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The Crystal Structure of the 2:1 Complex Between Antimony Tribromide and Pyrene

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The structure of the complex $2SbBr_3$ pyrene has been determined from three-dimensional X-ray data collected by counter methods. The unit cell is monoclinic, space group $P2_1/c$; $a = 10.669(4)$, $b = 13.001(4)$ and $c = 7.634(3)$ Å, $\beta = 90.00(12)°$, 2 molecules per unit cell. The structure was refined by full-matrix least-squares methods to a conventional $R = 0.079$. The structure consists of $SbBr_3$ molecules stacked in the bc plane and alternating with layers of pyrene molecules in the plane $x = 1/2$. Two $SbBr_3$ molecules are centrosymmetrically bonded to the pyrene molecule through the Sb atom. The antimony atom has distances of: 3.30 Å from the pyrene plane, 2.50 Å from two bromine atoms occupying equatorial positions in a plane almost parallel to the plane of pyrene (7°, 47′) 2.49 Å from the bromine atom accupyng the axial position opposite to the antimony-pyrene bond, 3.49 and 3.65 Å from two other bromine atoms of other complex units. The three intramolecular bonds and the three intermolecular contacts correspond to a distorted octahedral coordination.

Introduction

Molecular complexes between aromatic hydrocarbons and antimony trihalides have been isolated since the earliest work of Smith *et al.* [1,2] and Menshutkin [3]. Other works deal with the interpretation of these complexes, but only a few with a comparison of the complexing power of the different antimony halides. From the order of «melting point elevation», observed by thermal analysis of the binary systems, Shinomya [4] affirmed that $SbCl_3$ is more strongly additive than $SbBr_3$. A spectrophotometric study on the 1:1 complexes of pyrene witeh $SbCl_3$ and $SbBr_3$ in dichloromethane solution [5] showed that the stability constant is greater for the $SbBr_3$– than for the $SbCl_3$– complex. This different behaviour may be due either to a greater solvation of $SbCl_3$, which has a higher dipole moment than $SbBr_3$, or to greater acceptor properties of the bromine atom in $SbBr_3$.

Recently some crystal structure determinations have been carried out on the $SbCl_3$–complexes: 2:1 and 4:1 with dibenzyl [6]; 4:1 with stilbene [6]; 1:1 with aniline [7]; 2:1 with naphthalene [8]; 2:1 with phenanthrene [9]. It may be of interest to investigate the structure $SbBr_3$–arene complex and to compare the behaviour of the two halides in the solid compounds. As the complexes of pyrene have been extensively studied in solution [5], the $2SbBr_3$. Pyrene complex was chosen for this study.

Experimental Section

The complex $2SbBr_3$.Pyrene was prepared using the method previously described (5) and slowly recrystallized. Because of its hygroscopicity a small crystal (0.085×0.051×0.187 mm) was mounted under dry nitrogen in a Lindemann glass capillary.

Crystal Data. Bis antimony tribromide pyrene; $Sb_2Br_6C_{16}H_{10}$; Monoclinic $P2_1/c$ (C^5_{2h}); $a = 10.669(4)$ Å; $b = 13.001(4)$ Å; $c = 7.634(3)$ Å; $\beta = 90.00(12)°$; $D_c = 2.90$ g. cm^{-3} for, $Z = 2$ molecules per cell, $\mu = 145.58$ cm^{-1} for Mokα radiation $\lambda = 0.7107$ Å.

Space group data were determined from preliminary precession and Weissenberg photographs. The unit cell dimensions were measured on a Siemens four-circle automatic diffractometer using nickel filtered Cukα radiation (λ 1.54178 Å). Twenty medium to high angle reflections were accurately centered and used for least squares refinement of the lattice parameters using a program which is a part of the program package for the computer controlled diffractometer Siemens AED.

The intensities of the 3050 independent reflections in the Mo sphere with $\theta \leqslant 30°$ were obtained using the «five-values» measuring technique and the ω:2θ scan.

The reflections which passed the test: net count greater than $2\sigma_I$ were 1235, all the others treated as unobserved were given zero weight in the subsequent refinement.

The intensity of a reference reflection —4 5 1 recorded after each group of twenty reflections as a check of the stability of the instrument and of the crystal

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(1) Watson Smith, *J. Chem. Soc. (London)*, *35*, 309 (1879).
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Table I. Positional and thermal parameters (and their e.s.d's). For non-hydrogen atoms thermal parameters are defined by $T=\exp[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+\beta_{12}hk+\beta_{13}hl+\beta_{23}kl)]$.

	$x\ (\times 10^4)$	$y\ (\times 10^4)$	$z\ (\times 10^4)$	$B(\text{Å}^2)$
Sb	1644(1)	1233(1)	93(2)	
Br$_1$	3218(3)	1935(2)	2209(4)	
Br$_2$	687(3)	35(2)	2288(4)	
Br$_3$	153(3)	2686(2)	507(4)	
C$_1$	5421(25)	69(21)	691(36)	
C$_2$	5377(27)	—505(22)	2208(36)	
C$_3$	6269(31)	—285(25)	3551(36)	
C$_4$	7133(37)	399(33)	3415(45)	
C$_5$	7229(24)	963(26)	1861(49)	
C$_6$	6360(27)	859(22)	487(42)	
C$_7$	6464(33)	1395(29)	—1156(49)	
C$_8$	5602(33)	1226(26)	—2374(48)	
H$_3$	6215	—712	4732	4.3
H$_4$	7763	534	4464	5.6
H$_5$	7982	1488	1713	4.6
H$_7$	7213	1914	—1387	5.3
H$_8$	5653	1661	—3547	5.3

	$\beta_{11}(\times 10^4)$	$\beta_{22}(\times 10^4)$	$\beta_{33}(\times 10^4)$	$\beta_{12}(10^4)$	$\beta_{13}(10^4)$	$\beta_{23}(10^5)$
Sb	105(2)	39(1)	141(3)	—3(1)	6(2)	12(1)
Br$_1$	97(3)	54(2)	195(6)	—7(2)	—16(3)	—15(3)
Br$_2$	111(3)	40(1)	179(6)	—12(2)	—9(3)	11(2)
Br$_3$	133(3)	43(1)	174(6)	20(2)	—3(4)	6(2)
C$_1$	74(26)	48(16)	189(55)	22(18)	7(27)	—15(25)
C$_2$	96(31)	61(19)	199(59)	49(21)	69(35)	21(26)
C$_3$	119(35)	64(21)	123(55)	42(24)	—61(35)	1(27)
C$_4$	127(42)	95(30)	236(70)	59(31)	—101(43)	—46(38)
C$_5$	34(27)	84(25)	335(89)	—3(19)	4(35)	—55(38)
C$_6$	79(28)	46(16)	248(69)	23(18)	6(34)	21(27)
C$_7$	110(37)	85(28)	261(78)	—1(26)	20(44)	42(38)
C$_8$	126(37)	69(21)	285(81)	30(25)	125(48)	36(35)

specimen showed no evidence of any deterioration of the sample. The intensities were corrected for Lorentz and polarization effects but not for extinction or absorption.

All calculation were carried out on an IBM 360/44 computer using for Fourier calculations programs written by Immirzi[10], for full-matrix least squares a local version of the ORFLS[11], for Wilson plot, bond lengths and angles and least-squares planes Ahmed's programs[12].

Form factors for neutral Sb, Br, C, H were taken from F.H.Moore[13].

The effects of anomalous dispersion for Sb and Br were accounted for by adding. $\Delta f' = -0.6$ and -0.3 electrons to the scattering curve of antimony and of bromine. The effets of $\Delta f'' = 2.0$, 2.6 electrons respectively were neglected for this centric structure.

The approximate positional parameters of the antimony and the three bromine atoms were obtained from a three-dimensional Patterson synthesis. A structure factor calculation followed by a difference Fourier synthesis phased by the Sb and Br atoms revealed the position of all the carbon atoms. Four cycles of full matrix least-squares refinement with individual isotropic temperature factors and unit weights resulted in a residual $R = \Sigma \mid \mid F_o \mid - \mid F_o \mid \mid / \Sigma \mid F_o \mid$ of 0.136. Hydrogen atom positions were calculated and included with isotropic temperature factors equal to those of the carbon atom to which they were attached. At this point the Mills and Rollet weighting scheme in the form.

$$w=[1+(\frac{|F_o|-b}{a})^2]^{-1} \text{ was used with } a = 40,\ b = 60.$$

A final five cycles of anisotropic refinement of all the non hydrogen atoms (hydrogen parameters were not refined) yielded a residual R of 0.079 and R weighted of 0.097 for all the observed reflections.

The changes in all refined parameters were < 0.15. A three-dimensional difference Fourier calculated at the end of refinement was relatively featurless except for same positive peaks of about 1 e /Å^3 around the Sb and the Br positions.

Results and Discussion

The final positional and thermal parameters, with their e.s.d's, are given in Table I; the F_o and F_c values in Table II. Interatomic distances and angles, with their e.s.d's, are given in Table III. Views of the 2SbBr$_3$ pyrene complex perpendicular to ring and along the Sb-Br(3) bond are given respectively in fig. 1 and fig. 2. The packing of the molecules as viewed down the c axis is given in fig. 3.

The distances of the Sb, Br and C atoms from the mean least-squares plane of the pyrene molecule are given in Table IV.

(10) A. Immirzi, *Ricerca Sci.*, 37, 850 (1967).
(11) W. R. Busing, K. O. Martin and H. A. Levy, ORNL TM 305, Oak Ridge National Laboratory, Tennesee, 1962.
(12) F. R. Hall, M. E. Pippy and C. P. Huber, NCR Crystallography Programs for the IBM/360 System, World List of Crystallographic Computer Programs, 1966.
13) F. H. Moore, *Acta Cryst.*, 16, 1169 (1963).

The pyrene molecule is centrosymmetric in the ½00 position and symmetrically bonded to two $SbBr_3$ molecules in general position. The structure consists of single layers of pyrene molecules inclined at about 45° on the plane x = ½ and double layers of antimony tribromide molecules parallel to the plane x = 0. The asymmetric unit corresponds to half a molecule of pyrene and one molecule of $SbBr_3$.

The antimony atom, the atoms Br(1) and Br(2) of an $SbBr_3$ molecule lie in a plane almost parallel to the plane of the pyrene molecule (angle of 7°,47′). The atom Br(3) points away from the pyrene molecule and the bond Sb-Br(3) is almost normal to the plane Sb-Br(1). A second $SbBr_3$ molecule, related to

Table II. Observed and calculated structure factors.

H,0,0		
15	224*	-5
14	218*	-22
13	327	222
12	360	314
11	208*	114
10	240	-244
9	301	-311
8	807	-769
7	393	356
6	1453	1535
5	159*	66
4	341	-326
3	1025	1105
2	359	427
1	1650	1742
H,1,0		
1	1815	-1912
2	764	-754
3	137*	-138
4	352	-340
5	840	878
6	155*	-23
7	1217	-1273
8	461	-459
9	181*	-23
10	195	-206
11	192*	118
12	201*	107
13	234	-254
14	218*	-106
H,2,0		
14	224*	94
13	208*	37
12	203*	-97
11	200*	162
10	254*	-266
9	692	-601
8	355	-327
7	813	-805
6	1380	-1430
5	615	-926
4	734	-727
3	1459	-1466
2	382	285
1	238	-217
H,3,0		
1	125*	-10
2	1687	-1562
3	154	-94
4	1662	1596
5	726	752
6	200	99
7	173*	-32
8	197	-248
9	197*	37
10	451	423
11	295	261
12	203*	118
13	210*	-34
14	222*	-39
H,4,0		
14	224*	47
13	222*	44
12	200*	-112
11	204*	-83
10	284*	266
9	392	444
8	175	16
7	486	-568
6	849	-888
5	449	-448
4	1302	1263
3	2515	2405
2	2489	2334
1	1220	1115
0	538	504
H,7,0		
1	158*	142
2	1439	1392
3	168*	25
4	1050	-1017
5	263	-281
6	188*	139
7	201*	131
8	547	534
9	197*	152
10	217	-203
11	218*	-53
12	222*	68
13	223*	79
H,8,0		
13	229*	106
12	235	160
11	281	257
10	216*	-211
9	535	-513
8	200*	-117
7	199*	180
6	211	194
5	603	644
4	181*	-153
3	1009	-977
2	768	734
1	1876	1808
0	1767	1710
H,9,0		
1	176*	-96
2	1044	-1071
3	280	-249
4	690	680
5	192*	46
6	272	-272
7	189*	-4
8	424	-417
9	242	-229
10	291	290
11	211*	72
12	222*	-48
13	224*	23
H,10,0		
12	230*	54
11	223*	-69
10	222*	-87
9	201*	-103
8	507	-483
7	360	-354
6	200*	-96
5	623	-617
4	334	-323
3	251	249
2	186*	-206
1	183*	122
0	889	889
H,11,0		
1	252*	-777
2	209*	-372
3	188*	-42
4	198*	42
5	455	459
6	200	-73
7	396	-401
8	266	-218
9	221*	36
10	226*	75
11	230*	136
12	229*	81
H,12,0		
11	226*	32
10	229*	85
9	224*	131
8	212*	112
7	402	-405
6	530	-591
5	203*	-214
4	256	300
3	588	622
2	722	687
1	193*	177
0	319	-341
H,13,0		
1	315	324
2	207*	232
3	199*	-35
4	250	-246
5	243	-224
6	204*	-127
7	212	167
8	219*	149
9	219*	42
10	227*	-62
H,14,0		
9	226*	-81
8	222*	-76
7	228*	-199
6	243	-242
5	201*	-132
4	210*	-18
3	194*	55
2	212*	284
1	278	268
0	216	169
H,15,0		
1	383	352
2	234	88
3	205*	-79
4	297	-286
5	306	-389
6	223*	-130
7	231*	131
8	228*	28
H,16,0		
7	228*	-1
6	264	178
5	221*	-66
4	230*	-229
3	228*	-246
2	210*	-114
1	243	227
0	526	608
H,17,0		
1	233*	-246
2	230*	-85
3	219*	43
4	236*	-19
5	240*	184
H,18,0		
2	246	182
1	267	234
0	247*	163
H,18,1		
-2	242*	184
-1	240*	181
0	224*	-28
1	240*	-211
2	250*	-208
H,17,1		
5	231*	-97
4	242*	-276
3	489	-580
2	286	-341
1	220*	-68
0	226*	111
-1	228*	75
-2	232*	-78
-3	224*	-212
-4	227*	-113
-5	226*	44
H,16,1		
-7	223*	23
-6	234*	-3
-5	218*	85
-4	248	54
-3	230*	-126
-2	222*	-107
-1	224*	-96
0	229*	-199
1	219*	-32
2	229*	-91
3	226*	-155
4	227*	-189
5	228*	-56
6	226*	-73
7	224*	-24
H,15,1		
8	241*	28
7	228*	60
6	230*	231
5	221*	76
4	280	-287
3	214*	-188
2	216*	72
1	206*	71
0	468	546
-1	562	606
-2	216*	182
-3	212*	174
-4	301	363
-5	232*	267
-6	230*	299
-7	232*	235
-8	220*	-13
H,14,1		
-9	227*	-1
-8	232*	-233
-7	248	-238
-6	214*	172
-5	276	201
-4	210*	206
-3	208*	106
-2	481	-526
-1	480	-505
0	203*	173
1	454	469
2	288	229
3	296	301
4	297	-236
5	230*	-291
6	226*	253
7	382	363
8	259	227
9	251	189
10	236*	6
H,13,1		
10	252	198
9	238	118
8	228*	37
7	222*	-86
6	575	-606
5	604	-619
4	203*	-113
3	230	-204
2	406	-408
1	387	-386
0	678	-714
-1	605	-633
-2	389	374
-3	362	385
-4	199*	16
-5	214	-31
-6	332	-339
-7	472	-465
-8	212*	3
-9	228*	8
-10	231*	-135
H,12,1		
-11	224*	94
-10	229*	76
-9	214*	12
-8	225*	257
-7	215*	163
-6	200*	-57
-5	203*	143
-4	199*	40
-3	245	-322
-2	199*	103
-1	195*	55
0	588	-597
1	208	-199
2	192*	-119
3	440	-490
4	199*	-167
5	201*	74
6	381	-369
7	250	-186
8	202*	22
9	213*	-96
10	225*	-56
11	225*	27
H,11,1		
11	224*	82
10	223*	112
9	398	327
8	266	241
7	274	-255
6	202*	-216
5	197*	-141
4	186*	-109
3	421	419
2	444	434
1	238	-233
0	191*	133
-1	572	577
-2	744	774
-3	1131	1189
-4	1073	1089
-5	265	241
-6	195*	8
-7	209*	153
-8	205*	36
-9	200*	79
-10	214*	112
-11	234*	-57
H,10,1		
-12	226*	-39
-11	254	-189
-10	271	-235
-9	217*	100
-8	268	262
-7	250	241
-6	193*	-13
-5	653	-666
-4	685	-694
-3	194*	170
-2	618	630
-1	508	522
0	240	255
1	784	-752
2	667	-637
3	454	409
4	666	781
5	722	729
6	293	345
7	191*	-120
8	201*	-166
9	284	226
10	289	290
11	302	216
12	232*	105
H,9,1		
12	279	193
11	216*	168
10	195*	23
9	211*	-150
8	197*	-178
7	193*	39
6	191*	99
5	403	-445
4	913	-907
3	1548	-1533
2	1180	-1213
1	339	-352
0	424	424
-1	173*	149
-2	299	-296
-3	533	-528
-4	365	-357
-5	216	223
-6	278	258
-7	197*	46
-8	365	-374
-9	478	-487
-10	373	-379
-11	202*	-62
-12	221*	-2
H,8,1		
-13	223*	11
-12	220*	58
-11	205*	101
-10	201*	119
-9	199*	167
-8	193*	113
-7	182*	120
-6	253	213
-5	181*	71
-4	176*	68
-3	173*	91
-2	312	-323
-1	469	-432
0	164*	23
1	426	-412
2	487	-462
3	206	-148
4	467	-491
5	409	-417
6	220	-137
7	183*	-88
8	193*	-159
9	194*	-119
10	201*	-53
11	210*	-60
12	218*	-56
13	226*	4
H,7,1		
13	227*	124
12	218*	108
11	214*	178
10	205*	152
9	226	-201
8	193*	-79
7	461	484
6	165*	152
5	197	-181
4	245	-217
3	1285	-1206
2	580	-539
1	989	947
0	1496	1413
-1	1129	1085
-2	1163	1140
-3	425	449
-4	391	318
-5	1133	1173
-6	921	939
-7	203	236
-8	187*	-7
-9	202*	-201
-10	350	-358
-11	212*	-18
-12	224*	115
-13	216*	-1
H,4,1		
-14	236*	-85
-13	229*	-138
-12	213*	-61
-11	258	312
-10	205*	188
-9	269	-327
-8	246	-286
-7	497	-500
-6	314	-363
-5	1029	1027
-4	1070	1058
-3	984	-897
-2	953	-893
-1	617	-566
0	621	-563
1	1502	1385
2	1938	1838
3	346	-284
4	666	-676
5	194	-51
6	183*	-34
7	666	655
8	976	979
9	199*	29
10	203*	-177
11	201*	34
12	210*	-37
13	222*	102
14	237*	153
H,5,1		
14	226*	43
13	220*	-43
12	209*	74
11	285*	45
10	201*	141
9	677	695
8	200	194
7	770	-754
6	765	-789
5	834	-833
4	1330	-1292
3	157*	117
2	203	163
1	2338	-2116
0	1515	-1429
-1	191	158
-2	195	182
-3	874	879
-4	1702	1671
-5	602	-613
-6	744	-799
-7	181*	-123
-8	286	-306
-9	187*	-53
-10	197*	83
-11	344	-293
-12	234*	-287
-13	223*	-15
-14	230*	-46
H,6,1		
-14	233*	-76
-13	218*	92
-12	217*	119
-11	216	-113
-10	200*	80
-9	424	385
-8	197*	-154
-7	180*	51
-6	593	619
-5	275	-258
-4	295	-316
-3	550	536
-2	149*	-85
-1	930	-875
0	758	693
1	758	-675
2	1049	-944
3	489	485
4	317	-324
5	803	-798
6	396	363
7	186*	-194
8	480	-499
9	199*	212
10	198*	25
11	247	-228
12	211*	46
13	211*	41
14	236*	-105
H,3,1		
14	229*	42
13	221*	69
12	210*	-137
11	197*	69
10	482	509
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12	214*	35
13	232*	-137
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6	732	766
7	195	-242
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12	297*	128
13	217*	-63
14	227*	-53
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12	216*	-49
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11	226*	80
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H,15,2		
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7	232*	101
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-6	232*	221
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3	237*	-113
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2	674	727
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8	236*	95
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-7	214*	-146
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3	308	345
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7	816	827
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9	196*	88
10	207*	-74
11	227*	-258
12	226*	47
13	226*	135
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6	512	-528
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-13	228*	-158
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3	755	-709
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7	350	-330
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12	221*	-37
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H,3,3		
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11	262	-237
10	210*	-214
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8	199*	148
7	327	-353
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6	243	233
7	331	-336
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10	412	407
11	204*	81
12	214*	23
13	227*	-56
14	234*	-104
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10	248	-160
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8	210	-145
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6	785	862
5	954	990
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3	187	-209
2	505	-534
1	627	694
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-12	223*	179
-13	226*	93
-14	232*	-36
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12	221*	103
11	282	-154
10	211*	-194
9	540	-561
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7	187*	79
6	518	539
5	213	-184
4	197	284
3	248	-251
2	641	-688
1	1400	1523
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-1	755	818
-2	472	422
-3	552	-618
-4	990	-1028
-5	181*	46
-6	856	861
-7	274	228
-8	216	-168
-9	204*	-40
-10	212*	-217
-11	220*	125
-12	405	348
-13	236*	178
H,1,4		
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-12	226*	-71
-11	354	-251
-10	201*	-58
-9	195*	34
-8	203*	2
-7	371	335
-6	232	-255
-5	1295	-1351
-4	496	-506
-3	169*	-49
-2	497	-502
-1	349	281
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1	1953	-2147
2	1205	-1193
3	161*	18
4	428	-464
5	183*	-49
6	180*	-47
7	841	-903
8	467	-536
9	195*	85
10	201*	-22
11	213*	-17
12	217*	64
13	231*	-122
H,2,4		
13	233*	-21
12	214*	59
11	218*	116
10	306	-214
9	202*	-116
8	187*	24
7	365	-375
6	195*	-196
5	406	459
4	173*	92
3	179*	144
2	1022	1018
1	467	504
0	165*	-2
-1	497	588
-2	167*	-74
-3	955	-964
-4	398	-311
-5	694	-646
-6	897	-883
-7	351	-337
-8	213*	-255
-9	396	-339
-10	210*	-48
-11	220*	30
-12	232*	-50
-13	239*	37
H,3,4		
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-12	231*	-42
-11	217*	-102
-10	218	-144
-9	202*	123
-8	481	524
-7	360	385
-6	191*	-7
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-4	183*	-66
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-2	1459	1548
-1	1016	1197
0	165*	109
1	254	208
2	175*	-74
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4	1255	1256
5	784	808
6	189*	48
7	191*	-11
8	192*	3
9	197*	21
10	280	336
11	349	205
12	214*	-16
13	230*	-39
H,4,4		
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12	230*	-179
11	222*	-199
10	203*	-81
9	204*	41
8	203*	-109
7	430	-466
6	891	-912
5	550	-549
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3	1299	1326
2	1079	1147
1	590	617
0	301	-344
-1	222	-277
-2	602	631
-3	982	1130
-4	456	481
-5	239	-364
-6	615	-604
-7	568	-561
-8	203*	97
-9	428	392
-10	362	351
-11	218*	51
-12	223*	-32
-13	234*	-20
H,5,4		
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-11	223*	82
-10	210*	70
-9	209*	-162
-8	236	-325
-7	274	-324
-6	201*	-158
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-4	187*	22
-3	422	-477
-2	707	-838
-1	899	-969
0	454	-517
1	310	328
2	182*	-114
3	621	-587
4	807	-809
5	805	-830
6	267	-249
7	195*	50
8	197*	34
9	204*	-155
10	212*	-175
11	218*	-179
12	216*	-32
13	222*	53
H,6,4		
13	238*	68
12	231*	36
11	220*	-104
10	204*	-31
9	218*	-72
8	296	-287
7	197*	-8
6	199	-153
5	196*	-189
4	205	219
3	511	518
2	240	245
1	586	622
0	430	429
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-2	183*	-125
-3	184*	-87
-4	494	-501
-5	562	-611
-6	280	-261
-7	444	-485
-8	258	-209
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-10	208*	-28
-11	216*	-55
-12	223*	58
-13	242*	-3
H,7,4		
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-11	232*	50
-10	222*	196
-9	195*	-22
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-7	208*	21
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-5	522	580
-4	610	681
-3	299	338
-2	560	-592
-1	187*	110
0	659	695
1	493	577
2	768	832
3	451	399
4	616	-628
5	198*	-118
6	508	546
7	211*	129
8	336	305
9	216*	196
10	222*	-172
11	266	-85
12	232*	130
H,8,4		
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11	220*	98
10	232	-265
9	461	-434
8	218*	-251
7	202*	-106
6	209*	116
5	671	683
4	232	-248
3	521	-519
2	411	376
1	630	668
0	851	897
-1	1167	1255
-2	187*	-15
-3	989	-1037
-4	225	-255
-5	195*	-39
-6	203*	90
-7	339	304
-8	214*	-36
-9	284	-348
-10	226*	-57
-11	230*	119
-12	232*	146
H,9,4		
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-9	217*	-16
-8	306	298
-7	199*	-59
-6	209*	-141
-5	197*	-101
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-3	208*	-134
-2	539	593
-1	189*	109
0	469	-499
1	321	-288
2	618	-614
3	434	-428
4	281	276
5	224	108
6	357	-342
7	224	-265
8	214*	-178
9	228*	-229
10	228*	106
11	229*	94
H,10,4		
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10	230*	35
8	408	-389
7	202*	-23
6	216*	-46
5	211*	-105
4	208*	182
3	341	373
2	238	-138
1	345	355
0	517	511
-1	196*	-31
-2	201*	54
-3	199*	-12
-4	401	-457
-5	216*	-280
-7	265	-201
-8	220*	-66
-6	206*	-70
-9	220*	-26
-10	222*	-44
-11	236*	-6
H,11,4		
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-9	238*	42
-8	232*	209
-7	273	263
-6	211*	43
-5	272	-317
-4	203*	19
-3	317	345
-2	364	366
-1	469	451
0	199*	117
1	520	-522
2	281	-258
3	333	337
4	212*	201
5	219*	182
6	216	108
7	289	-278
8	230*	-137
9	226*	135
10	230*	114
H,12,4		
9	231*	108
8	232*	47
7	234*	-219
6	288	-322
5	214*	-110

Table II. (continued)

	H,12,4	
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2	597	613
1	205*	116
0	263	-261
-1	204*	-51
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-3	288	295
-4	241	207
-5	262	-253
-6	392	-494
-7	353	-312
-8	232*	53
-9	238*	66
	H,13,4	
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-5	232*	224
-4	226*	228
-3	214*	-10
-2	228*	-175
-1	213*	-177
0	208*	-3
1	251	222
2	242	180
3	205*	-98
4	234*	-207
5	234*	-221
6	226*	-99
7	239*	57
8	236*	85
	H,14,4	
7	237*	-88
6	241*	-191
5	238*	-56
4	225*	-19
3	236	102
2	224*	222
1	228*	237
0	220*	67
-1	219*	65
-2	218*	14
-3	222*	-32
-4	221*	-1
-5	235*	-106
-6	232*	-127
-7	239*	-87
	H,15,4	
-6	246*	95
-5	355	277
-4	238	145
-3	234*	-49
-2	235*	-159
-1	247*	-201
0	219*	10
1	242*	295
2	226*	64
3	234*	-191
4	242*	-164
5	245*	-210
6	235*	-39
	H,16,4	
4	265*	7
3	236*	-61
2	231*	-82
1	239*	235
0	477	445
-1	236*	152
-2	241*	-80
-3	256*	-238
-4	247*	-309
	H,16,5	
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-1	235*	-72
0	249*	-146
1	250*	-114
2	241*	-100
	H,15,5	
5	232*	-108
4	249*	-253
3	246*	-178
2	244*	-137
1	242*	44
0	268	308
-1	244*	217
-2	242*	25
-3	239*	30
-4	242*	15
-5	240*	45
	H,14,5	
-6	264	242
-5	308	360
-4	228*	196
-3	238*	116
-2	232*	-163
-1	245*	-190
0	240*	206
1	397	495
2	241*	193
3	240*	69
4	239*	-65
5	241*	-157
6	248*	118
	H,13,5	
7	250*	13
6	353	-313
5	313	-195
4	231*	70
3	226*	88
2	230*	176
1	228*	222
0	248	-263
-1	222*	-111
-2	323	322
-3	289	259
-4	228*	194
-5	234*	37
-6	361	-266
-7	305	-278
	H,12,5	
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-7	229	42
-6	237*	-176
-5	232*	-147
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-3	236*	-227
-2	248	-222
-1	219*	-125
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1	341	-373
2	226*	-96
3	270	-243
4	226*	-177
5	223*	-17
6	270	-197
7	242*	-151
8	238*	44
	H,11,5	
9	240*	96
8	232*	-45
7	380	-342
6	284	-322
5	357	-390
4	360	-291
3	229*	205
2	221*	-3
1	221*	-177
0	207*	-55
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-6	266	-100
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-9	246*	179
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-7	327	291
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-5	252	-223
-4	222*	-140
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-2	692	653
-1	487	465
0	232	170
1	252	-305
2	256	-252
3	339	361
4	637	581
5	363	313
6	220*	115
7	230*	-97
8	241*	-159
9	231*	103
10	248*	198
	H,9,5	
11	240*	147
10	238*	104
9	230*	-85
8	226*	-103
7	214*	74
6	313	158
5	210*	91
4	203*	-152
3	379	-396
2	399	-386
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0	649	625
-1	615	627
-2	204*	168
-3	205*	-136
-4	283	-254
-5	207*	35
-6	216*	117
-7	226*	41
-8	240*	-169
-9	329	-316
-10	307	-209
-11	265*	-69
	H,8,5	
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-9	223*	9
-8	218*	-41
-7	216*	-96
-6	217*	-10
-5	220*	-80
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-2	426	-379
-1	437	-393
0	256	-265
1	214*	-235
2	421	-411
3	357	-337
4	218*	-171
5	311	-271
6	233*	-53
7	227*	42
8	295	-93
9	230*	-73
10	240*	34
11	242*	-3
	H,7,5	
11	244*	97
10	238*	-37
9	351	-311
8	235*	-169
7	210*	-89
6	285	-288
5	213*	-96
4	460	-465
3	1017	-914
2	400	-390
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-6	247	274
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-8	229*	-16
-9	293	-217
-10	242*	-156
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-11	257*	192
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-9	233*	-143
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-7	212*	-15
-6	221*	149
-5	746	733
-4	833	796
-3	209*	-179
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3	268*	-79
4	578	-525
5	201*	-100
6	218*	241
7	222*	269
8	395	416
9	224*	37
10	232*	-232
11	231*	-41
12	231*	43
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11	234*	-46
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9	379	430
8	222*	98
7	327	-311
6	276	-269
5	526	-481
4	547	-510
3	829	760
2	485	426
1	350	-338
0	198*	53
-1	200*	65
-2	202*	73
-3	1121	1060
-4	761	691
-5	426	-406
-6	264	-244
-7	410	-404
-8	446	-318
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-10	229*	69
-11	259	-164
-12	243*	-120
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-10	222*	-64
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-8	280	-79
-7	227*	-139
-5	210	-146
-4	403	-446
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-2	226	-126
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1	195*	-85
2	772	-705
3	196*	-31
4	275	254
5	616	-585
6	198*	-23
7	216*	167
8	214*	-240
9	214*	5
10	224*	153
11	227*	-88
12	232*	-13
	H,3,5	
13	235*	35
12	228*	-108
11	220*	44
10	228*	161
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0	361	-379
1	1070	-944
2	191	-154
3	184*	35
4	692	690
5	729	754
6	202*	-157
7	390	-481
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8	201*	84
7	211*	-200
6	1007	-1052
5	584	-561
4	210	-127
3	199*	-119
2	299	267
1	271	245
0	695	-624
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-3	753	761
-4	616	600
-5	217*	262
-6	369	-345
-7	548	-516
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-13	252*	-69
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-13	252*	76
-12	266	-116
-11	259	-153
-10	228*	-92
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-8	382	354
-7	564	562
-6	203*	-312
-5	618	-672
-4	194*	-92
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-2	879	872
8	209*	-93
9	212*	28
10	221*	135
11	242*	208
12	238*	1
13	232*	-131
	H,1,5	
13	255*	79
12	245*	199
11	230*	127
10	228*	13
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8	326	-331
7	212*	-89
6	209	194
5	202*	-74
4	674	-689
3	611	-636
2	549	-511
1	181*	79
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-2	214	199
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-4	202*	-32
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-6	450	343
-7	226	186
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-9	489	-409
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-11	238*	-81
-12	270	69
-13	240*	64
	H,0,6	
12	246*	112
11	232*	174
10	233*	-166
9	232*	-172
8	214*	-17
7	212*	-107
6	278	261
5	361	329
4	807	-818
3	1104	-1144
2	927	-981
1	525	-503
0	231*	81
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-2	226	-274
-3	625	-672
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-5	316	298
-6	564	516
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-9	404	-389
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-11	252	-33
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-11	240*	-116
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-8	225*	198
-7	211*	-35
-6	471	-473
-5	427	-426
-4	630	-631
-3	435	-422
-2	413	415
-1	205*	-54
0	977	-913
1	612	-576
2	577	-531
3	542	-570
4	331	398
5	207*	219
6	434	-494
7	218*	-217
8	216*	-92
9	220*	-156
10	224*	130
11	236*	131
12	241*	-74
	H,2,6	
12	242*	29
11	240*	86
10	255	268
9	237	189
8	217*	164
7	430	445
6	217*	217
5	202*	-51
4	230	188
3	190*	51
2	665	-643
1	193*	56
0	189*	-8
-1	237	-303
-2	244	233
-3	394	353
-4	204*	17
-5	262	237
-6	363	308
-7	218*	-36
-8	213*	52
-9	222*	-20
-10	235*	-81
-11	240*	-103
-12	240*	-21
	H,3,6	
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-11	256*	-124
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-9	241	211
-8	303	235
-7	406	343
-6	221*	97
-5	277	-285
-4	212*	10
-3	597	593
-2	651	687
-1	636	625
0	353	299
1	312	-299
2	205*	30
3	559	481
4	659	589
5	380	394
6	215*	120
7	222*	-166
8	224*	-120
9	227*	148
10	233*	134
11	258	32
12	245*	22
	H,4,6	
12	236*	-103
11	224*	-71
10	238*	66
9	313	263
8	299	242
7	216*	-149
6	508	-457
5	487	-489
4	375	-361
3	214*	188
2	207*	-56
1	750	-672
0	1051	-1004
-1	685	-675
-2	205*	33
-3	671	711
-4	733	705
-5	220*	158
-6	250	-150
-7	217*	-149
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-9	240*	266
-10	252*	151
-11	249*	-23
-12	248*	-113
	H,5,6	
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-10	244*	40
-9	232*	-113
-8	321	-280
-7	292	-295
-6	228*	-16
-5	221*	42
-4	212*	-22
-3	428	-371
-2	788	-747
-1	615	-623
0	213*	-97
1	207*	57
2	207*	109
3	218*	-250
4	571	-533
5	361	-300
6	208*	-30
7	209*	80
8	216*	112
9	222*	-16
10	238*	-150
11	235*	-83
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11	242*	96
10	244*	78
9	236*	173
8	266	309
7	216	134
6	210*	127
5	210*	147
4	213	-203
3	217*	-158
2	201*	-3
1	212*	-220
0	256	-274
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-2	107*	-24
-3	215*	106
-4	341	332
-5	220*	234
-6	219*	74
-7	222*	96
-8	228*	29
-9	237*	-52
-10	230*	-14
-11	250*	-48
	H,7,6	
-11	250*	187
-10	240*	66
-9	228*	-50
-8	226*	-19
-7	226*	-124
-6	230	162
-5	562	533
-4	274	243
-3	214*	-170
-2	199*	-66
-1	211*	-135
0	262	222
1	784	774
2	514	463
3	204*	-130
4	206*	-27
5	200*	37
6	216*	34
7	343	375
8	234*	246
9	232*	-105
10	242*	-54
11	238*	6
	H,8,6	
10	246*	84
9	238*	-115
8	236*	-192
7	226	228
6	335	308
5	218*	-56
4	224*	-148
3	684	-638
2	996	-924
1	201*	-37
0	334	320
-1	202*	98
-2	215*	-28
-3	214*	-178
-4	420	-364
-5	293	271
-6	548	539
-7	257	225
-8	233*	57
-9	248*	-135
-10	248*	-166
	H,9,6	
-10	239*	-35
-9	248*	42
-8	238*	26
-7	241*	93
-6	224*	-103
-5	455	-446
-4	250	-310
-3	216*	73
-2	240	-62
-1	222*	56
0	215*	27
1	645	-578
2	394	-344
3	218*	150
4	223*	35
5	230*	71
6	230*	78
7	244*	-227
8	242*	-176
9	237*	44
10	253*	26
	H,10,6	
9	258*	118
8	230*	127
7	234*	-40
6	232*	83
5	244	151
4	232*	-161
3	244	-202
2	224*	-110
1	341	-317
0	232*	-195
-1	231*	208
-2	224*	-6
-3	228*	37
-4	235*	286
-5	229*	92
-6	235*	72
-7	240*	178
-8	237*	48
-9	256*	-62
	H,11,6	
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-7	235*	98
-6	243*	-145
-5	238*	-131
-4	249	-194
-3	228*	81
-2	333	350
-1	256	204
0	266	-196
1	218*	-149
2	218*	-26
3	224*	79
4	388	364
5	265	286
6	233*	-91
7	238*	-86
8	241*	55
	H,12,6	
7	239*	46
6	243*	-188
5	244	-211
4	227*	54
3	235*	128
2	221*	24
1	228*	-142
0	479	-431
-1	388	-351
-2	232*	125
-3	347	365
-4	254	267
-5	236*	91
-6	245*	-109
-7	252*	-123
	H,13,6	
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-5	244*	93
-4	240*	28
-3	232*	-45
-2	257	-227
-1	231*	-177
0	230*	-9
1	237*	108
2	242*	108
3	235*	11
4	244*	-113
5	236*	-135
6	244*	3
	H,14,6	
4	246*	-138
3	241*	-82
2	236*	-103
1	245*	-88
0	228*	-96
-1	238*	-109
-2	253*	-18
-3	250*	104
-4	244*	111
	H,15,6	
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0	244*	78
1	242*	136
	H,13,7	
3	359	344
2	239*	187
1	247*	-32
0	254*	-107
-1	250*	-215
-2	244*	-116
-3	250*	172
	H,12,7	
-5	252*	-89
-4	243*	-155
-3	242*	12
-2	244*	-9
-1	245*	-157
0	242*	-87
1	236*	-26
2	241*	-100
3	238*	33
4	232*	67
5	244*	-113
	H,11,7	
6	250*	-181
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4	238*	97
3	232*	23
2	223*	2
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-2	236*	-61
-3	234*	-17
-4	241*	30
-5	245*	9
-6	250*	-128
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-4	240*	-45
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-2	422	441
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0	226*	-22
1	262	-185
2	221*	-31
3	234*	156
4	280	289
5	235*	229
6	274	-38
7	251*	-219
	H,9,7	
8	248*	23
7	236*	167
6	355	352
5	367	420
4	230*	186
3	226*	-11
2	217*	-101
1	220*	10
0	222	203
-1	277	187
-2	230*	-103
-3	279	-290
-4	237*	-208
-5	234*	-14
-6	291	208
-7	273	204
-8	242*	63
	H,8,7	
-9	254*	-95
-8	240*	-93
-7	246*	-67
-6	242*	-114
-5	235*	-99
-4	228*	-104
-3	224*	-178
-2	228*	-172
-1	215*	-42
0	216*	-5
1	220*	-71
2	226*	-66
3	215*	-42
4	223*	-127
5	232*	-12
6	227*	95
7	232*	-47
8	236*	-17
9	252*	23
	H,7,7	
9	250*	-104
8	242*	-129
7	242*	90
6	265	285
5	225*	96
4	226*	-96
3	224*	-178
2	340	-413
1	226*	-205
0	229*	98
-1	241	-113
-2	359	-411
-3	373	-338
-4	305	-292
-5	232*	-40
-6	319	272
-7	265*	197
-8	246*	58
-9	237*	-26
	H,6,7	
-10	257*	42
-9	248*	-27
-8	255*	-173
-7	250*	-171
-6	301	249
-5	467	472
-4	233*	210
-3	228*	-16
-2	227*	-179
-1	274	-307
0	498	376
1	731	718
2	230*	208
3	215*	-12
4	222*	-197
5	253	-301
6	226*	92
7	246*	303
8	238*	45
9	233*	-75
10	245*	-84
	H,5,7	
10	243*	42
9	236*	61
8	301	336
7	226*	202
6	216*	-121
5	226*	187
4	394	375
3	298	264
2	493	476
1	222*	109
0	685	-683
-1	359	-368
-2	214*	-40
-3	217	42
-4	220*	192
-5	222*	149
-6	246	-255
-7	232*	-127
-8	234*	143
-9	244*	135
-10	258*	109
	H,4,7	
-10	252*	25
-9	247*	-78
-8	237*	-47
-7	234*	8
-6	218*	-174
-5	232*	-170
-4	224*	111
-3	227*	-186
-2	218*	-168
-1	220*	165
0	220	-197
1	296	-257
2	218*	204
3	211*	15
4	220*	-231
5	218*	151
6	220*	16
7	218*	-176
8	228*	81
9	220*	74
10	236*	-73
	H,3,7	
11	246*	-159
10	232*	-16
9	236*	202
8	219*	63
7	209*	-19
6	213*	61
5	208*	-131
4	199*	62
3	474	498
2	195*	86
1	430	-387
0	477	-528
-1	513	-557
-2	402	-445
-3	216*	279
-4	218*	138
-5	222*	-158
-6	219*	-86
-7	222*	-42
-8	232*	20
-9	309	243
-10	240*	178
-11	244*	-27
	H,2,7	
-11	250*	-159
-10	243*	-75
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-8	376	288
-7	218*	102
-6	221*	-84
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-4	327	-319
-3	342	309
-2	637	692
-1	288	280
0	205*	-163
1	297	-336
2	446	-423
3	209*	209
4	562	567
5	202*	143
6	210*	-100
7	225	-168
8	272	-245
9	226*	27
10	226*	189
11	228*	30
	H,1,7	
11	230*	22
10	229*	-42
9	230*	-112
8	222*	6
7	228*	207
6	393	361
5	437	481
4	235	227
3	293	-321
2	310	-321
1	205*	148
0	213*	-66
-1	215*	136
-2	225*	-202
-3	586	-574
-4	396	-396
-5	219*	72
-6	303	259
-7	259	261
-8	230*	132
-9	244*	-94
-10	249*	-40
-11	252*	12
	H,0,8	
10	245*	-23
9	365	-307
8	275	-327
7	220*	2
6	226*	102
5	222*	47
4	227*	63
3	368	-332
2	422	-446
1	214*	142
0	224*	313
-1	254	71
-2	222*	-132
-3	475	-499
-4	691	-699
-5	242*	-89
-6	236*	130
-7	239*	71
-8	252*	-8
-9	246*	-84
-10	258*	-143
	H,1,8	
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-8	236*	35
-7	246*	4
-6	233*	-113
-5	438	-420
-4	241	-250
-3	227*	124
-2	220*	55
-1	217*	10
0	210*	-81
1	383	-453
2	320	-337
3	211*	208
4	215*	158
5	212*	1
6	220*	54
7	221*	-130
8	234*	-154
9	240*	107
	H,2,8	
9	235*	6
8	224*	36
7	210*	-56
6	223*	176
5	234*	292
4	217*	159
3	344	373
2	422	480
1	220*	170
0	218*	239
-1	284	342
-2	224*	-56
-3	229*	-3
-4	224*	3
-5	234*	-89
-6	239*	-98
-7	240*	54
-8	250*	-14
-9	249*	1
	H,3,8	
-9	247*	86
-8	287	224
-7	319	139
-6	238*	-50
-5	233*	-91
-4	226*	37
-3	230*	205
-2	365	425
-1	228*	346
0	214*	-144
1	214*	-164
2	219*	-37
3	211*	71
4	297	283
5	222*	159
6	226*	-148
7	230*	-128
8	240*	-60
9	234*	-17
	H,4,8	
9	245*	-23
8	228*	16
7	244*	-144
6	318	-318
5	230*	-251
4	217*	39
3	270	319
2	227	324
1	213*	-28
0	312	-425
-1	286	-409
-2	218*	-195
-3	219*	152
-4	226*	49
-5	229*	-145
-6	301	-349
-7	246*	-270
-8	244*	-20
-9	244*	120
	H,5,8	
-9	254*	-84
-8	252*	-169
-7	236*	-126
-6	236*	4
-5	233*	148
-4	224*	49
-3	220*	-145
-2	310	-330
-1	218*	-201
0	217*	-17
1	228*	194
2	220*	89
3	224*	-160
4	223*	-179
5	263	-165
6	232*	-27
7	279	162
8	242*	67
9	243*	-42
	H,6,8	
8	245*	3
7	243*	78
6	227*	79
5	231*	71
4	260	211
3	235*	287
2	224*	216
1	273	320
0	224*	211
-1	227*	0
-2	226*	-0
-3	225*	41
-4	231*	-97
-5	244*	-15
-6	246*	-12
-7	243*	-76
-8	255*	9
	H,7,8	
-8	254*	-137
-7	256*	5
-6	246*	188
-5	278	214
-4	229*	156
-3	220*	70
-2	235*	-244
-1	229*	-41
0	259	382
1	233*	241
2	238*	95
3	224*	7
4	234*	-195
5	232*	-163
6	238*	144
7	237*	123
8	232*	-6
	H,8,8	
7	246*	-129
6	238*	143
5	235*	241
4	267	-108
3	230*	-169
2	225*	-85
1	232*	-13
0	297	253
-1	258	285
-2	240*	-188
-3	378	-392
-4	349	-285
-5	246*	-153
-6	254*	76
-7	252*	146
	H,9,8	
-6	242*	-108
-5	232*	-89
-4	238*	-105
-3	224*	-23
-2	244	218
-1	234*	141
0	226*	-186
1	230*	-142
2	242*	-121
3	234*	-126
4	244*	143
5	234*	99
6	238*	-117
	H,10,8	
5	234*	72
4	242*	221
3	230*	184
2	232*	18
1	255	173
0	228*	61
-1	228*	18
-2	240*	42
-3	242*	-32
-4	236*	-151
-5	237*	-50
	H,11,8	
-4	242*	-32
-3	249*	189
-2	246*	195
-1	247*	88
0	236*	-14
1	291	-176
2	248*	-88
3	249*	135
4	240*	157
	H,12,8	
1	240*	24
0	246*	-165
-1	251*	-139
	H,9,9	
3	234*	-64
2	248*	-46
1	238*	137
0	256*	258
-1	348	302
-2	238*	148
-3	256	-13
	H,8,9	
-4	238*	-74
-3	238*	-69
-2	246*	-17
-1	229*	-42
0	232*	-1
1	232*	20
2	234*	-34
3	248*	-68
4	227*	14
	H,7,9	
5	235*	9
4	242*	-143
3	237*	-239
2	228*	-109
1	230*	37
0	226*	120
-1	238*	103
-2	232*	-1
-3	252*	-157
-4	252*	-154
-5	244*	-2
	H,6,9	
-6	243*	122
-5	256*	228
-4	254*	163
-3	242*	-72
-2	287	-298
-1	241*	-78
0	239*	137
1	244*	153
2	229*	175
3	230*	-111
4	335	-298
5	239*	-76
6	247*	63
	H,5,9	
7	229*	-30
6	238*	-70
5	245*	-235
4	236*	-7
3	284	294
2	232*	180
1	262	141
0	238*	96
-1	240*	-68
-2	227*	73
-3	341	341
-4	248*	172
-5	250*	2
-6	246*	-83
-7	255*	-143
	H,4,9	
-7	251*	-48
-6	249*	-18
-5	240*	28
-4	248*	-94
-3	241*	32
-2	237*	48
-1	238*	-125
0	230*	-47
1	230*	60
2	234*	-51
3	231*	-22
4	230*	114
5	238*	-22
6	233*	-54
7	308	74
	H,3,9	
7	248*	-110
6	291	-268
5	265	-177
4	228*	-24
3	217*	27
2	234*	183
1	230*	87
0	225*	-208
-1	236*	-54
-2	233*	118
-3	249*	121
-4	252*	152
-5	248*	15
-6	260*	-229
-7	258*	-144
	H,2,9	
-8	256*	141
-7	250*	128
-6	242*	-120
-5	252*	-234
-4	242*	-61
-3	238*	153
-2	246*	252
-1	234*	204
0	228	-138
1	302	-372
2	221*	-98
3	229*	116
4	226*	154
5	234*	150
6	231*	-69
7	263	-212
8	230*	-50
	H,1,9	
8	242*	-126
7	238*	-44
6	239*	84
5	235*	-9
4	228*	-38
3	232*	-113
2	222*	-178
1	234*	104
0	325	377
-1	302	296
-2	242*	105
-3	236*	-55
-4	362	-164
-5	250*	-19
-6	256*	79
-7	266*	91
-8	300	-53
	H,0,10	
5	230*	61
4	237*	-179
3	236*	-312
2	240*	-268
1	256	-208
0	232*	76
-1	260*	200
-2	259*	-89
-3	260*	-169
-4	256*	-131
-5	262*	-59
	H,1,10	
-5	263*	-113
-4	254*	-58
-3	251*	12
-2	267*	162
-1	254*	105
0	240*	-129
1	236*	-128
2	231*	7
3	232*	38
4	240*	165
5	226*	140
	H,2,10	
5	236*	-3
	H,5,10	
4	228*	-86
	H,2,10	
3	226*	-64
2	234*	-14
1	242*	83
0	248*	23
-1	246*	84
-2	259*	164
-3	261*	119
-4	254*	78
-5	262*	111
	H,3,10	
-4	263*	-51
-3	254*	115
-2	251*	168
-1	236*	28
0	244*	-65
1	246*	-170
2	234*	-102
3	243	81
4	238*	100
	H,4,10	
4	243*	-104
3	230*	14
2	250*	41
1	246*	-111
0	264	-261
-1	250*	-223
-2	258*	-45
-3	254*	155
-4	249*	164
	H,5,10	
-3	250*	-81
-2	271	-149
-1	242*	-82
0	232*	66
1	246*	117
2	244*	92
3	247*	-7
	H,6,10	
2	250*	40
1	237*	7
0	247*	40
-1	252*	78
-2	242*	30

the first by the center of symmetry of the pyrene molecule, is linked in the same way on the opposite side of the pyrene molecule.

The structure is similar to that of 2SbCl$_3$.Naphthalene[8] and different from the structure of 2SbCl$_3$.Phe-

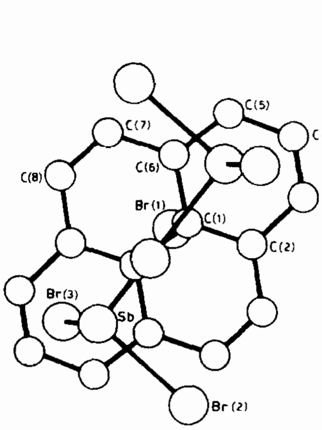

Figure 1. View of the complex perpendicular to the pyrene molecule.

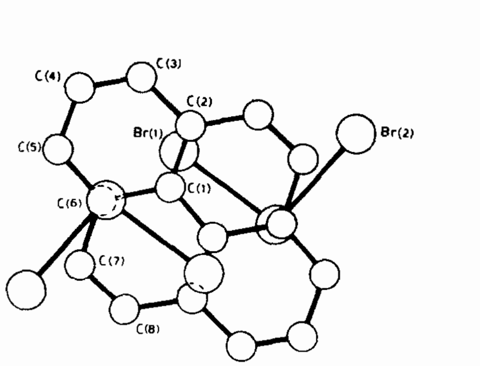

Figure 2. View of the complex along the Sb-Br(3) Bond.

Table III. Interatomic distances and angels (and their e.s.d's.).

Sb-Br(1)	2.502(3)Å	C(1)-C(1′)	1.40(4)Å
Sb-Br(2)	2.505(3)	C(1)-C(2)	1.38(4)
Sb-Br(3)	2.490(3)	C(2)-C(3)	1.43(4)
Sb-C(1′)	3.61(3)	C(3)-C(4)	1.29(4)
Sb-C(2′)	3.75(3)	C(4)-C(5)	1.40(4)
Sb-C(3′)	3.77(3)	C(5)-C(6)	1.41(4)
Sb-C(4′)	3.66(3)	C(6)-C(7)	1.44(4)
Sb-C(5′)	3.44(3)	C(7)-C(8)	1.33(4)
Sb-C(6′)	3.48(3)	C(8)-C(2′)	1.41(4)
Br(1)-Sb-Br(2)	93.9(1)°	C(2)-C(3)-C(4)	124(2)°
Br(1)-Sb-Br(3)	94.0(1)	C(3)-C(4)-C(5)	119(2)
Br(2)-Sb-Br(3)	97.3(1)	C(4)-C(5)-C(6)	122(2)
C(1′)-C(1)-C(2)	123(2)	C(5)-C(6)-C(7)	123(2)
C(1′)-C(1)-C(6)	117(2)	C(5)-C(6)-C(1)	117(2)
C(2)-C(1)-C(6)	120(2)	C(7)-C(6)-C(1)	120(2)
C(1)-C(2)-C(3)	118(2)	C(6)-C(7)-C(8)	118(2)
C(1)-C(2)-C(8′)	117(2)	C(7)-C(8)-C(2′)	124(2)
C(3)-C(2)-C(8′)	124(2)		
Bromine contacts.			
Sb-Br(2″)	3.494(3)Å	Br(2″)-Sb-Br(1)	170.3(1)°
Sb-Br(1‴)	3.652(3)	Br(2″)-Sb-Br(2)	76.4(1)
Br(3)-Br(2⁗)	3.600(4)	Br(2″)-Sb-Br(3)	88.2(1)
Br(2)-Br(2″)	3.790(4)	Sb-Br(2)-Sb″	103.6(1)
Br(3)-Br(3⁗′)	3.848(4)	Br(1‴)-Sb-Br(1)	81.0(1)
Br(2)-Br(3⁗′)	3.891(4)	Br(1‴)-Sb-Br(2)	174.9(1)
Br(1)-C(8⁗′)	3.51(3)	Br(1‴)-Sb-Br(3)	82.8(1)
		Br(1‴)-Sb-Br(2″)	108.7(1)
		Sb-Br(1‴)-Sb‴	108.6(1)

Asymmetric units: ( )=x,y,z; (′)=1−x,$\bar{y}$,$\bar{z}$; (″)=$\bar{x}$,$\bar{y}$,$\bar{z}$; (‴)=x,½−y,z−½; (⁗)=−x,½+y,½−z; (⁗′)=x,½−y,½+z.

Table IV. Distances from the mean least-squares plane of the pyrene molecule: 0.6049x—0.6907y—0.3963z—3.2266=0.

Sb	—3.301	Br(2)	—3.507
Br(1)	—3.356	Br(3)	—5.693
C(1)	—0.001	C(5)	—0.011
C(2)	—0.029	C(6)	0.040
C(3)	—0.001	C(7)	—0.042
C(4)	0.015	C(8)	—0.006

nanthrene[9]. In this last structure two crystallographically non-equivalent $SbCl_3$ molecules are bonded from the same side to the phenonthrene molecule. The following distances in the three complexes may be compared:

	Sb— distance (Å) in the plane X-Sb-X	Sb— distance (Å) ⊥ to the plane X-Sb-X	Distances (Å) of the Sb atom from the arene mean plane
$2SbCl_3 \cdot$ Naphthalene[8]	2.348(2) 2.347(2)	2.367(2)	3.223
$2SbCl_3 \cdot$ Phenanthrene[9]	2.350(4) 2.349(4)	2.359(3)	3.27
	2.338(3) 2.359(3)	2.398(3)	2.94
$2SbBr_3 \cdot$ Pyrene (this work)	2.500(3) 2.505(3)	2.490(3)	3.301

In both the $SbCl_3$ complexes the Sb-Cl bonds, normal to the ClSbCl plane, are a little but significantly longer than the Sb-Cl bonds lying in the plane. In the $2SbBr_3$.Pyrene complex the three bonds have almost equal values, very close to the mean Sb-Br distance (2.49 Å) found in the solid $SbBr_3$[14], the Sb-Br(3)bond normal to the BrSbBr plane being a little shorter than the other two. In the phenanthrene complex the shorter Sb-arene contact is opposite to the longer Sb-Cl distance normal to the ClSbCl plane.[9] This seems to suggest some dependency of this last bond from the strength of the Sb-arene bond.

In the $2SbBr_3$.Pyrene complex the shortest Sb-C distances, Sb-C(5′) = 3.44(3) and Sb-C(6′) = 3.48(3)Å (Table III), concern carbon atoms which are not involved in the shortest C-C distances, C(3)′)–C(4′) = 1.29(4) and C(7′)–C(8′) = 1.33(4)Å, observed in the coordinated pyrene molecule.

These C-C bonds are also the shortest in the free pyrene molecule (15): C(3)–C(4) = 1.344 and C(7)–C(8) = 1.315 A. On the contrary in the $2SbCl_3$. Naphthalene complex (8) the most significant change in the naphthalene bonds regards two adjacent C-C bonds which are the closest to the antimony atom and are the shortest in the complex molecule. This seems

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(15) A. Camerman and J. Trotter, *Acta Cryst.*, *18*, 636 (1965).

to indicate a weaker Sb-arene bond in the $2SbBr_3$.Pyrene complex.

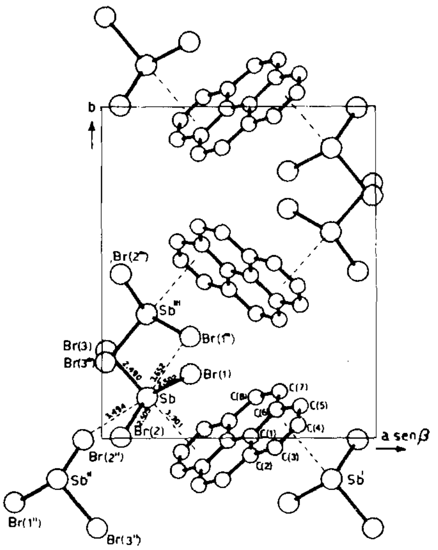

Figure 3. Packing of the molecules as viewed down the c axis and environment of the Sb atom showing a distorted octahedral coordination.

On the other side the shortest Br-C contact, Br(1)–C(8''''') = 3.51(3)Å, regards a carbon atom involved in one of the two shortest C-C bonds, C(8)–C(7) = 1.33(4)Å, observed in the coordinated pyrene molecule. This could suggest a weak interaction of the bromine atom with the aromatic ring[16].

Unlike $2SbCl_3$.Phenanthrene there are Sb...Cl contacts (3.26, 3.49, 3.41, 3.55 Å) which were considered sufficiently shorter than the sum of the Van der Waals radii to complete the distorted octahedral coordination around antimony[9]. Si milarly in the crystal structure of $2SbBr_3$.Pyrene the two shortest Sb...Br contacts, Sb-Br(2'') = 3.494(3) and Sb-Br(1''') = 3.652(3)Å (Table III), make angles witeh the other Sb-Br bonds (Table III) which correspond to a deformed octahedral coordination of five bromine atoms and the arene molecule around the antimony atom (Figure 1).

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