1366. *The Crystal Structure of Tris-(o-diphenylarsinophenyl)-arsineruthenium Dibromide*

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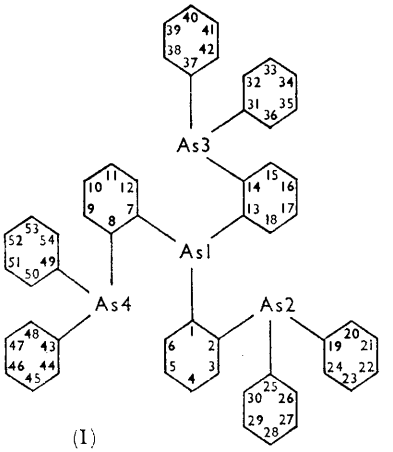
A three-dimensional crystal structure analysis shows that the ruthenium(II) atom in a six-co-ordinated complex has bonds in an arrangement not greatly distorted from the octahedral in spite of stereochemical difficulties to be expected with the quadridentate ligand that it contains. This is made possible by considerable distortions of bond angles in the ligand.

The ligand tris-(*o*-diphenylarsinophenyl)arsine [QAS = (I)] reacts with nitrosoruthenium compounds to form complexes of the type $RuQASX_2$ (X = Cl, Br, I, CNS, or NO_3) which are monomeric, diamagnetic, and non-electrolytes in nitrobenzene solution. So far as is known all finite hexa-co-ordinated complexes, including those of Ru^{II} are octahedral, but it seemed unlikely that an octahedral configuration could be preserved in the $RuQASX_2$ series, in view of the stereochemical limitations of the quadridentate ligand QAS. Indeed, were the ruthenium octahedrally co-ordinated then either the bonds between the ruthenium and the ligand or the bonds within the ligand itself must be considerably distorted and yet

when X = Cl or Br the compound remains thermally stable at over 380°. To determine the environment of the ruthenium atoms in these compounds, the crystal structure of one member $RuQASBr_2$, has been examined.

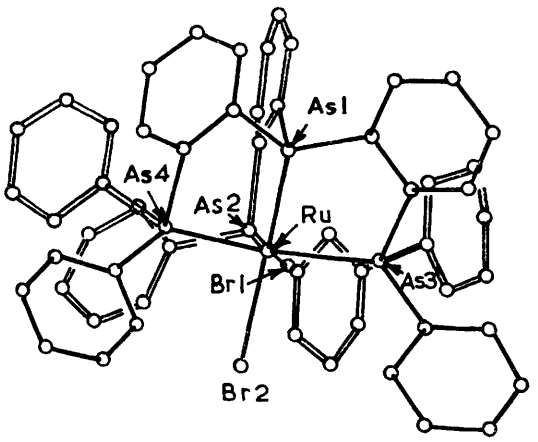
Crystal Data—$RuQASBr_2$, $M = 1251{\cdot}5$; orthorhombic, $a = 31{\cdot}53 \pm 0{\cdot}08$, $b = 11{\cdot}40 \pm 0{\cdot}10$, $c = 13{\cdot}03 \pm 0{\cdot}02$ Å; $U = 4684{\cdot}2$ Å^3; $D_m = 1{\cdot}79$ (by flotation); $Z = 4$, $D_c = 1{\cdot}76$; Space group $Pna2_1$ (C^9_{2v} No. 33); Cu-K_α radiation, single crystal photographs.

Structure Determination.—Over 2500 independent values of $F^2(hkl)$ were obtained from intensity measurements made from photographs taken by the equi-inclination Weissenberg method. Corrections were made for the Lorenz and polarisation factors but not for absorption or extinction. A three-dimensional Patterson map was computed from values of $F^2(hkl)$ sharpened to point atoms at rest.



(I)

The numbers represent the number of the carbon atom referred to in the Tables.



The space groups $Pna2_1$ and *Pnam* are both compatible with the absent spectra, but since there are only four molecules in the unit cell *Pnam* would require the molecule to have a mirror plane of symmetry passing through the ruthenium atom. The position of the vectors could not be reconciled both with this requirement and with the known chemical formula. A trial structure based on $Pna2_1$ of four octahedra whose positions were determined from the vector map gave an R value of 0·38. Application of shifts, obtained from a difference map, to the positional and isotropic thermal parameters of the heavy atoms reduced R to 0·29. Two rounds of least-squares refinement on the positional and isotropic thermal parameters of the heavy atoms further reduced R to 0·20. The least-squares refinement employed the block diagonal approximation and a weighting scheme such that $1/w = 1 + [(F_o - b)/a]^2$ where $a = 70$ and $b = 30$.

At this stage a second difference synthesis showed the position of all 54 carbon atoms and two more rounds of least-squares refinement on the positional and isotropic thermal parameters of all except the hydrogen atoms reduced R to 0·087.

Discussion

The purpose of the structure determination was to discover the environment of the heavy atoms and not to examine the detail of the phenyl groups. In the case of the carbon atoms the standard deviations are naturally higher than those in the positional parameters of the heavy atoms, but even so the bond angles and distances within the phenyl groups are not unreasonable.

Hartley and Venanzi [1] reported that a molecular model showed that considerable

[1] Hartley and Venanzi, *J.*, 1962, 182.

distortion of the bond angles and distances would be necessary to form a complex in which the co-ordination of the ruthenium atom could be considered as approaching the octahedral. Nevertheless the co-ordinates of the heavy atoms establish that the bonds from ruthenium retain an octahedral configuration depiste the restraints and limitations imposed by the ligand.

The trigonal symmetry [2] of the trigonal-bipyramidal ion $[PtQASI)^+$ enables the bond angles at the apical arsenic atom As_1 to remain close to the tetrahedral, but it is not obvious how in the octahedral system the average deviation of the bonds at As_1 from the ideal tetrahedral can be as little as 2·5°, no greater than the average deviation (3·0°) in $[PtQASI]^+$.

If the bonds from ruthenium were exactly octahedrally orientated and if the ruthenium atom were coplanar with each of the three bridging benzene rings, as is the platinum atom in $[PtQASI]^+$, then the bond angles at As1 would not be as close to the tetrahedral as they are found to be and overcrowding would occur among the free phenyl groups.

The actual orientation found differs from the ideal octahedral in that the bonds from ruthenium to As3 and As4 are bent 7° towards Br1 and 7° towards As1 and the bond to As2 is bent 3° towards As1. The benzene ring forming the bridge between As1 and As2 is found to be coplanar with Ru, As1, As2, Br1, and Br2. The plane containing these atoms forms an approximate mirror plane of symmetry within the molecule. Because the bonds from As1 are almost exactly tetrahedrally orientated the benzene rings forming the bridges from As1 to As3 and As4 though they are coplanar with the arsenic atoms to which they are attached are not coplanar with ruthenium (see Figure). The potential overcrowding mentioned above is avoided partly by the effects of the distortions necessary to provide tetrahedral bonds at As1 and partly by the distortions of the bond angles at As2, As3, and As4 which involve also the non-bridging phenyl groups. The deviations in the angles at As2, As3, and As4 from the tetrahedral can be seen in Table 2. The largest deviations are found when bonds to non-bridging phenyls are involved. The occurrence of such deviations, which are geometrically impossible in the bridges, makes possible the retention of the octahedral form.

The bond from ruthenium to As1 is short compared with those to As2, As3, and As4. In the $[PtQASI]^+$ ion the bond to As1 from platinum is also short (2·31 Å) compared with those to As2 (2·49 Å), As3 (2·45 Å), and As4 (2·43 Å). The shortening might be due to restrictions imposed by the ligand which in order to reduce the strain at As1 requires that the angles Ru–As1–C be slightly greater than the ideal tetrahedral.

The general conclusion from this structure is that the ruthenium bond angles are distorted from the octahedral about as much as they might be by the bridging requirements of a bidentate ligand. What seemed a possible way of preventing octahedral co-ordination fails because the valency angles at the arsenic atoms are not all sufficiently restricted by bridging.

Experimental

Preparation.—Samples were supplied by Dr. L. M. Venanzi, and had been recrystallised from tetrahydrofurfuryl alcohol. The yellow-orange crystals were about 0·25 mm. long.

X-Ray Photography.—The unit-cell dimensions were measured from zero layer Weissenberg photographs taken about the *b* and *c* axes. The intensities were estimated visually by the multiple film technique from equi-inclination Weissenberg photographs taken about the *b* axis. The layer scale factors were obtained by comparison of $F^2(hkO)$ values with those observed on a [001] zero layer Weissenberg photograph.

Calculations.—The main programmes used were written by J. S. Rollett (structure factor calculations and least-squares refinement), O. S. Mills (Fourier summations), G. A. Mair (standard deviations by procedures of Cruickshank [3] and Darlow [4]). Final structure factors are

[2] Mair, Powell, and Venanzi, *Proc. Chem. Soc.*, 1961, 170.
[3] Ahmed and Cruickshank, *Acta Cryst.*, 1953, **6**, 385.
[4] Darlow, *Acta Cryst.*, 1960, **13**, 683.

TABLE 1

Structure factors in absolute units with (90 — α) in degrees, given in every sixth column

k	h	l	F_o	F_c		k	h	l	F_o	F_c		k	h	l	F_o	F_c		k	h	l	F_o	F_c	
0	0	4	375	383	82			11	43	45	142			1	32	24	275			6	86	83	38
		6	315	349	80			12	49	34	330			2	60	57	125			7	53	46	235
		8	61	64	237			13	37	36	106			4	35	26	59			8	27	23	306
		10	32	31	270			15	35	48	212			5	33	34	309			9	85	91	36
		12	42	48	292	0	16	0	195	200	90			6	51	52	134			10	79	76	10
		14	53	65	247			1	112	123	176			7	40	50	272			11	95	100	353
0	2	3	509	461	9			2	236	254	40			8	31	31	166			12	32	31	90
		4	213	206	10			3	187	199	203	0	36	1	61	64	22	1	9	0	129	134	270
		5	452	453	355			4	142	141	101			3	48	48	17			1	132	148	273
		6	176	185	6			5	163	176	271			4	25	30	323			2	89	86	256
		7	119	121	4			6	129	137	39			5	28	21	10			3	44	39	312
		8	101	108	351			7	85	89	252			7	30	41	54			4	50	47	135
		9	73	72	140			8	61	68	350	0	38	0	51	50	270			5	48	48	336
		10	115	122	353			9	82	83	248			1	28	33	126			6	84	94	98
		11	75	76	317			10	42	34	86			2	49	55	285			7	81	79	276
		12	42	25	6			11	71	80	294			3	26	25	206			8	43	52	96
		13	57	68	164			12	32	35	330			4	33	37	275			9	29	32	347
		15	28	27	138	0	18	0	88	82	90			5	24	26	223			10	73	85	105
0	4	2	178	183	261			1	253	270	343	1	0	3	98	105	7			12	50	55	90
		3	282	293	257			2	201	213	86			5	256	268	355	1	10	0	50	42	270
		4	321	313	287			3	139	155	11			7	64	64	2			1	24	34	73
		5	319	339	280			4	108	109	116			9	39	39	132			2	101	99	157
		6	168	194	266			5	142	150	7			11	70	63	323			3	52	60	193
		7	246	261	275			6	54	58	162	1	1	2	28	22	1			4	107	112	10
		8	65	68	314			7	60	72	272			3	65	64	109			5	44	48	359
		9	166	188	257			8	33	31	92			4	36	39	51			6	88	81	205
		10	68	83	284			10	48	56	184			5	84	88	354			7	63	63	52
		11	106	111	278			12	37	38	247			6	42	47	59			8	44	49	251
		12	59	54	252			13	53	44	203			9	44	45	140			10	119	121	295
		14	37	34	7	0	20	0	241	237	270	1	2	2	89	83	275			11	39	37	326
0	6	0	142	147	270			1	101	108	324			3	73	69	167			12	55	57	229
		2	326	328	163			2	164	171	267			4	181	192	263	1	11	0	60	63	270
		3	173	175	305			3	170	189	355			5	97	98	308			1	73	80	320
		4	324	322	173			4	152	165	308			6	230	238	255			2	110	114	186
		5	164	172	205			5	49	57	344			7	55	48	257			3	46	47	59
		6	301	319	195			6	91	95	274			8	55	53	29			4	47	55	263
		7	129	133	186			7	58	60	271			9	52	53	261			5	28	32	61
		8	137	148	180			8	54	60	1			10	30	30	253			6	104	113	200
		9	118	131	214			9	42	42	331			11	44	41	266			7	62	58	0
		10	169	184	176			11	39	38	152			13	39	32	236			8	72	71	190
		11	141	151	178	0	22	0	30	28	270	1	3	2	65	71	6			9	60	66	22
		12	48	55	248			1	159	171	191			3	85	81	247			11	39	45	12
		13	40	44	171			2	124	124	243			4	188	202	352	1	12	1	116	123	86
		15	48	66	184			3	88	86	247			5	105	111	328			2	80	81	3
0	8	0	87	105	270			4	71	71	242			6	34	39	337			3	32	34	351
		1	282	298	267			5	146	157	212			8	32	39	42			4	65	68	9
		2	211	209	304			6	62	59	180			12	32	28	163			5	95	100	221
		3	252	271	71			7	59	58	239	1	4	2	82	54	128			6	69	79	338
		4	179	180	183			8	72	92	216			3	117	119	263			7	121	113	101
		5	185	188	95			9	63	73	273			4	93	91	153			8	84	77	333
		6	67	71	52			10	32	25	179			5	191	197	178			9	91	92	201
		7	73	76	96			11	30	28	191			6	161	162	206			10	32	39	301
		8	58	65	96	0	24	0	125	136	90			7	109	107	172			11	71	77	176
		9	96	109	92			2	39	50	207			8	55	57	165			12	38	32	308
		10	181	204	109			3	61	67	119			9	49	53	245	1	13	0	65	65	270
		11	72	80	130			4	78	73	139			10	107	110	166			1	92	95	104
		12	90	105	68			5	71	77	81			11	92	90	165			2	111	126	246
		14	75	96	96			6	108	113	119			12	39	39	223			3	85	92	155
0	10	0	123	111	270			7	64	73	128	1	5	0	165	176	270			4	96	100	284
		1	265	284	220			8	63	71	188			1	148	146	97			5	104	103	105
		2	165	172	229			9	61	63	129			3	38	32	354			6	58	50	252
		3	154	156	168			10	48	54	120			4	77	75	187			7	101	107	90
		4	31	33	322			12	33	32	103			5	81	91	247			8	29	23	262
		5	41	54	42	0	26	0	78	71	270			6	67	71	243			9	31	35	160
		6	109	106	135			2	33	36	285			7	48	50	290			10	32	38	293
		7	76	89	282			3	79	74	160			8	26	23	340	1	14	0	50	52	90
		8	59	58	170			4	63	61	2			10	43	46	253			1	64	73	258
		9	145	150	10			5	72	74	20			12	32	32	268			2	120	123	21
		10	58	63	46			6	34	39	9	1	6	0	83	90	90			3	90	97	221
		11	138	150	353			7	41	49	33			1	69	76	218			4	107	107	131
		12	53	57	101			8	61	69	48			2	164	161	6			5	78	79	272
		13	71	88	348			9	43	43	84			3	174	189	81			6	81	86	50
		15	65	95	10			10	40	53	52			4	119	129	157			7	84	85	239
0	12	0	115	123	90			11	50	63	353			5	190	201	99			8	73	68	24
		1	153	159	84			12	32	41	77			6	90	100	94			9	76	74	249
		2	166	171	163	0	28	0	48	43	270			7	51	60	117			10	78	81	104
		3	126	135	123			1	48	43	172			8	32	33	101			11	50	50	243
		4	79	74	68			2	48	46	94			9	103	103	73			12	43	43	34
		5	160	157	94			4	42	48	221			10	101	104	106	1	15	0	97	101	44
		6	129	135	202			6	57	60	348			11	63	63	112			2	81	85	351
		7	135	151	72			7	39	37	353			12	50	55	73			3	123	133	136
		8	97	110	213			9	40	37	318	1	7	1	69	70	83			5	70	76	184
		9	94	96	65			10	36	41	269			2	50	50	206			6	64	65	24
		10	135	139	288			11	37	47	341			3	115	115	356			7	54	55	102
		11	42	42	43	0	30	2	24	35	14			4	86	89	178	1	16	1	155	158	313
		12	71	79	227			3	53	49	24			5	69	70	183			2	95	94	75
		13	44	44	8			5	46	51	129			6	48	40	11			3	109	116	359
		14	58	69	276			7	37	41	99			7	35	47	166			4	122	133	149
0	14	0	110	102	90			8	34	24	300			8	33	34	84			5	108	114	359
		1	162	167	103			9	25	12	135			9	35	48	206			6	83	80	175
		2	135	154	306			10	26	23	238			10	48	58	118			7	111	107	281
		3	69	58	211	0	32	1	46	49	230			11	63	73	182			8	61	68	133
		4	194	210	352			2	51	49	335			12	39	36	358			9	63	64	14
		5	115	115	163			4	31	25	348	1	8	0	108	112	90			10	60	63	159
		6	156	170	346			5	30	29	208			1	67	64	197			11	31	29	332
		7	181	190	92			6	54	58	24			2	109	104	213			12	30	21	174
		8	130	138	350			7	43	44	232			3	44	48	47	1	17	0	123	138	90
		9	81	77	179			8	34	40	355			4	153	157	4			1	41	36	298
		10	76	84	346	0	34	0	61	60	90			5	98	100	38			2	160	167	70

TABLE 1 (*Continued*)

k	h	l	F_o	F_c	
		4	97	106	104
		5	33	36	43
		6	40	36	56
		11	31	30	46
		12	29	27	306
1	13	0	208	224	279
		1	81	80	321
		2	137	142	241
		3	123	130	6
		4	110	125	293
		5	74	81	75
		6	109	107	229
		8	31	31	226
		9	60	63	26
		10	32	38	284
		11	46	46	96
		12	28	28	162
1	19	0	31	32	270
		1	96	96	5
		2	82	91	61
		3	92	99	11
		4	67	71	358
		5	35	39	17
		6	56	55	321
		7	31	23	309
		8	39	45	359
		10	31	33	323
1	20	0	41	41	270
		1	170	182	160
		2	93	99	257
		3	85	92	199
		4	98	104	282
		5	136	145	181
		7	31	29	150
		8	55	53	241
		11	29	27	139
1	21	0	27	28	270
		1	33	34	244
		2	28	30	219
		3	85	92	315
		4	50	55	328
		5	60	62	245
		6	31	30	293
		7	50	64	270
		9	39	44	283
		10	31	28	289
		11	29	27	172
1	22	0	167	185	90
		1	80	81	153
		2	67	71	97
		3	103	116	172
		4	82	84	111
		5	31	28	129
		6	86	95	94
		7	45	48	125
		9	38	44	137
		10	30	29	128
1	23	0	36	36	90
		2	29	36	225
		3	30	26	337
		4	43	46	186
		5	31	33	243
		6	39	38	152
		8	39	44	217
		9	38	43	216
		11	42	44	185
1	24	0	36	30	90
		1	92	97	6
		2	60	65	74
		3	37	41	118
		4	73	76	52
		5	92	98	338
		6	33	38	15
		7	45	43	32
		8	57	59	40
		9	37	41	83
		10	35	33	30
		11	41	41	353
1	25	0	31	20	270
		1	57	56	357
		3	33	36	243
		4	31	23	183
		6	32	35	107
		8	31	30	122
		9	30	27	187
		10	34	38	93
		12	38	38	91
1	26	0	73	80	270
		2	31	30	74
		3	32	32	303
		4	38	30	332
		5	55	56	296
		6	67	76	282
		7	44	46	315
		8	37	41	17
		9	40	47	308
		10	32	39	283
		11	23	21	307
1	27	0	30	45	270
		2	32	38	219
		4	30	35	199
		5	32	27	351
		6	45	40	200
		7	33	31	357
		8	36	37	136
		9	28	27	3
		10	30	33	354
		11	60	57	326
1	28	4	32	36	194
		5	45	43	194
		6	38	34	237
		7	33	30	241
		9	26	28	273
		10	29	30	219
		11	99	131	116
1	29	0	30	46	270
		1	64	53	119
		4	39	37	203
		5	44	44	114
		6	43	49	245
		7	50	47	74
		9	25	18	61
		10	27	23	237
1	30	0	54	52	90
		1	32	29	241
		2	39	37	272
		5	30	27	143
		6	36	36	77
		7	28	25	222
		9	23	18	144
		10	24	27	94
1	31	1	59	56	179
		2	31	29	335
		3	38	36	136
		5	55	53	143
		6	35	27	6
		7	33	27	136
		8	24	21	337
		9	21	12	111
1	32	2	37	37	166
		5	28	21	326
		6	38	43	124
		7	31	29	271
		8	23	23	147
1	33	0	70	67	90
		1	30	31	220
		2	55	50	83
		3	29	20	174
		4	40	32	60
		6	36	33	62
1	34	1	35	37	53
		2	34	37	170
		4	27	19	309
		5	25	23	24
		6	33	36	195
		7	37	43	51
		8	18	17	187
1	35	0	38	36	90
		1	43	38	358
		2	32	28	96
		3	32	27	4
		4	25	28	24
		5	23	24	1
1	36	0	31	29	270
		1	31	32	120
		2	39	39	308
		5	21	20	175
		6	30	35	305
		7	27	33	89
1	37	1	23	20	20
		2	28	17	282
		3	27	24	316
		4	21	23	336
		5	23	27	280
		6	19	14	324
1	38	0	21	26	90
		1	33	35	194
		2	29	30	31
		3	27	35	184
		4	22	29	129
		5	19	23	188
2	0	2	158	171	72
		4	56	53	198
		6	156	168	257
		8	30	35	299
		10	69	84	255
		12	47	52	261
2	1	2	33	28	305
		3	89	93	204
		4	35	43	257
		5	132	133	336
		6	111	110	245
		7	44	42	21
		9	26	30	32
		10	75	80	249
		11	86	87	349
2	2	1	82	84	156
		2	171	172	18
		3	70	70	328
		4	65	62	30
		5	125	118	152
		6	55	60	325
		7	77	80	170
		8	52	56	4
		9	19	23	218
		11	81	92	168
2	3	1	144	148	152
		2	85	88	3
		3	51	52	318
		4	30	31	91
		5	89	85	182
		6	187	186	270
		7	109	102	99
		8	55	53	360
		9	27	31	176
		10	49	48	286
		11	63	65	144
		12	63	65	268
2	4	0	28	20	90
		1	65	56	156
		2	109	100	29
		3	70	75	299
		4	83	75	115
		5	74	81	258
		6	119	114	67
		7	79	86	265
		8	25	24	102
		9	19	16	321
		10	57	56	75
		12	30	40	68
2	5	0	67	74	90
		1	202	215	166
		2	172	183	8
		3	73	81	252
		4	76	80	151
		5	155	155	180
		6	121	123	39
		7	85	85	245
		8	61	56	21
		9	54	56	263
		10	60	61	84
		11	66	68	163
		12	36	48	23
2	6	0	80	90	90
		1	157	168	5
		2	95	92	156
		3	83	79	327
		5	106	105	355
		6	53	50	105
		7	43	47	292
		8	69	73	205
		9	19	18	38
		10	54	52	336
		11	30	32	332
2	7	0	191	216	90
		1	95	98	357
		2	101	108	117
		3	136	130	310
		4	132	122	113
		5	81	83	6
		6	152	145	103
		7	120	114	273
		8	51	55	171
		9	43	45	347
		10	58	53	113
		11	21	31	342
		12	30	38	80
2	8	0	183	202	270
		1	86	98	25
		2	151	157	246
		4	105	111	298
		5	76	78	322
		6	59	63	234
		9	39	42	212
		10	20	19	332
2	9	0	73	90	270
		1	172	182	351
		2	120	111	230
		3	81	82	58
		4	131	130	306
		5	163	172	5
		6	77	76	219
		7	93	94	356
		8	55	52	221
		9	34	45	54
		10	50	47	306
		11	42	47	9
		12	29	33	140
2	10	0	108	118	270
		1	113	124	172
		2	47	53	276
		3	98	107	194
		4	84	85	198
		5	108	110	231
		6	23	35	226
		7	67	55	75
		9	56	53	260
		10	36	39	179
2	11	0	195	203	270
		1	129	131	137
		2	147	148	246
		3	130	133	189
		4	147	152	292
		5	99	97	232
		6	79	78	265
		7	73	66	95
		8	46	45	244
		9	66	61	240
		10	55	57	224
2	12	0	46	56	90
		1	33	41	201
		2	37	43	52
		3	67	65	115
		4	117	129	169
		5	59	66	105
		6	63	67	133
		7	31	33	149
		10	59	57	127
2	13	0	95	100	90
		1	170	174	128
		2	45	45	36
		3	157	167	176
		4	157	157	147
		5	81	83	187
		6	24	31	96
		7	84	89	121
		8	28	24	140
		9	35	45	188
		10	59	61	145
		11	21	28	156
2	14	0	19	19	270
		1	52	48	260
		3	42	48	70
		5	81	82	72
		6	39	46	357
		7	32	24	300
		8	44	45	72
		9	94	102	39
		10	21	29	132
		11	29	40	11
2	15	0	129	139	90
		1	71	78	319
		2	84	88	46
		3	31	32	38
		4	105	115	105
		5	94	92	63
		6	83	83	15
		8	72	75	39
		9	59	58	80
		10	47	50	102
		11	36	40	50
2	16	1	62	67	213
		2	54	48	154
		3	28	21	250
		4	84	89	337
		5	43	42	100
		6	49	55	265
		8	29	34	248
		9	42	47	22
		10	56	65	287
		11	41	48	40
		12	27	30	243
2	17	0	61	63	270
		1	69	68	296
		2	28	36	60
		3	64	68	346
		4	75	70	352
		5	48	48	7
		6	42	41	308
		7	71	73	284
		8	36	44	22
		9	56	56	358
		10	47	51	333
		11	35	39	347
2	18	0	78	88	90
		1	61	64	118
		2	33	36	68
		4	59	57	329
		5	81	83	170
		6	43	46	22
		7	35	45	104
		8	62	63	280
		9	42	46	172
		10	55	64	310
		11	35	37	168
2	19	2	57	57	172
		3	83	91	333
		4	66	71	314
		5	47	45	183
		6	28	30	229
		8	42	44	233
		9	36	39	287
		10	51	55	281

TABLE 1 (*Continued*)

k	h	l	F_o	F_c
		11	34	42 170
		12	31	38 241
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		2	76	76 51
		3	58	58 216
		4	33	42 72
		5	48	54 270
		6	92	93 34
		7	29	27 241
		8	36	40 39
		9	42	44 199
		10	20	26 67
		11	19	23 236
		12	17	17 20
2	21	0	57	55 90
		1	32	32 89
		2	83	84 264
		4	27	27 258
		5	28	31 213
		6	41	48 73
		7	42	47 149
		8	30	29 254
		9	55	61 203
		10	20	26 77
		11	49	50 182
		12	29	32 54
2	22	0	59	54 90
		1	96	97 350
		2	57	55 89
		3	34	34 310
		4	56	54 119
		5	117	119 316
		7	36	43 295
		8	30	30 84
		11	18	25 315
2	23	0	33	36 90
		1	27	22 329
		3	66	74 179
		4	35	43 133
		5	62	64 310
		6	36	40 84
		8	29	30 135
		9	29	30 204
		10	47	55 105
		11	43	49 310
		12	34	35 86
2	24	0	122	126 270
		1	77	78 350
		2	35	37 216
		3	84	85 6
		4	41	41 240
		5	30	33 324
		6	63	64 252
		9	20	21 261
2	25	0	61	64 270
		1	54	58 4
		3	29	28 76
		4	42	36 161
		5	70	70 14
		6	60	57 213
		7	29	30 32
		8	35	42 129
		9	27	28 38
		10	25	28 190
		11	31	59 354
		12	22	28 189
2	26	0	80	84 270
		1	26	44 16
		2	69	66 269
		3	30	21 270
		4	66	63 234
		5	42	44 181
		6	30	26 225
		8	23	26 182
		9	26	28 296
		10	17	21 143
		11	21	28 163
2	27	0	96	96 270
		1	42	44 119
		2	59	52 291
		3	30	24 51
		4	42	44 274
		5	55	53 118
		6	65	69 275
		7	45	48 83
		8	27	22 340
		9	25	19 37
		10	23	23 265
		11	19	26 116
2	28	0	30	41 90
		1	52	50 176
		2	47	46 210
		3	36	39 159
		4	36	45 189
		5	36	38 126
		6	45	46 126
		8	32	38 188
		9	24	21 79
		10	15	22 141
2	29	1	89	92 185
		2	30	33 340
		3	36	33 185
		5	71	73 170
		6	34	37 23
		7	38	37 191
		8	25	25 311
2	30	3	36	40 122
		5	44	50 73
		6	27	23 85
		7	36	32 93
		9	26	30 86
2	31	0	99	99 90
		1	29	31 296
		2	61	53 90
		4	52	47 73
		6	61	66 78
		9	19	18 94
2	32	1	28	27 116
		4	33	29 359
		7	23	26 49
		9	17	14 12
2	33	1	67	68 4
		3	32	30 359
		4	41	47 353
		5	49	52 345
2	34	0	26	29 90
		2	26	33 45
		6	21	28 318
2	35	0	30	38 270
		2	24	26 253
		3	24	28 287
		4	28	22 283
		5	26	37 273
		6	24	28 251
2	36	2	23	29 18
		4	21	17 91
		6	21	28 7
2	37	4	29	39 181
2	38	1	27	29 305
3	0	3	54	48 9
		5	75	69 156
3	1	2	237	235 80
		3	190	191 14
		4	106	99 72
		5	87	83 131
		6	150	145 283
		7	91	85 122
		8	84	88 334
		9	74	82 173
		10	119	124 272
		11	116	132 162
		12	107	124 269
		13	55	65 174
		14	38	54 296
		15	39	55 189
		16	31	53 250
3	2	2	22	22 208
		3	63	54 14
		4	36	28 170
		5	45	43 219
		6	43	34 98
		9	28	25 101
3	3	1	80	90 263
		2	178	174 324
		3	213	202 309
		4	87	80 351
		5	148	138 205
		6	217	213 24
		7	150	154 247
		8	128	127 3
		9	100	108 249
		10	110	111 38
		11	109	122 184
		12	66	73 49
		13	52	59 210
		14	19	31 95
		15	22	36 174
		16	23	42 100
3	4	0	41	36 90
		1	46	42 335
		2	51	46 193
		3	28	29 151
		4	71	65 302
		5	31	30 327
		6	27	19 346
		8	19	26 156
3	5	0	295	315 90
		1	201	204 296
		2	137	143 148
		3	172	174 300
		4	144	153 152
		5	185	187 306
		6	210	207 123
		7	241	252 270
		8	158	163 188
		9	83	86 291
		10	56	56 131
		11	76	80 293
		12	44	49 104
		13	39	25 212
		14	19	24 180
		15	22	36 46
		16	21	35 46
3	6	0	28	15 90
		1	36	23 304
		2	66	61 181
		3	28	30 109
		4	22	26 336
		5	32	16 296
		9	20	29 244
3	7	0	148	160 270
		1	351	394 2
		2	259	259 224
		3	153	164 43
		4	144	144 249
		5	255	248 17
		6	207	206 195
		7	113	111 50
		8	143	138 185
		9	79	86 116
		10	30	29 251
		11	22	22 355
		12	48	61 150
		13	20	33 141
		16	14	22 337
3	8	0	26	16 90
		1	59	55 265
		2	49	39 93
		3	54	61 101
		4	69	69 212
		5	21	21 113
		6	16	17 269
		7	47	46 51
		8	39	35 143
3	9	0	420	452 270
		1	245	258 153
		2	311	313 260
		3	174	140 145
		4	254	248 286
		5	114	113 206
		6	145	148 272
		7	121	119 103
		9	29	35 235
		10	38	39 3
		12	30	35 111
		13	35	46 37
		14	25	39 74
3	10	0	17	13 270
		1	17	25 191
		2	18	15 294
		3	19	23 115
		4	57	53 209
		5	35	32 47
		6	17	23 43
		9	21	17 52
3	11	0	106	101 90
		1	302	310 171
		2	147	139 79
		3	240	243 178
		4	267	268 145
		5	183	189 175
		6	76	78 157
		7	90	89 125
		8	60	63 170
		9	21	27 198
		10	79	86 155
		11	22	21 65
		12	30	37 296
		13	34	46 10
3	12	0	35	38 90
		1	23	28 187
		2	31	30 155
		3	15	20 116
		4	22	26 354
		5	34	40 133
		9	30	28 58
3	13	0	165	170 90
		1	92	94 345
		2	205	207 57
		3	176	183 69
		4	153	155 97
		5	220	238 72
		6	115	119 39
		7	87	91 95
		8	80	80 30
		9	134	141 72
		10	31	43 104
		11	49	53 76
		12	29	33 350
3	14	0	39	36 90
		1	15	12 88
		2	55	49 131
		3	16	29 356
		4	24	24 28
		5	18	20 99
		9	22	23 155
		10	22	25 272
3	15	0	67	65 270
		1	113	114 273
		2	42	40 353
		3	62	61 340
		4	215	223 347
		5	52	52 5
		6	125	125 345
		7	128	123 236
		8	102	111 1
		9	95	104 354
		10	96	107 338
		11	37	53 348
		13	26	40 317
		15	28	48 8
3	16	1	28	27 63
		2	17	11 76
		3	17	19 213
		4	18	25 337
		7	21	15 80
		8	21	30 292
		10	22	28 345
3	17	0	107	108 90
		1	34	39 142
		2	102	95 144
		3	87	81 298
		4	26	35 352
		5	104	97 239
		6	60	55 192
		7	30	32 255
		8	84	86 240
		9	76	76 275
		10	100	108 274
		11	36	47 213
		12	58	70 241
		14	42	62 266
3	18	0	17	25 90
		1	25	26 340
		2	18	18 87
		3	18	22 231
		5	34	44 273
		7	21	33 227
		8	22	19 61
3	19	0	70	74 90
		1	137	140 32
		2	61	75 298
		3	60	52 349
		4	20	16 282
		5	20	29 256
		6	69	70 54
		7	75	76 127
		8	38	39 243
		9	90	101 184
		10	30	33 80
		11	72	85 136
		12	26	24 81
		13	46	68 159
3	20	1	46	42 337
		2	19	17 138
		3	20	33 14
		4	20	26 128
		5	36	39 303
3	21	0	34	22 270
		1	19	24 329
		2	65	59 299
		3	122	119 303
		5	114	115 298
		6	53	52 41
		7	73	71 277
		8	44	49 78
		9	30	32 230
		10	74	83 98
		11	46	60 313
		12	41	52 78
3	22	0	45	45 270
		1	28	33 300
		2	29	27 239
		3	36	32 6
		4	21	29 239
		7	22	22 353
3	23	0	41	48 270
		1	54	53 328
		2	80	74 118
		3	21	18 355
		4	88	90 165
		5	72	73 2
		6	114	122 202
		7	31	31 329
		8	61	62 137
		9	29	27 9
		10	55	64 195
		11	35	44 354
		12	26	38 214
3	24	0	30	25 270
		1	36	43 178
		2	21	24 272
		4	22	28 238
		5	22	29 129
3	25	0	156	169 270

TABLE 1 (*Continued*)

k	*h*	*l*	F_o	F_c	
		1	21	22	94
		2	86	84	265
		3	87	88	39
		4	76	71	282
		5	79	77	111
		6	62	62	259
		7	75	75	85
		9	34	41	66
		11	39	54	121
3	26	1	22	22	173
		3	22	20	152
		5	22	29	118
3	27	1	147	152	189
		2	62	55	298
		3	82	76	195
		4	22	29	307
		5	90	93	181
		6	57	60	29
		7	41	47	213
		8	28	33	308
3	28	2	22	22	69
3	29	0	142	151	90
		2	87	88	109
		3	31	35	155
		4	74	80	93
		5	21	27	45
		6	73	77	100
		8	25	32	171
		9	23	20	86
3	31	1	90	95	7
		3	41	38	23
		4	61	68	358
		5	68	76	6
		6	19	16	6
		7	39	48	29
		8	22	27	39
3	33	0	71	78	270
		3	38	43	268
		4	32	36	277
		5	56	58	256
		6	33	47	271
		7	21	23	328
		8	22	20	312
3	35	4	42	54	173
		5	21	26	180
4	0	2	65	64	102
		4	68	57	20
		6	78	71	238
		8	27	24	318
		10	71	76	270
		12	37	56	261
4	1	2	121	106	285
		3	197	192	341
		4	12	8	303
		5	136	123	191
		6	101	94	68
		7	84	78	226
		9	81	81	208
		10	107	106	77
		11	96	100	175
		12	72	78	66
		13	59	57	195
		14	26	33	101
		15	26	41	176
4	2	1	18	16	39
		2	54	54	10
		3	131	117	14
		4	65	59	343
		5	69	65	177
		6	77	76	8
		7	55	48	166
		8	64	54	21
		9	20	33	196
		11	58	70	168
4	3	0	86	94	90
		1	96	99	311
		2	146	145	205
		3	79	65	240
		4	31	33	185
		5	132	115	323
		6	177	171	114
		7	152	140	274
		8	123	115	180
		9	54	52	336
		10	86	88	107
		11	76	74	317
		12	89	93	95
		13	20	28	311
		14	26	36	128
		15	21	30	8
4	4	0	59	61	90
		1	46	41	270
		2	10	6	339
		3	72	66	276
		4	49	54	41
		5	105	104	264
		6	71	69	44
		7	74	72	267
		9	29	41	207
		10	43	42	93
4	5	0	111	111	270
		1	185	179	360
		2	211	209	212
		3	129	126	100
		4	97	95	279
		5	187	174	14
		6	186	175	204
		7	121	121	54
		8	129	115	177
		9	71	72	76
		10	57	57	207
		11	76	74	356
		12	37	48	177
		13	28	40	51
4	6	0	28	29	90
		1	131	137	337
		2	104	97	174
		3	45	46	15
		4	40	31	215
		5	65	64	0
		6	84	80	159
		7	59	53	288
		8	51	46	185
4	7	0	338	350	270
		1	199	208	152
		2	153	149	270
		3	140	132	143
		4	155	153	295
		5	138	130	146
		6	170	161	279
		7	197	192	93
		8	55	49	356
		9	29	30	158
		10	43	45	307
		11	22	29	94
		12	21	20	261
		13	28	41	42
4	8	0	181	181	270
		1	87	87	19
		2	91	85	259
		3	18	31	10
		4	115	107	285
		6	48	39	259
		7	18	25	71
		8	28	36	91
		9	30	31	178
4	9	0	138	138	90
		1	282	302	183
		2	212	213	41
		3	168	162	178
		4	165	159	122
		5	213	208	176
		6	98	97	25
		7	56	47	173
		8	28	37	19
		9	21	24	244
		10	31	37	113
		11	22	28	155
		12	30	39	311
4	10	0	77	75	270
		1	144	145	147
		2	44	45	257
		3	76	77	213
		4	64	62	220
		5	75	66	216
		6	56	45	206
		7	19	18	53
		9	21	24	250
		10	31	36	143
4	11	0	273	282	90
		1	109	110	315
		2	205	211	67
		3	145	140	29
		4	176	171	91
		5	114	114	62
		6	125	124	62
		7	27	41	309
		8	77	81	40
		9	88	92	57
		10	22	30	123
		12	21	29	305
4	12	0	50	43	90
		1	40	39	168
		2	52	50	85
		3	50	52	95
		4	100	97	149
		5	83	81	109
		7	28	45	95
		9	31	30	107
		10	22	32	155
4	13	0	71	68	270
		1	175	177	318
		2	34	33	281
		3	178	184	357
		4	204	197	339
		5	107	103	5
		6	71	70	345
		7	125	118	293
		8	79	83	349
		9	38	32	349
		10	96	99	329
		11	21	24	314
4	14	0	40	41	270
		2	27	30	351
		3	40	41	90
		4	42	38	5
		5	66	72	67
		6	27	28	2
		8	56	53	48
		9	22	40	47
		11	21	29	2
4	15	0	53	59	270
		1	58	57	120
		2	101	102	223
		3	106	103	284
		4	80	82	285
		5	168	173	246
		6	79	71	188
		7	55	55	269
		8	64	63	232
		9	88	88	254
		10	58	57	284
		11	51	56	237
		12	27	31	196
		14	19	28	256
4	16	0	29	26	90
		1	50	53	206
		2	38	31	104
		3	18	19	271
		4	52	53	7
		6	29	36	275
		9	22	34	348
		10	48	54	290
		11	21	26	22
		12	19	28	237
4	17	0	24	23	90
		1	80	80	55
		2	35	40	250
		3	18	31	203
		4	91	92	170
		5	34	43	269
		6	29	44	122
		7	56	57	118
		8	75	77	191
		9	76	73	180
		10	61	67	141
		11	41	48	171
		12	18	19	119
		13	27	41	137
4	18	0	62	61	90
		1	26	24	84
		2	26	17	44
		3	27	27	17
		5	29	34	156
		7	48	47	121
		8	38	46	281
		9	31	36	189
		10	30	39	302
		11	34	35	170
4	19	0	74	77	270
		1	32	41	330
		2	71	70	310
		3	75	78	159
		4	53	57	194
		5	36	39	344
		6	21	23	30
		8	38	47	77
		9	31	40	106
		10	72	73	108
		11	34	39	347
		12	46	54	71
4	20	1	19	10	15
		2	48	50	15
		3	20	24	248
		4	35	40	51
		5	30	26	267
		6	65	62	34
		7	31	27	224
		8	22	31	2
		9	37	38	211
		10	20	33	73
4	21	0	86	85	270
		1	63	67	223
		2	67	62	107
		3	29	40	149
		4	30	29	133
		5	30	33	60
		6	75	75	236
		7	31	33	325
		8	31	38	107
		9	42	49	15
		10	20	27	215
		11	51	53	3
		12	16	22	228
4	22	1	54	56	341
		2	36	47	99
		3	55	53	299
		4	43	42	143
		5	43	52	314
		6	38	39	160
		7	38	47	288
4	23	0	21	28	270
		3	60	65	26
		4	22	21	309
		5	76	88	130
		6	31	35	246
		7	44	47	72
		8	21	17	284
		9	35	42	44
		10	33	39	286
		11	47	54	118
		12	19	26	258
4	24	0	67	62	270
		1	56	56	8
		2	21	28	238
		3	65	67	5
		4	22	22	243
		6	62	58	224
4	25	0	65	69	90
		1	72	72	182
		2	31	38	296
		4	58	60	345
		5	58	58	173
		6	72	79	25
		7	30	24	199
		8	35	44	315
		10	30	38	10
		11	25	29	172
		12	15	26	7
4	26	0	79	77	270
		1	44	41	185
		2	62	58	272
		4	31	34	239
		5	38	42	183
4	27	0	114	119	90
		1	22	23	287
		2	58	62	95
		3	31	39	220
		4	53	50	82
		5	30	36	313
		6	59	62	94
		7	40	50	260
4	28	0	49	45	90
		1	38	39	179
		3	38	43	165
		4	30	38	160
		5	21	25	129
		6	20	24	133
		8	26	30	188
4	29	1	87	95	12
		2	22	34	139
		3	37	43	11
		5	65	74	349
		6	20	26	197
		7	41	45	15
		8	26	30	177
		9	87	97	12
4	30	3	21	28	97
		5	34	37	72
		7	18	23	84
4	31	0	97	106	270
		2	46	50	287
		3	20	27	320
		4	44	49	257
		5	27	32	252
		6	47	59	270
		8	15	15	326
4	32	6	24	19	335
4	33	1	47	55	188
		3	18	26	177
		4	43	54	176
		5	41	49	180
		7	19	27	188
4	34	0	18	18	90
		2	25	24	79
4	35	0	34	42	90
		1	17	24	261
		2	16	18	90
		3	16	23	89
		4	21	25	100
		5	24	34	90
		6	17	23	85
4	36	1	15	14	327
4	37	1	14	16	305
		4	16	33	2
5	0	3	123	116	394
		5	188	186	183
		7	75	67	182
		9	63	53	244
		11	47	50	158
5	1	2	57	45	215
		3	30	23	132
		4	41	30	70
		5	59	53	19
		6	66	53	80
		7	17	24	66
		8	46	36	200
		9	20	28	147

TABLE 1 (*Continued*)

k	h	l	F_o	F_c
		11	36	31 332
5	2	1	18	23 120
		2	97	94 89
		3	41	40 355
		4	105	96 113
		5	24	19 335
		6	163	145 85
		8	68	60 213
		9	20	19 79
		10	62	63 91
5	3	0	55	61 270
		1	44	45 360
		2	16	14 291
		3	39	35 168
		4	80	73 331
		5	92	86 330
		6	27	32 302
		7	30	21 39
		9	20	24 121
		10	29	29 308
		11	59	50 349
5	4	1	154	165 354
		2	82	78 230
		3	65	50 222
		4	87	82 346
		5	155	146 3
		6	32	30 111
		7	58	50 340
		8	33	31 311
		9	35	37 39
		10	36	34 45
		11	55	52 350
5	5	0	75	81 270
		1	76	75 126
		2	58	48 60
		3	78	71 248
		4	29	31 169
		5	75	66 230
		6	86	80 256
		7	18	14 125
		8	47	40 345
		10	30	32 256
		11	30	31 138
5	6	0	160	163 270
		1	24	22 124
		2	15	25 219
		3	55	52 203
		4	88	74 297
		5	88	73 296
		6	109	105 239
		9	54	55 251
		10	59	54 277
		11	36	39 308
5	7	0	31	28 90
		1	41	42 153
		2	59	59 35
		3	63	54 346
		4	69	65 134
		5	72	58 184
		6	29	29 45
		7	63	58 180
		8	47	49 21
		9	20	29 230
		10	47	47 126
		11	66	59 178
5	8	0	41	47 270
		1	97	103 118
		2	67	64 357
		3	55	44 208
		4	117	109 159
		5	78	73 184
		6	70	61 235
		7	69	73 85
		9	71	58 216
		10	21	29 161
		11	36	46 152
5	9	0	33	30 90
		1	112	103 287
		2	13	17 300
		3	58	57 338
		4	63	54 110
		5	28	36 325
		6	75	68 95
		7	89	83 287
		8	20	21 100
		9	29	37 346
		10	70	67 102
5	10	0	40	47 90
		1	71	67 179
		2	96	97 350
		3	25	31 122
		4	104	102 143
		5	72	65 108
		6	59	63 27
		8	20	26 37
		9	29	36 35
		10	56	55 96
5	11	0	13	23 270
		1	70	69 317
		2	76	81 206
		3	21	19 20
		4	54	50 263
		5	88	77 3
		6	76	72 197
		7	61	58 322
		8	64	62 206
		9	62	61 14
		10	30	33 294
5	12	0	48	56 90
		1	86	78 281
		2	15	22 128
		3	22	15 77
		4	40	36 75
		5	60	54 53
		6	26	22 141
		7	75	71 289
		8	20	30 102
		9	51	50 27
		11	54	51 358
5	13	0	48	52 270
		1	79	74 106
		2	128	132 252
		3	65	63 165
		4	93	76 293
		5	18	25 160
		6	62	62 233
		7	56	57 83
		8	29	39 222
		9	21	29 179
		10	30	27 294
5	14	2	57	54 175
		3	66	60 16
		4	99	86 330
		5	55	45 57
		6	51	46 215
		7	53	41 74
		8	21	38 274
		9	36	29 43
		10	75	74 291
		11	28	29 56
5	15	0	64	64 90
		1	127	129 159
		2	44	41 315
		3	122	124 175
		4	40	33 122
		5	70	66 193
		6	28	23 58
		7	41	51 85
		9	30	28 167
		10	29	30 138
5	16	1	80	86 120
		2	42	36 304
		3	18	32 230
		4	76	69 321
		5	76	80 216
		6	66	54 357
		7	62	53 134
		8	59	60 289
		9	47	48 207
		10	54	49 341
		11	33	43 162
5	17	0	83	89 90
		1	17	19 247
		2	119	122 67
		3	31	34 135
		4	92	85 120
		8	21	23 22
		9	36	37 86
		11	27	31 22
5	18	0	91	92 90
		1	18	14 107
		2	58	53 73
		3	92	88 197
		4	84	82 117
		5	72	60 272
		6	84	77 59
		7	36	41 202
		8	20	22 46
		9	55	48 219
		10	49	50 116
		11	26	31 255
5	19	0	41	33 270
		1	67	61 331
		2	56	56 84
		3	47	46 20
		4	56	60 10
		5	50	50 26
		6	36	36 320
		7	21	26 289
		8	47	51 16
		9	46	41 26
		10	19	22 310
5	20	1	139	129 343
		2	64	62 74
		3	79	70 351
		4	67	64 133
		5	92	87 356
		6	21	18 181
		7	36	29 306
		8	47	47 101
		10	27	30 130
		11	24	22 332
5	21	1	34	42 248
		3	73	74 331
		4	58	55 333
		5	47	41 230
		6	21	27 277
		7	36	40 258
		8	29	27 303
		9	28	35 308
		10	32	39 288
		11	23	27 156
5	22	0	153	141 270
		1	45	41 354
		2	81	71 254
		3	68	61 353
		4	66	57 276
		5	21	17 27
		6	81	81 254
		7	21	31 340
		8	20	8 138
		9	19	28 340
5	23	0	50	41 90
		2	21	29 212
		5	47	44 221
		6	21	23 88
		7	21	25 209
		8	28	34 233
		9	32	38 211
		11	33	39 185
5	24	0	21	15 270
		1	93	87 171
		2	72	70 271
		3	21	18 215
		4	36	45 236
		5	73	74 168
		6	29	28 224
		7	20	22 184
		8	34	40 217
		9	26	20 275
		10	16	17 194
		11	20	27 164
5	25	0	21	29 90
		1	39	40 3
		5	21	35 327
		6	35	40 88
		7	20	21 246
		8	27	30 129
		9	24	25 203
		10	31	39 94
		11	22	24 275
5	26	0	73	68 90
		2	36	37 165
		3	66	64 144
		4	21	24 129
		5	41	45 113
		6	53	54 91
		7	33	33 122
		8	18	26 184
		9	29	32 106
		10	14	22 103
5	27	0	42	46 270
		1	21	28 21
		2	21	28 211
		4	21	20 190
		5	40	42 346
		6	48	51 205
		7	32	32 2
		8	24	32 125
		9	22	18 12
		10	18	21 161
5	28	0	42	41 90
		2	21	23 71
		3	35	42 150
		4	35	39 18
		5	39	44 19
		6	27	31 57
		7	18	18 58
		8	16	25 27
		9	14	19 80
		10	16	19 12
5	29	0	68	65 270
		1	20	27 127
		2	29	25 274
		3	20	21 78
		4	44	41 235
		5	19	28 124
		6	51	53 246
		7	33	41 75
5	30	2	28	32 77
		4	19	23 10
		5	18	28 294
		6	17	20 283
		7	16	19 26
5	31	1	58	62 179
		2	19	23 338
		3	32	36 151
		5	45	50 143
		6	16	19 12
		7	25	28 149
		8	18	19 64
		9	26	27 326
5	33	0	65	71 90
		1	25	30 230
		2	30	32 86
		3	17	24 144
		4	36	36 61
		5	15	18 87
		6	30	35 66
5	34	5	13	14 208
		6	12	17 23
5	35	0	21	25 90
		1	30	34 349
		2	15	22 107
		3	20	23 19
		4	29	37 15
		5	16	19 1
5	36	1	19	26 306
		2	13	18 158
5	37	1	16	22 34
6	0	2	238	251 94
		4	183	181 97
		6	233	222 83
		8	64	53 228
6	1	1	42	51 358
		2	13	7 110
		4	18	21 217
		5	42	39 292
		6	16	17 216
6	2	1	263	339 360
		2	62	62 336
		3	148	142 13
		4	107	107 7
		5	228	224 3
		6	90	82 13
		7	76	66 8
		8	72	73 346
		9	54	46 132
		10	72	68 11
		11	55	45 318
		13	25	32 167
6	3	1	11	14 6
		2	35	28 42
		3	26	19 353
		4	33	34 197
		5	15	15 222
		6	23	30 249
6	4	0	224	272 270
		1	12	20 2
		2	92	88 266
		3	135	136 256
		4	117	114 250
		5	184	189 278
		6	157	145 260
		7	119	118 281
		8	39	40 345
		9	104	99 259
		10	72	62 288
		11	71	69 294
		12	28	34 235
6	5	0	30	36 270
		1	19	25 131
		4	44	42 214
		5	15	16 172
		7	18	22 238
		10	21	29 127
6	6	0	14	26 270
		1	50	48 121
		2	57	47 135
		3	58	50 301
		4	178	176 169
		5	113	107 201
		6	147	143 204
		7	69	69 167
		8	99	93 185
		9	77	79 208
		10	93	92 182
		11	84	88 173
		12	33	40 234
		13	30	34 172
6	7	0	27	21 90
		1	32	27 264
		2	40	36 176
		4	21	21 150
		5	28	33 63
		6	25	26 137
6	8	0	58	58 270
		1	21	28 284
		2	98	102 298
		3	98	93 46
		4	67	56 165
		5	146	136 101
		6	59	52 61
		7	57	54 142
		8	49	50 77
		9	51	53 87

TABLE 1 (*Continued*)

k	*h*	*l*	F_o	F_c
		10	127	125 105
		11	54	60 137
		12	68	76 72
		13	17	26 213
6	9	1	22	14 337
		2	23	24 223
		3	45	43 124
		4	27	25 260
		5	47	46 34
		6	25	28 200
		7	19	28 34
		8	20	27 201
6	10	1	136	138 240
		2	44	47 226
		3	76	78 169
		4	16	12 308
		5	51	42 33
		6	45	42 115
		7	89	87 290
		8	41	41 170
		9	98	92 7
		10	29	31 43
		11	89	91 357
		12	37	42 95
		13	43	55 342
6	11	1	49	42 125
		2	21	18 252
		3	62	62 174
		4	29	24 310
		6	19	26 309
		7	28	35 106
6	12	0	39	38 90
		1	59	62 74
		2	106	114 167
		3	82	81 85
		4	66	59 322
		5	70	63 79
		6	91	97 190
		7	111	101 77
		8	68	67 216
		9	55	55 60
		10	94	90 285
		11	20	23 46
		12	47	56 229
6	13	0	63	61 90
		1	51	47 139
		2	23	26 63
		3	41	39 179
		4	30	32 77
6	14	0	39	34 270
		1	102	105 116
		2	78	76 316
		3	45	47 139
		4	126	125 340
		5	70	65 162
		6	126	117 353
		7	93	101 104
		8	75	76 341
		9	59	57 182
		10	53	52 349
		11	42	44 165
		12	17	21 345
6	15	0	33	36 90
		1	17	23 307
		2	60	58 77
		3	25	30 354
		4	32	35 80
		8	21	31 354
6	16	0	140	143 90
		1	74	72 155
		2	108	106 50
		3	75	120 206
		4	104	100 111
		5	121	107 252
		6	88	80 52
		7	51	47 265
		8	42	43 14
		9	62	56 244
		10	34	37 114
		11	41	48 293
		12	16	31 344
6	17	0	26	30 270
		1	26	42 332
		2	26	34 89
		3	42	45 331
		4	27	24 352
		7	29	36 246
		8	21	18 334
6	18	0	76	67 90
		1	154	166 342
		2	121	112 91
		3	106	95 15
		4	93	88 117
		5	118	112 17
		7	42	50 294
		8	29	29 109
		9	28	27 79
		10	27	33 182
		11	17	5 306
		13	21	31 249
6	19	2	19	29 195
		3	34	37 327
		5	21	20 267
		7	21	31 243
		11	17	20 189
6	20	0	166	176 270
		1	83	74 341
		2	110	101 272
		3	105	108 351
		4	121	117 298
		6	63	63 281
		7	21	33 282
		8	29	36 26
		9	19	27 352
		10	18	24 319
6	21	2	29	42 234
		4	21	21 201
		11	15	11 200
6	22	1	114	108 176
		2	74	77 231
		3	62	54 232
		4	36	40 250
		5	93	97 211
		6	29	34 190
		7	35	39 224
		8	52	59 216
		9	41	45 274
		10	17	19 217
6	23	2	21	22 265
		4	21	27 195
		11	18	12 324
6	24	0	93	96 90
		2	21	24 185
		3	47	45 122
		4	59	53 153
		5	41	41 106
		6	70	73 106
		7	48	50 114
		8	49	50 188
		9	41	48 131
		10	26	33 119
6	25	10	14	15 178
6	26	0	21	25 270
		2	21	17 308
		3	58	56 155
		4	45	46 355
		5	53	58 6
		6	33	38 18
		7	26	28 44
		8	38	45 51
		9	15	26 80
		10	28	36 51
6	27	1	21	26 165
		5	27	28 108
		7	17	22 82
6	28	0	20	30 270
		2	35	40 93
		3	20	25 240
		5	19	26 286
		6	35	47 235
		7	23	24 346
		8	15	12 26
		9	22	28 315
6	29	1	20	29 189
		5	18	14 156
		6	17	22 31
6	30	1	19	23 94
		2	19	17 21
		3	32	38 19
		5	24	35 133
		6	16	21 287
		7	20	27 93
		8	21	19 295
6	31	0	36	35 90
		2	25	24 81
		4	24	22 40
		6	15	22 60
6	32	1	24	35 216
		2	29	34 325
		5	15	16 185
		6	29	41 22
		7	24	36 232
6	33	1	23	25 360
		3	15	21 328
		5	13	19 315
6	34	0	39	42 90
		1	26	30 277
		2	32	40 133
		4	25	23 89
		5	16	21 328
6	35	3	17	19 296
6	36	1	39	43 23
		2	18	24 199
		3	23	34 14
7	0	3	112	114 352
		5	232	224 351
		7	62	52 330
		9	21	24 159
		11	35	41 305
7	1	1	67	92 0
		2	65	73 72
		3	62	59 25
		4	57	52 96
		5	59	47 49
		6	35	33 60
		9	21	29 144
7	2	1	37	49 359
		2	137	157 269
		3	68	64 274
		4	126	127 264
		5	100	97 275
		6	178	173 253
		7	71	65 281
		8	35	31 48
		9	59	58 246
		11	29	37 264
7	3	0	63	90 270
		1	58	72 358
		2	38	35 315
		3	50	48 312
		4	74	69 326
		5	55	46 298
		6	61	52 342
		7	54	48 297
		8	28	34 356
7	4	0	63	92 270
		1	128	155 176
		2	38	41 197
		3	42	38 233
		4	144	137 186
		5	160	149 186
		6	109	106 204
		7	66	59 178
		8	105	104 162
		9	42	36 236
		10	80	82 166
		11	49	52 162
7	5	0	22	26 270
		2	26	28 135
		3	71	65 252
		4	39	37 207
		5	59	56 242
		6	64	57 213
		7	47	41 270
		9	21	28 261
7	6	0	51	54 90
		1	42	46 188
		2	39	38 297
		3	92	92 77
		4	80	79 151
		5	154	158 103
		6	83	77 89
		7	67	57 97
		8	50	41 140
		9	83	85 69
		10	95	93 110
		11	56	65 105
7	7	0	20	17 270
		1	50	45 17
		2	18	16 222
		3	59	54 29
		4	49	37 179
		6	26	28 146
		7	48	40 132
		10	21	27 152
		11	20	36 169
7	8	0	40	43 90
		1	84	87 221
		2	41	43 235
		3	92	84 130
		4	111	114 343
		5	78	70 59
		6	67	64 37
		7	34	34 348
		9	88	89 30
		10	36	45 4
		11	73	83 359
7	9	0	50	44 270
		1	24	29 251
		2	54	44 284
		3	15	19 159
		4	88	39 262
		6	19	28 21
		8	36	34 116
		10	20	37 81
7	10	0	45	40 90
		1	45	50 114
		2	87	80 124
		3	53	55 162
		4	93	88 358
		6	19	23 177
		7	64	57 52
		8	36	37 265
		10	93	95 292
		11	19	33 352
7	11	1	50	47 194
		2	49	43 140
		4	30	34 188
		5	18	25 47
		6	28	29 214
		8	36	37 186
		9	29	31 10
7	12	0	22	32 90
		1	101	109 80
		2	61	58 25
		4	62	63 358
		5	53	49 214
		6	103	92 355
		7	77	74 101
		8	66	62 344
		9	46	47 186
		10	20	33 303
		11	49	57 177
7	13	0	16	33 270
		1	23	20 99
		3	43	41 78
		4	41	36 317
		5	67	58 104
		7	68	62 88
7	14	0	66	65 90
		2	84	89 15
		3	79	80 250
		4	75	70 113
		5	90	81 270
		6	84	91 18
		7	78	77 255
		8	55	60 28
		9	61	64 237
		10	52	51 107
		11	31	38 243
7	15	1	62	62 168
		2	31	38 22
		3	19	26 222
		4	27	21 341
		5	28	31 190
		6	54	49 23
		8	36	36 1
7	16	0	18	23 90
		1	113	126 321
		2	56	51 94
		3	72	77 350
		4	79	76 144
		5	78	74 348
		6	55	53 169
		7	83	88 287
		8	41	48 133
		10	38	46 161
7	17	0	73	65 90
		2	74	70 83
		4	53	51 122
7	18	0	136	153 270
		1	65	64 335
		2	96	101 248
		3	106	117 360
		4	98	101 278
		5	21	37 70
		6	63	62 236
		9	27	32 35
7	19	1	72	64 357
		3	35	38 8
		5	29	39 17
7	20	0	40	48 270
		1	120	124 164
		2	100	108 250
		3	68	66 198
		4	66	68 278
		5	75	83 192
		7	20	33 150
		8	28	38 225
		9	18	19 261
7	21	0	54	48 270
		2	29	28 283
		3	21	30 285
		5	21	32 246
		7	20	19 269
		9	18	23 282
7	22	0	108	117 90
		1	36	50 178
		2	29	33 110
		3	78	78 159
		4	63	61 119
		6	57	66 101
		7	34	47 113
		8	26	29 185
		9	24	33 141
7	23	4	29	37 171
		6	20	21 165
		8	25	27 200
7	24	1	42	49 1
		2	42	49 62
		3	36	46 117
		4	35	40 50
		5	63	71 19
		6	28	31 17
		7	32	41 47
		8	30	42 43

TABLE 1 (*Continued*)

k	*h*	*l*	F_o	F_c	
		9	26	34	81
7	26	0	35	46	270
		3	20	27	282
		6	44	51	286
		7	29	29	317
		8	22	35	9
		9	18	33	314
7	28	3	27	46	343
		5	25	34	171
8	0	2	36	33	242
		4	76	62	245
		6	125	117	251
8	1	1	53	66	352
		4	28	35	294
		5	73	63	332
		6	24	36	228
8	2	0	18	24	270
		1	88	108	176
		4	20	33	213
		5	142	126	167
8	3	0	94	130	270
		1	39	46	107
		3	35	36	317
		4	28	34	236
		6	73	66	243
8	4	0	105	136	90
		1	63	65	218
		2	22	29	99
		4	79	69	95
		6	98	84	62
8	5	0	20	32	90
		1	67	72	189
		2	44	42	294
		4	47	43	157
		5	76	69	177
8	6	0	89	97	90
		1	71	78	328
		2	17	18	155
		4	56	52	357
		5	84	73	7
		6	25	42	71
8	7	0	78	78	90
		1	64	65	272
		2	18	24	182
		3	20	30	69
		4	38	47	133
		6	76	69	103
8	8	0	47	48	270
		1	65	61	42
		2	19	22	241
		3	29	40	262
		4	74	70	324
		5	42	50	300
8	9	0	27	37	270
		1	33	42	345
		2	28	33	188
		3	37	38	66
		4	46	48	320
		5	73	67	40
8	10	1	64	63	116
		2	21	23	350
		3	54	46	243
		4	33	44	190
		5	70	64	254
8	11	0	51	42	270
		1	82	74	128
		2	31	38	252
		3	40	44	186
		4	89	81	161
8	13	0	64	63	90
		1	73	71	146
		2	62	62	48
		3	60	51	179
		4	44	53	128
		5	64	61	198
		6	27	38	40
8	14	0	33	53	270
		1	41	52	270
		3	25	31	75
		5	38	47	45
8	15	0	65	58	90
		1	60	61	323
		2	86	84	60
		4	59	57	111
		5	38	35	15
		6	38	43	34
8	16	1	25	35	211
		2	44	51	201
		4	38	37	309
		5	27	31	104
		6	27	40	229
8	17	0	26	32	270
		1	68	61	341
		3	46	50	350
		4	27	22	350
		5	38	42	335
8	18	1	59	60	152
		3	27	34	168
		4	27	29	334
		5	39	42	104
8	19	0	27	33	270
		2	47	48	224
		3	38	33	330
		4	27	31	283
		5	38	34	222
		6	27	34	234
8	20	0	66	70	90
		2	38	51	53
		3	47	60	188
		4	47	46	75
		6	46	58	46
8	21	2	27	42	259
		4	38	32	211
8	22	1	55	63	350
		2	61	63	81
		4	38	35	108
		5	53	59	339
8	23	3	38	46	165
8	24	0	54	61	270
		1	38	42	355
		3	53	53	343
		6	34	44	260
8	25	5	24	30	30
8	26	0	36	38	270
		1	36	33	198
		2	25	39	265
		5	38	35	198
8	27	0	25	38	270
		5	22	27	125
8	28	0	24	27	90
		5	21	20	114
8	29	1	32	40	184
		5	27	37	169
8	31	0	44	52	90
		2	19	28	86

TABLE 2

$RuQASBr_2$

Some distances in Å and standard deviations in Å × 10^3 shown in parentheses

Within the bridging groups

Ru–As1	2·308(5)	As3–C14	1·974(30)	C7–C8	1·438(57)
Ru–As2	2·398(5)	As3–C31	1·945(40)	C8–C9	1·438(56)
Ru–As3	2·465(5)	As3–C37	1·901(40)	C9–C10	1·532(57)
Ru–As4	2·472(5)	As4–C8	1·947(42)	C10–C11	1·369(65)
Ru–Br1	2·610(5)	As4–C43	1·938(40)	C11–C12	1·369(55)
Ru–Br2	2·615(5)	As4–C49	1·991(40)	C12–C7	1·413(47)
As1–C1	1·940(40)	C1–C2	1·400(47)	C13–C14	1·398(51)
As1–C7	1·960(29)	C2–C3	1·441(52)	C14–C15	1·419(51)
As1–C13	1·947(39)	C3–C4	1·489(57)	C15–C16	1·417(52)
As2–C2	1·915(36)	C4–C5	1·365(51)	C16–C17	1·458(58)
As2–C19	2·049(38)	C5–C6	1·420(59)	C17–C18	1·369(57)
As2–C25	1·966(39)	C6–C1	1·448(60)	C18–C13	1·459(51)

In the phenyl groups

C–C Average 1·41; average deviation 0·04; maximum deviation 0·10 Å

Some angles in degrees and standard deviations in degrees × 10 shown in parentheses

As1–Ru–As2	86·7(2)	Ru–As2–C2	106·1(10)	As2–C2–C1	121·5(28)
As1–Ru–As3	82·7(2)	Ru–As2–C19	120·3(27)	As3–C14–C13	117·8(24)
As1–Ru–As4	82·7(2)	Ru–As2–C25	120·7(11)	As4–C8–C7	121·9(28)
As2–Ru–As3	96·6(2)	C2–As2–C19	108·9(25)	C6–C1–C2	123·2(36)
As2–Ru–As4	97·1(2)	C2–As2–C25	150·5(15)	C1–C2–C3	116·4(33)
As3–Ru–As4	159·3(2)	C19–As2–C25	94·2(36)	C2–C3–C4	120·9(30)
Br1–Ru–As1	88·1(2)	Ru–As3–C14	103·5(9)	C3–C4–C5	118·0(37)
Br1–Ru–As2	174·8(2)	Ru–As3–C31	123·8(11)	C4–C5–C6	122·7(37)
Br1–Ru–As3	82·5(2)	Ru–As3–C37	123·9(12)	C5–C6–C1	117·3(35)
Br1–Ru–As4	82·5(2)	C14–As3–C31	97·2(16)	C12–C7–C8	121·7(31)
Br1–Ru–Br2	92·4(2)	C14–As3–C37	104·9(15)	C7–C8–C9	120·1(35)
Br2–Ru–As1	178·9(2)	C31–As3–C37	99·2(16)	C8–C9–C10	115·3(36)
Br2–Ru–As2	92·8(2)	Ru–As4–C8	102·6(13)	C9–C10–C11	119·2(38)
Br2–Ru–As3	98·4(2)	Ru–As4–C43	123·9(12)	C10–C11–C12	124·4(38)
Br2–Ru–As4	96·4(2)	Ru–As4–C49	122·3(11)	C11–C12–C7	118·6(36)
Ru–As1–C1	110·3(11)	C8–As4–C43	107·2(17)	C18–C13–C14	119·7(34)
Ru–As1–C7	114·0(10)	C8–As4–C49	96·6(17)	C13–C14–C15	121·5(30)
Ru–As1–C13	111·5(12)	C43–As4–C49	100·2(16)	C14–C15–C16	118·4(34)
C1–As1–C7	104·0(15)	As1–C1–C2	115·3(28)	C15–C16–C17	120·4(35)
C1–As1–C13	109·5(17)	As1–C7–C8	109·2(24)	C16–C17–C18	120·2(35)
C7–As1–C13	107·1(13)	As1–C13–C14	114·5(26)	C17–C18–C13	119·7(35)

C–C–C in phenyl groups; average 119·9°; average deviation 3·9°; maximum deviation 10°.

TABLE 3

$RuQASBr_2$

Atomic co-ordinates in fractions of the unit cell lengths, *b*, *a*, and *c* and isotropic thermal factors in $Å^{-2}$

	Y	*X*	*Z*	*B*		*Y*	*X*	*Z*	*B*
Ru	0·17175	0·12016	0·00075	3·612	C25	0·3350	0·2004	−0·1634	4·245
Br1	0·02127	0·05987	0·03928	4·606	C26	0·2254	0·2143	−0·2056	9·166
As1	0·31962	0·07205	0·03372	3·556	C27	0·2355	0·2429	−0·2884	9·655
As2	0·32378	0·17107	−0·03054	3·756	C28	0·3344	0·2541	−0·3448	5·363
Br2	0·00548	0·17469	−0·04045	4·587	C29	0·4313	0·2381	−0·3023	9·490
As3	0·17119	0·12685	0·18927	3·525	C30	0·4422	0·2092	−0·2172	8·916
As4	0·17533	0·08630	−0·17039	3·860	C31	0·2809	0·1620	0·2656	4·782
C1	0·4717	0·0983	0·0128	5·002	C32	0·3960	0·1473	0·2693	5·172
C2	0·4688	0·1411	−0·0151	3·365	C33	0·4818	0·1741	0·3259	5·047
C3	0·5798	0·1630	−0·0163	5·072	C34	0·4440	0·2131	0·3691	6·528
C4	0·6920	0·1392	−0·0063	7·237	C35	0·3283	0·2269	0·3618	6·050
C5	0·6863	0·0970	0·0164	5·478	C36	0·2462	0·2013	0·3034	6·555
C6	0·5789	0·0758	0·0369	7·388	C37	0·0339	0·1366	0·2697	3·892
C7	0·3208	0·0232	−0·0591	3·915	C38	0·0427	0·1428	0·3768	5·832
C8	0·2376	0·0302	−0·1404	5·316	C39	−0·0694	0·1532	0·4318	6·497
C9	0·2105	−0·0034	−0·2112	5·214	C40	−0·1694	0·1560	0·3806	7·544
C10	0·2874	−0·0431	−0·2021	7·063	C41	−0·1803	0·1474	0·2715	5·441
C11	0·3624	−0·0468	−0·1206	5·876	C42	−0·0736	0·1390	0·2121	4·798
C12	0·3842	−0·0152	−0·0510	5·257	C43	0·0378	0·0785	−0·2556	5·046
C13	0·3100	0·0500	0·1730	5·261	C44	−0·0660	0·0904	−0·2152	6·875
C14	0·2305	0·0713	0·2363	3·764	C45	−0·1653	0·0823	−0·2721	5·823
C15	0·2049	0·0568	0·3369	5·093	C46	−0·1701	0·0683	−0·3705	7·540
C16	0·2635	0·0202	0·3734	5·670	C47	−0·0599	0·0550	−0·4153	5·600
C17	0·3464	−0·0023	0·3080	5·942	C48	0·0426	0·0623	−0·3556	6·083
C18	0·3680	0·0117	0·2104	5·016	C49	0·2931	0·1017	−0·2769	5·573
C19	0·3313	0·2259	0·0536	6·770	C50	0·4008	0·0864	−0·2635	6·868
C20	0·2269	0·2474	0·0520	6·112	C51	0·4850	0·1008	−0·3423	8·192
C21	0·2305	0·2867	0·1119	8·380	C52	0·4606	0·1239	−0·4243	6·469
C22	0·3363	0·2986	0·1583	6·681	C53	0·3406	0·1389	−0·4344	6·757
C23	0·4306	0·2752	0·1622	5·911	C54	0·2588	0·1291	−0·3604	5·930
C24	0·4382	0·2356	0·1047	5·071					

given in Table 1, positional and thermal parameters in Table 3 and bond angles and distances together with the estimated standard deviations in Table 2.

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