11)	58.1(2)
C(1)*	C(13)	C(12)	H(21)	-62.39
C(1)*	C(13)	C(12)	H(22)	178.50
C(2)	C(1)	C(13)	C(12)	-58.0(2)
C(2)	C(1)	C(13)	H(23)	62.64
C(2)	C(1)	C(13)	H(24)	-178.65
C(2)	C(3)	C(4)	C(5)	-176.4(1)
C(2)	C(3)	C(4)	H(5)	-55.78
C(2)	C(3)	C(4)	H(6)	62.88
C(3)	C(2)	C(1)	C(13)	163.3(1)
C(3)	C(4)	C(5)	C(6)	-175.6(1)
C(3)	C(4)	C(5)	H(7)	-54.80
C(3)	C(4)	C(5)	H(8)	63.60
C(4)	C(3)	C(2)	H(1)	170.10
C(4)	C(3)	C(2)	H(2)	51.86
C(4)	C(5)	C(6)	C(7)	176.2(1)
C(4)	C(5)	C(6)	H(9)	-63.28
C(4)	C(5)	C(6)	H(10)	55.64
C(5)	C(4)	C(3)	H(3)	62.93
C(5)	C(4)	C(3)	H(4)	-55.81
C(5)	C(6)	C(7)	C(8)	-177.0(1)
C(5)	C(6)	C(7)	H(11)	-56.15
C(5)	C(6)	C(7)	H(12)	62.11
C(6)	C(5)	C(4)	H(5)	63.73
C(6)	C(5)	C(4)	H(6)	-54.93
C(6)	C(7)	C(8)	C(9)	176.8(1)
C(6)	C(7)	C(8)	H(13)	-62.65
C(6)	C(7)	C(8)	H(14)	56.32
C(7)	C(6)	C(5)	H(7)	55.37
C(7)	C(6)	C(5)	H(8)	-63.03
C(7)	C(8)	C(9)	C(10)	-175.1(1)
C(7)	C(8)	C(9)	H(15)	-54.19
C(7)	C(8)	C(9)	H(16)	63.98
C(8)	C(7)	C(6)	H(9)	62.43
C(8)	C(7)	C(6)	H(10)	-56.49
C(8)	C(9)	C(10)	C(11)	-65.6(2)
C(8)	C(9)	C(10)	H(17)	55.15
C(8)	C(9)	C(10)	H(18)	173.72
C(9)	C(8)	C(7)	H(11)	55.95
C(9)	C(8)	C(7)	H(12)	-62.30
C(9)	C(10)	C(11)	C(12)	-177.9(1)
C(9)	C(10)	C(11)	H(19)	-57.22
C(9)	C(10)	C(11)	H(20)	61.39

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Torsion or Conformation Angles (cont.)

(1)	(2)	(3)	(4)	angle
C(10)	C(9)	C(8)	H(13)	64.37
C(10)	C(9)	C(8)	H(14)	-54.60
C(10)	C(11)	C(12)	C(13)	-171.2(1)
C(10)	C(11)	C(12)	H(21)	-50.80
C(10)	C(11)	C(12)	H(22)	68.32
C(11)	C(10)	C(9)	H(15)	173.51
C(11)	C(10)	C(9)	H(16)	55.35
C(11)	C(12)	C(13)	H(23)	178.69
C(11)	C(12)	C(13)	H(24)	-62.58
C(12)	C(11)	C(10)	H(17)	61.37
C(12)	C(11)	C(10)	H(18)	-57.20
C(13)	C(1)	C(2)	H(1)	-75.85
C(13)	C(1)	C(2)	H(2)	42.40
C(13)	C(12)	C(11)	H(19)	68.06
C(13)	C(12)	C(11)	H(20)	-50.55
H(1)	C(2)	C(3)	H(3)	-69.27
H(1)	C(2)	C(3)	H(4)	49.46
H(2)	C(2)	C(3)	H(3)	172.49
H(2)	C(2)	C(3)	H(4)	-68.78
H(3)	C(3)	C(4)	H(5)	-176.41
H(3)	C(3)	C(4)	H(6)	-57.75
H(4)	C(3)	C(4)	H(5)	64.86
H(4)	C(3)	C(4)	H(6)	-176.49
H(5)	C(4)	C(5)	H(7)	-175.47
H(5)	C(4)	C(5)	H(8)	-57.07
H(6)	C(4)	C(5)	H(7)	65.88
H(6)	C(4)	C(5)	H(8)	-175.72
H(7)	C(5)	C(6)	H(9)	175.92
H(7)	C(5)	C(6)	H(10)	-65.16
H(8)	C(5)	C(6)	H(9)	57.52
H(8)	C(5)	C(6)	H(10)	176.43
H(9)	C(6)	C(7)	H(11)	-176.69
H(9)	C(6)	C(7)	H(12)	-58.44
H(10)	C(6)	C(7)	H(11)	64.39
H(10)	C(6)	C(7)	H(12)	-177.36
H(11)	C(7)	C(8)	H(13)	176.47
H(11)	C(7)	C(8)	H(14)	-64.56
H(12)	C(7)	C(8)	H(13)	58.22
H(12)	C(7)	C(8)	H(14)	177.19
H(13)	C(8)	C(9)	H(15)	-174.71
H(13)	C(8)	C(9)	H(16)	-56.55
H(14)	C(8)	C(9)	H(15)	66.32
H(14)	C(8)	C(9)	H(16)	-175.52
H(15)	C(9)	C(10)	H(17)	-65.78
H(15)	C(9)	C(10)	H(18)	52.80
H(16)	C(9)	C(10)	H(17)	176.07
H(16)	C(9)	C(10)	H(18)	-65.36
H(17)	C(10)	C(11)	H(19)	-177.93
H(17)	C(10)	C(11)	H(20)	-59.32
H(18)	C(10)	C(11)	H(19)	63.50
H(18)	C(10)	C(11)	H(20)	-177.90
H(19)	C(11)	C(12)	H(21)	-171.50

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Torsion or Conformation Angles (cont.)

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
H(19)	C(11)	C(12)	H(22)	-52.38					
H(20)	C(11)	C(12)	H(21)	69.90					
H(20)	C(11)	C(12)	H(22)	-170.99					
H(21)	C(12)	C(13)	H(23)	58.24					
H(21)	C(12)	C(13)	H(24)	176.97					
H(22)	C(12)	C(13)	H(23)	-60.87					
H(22)	C(12)	C(13)	H(24)	57.86					

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Intermolecular Distances Involving the Nonhydrogen Atoms

atom	atom	distance	ADC(*)	atom	atom	distance	ADC(*)
O(1)	C(1)	3.313(2)	54502	O(1)	C(2)	3.561(2)	54502
O(1)	C(13)	3.363(2)	54404				

Non-bonded Distances Involving Hydrogen Atoms

atom	atom	distance	ADC(*)	atom	atom	distance	ADC(*)
O(1)	H(23)	2.65	54404	H(1)	O(1)	2.88	2
O(1)	H(1)	2.86	54501	H(3)	O(1)	2.59	1
O(1)	H(1)	2.88	54502	H(5)	O(1)	3.81	1
H(2)	H(19)	2.64	56603	H(6)	O(1)	2.73	1
H(7)	H(17)	2.49	65603	H(19)	O(1)*	3.78	1
H(18)	H(23)	2.62	65602	H(20)	O(1)*	3.09	1
H(19)	H(22)	2.63	65602				

Contacts out to 3.60 angstroms. Estimated standard deviations in the least significant figure are given in parentheses.