Crystal structure of 5-chloro-7-(diphenylmethylene)-5,6-(*endo,endo*)-bis(phenylsulfonyl)-bicyclo[2.2.1]hept-2-ene, $C_{32}H_{25}O_4S_2Cl$

K. Peters, E.-M. Peters

Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70506 Stuttgart, Germany

S. Cossu and O. De Lucchi

Universitá di Venezia, Dipartimento di Chimica, Dorsoduro 2137, I-30123 Venezia, Italia

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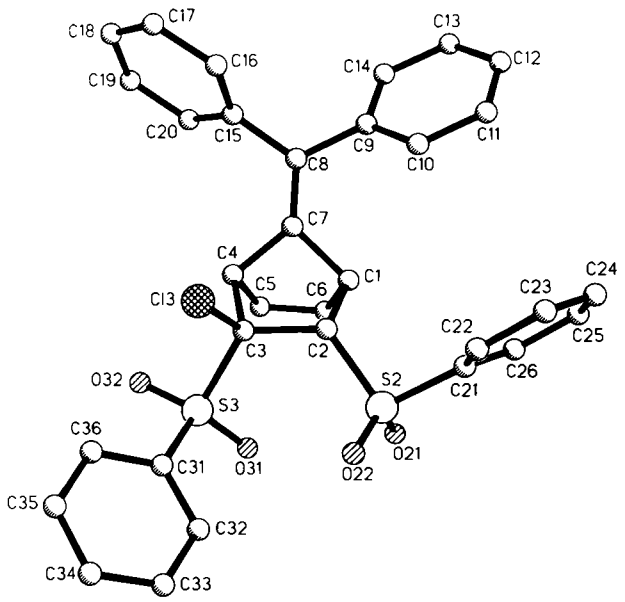

Table 1. Parameters used for the X-ray data collection

Crystal:	colorless prism, size 0.35 x 0.45 x 0.7 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	3.20 cm^{-1}
Diffractometer:	Siemens-P4
Scan mode:	ω
$T_{measurement}$:	293 K
$2\theta_{max}$:	55°
$N(hkl)_{unique}$:	6532
Criterion for F_o:	$F_o > 3\ \sigma(F_o)$
$N(param)_{refined}$:	352
Program:	SHELXTL-plus

Source of material: The title compound was prepared by reaction of (*E*)-1-chloro-1,2-bis(phenylsulphonyl) with diphenylfulvene in refluxing toluene (24 h) (see ref. 1).

$C_{32}H_{25}ClO_4S_2$, monoclinic, $P2_1/c$ (No. 14), a =19.314(2) Å, b =12.617(2) Å, c =12.044(2) Å, β =104.46(1)°, V =2842.0 $Å^3$, Z =4, $R(F)$ =0.046, $R_w(F)$ =0.048.

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

Atom	Site	x	y	z	U_{iso}
H(1)	4*e*	0.76940(9)	1.3067(1)	0.0894(2)	0.08
H(2)	4*e*	0.79785(9)	1.2165(1)	0.2844(1)	0.08
H(4)	4*e*	0.6389(1)	1.0583(1)	0.1173(2)	0.08
H(5)	4*e*	0.6931(1)	1.0280(2)	–0.0474(2)	0.08
H(6)	4*e*	0.7748(1)	1.1739(2)	–0.0574(2)	0.08
H(10)	4*e*	0.7308(1)	1.4097(2)	0.2545(2)	0.08
H(11)	4*e*	0.7519(1)	1.5926(2)	0.2420(2)	0.08
H(12)	4*e*	0.6764(1)	1.6937(2)	0.1011(3)	0.08
H(13)	4*e*	0.5780(1)	1.6172(2)	–0.0223(3)	0.08
H(14)	4*e*	0.5544(1)	1.4354(2)	–0.0084(2)	0.08
H(16)	4*e*	0.5539(1)	1.3344(2)	0.2781(2)	0.08
H(17)	4*e*	0.4409(2)	1.2732(3)	0.2930(3)	0.08
H(18)	4*e*	0.3790(2)	1.1489(3)	0.1643(3)	0.08
H(19)	4*e*	0.4211(1)	1.0986(2)	0.0095(3)	0.08
H(20)	4*e*	0.5340(1)	1.1565(2)	–0.0061(2)	0.08
H(22)	4*e*	0.9070(1)	1.3083(2)	0.4271(2)	0.08
H(23)	4*e*	0.9211(1)	1.4925(2)	0.4616(2)	0.08
H(24)	4*e*	0.9332(2)	1.6043(2)	0.3134(3)	0.08
H(25)	4*e*	0.9269(2)	1.5383(2)	0.1320(3)	0.08
H(26)	4*e*	0.9086(1)	1.3541(2)	0.0946(2)	0.08
H(32)	4*e*	0.9251(1)	0.9172(2)	0.3215(2)	0.08
H(33)	4*e*	0.9797(1)	0.8100(2)	0.4801(2)	0.08
H(34)	4*e*	0.9098(2)	0.7160(2)	0.5761(2)	0.08
H(35)	4*e*	0.7860(2)	0.7257(2)	0.5183(3)	0.08
H(36)	4*e*	0.7297(1)	0.8311(2)	0.3605(3)	0.08

Table 3. Final 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}
Cl(3)	4*e*	0.72069(3)	1.07650(4)	0.34889(4)	0.0677(3)	0.0413(2)	0.0523(3)	–0.0049(2)	0.0235(2)	0.0017(2)
S(2)	4*e*	0.88963(2)	1.18019(4)	0.23160(4)	0.0378(2)	0.0408(2)	0.0476(3)	0.0017(2)	0.0068(2)	–0.0022(2)
S(3)	4*e*	0.78190(3)	0.94469(3)	0.19712(4)	0.0565(3)	0.0276(2)	0.0524(3)	0.0025(2)	0.0029(2)	–0.0043(2)
O(21)	4*e*	0.90865(8)	1.1552(1)	0.1275(1)	0.0552(9)	0.0668(9)	0.0646(9)	0.0048(7)	0.0238(7)	–0.0135(8)
O(22)	4*e*	0.92019(8)	1.1218(1)	0.3344(1)	0.0537(8)	0.0496(8)	0.0635(9)	0.0051(7)	–0.0058(7)	0.0065(7)

Table 3. (Continued)

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(31)	4*e*	0.83440(9)	0.9564(1)	0.1332(1)	0.079(1)	0.0459(7)	0.0542(9)	0.0162(7)	0.0228(8)	−0.0036(6)
O(32)	4*e*	0.71782(9)	0.8861(1)	0.1483(1)	0.071(1)	0.0326(7)	0.090(1)	−0.0038(7)	−0.0137(9)	−0.0115(7)
C(1)	4*e*	0.75204(9)	1.2373(1)	0.1011(2)	0.0385(9)	0.0346(8)	0.046(1)	−0.0002(7)	0.0065(7)	0.0050(7)
C(2)	4*e*	0.79403(9)	1.1807(1)	0.2128(1)	0.0368(8)	0.0287(7)	0.0393(9)	−0.0015(6)	0.0067(7)	−0.0030(6)
C(3)	4*e*	0.74799(9)	1.0791(1)	0.2179(2)	0.0425(9)	0.0281(8)	0.0409(9)	−0.0005(7)	0.0073(7)	−0.0016(6)
C(4)	4*e*	0.6804(1)	1.0992(1)	0.1145(2)	0.0399(9)	0.0323(8)	0.052(1)	−0.0029(7)	0.0019(8)	0.0013(7)
C(5)	4*e*	0.7060(1)	1.0848(2)	0.0068(2)	0.060(1)	0.045(1)	0.044(1)	0.0006(9)	−0.0028(9)	−0.0033(8)
C(6)	4*e*	0.7493(1)	1.1643(2)	0.0009(2)	0.053(1)	0.051(1)	0.039(1)	0.0029(9)	0.0046(8)	0.0047(8)
C(7)	4*e*	0.67753(9)	1.2193(1)	0.1169(2)	0.0386(9)	0.0333(8)	0.048(1)	−0.0028(7)	0.0030(8)	0.0047(7)
C(8)	4*e*	0.6270(1)	1.2877(1)	0.1266(2)	0.0405(9)	0.0372(9)	0.048(1)	−0.0010(7)	0.0051(8)	0.0049(7)
C(9)	4*e*	0.6405(1)	1.4043(1)	0.1241(2)	0.0389(9)	0.0374(9)	0.057(1)	0.0031(7)	0.0132(8)	0.0015(8)
C(10)	4*e*	0.6990(1)	1.4521(2)	0.1976(2)	0.056(1)	0.047(1)	0.060(1)	−0.0007(9)	0.008(1)	−0.0044(9)
C(11)	4*e*	0.7121(1)	1.5596(2)	0.1895(2)	0.066(1)	0.048(1)	0.092(2)	−0.010(1)	0.018(1)	−0.018(1)
C(12)	4*e*	0.6669(1)	1.6196(2)	0.1078(3)	0.069(2)	0.034(1)	0.124(2)	−0.000(1)	0.039(2)	0.003(1)
C(13)	4*e*	0.6091(1)	1.5745(2)	0.0352(3)	0.068(2)	0.044(1)	0.119(2)	0.014(1)	0.015(2)	0.025(1)
C(14)	4*e*	0.5952(1)	1.4672(2)	0.0428(2)	0.044(1)	0.045(1)	0.091(2)	0.0054(9)	0.003(1)	0.014(1)
C(15)	4*e*	0.5554(1)	1.2506(2)	0.1354(2)	0.040(1)	0.0452(9)	0.057(1)	−0.0007(8)	0.0067(8)	0.0079(9)
C(16)	4*e*	0.5272(1)	1.2851(2)	0.2229(2)	0.062(1)	0.101(2)	0.074(2)	−0.023(1)	0.024(1)	−0.019(2)
C(17)	4*e*	0.4612(2)	1.2475(3)	0.2331(3)	0.086(2)	0.147(3)	0.096(2)	−0.040(2)	0.051(2)	−0.021(2)
C(18)	4*e*	0.4230(2)	1.1781(3)	0.1546(3)	0.058(1)	0.111(2)	0.106(2)	−0.030(2)	0.023(2)	0.007(2)
C(19)	4*e*	0.4492(1)	1.1448(2)	0.0666(3)	0.054(1)	0.074(2)	0.095(2)	−0.017(1)	0.006(1)	−0.003(1)
C(20)	4*e*	0.5154(1)	1.1808(2)	0.0563(2)	0.044(1)	0.059(1)	0.068(1)	−0.0054(9)	0.004(1)	−0.001(1)
C(21)	4*e*	0.90633(9)	1.3173(2)	0.2584(2)	0.0349(9)	0.045(1)	0.051(1)	−0.0071(7)	0.0089(8)	−0.0004(8)
C(22)	4*e*	0.9103(1)	1.3563(2)	0.3668(2)	0.048(1)	0.050(1)	0.055(1)	−0.0067(9)	0.0055(9)	−0.0044(9)
C(23)	4*e*	0.9196(1)	1.4639(2)	0.3872(2)	0.068(2)	0.056(1)	0.086(2)	−0.016(1)	0.011(1)	−0.021(1)
C(24)	4*e*	0.9258(2)	1.5298(2)	0.2993(3)	0.080(2)	0.048(1)	0.128(3)	−0.022(1)	0.021(2)	−0.011(2)
C(25)	4*e*	0.9222(2)	1.4907(2)	0.1919(3)	0.093(2)	0.060(2)	0.111(2)	−0.022(1)	0.038(2)	0.023(2)
C(26)	4*e*	0.9122(1)	1.3827(2)	0.1697(2)	0.067(1)	0.063(1)	0.068(1)	−0.013(1)	0.026(1)	0.007(1)
C(31)	4*e*	0.8227(1)	0.8828(1)	0.3281(2)	0.053(1)	0.0283(8)	0.058(1)	0.0026(8)	0.0091(9)	0.0057(8)
C(32)	4*e*	0.8964(1)	0.8780(2)	0.3619(2)	0.054(1)	0.041(1)	0.066(1)	0.0017(9)	0.011(1)	0.0062(9)
C(33)	4*e*	0.9285(1)	0.8150(2)	0.4556(2)	0.061(1)	0.054(1)	0.077(2)	0.009(1)	0.001(1)	0.011(1)
C(34)	4*e*	0.8872(2)	0.7589(2)	0.5114(2)	0.095(2)	0.054(1)	0.074(2)	0.015(1)	0.014(1)	0.026(1)
C(35)	4*e*	0.8142(2)	0.7646(2)	0.4770(3)	0.093(2)	0.069(2)	0.115(2)	0.013(1)	0.040(2)	0.051(2)
C(36)	4*e*	0.7809(1)	0.8269(2)	0.3849(3)	0.062(1)	0.054(1)	0.112(2)	0.004(1)	0.023(1)	0.036(1)

References

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