order in the structure. The same thing is true of the oxygen atoms of the water molecules. The hydrogen atoms attached to the nitrogen ligands have (except for H(4)) reasonable *B* values, comparable to those of the nitrogen atoms to which they are attached; the same is true of the water hydrogen atoms.

This compound is nearly isostructural with $(NH_3)_4Co(OH)(OH)Co(NH_3)_4Cl_4\cdot 4H_2O$, the structure of which has been reported by both Vannerberg[13] and Prout.[14] The two cations are of nearly the same size and shape, and therefore the crystal forces must be very similar in the two cases. Evidently, with ions this large, the exact charge distribution in the ion is not as important in determining the structure of the crystal as is the general shape of and overall charge on the ion. The comparison between these two compounds is striking. The two formulas are nearly identical as are the cell dimensions and the overall structure. Table VII lists the cell parameters for the two compounds; the length of our *c* axis has been halved to account for the disorder in our compound, and *a* and *b* of the di-μ-hydroxo compound have been interchanged to afford a direct comparison. The only significant difference between these dimensions is in the length of *c*, which reflects the different Co–Co distances in the two compounds. In the Cl- and NH_2-bridged cation, the Co–Co distance is 3.151 (1) Å, while it is approximately 2.97 (1) Å in the $(OH)_2$-bridged species.

TABLE VII

	μ-Cl-μ-NH_2	Di-μ-OH		μ-Cl-μ-NH_2	Di-μ-OH
a, Å	7.812	7.79	α, deg	107.02	106.5
b, Å	6.666	6.69	β, deg	90.52	92.5
c, Å	10.289	10.05	γ, deg	107.14	106.6

Acknowledgments.—We thank Professor Carl Brubaker for telling us of Dr. Chester's work. We particularly appreciate the efforts of Dr. Sten Samson in designing and maintaining the X-ray equipment which we used. This research was partially supported by NSF Grant GP-5768 to the California Institute of Technology.

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CONTRIBUTION FROM THE DEPARTMENT OF CHEMISTRY,
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The Crystal Structure of Tetrafluorocyclobutenebis(dimethylarsine)triiron Decacarbonyl, $(CH_3)_2As\overline{C{=}C(As(CH_3)_2)CF_2C}F_2\cdot Fe_3(CO)_{10}$

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Received December 11, 1969

Tetrafluorocyclobutenebis(dimethylarsine)triiron decacarbonyl, $(CH_3)_2As\overline{C{=}C(As(CH_3)_2)CF_2C}F_2\cdot Fe_3(CO)_{10}$, crystallizes in the monoclinic space group $P2_1/c$, with a = 11.60 (2) Å, b = 20.04 (2) Å, c = 22.11 (2) Å, β = 93.7 (2)°, and Z = 8 (two molecules per asymmetric unit). The structure was determined with Mo Kα diffractometer data by a combination of direct, Patterson, and electron density methods and was refined by least-squares procedures to a final *R* of 0.09 for 2524 observed (of a total of 3234) reflections. The molecule is best described as a derivative of $Fe_3(CO)_{12}$, in which one terminal carbonyl group on each of the two equivalent iron atoms is replaced by an arsenic atom of the diarsine ligand. The central Fe_3As_2 cluster is significantly folded in one of the molecules of the asymmetric unit but is more nearly planar in the other molecule. The Fe–Fe bond distances in the iron triangle (2.53, 2.65, 2.65 Å) do not different significantly from those in the parent compound.

Complexes of metal carbonyls with ditertiary arsines have been extensively studied.[2,3] The diarsine derivative[4] $LFe_3(CO)_{10}$, $L = (CH_3)_2As\overline{C{=}C(As(CH_3)_2)CF_2C}F_2$, is of particular structural interest both in terms of the manner of attachment of the ligand, L, and of possible distortions of the skeleton of the parent $Fe_3(CO)_{12}$, whose structure is known from X-ray studies on disordered crystals of $Fe_3(CO)_{12}$ itself[5] and on the derivatives $(C_2H_5)_3NH)(HFe_3(CO)_{11}$[6] and $(C_6H_5)_3PFe_3(CO)_{11}$.[7]

The infrared, nmr, and Mössbauer spectra of $LFe_3(CO)_{10}$ suggest a structure in which two terminal carbonyl groups of the two equivalent iron atoms of $Fe_3(CO)_{12}$ are replaced by the arsenic atoms of the diarsine ligand.[4] The presence of only one ^{19}F resonance in the nmr spectrum indicates that all the fluorine atoms are equivalent, so that the diarsine ligand would be expected to be planar, in contrast to the previously determined structure of $LFe_2(CO)_6$, in which the ligand is bent as a result of the formation of a π bond from the cyclobutene system to one of the iron atoms.[8]

An X-ray crystal analysis of $LFe_3(CO)_{10}$ has been

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TABLE I

MEASURED AND CALCULATED STRUCTURE FACTORS[a]

**** H = 0****

0	2	17*	8
0	4	172	193
0	6	45	48
0	8	300	280
0	10	0*	54
0	12	268	271
0	14	24*	55
0	16	102	109
0	18	46	56
1	1	100	51
1	2	198	203
1	3	203	195
1	4	157	158
1	5	73	76
1	6	109	108
1	7	282	289
1	8	147	151
1	9	191	190
1	10	197	197
1	11	86	85
1	12	51	59
1	13	59	54
1	14	19*	25
1	15	72	90
1	16	162	165
1	17	0*	5
1	18	0*	15
2	0	51	52
2	1	161	165
2	2	844	829
2	3	376	350
2	4	57	55
2	5	76	76
2	6	208	217
2	7	74	59
2	8	91	89
2	9	84	68
2	10	76	63
2	11	233	249
2	12	43	31
2	13	47	47
2	14	157	156
2	15	101	103
2	16	78	77
2	17	0*	47
2	18	0*	10
3	1	207	204
3	2	100	98
3	3	0*	93
3	4	243	237
3	5	42	51
3	6	15*	32
3	7	77	80
3	8	48	37
3	9	136	135
3	10	80	75
3	11	184	196
3	12	44	44
3	13	98	99
3	14	76	80
3	15	52	31
3	16	58	66
3	17	61	48
3	18	75	70
4	0	180	192
4	1	203	196
4	2	69	64
4	3	93	95
4	4	41	40
4	5	152	178
4	6	39	34
4	7	110	115
4	8	57	47
4	9	137	139
4	10	45	45
4	11	61	57
4	12	41	11
4	13	98	97
4	14	0*	23
4	15	59	45
4	16	25*	1
4	17	105	103
4	18	110	116
5	1	120	122
5	2	264	274
5	3	54	49
5	4	71	84
5	5	28	30
5	6	29	25
5	7	14*	13
5	8	45	43
5	9	59	51
5	10	43	32
5	11	33	19
5	12	29	15
5	13	61	68
5	14	137	135
5	15	9*	4
5	16	47	27
5	17	98	111
6	0	59	54
6	1	115	120
6	2	114	125
6	3	56	41
6	4	122	112
6	5	5*	25
6	6	71	80
6	7	269	266
6	8	33	49
6	9	90	95
6	10	68	65
6	11	96	93
6	12	96	96
6	13	45	41
6	14	16*	15
6	15	21*	9
6	16	94	92
6	17	45	64
7	1	165	158
7	2	136	126
7	3	255	260
7	4	136	130
7	5	87	83
7	6	0*	1
7	7	48	44
7	8	23*	14
7	9	48	55
7	10	73	74
7	11	8*	8
7	12	0*	22
7	13	54	57
7	14	21*	5
7	15	83	92
7	16	25*	26
8	0	210	218
8	1	175	181
8	2	109	99
8	3	112	109
8	4	0*	16
8	5	39	43
8	6	32	38
8	7	0*	1
8	8	80	82
8	9	150	183
8	10	42	40
8	11	34	48
8	12	83	84
8	13	50	45
8	14	45	34
8	15	50	57
8	16	12*	7
9	1	236	228
9	2	65	68
9	3	103	97
9	4	51	50
9	5	12*	36
9	6	0*	40
9	7	107	115
9	8	47	50
9	9	53	61
9	10	70	75
9	11	45	43
9	12	61	67
9	13	36	34
9	14	0*	11
9	15	77	70
10	0	65	32
10	1	207	214
10	2	42	42
10	3	131	134
10	4	112	106
10	5	22*	13
10	6	29	8
10	7	41	55
10	8	34	33
10	9	12*	24
10	10	0*	2
10	11	92	95
10	12	71	81
10	13	38	26
10	14	53	75
10	15	78	61
11	1	143	153
11	2	0*	0
11	3	16*	18
11	4	205	202
11	5	85	87
11	6	44	50
11	7	23*	47
11	8	41	36
11	9	40	34
11	10	21*	24
11	11	36	34
11	12	70	78
11	13	90	98
11	14	65	53
12	0	52	38
12	1	23*	32
12	2	169	174
12	3	89	82
12	4	60	57
12	5	0*	40
12	6	41	17
12	7	55	54
12	8	25*	22
12	9	32	9
12	10	112	116
12	11	28*	30
12	12	51	12
12	13	59	51
13	1	0*	21
13	2	104	111
13	3	99	104
13	4	42	47
13	5	38	30
13	6	57	51
13	7	47	42
13	8	80	81
13	9	24*	1
13	10	82	72
13	11	57	46
14	0	153	159
14	1	148	144
14	2	54	42
14	3	51	40
14	4	70	70
14	5	47	29
14	6	21*	53
14	7	84	81
14	8	102	102
14	9	47	13
14	10	65	55
15	1	0*	33
15	2	37	15
15	3	4*	2
15	4	87	86
15	5	25*	22
15	6	77	79
15	7	14*	26
15	8	0*	20
16	0	0*	9
16	1	121	119
16	2	52	47
16	3	95	93
16	4	51	49
16	5	97	89
16	6	31*	36

**** H = 1****

0	0	62	63
0	-2	474	396
0	2	346	301
0	-4	320	293
0	4	199	193
0	-6	261	246
0	6	448	459
0	-8	184	178
0	8	199	179
0	-10	51	68
0	10	77	67
0	-12	207	207
0	12	97	89
0	-14	184	185
0	14	132	127
0	-16	42	49
0	16	15*	37
0	-18	43	32
0	18	75	61
1	0	26	66
1	-1	348	324
1	1	189	190
1	-2	110	121
1	2	333	317
1	-3	35	25
1	3	35	23
1	-4	48	80
1	4	220	223
1	-5	193	196
1	5	79	76
1	-6	62	61
1	6	0*	5
1	-7	98	97
1	7	0*	6
1	-8	165	153
1	8	277	269
1	-9	247	225
1	9	105	103
1	-10	178	174
1	10	0*	20
1	-11	24*	29
1	11	48	48
1	-12	0*	7
1	12	154	157
1	-13	198	203
1	13	113	116
1	-14	55	51
1	14	212	214
1	-15	135	136
1	15	28*	39
1	-16	22*	27
1	16	110	111
1	-17	51	8
1	17	27*	25
1	-18	12*	14
1	18	53	42
2	0	386	344
2	-1	127	120
2	1	72	51
2	-2	256	244
2	2	219	217
2	-3	251	241
2	3	117	109
2	-4	0*	20
2	4	13*	13
2	-5	182	190
2	5	153	151
2	-6	179	172
2	6	32	32
2	-7	267	255
2	7	110	112
2	-8	45	55
2	8	168	157
2	-9	73	66
2	9	188	183
2	-10	202	194
2	10	101	104
2	-11	8*	11
2	11	65	68
2	-12	95	84
2	12	95	113
2	-13	79	72
2	13	97	94
2	-14	23*	19
2	14	33	13
2	-15	65	58
2	15	44	54
2	-16	0*	2
2	16	32	31
2	-17	129	124
2	17	0*	34
2	-18	58	51
2	18	53	67
3	0	360	341
3	-1	27	11
3	1	17*	9
3	-2	245	226
3	2	422	408
3	-3	30	31
3	3	75	86
3	-4	55	56
3	4	114	120
3	-5	130	140
3	5	122	123
3	-6	146	146
3	6	262	254
3	-7	235	235
3	7	50	36
3	-8	11*	5
3	8	5*	3
3	-9	15*	15
3	9	87	70
3	-10	38	27
3	10	144	143
3	-11	83	83
3	11	51	48
3	-12	71	59
3	12	76	71
3	-13	0*	7
3	13	58	75
3	-14	23*	0
3	14	88	87
3	-15	107	101
3	15	27*	6
3	-16	79	86
3	16	56	61
3	-17	46	52
3	17	75	82
3	-18	19*	17
3	18	43	41
4	0	56	82
4	-1	138	144
4	1	37	30
4	-2	20*	36
4	2	18*	9
4	-3	220	233
4	3	176	170
4	-4	239	254
4	4	0*	1
4	-5	90	97
4	5	32	19
4	-6	197	196
4	6	104	94
4	7	156	141
4	-7	27	15
4	-8	42	43
4	8	126	117
4	-9	52	43
4	9	57	64
4	-10	16*	13
4	10	56	64
4	-11	60	72
4	11	157	150
4	-12	108	106
4	12	41	38
4	-13	81	76
4	13	0*	3
4	-14	72	82
4	14	12*	22
4	-15	114	110
4	15	40	33
4	-16	120	115
4	16	40	21
4	-17	71	78
4	17	52	29
4	-18	34	11
5	0	43	48
5	-1	108	121
5	1	27	25
5	-2	90	77
5	2	145	141
5	-3	61	63
5	3	213	210
5	-4	246	272
5	4	297	299
5	-5	149	151
5	5	133	190
5	-6	83	89
5	6	41	37
5	-7	115	116
5	7	15*	27
5	-8	44	53
5	8	94	114
5	-9	29	15
5	9	64	66
5	-10	29	20
5	10	71	69
5	-11	57	47
5	11	103	106
5	-12	58	27
5	12	123	116
5	-13	0*	35
5	13	86	82
5	-14	80	84
5	14	74	75
5	-15	0*	23
5	15	0*	4
5	-16	85	87
5	16	67	45
5	-17	54	52
5	17	72	69
6	0	136	148
6	-1	97	98
6	1	56	66
6	-2	164	161
6	2	68	57
6	3	107	96
6	-3	79	65
6	-4	72	71
6	4	36	27
6	-5	153	153
6	5	213	204
6	-6	237	238
6	6	99	99
6	-7	106	102
6	7	61	55
6	-8	125	132
6	8	86	78
6	-9	24*	4
6	9	41	18
6	-10	26*	1
6	10	0*	4
6	-11	69	60
6	11	46	26
6	-12	118	119
6	12	0*	23
6	-13	86	97
6	13	125	109
6	-14	59	62
6	14	32	62
6	-15	99	115
6	15	89	96
6	-16	64	81
6	16	41	29
6	-17	43	32
6	17	39	22
7	0	19*	32
7	-1	70	73
7	1	453	453
7	-2	351	326
7	2	104	96
7	-3	3*	1
7	3	96	89
7	-4	91	80
7	4	142	139
7	-5	0*	17
7	5	126	119
7	-6	0*	23
7	6	82	101
7	-7	126	128
7	7	210	201
7	-8	27	44
7	8	42	49
7	-9	0*	18
7	9	70	67
7	-10	69	77
7	10	92	87
7	-11	0*	13
7	11	91	104
7	-12	45	35
7	12	78	59
7	-13	27*	20
7	13	29*	35
7	-14	98	96
7	14	57	69
7	-15	58	53
7	15	140	137
7	-16	35	12
7	16	27*	0
8	0	29	21
8	-1	224	225
8	1	37	37
8	-2	153	154
8	2	38	33
8	-3	17*	1
8	3	115	111
8	-4	60	49
8	4	68	57
8	-5	36	38
8	5	72	65
8	-6	80	93
8	6	93	81
8	-7	91	89
8	7	81	75
8	-8	0*	10
8	8	29*	33
8	-9	132	140
8	9	28	13
8	-10	46	42
8	10	8*	16
8	-11	47	50
8	11	45	48
8	-12	37	37
8	12	38	36
8	-13	47	48
8	13	70	75
8	-14	89	79
8	14	37	11
8	-15	90	99
8	15	46	49
8	-16	54	28
8	16	59	48
9	0	84	87
9	-1	141	144
9	1	203	196
9	-2	80	68
9	2	35	36
9	-3	94	94
9	3	57	56
9	-4	43	41
9	4	178	190
9	-5	17*	11
9	5	104	106
9	-6	29	14
9	6	115	125
9	-7	32	27
9	7	31	24
9	-8	44	9
9	8	60	55
9	-9	102	100
9	9	48	35
9	-10	0*	14
9	10	31	5
9	-11	44	42
9	11	25*	18
9	-12	56	52
9	12	118	129
9	-13	0*	10
9	13	171	183
9	-14	66	68
9	14	52	54
9	-15	37	20
9	15	0*	3
10	0	70	56
10	-1	32	39
10	1	84	74
10	-2	0*	36
10	2	10*	2
10	-3	110	114
10	3	22*	29
10	-4	57	58
10	4	87	89
10	-5	50	37
10	5	41	34
10	-6	67	69
10	6	97	83
10	-7	14*	27
10	7	18*	9
10	-8	61	65
10	8	0*	9
10	-9	50	52
10	9	0*	26
10	-10	0*	6
10	10	109	110
10	-11	64	66
10	11	83	90
10	-12	0*	28
10	12	0*	3
10	-13	26*	32
10	13	28*	35
10	-14	0*	4
10	14	52	51
10	-15	104	101
11	0	17*	43
11	-1	109	112
11	1	163	160
11	-2	59	45
11	2	214	217
11	-3	112	101
11	3	129	124
11	-4	44	35
11	4	66	65
11	-5	0*	21
11	5	40	55
11	-6	132	109
11	6	127	121
11	-7	52	58
11	7	56	39
11	-8	73	82
11	8	44	27
11	-9	0*	27
11	9	104	110
11	-10	66	61
11	10	124	125
11	-11	99	110
11	11	45	36
11	-12	15*	2
11	12	38	33
11	-13	39	16
11	13	0*	23
11	-14	38	37
12	0	67	66
12	1	122	101
12	-1	97	109
12	-2	62	62
12	2	26*	6
12	-3	68	71
12	3	53	54
12	-4	38	16
12	4	130	125
12	-5	66	69
12	5	71	69
12	-6	41	35
12	6	73	74
12	-7	75	57
12	7	18*	9
12	-8	41	54
12	8	106	101
12	-9	39	47
12	9	66	46
12	-10	35	35
12	10	45	22
12	-11	48	44
12	11	52	37
12	-12	30*	19
12	12	127	127
12	-13	60	77
13	0	18*	20
13	-1	18*	83
13	1	108	116
13	-2	105	111
13	2	46	41
13	-3	18*	41
13	3	207	210
13	-4	91	95
13	4	55	43
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TABLE I (*Continued*)

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2	-4	22*	13
2	4	92	83
2	-5	27*	14
2	5	0*	17
2	-6	28*	1
2	-7	20*	7
2	-8	26*	17
3	0	27*	27
3	-1	38	46
3	1	43	15
3	-2	17*	13
3	2	8*	20
3	-3	22*	35
3	3	40	23
3	-4	106	108
3	4	94	103
3	-5	31*	9
3	5	59	77
3	-6	58	46
3	-7	0*	32
4	0	38	23
4	-1	41	34
4	1	85	70
4	-2	74	76
4	2	54	30
4	-3	0*	1
4	3	86	88
4	-4	0*	6
4	4	75	68
4	-5	47	35
4	-6	0*	11
4	-7	21*	37
5	0	41	45
5	-1	37	56
5	1	57	42
5	-2	84	80
5	2	112	127
5	-3	0*	10
5	3	1*	6
5	-4	56	37
5	-5	64	63
5	-6	59	72
6	0	34	34
6	-1	49	64
6	1	21*	10
6	-2	30*	4
6	2	40	34
6	-3	56	56
6	-4	41	46

[a] Columns are k, l, $|F_o|$, $|F_c|$; unobserved reflections are indicated by an asterisk after the $|F_o|$ value.

undertaken to determine the structure and to compare it with that of the parent compound.

Experimental Section

$LFe_3(CO)_{10}$ was obtained by chromatography of the mixture of products formed by ultraviolet irradiation of $Fe_3(CO)_{12}$ and the diarsine.[4] The crystals are black needles elongated along a. Unit cell and space group data were obtained by photographic and diffractometer methods, the lattice parameters being determined by least-squares treatment of the θ values for 30 reflections, measured with Mo Kα radiation.

Crystal Data (λ(Mo Kα) 0.7107 Å).—The following data were obtained for $C_{18}H_{12}As_2F_4Fe_3O_{10}$ of mol wt 782 and mp ~160° dec: monoclinic, $a = 11.60$ (2) Å, $b = 20.04$ (2) Å, $c = 22.11$ (2) Å, $\beta = 93.7$ (2)° (standard deviations in parentheses), $V = 5129$ (19) Å^3, $D_m = 2.01 \pm 0.02$ (flotation in carbon tetrachloride–methyl iodide), $Z = 8$, $D_x = 2.02$ (1), $F(000) = 3040$; absorption coefficient, μ(Mo Kα) = 45 cm^{-1}. Absent spectra: $h0l$ when l is odd; $0k0$ when k is odd. Space group is $P2_1/c$ (C_{2h}^5).

The intensities of the reflections were measured on a Datex-automatic General Electric XRD 6 diffractometer, with a scintillation counter, Mo Kα radiation (Zr filter and pulse-height analyzer), and a θ–2θ scan. The scan range in 2θ was $(1.80 + 0.86 \tan \theta)°$ at a scan speed of 4°/min, and backgrounds were measured for 10 sec at both ends of each scan. The standard deviation of an intensity was calculated from the counting statistics: $\sigma^2(I) = S + B + (dS)^2$, where S is the scan count, B is the background, corrected to time of scan, $I = S - B$, and d is an empirical constant which allows for unknown experimental errors, taken as 0.04. Of 3234 reflections with 2θ (Mo Kα) $\leq$ 35° (minimum interplanar spacing, 1.18 Å) 710 had intensities less than 1σ and were classified as unobserved. The crystal used to record the intensities was a needle, of length 0.3 mm along a and cross section 0.03 × 0.04 mm, and was mounted with a^* parallel to the ϕ axis of the goniostat. The maximum error in $|F_o|$ as a result of absorption is only about 2%, and no absorption correction was made. Lorentz and polarization factors were applied, and the structure amplitudes were derived.

Structure Analysis

The asymmetric unit contains two molecules, so that, with ten heavy atoms, the Patterson function was complicated. Two possible molecular orientations appeared in the origin region, but, as a result of the large number of peaks, it was not immediately possible to derive any further information.

An effort was then made to determine the structure

TABLE II

FINAL POSITIONAL (FRACTIONAL, $\times 10^4$) AND THERMAL PARAMETERS[a]

	Molecule 1				Molecule 2			
Atom	x	y	z	B, Å^2	x	y	z	B, Å^2
Fe(1)	3759(3)	0773(2)	1986(2)		8370(4)	2441(3)	0695(2)	
Fe(2)	1932(3)	0822(2)	2646(2)		6462(4)	3155(2)	0738(2)	
Fe(3)	1871(4)	0053(2)	1738(2)		6492(4)	2248(2)	−0048(2)	
As(4)	0196(3)	0762(2)	3092(1)		4616(3)	3527(2)	0792(1)	
As(5)	0123(3)	−0490(2)	1633(1)		4683(3)	2109(2)	−0529(1)	
C(6)	4694(31)	1330(18)	2313(16)	5.7(8)	9362(36)	2764(20)	1247(19)	7.5(10)
C(7)	4249(33)	0122(20)	2501(18)	6.7(10)	7881(31)	1830(19)	1184(17)	6.3(9)
C(8)	3046(30)	1380(19)	1537(17)	6.2(9)	8602(28)	3035(18)	0172(16)	5.4(8)
C(9)	4546(25)	0498(15)	1421(14)	4.0(7)	9233(33)	1892(20)	0354(17)	6.7(10)
C(10)	1994(27)	1685(17)	2609(14)	4.5(8)	7087(25)	3905(16)	0714(13)	3.9(7)
C(11)	2881(25)	0779(15)	3292(14)	4.1(7)	6759(29)	3031(18)	1546(18)	6.3(9)
C(12)	2732(26)	−0627(15)	1691(13)	3.6(7)	6756(29)	1425(20)	0014(15)	5.6(9)
C(13)	1908(27)	0271(16)	0975(16)	4.9(8)	7265(34)	2323(20)	−0694(19)	7.4(10)
C(14)	1945(29)	−0133(18)	2620(16)	5.2(8)	5772(27)	2228(16)	0699(15)	4.7(8)
C(15)	0999(27)	0868(16)	1849(14)	4.6(7)	6281(27)	3266(17)	−0138(15)	4.6(8)
C(16)	0063(31)	−1445(19)	1706(17)	7.1(10)	3993(31)	1239(18)	−0461(16)	6.6(9)
C(17)	−0819(30)	−0300(18)	0884(16)	6.4(9)	4406(33)	2319(19)	−1404(17)	7.2(10)
C(18)	0165(29)	0405(17)	3903(16)	5.8(9)	3900(27)	3356(16)	1546(14)	5.1(8)
C(19)	−0710(32)	1564(19)	3118(17)	7.3(10)	4256(29)	4471(17)	0625(15)	5.7(9)
C(20)	−0903(21)	0172(12)	2681(12)	2.3(6)	3474(29)	3127(18)	0239(16)	5.9(9)
C(21)	−0919(25)	−0222(14)	2224(13)	3.9(7)	3508(24)	2691(15)	−0202(13)	3.7(7)
C(22)	−2184(29)	−0009(18)	2810(16)	5.3(8)	2143(31)	3240(19)	0099(17)	6.1(9)
C(23)	−2172(35)	−0456(21)	2266(18)	7.2(10)	2195(28)	2755(18)	−0377(16)	5.1(8)
F(24)	−2237(19)	−0284(11)	3355(11)	8.5(6)	1544(17)	3078(10)	0555(9)	7.6(5)
F(25)	−2908(19)	0507(11)	2770(10)	8.6(6)	1874(18)	3854(11)	−0066(10)	8.1(6)
F(26)	−2951(19)	−0304(11)	1840(10)	8.5(6)	1897(17)	2950(10)	−0961(10)	7.6(5)
F(27)	−2341(17)	−1098(11)	2398(9)	7.7(5)	1612(18)	2176(11)	−0322(10)	8.2(6)
O(28)	5359(21)	1724(12)	2543(11)	6.9(6)	9953(25)	3063(15)	1584(13)	9.3(8)
O(29)	4592(21)	−0263(13)	2820(12)	7.1(6)	7668(22)	1444(14)	1560(12)	8.2(7)
O(30)	2664(19)	1789(12)	1218(10)	5.8(5)	8924(22)	3447(14)	−0155(12)	8.0(7)
O(31)	5040(20)	0279(11)	1018(11)	6.2(6)	9752(21)	1455(14)	0158(11)	7.5(6)
O(32)	3328(21)	−1087(13)	1590(11)	7.1(6)	6905(21)	0838(14)	0083(11)	7.4(6)
O(33)	1875(20)	0403(12)	0464(12)	6.8(6)	7665(25)	2401(14)	−1167(14)	9.2(8)
O(34)	3426(20)	0789(12)	3745(11)	6.6(6)	6826(20)	2973(12)	2062(12)	7.2(6)
O(35)	1945(20)	2253(13)	2615(10)	6.6(6)	7446(21)	4475(13)	0667(11)	7.1(6)
O(36)	1916(19)	−0608(12)	2926(10)	6.1(6)	5238(18)	1911(11)	1023(10)	5.3(5)
O(37)	0301(18)	1215(9)	1602(9)	4.8(5)	6110(19)	3625(12)	−0531(11)	6.3(6)

	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}[b]
			Molecule 1			
Fe(1)	53	26	22	−4	4	0
Fe(2)	44	27	21	−6	4	−10
Fe(3)	56	30	17	−6	4	−5
As(4)	48	21	20	−4	5	−6
As(5)	59	24	21	−10	0	−7
			Molecule 2			
Fe(1)	48	41	26	0	−1	3
Fe(2)	66	27	31	−1	−6	−8
Fe(3)	54	30	26	3	2	−6
As(4)	65	21	23	1	5	−3
As(5)	71	26	19	−2	−4	−3
Mean σ	4	1	1	2	2	1

[a] Standard deviations are given in parentheses. [b] Coefficients in the temperature expression: $\exp[-10^4(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + 2b_{12}hk + 2b_{13}hl + 2b_{23}kl)]$.

by direct methods. The a-axis projection was examined, and the signs of the 34 $0kl$ reflections with a normalized structure factor,[9] $|E|, \geq 1.4$ were determined with a computer program,[10] which uses Sayre relationships[11] in the Vand and Pepinsky version[12] of the Cochran and Douglas procedure.[13] The program discriminates among the large number of possible solutions by a novel test,[10b] which rejects solutions in which Sayre relations for any reflections indicate a sign opposite to that in the solution to a probability of greater than 0.985. One possible solution was outstanding in having the lowest probability in the opposite-indication-of-sign test, and the E map computed with this set

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[9] M. M. Woolfson, "Direct Methods in Crystallography," Clarendon Press, Oxford, 1961, pp 8–14.

[10] (a) R. Hoge and J. Trotter, *J. Chem. Soc. A*, 2165 (1969); (b) R. Hoge, Ph.D. Thesis, University of British Columbia, 1969.

[11] D. Sayre, *Acta Crystallogr.*, **5**, 60 (1952).

[12] See ref 9, pp 101–106.

[13] (a) J. S. Rollett, "Computing Methods in Crystallography," Pergamon Press, Oxford, 1965, pp 167–171; (b) see ref 9, pp 94–100.

TABLE III

EQUATIONS OF MEAN PLANES IN THE FORM $lX' + mY + nZ' = p$, WHERE X', Y, Z' ARE COORDINATES IN Å, REFERRED TO ORTHOGONAL AXES a, b, c^*

	l	m	n	p	Maximum displacement, Å
		Iron triangle (3 Fe atoms)			
Molecule 1	0.3477	−0.7384	0.5778	2.8059	0
Molecule 2	0.3921	0.6513	−0.6497	5.9574	0
		Diarsine ligand (2 As and 4 C atoms)			
Molecule 1	0.2872	−0.7502	0.5956	2.8559	0.009
Molecule 2	0.2296	0.7076	−0.6683	5.0354	0.037

of signs revealed the positions, in projection, of the ten heavy atoms in the asymmetric unit.

With this information on the y and z parameters of the heavy atoms, attention was refocused on the Patterson function, and the three-dimensional structure of the two heavy-atom units was derived. Sixty-one of the sixty-four carbon, oxygen, and fluorine atoms were located from a Fourier summation with phases based on the iron and arsenic atoms, and the remaining three atoms were found on a subsequent electron density map.

Preliminary least-squares refinement of parameters utilized the block-diagonal approximation and reduced R to 0.11. At this stage a three-dimensional difference map showed electron density fluctuations around the iron and arsenic atoms which indicated anisotropic thermal motion. Refinement was continued using a modified full-matrix procedure. The function minimized was $\Sigma w(F_o - kF_c)^2$, with $w = 0$ for the unobserved reflections and $w = [A + B|F| + C|F|^2 + D|F|^3]^{-1}$ for the observed reflections. The coefficients A, B, C, and D were adjusted to achieve best constancy of local averages of $\Sigma w(F_o - F_c)^2$ over the full range of $|F_o|$, the final values being 600, 0.3, −0.06, and 0.00027, respectively. Scattering factors were from ref 14 and included the real part of the dispersion correction. The variables refined were the positional parameters, anisotropic thermal parameters for the ten heavy atoms, isotropic thermal parameters for the other atoms, and a single overall scale factor, a total of 347 variables. Since the dimensions of the computer program used were limited to 249 variables, it was necessary to vary different combinations of parameters in successive cycles. No parameter correlation coefficients greater than 0.35 were observed, and full convergence was reached after six cycles. Final values of R and R_w were 0.090 and 0.096, respectively, for the 2524 observed reflections (the values were 0.131 and 0.117 for all 3234 reflections, with $|F_o|$ for the unobserved reflections taken as the actual measured values) ($R = \Sigma|F_o - F_c|/\Sigma|F_o|$; $R_w = (\Sigma w(F_o - F_c)^2/\Sigma wF_o^2)^{1/2}$). Measured and calculated structure factors are listed in Table I. A final difference synthesis showed maximum fluctuations of ±0.8 e Å^{-3}.

Final positional and thermal parameters are given in Table II, together with their standard deviations

TABLE IV

BOND DISTANCES (Å) AND VALENCY ANGLES (DEG)[a]

Distances

	Molecule 1	Molecule 2		Molecule 1	Molecule 2
Fe(1)–Fe(2)	2.652 (8)	2.643 (7)	As(4)–C(20)	1.92	1.92
Fe(1)–Fe(3)	2.651 (7)	2.671 (9)	As(5)–C(21)	1.91	1.97
Fe(2)–Fe(3)	2.527 (6)	2.517 (7)			
Fe(2)–As(4)	2.301 (7)	2.278 (6)	C(20)–C(21)	1.28	1.31
Fe(3)–As(5)	2.300 (6)	2.307 (7)	C(20)–C(22)	1.58	1.57
			C(21)–C(23)	1.54	1.55
Fe(1)–C(6)	1.69	1.75	C(22)–C(23)	1.50	1.44
Fe(1)–C(7)	1.80	1.75			
Fe(1)–C(8)	1.74	1.69	C(22)–F(24)	1.33	1.30
Fe(1)–C(9)	1.69	1.70	C(22)–F(25)	1.33	1.32
Fe(2)–C(10)	1.73	1.67	C(23)–F(26)	1.30	1.37
Fe(2)–C(11)	1.75	1.81	C(23)–F(27)	1.34	1.35
Fe(3)–C(12)	1.70	1.68			
Fe(3)–C(13)	1.75	1.74	Av C–F	1.33	
Av Fe–C$_{term}$	1.73		C(6)–O(28)	1.19	1.15
			C(7)–O(29)	1.10	1.17
Fe(2)–C(14)	1.91	2.02	C(8)–O(30)	1.15	1.17
Fe(2)–C(15)	2.01	1.95	C(9)–O(31)	1.18	1.16
Fe(3)–C(14)	1.98	1.90	C(10)–O(35)	1.14	1.22
Fe(3)–C(15)	1.94	2.06	C(11)–O(34)	1.15	1.14
			C(12)–O(32)	1.18	1.20
As(4)–C(18)	1.93	1.94	C(13)–O(33)	1.16	1.18
As(4)–C(19)	1.92	1.97	C(14)–O(36)	1.17	1.17
As(5)–C(16)	1.92	1.93	C(15)–O(37)	1.18	1.13
As(5)–C(17)	1.96	1.98			
			Av C–O	1.16	
Av As–CH$_3$	1.94				

Angles

	Molecule 1	Molecule 2		Molecule 1	Molecule 2
C(6)–Fe(1)–C(7)	92	93	Fe(2)–As(4)–C(18)	119	116
C(6)–Fe(1)–C(8)	93	95	Fe(2)–As(4)–C(19)	118	120
C(6)–Fe(1)–C(9)	100	100	Fe(2)–As(4)–C(20)	114	116
C(6)–Fe(1)–Fe(2)	105	107	C(18)–As(4)–C(19)	104	104
C(7)–Fe(1)–C(9)	94	93	C(18)–As(4)–C(20)	99	99
C(7)–Fe(1)–Fe(2)	85	93	C(19)–As(4)–C(20)	100	99
C(7)–Fe(1)–Fe(3)	88	90	Fe(3)–As(5)–C(16)	120	116
C(8)–Fe(1)–C(9)	94	92	Fe(3)–As(5)–C(17)	116	121
C(8)–Fe(1)–Fe(2)	86	79	Fe(3)–As(5)–C(21)	113	113
C(8)–Fe(1)–Fe(3)	85	81	C(16)–As(5)–C(17)	104	103
C(9)–Fe(1)–Fe(3)	96	97	C(16)–As(5)–C(21)	101	99
Fe(2)–Fe(1)–Fe(3)	56.9 (2)	56.5 (2)	C(17)–As(5)–C(21)	100	102
C(10)–Fe(2)–C(11)	94	96	As(4)–C(20)–C(21)	137	134
C(10)–Fe(2)–C(15)	86	83	As(4)–C(20)–C(22)	131	134
C(10)–Fe(2)–As(4)	97	97	C(21)–C(20)–C(22)	92	92
C(11)–Fe(2)–C(14)	88	88	As(5)–C(21)–C(20)	137	136
C(11)–Fe(2)–As(4)	100	96	As(5)–C(21)–C(23)	127	130
C(14)–Fe(2)–Fe(3)	51	48	C(20)–C(21)–C(23)	96	93
C(14)–Fe(2)–As(4)	88	86			
C(15)–Fe(2)–Fe(3)	49	53	C(20)–C(22)–F(24)	111	112
C(15)–Fe(2)–As(4)	87	89	C(20)–C(22)–F(25)	114	114
Fe(1)–Fe(2)–C(10)	89	97	C(20)–C(22)–C(23)	86	88
Fe(1)–Fe(2)–C(11)	88	82	F(24)–C(22)–C(23)	119	117
Fe(1)–Fe(2)–C(14)	87	80	F(24)–C(22)–F(25)	109	109
Fe(1)–Fe(2)–C(15)	86	94	F(25)–C(22)–C(23)	117	117
Fe(1)–Fe(2)–Fe(3)	61.5 (2)	62.3 (2)			
Fe(3)–Fe(2)–As(4)	109.1 (2)	109.1 (2)	C(21)–C(23)–F(26)	120	116
			C(21)–C(23)–F(27)	118	113
C(12)–Fe(3)–C(13)	95	93	C(21)–C(23)–C(22)	86	88
C(12)–Fe(3)–C(14)	86	90	F(26)–C(23)–C(22)	114	119
C(12)–Fe(3)–As(5)	97	94	F(26)–C(23)–F(27)	106	103
C(13)–Fe(3)–C(15)	88	84	F(27)–C(23)–C(22)	113	118
C(13)–Fe(3)–As(5)	96	98			
C(14)–Fe(3)–Fe(2)	48	52	Fe(1)–C(6)–O(28)	180	170
C(14)–Fe(3)–As(5)	90	88	Fe(1)–C(7)–O(29)	177	172
C(15)–Fe(3)–Fe(2)	51	49	Fe(1)–C(8)–O(30)	174	170
C(15)–Fe(3)–As(5)	87	89	Fe(1)–C(9)–O(31)	176	171
Fe(1)–Fe(3)–C(12)	88	87	Fe(2)–C(10)–O(35)	174	174
Fe(1)–Fe(3)–C(13)	90	93	Fe(2)–C(11)–O(34)	173	173
Fe(1)–Fe(3)–C(14)	85	82	Fe(3)–C(12)–O(32)	173	177
Fe(1)–Fe(3)–C(15)	87	90	Fe(3)–C(13)–O(33)	176	172
Fe(1)–Fe(3)–Fe(2)	61.6 (2)	61.2 (2)			
Fe(2)–Fe(3)–As(5)	110.4 (3)	110.7 (2)	Fe(2)–C(14)–O(36)	143	134
			Fe(3)–C(14)–O(36)	136	146
			Fe(2)–C(15)–O(37)	139	147
			Fe(3)–C(15)–O(37)	142	136

[a] Unless otherwise specified, standard deviations are as follows: bond lengths, 0.03–0.04 Å; Fe(As)–Fe(As)–C, 0.8–1.3°; C–Fe(As)–C, 1.3–1.8°; angles at C, 2–3°.

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(14) "International Tables for X-Ray Crystallography," Vol. III, Kynoch Press, Birmingham, England, 1962.

calculated from the inverse matrix of the last refinement cycle. The mean planes of the iron triangle and diarsine ligand of each molecule are given in Table III, and the bond distances and valency angles are in Table IV.

Discussion

The molecule (Figure 1) is best described as a derivative of $Fe_3(CO)_{12}$,[5] with one equatorial carbonyl group on each of the two equivalent iron atoms replaced by the arsenic atoms of the diarsine ligand. In each of the two molecules in the asymmetric unit the arsenic and carbon atoms of the ligand are coplanar (Table III) in contrast to the nonplanarity in $LFe_2(CO)_6$.[8] Presumably the deviation from planarity in the latter compound is associated with the involvement of the cyclobutene π electrons in bonding to one of the iron atoms; this bonding is not present in $LFe_3(CO)_{10}$, so that planarity of the ligand is not unexpected. The difference in bonding in the two compounds is further indicated by the C=C bond lengths; the distance (Table IV) in $LFe_3(CO)_{12}$ is 1.30 (3) Å (standard deviation in parentheses), indicating retention of double bond character, while the corresponding length in $LFe_2(CO)_6$ is 1.51 (4) Å, consistent with the involvement of the π electrons in bonding to an iron atom.

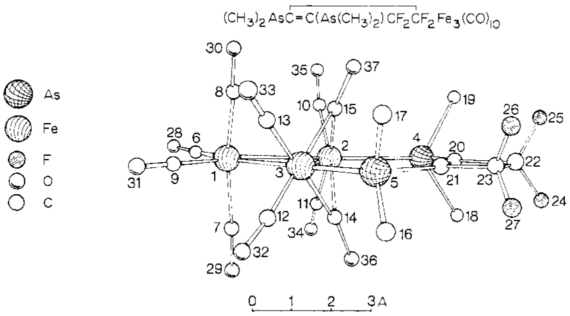

Figure 1.—View of the molecule.

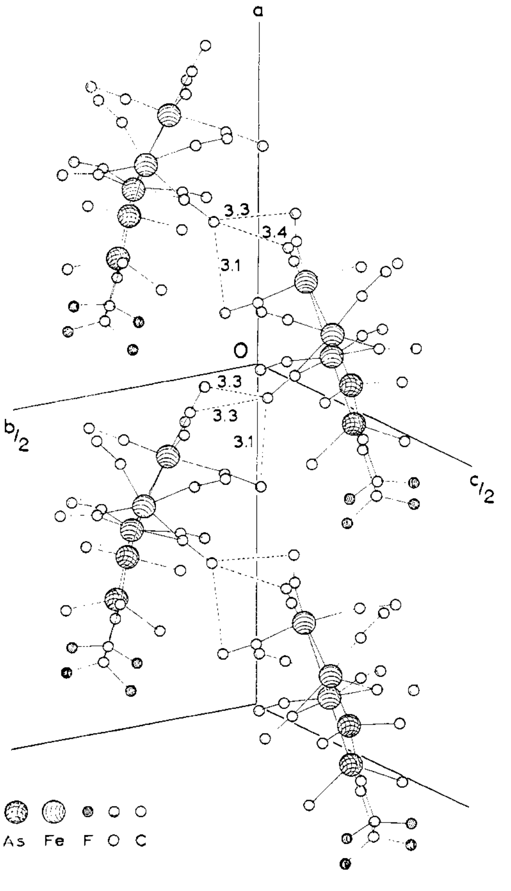

Figure 2.—View of two asymmetric units showing the relationship between molecules.

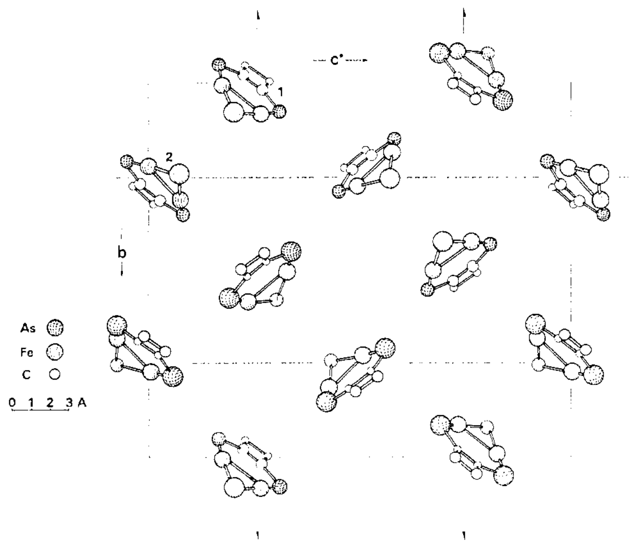

Figure 3.—Projection of the structure along *a*. Only the heavy-atom cluster and cyclobutene ring are shown.

In each of the two $LFe_3(CO)_{10}$ molecules in the asymmetric unit, the ligand is not quite coplanar with the iron triangle, and the amount of folding is slightly different in the two molecules. In molecule 1 the angle between the triangle and ligand planes is only 3.7°, but molecule 2 is more significantly bent, the angle being 9.9°. Since the angle is different in the two molecules, the small deviations from planarity are probably a result of crystal packing forces.

The bond lengths and valency angles in the two $LFe_3(CO)_{10}$ molecules in the asymmetric unit are not significantly different (Table IV). The Fe–Fe distances in the isosceles iron triangle are 2.65 (1) Å for the equivalent bonds and 2.53 (1) Å for the carbonyl-bridged bond. These lengths are close to the distances of 2.67 (1) and 2.56 (1) Å for the parent $Fe_3(CO)_{12}$ molecule,[5] so that the replacement of two terminal carbonyl groups by the diarsine ligand has apparently proceeded with little disturbance of the bonding in the iron triangle.

The mean Fe–C(terminal) distance is 1.73 (1) Å, close to the distance found in related compounds,[7,8] and all the Fe–C–O groupings are close to linear. The Fe–C(bridging) distances are considerably longer, and the bridges appear to be slightly asymmetric. The mean of the four longer Fe–C(bridging) bonds (with standard deviation of the mean) is 2.02 (2) Å, while the average of the shorter bonds is 1.93 (2) Å, the difference being 3σ and probably significant. This asymmetry is similar to although not as pronounced as that found in $(C_6H_5)_3$-

PFe$_3$(CO)$_{11}$ (average Fe–C(bridging), 2.04 and 1.87 Å).[7] As Dahm and Jacobson pointed out,[7] this asymmetry need not be the result of crystal packing forces but could be inherent in the bonding of the parent Fe$_3$(CO)$_{12}$, in which there is some evidence for unsymmetrical bridging carbonyl groups.[5] The C–O bond lengths average 1.17 Å, and the distances in the bridging carbonyl groups are not significantly longer than the average.

All the other bond lengths and valency angles (Table IV) are quite similar to those in related molecules. The angles in the Fe$_3$(CO)$_{10}$ moiety are similar to those in (C$_6$H$_5$)$_3$PFe$_3$(CO)$_{11}$,[7] and the dimensions of the diarsine ligand are quite close to those in LFe$_2$(CO)$_6$,[8] apart from the differences caused by the nonplanarity of the ligand in the latter compound. The valency angles at arsenic show deviations from the exact tetrahedral value, the Fe–As–C angles (113–121°) being larger than the C–As–C angles (99–104°).

The magnitudes of the principal axes of the thermal vibration ellipsoids of the iron and arsenic atoms are given in Table V. The largest vibrations are approximately perpendicular to the plane of the iron triangle.

TABLE V

MAGNITUDES (Å, σ = 0.005–0.008 Å) OF THE PRINCIPAL AXES OF THE THERMAL VIBRATION ELLIPSOIDS OF THE IRON AND ARSENIC ATOMS

	Molecule 1			Molecule 2		
	Axis 1	Axis 2	Axis 3	Axis 1	Axis 2	Axis 3
Fe(1)	0.186	0.233	0.235	0.179	0.249	0.292
Fe(2)	0.165	0.175	0.277	0.195	0.223	0.298
Fe(3)	0.190	0.192	0.261	0.190	0.222	0.273
As(4)	0.177	0.179	0.249	0.194	0.212	0.243
As(5)	0.166	0.218	0.260	0.193	0.232	0.240

All the intermolecular distances correspond to normal van der Waals interactions, the closest approaches being about 3.1 Å. The molecules are arranged (Figure 2) so that an oxygen atom of a bridging carbonyl group of each molecule in the asymmetric unit is approximately equidistant from three of the four terminal carbonyl groups of the unique iron atom of the other molecule. Another, simplified view of the molecular packing is shown in Figure 3.

Acknowledgments.—We thank Dr. W. R. Cullen for crystals, the National Research Council of Canada for financial support, and the University of British Columbia Computing Centre for assistance.

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Some Reactions of the Octahalodirhenate(III) Ions. VIII. Definitive Structural Characterization of the Octabromodirhenate(III) Ion[1]

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Received March 9, 1970

The compound Cs$_2$Re$_2$Br$_8$ has been prepared and its structure investigated by single-crystal X-ray diffractometry. The existence of the Re$_2$Br$_8^{2-}$ ion with virtual D_{4h} symmetry is confirmed. The Re–Re bond has a length of 2.228 (4) Å, very similar to that found in related compounds. The Re–Br bonds have an average length of 2.478 ± 0.006 Å. The set of eight bromine atoms defines a right, square parallelepiped with mean basal edge 3.39 ± 0.02 Å and mean vertical edge 3.48 ± 0.04 Å. Each cesium ion is surrounded by 11 bromine atoms (Cs · · · Br distances in the range 3.63–4.17 Å), while each Re$_2$Br$_8^{2-}$ ion has a cesium ion in approximately symmetrical contact with each of its four vertical faces. The space group is Pbca with $a = 12.625 \pm 0.004$ Å, $b = 12.953 \pm 0.004$ Å, and $c = 10.141 \pm 0.003$ Å. For $Z = 4$, d(calcd) = 5.11 g cm^{-3} (d(measd) = 5.10 g cm^{-3}) and the Re$_2$Br$_8^{2-}$ units are required to have $\bar{1}$ symmetry. The structure was solved using 770 reflections within the sphere bounded by $2\theta = 40°$ (Mo Kα) collected with a counter diffractometer and refined by full-matrix least-squares methods with anisotropic temperature parameters to a conventional R factor of 7.1% and a weighted R of 5.4%.

Introduction

A number of molecules and ions containing a quadruple Re–Re bond are known[2] and several have been structurally characterized with high accuracy by X-ray crystallography. Among these are the Re$_2$Cl$_8^{2-}$ ion[3–5] in which the Re–Re distance is 2.241 (7) Å, the Re$_2$Cl$_6$[P(C$_2$H$_5$)$_3$]$_2$ molecule[6] in which Re–Re = 2.222 (3) Å, and the (C$_3$H$_7$CO$_2$)$_4$Re$_2$(ReO$_4$)$_2$ and (C$_6$H$_5$CO$_2$)$_4$Re$_2$Cl$_2$ molecules[7] in which the Re–Re distances are 2.251 (2) and 2.235 (2) Å, respectively. In Re$_2$Cl$_4$(O$_2$CCH$_3$)$_2$(H$_2$O)$_2$, where the four oxygen atoms of the bridging acetato groups lie on one vertical face of the Re$_2$X$_8$ parallelepiped and the four Cl atoms define the opposite, parallel vertical face, with approximately the same nonbonded distances as in the Re$_2$Cl$_8^{2-}$ ion itself, the Re–Re distance is reported[8] to be 2.224 (5) Å. In these species, then, the bond length is relatively in-

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(1) Supported in part by the U. S. Atomic Energy Commission.

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