Crystal structure of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis-[((*R*)-2-*O*- acetylpropanoyl)oxy]calix[4]arene, $C_{64}H_{80}O_{16}$

S. Ben Sdira[I], M. B. Guidicelli[I], C. Bavoux*,[II], R. Lamartine[I] and M. Perrin[II]

[I] Universite Claude Bernard Lyon 1, CNRS UMR 5078, Laboratoire de Chimie Industrielle, 43 Boulvard du 11 Novembre 1918, 69622 Villeurbanne Cedex, France

[II] Universite Claude Bernard Lyon 1, CNRS UMR 5078, Laboratoire de Cristallographie,43 Boulvard du 11 Novembre 1918, 69622 Villeurbanne Cedex, France

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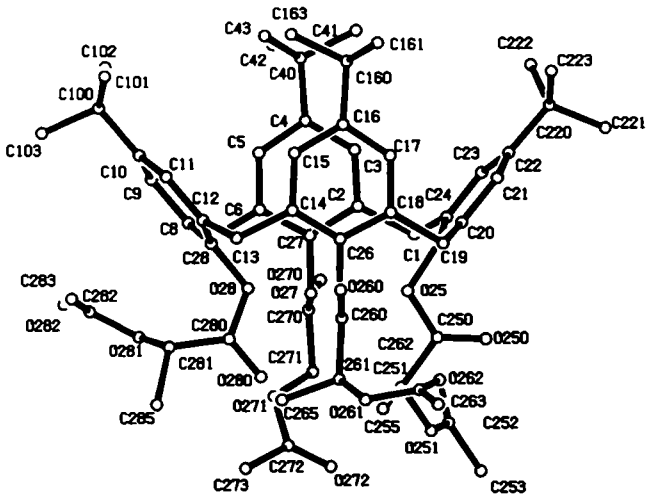

Abstract

$C_{64}H_{80}O_{16}$, monoclinic, $P2_1$ (No. 4), a = 11.534(2) Å, b = 15.352(3) Å, c = 18.568(4) Å, β = 107.09(3)°, V = 3142.7 Å^3, Z = 2, $R_{gt}(F)$ = 0.067, $wR_{ref}(F^2)$ = 0.15, T = 223 K.

Source of material

The title compound is obtained from the reaction of *R-O*-acetyl lacric acid chlorid with *p-tert*-butylcalix[4]arene which yields a chiral cone *p-tert*-butylcalix[4]arene functionalized at the lower rim with *R-O*-acetyl lactic acid unit (3,64 %), with retention of configuration on the asymmetric centre. Only the tetra-substituted product was obtained, as is established via NMR experiments (^{1}H, ^{13}C) and X-ray analysis.

Suitable crystals for X-ray investigation were obtained from slow evaporation of a solution of the title compound in an ether-petrol ether mixture. Because the crystals were very fragil, it was not possible to cut them into smaller ones. Thus, the selected crystal for this study has a large dimension.

Discussion

The calixarene crystallizes in a flattened cone conformation: angles between the best plane of the methylene groups and the two almost parallel rings are 91.6(1)° and 91.0(1)°; with the two splayed outward rings values of 129.4(2)° and 128.5(2)° are obtained. Three diester groups are oriented in the prolongation of the C—O bond; the other one makes a loop and is bent outward of the macrocycle; this orientation is due to the steric hindrance induces by the orientation of the two splayed outward rings.

* Correspondence author (e-mail: bavoux@cdl1lyon.univ-lyon1.fr)

Table 1. Data collection and handling.

Crystal:	colourless plate, size 0.2 × 0.8 × 1.4 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.83 cm^{-1}
Diffractometer, scan mode:	Nonius KappaCCD, 195 images, $\Delta\omega$ = 1.5°
$2\theta_{max}$:	46.14°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	15620, 8760
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 4836
$N(param)_{refined}$:	745
Programs:	SHELXL-97 [1], PLATON[2]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	Occ.	x	y	z	U_{iso}
H(1A)	2*a*		0.4577(5)	0.0283(5)	0.5774(3)	0.062
H(1B)	2*a*		0.4431(5)	−0.0730(5)	0.5843(3)	0.062
H(3)	2*a*		0.4743(5)	−0.1186(4)	0.7273(3)	0.059
H(5)	2*a*		0.7635(5)	−0.0146(4)	0.8755(3)	0.058
H(7A)	2*a*		0.7963(5)	0.1640(4)	0.7617(3)	0.054
H(7B)	2*a*		0.8850(5)	0.1025(4)	0.8206(3)	0.054
H(9)	2*a*		0.8907(5)	0.1088(4)	0.9528(3)	0.050
H(11)	2*a*		0.6546(5)	0.2520(4)	1.0223(3)	0.053
H(13A)	2*a*		0.5067(5)	0.3517(4)	0.8514(3)	0.055
H(13B)	2*a*		0.5038(5)	0.3419(4)	0.9351(3)	0.055
H(15)	2*a*		0.4435(5)	0.1786(4)	0.9612(3)	0.055
H(17)	2*a*		0.1594(5)	0.0821(4)	0.8040(4)	0.059
H(19A)	2*a*		0.0661(5)	0.1849(4)	0.6821(3)	0.062
H(19B)	2*a*		0.1724(5)	0.2258(4)	0.6561(3)	0.062
H(21)	2*a*		0.0390(5)	0.0252(5)	0.6763(3)	0.065
H(23)	2*a*		0.2747(6)	−0.1297(5)	0.6214(3)	0.065
H(41A)	2*a*		0.5075(6)	−0.2363(5)	0.7959(4)	0.125
H(41B)	2*a*		0.4429(6)	−0.1775(5)	0.8415(4)	0.125
H(41C)	2*a*		0.5204(6)	−0.2576(5)	0.8805(4)	0.125
H(42A)	2*a*		0.7075(8)	−0.0783(6)	0.9608(4)	0.129
H(42B)	2*a*		0.6435(8)	−0.1604(6)	0.9820(4)	0.129
H(42C)	2*a*		0.5660(8)	−0.0802(6)	0.9429(4)	0.129
H(43A)	2*a*		0.7367(6)	−0.2348(5)	0.8281(4)	0.113
H(43B)	2*a*		0.7471(6)	−0.2543(5)	0.9127(4)	0.113
H(43C)	2*a*		0.8116(6)	−0.1724(5)	0.8916(4)	0.113
H(10A)	2*a*		0.7462(8)	0.2225(8)	1.1320(4)	0.194
H(10B)	2*a*		0.8159(8)	0.1475(8)	1.1843(4)	0.194
H(10C)	2*a*		0.7000(8)	0.1262(8)	1.1175(4)	0.194
H(10D)	2*a*		0.932(1)	0.0429(7)	1.0571(5)	0.203
H(10E)	2*a*		0.809(1)	0.0204(7)	1.0734(5)	0.203

Table 2. Continued.

Atom	Site	Occ.	x	y	z	U_{iso}
H(10F)	2a		0.925(1)	0.0417(7)	1.1402(5)	0.203
H(10G)	2a		1.0120(9)	0.1958(9)	1.0779(5)	0.227
H(10H)	2a		1.0059(9)	0.1867(9)	1.1608(5)	0.227
H(10I)	2a		0.9402(9)	0.2645(9)	1.1105(5)	0.227
H(16A)	2a		0.0906(6)	0.0642(6)	0.9171(5)	0.142
H(16B)	2a		0.1581(6)	0.1189(6)	0.9884(5)	0.142
H(16C)	2a		0.1425(6)	0.0181(6)	0.9953(5)	0.142
H(16D)	2a		0.2140(8)	−0.0414(5)	0.8620(4)	0.131
H(16E)	2a		0.2600(8)	−0.0845(5)	0.9419(4)	0.131
H(16F)	2a		0.3535(8)	−0.0511(5)	0.9017(4)	0.131
H(16G)	2a		0.3783(6)	0.1046(5)	1.0448(4)	0.117
H(16H)	2a		0.4533(6)	0.0378(5)	1.0128(4)	0.117
H(16I)	2a		0.3598(6)	0.0043(5)	1.0530(4)	0.117
H(22A)	2a		0.017(1)	−0.1664(7)	0.5385(5)	0.229
H(22B)	2a		−0.078(1)	−0.1086(7)	0.5622(5)	0.229
H(22C)	2a		−0.074(1)	−0.2093(7)	0.5767(5)	0.229
H(22D)	2a		0.1990(8)	−0.2120(6)	0.7281(6)	0.184
H(22E)	2a		0.1884(8)	−0.2381(6)	0.6448(6)	0.184
H(22F)	2a		0.0935(8)	−0.2731(6)	0.6833(6)	0.184
H(22G)	2a		0.0502(9)	−0.1235(7)	0.7565(6)	0.187
H(22H)	2a		−0.0536(9)	−0.1835(7)	0.7080(6)	0.187
H(22I)	2a		−0.0580(9)	−0.0828(7)	0.6936(6)	0.187
H(251)	2a		0.4727(6)	0.2331(4)	0.5573(3)	0.061
H(25A)	2a		0.334(1)	0.2639(7)	0.3233(4)	0.172
H(25B)	2a		0.303(1)	0.1651(7)	0.3066(4)	0.172
H(25C)	2a		0.436(1)	0.1987(7)	0.3181(4)	0.172
H(25D)	2a		0.4163(7)	0.3794(5)	0.5488(4)	0.106

Table 2. Continued.

Atom	Site	Occ.	x	y	z	U_{iso}
H(25E)	2a		0.3731(7)	0.3353(5)	0.6126(4)	0.106
H(25F)	2a		0.2798(7)	0.3535(5)	0.5337(4)	0.106
O(260)	2a		0.2153(6)	0.4026(5)	0.7990(4)	0.113(2)
H(261)	2a		0.2835(6)	0.4408(5)	0.6532(4)	0.072
H(26D)	2a		0.3906(7)	0.5664(6)	0.7007(7)	0.200
H(26E)	2a		0.4585(7)	0.4852(6)	0.7447(7)	0.200
H(26F)	2a		0.3811(7)	0.5450(6)	0.7813(7)	0.200
H(26A)	2a	0.5	−0.001(2)	0.597(2)	0.687(2)	0.118
H(26B)	2a	0.5	−0.097(2)	0.522(2)	0.664(2)	0.118
H(26C)	2a	0.5	−0.068(2)	0.578(2)	0.601(2)	0.118
H(46A)	2a	0.5	0.004(3)	0.606(3)	0.616(5)	0.255
H(46B)	2a	0.5	−0.096(3)	0.540(3)	0.622(5)	0.255
H(46C)	2a	0.5	−0.046(3)	0.536(3)	0.553(5)	0.255
H(271)	2a		0.6435(7)	0.1367(6)	0.5082(4)	0.083
H(27A)	2a		0.8077(9)	0.3583(6)	0.6213(5)	0.168
H(27B)	2a		0.6894(9)	0.4045(6)	0.5727(5)	0.168
H(27C)	2a		0.8031(9)	0.3987(6)	0.5430(5)	0.168
H(27D)	2a		0.8179(8)	0.1419(6)	0.4683(5)	0.149
H(27E)	2a		0.7912(8)	0.0450(6)	0.4850(5)	0.149
H(27F)	2a		0.8935(8)	0.0972(6)	0.5433(5)	0.149
H(281)	2a		0.7289(6)	0.3898(4)	0.8598(4)	0.072
H(28A)	2a		1.0416(6)	0.2725(6)	0.8404(4)	0.123
H(28B)	2a		1.0653(6)	0.2510(6)	0.9261(4)	0.123
H(28C)	2a		1.1203(6)	0.3356(6)	0.9019(4)	0.123
H(28D)	2a		0.8139(7)	0.5130(5)	0.8191(5)	0.141
H(28E)	2a		0.6745(7)	0.5100(5)	0.7772(5)	0.141
H(28F)	2a		0.7681(7)	0.4805(5)	0.7355(5)	0.141

Table 3. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	Occ.	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(25)	2a		0.3450(3)	0.1506(3)	0.6198(2)	0.050(2)	0.040(3)	0.043(2)	−0.003(2)	−0.001(2)	0.003(2)
O(26)	2a		0.3239(3)	0.3206(3)	0.7453(2)	0.046(2)	0.039(3)	0.059(3)	0.010(2)	0.013(2)	0.007(2)
O(27)	2a		0.6467(4)	0.1026(3)	0.6487(2)	0.050(2)	0.047(3)	0.045(2)	−0.002(2)	0.009(2)	0.001(2)
O(28)	2a		0.6181(3)	0.2549(3)	0.7786(2)	0.046(2)	0.056(3)	0.041(2)	−0.004(2)	−0.001(2)	0.008(2)
C(1)	2a		0.4423(5)	−0.0176(5)	0.6093(3)	0.060(4)	0.046(4)	0.042(3)	0.004(3)	0.004(3)	−0.005(3)
C(2)	2a		0.5408(5)	−0.0169(4)	0.6858(3)	0.040(3)	0.042(4)	0.049(4)	0.000(3)	0.009(3)	−0.003(4)
C(3)	2a		0.5373(5)	−0.0782(4)	0.7390(3)	0.041(3)	0.041(4)	0.064(4)	−0.002(3)	0.012(3)	0.000(4)
C(4)	2a		0.6237(5)	−0.0832(4)	0.8103(3)	0.042(3)	0.032(4)	0.053(4)	0.002(3)	0.006(3)	0.001(3)
C(5)	2a		0.7084(5)	−0.0162(4)	0.8275(3)	0.047(4)	0.053(5)	0.038(3)	−0.002(4)	0.003(3)	−0.002(4)
C(6)	2a		0.7148(5)	0.0483(4)	0.7768(3)	0.036(3)	0.044(4)	0.054(4)	0.001(3)	0.008(3)	−0.003(4)
C(7)	2a		0.8023(5)	0.1240(4)	0.8031(3)	0.043(3)	0.044(4)	0.048(4)	−0.002(3)	0.010(3)	0.006(3)
C(8)	2a		0.7693(5)	0.1703(4)	0.8669(3)	0.040(3)	0.046(4)	0.046(4)	−0.012(3)	0.012(3)	0.002(3)
C(9)	2a		0.8244(5)	0.1462(4)	0.9420(3)	0.033(3)	0.045(4)	0.047(4)	0.003(3)	0.010(3)	−0.003(3)
C(10)	2a		0.7831(5)	0.1766(4)	1.0018(3)	0.038(3)	0.045(4)	0.041(3)	−0.004(3)	0.007(3)	0.003(3)
C(11)	2a		0.6840(5)	0.2317(4)	0.9838(3)	0.036(3)	0.057(5)	0.038(3)	−0.007(3)	0.010(3)	−0.007(3)
C(12)	2a		0.6261(5)	0.2581(4)	0.9097(3)	0.039(3)	0.042(4)	0.050(4)	−0.002(3)	0.006(3)	−0.003(3)
C(13)	2a		0.5085(5)	0.3100(4)	0.8909(3)	0.046(3)	0.043(4)	0.049(4)	−0.003(3)	0.014(3)	0.006(3)
C(14)	2a		0.4001(5)	0.2479(4)	0.8648(3)	0.040(3)	0.045(4)	0.047(4)	0.005(3)	0.015(3)	0.001(3)
C(15)	2a		0.3878(5)	0.1820(4)	0.9135(3)	0.039(3)	0.047(4)	0.052(4)	0.007(3)	0.014(3)	0.004(4)
C(16)	2a		0.2948(5)	0.1210(4)	0.8931(3)	0.038(3)	0.037(4)	0.054(4)	0.006(3)	0.014(3)	0.000(3)
C(17)	2a		0.2194(5)	0.1244(4)	0.8195(4)	0.043(3)	0.036(4)	0.070(4)	−0.002(3)	0.020(3)	0.002(4)
C(18)	2a		0.2283(5)	0.1872(4)	0.7678(3)	0.037(3)	0.044(4)	0.052(4)	0.005(3)	0.009(3)	0.006(4)
C(19)	2a		0.1515(5)	0.1798(4)	0.6859(3)	0.041(3)	0.045(4)	0.059(4)	0.001(3)	0.001(3)	0.008(4)
C(20)	2a		0.1771(5)	0.0923(4)	0.6578(3)	0.042(4)	0.041(4)	0.039(3)	0.003(3)	−0.003(3)	0.001(3)
C(21)	2a		0.1096(5)	0.0180(5)	0.6625(3)	0.038(3)	0.055(5)	0.060(4)	−0.001(4)	0.002(3)	0.003(4)
C(22)	2a		0.1413(6)	−0.0646(5)	0.6479(4)	0.044(4)	0.041(5)	0.061(4)	−0.004(4)	−0.008(3)	0.004(4)
C(23)	2a		0.2492(6)	−0.0740(5)	0.6294(3)	0.049(4)	0.040(4)	0.058(4)	−0.004(3)	−0.007(3)	0.000(3)
C(24)	2a		0.3194(5)	−0.0035(4)	0.6226(3)	0.039(3)	0.041(5)	0.041(3)	−0.004(3)	−0.005(3)	0.002(3)
C(25)	2a		0.2798(6)	0.0778(4)	0.6339(3)	0.050(4)	0.039(5)	0.046(4)	−0.011(4)	0.001(3)	0.000(3)
C(26)	2a		0.3178(5)	0.2519(4)	0.7942(3)	0.041(3)	0.035(4)	0.050(4)	0.003(3)	0.010(3)	0.008(3)
C(27)	2a		0.6323(5)	0.0439(4)	0.7047(3)	0.040(3)	0.043(4)	0.046(4)	0.010(3)	0.013(3)	0.006(3)
C(28)	2a		0.6740(5)	0.2293(4)	0.8540(3)	0.040(3)	0.040(4)	0.040(4)	0.003(3)	−0.001(3)	0.002(3)
C(40)	2a		0.6258(5)	−0.1540(5)	0.8689(4)	0.048(4)	0.048(4)	0.064(4)	−0.001(3)	0.017(3)	0.012(4)
C(41)	2a		0.5138(6)	−0.2117(5)	0.8445(4)	0.076(5)	0.081(7)	0.084(5)	−0.001(5)	0.010(4)	0.031(5)

Table 3. Continued.

Atom	Site	Occ.	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(42)	2a		0.6367(8)	−0.1146(6)	0.9457(4)	0.107(6)	0.091(7)	0.066(5)	−0.013(5)	0.035(4)	0.007(5)
C(43)	2a		0.7413(6)	−0.2091(5)	0.8760(4)	0.072(5)	0.065(6)	0.088(5)	0.022(4)	0.023(4)	0.034(5)
C(100)	2a		0.8479(5)	0.1494(5)	1.0828(3)	0.046(3)	0.063(5)	0.044(4)	0.007(3)	0.007(3)	0.002(3)
C(101)	2a		0.7706(8)	0.1626(8)	1.1337(4)	0.094(6)	0.24(1)	0.069(5)	0.052(8)	0.039(5)	0.059(7)
C(102)	2a		0.881(1)	0.0552(7)	1.0889(5)	0.22(1)	0.092(8)	0.065(6)	0.047(9)	0.003(6)	0.000(6)
C(103)	2a		0.9620(9)	0.2041(9)	1.1106(5)	0.128(8)	0.21(1)	0.076(6)	−0.091(9)	−0.028(6)	0.030(7)
C(160)	2a		0.2776(5)	0.0486(4)	0.9461(3)	0.052(4)	0.044(5)	0.054(4)	0.004(3)	0.014(3)	0.012(4)
C(161)	2a		0.1556(6)	0.0639(6)	0.9634(5)	0.066(5)	0.111(8)	0.124(7)	0.013(5)	0.056(5)	0.045(6)
C(162)	2a		0.2761(8)	−0.0403(5)	0.9096(4)	0.118(7)	0.047(5)	0.078(5)	0.009(5)	−0.002(5)	0.009(4)
C(163)	2a		0.3763(6)	0.0488(5)	1.0211(4)	0.076(5)	0.066(6)	0.086(5)	−0.007(4)	0.013(4)	0.026(5)
C(220)	2a		0.0634(6)	−0.1446(5)	0.6511(4)	0.062(4)	0.053(5)	0.079(5)	−0.017(4)	0.009(4)	0.016(4)
C(221)	2a		−0.026(1)	−0.1585(7)	0.5754(5)	0.18(1)	0.13(1)	0.101(7)	−0.104(9)	−0.034(7)	0.021(7)
C(222)	2a		0.1436(8)	−0.2244(6)	0.6795(6)	0.090(6)	0.067(7)	0.21(1)	−0.011(5)	0.034(7)	0.042(7)
C(223)	2a		−0.0058(9)	−0.1325(7)	0.7074(6)	0.123(8)	0.090(8)	0.17(1)	−0.049(7)	0.051(7)	0.008(7)
C(250)	2a		0.3047(6)	0.1802(4)	0.5478(4)	0.046(4)	0.038(4)	0.055(4)	0.002(3)	0.002(3)	0.002(4)
O(250)	2a		0.2140(4)	0.1565(4)	0.5027(3)	0.060(3)	0.101(5)	0.061(3)	−0.017(3)	−0.011(3)	0.016(3)
C(251)	2a		0.3880(6)	0.2490(4)	0.5326(3)	0.056(4)	0.044(5)	0.046(4)	0.002(3)	0.005(3)	0.006(3)
O(251)	2a		0.3680(4)	0.2567(3)	0.4528(2)	0.084(3)	0.049(3)	0.053(3)	0.001(3)	0.016(2)	0.010(3)
C(252)	2a		0.3936(8)	0.1880(6)	0.4165(4)	0.095(6)	0.059(6)	0.058(5)	−0.011(5)	0.018(4)	−0.001(5)
O(252)	2a		0.4329(5)	0.1213(4)	0.4474(3)	0.093(4)	0.071(4)	0.073(4)	0.007(3)	0.012(3)	−0.002(3)
C(253)	2a		0.364(1)	0.2055(7)	0.3337(4)	0.179(9)	0.108(8)	0.064(5)	0.001(7)	0.044(6)	−0.008(6)
C(255)	2a		0.3620(7)	0.3373(5)	0.5594(4)	0.089(5)	0.056(5)	0.061(4)	0.002(4)	0.015(4)	−0.002(4)
C(260)	2a		0.2658(7)	0.3927(5)	0.7508(4)	0.079(5)	0.047(5)	0.068(5)	0.012(4)	0.033(4)	0.014(4)
C(261)	2a		0.2772(6)	0.4652(5)	0.7007(4)	0.070(5)	0.043(5)	0.071(4)	0.013(4)	0.024(4)	0.011(4)
C(265)	2a		0.3867(7)	0.5204(6)	0.7349(7)	0.057(5)	0.069(7)	0.25(1)	0.006(5)	0.015(7)	0.037(8)
O(261)	2a		0.1757(4)	0.5222(3)	0.6848(3)	0.066(3)	0.036(3)	0.084(3)	0.004(3)	0.004(3)	0.006(3)
C(262)	2a		0.0695(9)	0.4853(8)	0.6468(7)	0.078(6)	0.067(8)	0.15(1)	−0.002(6)	−0.029(6)	−0.001(8)
O(262)	2a	0.5	0.081(4)	0.420(2)	0.614(2)	0.20(3)	0.06(2)	0.11(2)	−0.04(2)	0.00(1)	−0.02(1)
C(263)	2a	0.5	−0.035(2)	0.552(2)	0.650(2)	0.06(1)	0.05(1)	0.10(2)	−0.008(9)	−0.02(1)	0.01(1)
C(463)	2a	0.5	−0.025(3)	0.547(3)	0.606(5)	0.12(2)	0.13(3)	0.23(5)	0.06(2)	0.01(3)	0.11(3)
O(462)	2a	0.5	0.051(2)	0.405(2)	0.642(3)	0.08(1)	0.04(1)	0.22(3)	−0.023(8)	−0.03(1)	0.04(1)
C(270)	2a		0.7157(8)	0.0697(7)	0.6074(5)	0.070(6)	0.102(9)	0.082(6)	0.029(6)	0.037(5)	0.041(6)
O(270)	2a	0.57	0.735(5)	−0.010(1)	0.601(2)	0.16(3)	0.06(1)	0.11(2)	0.05(1)	0.09(2)	0.02(1)
O(470)	2a	0.43	0.804(4)	0.028(4)	0.644(3)	0.11(2)	0.13(3)	0.12(3)	0.08(2)	0.07(2)	0.07(3)
C(271)	2a		0.7234(7)	0.1322(6)	0.5456(4)	0.069(5)	0.077(6)	0.065(5)	−0.002(4)	0.023(4)	0.024(5)
O(271)	2a		0.7584(4)	0.2164(4)	0.5787(3)	0.081(3)	0.074(4)	0.062(3)	−0.016(3)	0.017(2)	0.008(3)
C(272)	2a		0.7130(8)	0.2864(6)	0.5344(5)	0.084(6)	0.066(7)	0.083(6)	−0.011(5)	0.040(5)	0.020(6)
O(272)	2a		0.6477(5)	0.2776(4)	0.4713(4)	0.099(4)	0.094(5)	0.110(5)	−0.013(4)	−0.005(4)	0.044(4)
C(273)	2a		0.7571(9)	0.3690(6)	0.5710(5)	0.141(8)	0.081(8)	0.121(8)	−0.024(7)	0.050(6)	0.002(7)
C(275)	2a		0.8149(8)	0.1013(6)	0.5070(5)	0.124(7)	0.107(8)	0.086(6)	0.017(6)	0.060(6)	0.028(6)
C(280)	2a		0.6478(6)	0.3341(5)	0.7569(4)	0.060(4)	0.055(5)	0.061(5)	−0.001(4)	0.013(4)	0.021(4)
O(280)	2a		0.5964(5)	0.3572(4)	0.6933(3)	0.086(4)	0.124(5)	0.072(3)	−0.020(4)	−0.001(3)	0.043(4)
C(281)	2a		0.7452(6)	0.3879(4)	0.8110(4)	0.048(4)	0.046(5)	0.079(5)	0.005(4)	0.009(3)	0.011(4)
O(281)	2a		0.8572(4)	0.3430(3)	0.8196(2)	0.048(3)	0.068(3)	0.060(3)	−0.001(2)	0.018(2)	−0.001(3)
C(282)	2a		0.9407(6)	0.3462(5)	0.8895(5)	0.058(4)	0.046(5)	0.072(5)	−0.009(4)	0.012(4)	−0.004(4)
O(282)	2a		0.9214(5)	0.3848(4)	0.9405(3)	0.081(4)	0.089(5)	0.077(4)	−0.001(3)	0.015(3)	−0.019(3)
C(283)	2a		1.0518(6)	0.2970(6)	0.8895(4)	0.047(4)	0.097(7)	0.098(6)	−0.007(5)	0.014(4)	−0.009(5)
C(285)	2a		0.7510(7)	0.4816(5)	0.7831(5)	0.085(6)	0.063(6)	0.124(7)	−0.007(5)	0.018(5)	0.035(5)

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