JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
J. Am. Chem. Soc., 1998, 120(15), 3641-3649, DOI:10.1021/ja974072a

Data Collection and Reduction.

Diffractometer type	Siemens P4
Radiation source	rotating-anode
Monochromator type	graphite
Radiation	MoKα
Wavelength	0.71073 Å
Temperature	158 K
Cell measurement reflections	30 ($4.18^{\circ} < \theta < 13.39^{\circ}$)
Intensity measurement method	ω scans
θ range for data collection	2.78 to 27.50°
Limiting indices	$0 \leq h \leq 6$, $0 \leq k \leq 7$, $-38 \leq l \leq 38$
Scan width (in ω)	1.2° plus α_1,α_2 separation
Scan speed (in ω)	4.0°/min
Reflections collected	2218
Independent reflections	1988 (R_{int} = 0.0337)
Observed reflections	1309 (I >2sigma(I))
Number of standards	2
Interval between standards	98
Decay of standards	< 1.0
Absorption correction	None

Unit cell refinement and data collection were carried out by use of the Siemens XSCAnS system, Version 2.10b. Data were processed with a local version of CARESS (R.W. Broach et al.), which employs a modified version of the Lehman-Larsen algorithm to obtain integrated intensities and standard deviations from the measured 96-step peak profiles.

Structure Solution and Refinement.

Structure solution method	direct methods
Refinement method	Full-matrix least-squares on F^2
Scattering Factor Source	International Tables Vol C Tables 4.2.6.8 and 6.1.1.4
Final refinement: Data	1988
Restraints	0
Parameters	162
Final R indices [$I>2\sigma(I)$]	R1 = 0.0591, wR2 = 0.1453
R indices (all data)	R1 = 0.0948, wR2 = 0.1718
Goodness-of-fit on F^2	1.068
Extinction coefficient	0.011(5)
Largest diff. peak and hole	0.399 and −0.375 $e\text{Å}^{-3}$
Maximum Δ/σ in final cycle	0.000
Mean Δ/σ in final cycle	0.000

Final weighting scheme:

calc $w=1/[\sigma^2(Fo^2)+(0.1028P)^2+0.0233P]$

where $P=(Fo^2+2Fc^2)/3$

R-factor definitions:

$R1 = \sum||F_o|-|F_c||/\sum|F_o|$

$wR2 = [\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]]^{1/2}$

Structure solution, refinement, and generation of figures and tables were carried out by use of Version 5.03 of the Siemens SHELXTL program package.

Table 3. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	8983(5)	6350(4)	4654(1)	20(1)
C(2)	7922(5)	4250(4)	4691(1)	17(1)
C(3)	8968(5)	2925(4)	5044(1)	21(1)
C(4)	5758(5)	3369(4)	4382(1)	20(1)
C(5)	4610(5)	4398(4)	4026(1)	19(1)
C(6)	2445(5)	3584(4)	3711(1)	17(1)
C(7)	1557(5)	4890(4)	3345(1)	21(1)
C(8)	-527(5)	4287(5)	3041(1)	24(1)
C(9)	-1823(5)	2310(5)	3090(1)	24(1)
C(10)	-1003(6)	966(4)	3445(1)	24(1)
C(11)	1085(5)	1586(4)	3741(1)	20(1)
F(1)	2776(3)	6827(3)	3279(1)	32(1)
F(2)	-1305(4)	5621(3)	2699(1)	37(1)
F(3)	-3866(3)	1707(3)	2802(1)	34(1)
F(4)	-2301(4)	-943(3)	3506(1)	36(1)
F(5)	1752(4)	194(3)	4082(1)	31(1)

Table 4. Bond lengths [Å] and angles [°] for 1.

C(1)-C(3)#1	1.387(3)	C(1)-C(2)	1.394(4)
C(2)-C(3)	1.401(3)	C(2)-C(4)	1.471(3)
C(3)-C(1)#1	1.387(3)	C(4)-C(5)	1.331(3)
C(5)-C(6)	1.469(3)	C(6)-C(11)	1.396(4)
C(6)-C(7)	1.399(3)	C(7)-F(1)	1.344(3)
C(7)-C(8)	1.380(3)	C(8)-F(2)	1.341(3)
C(8)-C(9)	1.377(4)	C(9)-F(3)	1.337(3)
C(9)-C(10)	1.378(4)	C(10)-F(4)	1.345(3)
C(10)-C(11)	1.371(3)	C(11)-F(5)	1.349(3)
C(1)-H(1)	0.97(3)	C(3)-H(3)	0.96(3)
C(4)-H(4)	0.93(3)	C(5)-H(5)	0.95(3)

C(3)#1-C(1)-C(2)	120.5(2)	C(1)-C(2)-C(3)	117.9(2)
C(1)-C(2)-C(4)	123.5(2)	C(3)-C(2)-C(4)	118.6(2)
C(1)#1-C(3)-C(2)	121.6(2)	C(5)-C(4)-C(2)	125.9(2)
C(4)-C(5)-C(6)	127.6(2)	C(11)-C(6)-C(7)	114.6(2)
C(11)-C(6)-C(5)	126.1(2)	C(7)-C(6)-C(5)	119.3(2)
F(1)-C(7)-C(8)	117.5(2)	F(1)-C(7)-C(6)	119.3(2)
C(8)-C(7)-C(6)	123.2(2)	F(2)-C(8)-C(9)	119.8(2)
F(2)-C(8)-C(7)	120.4(2)	C(9)-C(8)-C(7)	119.8(2)
F(3)-C(9)-C(8)	120.7(2)	F(3)-C(9)-C(10)	120.4(3)
C(8)-C(9)-C(10)	118.9(2)	F(4)-C(10)-C(11)	119.9(2)
F(4)-C(10)-C(9)	119.7(2)	C(11)-C(10)-C(9)	120.4(2)
F(5)-C(11)-C(10)	116.9(2)	F(5)-C(11)-C(6)	120.0(2)
C(10)-C(11)-C(6)	123.1(2)	C(3)#1-C(1)-H(1)	117(2)
C(2)-C(1)-H(1)	122(2)	C(1)#1-C(3)-H(3)	122(2)
C(2)-C(3)-H(3)	117(2)	C(5)-C(4)-H(4)	119(2)
C(2)-C(4)-H(4)	115(2)	C(4)-C(5)-H(5)	120(2)
C(6)-C(5)-H(5)	112(2)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z+1

Table 5. Anisotropic displacement parameters [$Å^2$ x 10^3] for 1.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
C(1)	25(1)	19(1)	15(1)	3(1)	-10(1)	-2(1)
C(2)	20(1)	20(1)	12(1)	-1(1)	-6(1)	0(1)
C(3)	26(1)	15(1)	20(1)	0(1)	-8(1)	-3(1)
C(4)	23(1)	16(1)	19(1)	-2(1)	-7(1)	-4(1)
C(5)	22(1)	18(1)	17(1)	-1(1)	-8(1)	-3(1)
C(6)	19(1)	19(1)	14(1)	-3(1)	-5(1)	-2(1)
C(7)	23(1)	21(1)	19(1)	2(1)	-6(1)	-3(1)
C(8)	26(1)	30(2)	16(1)	5(1)	-11(1)	-2(1)
C(9)	21(1)	33(2)	16(1)	-6(1)	-10(1)	-3(1)
C(10)	27(1)	22(1)	22(1)	-4(1)	-5(1)	-7(1)
C(11)	24(1)	20(1)	16(1)	1(1)	-6(1)	-1(1)
F(1)	37(1)	25(1)	32(1)	12(1)	-17(1)	-11(1)
F(2)	38(1)	45(1)	28(1)	16(1)	-20(1)	-5(1)
F(3)	29(1)	47(1)	27(1)	-6(1)	-18(1)	-10(1)
F(4)	40(1)	27(1)	40(1)	-1(1)	-15(1)	-17(1)
F(5)	42(1)	23(1)	28(1)	10(1)	-18(1)	-11(1)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(1)	8380(55)	7342(47)	4416(10)	15(7)
H(3)	8260(62)	1470(52)	5057(10)	29(8)
H(4)	5301(62)	1924(55)	4432(11)	32(9)
H(5)	5084(56)	5866(52)	3964(10)	21(7)

$$C_6F_5 - CH = CH - C_6H_4 - CH = CH - C_6F_5 \cdot C_6H_4(CH_3)_2$$

trans, trans − 1, 4 − bis(pentafluorophenylvinyl)benzene · o − xylene

Solution and Refinement:

There was some anisotropic movement and/or decay of the crystal. A number of reflections, particularly near the end of data collection, had one large background. Therefore a background function of θ was calculated for weak reflections excluding those with anomalous backgrounds and then applied to all the data. When the data were merged, some of these reflections were still significantly weak and thus deleted. During refinement other much-smaller-than-calculated reflections were deleted. A total of approximately 200 reflections were thereby removed.

The structure was solved with SHELXS-86. The hydrogen atoms were placed initially at calculated positions. Their coordinates and isotropic displacement parameters were then refined. Refinement, including hydrogen atom coordinates and isotropic displacement parameters, was full-matrix least-squares using CRYM programs.

The GOF value of 3.19 is still high, but there seem to be no ill effects on the structure. Indeed, much of the magnitude of the GOF can be attributed to the intensity of the data set.

Weights w are calculated as $1/\sigma^2(F_o^2)$; variances ($\sigma^2(F_o^2)$) were derived from counting statistics plus an additional term, $(0.014I)^2$; variances of the merged data were obtained by propagation of error plus another additional term, $(0.014\bar{I})^2$.

Definitions:

$$R = \frac{\Sigma||F_o| - |F_c||}{\Sigma F_o}; \quad R_w = \left\{\frac{\Sigma w(F_o^2 - F_c^2)^2}{\Sigma w(F_o^2)^2}\right\}^{\frac{1}{2}}$$

$$S = \left\{\frac{\Sigma w(F_o^2 - F_c^2)^2}{n - p}\right\}^{\frac{1}{2}}$$

where n = number of data,

p = number of parameters refined.

References

The CRYM Crystallographic Computing System

Duchamp, D. J. (1964). Am. Crystallogr. Assoc. Meet., Bozeman, Montana, Paper B14, p. 29-30.

SHELXS-86

Sheldrick, G. M. (1990). *Acta Cryst.* **A46,** 467-473.

ORTEP

Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA.

Scattering Factors and f′, f″:

Cromer, D. T. & Waber, J. T. (1974). *International Tables For X-ray Crystallography*, Vol. IV, pp. 99–101. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

Creagh, D. C. & McAuley, W. J. (1992). *International Tables For Crystallography*, Vol. C, pp. 219–222. Dordrecht: Kluwer Academic Publishers.)

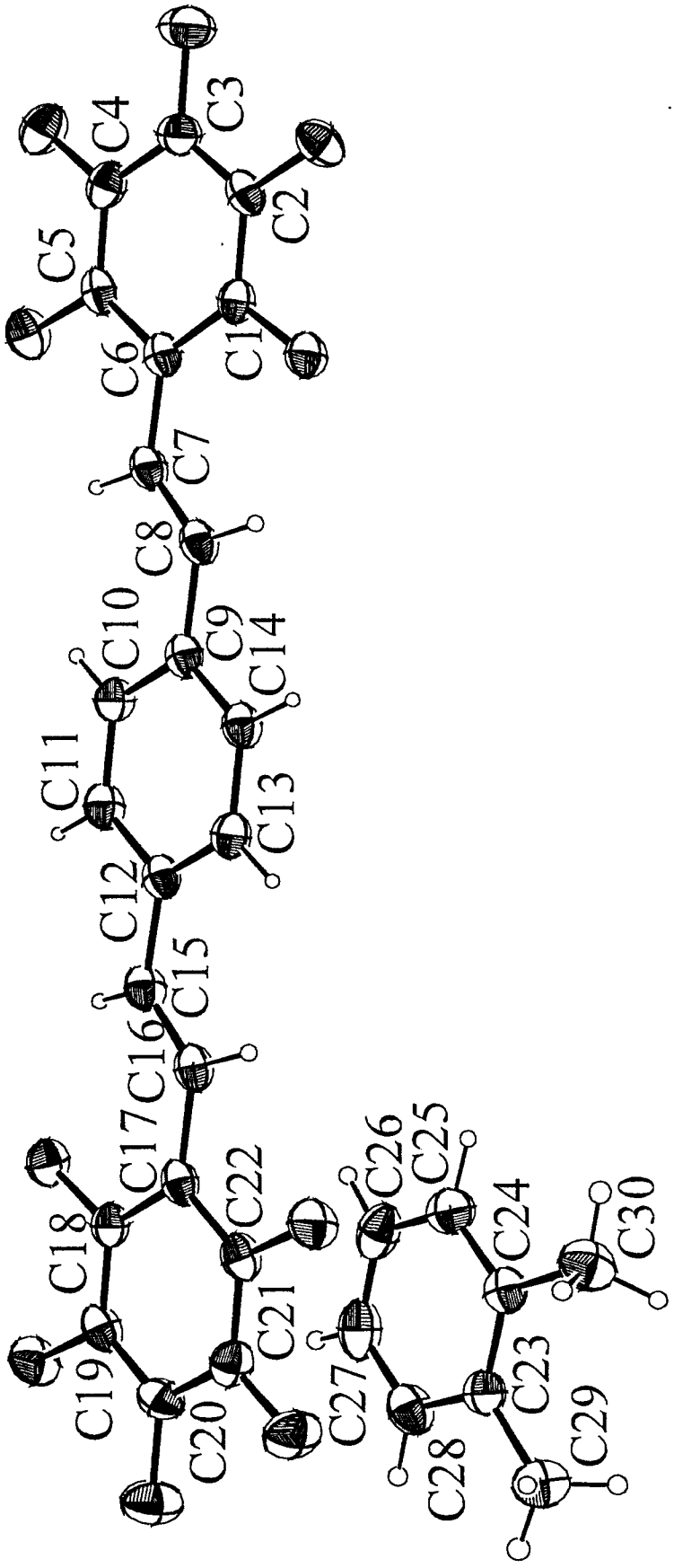
C3
C4
C2
C5
C1
C6
C7
C8
C10
C9
C14
C11
C13
C12
C15
C16
C17
C22
C26
C25
C18
C24
C30
C21
C27
C23
C19
C20
C29
C28

Table 1. Crystal and Intensity Collection Data for

$C_6F_5 - CH = CH - C_6H_4 - CH = CH - C_6F_5 \cdot C_6H_4(CH_3)_2$

Formula: $C_{30}H_{18}F_{10}$	Formula weight: 568.46
Crystal color: Very pale yellow	Habit: Needle
Crystal size: $0.30 \times 0.46 \times 0.55$ mm	$\rho_{calc} = 1.563$ g cm^{-3}
Crystal System: Triclinic	Space group: $P\bar{1}$ (#2)
$a = 7.220(4)$Å	$\alpha = 83.25(4)°$
$b = 7.926(3)$Å	$\beta = 83.94(5)°$
$c = 23.118(13)$Å	$\gamma = 67.11(4)°$
V = 1207.7(11)Å^3	$Z = 2$
Lattice parameters: 25 reflections,	$11° \leq \theta \leq 13°$
$\mu = 1.44$ cm^{-1} ($\mu r_{max} = 0.06$)	
CAD-4 diffractometer	ω scan
MoKα, $\lambda = 0.7107$Å	Graphite monochromator
2θ range: 2°–50°	$-8 \leq h \leq 8, -9 \leq k \leq 9, -27 \leq l \leq 27$
T = 160K	$F_{000} = 576$
Number of reflections measured: 9381	Number of independent reflections: 4239
Number with $F_o^2 > 0$: 3853	Number with $F_o^2 > 3\sigma(F_o^2)$: 3194
Standard reflections: 3 every 1 hr	Variation: No decay
GOF_{merge} : 1.31 for 4214 multiples	R_{merge} : 0.026 for 3491 duplicates
Number used in refinement: 4238	Criterion: All reflections (some deleted)

Final R(F_o): 0.054 for 3194 reflections with $F_o^2 > 3\sigma(F_o^2)$

Final R(F_o): 0.064 for 3853 reflections with $F_o^2 > 0$

Final weighted R(F_o^2) : 0.119 for 4238 reflections

Final goodness of fit: 3.19 for 433 parameters and 4238 reflections

$(\Delta/\sigma)_{max}$ in final least squares cycle: 0.01

$\Delta\rho_{max}$: 0.34 eÅ^{-3}, $\Delta\rho_{min}$: -0.43 eÅ^{-3} in final difference map

Table 2. Final Heavy Atom Parameters for

$C_6F_5 - CH = CH - C_6H_4 - CH = CH - C_6F_5 \cdot C_6H_4(CH_3)_2$

x, y, z and $U_{eq}{}^a \times 10^4$

Atom	x	y	z	U_{eq}
C1	3402(3)	6964(3)	−540(1)	265(5)
C2	4033(4)	5696(3)	−950(1)	283(5)
C3	4643(4)	6174(3)	−1505(1)	312(6)
C4	4604(4)	7914(3)	−1643(1)	308(6)
C5	3971(3)	9164(3)	−1226(1)	272(5)
C6	3350(3)	8740(3)	−655(1)	261(5)
C7	2716(4)	10134(3)	−236(1)	281(6)
C8	2177(4)	9948(3)	329(1)	294(6)
C9	1541(3)	11363(3)	739(1)	261(5)
C10	1376(4)	13168(3)	583(1)	285(6)
C11	763(4)	14443(3)	993(1)	297(6)
C12	299(3)	13980(3)	1578(1)	274(6)
C13	480(4)	12173(3)	1733(1)	297(6)
C14	1086(4)	10901(3)	1323(1)	287(6)
C15	−314(4)	15397(3)	1991(1)	303(6)
C16	−814(4)	15197(3)	2555(1)	298(6)
C17	−1438(4)	16581(3)	2979(1)	273(5)
C18	−1580(3)	18389(3)	2864(1)	275(5)
C19	−2197(4)	19627(3)	3280(1)	306(6)

Table 2. (Cont.)

Atom	x	y	z	U_{eq}
C20	−2682(4)	19103(3)	3842(1)	326(6)
C21	−2545(4)	17330(3)	3980(1)	324(6)
C22	−1946(4)	16117(3)	3557(1)	303(6)
F1	2824(2)	6384(2)	−6(1)	322(3)
F2	4070(2)	3993(2)	−808(1)	373(4)
F3	5272(2)	4938(2)	−1903(1)	456(4)
F4	5204(2)	8392(2)	−2187(1)	398(4)
F5	3963(2)	10845(2)	−1384(1)	368(4)
F18	−1109(2)	18999(2)	2322(1)	345(3)
F19	−2335(2)	21367(2)	3135(1)	406(4)
F20	−3263(3)	20295(2)	4252(1)	483(4)
F21	−3002(2)	16801(2)	4531(1)	460(4)
F22	−1835(2)	14393(2)	3716(1)	406(4)
C23	−7691(4)	17797(3)	4140(1)	324(6)
C24	−7101(4)	16371(3)	3775(1)	317(6)
C25	−6660(4)	16720(4)	3186(1)	392(7)
C26	−6779(4)	18440(4)	2954(1)	438(8)
C27	−7368(4)	19850(4)	3314(1)	448(8)
C28	−7815(4)	19530(4)	3903(1)	405(7)

Table 2. (Cont.)

Atom	x	y	z	U_{eq}
C29	−8150(5)	17471(5)	4780(1)	457(8)
C30	−6922(5)	14461(4)	4012(2)	457(8)

[a] $U_{eq} = \frac{1}{3}\sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

Table 3. Selected Distances and Angles for

$$C_6F_5 - CH = CH - C_6H_4 - CH = CH - C_6F_5 \cdot C_6H_4(CH_3)_2$$

	Distance(Å)		Distance(Å)
C1 –C2	1.375(3)	C18 –C19	1.370(3)
C1 –C6	1.388(3)	C19 –C20	1.368(4)
C2 –C3	1.370(4)	C20 –C21	1.371(4)
C3 –C4	1.369(4)	C21 –C22	1.369(4)
C4 –C5	1.378(4)	C23 –C24	1.395(4)
C5 –C6	1.394(3)	C23 –C28	1.391(4)
C6 –C7	1.461(3)	C23 –C29	1.495(4)
C7 –C8	1.329(4)	C24 –C25	1.386(4)
C8 –C9	1.458(3)	C24 –C30	1.509(4)
C9 –C10	1.395(3)	C25 –C26	1.378(4)
C9 –C14	1.396(3)	C26 –C27	1.377(4)
C10 –C11	1.380(4)	C27 –C28	1.383(4)
C11 –C12	1.400(4)		
C12 –C13	1.393(4)		
C12 –C15	1.465(4)		
C13 –C14	1.378(4)		
C15 –C16	1.324(4)		
C16 –C17	1.464(4)		
C17 –C18	1.392(3)		
C17 –C22	1.392(3)		

Table 3. (Cont.)

	Angle(°)		Angle(°)
C6 –C1 –C2	123.4(2)	C16 –C15 –C12	126.5(2)
C3 –C2 –C1	119.7(2)	C17 –C16 –C15	127.9(2)
C4 –C3 –C2	119.3(2)	C18 –C17 –C16	125.9(2)
C5 –C4 –C3	120.1(2)	C22 –C17 –C16	119.6(2)
C6 –C5 –C4	122.7(2)	C22 –C17 –C18	114.5(2)
C5 –C6 –C1	114.7(2)	C19 –C18 –C17	123.2(2)
C7 –C6 –C1	125.8(2)	C20 –C19 –C18	120.1(2)
C7 –C6 –C5	119.5(2)	C21 –C20 –C19	119.1(2)
C8 –C7 –C6	127.7(2)	C22 –C21 –C20	120.0(2)
C9 –C8 –C7	126.8(2)	C21 –C22 –C17	123.2(2)
C10 –C9 –C8	123.6(2)	C28 –C23 –C24	119.0(2)
C14 –C9 –C8	118.8(2)	C29 –C23 –C24	120.9(2)
C14 –C9 –C10	117.5(2)	C29 –C23 –C28	120.2(3)
C11 –C10 –C9	120.8(2)	C25 –C24 –C23	119.2(2)
C12 –C11 –C10	121.7(2)	C30 –C24 –C23	121.1(2)
C13 –C12 –C11	117.4(2)	C30 –C24 –C25	119.7(3)
C15 –C12 –C11	118.7(2)	C26 –C25 –C24	121.5(3)
C15 –C12 –C13	123.9(2)	C27 –C26 –C25	119.4(3)
C14 –C13 –C12	120.9(2)	C28 –C27 –C26	120.0(3)
C13 –C14 –C9	121.7(2)	C27 –C28 –C23	120.9(3)

Table 4. Anisotropic Displacement Parameters for

$C_6F_5 - CH = CH - C_6H_4 - CH = CH - C_6F_5 \cdot C_6H_4(CH_3)_2$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C1	247(13)	273(13)	271(13)	−110(11)	−31(10)	39(10)
C2	298(14)	216(12)	357(14)	−119(11)	−72(11)	11(11)
C3	272(14)	326(14)	336(14)	−94(11)	−32(11)	−77(11)
C4	263(14)	369(15)	279(13)	−125(12)	−27(10)	47(11)
C5	248(13)	240(13)	350(14)	−124(11)	−74(11)	51(11)
C6	232(13)	245(13)	309(13)	−94(10)	−63(10)	20(10)
C7	291(14)	211(13)	356(14)	−117(11)	−47(11)	22(11)
C8	281(14)	212(13)	399(15)	−107(11)	−44(11)	−2(11)
C9	218(13)	241(13)	323(13)	−85(10)	−54(10)	8(10)
C10	288(14)	275(14)	290(14)	−114(11)	−36(11)	26(11)
C11	315(15)	220(13)	348(15)	−108(11)	−34(11)	34(11)
C12	223(13)	241(13)	354(14)	−85(11)	−49(11)	1(10)
C13	304(14)	290(14)	301(14)	−132(11)	−16(11)	26(11)
C14	285(14)	221(13)	354(14)	−104(11)	−31(11)	13(11)
C15	313(15)	207(13)	382(15)	−97(11)	−32(11)	6(11)
C16	316(14)	242(13)	349(14)	−132(11)	−38(11)	30(11)
C17	260(13)	218(12)	351(14)	−106(10)	−52(10)	19(10)
C18	265(14)	267(13)	299(13)	−119(11)	−39(10)	39(10)
C19	322(14)	186(12)	417(15)	−105(11)	−81(12)	22(11)
C20	337(15)	264(13)	367(15)	−87(11)	−61(11)	−57(11)
C21	326(15)	350(15)	291(14)	−134(12)	−39(11)	27(11)
C22	343(15)	224(13)	362(14)	−139(11)	−62(11)	49(11)
F1	415(9)	277(7)	302(8)	−182(7)	4(6)	24(6)
F2	462(9)	237(7)	445(9)	−162(7)	−43(7)	−14(6)
F3	552(10)	432(9)	398(9)	−187(8)	29(7)	−146(7)
F4	405(9)	473(9)	293(8)	−172(7)	3(6)	45(7)
F5	451(9)	267(8)	395(8)	−173(7)	−42(7)	76(6)
F18	440(9)	268(7)	349(8)	−186(7)	18(6)	37(6)
F19	513(10)	212(7)	502(9)	−152(7)	−40(7)	−14(6)
F20	639(11)	357(9)	425(9)	−141(8)	−9(8)	−119(7)
F21	655(11)	423(9)	293(8)	−217(8)	5(7)	19(7)
F22	611(11)	277(8)	371(8)	−239(7)	−4(7)	34(6)
C23	288(14)	330(14)	350(14)	−112(12)	−41(11)	−10(11)

Table 4. (Cont.)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C24	264(14)	305(14)	365(14)	−87(11)	−52(11)	−5(11)
C25	341(16)	447(17)	377(16)	−127(13)	−32(12)	−66(13)
C26	322(16)	589(20)	391(17)	−189(14)	−54(13)	90(15)
C27	379(17)	390(17)	567(20)	−174(14)	−95(14)	142(15)
C28	385(17)	306(15)	522(18)	−121(13)	−66(13)	−27(13)
C29	507(21)	459(19)	380(17)	−155(17)	−9(15)	−66(14)
C30	530(21)	334(16)	485(19)	−137(15)	−64(16)	−20(14)

$U_{i,j}$ values have been multiplied by 10^4

The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*^2} + U_{22}k^2b^{*^2} + U_{33}\ell^2c^{*^2} + 2U_{12}hka^*b^* + 2U_{13}h\ell a^*c^* + 2U_{23}k\ell b^*c^*)$$

Table 5. Refined Hydrogen Parameters for

$C_6F_5 - CH = CH - C_6H_4 - CH = CH - C_6F_5 \cdot C_6H_4(CH_3)_2$

x, y and $z \times 10^4$

Atom	x	y	z	B
H7	2754(34)	11273(32)	−400(10)	2.8(6)
H8	2088(36)	8816(34)	494(11)	3.4(6)
H10	1675(37)	13506(33)	195(11)	2.9(6)
H11	681(34)	15633(33)	889(10)	2.3(5)
H13	199(35)	11797(32)	2125(11)	2.5(5)
H14	1148(34)	9713(33)	1446(10)	2.5(5)
H15	−405(37)	16529(34)	1817(10)	3.1(6)
H16	−878(38)	14065(36)	2714(11)	3.6(6)
H25	−6265(38)	15665(35)	2940(11)	3.5(6)
H26	−6495(41)	18581(38)	2552(12)	4.3(7)
H27	−7520(43)	21012(40)	3150(12)	4.8(7)
H28	−8274(44)	20541(39)	4136(13)	5.0(8)
H29a	−8534(50)	18576(46)	4973(14)	6.7(9)
H29b	−9302(47)	17148(39)	4869(12)	4.8(8)
H29c	−6981(42)	16531(38)	4952(12)	3.9(7)
H30a	−6711(49)	13700(45)	3710(15)	6.2(9)
H30b	−5831(46)	13933(39)	4268(13)	4.8(7)
H30c	−8160(46)	14490(37)	4238(12)	4.3(7)

Table 6. Complete Distances and Angles for

$C_6F_5 - CH = CH - C_6H_4 - CH = CH - C_6F_5 \cdot C_6H_4(CH_3)_2$

	Distance(Å)		Distance(Å)
C1 –C2	1.375(3)	C20 –C21	1.371(4)
C1 –C6	1.388(3)	C20 –F20	1.337(3)
C1 –F1	1.349(3)	C21 –C22	1.369(4)
C2 –C3	1.370(4)	C21 –F21	1.342(3)
C2 –F2	1.342(3)	C22 –F22	1.346(3)
C3 –C4	1.369(4)	C23 –C24	1.395(4)
C3 –F3	1.339(3)	C23 –C28	1.391(4)
C4 –C5	1.378(4)	C23 –C29	1.495(4)
C4 –F4	1.346(3)	C24 –C25	1.386(4)
C5 –C6	1.394(3)	C24 –C30	1.509(4)
C5 –F5	1.338(3)	C25 –C26	1.378(4)
C6 –C7	1.461(3)	C25 –H25	1.00(3)
C7 –C8	1.329(4)	C26 –C27	1.377(4)
C7 –H7	0.95(3)	C26 –H26	0.93(3)
C8 –C9	1.458(3)	C27 –C28	1.383(4)
C8 –H8	0.96(3)	C27 –H27	0.92(3)
C9 –C10	1.395(3)	C28 –H28	0.95(3)
C9 –C14	1.396(3)	C29 –H29a	0.96(4)
C10 –C11	1.380(4)	C29 –H29b	0.96(3)
C10 –H10	0.93(3)	C29 –H29c	0.97(3)
C11 –C12	1.400(4)	C30 –H30a	0.94(4)
C11 –H11	0.93(2)	C30 –H30b	0.96(3)
C12 –C13	1.393(4)	C30 –H30c	0.98(3)
C12 –C15	1.465(4)		
C13 –C14	1.378(4)		
C13 –H13	0.95(3)		
C14 –H14	0.94(2)		
C15 –C16	1.324(4)		
C15 –H15	0.92(3)		
C16 –C17	1.464(4)		
C16 –H16	0.94(3)		
C17 –C18	1.392(3)		
C17 –C22	1.392(3)		
C18 –C19	1.370(3)		
C18 –F18	1.347(3)		
C19 –C20	1.368(4)		
C19 –F19	1.347(3)		

Table 6. (Cont.)

	Angle(°)		Angle(°)
C6 –C1 –C2	123.4(2)	H13 –C13 –C12	120.2(15)
F1 –C1 –C2	115.9(2)	H13 –C13 –C14	118.9(15)
F1 –C1 –C6	120.7(2)	C13 –C14 –C9	121.7(2)
C3 –C2 –C1	119.7(2)	H14 –C14 –C9	120.4(15)
F2 –C2 –C1	120.3(2)	H14 –C14 –C13	117.8(15)
F2 –C2 –C3	119.9(2)	C16 –C15 –C12	126.5(2)
C4 –C3 –C2	119.3(2)	H15 –C15 –C12	113.0(16)
F3 –C3 –C2	119.8(2)	H15 –C15 –C16	120.4(16)
F3 –C3 –C4	120.9(2)	C17 –C16 –C15	127.9(2)
C5 –C4 –C3	120.1(2)	H16 –C16 –C15	118.7(17)
F4 –C4 –C3	119.6(2)	H16 –C16 –C17	113.3(17)
F4 –C4 –C5	120.3(2)	C18 –C17 –C16	125.9(2)
C6 –C5 –C4	122.7(2)	C22 –C17 –C16	119.6(2)
F5 –C5 –C4	117.6(2)	C22 –C17 –C18	114.5(2)
F5 –C5 –C6	119.7(2)	C19 –C18 –C17	123.2(2)
C5 –C6 –C1	114.7(2)	F18 –C18 –C17	120.1(2)
C7 –C6 –C1	125.8(2)	F18 –C18 –C19	116.8(2)
C7 –C6 –C5	119.5(2)	C20 –C19 –C18	120.1(2)
C8 –C7 –C6	127.7(2)	F19 –C19 –C18	119.9(2)
H7 –C7 –C6	113.1(15)	F19 –C19 –C20	119.9(2)
H7 –C7 –C8	119.2(15)	C21 –C20 –C19	119.1(2)
C9 –C8 –C7	126.8(2)	F20 –C20 –C19	120.5(2)
H8 –C8 –C7	119.5(16)	F20 –C20 –C21	120.4(2)
H8 –C8 –C9	113.5(16)	C22 –C21 –C20	120.0(2)
C10 –C9 –C8	123.6(2)	F21 –C21 –C20	119.4(2)
C14 –C9 –C8	118.8(2)	F21 –C21 –C22	120.6(2)
C14 –C9 –C10	117.5(2)	C21 –C22 –C17	123.2(2)
C11 –C10 –C9	120.8(2)	F22 –C22 –C17	119.2(2)
H10 –C10 –C9	118.9(16)	F22 –C22 –C21	117.6(2)
H10 –C10 –C11	120.3(16)	C28 –C23 –C24	119.0(2)
C12 –C11 –C10	121.7(2)	C29 –C23 –C24	120.9(2)
H11 –C11 –C10	120.4(15)	C29 –C23 –C28	120.2(3)
H11 –C11 –C12	117.8(15)	C25 –C24 –C23	119.2(2)
C13 –C12 –C11	117.4(2)	C30 –C24 –C23	121.1(2)
C15 –C12 –C11	118.7(2)	C30 –C24 –C25	119.7(3)
C15 –C12 –C13	123.9(2)	C26 –C25 –C24	121.5(3)
C14 –C13 –C12	120.9(2)	H25 –C25 –C24	116.5(16)

Table 6. (Cont.)

			Angle(°)
H25	–C25	–C26	122.1(16)
C27	–C26	–C25	119.4(3)
H26	–C26	–C25	116.7(18)
H26	–C26	–C27	123.8(18)
C28	–C27	–C26	120.0(3)
H27	–C27	–C26	118.6(19)
H27	–C27	–C28	121.3(19)
C27	–C28	–C23	120.9(3)
H28	–C28	–C23	121.0(19)
H28	–C28	–C27	118.0(19)
H29a	–C29	–C23	111.3(21)
H29b	–C29	–C23	113.7(19)
H29c	–C29	–C23	109.7(17)
H29b	–C29	–H29a	102.2(28)
H29c	–C29	–H29a	109.5(27)
H29c	–C29	–H29b	110.1(26)
H30a	–C30	–C24	111.4(21)
H30b	–C30	–C24	109.9(19)
H30c	–C30	–C24	110.9(18)
H30b	–C30	–H30a	109.8(28)
H30c	–C30	–H30a	107.0(28)
H30c	–C30	–H30b	107.8(26)

Table 7. Torsion Angles for

$C_6F_5 - CH = CH - C_6H_4 - CH = CH - C_6F_5 \cdot C_6H_4(CH_3)_2$

				Angle(°)
C6	–C7	–C8	–C9	–179.8(2)
C5	–C6	–C7	–H7	1.5(16)
C5	–C6	–C7	–C8	–176.4(3)
C1	–C6	–C7	–H7	181.5(16)
C1	–C6	–C7	–C8	3.6(4)
C7	–C8	–C9	–C10	1.3(4)
C7	–C8	–C9	–C14	–178.1(3)
H7	–C8	–C9	–C10	2.3(8)
H7	–C8	–C9	–C14	–177.0(8)
C12	–C15	–C16	–C17	–179.8(2)
C11	–C12	–C15	–H15	3.2(18)
C11	–C12	–C15	–C16	–180.5(3)
C13	–C12	–C15	–H15	182.2(17)
C13	–C12	–C15	–C16	–1.5(4)
C15	–C16	–C17	–C18	–1.4(4)
C15	–C16	–C17	–C22	–181.2(3)
H16	–C16	–C17	–C18	183.0(18)
H16	–C16	–C17	–C22	3.2(18)