Crystal structure of 5,11,17,23-tetra-*t*-butyl-25,27-dihydroxy-26,28-di-tosyl-oxy-calix[4]arene, $C_{58}H_{68}O_8S_2$

E. F. Paulus*,[I], W. Joswig[I], V. Böhmer[II], M. Saadioui[II], M. Krilow[#,I], M. Peikert-Regelien[#,I] and B. Urschel[#,I]

[I] Johann Wolfgang Goethe-Universität, Institut für Mineralogie/Kristallographie, Senckenberganlage 30, D-60325 Frankfurt/Main, Germany
[II] Johannes Gutenberg-Universität, Fachbereich Chemie und Pharmazie, Abteilung Lehramt Chemie, Duisbergweg 10-14, D-55099 Mainz, Germany

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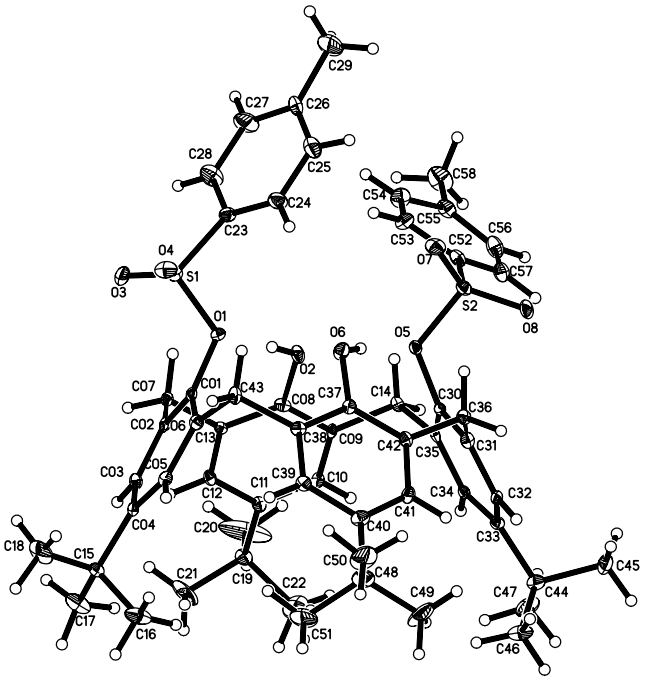

Abstract

$C_{58}H_{68}O_8S_2$, monoclinic, *C*1*c*1 (No. 9), a = 23.888(5) Å, b = 11.225(2) Å, c = 21.431(4) Å, β = 112.41(3)°, V = 5312.7 Å^3, Z = 4, $R_{gt(F)}$ = 0.041, $wR_{ref(F^2)}$ = 0.105, T = 293 K.

Source of material

To a solution of p-*tert*-butylcalix[4]arene (3 g, 4.61 mmol) and tosyl chloride (8.78 g, 46.1 mmol) in dichloromethane (70 mL) was added triethylamine (5 mL). After 24 h of stirring at room temperature the precipitate was filtered and carefully washed with methanol to remove the triethylamine hydrochloride (yield 78 % of a white powder; mp 553 K – 554 K). Single crystals were grown by slow evaporation of a solution in dichloromethane/ethanol.

Experimental details

The average I/σ of the measured X-ray intensities is 33.8. The largest difference peak and hole were 0.205 e/Å^3 and –0.173 e/Å^3, respectively. Nevertheless the measurement is 100% complete for θ = 19.97°, the ratio *N(hkl)/N(param)* is only 3.50 for $I > 2\sigma(I)$ and 4.10 for all the reflections as usual for non-centrosymmetric structures. With such a large molecule and such a small crystal it is not worthwhile to measure to higher theta, because the reflections are relatively weak. The Flack parameter of -0.04(14) is significant, what means that our measurements are accurate enough.

Discussion

Although easy to prepare, the title compound was not found in the literature. Similar 1,3-ditosylates were described only for the p-unsubstituted calix[4]arene [1] and for tetrathia *t*-butyl calix[4]arene [2].The crystal structure might be compared with that of the ditosylate of the analogous tetra-thia-calix[4]arene [2-4], whose molecule lies on a crystallographic twofold axis. The differences in the size and shape of the calix[4]arene skeletons can be characterized by the diagonals and the sides of the quadrilaterals of the four bridging sulphur atoms (7.81 Å and 8.97 Å, 5.538 Å and 5.505 Å) and of the analogous four bridging methylenes(7.125 Å and 7.268 Å, 5.080 Å, 5.097 Å, 5.076 Å and 5.115 Å); further on are the lengths of the four sides (2.819 Å, 2.810 Å, 2.805 Å, 2.983 Å) and of the two diagonals (4.322 Å, 3.695 Å) of the quadrilateral of the four phenolic oxygens in the present compound much more similar to those in a regular square (with the fixed intramolecular hydrogen bonds O2H···O1 [2.819 Å] and O6H···O5 [2.805 Å]) than this is the case in the thia-compound (sides: 3.564 Å, 2.997 Å; diagonals: 5.380 Å, 3.681 Å). The discussed distances are at least partly the reason and the result of quite different conformations of the two calixarenes. The dihedral angles between the least square plane of the four bridging sulphur atoms and the four phenolic rings are extremely different (89.2° and 40.7°) in the thia-compound, whereas in the present study these angles are much more similar (64.8°, 50.7°, 58.4°, 57.1°). Only in the former case the oxygen quadrangular is wide enough, that one of the dihedral angles can be as small as 40.7°, which results into a diagonal oxygen —oxygen distance of 3.680 Å. Strong differences show the relative positions of the two tosyl rings. In the thia-compound they have a dihedral angle of 97.0° with one another, whereas in the other case this dihedral angle is 36.5°, what is achieved by turning one tosyl group around O1—S1 by about 80°: The narrow rim is barred, the tosyl group closes it like a lid. These conformations together with the smaller diameter of the narrow rim do not allow to form channels with disordered dichloro-methane molecules like in the thia-compound [2]. Of course, it is an open question, whether such large conformational differences should be at least partly preformed in solution (a solution memory effect?). The average e.s.d. for a C—C bond is 0.008 Å, for a C—O bond 0.006 Å, for a C—S bond 0.005 Å, for an O—S bond 0.004 Å and for the O—H bond 0.05 Å, for bond angles 0.4° and for torsion angles 0.5°.

* Correspondence author (e-mail: e.paulus@kristall.uni-frankfurt.de)
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Table 1. Data collection and handling.

Crystal:	colourless block, size 0.1 × 0.1 × 0.4 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	1.53 cm^{-1}
Diffractometer, scan mode:	Nonius CAD4, $\omega/2\theta$
$2\theta_{max}$:	39.94°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4958, 2571
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2192
$N(param)_{refined}$:	634
Programs:	SHELXS-97 [5], SHELXL-97 [6], SHELXTL-plus [7]

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(03A)	4*a*	0.8960	0.3161	0.8674	0.045
H(05A)	4*a*	1.0508	0.3260	0.8422	0.047
H(07A)	4*a*	0.8308	0.4944	0.8459	0.041
H(07B)	4*a*	0.8412	0.5965	0.8015	0.041
H(10A)	4*a*	0.6766	0.3215	0.5928	0.040
H(12A)	4*a*	0.7652	0.3296	0.7926	0.045
H(14A)	4*a*	0.7357	0.5856	0.5572	0.044
H(14B)	4*a*	0.6861	0.4888	0.5232	0.044
H(16A)	4*a*	1.0374	0.0283	0.8921	0.143
H(16B)	4*a*	1.0597	0.1364	0.8613	0.143
H(16C)	4*a*	0.9946	0.0841	0.8233	0.143
H(17A)	4*a*	0.9628	0.0466	0.9351	0.140
H(17B)	4*a*	0.9156	0.1150	0.8738	0.140
H(17C)	4*a*	0.9364	0.1687	0.9467	0.140
H(18A)	4*a*	1.0362	0.2822	0.9928	0.222
H(18B)	4*a*	1.0836	0.2533	0.9606	0.222
H(18C)	4*a*	1.0632	0.1535	0.9987	0.222
H(20A)	4*a*	0.5856	0.1930	0.6851	0.345
H(20B)	4*a*	0.6001	0.3059	0.6509	0.345
H(20C)	4*a*	0.6159	0.3045	0.7290	0.345
H(21A)	4*a*	0.7004	0.1907	0.8033	0.203
H(21B)	4*a*	0.7411	0.1200	0.7735	0.203
H(21C)	4*a*	0.6770	0.0710	0.7644	0.203
H(22A)	4*a*	0.6558	0.0384	0.6632	0.262
H(22B)	4*a*	0.6999	0.1081	0.6377	0.262
H(22C)	4*a*	0.6303	0.1357	0.6069	0.262
H(24A)	4*a*	0.9663	0.8397	0.7018	0.084
H(25A)	4*a*	0.9279	1.0033	0.6340	0.105
H(27A)	4*a*	0.8271	1.0849	0.7347	0.118
H(28A)	4*a*	0.8579	0.9159	0.7985	0.102
H(29A)	4*a*	0.8822	1.2472	0.6670	0.224
H(29B)	4*a*	0.8159	1.1980	0.6350	0.224
H(29C)	4*a*	0.8610	1.1762	0.5989	0.224
H(32A)	4*a*	0.8709	0.2828	0.4538	0.044
H(34A)	4*a*	0.7174	0.2976	0.4863	0.042
H(36A)	4*a*	0.9259	0.5641	0.5160	0.047
H(36B)	4*a*	0.9388	0.4516	0.4803	0.047
H(39A)	4*a*	1.0910	0.3272	0.7423	0.056
H(41A)	4*a*	0.9958	0.2877	0.5463	0.051
H(43A)	4*a*	1.0821	0.5100	0.7994	0.047
H(43B)	4*a*	1.0322	0.6044	0.7614	0.047
H(45A)	4*a*	0.7277	0.2545	0.3277	0.135
H(45B)	4*a*	0.7493	0.1273	0.3166	0.135
H(45C)	4*a*	0.7966	0.2302	0.3450	0.135
H(46A)	4*a*	0.7991	–0.0030	0.4135	0.136
H(46B)	4*a*	0.8215	0.0485	0.4870	0.136
H(46C)	4*a*	0.8505	0.0934	0.4367	0.136
H(47A)	4*a*	0.6771	0.1771	0.4012	0.131
H(47B)	4*a*	0.7117	0.0902	0.4607	0.131
H(47C)	4*a*	0.6941	0.0487	0.3858	0.131
H(49A)	4*a*	1.0817	0.0295	0.5878	0.248
H(49B)	4*a*	1.0656	0.1485	0.5464	0.248
H(49C)	4*a*	1.0182	0.0889	0.5709	0.248
H(50A)	4*a*	1.1750	0.1440	0.6628	0.187
H(50B)	4*a*	1.1645	0.2647	0.6935	0.187
H(50C)	4*a*	1.1483	0.2538	0.6156	0.187
H(51A)	4*a*	1.0568	0.0574	0.7019	0.204
H(51B)	4*a*	1.1047	0.1495	0.7465	0.204
H(51C)	4*a*	1.1254	0.0410	0.7144	0.204
H(53A)	4*a*	0.7938	0.8637	0.5874	0.070
H(54A)	4*a*	0.6997	0.9362	0.5806	0.083
H(56A)	4*a*	0.6177	0.7780	0.4043	0.083
H(57A)	4*a*	0.7091	0.7014	0.4081	0.068
H(58A)	4*a*	0.5875	1.0049	0.4685	0.159
H(58B)	4*a*	0.5908	0.9292	0.5312	0.159
H(58C)	4*a*	0.5576	0.8783	0.4582	0.159
H(2)	4*a*	0.8430	0.6100	0.7000	0.040
H(6)	4*a*	0.9290	0.6080	0.6230	0.090

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

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(01)	4*a*	0.9452(2)	0.5209(4)	0.7990(2)	0.033(2)	0.036(3)	0.020(2)	–0.005(2)	0.005(2)	–0.003(2)
C(02)	4*a*	0.9046(2)	0.4626(4)	0.8207(2)	0.036(2)	0.044(3)	0.015(2)	–0.007(2)	0.008(2)	–0.006(2)
C(03)	4*a*	0.9227(2)	0.3558(4)	0.8526(2)	0.037(2)	0.047(3)	0.033(2)	–0.002(2)	0.019(2)	0.003(2)
C(04)	4*a*	0.9770(2)	0.3034(4)	0.8641(2)	0.046(3)	0.038(3)	0.024(2)	–0.003(2)	0.014(2)	–0.002(2)
C(05)	4*a*	1.0140(2)	0.3611(4)	0.8370(2)	0.035(2)	0.046(3)	0.035(3)	0.002(2)	0.012(2)	–0.007(2)
C(06)	4*a*	0.9989(2)	0.4684(4)	0.8024(2)	0.031(3)	0.044(3)	0.036(3)	–0.003(2)	0.005(2)	–0.002(2)
C(07)	4*a*	0.8412(2)	0.5108(4)	0.8072(2)	0.039(2)	0.039(3)	0.031(2)	–0.006(2)	0.021(2)	–0.003(2)
C(08)	4*a*	0.7829(2)	0.4991(4)	0.6794(2)	0.039(2)	0.033(3)	0.059(3)	0.002(2)	0.042(2)	0.006(2)
C(09)	4*a*	0.7383(2)	0.4491(4)	0.6218(2)	0.023(2)	0.040(3)	0.019(2)	0.006(2)	0.001(2)	–0.002(2)
C(10)	4*a*	0.7056(2)	0.3559(4)	0.6309(2)	0.025(2)	0.045(3)	0.030(3)	–0.010(2)	0.012(2)	–0.004(2)
C(11)	4*a*	0.7128(2)	0.3099(4)	0.6924(2)	0.033(2)	0.046(3)	0.036(3)	–0.005(2)	0.012(2)	0.003(2)
C(12)	4*a*	0.7586(2)	0.3606(4)	0.7502(2)	0.041(2)	0.046(3)	0.033(3)	0.001(2)	0.021(2)	0.006(2)
C(13)	4*a*	0.7936(2)	0.4556(4)	0.7446(2)	0.029(2)	0.028(3)	0.035(2)	0.002(2)	0.018(2)	0.004(2)
C(14)	4*a*	0.7281(2)	0.5006(4)	0.5528(2)	0.034(2)	0.044(3)	0.030(3)	0.002(2)	0.012(2)	0.008(2)
C(15)	4*a*	0.9997(2)	0.1883(4)	0.9054(2)	0.060(3)	0.038(3)	0.044(3)	–0.003(3)	0.019(3)	0.007(3)
C(16)	4*a*	1.0253(3)	0.1009(5)	0.8669(4)	0.113(4)	0.054(4)	0.150(5)	0.024(4)	0.084(4)	0.030(4)
C(17)	4*a*	0.9491(3)	0.1238(6)	0.9162(4)	0.092(4)	0.077(4)	0.120(5)	0.014(4)	0.051(4)	0.043(4)
C(18)	4*a*	1.0503(4)	0.2224(7)	0.9702(4)	0.167(8)	0.105(6)	0.076(5)	–0.012(6)	–0.061(5)	0.040(5)
C(19)	4*a*	0.6728(2)	0.2093(5)	0.7018(3)	0.040(3)	0.051(3)	0.054(3)	–0.018(3)	0.012(2)	0.004(3)
C(20)	4*a*	0.6136(3)	0.2572(7)	0.6908(7)	0.115(4)	0.094(6)	0.55(1)	0.001(5)	0.204(6)	0.107(7)

Table 3. Continued.

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(21)	4*a*	0.7002(4)	0.1417(6)	0.7665(4)	0.140(6)	0.116(5)	0.115(6)	–0.066(5)	0.009(5)	0.070(5)
C(22)	4*a*	0.6639(5)	0.1139(7)	0.6473(5)	0.318(9)	0.102(6)	0.149(7)	–0.124(6)	0.139(6)	–0.042(5)
C(23)	4*a*	0.9171(2)	0.8617(4)	0.7572(3)	0.050(3)	0.040(3)	0.055(3)	0.004(3)	0.023(3)	–0.001(3)
C(24)	4*a*	0.9377(3)	0.8881(5)	0.7089(3)	0.094(4)	0.053(4)	0.080(4)	0.018(3)	0.053(3)	0.011(3)
C(25)	4*a*	0.9158(3)	0.9891(6)	0.6697(3)	0.118(5)	0.087(5)	0.066(4)	0.007(4)	0.046(4)	0.019(4)
C(26)	4*a*	0.8778(3)	1.0677(6)	0.6807(3)	0.114(5)	0.074(4)	0.035(3)	0.013(4)	0.015(3)	0.016(3)
C(27)	4*a*	0.8558(3)	1.0360(6)	0.7281(4)	0.092(4)	0.076(5)	0.119(6)	0.043(4)	0.032(4)	0.028(4)
C(28)	4*a*	0.8741(3)	0.9350(6)	0.7666(4)	0.077(4)	0.092(5)	0.107(5)	0.005(4)	0.058(3)	0.025(4)
C(29)	4*a*	0.8574(4)	1.1828(7)	0.6418(5)	0.221(9)	0.090(5)	0.121(7)	0.076(6)	0.048(6)	0.041(5)
C(30)	4*a*	0.8232(2)	0.4918(4)	0.5244(2)	0.039(3)	0.032(3)	0.025(2)	–0.004(2)	0.011(2)	0.002(2)
C(31)	4*a*	0.8641(2)	0.4328(5)	0.5027(2)	0.033(2)	0.052(3)	0.037(3)	0.010(2)	0.019(2)	0.005(3)
C(32)	4*a*	0.8452(2)	0.3241(4)	0.4697(2)	0.048(3)	0.036(3)	0.027(2)	0.008(2)	0.017(2)	–0.002(2)
C(33)	4*a*	0.7881(2)	0.2755(4)	0.4600(2)	0.037(3)	0.034(3)	0.040(3)	0.000(2)	0.017(2)	0.003(2)
C(34)	4*a*	0.7532(2)	0.3334(4)	0.4886(2)	0.047(3)	0.033(3)	0.028(2)	–0.009(2)	0.017(2)	0.003(2)
C(35)	4*a*	0.7687(2)	0.4437(4)	0.5208(2)	0.032(2)	0.053(3)	0.023(2)	0.009(2)	0.015(2)	0.015(2)
C(36)	4*a*	0.9266(2)	0.4777(4)	0.5164(2)	0.043(3)	0.043(3)	0.042(3)	0.001(2)	0.028(2)	0.004(2)
C(37)	4*a*	0.9856(2)	0.4979(4)	0.6435(2)	0.017(2)	0.041(3)	0.034(3)	0.002(2)	0.008(2)	–0.001(2)
C(38)	4*a*	1.0286(2)	0.4563(4)	0.7026(2)	0.032(2)	0.038(3)	0.048(3)	0.000(2)	0.027(2)	0.000(2)
C(39)	4*a*	1.0608(2)	0.3531(5)	0.7025(3)	0.051(3)	0.045(3)	0.046(3)	–0.001(3)	0.020(2)	0.002(3)
C(40)	4*a*	1.0479(2)	0.2869(5)	0.6422(3)	0.038(3)	0.047(3)	0.065(4)	0.009(3)	0.018(3)	–0.004(3)
C(41)	4*a*	1.0050(2)	0.3306(5)	0.5861(2)	0.043(3)	0.055(3)	0.037(3)	0.004(3)	0.022(2)	–0.006(2)
C(42)	4*a*	0.9734(2)	0.4356(4)	0.5835(2)	0.032(2)	0.049(3)	0.036(3)	0.004(2)	0.022(2)	0.006(2)
C(43)	4*a*	1.0401(2)	0.5199(5)	0.7694(2)	0.028(2)	0.060(3)	0.034(3)	–0.005(3)	0.017(2)	0.000(3)
C(44)	4*a*	0.7676(2)	0.1622(5)	0.4171(3)	0.054(3)	0.044(3)	0.061(4)	–0.003(3)	0.020(3)	–0.005(3)
C(45)	4*a*	0.7596(3)	0.1968(6)	0.3448(3)	0.138(5)	0.081(5)	0.045(3)	–0.036(4)	0.029(4)	–0.020(3)
C(46)	4*a*	0.8137(3)	0.0669(5)	0.4406(4)	0.103(5)	0.044(4)	0.122(6)	0.000(4)	0.040(4)	–0.011(4)
C(47)	4*a*	0.7070(3)	0.1151(6)	0.4161(4)	0.088(4)	0.075(4)	0.112(5)	–0.044(4)	0.051(4)	–0.043(4)
C(48)	4*a*	1.0850(3)	0.1725(6)	0.6452(3)	0.086(4)	0.061(4)	0.101(5)	0.034(3)	0.045(4)	0.005(4)
C(49)	4*a*	1.0605(4)	0.1039(7)	0.5821(4)	0.202(8)	0.107(5)	0.111(6)	0.099(6)	–0.026(6)	–0.062(5)
C(50)	4*a*	1.1492(3)	0.2125(7)	0.6552(5)	0.126(6)	0.107(6)	0.140(7)	0.059(5)	0.051(5)	–0.018(5)
C(51)	4*a*	1.0938(4)	0.0982(7)	0.7078(5)	0.189(8)	0.070(5)	0.149(8)	0.061(5)	0.064(6)	0.030(5)
C(52)	4*a*	0.7596(2)	0.7775(5)	0.4958(3)	0.042(3)	0.053(3)	0.046(3)	0.007(3)	0.012(2)	0.016(3)
C(53)	4*a*	0.7587(3)	0.8475(5)	0.5501(3)	0.057(3)	0.052(3)	0.062(4)	–0.003(3)	0.018(3)	–0.014(3)
C(54)	4*a*	0.7020(2)	0.8914(6)	0.5451(3)	0.062(3)	0.076(4)	0.075(4)	0.015(3)	0.031(3)	–0.001(3)
C(55)	4*a*	0.6499(2)	0.8703(5)	0.4895(3)	0.050(3)	0.066(4)	0.067(4)	0.023(3)	0.031(3)	0.021(3)
C(56)	4*a*	0.6532(2)	0.7974(6)	0.4405(3)	0.049(4)	0.094(5)	0.053(4)	0.007(3)	0.007(3)	0.020(4)
C(57)	4*a*	0.7080(2)	0.7504(5)	0.4426(3)	0.047(3)	0.073(4)	0.046(3)	0.006(3)	0.015(3)	0.009(3)
C(58)	4*a*	0.5910(3)	0.9258(7)	0.4866(4)	0.078(4)	0.126(6)	0.122(6)	0.033(4)	0.047(4)	0.033(5)
O(1)	4*a*	0.9289(1)	0.6347(3)	0.7689(2)	0.037(2)	0.030(2)	0.040(2)	–0.003(2)	0.014(1)	–0.005(2)
O(2)	4*a*	0.8130(2)	0.5955(3)	0.6686(2)	0.048(2)	0.063(2)	0.034(2)	–0.020(2)	0.013(2)	0.007(2)
O(3)	4*a*	0.9248(2)	0.7455(4)	0.8666(2)	0.117(3)	0.068(3)	0.049(2)	–0.013(2)	0.044(2)	–0.015(2)
O(4)	4*a*	1.0148(2)	0.7581(3)	0.8362(2)	0.039(2)	0.053(2)	0.088(3)	–0.003(2)	0.003(2)	–0.005(2)
O(5)	4*a*	0.8398(1)	0.6085(3)	0.5520(2)	0.041(2)	0.039(2)	0.032(2)	0.003(2)	0.018(1)	0.005(2)
O(6)	4*a*	0.9593(2)	0.6030(3)	0.6472(2)	0.049(2)	0.058(2)	0.046(2)	0.020(2)	0.012(2)	–0.006(2)
O(7)	4*a*	0.8755(2)	0.8004(3)	0.5372(2)	0.058(2)	0.051(2)	0.078(3)	–0.020(2)	0.025(2)	0.003(2)
O(8)	4*a*	0.8220(2)	0.6812(3)	0.4351(2)	0.089(2)	0.069(3)	0.042(2)	0.014(2)	0.043(2)	0.012(2)
S(1)	4*a*	0.95083(6)	0.7495(1)	0.81673(7)	0.0531(8)	0.0395(7)	0.0435(8)	–0.0021(7)	0.0112(6)	–0.0030(7)
S(2)	4*a*	0.82775(6)	0.7218(1)	0.50041(6)	0.0500(7)	0.0423(7)	0.0471(8)	0.0018(7)	0.0250(6)	0.0095(7)

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