Crystal data#1

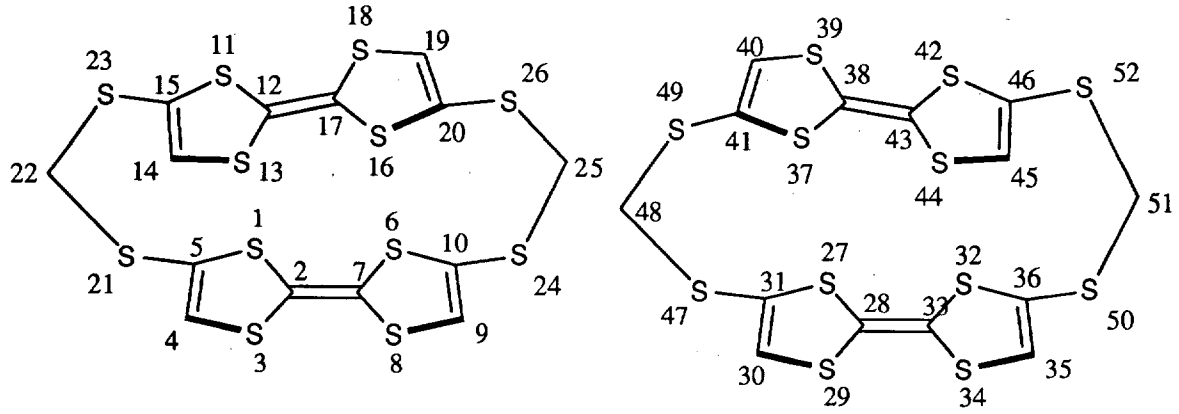
	6b	**7a**	**7c**	**8c**•$CHCl_3$	**9a**•$(CS_2)_2$	**9c**•$CHCl_3$
chemical formura	$C_{14}H_{16}S_{12}$	$C_{16}H_{12}S_{12}$	$C_{16}H_{12}S_{12}$	$C_{19}H_{16}S_{12}Cl_3$	$C_{22}H_{21}S_{16}$	$C_{21}H_{21}S_{12}Cl_3$
formula weight	571.02	589.04	589.04	735.46	797.36	768.48
crystal system	triclinic	orthorhombic	monoclinic	orthorhombic	triclinic	monoclinic
space group	P $\bar{1}$	Pbca	P2/m	Aba2	P $\bar{1}$	$P2_1/n$
color of crystals	orange	yellow	orange	orange	yellow	orange
dmensions of crystal/mm^3	0.50×0.15×0.16	0.30×0.28×0.05	0.44×0.33×0.07	0.22×0.20×0.10	0.90×0.20×0.08	0.20×0.15×0.03
a/Å	12.145 (6)	22.446 (3)	17.173 (2)	16.304 (1)	8.987 (4)	10.995 (2)
b/Å	16.734 (4)	12.290 (2)	7.977 (1)	20.238 (3)	12.150 (5)	11.147 (3)
c/Å	11.457 (6)	8.310 (2)	17.719 (3)	9.104 (1)	8.329 (3)	26.230 (2)
α/°	96.83 (4)				99.83 (3)	
β/°	112.86 (3)		106.21 (1)		96.53 (4)	94.40 (1)
γ/°	82.71 (3)				76.71 (3)	
V/$Å^3$	2121 (1)	2292.5 (6)	2330.8 (6)	3003.8 (6)	869.5 (6)	3205.4 (9)
Z	4	4	4	4	1	4
linear absorption coefficient / cm^{-1}	114.75	103.37	101.67	103.46	10.1	125.14
range of transmission factors	0.47-1.00	-	-	-	0.92-1.00	0.40-1.00
temperature / K	295	295	295	295	295	295
wave lengths of raddiation / Å	1.54178 (*Cu Kα*)	1.54178 (*Cu Kα*)	1.54178 (*Cu Kα*)	1.54178 (*Cu Kα*)	0.71069(*MoKα*)	1.54178 (*Cu Kα*)
2θ max / °	126.1	126.1	157.9	126.1	55.0	126.3
number of data and cut-off	4126	1587	2716	1514	2898	1978
	(I ≥3.0σ(I))	(|Fo| ≥1.0σ(|Fo|)	(|Fo| ≥3.0σ(|Fo|)	(|Fo| ≥1.0σ(|Fo|)	(I ≥3.0σ(I))	(I ≥3.0σ(I))
number of parameteers refined	469	127	253	158	206	326
calculated density /g cm^{-3}	1.787	1.707	1.679	1.627	1.523	1.980
Intensity measurement method	ω-2θ	ω-2θ	ω-2θ	ω-2θ	ω-2θ	ω-2θ
R [a], R_W [b]	0.065, 0.052	0.073, 0.067	0.071, 0.071	0.072, 0.069	0.066, 0.057	0.050, 0.052

[a] $R = \Sigma (|F_o| - |F_c|)/\Sigma |F_o|$. [b] $R_w = \{\Sigma w(|F_o| - |F_c|)^2/\Sigma w|F_o|^2\}^{1/2}$.

Crystal data#2

	6•PF_6	**7**•ClO_4	**7**•I_3	**7**•I_3	**8**•PF_6
chemical formula	$C_{14}H_8S_{12}P_2F_{12}$	$C_{48}H_{36}S_{36}Cl_4O_{16}$	$C_{16}H_{12}S_{12}I_6$	$C_{16}H_{12}S_{12}I_6$	$C_{18}H_{16}S_{12}PF_6$
formula weight	705.90	2164.77	1350.42	1350.42	762.01
crystal system	monoclinic	monoclinic	monoclinic	triclinic	triclinic
space group	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P\bar{1}$	$P\bar{1}$
color of crystal	black	black	black	black	black
dimensions of crystal / mm^3	0.25×0.15×0.01	0.75×0.30×0.02	0.48×0.05×0.03	0.16×0.10×0.01	0.35×0.35×0.01
a/Å	9.027 (8)	7.834 (5)	15.420 (1)	13.529 (3)	7.929 (1)
b/Å	15.513 (3)	23.891 (4)	10.106 (1)	13.540 (3)	12.467 (3)
c/Å	10.427 (2)	20.897 (3)	11.546 (1)	8.177 (1)	7.618 (3)
α/°				90.33 (2)	109.37 (2)
β/°	109.94 (3)	99.08 (2)	108.475 (7)	99.84 (2)	90.22 (2)
γ/°				145.21 (1)	94.60 (1)
V/$Å^3$	1372 (1)	3682 (2)	1706.4 (3)	813.0 (5)	707.8 (3)
Z	2	2	2	1	1
linear absorption coefficient / cm^{-1}	98.69	110.29	498.30	522.96	96.22
range of transmission factors	-	0.67-1.00	-	0.44-1.00	-
temperature / K	295	295	295	295	295
wave lengths of raddiation / Å	1.54178 (*Cu Kα*)	1.54178 (*Cu Kα*)	1.54178 (*Cu Kα*)	1.54178 (*Cu Kα*)	1.54178 (*Cu Kα*)
2θ max / °	126.1	126.1	125.9	126.1	126.1
number of data and cut-off	688	3677	1893	1650	1905
	(I ≥3.0σ(I))	(I ≥3.0σ(I))	(I ≥2.0σ(I))	(I ≥2.0σ(I))	(|Fo| ≥3.0σ(|Fo|)
number of parameteers refined	182	483	155	160	170
calculated density /g cm^{-3}	1.708	1.861	2.628	2.758	1.780
Intensity measurement method	ω-2θ	ω-2θ	ω-2θ	ω-2θ	ω-2θ
Ra, R_w[b]	0.064, 0.073	0.075, 0.075	0.078, 0.224[c]	0.105, 0.315[c]	0.0813, 0.089

[a] $R = \Sigma (|F_o| - |F_c|)/\Sigma |F_o|$. [b] $R_w = \{\Sigma w(|F_o| - |F_c|)^2/\Sigma w|F_o|^2\}^{1/2}$. [c] $R_w = \{\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2\}^{1/2}$ for all data.



Atomic numbering scheme of tetrathafulvalenophane **6b**

Positional parameters and B(eq) for **6b**

Atom	*x*	*y*	*z*	B_{eq}/Å^2
S1	0.1443(3)	0.0892(2)	0.1795(3)	5.44(9)
S3	0.2586(3)	0.1730(2)	0.0495(3)	5.55(9)
S6	0.3855(3)	-0.0401(2)	0.2701(3)	5.07(9)
S8	0.4908(3)	0.0497(2)	0.1398(3)	5.52(9)
S11	-0.0394(3)	-0.0507(2)	0.2346(3)	5.28(9)
S13	0.1047(3)	0.0456(2)	0.4653(3)	5.39(9)
S16	0.3182(3)	-0.1011(2)	0.5308(3)	5.52(9)
S18	0.1739(3)	-0.1953(2)	0.2988(3)	6.02(10)
S21	-0.0801(3)	0.2046(2)	0.0956(3)	5.38(9)
S23	-0.2252(3)	0.0886(2)	0.1418(4)	6.6(1)
S24	0.5924(3)	-0.1705(2)	0.3331(3)	5.54(9)
S26	0.5444(3)	-0.2101(2)	0.5586(3)	6.4(1)
S27	0.3332(3)	0.5798(2)	0.8194(3)	5.71(10)
S29	0.4355(3)	0.6470(2)	0.6618(4)	7.1(1)
S32	0.2270(3)	0.4389(2)	0.5921(3)	6.09(10)
S34	0.3336(3)	0.5053(2)	0.4391(3)	7.6(1)
S37	0.3013(3)	0.4569(2)	1.0593(3)	5.62(9)
S39	0.0775(3)	0.5586(2)	0.9368(3)	6.1(1)
S42	-0.0174(3)	0.4100(2)	0.7166(4)	6.4(1)
S44	0.2086(3)	0.3126(2)	0.8415(3)	5.92(10)
S47	0.4198(3)	0.7106(2)	1.0316(3)	6.4(1)
S49	0.4284(3)	0.5973(2)	1.2248(3)	6.13(10)
S50	0.1136(3)	0.3112(2)	0.3834(3)	6.8(1)
S52	-0.0857(3)	0.3007(2)	0.4773(4)	7.5(1)
C2	0.2716(9)	0.0920(6)	0.1437(10)	4.5(3)
C4	0.1109(9)	0.2071(6)	0.031(1)	4.9(3)
C5	0.0594(9)	0.1697(6)	0.0878(10)	4.2(3)
C7	0.3668(9)	0.0417(6)	0.1788(10)	4.5(3)
C9	0.5746(9)	-0.0385(6)	0.208(1)	4.6(3)
C10	0.5268(9)	-0.0788(6)	0.265(1)	4.5(3)
C12	0.0935(10)	-0.0448(6)	0.3651(10)	4.4(3)
C14	-0.026(1)	0.0942(7)	0.362(1)	5.1(4)
C15	-0.097(1)	0.0515(6)	0.256(1)	4.9(3)
C17	0.1853(10)	-0.1062(6)	0.3971(10)	4.3(3)
C19	0.323(1)	-0.2295(7)	0.365(1)	5.1(4)
C20	0.390(1)	-0.1870(6)	0.469(1)	5.1(4)
C22	-0.1713(9)	0.1174(6)	0.025(1)	4.8(3)
C25	0.6187(9)	-0.1418(6)	0.5014(10)	4.7(3)
C28	0.3512(10)	0.5710(7)	0.674(1)	5.5(4)
C30	0.457(1)	0.6981(7)	0.809(1)	6.3(4)
C31	0.4116(10)	0.6680(7)	0.884(1)	5.5(4)

C33	0.308(1)	0.5142(8)	0.579(1)	5.6(4)
C35	0.2431(10)	0.4249(7)	0.364(1)	6.2(4)
C36	0.198(1)	0.3951(7)	0.437(1)	5.7(4)
C38	0.1620(9)	0.4628(7)	0.934(1)	4.6(3)
C40	0.1979(9)	0.6074(6)	1.054(1)	4.5(3)
C41	0.2976(10)	0.5621(6)	1.1088(10)	4.5(3)
C43	0.1239(9)	0.4059(6)	0.846(1)	4.4(3)
C45	0.1187(9)	0.2765(6)	0.687(1)	5.0(3)
C46	0.019(1)	0.3227(6)	0.632(1)	5.2(4)
C48	0.5065(9)	0.6266(6)	1.1313(10)	4.7(3)
C51	-0.0328(10)	0.3560(6)	0.382(1)	6.2(4)

Bond lengths and angles of **6b**

Atoms	Length/Å	Atoms	Length/Å
S1-C2	1.75(1)	S29-C28	1.78(1)
S1-C5	1.77(1)	S29-C30	1.73(1)
S3-C2	1.79(1)	S32-C33	1.75(1)
S3-C4	1.75(1)	S32-C36	1.76(1)
S6-C7	1.76(1)	S34-C33	1.73(1)
S6-C10	1.78(1)	S34-C35	1.77(1)
S8-C7	1.754(9)	S37-C38	1.74(1)
S8-C9	1.76(1)	S37-C41	1.78(1)
S11-C12	1.73(1)	S39-C38	1.80(1)
S11-C15	1.79(1)	S39-C40	1.77(1)
S13-C12	1.77(1)	S42-C43	1.78(1)
S13-C14	1.74(1)	S42-C46	1.77(1)
S16-C17	1.74(1)	S44-C43	1.76(1)
S16-C20	1.81(1)	S44-C45	1.76(1)
S18-C17	1.74(1)	S47-C31	1.73(1)
S18-C19	1.72(1)	S47-C48	1.86(1)
S21-C5	1.752(9)	S49-C41	1.75(1)
S21-C22	1.86(1)	S49--C48	1.822(9)
S23-C15	1.70(1)	S50C36	1.75(1)
S23-C22	1.84(1)	S50-C51	1.83(1)
S24-C10	1.76(1)	S52-C46	1.76(1)
S24-C25	1.84(1)	S52-C51	1.84(1)
S26-C20	1.77(1)	C2-C7	1.30(1)
S26-C25	1.858(9)	C4-C5	1.31(1)
S27-C28	1.76(1)	C9-C10	1.31(1)
S27-C31	1.78(1)	C12-C17	1.38(1)
C14-C15	1.36(1)	C19-C20	1.34(1)
C28-C33	1.34(1)	C30-C31	1.36(1)
C35-C36	1.33(1)	C38-C43	1.29(1)
C40-C41	1.31(1)	C45-C46	1.32(1)

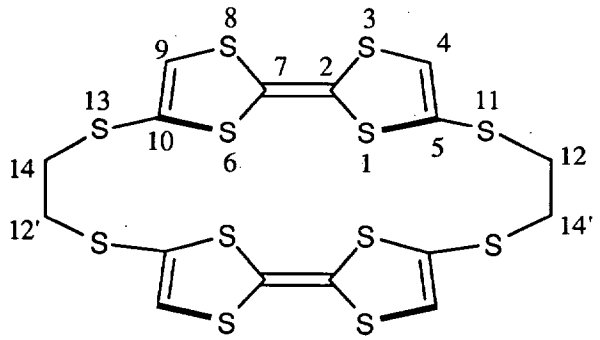
Atoms	Angle/°	Atoms	Angle/°
C2-S1-C5	95.6(5)	S3-C2-C7	121.4(8)
C2-S3-C4	95.7(5)	S3-C4-C5	117.6(8)
C7-S6-C10	95.0(5)	S1-C5-S21	118.5(5)
C7-S8-C9	96.5(5)	S1-C5-C4	117.9(8)
C12-S11-C15	95.6(6)	S21-C5-C4	123.0(8)
C12-S13-C14	94.4(6)	S6-C7-S8	113.4(6)
C17-S16-C20	92.0(6)	S6-C7-C2	124.0(8)
C17-S18-C19	96.0(5)	S8-C7-C2	122.6(8)
C5-S21-C22	103.5(5)	S8-C9-C10	116.6(8)
C15-S23-C22	102.6(5)	S6-C10-S24	117.8(6)
C10-S24-C25	101.2(5)	S6-C10-C9	118.3(8)
C20-S26-C25	103.1(5)	S24-C10-C9	123.9(8)

C28-S27-C31	96.5(6)	S11-C12-S13	115.5(7)
C28-S29-C30	97.2(6)	S11-C12-C17	124.4(8)
C33-S32-C36	94.4(6)	S13-C12-C17	120.0(8)
C33-S34-C35	96.8(6)	S13-C14-C15	118.9(9)
C38-S37-C41	95.6(5)	S11-C15-S23	119.1(7)
C38-S39-C40	95.4(5)	S11-C15-C14	114.8(9)
C43-S42-C46	94.6(6)	S23-C15-C14	125.9(9)
C43-S44-C45	97.3(6)	S16-C17-S18	115.5(7)
C31-S47-C48	100.1(5)	S16-C17-C12	124.5(8)
C41-S49-C48	102.9(5)	S18-C17-C12	120.0(8)
C36-S50-C51	101.2(5)	S18-C19-C20	116.3(9)
C46-S52-C51	101.4(5)	S16-C20-S26	115.7(7)
S1-C2-S3	113.0(6)	S16-C20-C19	118.2(9)
S1-C2-C7	125.6(8)	S26-C20-C19	126.0(9)
S21-C22-S23	108.5(6)	S44-C45-C46	115.0(9)
S24-C25-S26	109.6(5)	S42-C46-S52	116.3(7)
S27-C28-S29	112.7(8)	S42-C46-C45	119(1)
S27-C28-C33	125.6(9)	S52-C46-C45	124.1(9)
S29-C28-C33	121.7(9)	S47-C48-S49	111.6(5)
S29-C30-C31	117(1)	S50-C51-S52	111.3(6)
S27-C31-S47	118.8(7)	S27-C31-C30	116(1)
S47-C31-C30	125(1)	S32-C33-S34	114.6(7)
S32-C33-C28	121.4(9)	S34-C33-C28	123.9(9)
S34-C35C36	114(1)	S32-C36-S50	118.8(7)
S32-C36C35	120(1)	S50-C36-C35	122(1)
S37-C38-S39	112.8(7)	S37-C38-C43	124.4(9)
S39-C38-C43	122.8(9)	S39-C40-C41	116.9(9)
S37-C41-S49	117.2(6)	S37-C41-C40	117.8(9)
S49-C41-C40	125.0(9)	S42-C43-S44	111.9(7)
S42-C43-C38	125.4(8)	S44-C43-C38	122.6(9)

Anisotropic displacement parameters for **6b**

atom	U11	U22	U33	U12	U13	U23
S1	0.058(2)	0.070(2)	0.101(3)	0.012(2)	0.052(2)	0.032(2)
S3	0.061(2)	0.073(2)	0.098(3)	0.007(2)	0.048(2)	0.032(2)
S6	0.057(2)	0.064(2)	0.092(2)	0.011(2)	0.049(2)	0.024(2)
S8	0.065(2)	0.077(2)	0.094(3)	0.009(2)	0.057(2)	0.022(2)
S11	0.068(2)	0.055(2)	0.091(3)	-0.005(2)	0.047(2)	-0.007(2)
S13	0.086(2)	0.056(2)	0.084(2)	-0.010(2)	0.058(2)	-0.011(2)
S16	0.077(2)	0.067(2)	0.077(2)	0.001(2)	0.046(2)	-0.003(2)
S18	0.074(2)	0.060(2)	0.103(3)	-0.004(2)	0.048(2)	-0.015(2)
S21	0.063(2)	0.057(2)	0.102(3)	0.013(2)	0.053(2)	0.013(2)
S23	0.057(2)	0.078(2)	0.134(3)	0.001(2)	0.056(2)	0.015(2)
S24	0.073(2)	0.053(2)	0.098(3)	0.013(2)	0.052(2)	0.006(2)
S26	0.076(3)	0.078(2)	0.103(3)	0.013(2)	0.047(2)	0.032(2)
S27	0.078(2)	0.071(2)	0.087(3)	-0.018(2)	0.048(2)	0.007(2)
S29	0.085(3)	0.105(3)	0.104(3)	-0.026(2)	0.047(2)	0.031(3)
S32	0.083(3)	0.084(2)	0.081(3)	-0.019(2)	0.046(2)	0.004(2)
S34	0.080(3)	0.147(4)	0.088(3)	-0.016(3)	0.054(2)	0.017(3)
S37	0.086(3)	0.057(2)	0.085(3)	0.021(2)	0.054(2)	0.015(2)
S39	0.065(2)	0.061(2)	0.126(3)	0.015(2)	0.061(2)	0.010(2)
S42	0.065(2)	0.058(2)	0.134(3)	0.009(2)	0.059(2)	-0.005(2)
S44	0.083(2)	0.054(2)	0.114(3)	0.017(2)	0.066(2)	0.023(2)
S47	0.085(3)	0.057(2)	0.113(3)	0.004(2)	0.055(2)	0.000(2)
S49	0.090(3)	0.072(2)	0.076(2)	0.020(2)	0.046(2)	0.001(2)
S50	0.085(3)	0.069(2)	0.109(3)	0.010(2)	0.052(2)	-0.012(2)
S52	0.066(2)	0.062(2)	0.159(4)	-0.003(2)	0.053(3)	-0.022(2)

C2	0.056(8)	0.062(8)	0.069(8)	0.006(6)	0.040(7)	0.018(7)
C4	0.053(8)	0.057(8)	0.088(9)	0.010(6)	0.044(7)	0.011(7)
C5	0.046(7)	0.055(7)	0.072(8)	0.012(6)	0.039(6)	0.017(6)
C7	0.051(8)	0.071(8)	0.067(8)	0.001(6)	0.041(6)	0.019(7)
C9	0.069(8)	0.051(7)	0.070(9)	-0.005(6)	0.044(7)	-0.001(6)
C10	0.050(8)	0.051(7)	0.076(9)	0.011(6)	0.035(7)	0.004(6)
C12	0.072(9)	0.054(7)	0.053(8)	-0.022(7)	0.037(7)	-0.016(6)
C14	0.069(9)	0.061(8)	0.09(1)	0.004(7)	0.060(8)	0.012(7)
C15	0.065(9)	0.047(7)	0.09(1)	-0.006(6)	0.056(8)	-0.005(7)
C17	0.067(8)	0.055(7)	0.050(8)	-0.009(6)	0.033(7)	-0.013(6)
C19	0.066(9)	0.059(8)	0.080(10)	-0.017(7)	0.037(7)	0.003(7)
C20	0.074(9)	0.053(8)	0.09(1)	0.020(7)	0.061(8)	0.030(7)
C22	0.060(8)	0.050(7)	0.081(9)	-0.012(6)	0.033(7)	0.001(7)
C25	0.071(8)	0.061(8)	0.056(8)	-0.012(6)	0.031(6)	0.005(6)
C28	0.065(9)	0.081(10)	0.09(1)	-0.002(7)	0.049(8)	0.033(8)
C30	0.09(1)	0.075(9)	0.09(1)	0.000(8)	0.049(9)	0.016(8)
C31	0.061(8)	0.061(8)	0.08(1)	-0.005(7)	0.026(7)	-0.008(7)
C33	0.068(9)	0.10(1)	0.066(10)	-0.017(8)	0.040(7)	0.008(8)
C35	0.052(8)	0.10(1)	0.09(1)	-0.005(8)	0.036(8)	0.001(9)
C36	0.075(9)	0.071(9)	0.08(1)	0.004(7)	0.041(8)	0.002(8)
C38	0.055(8)	0.061(8)	0.078(10)	0.015(6)	0.051(7)	0.008(7)
C40	0.046(7)	0.066(8)	0.068(8)	0.012(6)	0.036(6)	0.008(7)
C41	0.075(9)	0.047(7)	0.065(8)	0.009(6)	0.049(7)	0.006(6)
C43	0.053(8)	0.050(7)	0.081(10)	0.014(6)	0.047(7)	0.010(7)
C45	0.043(8)	0.056(8)	0.10(1)	0.006(6)	0.042(7)	0.011(7)
C46	0.060(8)	0.048(7)	0.10(1)	-0.009(6)	0.048(8)	-0.022(7)
C48	0.048(7)	0.063(8)	0.079(9)	0.013(6)	0.032(6)	0.029(7)
C51	0.061(8)	0.072(8)	0.11(1)	0.023(7)	0.052(8)	0.013(8)



Atomic numbering scheme of tetrathafulvalenophane **7a**

Positional parameters and B(eq) for **7a**

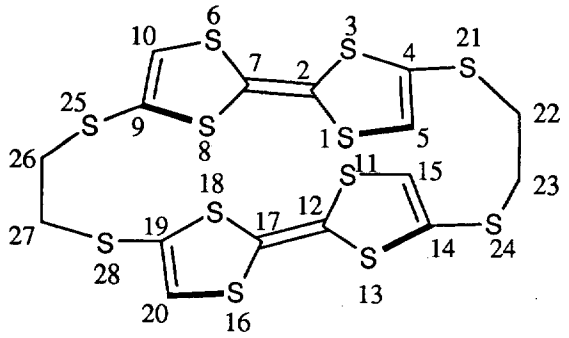
Atom	*x*	*y*	*z*	B_{eq}/Å^2
S(1)	0.13383(7)	0.00160(15)	0.38620(25)	5.15(10)
C(2)	0.11605(31)	0.13862(57)	0.34474(90)	4.40(21)
S(3)	0.16926(7)	0.23151(16)	0.41959(25)	5.23(10)
C(4)	0.20510(32)	0.13699(63)	0.54522(93)	4.92(23)
C(5)	0.18975(29)	0.03311(62)	0.52962(90)	4.66(23)
S(6)	0.01409(7)	0.08066(15)	0.18781(26)	5.26(10)
C(7)	0.06739(29)	0.17104(53)	0.26857(89)	4.15(20)
S(8)	0.05122(9)	0.30856(14)	0.23300(28)	5.22(10)
C(9)	-0.01647(32)	0.28681(57)	0.14071(93)	4.81(23)
C(10)	-0.03411(29)	0.18221(56)	0.12096(87)	4.29(21)
S(11)	0.22818(7)	-0.07356(19)	0.62170(28)	5.87(11)
C(12)	0.16936(32)	-0.14169(57)	0.73897(99)	4.98(23)
S(13)	-0.09514(9)	0.14529(16)	0.00059(25)	5.20(10)
C(14)	-0.14170(31)	0.06595(59)	0.13978(92)	4.72(22)

Bond lengths and angles of **7a**

Atoms	Length/Å	Atoms	Length/Å
S(1)–C(2)	1.764(7)	S(1)–C(5)	1.774(7)
C(2)–S(3)	1.765(7)	C(2)–C(7)	1.324(10)
S(3)–C(4)	1.756(8)	C(4)–C(5)	1.329(11)
C(5)–S(11)	1.746(8)	S(6)–C(7)	1.765(7)
S(6)–C(10)	1.743(7)	C(7)–S(8)	1.754(7)
S(8)–C(9)	1.723(8)	C(9)–C(10)	1.355(10)
C(10)–S(13)	1.756(7)	S(11)–C(12)	1.842(8)
C(12)–S(14')	1.506(11)	C(13)–S(14)	1.838(8)
Atoms	**Angle/°**	**Atoms**	**Angle/°**
C(2)–S(1)–C(5)	94.7(4)	S(1)–C(2)–S(3)	113.3(4)
S(1)–C(2)–C(7)	124.6(6)	S(3)–C(2)–C(7)	122.1(6)
C(2)–S(3)–C(4)	95.3(4)	S(3)–C(4)–C(5)	117.3(6)
S(1)–C(5)–C(4)	117.3(6)	C(1)–C(5)–S(11)	118.7(4)
C(4)–C(5)–S(11)	123.4(6)	C(7)–S(6)–C(10)	95.2(3)
S(6)–C(7)–S(8)	113.7(4)	S(6)–C(7)–C(2)	123.5(5)
S(8)–C(7)–C(2)	122.8(5)	C(7)–S(8)–C(9)	96.2(3)
S(8)–C(9)–C(10)	117.3(6)	S(6)–C(10)–C(9)	117.3(5)
S(6)–C(10)–C(13)	118.7(4)	S(9)–C(10)–C(13)	122.8(6)
S(5)–C(11)–C(12)	102.6(3)	S(11)–C(12)–C(14')	111.6(5)
C(10)–S(13)–C(14)	102.8(3)	S(13)–C(14)–S(12')	109.1(5)

Anisotropic displacement parameters for **7a**

Atom	U11	U22	U33	U12	U13	U23
S1	0.054(1)	0.052(4)	0.090(2)	-0.0064(9)	-0.015(1)	0.001(1)
C2	0.052(4)	0.050(5)	0.066(5)	-0.006(3)	0.003(4)	-0.003(4)
S3	0.052(1)	0.060(4)	0.084(2)	-0.0124(9)	-0.003(1)	-0.004(1)
C4	0.042(4)	0.066(6)	0.070(5)	-0.008(4)	0.010(4)	0.001(4)
C5	0.057(1)	0.067(6)	0.068(5)	-0.005(4)	-0.001(4)	0.005(4)
S6	0.047(4)	0.043(4)	0.099(2)	0.0011(9)	-0.021(1)	0.002(1)
C7	0.047(2)	0.046(5)	0.065(5)	-0.0002(31)	0.003(4)	-0.008(4)
S8	0.060(1)	0.046(4)	0.093(2)	-0.0024(9)	0.004(1)	-0.001(1)
C9	0.054(4)	0.056(6)	0.072(5)	0.009(4)	0.011(4)	-0.004(4)
C10	0.044(4)	0.054(6)	0.065(5)	0.008(3)	0.004(4)	0.008(4)
S11	0.046(1)	0.084(4)	0.092(2)	0.008(1)	-0.004(1)	0.011(1)
C12	0.059(4)	0.053(6)	0.077(5)	0.002(4)	0.008(4)	-0.0008(40)
S13	0.058(1)	0.068(4)	0.072(1)	0.008(1)	-0.011(1)	0.005(1)
C14	0.049(4)	0.056(6)	0.075(5)	-0.003(4)	0.0006(40)	-0.004(4)



Atomic numbering scheme of tetrathafulvalenophane **7c**

Positional parameters and B(eq) for **7c**

Atom	*x*	*y*	*z*	B_{eq}/Å^2
S(1)	0.3897(1)	0.8474(4)	0.8858(1)	7.90(11)
C(2)	0.4095(5)	0.8823(11)	0.7958(5)	6.41(27)
S(3)	0.5124(1)	0.8655(4)	0.7988(1)	8.10(11)
C(4)	0.5463(4)	0.8490(11)	0.9017(5)	6.67(28)
C(5)	0.4919(5)	0.8398(12)	0.9400(5)	7.05(29)
S(6)	0.3706(2)	0.9453(4)	0.6382(1)	9.33(12)
C(7)	0.3523(5)	0.9149(12)	0.7298(5)	6.66(27)
S(8)	0.2480(1)	0.9293(4)	0.7254(1)	7.55(10)
C(9)	0.2134(5)	0.9834(11)	0.6245(5)	6.35(26)
C(10)	0.2701(6)	0.9934(15)	0.5879(5)	8.46(35)
S(11)	0.4695(1)	0.3990(4)	0.6945(1)	7.67(10)
C(12)	0.4049(4)	0.3930(12)	0.7560(5)	6.54(27)
S(13)	0.4549(1)	0.3513(4)	0.8545(1)	7.58(10)
C(14)	0.5518(4)	0.3425(10)	0.8416(4)	5.74(24)
C(15)	0.5573(5)	0.3674(12)	0.7691(5)	6.65(28)
S(16)	0.2606(1)	0.4197(4)	0.7918(1)	8.32(11)
C(17)	0.3255(5)	0.4219(12)	0.7307(5)	6.82(28)
S(18)	0.2755(1)	0.4566(4)	0.6313(1)	7.85(10)
C(19)	0.1779(4)	0.4625(11)	0.6433(5)	6.28(27)
C(20)	0.1719(5)	0.4476(12)	0.7163(6)	7.53(32)
S(21)	0.6512(1)	0.8491(4)	0.9469(2)	8.52(11)
C(22)	0.6746(5)	0.6365(12)	0.9233(6)	7.48(32)
C(23)	0.6420(5)	0.5099(13)	0.9706(5)	7.35(31)
S(24)	0.6341(1)	0.3026(3)	0.9241(1)	7.47(10)
S(25)	0.1108(2)	1.0200(3)	0.5838(1)	7.53(10)
C(26)	0.0729(4)	0.8071(12)	0.5885(5)	6.87(29)
C(27)	0.1033(5)	0.6971(11)	0.5339(5)	6.71(28)
S(28)	0.0951(1)	0.4760(3)	0.5592(2)	7.70(10)

Bond lengths and angles of **7c**

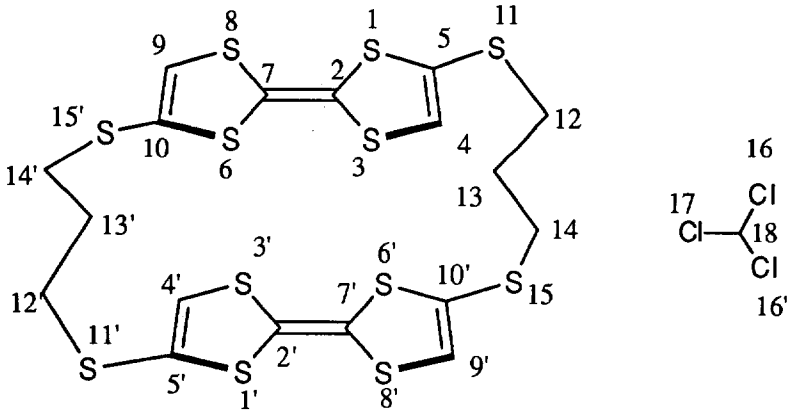
Atoms	Length/Å	Atoms	Length/Å
S(1)–C(2)	1.744(10)	S(1)–C(5)	1.751(8)
C(2)–S(3)	1.757(9)	C(2)–C(7)	1.326(10)
S(3)–C(4)	1.756(9)	C(4)–C(5)	1.302(13)
C(4)–S(21)	1.755(7)	S(6)–C(7)	1.755(10)
S(6)–C(10)	1.750(10)	C(7)–S(8)	1.775(8)
S(8)–C(9)	1.772(8)	C(9)–C(10)	1.314(15)
C(9)–S(25)	1.732(8)	S(11)–C(12)	1.758(9)
S(11)–C(15)	1.724(7)	C(12)–S(13)	1.750(8)
C(12)–C(17)	1.332(11)	S(13)–C(14)	1.744(8)
C(14)–C(15)	1.330(12)	C(14)–S(24)	1.756(7)
S(16)–C(17)	1.757(10)	S(16)–C(20)	1.738(8)
C(17)–S(18)	1.753(8)	S(18)–C(19)	1.748(9)
C(19)–C(20)	1.331(14)	C(19)–S(28)	1.752(7)
S(21)–C(22)	1.818(10)	C(22)–S(23)	1.515(14)
C(23)–S(24)	1.835(10)	S(25)–C(26)	1.830(10)
C(26)–C(27)	1.503(14)	C(27)–S(28)	1.836(9)

Atoms	Angle/°	Atoms	Angle/°
C(2)–S(1)–C(5)	94.9(4)	S(1)–C(2)–S(3)	114.3(4)
S(1)–C(2)–C(7)	123.4(7)	S(3)–C(2)–C(7)	122.3(8)
C(2)–S(3)–C(4)	94.4(4)	S(3)–C(4)–C(5)	117.9(6)
S(3)–C(4)–S(21)	118.4(5)	C(5)–C(4)–S(21)	123.8(7)
S(1)–C(5)–C(4)	117.9(7)	C(7)–S(6)–C(10)	95.5(4)
S(6)–C(7)–S(8)	112.9(4)	S(6)–C(7)–C(2)	124.2(7)
S(8)–C(7)–C(2)	122.9(8)	C(7)–S(8)–C(9)	96.3(4)
S(8)–C(9)–C(10)	115.3(6)	S(8)–C(9)–S(25)	118.5(6)
C(10)–C(9)–S(25)	126.3(7)	S(6)–C(10)–C(9)	119.8(7)
C(12)–S(11)–C(15)	95.1(4)	S(11)–C(12)–S(13)	113.9(4)
S(11)–C(12)–C(17)	123.4(7)	S(13)–C(12)–C(17)	122.7(7)
C(12)–S(13)–C(14)	95.5(4)	S(13)–C(14)–C(15)	116.7(5)
S(13)–C(14)–S(24)	118.3(5)	C(15)–C(14)–S(24)	125.0(6)
S(11)–C(15)–C(14)	118.6(6)	C(17)–S(16)–C(20)	95.4(5)
S(16)–C(17)–S(18)	113.8(5)	S(16)–C(17)–C(12)	123.8(7)
S(18)–C(17)–C(12)	122.3(8)	C(17)–S(18)–C(19)	95.7(4)
S(18)–C(19)–C(20)	116.9(6)	S(18)–C(19)–S(28)	118.4(5)
C(20)–C(19)–S(28)	124.6(7)	S(16)–C(20)–C(19)	118.1(7)
S(4)–C(21)–S(22)	99.1(4)	S(21)–C(22)–C(23)	110.8(7)
C(22)–C(23)–S(24)	110.2(7)	C(14)–S(24)–C(23)	98.8(4)
C(9)–S(25)–C(26)	99.1(4)	S(25)–C(26)–C(27)	108.7(7)
C(26)–C(27)–S(28)	109.8(7)	C(19)–S(28)–C(27)	99.6(4)

Anisotropic displacement parameters for **7c**

Atom	U11	U22	U33	U12	U13	U23
S1	0.063(1)	0.160(4)	0.070(1)	0.005(1)	0.014(1)	0.010(2)
C2	0.061(5)	0.104(7)	0.073(5)	0.0002(43)	0.020(4)	0.00003(484)
S3	0.065(1)	0.154(4)	0.083(1)	-0.014(1)	0.023(1)	-0.0003(2)
C4	0.054(4)	0.103(7)	0.087(6)	-0.011(4)	0.010(4)	-0.021(5)
C5	0.062(5)	0.113(8)	0.082(6)	-0.001(5)	0.010(4)	-0.006(5)
S6	0.085(2)	0.189(4)	0.074(1)	-0.023(2)	0.023(1)	0.009(2)
C7	0.064(4)	0.107(7)	0.075(5)	-0.004(4)	0.019(4)	-0.0002(51)
S8	0.069(1)	0.147(4)	0.063(1)	0.009(1)	0.012(1)	0.006(1)
C9	0.079(5)	0.096(7)	0.058(4)	-0.001(4)	0.009(4)	-0.0007(45)
C10	0.093(6)	0.16(1)	0.061(5)	-0.010(6)	0.005(5)	0.015(6)
S11	0.072(1)	0.153(4)	0.060(1)	-0.012(1)	0.0014(1)	-0.003(1)

C12	0.060(4)	0.115(7)	0.066(5)	-0.004(4)	0.008(4)	0.002(5)
S13	0.065(1)	0.152(4)	0.064(1)	0.008(1)	0.013(1)	0.015(1)
C14	0.061(4)	0.089(6)	0.060(5)	0.005(4)	0.007(4)	-0.001(4)
C15	0.070(5)	0.104(8)	0.070(5)	-0.0007(43)	0.013(4)	-0.006(5)
S16	0.074(1)	0.161(4)	0.075(1)	0.002(1)	0.022(1)	0.010(1)
C17	0.079(5)	0.107(7)	0.065(5)	-0.011(5)	0.013(4)	0.002(5)
S18	0.068(1)	0.160(4)	0.061(1)	-0.003(1)	0.006(1)	0.001(1)
C19	0.065(4)	0.090(7)	0.073(5)	-0.009(4)	0.005(4)	-0.006(5)
C20	0.089(6)	0.102(8)	0.086(6)	-0.007(5)	0.021(5)	0.007(6)
S21	0.063(1)	0.125(4)	0.121(2)	-0.010(1)	0.003(1)	-0.029(2)
C22	0.063(5)	0.114(8)	0.101(7)	-0.002(5)	0.026(5)	-0.007(6)
C23	0.074(5)	0.126(9)	0.067(5)	0.011(5)	0.0008(43)	-0.011(5)
S24	0.072(1)	0.116(3)	0.085(1)	0.023(1)	0.007(1)	0.013(1)
S25	0.091(2)	0.100(3)	0.081(1)	0.015(1)	0.002(1)	0.011(1)
C26	0.063(5)	0.098(7)	0.089(6)	0.003(4)	0.007(4)	-0.003(5)
C27	0.085(5)	0.092(7)	0.068(5)	0.003(5)	0.008(4)	-0.001(5)
S28	0.070(1)	0.109(3)	0.096(2)	-0.006(1)	-0.013(1)	-0.009(1)



Atomic numbering scheme of tetrathafulvalenophane **8c**

Positional parameters and B(eq) for **8c**

Atom	*x*	*y*	*z*	B_{eq}/Å^2
S(1)	1.2327(2)	0.0250(2)	0.9029	4.14
C(2)	1.1740(7)	-0.0377(6)	0.825(1)	3.18
S(3)	1.1116(2)	-0.0113(2)	0.6782(6)	3.71
C(4)	1.1265(8)	0.0745(7)	0.711(1)	3.81
C(5)	1.1816(8)	0.0906(6)	0.811(2)	3.82
S(6)	0.8866(2)	0.1639(2)	0.7988(5)	3.62
C(7)	0.8270(7)	0.1001(6)	0.874(2)	2.95
S(8)	0.7674(2)	0.1259(2)	1.0250(6)	4.57
C(9)	0.8308(7)	0.1941(6)	1.064(2)	3.34
C(10)	0.8864(7)	0.2129(6)	0.961(1)	3.10
S(11)	1.2115(2)	0.1700(2)	0.8581(6)	4.06
C(12)	1.1644(7)	0.1815(7)	1.037(2)	3.91
C(13)	1.0706(8)	0.1930(7)	1.031(2)	3.67
C(14)	1.0487(7)	0.2501(6)	0.934(2)	3.69
S(15)	0.9445(2)	0.2824(2)	0.9719(6)	3.90
Cl(16)	0.5000	-0.5000	0.0460(10)	9.41
Cl(17)	0.0110(9)	0.0683(3)	0.3159(9)	20.41
C(18)	0.552(2)	0.508(3)	0.213(10)	14.61

Bond lengths and angles of **8c**

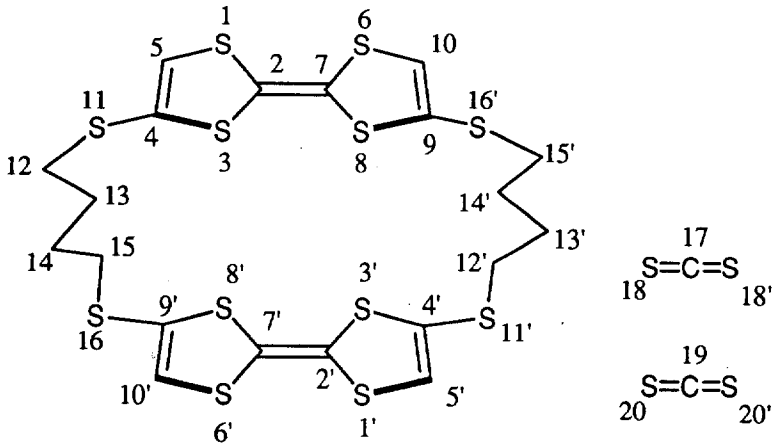
Atoms	Length/ Å	Atoms	Length/ Å
S(1)–C(2)	1.74(1)	C(9)-C(10)	1.36(2)
S(1)-C(5)	1.77(1)	C(10)-S(15)	1.70(1)
C(2)-S(3)	1.76(1)	S(11)-C(12)	1.82(1)
C(2)-C(7)	1.34(2)	C(12)-C(13)	1.55(2)
S(3)-C(4)	1.78(1)	C(13)-C(14)	1.50(2)
C(4)-C(5)	1.32(2)	C(14)-S(15)	1.85(1)
C(5)-S(11)	1.73(1)	Cl(16)-C(18)	1.75(8)
S(6)-C(7)	1.75(1)	Cl(16)-C(18)	1.75(8)
S(6)-C(10)	1.78(1)	Cl(17)-C(18)	1.93(7)
C(7)-S(8)	1.76(1)	Cl(17)-C(18)	1.85(6)
S(8)-C(9)	1.76(1)	C(18)-C(18)	1.74(8)

Atoms	Angle/°	Atoms	Angle/°
C(2)-S(1)-C(5)	95.5(6)	S(6)-C(7)-S(8)	113.0(7)
S(1)-C(2)-S(3)	113.9(6)	C(7)-S(8)-C(9)	93.8(6)
S(1)-C(2)-C(7)	124(1)	S(8)-C(9)-C(10)	118(1)
S(3)-C(2)-C(7)	121.9(9)	S(6)-C(10)-C(9)	114.7(9)
C(2)-S(3)-C(4)	95.1(6)	S(6)-C(10)-S(15)	120.4(7)
S(3)-C(4)-C(5)	117(1)	C(9)-C(10)-S(15)	124(1)

S(1)-C(5)-C(4)	117(1)	C(5)-S(11)-C(12)	102.7(7)
S(1)-C(5)-S(11)	116.5(8)	S(11)-C(12)-C(13)	114(1)
C(4)-C(5)-S(11)	126(1)	C(12)-C(13)-C(14)	112(1)
C(7)-S(6)-C(10)	94.9(6)	C(13)-C(14)-S(15)	112.4(9)
C(2)-C(7)-S(6)	125(1)	C(10)-S(15)-C(14)	102.0(6)
C(2)-C(7)-S(8)	122(1)	Cl(16)-C(18)-Cl(17)	103(2)

Anisotropic displacement parameters for **8c**

Atom	U11	U22	U33	U12	U13	U23
S(1)	0.055(2)	0.023(6)	0.078(3)	0.002(15)	-0.021(2)	0.013(2)
C(2)	0.039(6)	0.02(1)	0.058(8)	0.014(5)	-0.004(6)	0.008(6)
S(3)	0.058(2)	0.033(6)	0.050(2)	0.0004(17)	-0.006(2)	0.013(2)
C(4)	0.055(7)	0.04(1)	0.050(8)	0.014(7)	-0.004(7)	0.004(7)
C(5)	0.044(7)	0.04(1)	0.065(8)	0.008(6)	0.003(7)	0.011(7)
S(6)	0.063(2)	0.030(7)	0.044(2)	-0.009(2)	0.003(2)	-0.005(2)
C(7)	0.040(6)	0.03(1)	0.038(6)	0.009(5)	0.006(5)	-0.005(6)
S(8)	0.062(2)	0.031(7)	0.080(3)	-0.009(2)	0.027(2)	-0.018(2)
C(9)	0.050(6)	0.017(9)	0.060(8)	0.003(6)	0.005(6)	-0.008(6)
C(10)	0.059(7)	0.015(9)	0.044(6)	0.006(6)	-0.001(6)	-0.013(6)
S(11)	0.055(2)	0.024(6)	0.075(2)	-0.0001(15)	0.015(2)	0.011(2)
C(12)	0.051(7)	0.04(1)	0.052(7)	-0.002(7)	-0.006(6)	0.0004(70)
C(13)	0.051(7)	0.04(1)	0.052(7)	-0.009(6)	-0.0006(59)	0.001(7)
C(14)	0.044(6)	0.02(1)	0.074(9)	-0.003(2)	0.001(6)	-0.007(7)
S(15)	0.054(2)	0.018(7)	0.076(2)	0.030(6)	0.008(2)	-0.010(2)
Cl(16)	0.19(1)	0.092(8)	0.074(5)	0.030(6)	0.0	0.0
Cl(17)	0.61(2)	0.075(8)	0.090(5)	-0.07(9)	0.038(8)	-0.03(4)
C(18)	0.10(3)	0.13(5)	0.3(1)	0.04(3)	-0.09(4)	-0.02(5)



Atomic numbering scheme of tetrathafulvalenophane **9a**

Positional parameters and B(eq) for **9a**

atom	x	y	z	B(eq)
S(1)	1.0227(1)	0.51424(9)	0.2323(1)	4.95(3)
S(3)	0.8163(1)	0.39027(8)	0.3431(1)	4.91(3)
S(6)	0.8155(1)	0.75511(9)	0.3873(1)	4.86(3)
S(8)	0.6071(1)	0.63388(8)	0.4992(1)	5.12(3)
S(11)	0.9906(1)	0.16024(8)	0.1957(1)	4.58(2)
S(16)	0.6293(1)	0.15017(9)	-0.5855(1)	4.54(2)
S(18)	0.4052(4)	0.4417(5)	0.0675(5)	23.5(2)
S(20)	0.3849(2)	0.1108(2)	0.9984(3)	11.21(7)
C(2)	0.8585(4)	0.5228(3)	0.3331(4)	3.96(8)
C(4)	0.9647(4)	0.3093(3)	0.2264(4)	3.97(8)
C(5)	1.0549(5)	0.3675(4)	0.1780(5)	4.84(10)
C(7)	0.7714(4)	0.6227(3)	0.3975(4)	3.98(8)
C(9)	0.5463(4)	0.7826(3)	0.5064(4)	3.99(8)
C(10)	0.6438(5)	0.8344(3)	0.4561(5)	4.68(10)
C(12)	0.8410(5)	0.1404(4)	0.0353(5)	4.39(9)
C(13)	0.8655(5)	0.1720(4)	-0.1247(5)	4.68(10)
C(14)	0.7454(5)	0.1448(4)	-0.2597(5)	4.56(10)
C(15)	0.7621(5)	0.1873(4)	-0.4143(5)	4.8(1)
C(17)	0.5000	0.5000	0.0000	9.0(3)
C(19)	0.5000	0.0000	1.0000	6.2(2)
H(5)	1.140(4)	0.335(3)	0.118(4)	3.0000
H(10)	0.635(4)	0.899(3)	0.450(4)	3.0000
H(12A)	0.835(4)	0.073(3)	0.033(4)	3.0000
H(12B)	0.745(4)	0.183(3)	0.080(4)	3.0000
H(13A)	0.962(4)	0.137(3)	-0.153(4)	3.0000
H(13B)	0.856(4)	0.262(3)	-0.107(4)	3.0000
H(14A)	0.753(4)	0.059(3)	-0.285(4)	3.0000
H(14B)	0.642(4)	0.179(3)	-0.236(4)	3.0000
H(15A)	0.864(5)	0.149(4)	-0.461(5)	5.8573
H(15B)	0.746(5)	0.266(4)	-0.394(5)	5.8573

Bond lengths and angles of **9a**

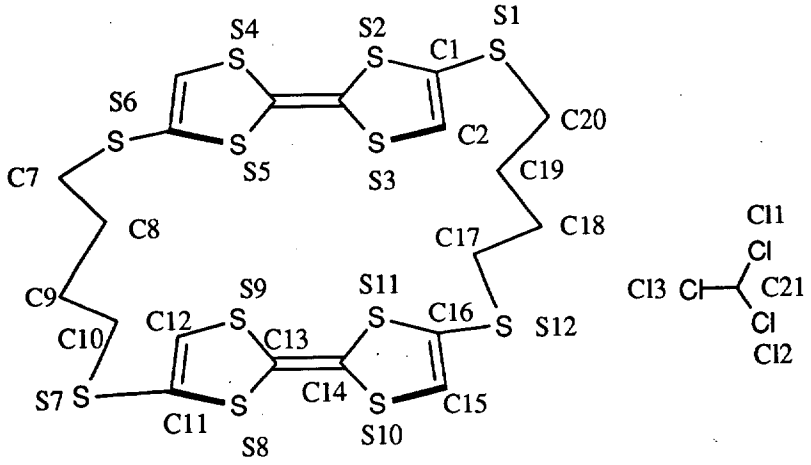
Atoms	Length/ Å	Atoms	Length/ Å
S(1)-C(2)	1.753(4)	S(16)-C(9)	1.747(4)
S(1)-C(5)	1.728(4)	S(16)-C(15)	1.817(4)
S(3)-C(2)	1.754(4)	S(18)-C(17)	1.438(3)
S(3)-C(4)	1.748(4)	S(20)-C(19)	1.499(2)
S(6)-C(7)	1.761(4)	C(2)-C(7)	1.346(5)
S(6)-C(10)	1.723(5)	C(4)-C(5)	1.324(6)
S(8)-C(7)	1.752(4)	C(9)-C(10)	1.329(6)

S(8)-C(9)	1.756(4)	C(12)-C(13)	1.501(6)
S(11)-C(4)	1.750(4)	C(13)-C(14)	1.517(6)
S(11)-C(12)	1.812(4)	C(14)-C(15)	1.501(6)

Atoms	Angle/°	Atoms	Angle/°
C(2)-S(1)-C(5)	94.2(2)	S(6)-C(7)-S(8)	114.0(2)
C(2)-S(3)-C(4)	95.2(2)	S(6)-C(7)-C(2)	122.0(3)
C(7)-S(6)-C(10)	94.2(2)	S(8)-C(7)-C(2)	124.0(3)
C(7)-S(8)-C(9)	95.1(2)	S(8)-C(9)-S(16)	118.4(2)
C(4)-S(11)-C(12)	100.6(2)	S(8)-C(9)-C(10)	115.6(3)
C(9)-S(16)-C(15)	100.9(2)	S(16)-C(9)-C(10)	125.9(3)
S(1)-C(2)-S(3)	114.6(2)	S(6)-C(10)-C(9)	119.8(3)
S(1)-C(2)-C(7)	122.9(3)	S(11)-C(12)-C(13)	114.4(3)
S(3)-C(2)-C(7)	122.5(3)	C(12)-C(13)-C(14)	112.8(4)
S(3)-C(4)-S(11)	118.4(2)	C(13)-C(14)-C(15)	112.3(3)
S(3)-C(4)-C(5)	115.9(3)	S(16)-C(15)-C(14)	114.8(3)
S(11)-C(4)-C(5)	125.5(3)	S(18)-C(17)-S(18)	180.00
S(1)-C(5)-C(4)	119.9(3)	S(20)-C(19)-S(20)	180.00

Anisotropic displacement parameters for **9a**

atom	U11	U22	U33	U12	U13	U23
S(1)	0.0763(7)	0.0548(6)	0.0626(6)	-0.0209(5)	0.0189(5)	0.0057(5)
S(3)	0.0754(7)	0.0415(5)	0.0728(7)	-0.0115(5)	0.0243(6)	0.0060(5)
S(6)	0.0599(6)	0.0454(5)	0.0840(8)	-0.0152(5)	0.0067(5)	0.0162(5)
S(8)	0.0707(7)	0.0420(5)	0.0865(8)	-0.0095(5)	0.0229(6)	0.0152(5)
S(11)	0.0668(7)	0.0439(5)	0.0572(6)	-0.0051(4)	0.0011(5)	0.0025(4)
S(16)	0.0659(6)	0.0521(6)	0.0501(6)	-0.0063(5)	0.0066(5)	0.0025(4)
S(18)	0.191(3)	0.518(7)	0.298(4)	-0.198(4)	-0.035(3)	0.242(5)
S(20)	0.101(1)	0.108(1)	0.208(2)	-0.013(1)	0.008(1)	0.014(1)
C(2)	0.060(2)	0.043(2)	0.048(2)	-0.012(2)	0.003(2)	0.008(2)
C(4)	0.059(2)	0.045(2)	0.045(2)	-0.009(2)	0.002(2)	0.003(2)
C(5)	0.063(3)	0.061(3)	0.059(2)	-0.013(2)	0.015(2)	-0.001(2)
C(7)	0.060(2)	0.042(2)	0.050(2)	-0.013(2)	0.002(2)	0.010(2)
C(9)	0.061(2)	0.043(2)	0.047(2)	-0.012(2)	-0.003(2)	0.007(2)
C(10)	0.070(3)	0.037(2)	0.071(3)	-0.012(2)	-0.001(2)	0.010(2)
C(12)	0.064(3)	0.048(2)	0.055(2)	-0.014(2)	0.010(2)	0.004(2)
C(13)	0.061(3)	0.063(3)	0.056(2)	-0.018(2)	0.003(2)	0.010(2)
C(14)	0.060(3)	0.062(3)	0.055(2)	-0.020(2)	0.005(2)	0.010(2)
C(15)	0.062(3)	0.068(3)	0.057(2)	-0.018(2)	0.004(2)	0.016(2)
C(17)	0.076(5)	0.181(10)	0.092(6)	-0.027(6)	0.001(4)	0.048(6)
C(19)	0.062(4)	0.106(6)	0.072(4)	-0.034(4)	0.008(3)	0.004(4)



Atomic numbering scheme of tetrathafulvalenophane **9c**

Positional parameters and B(eq) for **9c**

atom	x	y	z	B(eq)
Cl(1)	0.8916(5)	0.2952(6)	0.4533(2)	11.2(2)
Cl(2)	0.8706(6)	0.4592(6)	0.3699(2)	11.2(2)
Cl(3)	0.8992(5)	0.2113(5)	0.3514(2)	9.0(2)
S(1)	0.6133(4)	0.1884(4)	0.5832(2)	4.7(1)
S(2)	0.5520(4)	0.3346(4)	0.4880(2)	4.3(1)
S(3)	0.5665(4)	0.1256(4)	0.4198(2)	4.7(1)
S(4)	0.5143(4)	0.5096(4)	0.3869(2)	4.9(1)
S(5)	0.5302(4)	0.2965(4)	0.3210(2)	4.5(1)
S(6)	0.5495(4)	0.4415(5)	0.2262(2)	6.8(2)
S(7)	1.1727(4)	0.3888(4)	0.2148(2)	4.6(1)
S(8)	1.2126(4)	0.4047(4)	0.3290(2)	4.0(1)
S(9)	1.2302(4)	0.1432(3)	0.3413(2)	4.1(1)
S(10)	1.2322(4)	0.4323(4)	0.4539(2)	5.1(1)
S(11)	1.2375(4)	0.1700(4)	0.4633(2)	4.3(1)
S(12)	1.2393(4)	0.1741(4)	0.5774(2)	5.6(1)
C(1)	0.596(1)	0.193(1)	0.5145(6)	3.8(5)
C(2)	0.601(1)	0.097(1)	0.4848(6)	3.7(5)
C(3)	0.550(1)	0.281(1)	0.4249(6)	3.8(5)
C(4)	0.534(1)	0.353(1)	0.3838(6)	3.8(5)
C(5)	0.536(1)	0.538(1)	0.3203(6)	4.4(5)
C(6)	0.546(1)	0.439(2)	0.2921(6)	4.4(5)
C(7)	0.699(1)	0.361(2)	0.2184(6)	5.8(5)
C(8)	0.804(2)	0.459(1)	0.2219(6)	5.3(5)
C(9)	0.922(1)	0.379(1)	0.2166(6)	4.7(5)
C(10)	1.026(1)	0.470(1)	0.2178(6)	4.3(5)
C(11)	1.189(1)	0.316(1)	0.2735(5)	3.2(4)
C(12)	1.199(1)	0.195(1)	0.2792(5)	3.4(4)
C(13)	1.222(1)	0.283(1)	0.3703(6)	3.3(4)
C(14)	1.230(1)	0.293(1)	0.4226(6)	3.8(5)
C(15)	1.229(1)	0.375(2)	0.5163(6)	4.7(5)
C(16)	1.232(1)	0.254(2)	0.5201(6)	4.2(5)
C(17)	1.082(1)	0.108(1)	0.5752(6)	4.9(5)
C(18)	0.992(1)	0.210(1)	0.5886(6)	4.3(5)
C(19)	0.865(1)	0.149(1)	0.5827(6)	3.9(5)
C(20)	0.773(1)	0.251(1)	0.5947(6)	4.7(5)
C(21)	0.873(3)	0.319(2)	0.3926(8)	14(1)

Bond lengths and angles of **9c**

Atoms	Length/ Å	Atoms	Length/ Å

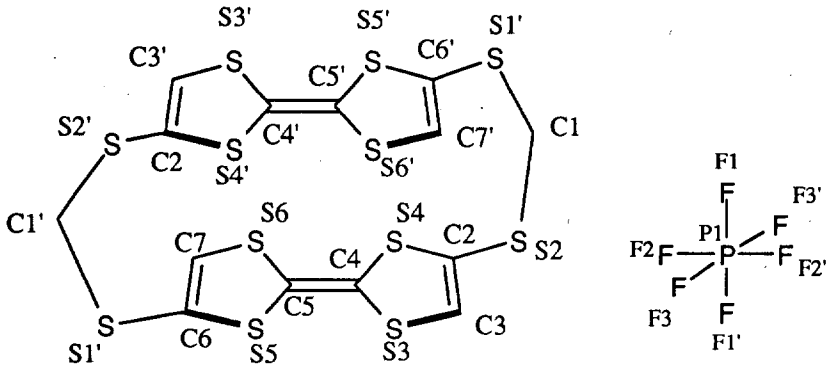
Cl(1)-C(21)	1.65(2)	S(12)-C(17)	1.86(2)
Cl(2)-C(21)	1.63(2)	C(1)-C(2)	1.31(2)
Cl(3)-C(21)	1.70(2)	S(1)-C(1)	1.77(1)
S(1)-C(20)	1.85(2)	C(3)-C(4)	1.34(2)
S(2)-C(1)	1.76(1)	C(5)-C(6)	1.30(2)
S(2)-C(3)	1.74(1)	S(3)-C(2)	1.72(1)
S(3)-C(3)	1.77(1)	C(7)-C(8)	1.50(2)
S(4)-C(4)	1.74(1)	S(4)-C(5)	1.77(2)
S(5)-C(4)	1.78(1)	C(8)-C(9)	1.55(2)
S(5)-C(6)	1.74(2)	S(6)-C(6)	1.75(1)
S(6)-C(7)	1.83(2)	S(7)-C(10)	1.83(1)
C(9)-C(10)	1.51(2)	S(7)-C(11)	1.76(1)
S(8)-C(11)	1.75(1)	S(8)-C(13)	1.75(1)
S(9)-C(12)	1.72(1)	S(9)-C(13)	1.75(1)
S(10)-C(14)	1.75(1)	S(10)-C(15)	1.73(1)
S(11)-C(14)	1.75(1)	C(11)-C(12)	1.30(2)
S(11)-C(16)	1.78(1)	S(12)-C(16)	1.74(1)
C(13)-C(14)	1.35(2)	C(15)-C(16)	1.32(2)
C(17)-C(18)	1.51(2)		

Atoms	Angle/°	Atoms	Angle/°
C(1)-S(1)-C(20)	99.9(6)	S(5)-C(4)-C(3)	121(1)
C(1)-S(2)-C(3)	94.4(6)	S(4)-C(5)-C(6)	119(1)
C(2)-S(3)-C(3)	93.9(6)	C(4)-S(4)-C(5)	93.7(7)
C(4)-S(5)-C(6)	94.5(6)	S(5)-C(6)-S(6)	117.9(9)
C(6)-S(6)-C(7)	101.5(7)	S(5)-C(6)-C(5)	117(1)
C(10)-S(7)-C(11)	101.8(6)	C(11)-S(8)-C(13)	94.2(6)
S(6)-C(6)-C(5)	125(1)	C(12)-S(9)-C(13)	93.6(6)
C(14)-S(10)-C(15)	94.8(7)	C(14)-S(11)-C(16)	95.0(6)
S(6)-C(7)-C(8)	112(1)	C(16)-S(12)-C(17)	100.5(7)
S(1)-C(1)-S(2)	117.5(8)	S(1)-C(1)-C(2)	125(1)
S(2)-C(1)-C(2)	117(1)	C(7)-C(8)-C(9)	108(1)
S(3)-C(2)-C(1)	120(1)	S(2)-C(3)-S(3)	114.5(7)
S(2)-C(3)-C(4)	123(1)	S(3)-C(3)-C(4)	122(1)
S(4)-C(4)-S(5)	113.7(6)	S(4)-C(4)-C(3)	125(1)
C(8)-C(9)-C(10)	110(1)	S(7)-C(11)-C(12)	125(1)
S(8)-C(11)-C(12)	116.7(9)	S(9)-C(12)-C(11)	120(1)
S(8)-C(13)-S(9)	114.6(6)	S(8)-C(13)-C(14)	124(1)
S(7)-C(10)-C(9)	113(1)	S(9)-C(13)-C(14)	121.8(9)
S(10)-C(14)-S(11)	114.7(7)	S(10)-C(14)-C(13)	123(1)
S(11)-C(14)-C(13)	122(1)	S(10)-C(15)-C(16)	120(1)
S(11)-C(16)-S(12)	116.7(8)	S(11)-C(16)-C(15)	115(1)
S(12)-C(16)-C(15)	128(1)	S(12)-C(17)-C(18)	113(1)
S(7)-C(11)-S(8)	117.9(7)	C(18)-C(19)-C(20)	110(1)
S(1)-C(20)-C(19)	111(1)	Cl(1)-C(21)-Cl(2)	121(2)
Cl(1)-C(21)-Cl(3)	119(1)	Cl(2)-C(21)-Cl(3)	118(1)

Anisotropic displacement parameters for **9c**

atom	U11	U22	U33	U12	U13	U23
Cl(1)	0.122(5)	0.240(7)	0.062(4)	0.008(5)	0.008(4)	0.020(5)
Cl(2)	0.183(7)	0.132(6)	0.115(5)	0.019(5)	0.044(5)	0.001(5)
Cl(3)	0.107(5)	0.125(5)	0.111(5)	-0.010(4)	0.017(4)	-0.009(4)
S(1)	0.062(3)	0.072(3)	0.046(3)	-0.002(3)	0.004(3)	0.013(3)
S(2)	0.067(3)	0.054(3)	0.040(3)	0.000(2)	-0.001(2)	0.001(2)
S(3)	0.079(4)	0.047(3)	0.052(3)	0.003(3)	0.005(3)	0.000(3)
S(4)	0.075(4)	0.048(3)	0.061(3)	0.001(3)	0.002(3)	0.000(3)
S(5)	0.063(3)	0.066(3)	0.042(3)	-0.002(3)	0.008(2)	0.000(3)
S(6)	0.060(4)	0.154(5)	0.046(3)	0.013(3)	0.007(3)	0.030(3)
S(7)	0.059(3)	0.076(3)	0.040(3)	0.004(3)	0.005(2)	0.014(3)

S(8)	0.056(3)	0.047(3)	0.048(3)	-0.002(2)	0.003(3)	0.005(2)
S(9)	0.068(3)	0.047(3)	0.041(3)	0.003(2)	0.003(2)	0.000(2)
S(10)	0.094(4)	0.051(3)	0.047(3)	-0.001(3)	0.007(3)	-0.005(3)
S(11)	0.074(4)	0.047(3)	0.043(3)	0.002(3)	0.006(2)	0.006(3)
S(12)	0.067(4)	0.107(4)	0.039(3)	0.007(3)	0.002(3)	0.014(3)
C(1)	0.03(1)	0.05(1)	0.07(1)	-0.005(9)	0.005(9)	0.02(1)
C(2)	0.03(1)	0.05(1)	0.06(1)	-0.016(9)	0.002(9)	-0.01(1)
C(3)	0.03(1)	0.07(1)	0.04(1)	-0.004(10)	-0.006(9)	0.01(1)
C(4)	0.03(1)	0.07(1)	0.05(1)	-0.008(9)	0.006(9)	0.01(1)
C(5)	0.03(1)	0.09(1)	0.05(1)	0.01(1)	0.001(10)	0.01(1)
C(6)	0.04(1)	0.08(1)	0.05(1)	0.01(1)	-0.006(10)	0.02(1)
C(7)	0.04(1)	0.11(2)	0.08(1)	0.02(1)	0.03(1)	0.00(1)
C(8)	0.04(1)	0.08(1)	0.08(1)	0.01(1)	0.01(1)	0.02(1)
C(9)	0.04(1)	0.07(1)	0.07(1)	-0.01(1)	0.01(1)	0.00(1)
C(10)	0.03(1)	0.05(1)	0.09(1)	0.020(9)	0.003(10)	0.03(1)
C(11)	0.03(1)	0.06(1)	0.026(9)	-0.004(10)	-0.005(8)	-0.01(1)
C(12)	0.04(1)	0.06(1)	0.04(1)	0.003(10)	-0.004(8)	0.00(1)
C(13)	0.04(1)	0.04(1)	0.04(1)	0.004(9)	0.002(9)	0.011(10)
C(14)	0.04(1)	0.05(1)	0.06(1)	0.011(9)	0.009(10)	0.00(1)
C(15)	0.05(1)	0.08(1)	0.05(1)	0.00(1)	0.000(10)	0.00(1)
C(16)	0.04(1)	0.09(1)	0.03(1)	0.00(1)	0.007(9)	0.00(1)
C(17)	0.05(1)	0.08(1)	0.06(1)	-0.02(1)	0.01(1)	0.02(1)
C(18)	0.03(1)	0.06(1)	0.07(1)	0.00(1)	-0.008(10)	0.00(1)
C(19)	0.04(1)	0.05(1)	0.06(1)	-0.003(10)	0.000(9)	0.010(9)
C(20)	0.04(1)	0.07(1)	0.06(1)	-0.027(10)	0.00(1)	0.00(1)
C(21)	0.35(4)	0.15(2)	0.06(2)	0.12(3)	0.05(2)	0.01(2)



Atomic numbering scheme of tetrathafulvalenophane **6**•PF_6

Positional parameters and B(eq) for **6**•PF_6

atom	x	y	z	B(eq)
S(1)	0.4868(9)	0.6757(6)	0.8889(8)	5.1(2)
S(2)	0.7035(8)	0.5271(6)	1.0157(7)	4.3(2)
S(3)	0.7398(9)	0.4789(5)	0.7609(7)	4.2(2)
S(4)	0.9501(9)	0.3793(5)	1.1711(7)	4.3(2)
S(5)	0.9905(9)	0.3320(5)	0.9161(6)	4.0(2)
S(6)	0.7648(9)	0.8041(5)	0.9547(7)	4.8(2)
P(1)	0.7401(10)	0.5979(6)	1.3987(7)	4.5(2)
F(1)	0.742(3)	0.691(1)	1.460(2)	8.9(7)
F(2)	0.740(3)	0.505(1)	1.340(2)	8.8(7)
F(3)	0.604(2)	0.625(2)	1.265(2)	8.9(7)
F(4)	0.876(2)	0.574(2)	1.533(2)	10.0(7)
F(5)	0.863(2)	0.629(2)	1.332(2)	9.0(7)
F(6)	0.613(2)	0.570(2)	1.465(2)	11.3(8)
C(1)	0.627(4)	0.742(2)	1.011(3)	5.7(9)
C(2)	0.602(3)	0.592(2)	0.873(3)	3.2(7)
C(3)	0.624(4)	0.564(2)	0.757(2)	5.0(8)
C(4)	0.794(3)	0.460(2)	0.934(2)	3.7(7)
C(5)	0.897(3)	0.399(2)	0.997(2)	2.8(6)
C(6)	1.078(3)	0.298(2)	1.179(3)	4.9(8)
C(7)	1.107(3)	0.277(2)	1.063(3)	5.1(8)
H(1)	0.5684	0.7828	1.0470	6.6218
H(2)	0.6864	0.7064	1.0866	6.6218
H(3)	0.5717	0.5941	0.6708	5.7967
H(4)	1.1308	0.2665	1.2635	5.5996

Bond lengths and angles of **6**•PF_6

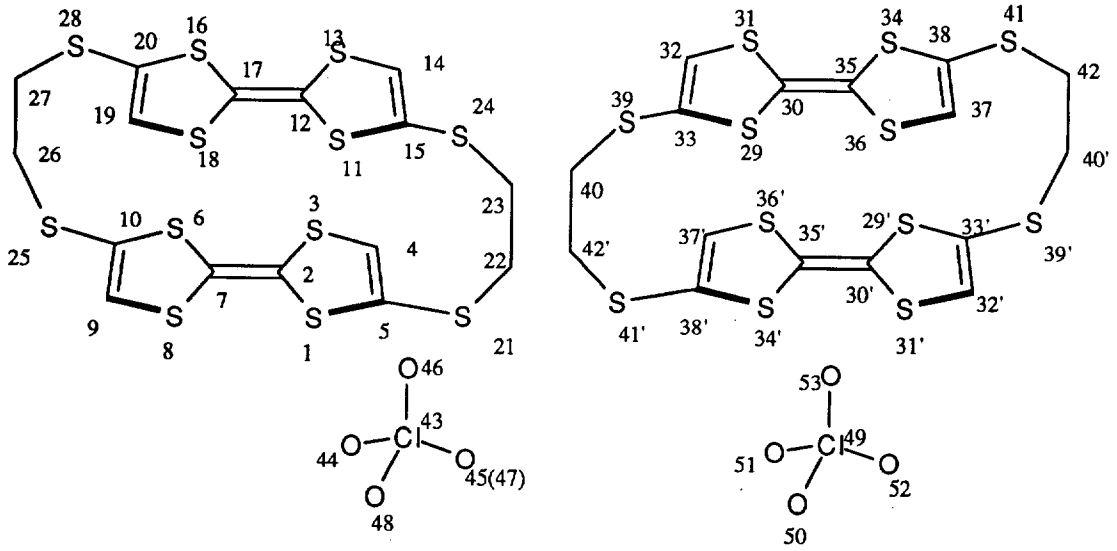
Atoms	Length/ Å	Atoms	Length/ Å
S(1)-C(1)	1.78(3)	S(6)-C(7)	1.76(3)
S(1)-C(2)	1.71(3)	P(1)-F(1)	1.58(2)
S(2)-C(2)	1.77(2)	P(1)-F(2)	1.56(2)
S(2)-C(4)	1.71(3)	P(1)-F(3)	1.57(2)
S(3)-C(3)	1.68(3)	P(1)-F(4)	1.56(2)
S(3)-C(4)	1.73(3)	P(1)-F(5)	1.57(2)
S(4)-C(5)	1.74(2)	P(1)-F(6)	1.59(2)
S(4)-C(6)	1.70(3)	C(2)-C(3)	1.36(3)
S(5)-C(5)	1.72(3)	C(4)-C(5)	1.34(3)
S(5)-C(7)	1.76(3)	C(6)-C(7)	1.36(4)
S(6)-C(1)	1.83(3)		

Atoms	Angle/°	Atoms	Angle/°
C(1)-S(1)-C(2)	102(1)	F(4)-P(1)-F(5)	91(1)

C(2)-S(2)-C(4)	97(1)	F(4)-P(1)-F(6)	90(1)
C(3)-S(3)-C(4)	96(1)	F(5)-P(1)-F(6)	178(2)
C(5)-S(4)-C(6)	97(1)	S(1)-C(1)-S(6)	118(1)
C(5)-S(5)-C(7)	97(1)	S(1)-C(2)-S(2)	121(1)
C(1)-S(6)-C(7)	102(2)	S(1)-C(2)-C(3)	127(2)
F(1)-P(1)-F(2)	179(1)	S(2)-C(2)-C(3)	112(2)
F(1)-P(1)-F(3)	91(1)	S(3)-C(3)-C(2)	120(2)
F(1)-P(1)-F(4)	87(1)	S(2)-C(4)-S(3)	114(2)
F(1)-P(1)-F(5)	90(1)	S(2)-C(4)-C(5)	124(2)
F(1)-P(1)-F(6)	89(1)	S(3)-C(4)-C(5)	122(2)
F(2)-P(1)-F(3)	90(1)	S(4)-C(5)-S(5)	114(2)
F(2)-P(1)-F(4)	92(1)	S(4)-C(5)-C(4)	122(2)
F(2)-P(1)-F(5)	91(1)	S(5)-C(5)-C(4)	124(2)
F(2)-P(1)-F(6)	91(1)	S(4)-C(6)-C(7)	118(2)
F(3)-P(1)-F(4)	178(2)	S(5)-C(7)-S(6)	118(2)
F(3)-P(1)-F(5)	89(1)	S(5)-C(7)-C(6)	115(2)
F(3)-P(1)-F(6)	90(1)	S(6)-C(7)-C(6)	127(2)

Anisotropic displacement parameters for **6**•PF_6

atom	U11	U22	U33	U12	U13	U23
S(1)	0.051(5)	0.080(7)	0.066(5)	0.015(5)	0.022(4)	0.004(5)
S(2)	0.043(5)	0.080(6)	0.043(4)	0.005(4)	0.021(4)	0.008(4)
S(3)	0.063(5)	0.058(5)	0.039(4)	0.002(5)	0.018(3)	0.001(4)
S(4)	0.049(5)	0.081(6)	0.038(4)	0.004(5)	0.020(3)	0.008(4)
S(5)	0.046(5)	0.068(6)	0.032(3)	0.008(5)	0.008(3)	0.002(4)
S(6)	0.062(5)	0.065(6)	0.053(4)	0.011(5)	0.016(4)	0.005(4)
P(1)	0.057(5)	0.070(7)	0.045(5)	-0.011(5)	0.020(4)	-0.004(5)
F(1)	0.12(2)	0.09(2)	0.13(2)	-0.02(2)	0.05(1)	-0.03(1)
F(2)	0.13(2)	0.11(2)	0.11(2)	-0.02(2)	0.05(1)	0.01(1)
F(3)	0.06(1)	0.19(2)	0.08(1)	0.03(1)	0.01(1)	0.03(1)
F(4)	0.07(1)	0.25(3)	0.05(1)	-0.01(2)	0.007(9)	0.02(1)
F(5)	0.08(1)	0.20(2)	0.08(1)	-0.05(2)	0.05(1)	-0.01(2)
F(6)	0.08(2)	0.29(3)	0.07(1)	-0.07(2)	0.04(1)	0.00(2)
C(1)	0.07(2)	0.12(3)	0.04(2)	0.00(2)	0.04(2)	0.00(2)
C(2)	0.05(2)	0.02(2)	0.06(2)	0.01(1)	0.02(1)	0.02(1)
C(3)	0.11(3)	0.06(2)	0.01(1)	-0.03(2)	0.01(2)	-0.01(1)
C(4)	0.06(2)	0.05(2)	0.04(1)	0.00(2)	0.01(1)	0.00(1)
C(5)	0.05(2)	0.03(2)	0.03(1)	0.00(2)	0.01(1)	0.00(1)
C(6)	0.05(2)	0.09(3)	0.05(2)	0.02(2)	0.02(2)	0.03(2)
C(7)	0.05(2)	0.08(3)	0.06(2)	0.04(2)	0.02(2)	0.03(2)



Atomic numbering scheme of tetrathafulvalenophane **7**•ClO_4

Positionalparametersand B(eq)for **7**•ClO_4

Atom	*x*	*y*	*z*	B_{eq}/Å^2
Cl(43)	0.1209(5)	0.2238(2)	0.7425(3)	5.7(1)
Cl(49)	-0.0880(5)	0.2470(1)	0.4833(2)	5.27(9)
S(1)	0.3716(4)	0.0379(1)	0.5699(1)	3.36(7)
S(3)	0.0841(4)	0.0996(1)	0.6083(2)	3.75(7)
S(6)	-0.1449(4)	-0.0091(1)	0.6009(1)	3.15(7)
S(8)	0.1301(4)	-0.0766(1)	0.5592(1)	3.07(6)
S(11)	0.4947(4)	-0.0019(1)	0.7261(1)	3.47(7)
S(13)	0.1987(4)	0.0544(1)	0.7663(1)	3.66(7)
S(16)	-0.0128(4)	-0.0637(1)	0.7514(1)	3.53(7)
S(18)	0.2883(4)	-0.1166(1)	0.7127(2)	3.73(7)
S(21)	0.5971(4)	0.1360(2)	0.5676(2)	4.67(8)
S(24)	0.7065(4)	0.0993(1)	0.7250(2)	4.21(8)
S(25)	-0.3926(4)	-0.1001(1)	0.5992(2)	3.71(7)
S(28)	-0.2280(4)	-0.1677(1)	0.7348(1)	4.04(8)
S(29)	0.7282(5)	0.0182(2)	0.8909(2)	4.89(9)
S(31)	0.4180(5)	0.0697(2)	0.9265(2)	5.27(9)
S(34)	0.2200(4)	-0.0470(2)	0.9138(2)	4.65(8)
S(36)	0.5210(5)	-0.1046(2)	0.8786(2)	5.38(10)
S(39)	0.9099(6)	0.1284(2)	0.8862(2)	6.9(1)
S(41)	0.0025(6)	-0.1511(2)	0.9044(2)	6.8(1)
O(44)	0.047(2)	0.1728(5)	0.7396(10)	11.7(6)
O(45)	0.021(5)	0.244(2)	0.685(2)	22(1)
O(46)	0.064(2)	0.2659(7)	0.774(1)	12.2(8)
O(47)	0.277(2)	0.2279(6)	0.727(2)	17(1)
O(48)	0.220(9)	0.215(2)	0.804(2)	18(1)
O(50)	-0.084(4)	0.228(1)	0.540(1)	26(1)
O(51)	-0.198(2)	0.2069(7)	0.453(1)	14.1(6)
O(52)	-0.147(2)	0.2987(6)	0.486(1)	15.0(7)
O(53)	0.076(2)	0.2454(5)	0.4718(9)	11.8(5)
C(2)	0.162(1)	0.0353(4)	0.5841(5)	2.7(2)
C(4)	0.264(2)	0.1379(5)	0.5990(6)	4.2(3)
C(5)	0.399(2)	0.1098(5)	0.5822(5)	3.4(3)
C(7)	0.062(1)	-0.0102(5)	0.5825(5)	2.9(3)
C(9)	-0.063(1)	-0.1103(5)	0.5648(5)	3.1(3)
C(10)	-0.188(1)	-0.0799(4)	0.5848(5)	2.8(2)
C(12)	0.290(1)	-0.0083(5)	0.7449(5)	3.2(3)
C(14)	0.376(1)	0.0940(5)	0.7609(5)	3.2(3)

C(15)	0.512(1)	0.0696(5)	0.7403(5)	3.4(3)
C(17)	0.198(1)	-0.0565(5)	0.7393(5)	3.1(3)
C(19)	0.112(2)	-0.1586(5)	0.7137(6)	4.0(3)
C(20)	-0.032(2)	-0.1333(5)	0.7307(5)	3.6(3)
C(22)	0.659(2)	0.1876(5)	0.6339(6)	4.7(3)
C(23)	0.636(2)	0.1703(5)	0.7024(6)	4.2(3)
C(26)	-0.388(2)	-0.1759(5)	0.6030(5)	3.6(3)
C(27)	-0.260(2)	-0.2032(5)	0.6551(5)	3.7(3)
C(30)	0.518(1)	0.0094(6)	0.9050(5)	4.3(3)
C(32)	0.580(2)	0.1148(7)	0.9134(7)	5.6(4)
C(33)	0.726(2)	0.0901(6)	0.8978(6)	4.6(3)
C(35)	0.431(2)	-0.0419(6)	0.8990(5)	3.8(3)
C(37)	0.343(2)	-0.1455(6)	0.8853(7)	5.5(4)
C(38)	0.204(2)	-0.1193(6)	0.9006(6)	5.1(4)
C(40)	0.954(3)	0.1644(9)	0.974(1)	11.1(8)
C(42)	-0.038(2)	-0.1254(7)	0.9955(9)	6.7(5)

Bond lengths and angles of **7**•ClO_4

Atoms	Length/ Å	Atoms	Length/ Å
Cl(43)-O(44)	1.35(1)	S(21)-C(22)	1.86(1)
Cl(43)-O(45)	1.41(3)	S(24)-C(15)	1.75(1)
Cl(43)-O(46)	1.32(1)	S(24)-C(23)	1.82(1)
Cl(43)-O(47)	1.32(1)	S(25)-C(10)	1.74(1)
Cl(43)-O(48)	1.41(3)	S(25)-C(26)	1.81(1)
Cl(49)-O(50)	1.26(2)	S(28)-C(20)	1.75(1)
Cl(49)-O(51)	1.37(1)	S(28)-C(27)	1.85(1)
Cl(49)-O(52)	1.32(1)	S(29)-C(30)	1.73(1)
Cl(49)-O(53)	1.34(1)	S(29)-C(33)	1.72(1)
S(1)-C(2)	1.71(1)	S(31)-C(30)	1.73(2)
S(1)-C(5)	1.75(1)	S(31)-C(32)	1.72(2)
S(3)-C(2)	1.76(1)	S(34)-C(35)	1.73(1)
S(3)-C(4)	1.71(1)	S(34)-C(38)	1.75(2)
S(6)-C(7)	1.72(1)	S(36)-C(35)	1.74(1)
S(6)-C(10)	1.75(1)	S(36)-C(37)	1.73(2)
S(8)-C(7)	1.77(1)	S(39)-C(33)	1.76(1)
S(8)-C(9)	1.73(1)	S(41)-C(38)	1.76(2)
S(11)-C(12)	1.72(1)	C(2)-C(7)	1.34(1)
S(11)-C(15)	1.73(1)	C(4)-C(5)	1.35(2)
S(13)-C(12)	1.75(1)	C(9)-C(10)	1.34(2)
S(13)-C(14)	1.70(1)	C(12)-C(17)	1.35(2)
S(16)-C(17)	1.72(1)	C(14)-C(15)	1.34(2)
S(16)-C(20)	1.72(1)	C(22)-C(23)	1.53(2)
S(18)-C(17)	1.73(1)	C(30)-C(35)	1.40(2)
S(18)-C(19)	1.71(1)	C(32)-C(33)	1.37(2)
S(21)-C(5)	1.74(1)	C(37)-C(38)	1.34(2)
C(19)-C(20)	1.38(2)	C(40)-C(42)	1.26(2)
C(26)-C(27)	1.51(2)		

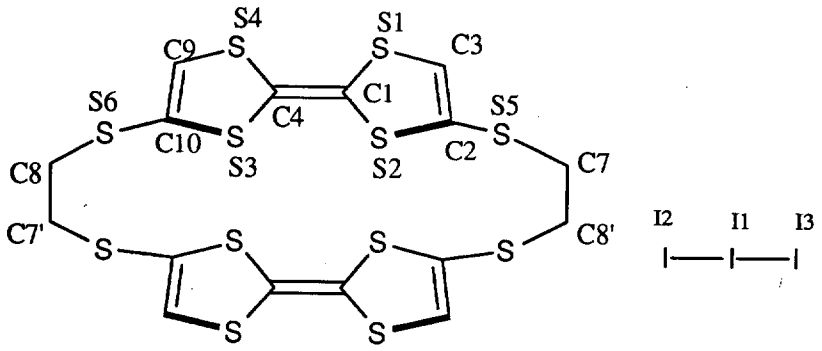
Atoms	Angle/°	Atoms	Angle/°
O(44)-Cl(43)O(45)	96(2)	C(10)-S(25)-C(26)	105.8(6)
O(44)-Cl(43)O(46)	122.2(9)	C(20)-S(28)-C(27)	99.6(6)
O(44)-Cl(43)O(47)	117.9(8)	C(30)-S(29)-C(33)	94.8(7)
O(44)-Cl(43)O(48)	95(2)	C(30)-S(31)-C(32)	95.9(7)
O(45)-Cl(43)O(46)	88(2)	C(35)-S(34)-C(38)	95.2(7)
O(45)-Cl(43)O(47)	101(2)	C(35)-S(36)-C(37)	95.9(7)
O(45)-Cl(43)O(48)	167(3)	Cl(43)O(45)-O(46)	44(1)
O(46)-Cl(43)O(47)	117.8(9)	Cl(43)O(46)-O(45)	48(2)
O(46)-Cl(43)O(48)	80(2)	Cl(43)O(46)-O(48)	52(1)

O(47)-Cl(43)O(48)	80(3)	O(45)-O(46)-O(48)	100(2)
O(50)-Cl(49)O(51)	96(2)	Cl(43)O(47)-O(48)	52(2)
O(50)-Cl(49)O(52)	105(2)	Cl(43)O(48)-O(46)	48(2)
O(50)-Cl(49)O(53)	106(2)	Cl(43)O(48)-O(47)	48(1)
O(51)-Cl(49)O(52)	118(1)	O(46)-O(48)-O(47)	80(2)
O(51)-Cl(49)O(53)	116.5(9)	Cl(49)O(50)-O(51)	44(1)
O(52)-Cl(49)O(53)	112.6(9)	Cl(49)O(51)-O(50)	39.9(8)
C(2)-S(1)-C(5)	96.3(6)	S(1)-C(2)-S(3)	113.9(6)
C(2)-S(3)-C(4)	96.0(6)	S(1)-C(2)-C(7)	126.8(8)
C(7)-S(6)-C(10)	95.9(5)	S(3)-C(2)-C(7)	119.1(8)
C(7)-S(8)-C(9)	95.3(5)	S(3)-C(4)-C(5)	117(1)
C(12)-S(11)-C(15)	95.7(6)	S(1)-C(5)-S(21)	114.9(7)
C(12)-S(13)-C(14)	95.1(5)	S(1)-C(5)-C(4)	116(1)
C(17)-S(16)-C(20)	96.2(6)	S(21)-C(5)-C(4)	129(1)
C(17)-S(18)-C(19)	96.3(6)	S(6)-C(7)-S(8)	114.3(6)
C(5)-S(21)-C(22)	104.0(6)	S(6)-C(7)-C(2)	123.5(9)
C(15)-S(24)-C(23)	100.7(6)	S(8)-C(7)-C(2)	122.2(8)
S(8)-C(9)-C(10)	117.3(9)	S(29)-C(33)-S(39)	119.2(9)
S(6)-C(10)-S(25)	112.9(6)	S(29)-C(33)-C(32)	118(1)
S(6)-C(10)-C(9)	117.2(9)	S(39)-C(33)-C(32)	123(1)
S(25)-C(10)-C(9)	129.9(9)	S(34)-C(35)-S(36)	114.9(8)
S(11)-C(12)-S(13)	114.5(7)	S(34)-C(35)-C(30)	121(1)
S(11)-C(12)-C(17)	124.1(9)	S(36)-C(35)-C(30)	124(1)
S(13)-C(12)-C(17)	121.2(9)	S(36)-C(37)-C(38)	117(1)
S(13)-C(14)-C(15)	118.6(9)	S(34)-C(38)-S(41)	118(1)
S(11)-C(15)-S(24)	114.4(7)	S(34)-C(38)-C(37)	117(1)
S(11)-C(15)-C(14)	115.9(9)	S(41)-C(38)-C(37)	125(1)
S(24)-C(15)-C(14)	130(1)	S(16)-C(17)-S(18)	114.6(7)
S(16)-C(17)-C(12)	125.7(9)	S(18)-C(17)-C(12)	119.6(9)
S(18)-C(19)-C(20)	116(1)	S(16)-C(20)-S(28)	118.9(8)
S(16)-C(20)-C(19)	116.6(9)	S(28)-C(20)-C(19)	124(1)
S(21)-C(22)-C(23)	117.6(9)	S(24)-C(23)-C(22)	114.7(9)
S(25)-C(26)-C(27)	118.0(8)	S(28)-C(27)-C(26)	115.6(8)
S(29)-C(30)-S(31)	115.2(9)	S(29)-C(30)-C(35)	124(1)
S(31)-C(30)-C(35)	120.9(9)	S(31)-C(32)-C(33)	116(1)

Anisotropic displacement parameters for **7**•ClO_4

atom	U11	U22	U33	U12	U13	U23
Cl(43)	0.065(2)	0.052(2)	0.107(4)	-0.011(2)	0.032(2)	-0.027(2)
Cl(49)	0.070(2)	0.052(2)	0.085(3)	0.001(2)	0.030(2)	-0.007(2)
S(1)	0.045(2)	0.047(2)	0.034(2)	0.002(1)	0.003(1)	0.007(1)
S(3)	0.048(2)	0.045(2)	0.047(2)	0.001(2)	0.003(1)	-0.007(1)
S(6)	0.045(2)	0.037(2)	0.037(2)	0.005(1)	0.005(1)	-0.002(1)
S(8)	0.044(2)	0.040(1)	0.034(2)	0.005(1)	0.009(1)	0.003(1)
S(11)	0.046(2)	0.050(2)	0.036(2)	0.003(1)	0.007(1)	0.002(1)
S(13)	0.046(2)	0.049(2)	0.046(2)	0.002(1)	0.012(1)	-0.001(1)
S(16)	0.042(2)	0.056(2)	0.036(2)	0.000(1)	0.005(1)	0.002(1)
S(18)	0.043(2)	0.047(2)	0.051(2)	0.005(1)	0.007(1)	0.008(1)
S(21)	0.053(2)	0.074(2)	0.053(2)	-0.012(2)	0.015(2)	-0.003(2)
S(24)	0.043(2)	0.063(2)	0.055(2)	0.000(2)	0.008(2)	0.009(2)
S(25)	0.044(2)	0.047(2)	0.052(2)	0.007(1)	0.015(1)	0.005(1)
S(28)	0.047(2)	0.067(2)	0.040(2)	-0.011(2)	0.010(1)	0.008(2)
S(29)	0.055(2)	0.082(3)	0.049(2)	-0.002(2)	0.008(2)	0.003(2)
S(31)	0.072(2)	0.079(3)	0.052(2)	-0.009(2)	0.018(2)	-0.012(2)
S(34)	0.057(2)	0.081(2)	0.041(2)	-0.013(2)	0.012(2)	-0.002(2)
S(36)	0.061(2)	0.081(3)	0.060(2)	0.017(2)	0.003(2)	0.010(2)
S(39)	0.095(3)	0.111(3)	0.062(3)	-0.037(3)	0.031(2)	-0.018(2)
S(41)	0.084(3)	0.114(3)	0.052(2)	-0.049(3)	-0.010(2)	0.007(2)
O(44)	0.078(10)	0.066(9)	0.31(3)	-0.013(7)	0.07(1)	-0.03(1)

O(45)	0.29(5)	0.34(5)	0.19(4)	-0.17(4)	-0.05(3)	0.09(3)
O(46)	0.11(1)	0.09(1)	0.29(3)	-0.022(10)	0.13(2)	-0.08(2)
O(47)	0.13(2)	0.09(1)	0.48(5)	-0.06(1)	0.19(2)	-0.15(2)
O(48)	0.48(9)	0.14(3)	0.07(2)	0.00(4)	-0.04(3)	0.00(2)
O(50)	0.38(4)	0.42(5)	0.23(3)	-0.10(4)	0.16(3)	0.11(3)
O(51)	0.081(10)	0.13(1)	0.32(3)	-0.036(9)	0.01(1)	-0.10(1)
O(52)	0.10(1)	0.073(9)	0.41(3)	0.022(8)	0.06(1)	-0.01(1)
O(53)	0.090(9)	0.080(9)	0.30(2)	-0.013(7)	0.10(1)	-0.05(1)
C(2)	0.045(7)	0.040(6)	0.014(5)	0.010(6)	-0.002(5)	-0.010(5)
C(4)	0.061(9)	0.060(8)	0.034(7)	0.008(7)	-0.003(6)	0.007(6)
C(5)	0.050(8)	0.050(7)	0.025(6)	-0.006(6)	-0.005(5)	0.007(5)
C(7)	0.040(7)	0.035(6)	0.033(6)	-0.004(5)	0.003(5)	-0.002(5)
C(9)	0.035(7)	0.050(7)	0.031(6)	0.002(6)	-0.001(5)	0.010(5)
C(10)	0.039(7)	0.035(6)	0.030(6)	0.001(5)	0.002(5)	0.003(5)
C(12)	0.038(7)	0.047(7)	0.033(7)	-0.006(6)	0.000(5)	-0.002(5)
C(14)	0.042(7)	0.050(7)	0.026(6)	0.005(6)	0.002(5)	-0.003(5)
C(15)	0.042(7)	0.053(7)	0.034(7)	0.002(6)	0.002(6)	0.002(6)
C(17)	0.038(7)	0.055(7)	0.025(6)	0.003(6)	0.000(5)	0.001(5)
C(19)	0.044(8)	0.064(8)	0.040(7)	-0.007(7)	-0.006(6)	0.020(6)
C(20)	0.053(8)	0.046(7)	0.032(7)	-0.005(6)	-0.006(6)	0.011(6)
C(22)	0.070(10)	0.054(8)	0.054(8)	-0.020(7)	0.001(7)	0.002(7)
C(23)	0.066(9)	0.036(7)	0.060(8)	0.000(6)	0.012(7)	-0.004(6)
C(26)	0.058(8)	0.040(7)	0.036(7)	0.003(6)	-0.005(6)	-0.007(6)
C(27)	0.059(8)	0.043(7)	0.036(7)	-0.007(6)	0.002(6)	0.001(6)
C(30)	0.034(7)	0.11(1)	0.015(6)	-0.003(8)	-0.007(5)	0.016(7)
C(32)	0.08(1)	0.09(1)	0.044(8)	-0.015(9)	0.009(8)	-0.004(8)
C(33)	0.066(9)	0.063(9)	0.042(8)	-0.013(7)	0.000(7)	-0.010(7)
C(35)	0.048(8)	0.071(9)	0.021(6)	-0.007(7)	-0.006(5)	0.006(6)
C(37)	0.08(1)	0.08(1)	0.050(9)	0.008(9)	-0.018(8)	0.011(8)
C(38)	0.08(1)	0.077(10)	0.029(7)	-0.016(9)	-0.016(7)	0.013(7)
C(40)	0.10(2)	0.10(2)	0.21(3)	-0.04(1)	-0.01(2)	0.03(2)
C(42)	0.07(1)	0.08(1)	0.10(1)	0.001(9)	0.000(10)	0.03(1)



Atomic numbering scheme of tetrathafulvalenophane **7**•I_3 (needle)

Positionalparametersand B(eq)for **7**•I_3 (needle)

Atom	*x*	*y*	*z*	B_{eq}/Å^2
I(1)	0.41313(7)	0.6580(1)	0.35786(9)	3.62(3)
I(2)	0.52846(8)	0.6578(1)	0.2025(1)	5.16(4)
I(3)	0.28168(9)	0.6415(1)	0.4906(1)	4.96(4)
S(1)	0.3161(3)	1.3139(4)	0.3969(4)	3.80(8)
S(2)	0.3174(3)	1.0258(4)	0.4069(4)	3.61(8)
S(3)	0.4685(3)	1.0299(4)	0.2556(4)	3.59(7)
S(4)	0.4530(3)	1.3155(4)	0.2463(4)	4.07(8)
S(5)	0.1759(2)	1.0184(4)	0.5393(3)	3.38(7)
S(6)	0.6010(3)	1.0267(5)	0.1093(3)	3.47(7)
C(1)	0.359(1)	1.169(2)	0.363(1)	3.2(3)
C(2)	0.246(1)	1.111(2)	0.474(1)	3.5(3)
C(3)	0.249(1)	1.239(2)	0.468(2)	3.9(3)
C(4)	0.421(1)	1.169(2)	0.294(1)	3.2(3)
C(7)	0.2616(10)	0.942(2)	0.671(1)	3.3(3)
C(8)	0.684(1)	0.950(2)	0.244(1)	3.6(3)
C(9)	0.525(1)	1.249(2)	0.177(2)	4.6(4)
C(10)	0.5345(10)	1.116(2)	0.181(1)	3.2(3)

Bond lengths and angles of **7**•I_3

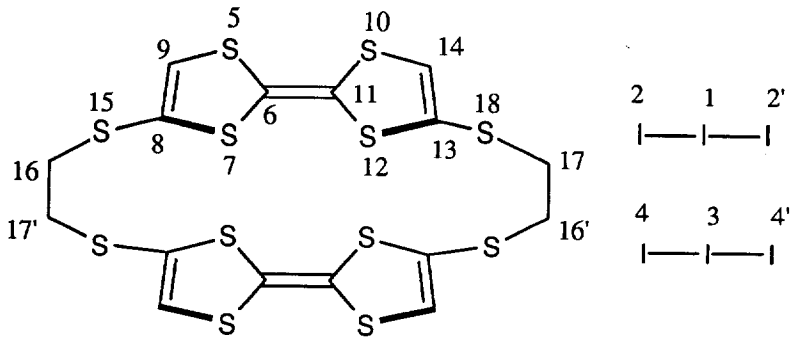
Atoms	Length/ Å	Atoms	Length/ Å
I(1)-I(2)	2.899(2)	S(4)-C(9)	1.70(2)
I(1)-I(3)	2.908(2)	S(5)-C(2)	1.76(2)
S(1)-C(1)	1.70(2)	S(5)-C(7)	1.84(1)
S(1)-C(3)	1.69(2)	S(6)-C(8)	1.84(1)
S(2)-C(1)	1.72(2)	S(6)-C(10)	1.75(2)
S(2)-C(2)	1.76(2)	C(1)-C(4)	1.42(3)
S(3)-C(4)	1.71(2)	C(2)-C(3)	1.31(3)
S(3)-C(10)	1.76(2)	C(7)-C(8)	1.53(2)
S(4)-C(4)	1.70(2)	C(9)-C(10)	1.36(3)

Atoms	Angle/°	Atoms	Angle/°
I(2)-I(1)-I(3)	173.23(5)	S(5)-C(2)-C(3)	126(2)
C(1)-S(1)-C(3)	94.1(9)	S(1)-C(3)-C(2)	121(2)
C(1)-S(2)-C(2)	93.8(9)	S(3)-C(4)-S(4)	116(1)
C(4)-S(3)-C(10)	94.8(8)	S(3)-C(4)-C(1)	124(1)
C(4)-S(4)-C(9)	96(1)	S(4)-C(4)-C(1)	120(1)
C(2)-S(5)-C(7)	101.4(7)	S(5)-C(7)-C(8)	110(1)
C(8)-S(6)-C(10)	99.8(7)	S(6)-C(8)-C(7)	110(1)
S(1)-C(1)-S(2)	116(1)	S(4)-C(9)-C(10)	117(2)
S(1)-C(1)-C(4)	120(1)	S(3)-C(10)-S(6)	119(1)
S(2)-C(1)-C(4)	123(1)	S(3)-C(10)-C(9)	116(1)
S(2)-C(2)-S(5)	119(1)	S(6)-C(10)-C(9)	125(1)

S(2)-C(2)-C(3)	115(1)

Anisotropic displacement parameters for **7**•I_3

atom	U11	U22	U33	U12	U13	U23
I(1)	0.0431(6)	0.0488(7)	0.0502(7)	-0.0030(4)	0.0210(5)	-0.0057(5)
I(2)	0.0522(7)	0.0744(9)	0.0854(9)	-0.0170(6)	0.0443(7)	-0.0162(7)
I(3)	0.0720(9)	0.0691(9)	0.0641(8)	-0.0032(6)	0.0457(7)	-0.0129(6)
S(1)	0.055(2)	0.044(2)	0.061(2)	0.007(2)	0.042(2)	-0.001(2)
S(2)	0.046(2)	0.052(2)	0.051(2)	0.005(2)	0.032(2)	0.002(2)
S(3)	0.044(2)	0.052(2)	0.053(2)	0.004(2)	0.034(2)	0.002(2)
S(4)	0.057(2)	0.046(2)	0.068(3)	0.000(2)	0.043(2)	0.002(2)
S(5)	0.028(2)	0.063(2)	0.042(2)	-0.002(2)	0.017(1)	0.003(2)
S(6)	0.041(2)	0.067(3)	0.031(2)	0.006(2)	0.022(2)	0.000(2)
C(1)	0.034(7)	0.044(9)	0.040(8)	0.005(7)	0.005(6)	-0.002(7)
C(2)	0.037(8)	0.07(1)	0.029(7)	-0.004(8)	0.015(6)	-0.005(8)
C(3)	0.036(8)	0.07(1)	0.052(10)	0.003(8)	0.030(8)	0.006(9)
C(4)	0.041(8)	0.045(9)	0.042(8)	-0.005(7)	0.020(7)	0.003(7)
C(7)	0.034(8)	0.042(9)	0.044(8)	0.002(6)	0.004(6)	0.002(7)
C(8)	0.041(8)	0.053(10)	0.041(8)	-0.002(7)	0.012(7)	-0.013(7)
C(9)	0.039(9)	0.08(1)	0.07(1)	0.003(9)	0.037(8)	0.00(1)
C(10)	0.028(7)	0.06(1)	0.032(7)	0.017(7)	0.012(6)	0.007(7)



Atomic numbering scheme of tetrathafulvalenophane **7**•I_3 (plate)

Positionalparametersand B(eq)for **7**•I3 (plate)

Atom	*x*	*y*	*z*	B_{eq}/Å^2
I(1)	0.0000	0.0000	1.0000	4.32(6)
I(2)	0.1899(3)	-0.0214(3)	0.9497(2)	5.86(6)
I(3)	1.0000	0.5000	1.0000	29.9(7)
I(4)	0.642(1)	0.158(1)	0.9961(5)	17.8(3)
S(5)	0.6159(7)	0.4721(7)	0.7839(7)	3.4(1)
S(7)	0.3127(7)	0.1825(6)	0.4743(8)	3.2(1)
S(10)	0.4724(8)	0.5693(8)	0.8108(7)	3.7(1)
S(12)	0.1642(7)	0.2872(7)	0.5010(8)	3.4(1)
S(15)	0.4574(7)	0.0971(7)	0.4330(9)	3.8(1)
S(18)	0.0619(7)	0.4226(8)	0.4950(9)	4.1(1)
C(6)	0.414(3)	0.346(3)	0.636(3)	2.7(4)
C(8)	0.470(2)	0.216(2)	0.555(3)	2.8(4)
C(9)	0.603(2)	0.347(3)	0.692(3)	2.6(4)
C(11)	0.351(2)	0.390(3)	0.654(3)	2.9(4)
C(13)	0.193(3)	0.429(3)	0.606(4)	3.8(5)
C(14)	0.326(3)	0.550(3)	0.749(3)	3.2(4)
C(16)	-0.222(2)	0.132(3)	0.610(3)	3.1(4)
C(17)	-0.171(3)	0.190(3)	0.456(3)	3.5(4)

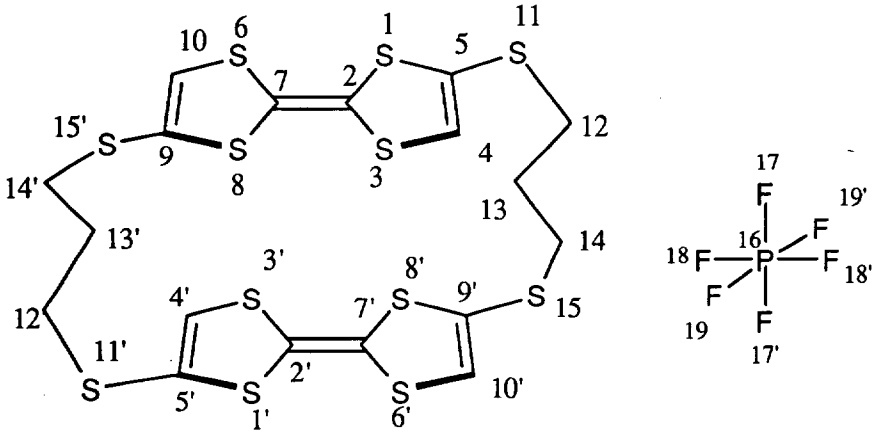
Bond lengths and angles of **7**•I3

Atoms	Length/ Å	Atoms	Length/ Å
S(5)-C(6)	1.74(3)	S(15)-C(8)	1.76(4)
S(5)-C(9)	1.70(4)	S(15)-C(16)	1.81(2)
S(7)-C(6)	1.70(3)	S(18)-C(13)	1.78(5)
S(7)-C(8)	1.77(4)	S(18)-C(17)	1.81(2)
S(10)-C(11)	1.71(3)	C(6)-C(11)	1.42(7)
S(10)-C(14)	1.74(5)	C(8)-C(9)	1.30(2)
S(12)-C(11)	1.73(3)	C(13)-C(14)	1.30(3)
S(12)-C(13)	1.79(5)	C(16)-C(17)	1.45(3)

Atoms	Angle/°	Atoms	Angle/°
C(6)-S(5)-C(9)	93(2)	S(15)-C(8)-C(9)	125(3)
C(6)-S(7)-C(8)	94(2)	S(5)-C(9)-C(8)	121(3)
C(11)-S(10)-C(14)	96(2)	S(10)-C(11)-S(12)	116(3)
C(11)-S(12)-C(13)	93(2)	S(10)-C(11)-C(6)	122(2)
C(8)-S(15)-C(16)	102(2)	S(12)-C(11)-C(6)	122(2)
C(13)-S(18)-C(17)	103(2)	S(12)-C(13)-S(18)	118(1)
S(5)-C(6)-S(7)	116(3)	S(12)-C(13)-C(14)	118(4)
S(5)-C(6)-C(11)	118(2)	S(18)-C(13)-C(14)	122(4)
S(7)-C(6)-C(11)	125(2)	S(10)-C(14)-C(13)	116(4)
S(7)-C(8)-S(15)	119(1)	S(15)-C(16)-C(17)	113(1)
S(7)-C(8)-C(9)	115(3)	S(18)-C(17)-C(16)	115(1)

Anisotropic displacement parameters for **7**•I_3

atom	U11	U22	U33	U12	U13	U23
I(1)	0.053(1)	0.059(1)	0.052(1)	0.049(1)	-0.0079(10)	-0.011(1)
I(2)	0.087(1)	0.107(2)	0.062(1)	0.091(1)	-0.0050(10)	-0.0115(10)
I(3)	0.68(2)	0.66(2)	0.122(5)	0.66(2)	-0.216(8)	-0.210(7)
I(4)	0.50(1)	0.52(1)	0.053(2)	0.50(1)	0.048(4)	0.050(4)
S(5)	0.041(3)	0.048(3)	0.048(3)	0.040(3)	0.003(2)	0.004(2)
S(7)	0.034(2)	0.031(2)	0.055(3)	0.029(2)	0.004(2)	0.008(2)
S(10)	0.053(3)	0.054(3)	0.045(3)	0.047(3)	0.010(3)	0.008(3)
S(12)	0.030(2)	0.038(3)	0.062(4)	0.029(2)	0.006(2)	0.009(2)
S(15)	0.043(3)	0.038(3)	0.076(4)	0.034(3)	0.031(3)	0.022(3)
S(18)	0.038(3)	0.049(3)	0.088(5)	0.040(3)	0.024(3)	0.033(3)
C(6)	0.034(10)	0.04(1)	0.04(1)	0.030(9)	0.021(9)	0.018(9)
C(8)	0.025(9)	0.022(9)	0.07(1)	0.021(9)	0.009(10)	0.003(9)
C(9)	0.022(9)	0.04(1)	0.05(1)	0.027(9)	0.019(9)	0.033(10)
C(11)	0.024(9)	0.04(1)	0.04(1)	0.028(9)	0.001(9)	0.001(9)
C(13)	0.026(10)	0.03(1)	0.09(2)	0.023(9)	0.02(1)	0.01(1)
C(14)	0.06(1)	0.04(1)	0.05(1)	0.05(1)	0.04(1)	0.03(1)
C(16)	0.024(9)	0.03(1)	0.03(1)	0.018(9)	0.013(8)	0.001(9)
C(17)	0.04(1)	0.05(1)	0.05(1)	0.04(1)	0.01(1)	0.02(1)



Atomic numbering scheme of tetrathafulvalenophane **8**•PF_6

Positional parameters and B(eq) for **8**•PF_6

Atom	x	y	z	Beq/Å2
S1	0.2604(2)	0.0333(2)	0.2140(3)	4.01
C2	0.4776(9)	0.0285(6)	0.2433(11)	2.99
S3	0.5404(2)	-0.1071(2)	0.2113(3)	3.91
C4	0.3376(9)	-0.176O(7)	0.1618(12)	3.62
C5	0.7897(9)	0.1129(7)	0.8352(11)	3.26
S6	0.5189(3)	0.2568(2)	0.3067(4)	4.37
C7	0.5861(9)	0.1231(6)	0.2831(11)	2.93
S8	0.8050(3)	0.1223(2)	0.3106(3)	3.79
C9	0.8508(10)	0.2681(7)	0.3538(12)	3.44
C10	0.7170(10)	0.3286(7)	0.3545(13)	3.89
S11	1.0055(2)	0.1538(2)	0.8825(3)	4.02
C12	1.0182(10)	0.3071(7)	0.9276(12)	3.78
C13	0.9919(10)	0.5448(7)	0.7614(11)	3.52
C14	1.1146(10)	0.2937(8)	0.6039(11)	3.91
S15	1.O623(3)	0.3264(2)	0.395312)	3.94
P16	0.5000(0)	0.5000(0)	1.0000(0)	4.24
F17	0.5175(7)	0.5330(5)	0.9651(12)	7.95
F18	0.5659(9)	0.6280(5)	1.0773(15)	10.43
F19	0.4567(15)	0.5011(2)	1.1960(14)	14.20

Bond lengths and angles of **8**•PF_6

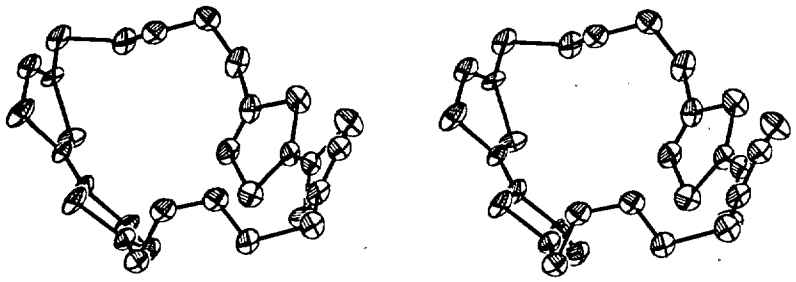
Atoms	Length/Å	Atoms	Length/Å
S(1)-C(2)	1.744(7)	S(8)-C(9)	1.743(8)
S(1)-C(5)	1.745(8)	C(9)-C(10)	1.35(1)
C(2)-C(7)	1.35(1)	C(9)-S(15)	1.758(8)
C(2)-S(3)	1.740(8)	S(11)-C(12)	1.820(9)
S(3)-C(4)	1.738(7)	C(12)-C(13)	1.51(1)
C(4)-C(5)	1.33(1)	C(13)-C(14)	1.55(1)
C(5)-S(11)	1.747(7)	C(14)-S(15)	1.82(1)
S(6)-C(10)	1.719(8)	P(16)-F(17)	1.581(6)
S(6)-(C7)	1.742(8)	P(16)-F(18)	1.551(6)
C(7)-S(8)	1.749(7)	P(16)-F(19)	1.53(1)

Atoms	Angles/°	Atoms	Angles/°
C(2)-S(1)-C(5)	95.3(4)	C(10)-C(9)-S(15)	124.6(6)
C(7)-C(2)-S(3)	123.8(6)	S(8)-C(9)-S(15)	119.2(5)
C(7)-C(2)-S(1)	121.786)	C(9)-C(10)-S(6)	118.3(6)
S(3)-C(2)-S(1)	114.5(4)	C(5)-S(11)-C(12)	103.0(4)
C(4)-S(3)-C(2)	95.3(4)	C(13)-C(12)-S(11)	116.4(5)
S(3)-C(4)-C(5)	117.8(6)	C(12)-C(13)-C(14)	112.5(8)

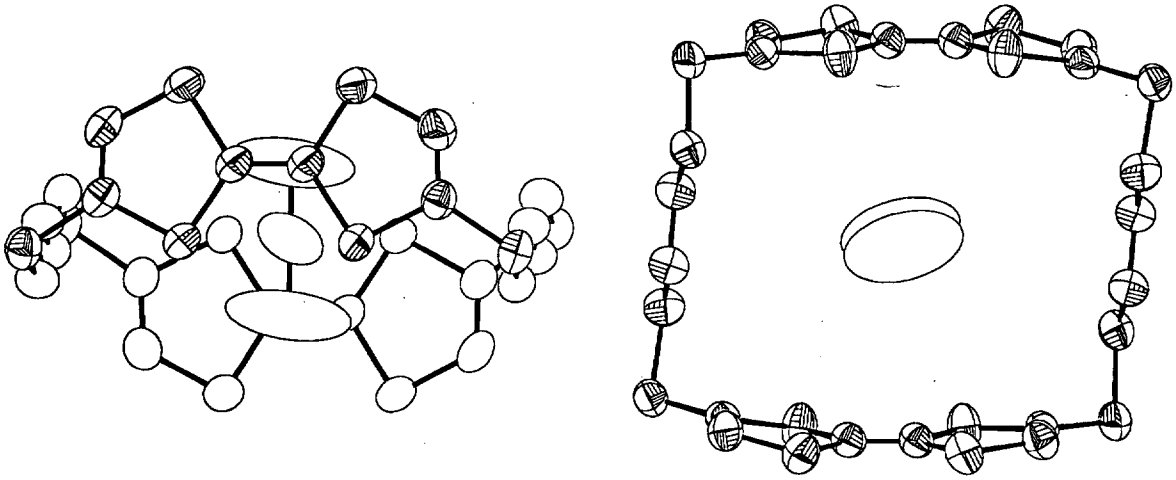
S(11)-C(5)-C(2)	129.8(6)	C(13)-C(14)-S(15)	111.3(7)
S(11)-C(5)-S(1)	113.1(5)	C(9)-S(15)-C(14)	100.4(4)
C(4)-C(5)-S(1)	117.1(6)	F(19)-P(16)-F(18)	90.7(7)
C(10)-S(6)-C(7)	95.6(4)	F(19)-P(16)-F(17)	91.8(6)
C(2)-C(7)-S(6)	122.4(6)	F(18)-P(16)-F(17)	90.6(3)
C(2)-C(7)-S(8)	123.3(6)	F(18)-P(16)-F(19)	89.3(7)
S(6)-C(7)-S(8)	114.3(4)	F(17)-P(16)-F(19)	88.2(6)
C(9)-S(8)-C(7)	95.7(4)	F(17)-P(16)-F(18)	89.4(3)
C(10)-C(9)-S(8)	116.1(6)		

Anisotropic Displacement Parameters for **8** •PF_6

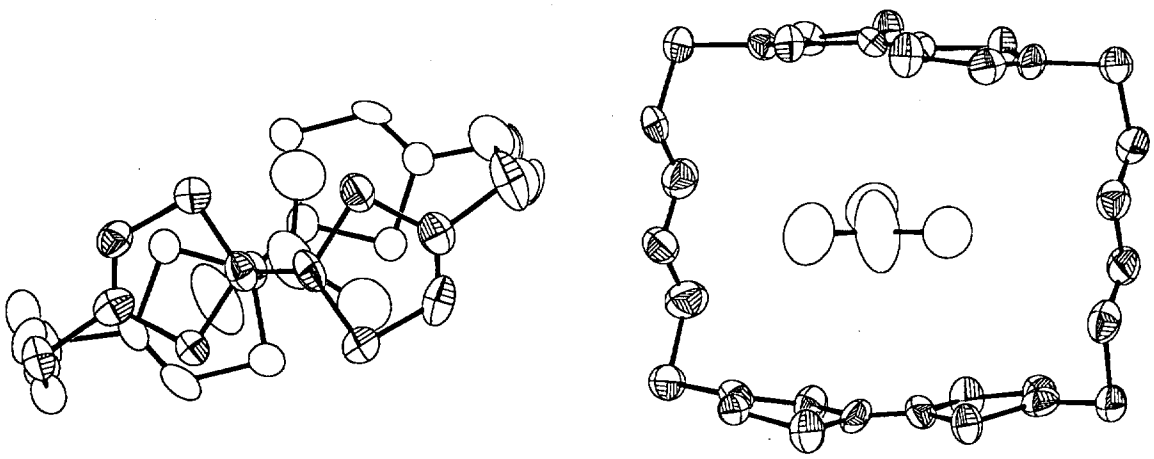
Atom	U11	U22	U33	U12	U13	U23
C1	0.01085	0.005810	0.028640	0.002140	-0.001780	0.006990
C2	0.00828	0.005640	0.018390	-0.000310	-0.001620	0.007050
S3	0.00946	0.006650	0.028580	0.000610	-0.003540	0.011080
C4	0.01011	0.006250	0.022980	-0.002110	-0.001600	0.007650
C5	0.01050	0.006260	0.019560	0.001400	0.002930	0.009820
S6	0.01207	0.006420	0.030930	0.001990	0.000670	0.008120
C7	0.00908	0.005490	0.016640	0.000520	-0.003090	0.005960
S8	0.01135	0.006360	0.024440	-0.000700	-0.004520	0.008920
C9	0.01432	0.005620	0.017660	-0.000620	-0.002210	0.007210
C10	0.01376	0.006310	0.022050	-0.002720	-0.001400	0.007300
S11	0.00961	0.007140	0.028490	0.000820	-0.001090	0.010970
C12	0.01455	0.006140	0.019460	-0.003080	-0.003040	0.005980
C13	0.01531	0.006900	0.013890	0.002700	0.004650	0.005770
C14	0.01281	0.009620	0.014770	-0.000630	-0.004300	0.007400
S15	0.01310	0.008100	0.019330	-0.004540	-0.001560	0.009140
P16	0.01112	0.005740	0.032650	0.000980	-0.009650	0.009550
F17	0.01427	0.008340	0.073600	-0.000260	-0.027120	0.016170
F18	0.01948	0.006490	0.104000	-0.000960	-0.042560	0.014610
F19	0.06449	0.035990	0.046640	0.026090	0.036540	0.047210



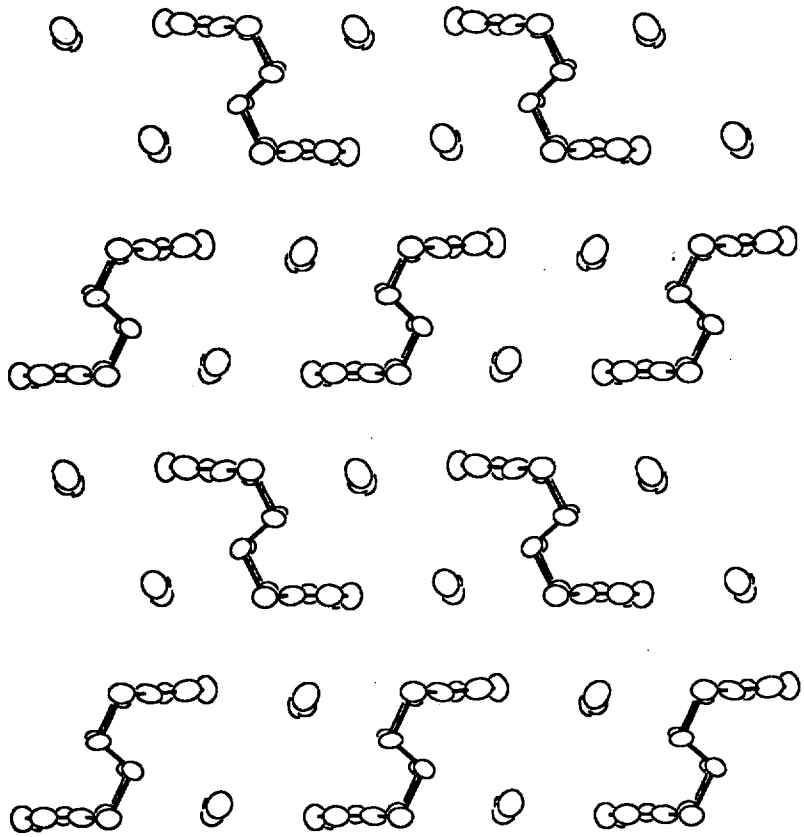
Stereo view of **8c** (trans/trans): The solvent of crystallization ($CHCl_3$) occupying the interstitial position is omitted for clarity).



ORTEP drawing of **9a** (cis/cis): (left) top view and (right) side view. One of two solvent molecules (CS_2) is omitted, and the other is included in the cavity.



ORTEP drawing of **9c** (trans/trans): The solvent molecule ($CHCl_3$) is included in the cavity. (left) top view and (right) side view.



Packing diagram of **7**•I_3 (insulator salt): no S••••S contact is observed.