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The Crystal Structure of Mercury(I) Hexafluorosilicate Dihydrate *

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The structure of mercury(I) hexafluorosilicate dihydrate is monoclinic with the unit cell dimensions $a=5.642\pm 1$, $b=8.601\pm 2$, $c=8.822\pm 2$, $\beta=123.76\pm 0.02°$. The cell contains 2 formula units, and the space group is $P2_1/c$. The structure contains $H_2O-Hg-Hg-H_2O$ groups with an Hg–Hg distance of 2.495 ± 3 Å, and equivalent Hg–O distances of 2.20 ± 3 Å. The angle Hg–Hg–O is $170.9\pm 0.9°$. No deviation from a normal SiF_6 anion could be detected. The mean Si–F distance is 1.70 ± 2 Å. The distances from the water molecules to two neighbouring fluorine atoms are 2.58 ± 4 Å, and 2.65 ± 4 Å indicating hydrogen bonding.

The occurrence of complexes of the type $[H_2O-Hg-Hg-H_2O]^{2+}$ and Hg_2OH^+ in water solutions of mercurous salts has been established;[1,2] the former complex has also been found in solid perchlorate [2] and nitrate.[3] These compounds, $Hg(ClO_4)_2.4H_2O$ and $Hg_2(NO_3)_2.2H_2O$ were, however, determined with relatively low accuracy, especially in the Hg–O distances. The present investigation was undertaken in order to provide data concerning the dimensions of the $H_2O-Hg-Hg-H_2O$ group suitable for comparison with results obtained by the present author for some salts containing O–Hg–Hg–O elements.

EXPERIMENTAL

$Hg_2SiF_6.2H_2O$ was easily prepared by use of the equilibrium $Hg^{2+}+Hg \rightleftharpoons Hg_2^{2+}$.[4] HgO was dissolved in H_2SiF_6 (~40 %), and a drop of mercury was placed in the solution. The compound crystallized during slow evaporation, as large prismatic colourless crystals. The density was calculated from the loss of weight in benzene after a careful separation from excess mercury. The density of $Hg_2SiF_6.2H_2O$ as well as the solubility of the compound is not in agreement with values for a compound with the same formula given in *Handbook of Physics and Chemistry*, 46th Ed. Since the result of the structure determination was unambiguous, an analysis of the compound was regarded as unnecessary.

The very strong tendency of the Hg_2^{2+} ion to coordinate water molecules in the presence of the SiF_6 anion was strikingly demonstrated, when attempts were made to

* Structural Studies on Mercury(I) Compounds VII.

prepare the anhydrous compound, which should contain Hg – F contacts. Reactions between Hg_2F_2(s) and SiF_4(g) were carried out both at room temperature and at liquid air temperature. In both cases, slight impurities of water gave the dihydrate compound.

X-Ray data collection was carried out, using an integrating single crystal Weissenberg camera and Ni-filtered Cu$K\alpha$ radiation. A crystal of approximate size $0.07 \times 0.05 \times 0.03$ mm^3 was rotated around the b axis, and altogether 341 independent reflections, $h0l - h5l$, were registered. The multiple film technique was applied. An overexposed recording of the $0kl$ reflections was then made to establish the non-existence of reflections $0k0$ with $k=2n+1$. The intensities were measured with a photometric SAAB Abrahamsson type film scanner [5] on line with an IBM 1800 process controller.[6] Correction for absorption was included in the data processing.

DETERMINATION OF THE STRUCTURE

The Weissenberg photographs showed monoclinic symmetry with the extinctions characteristic for the unambiguously determined space group $P2_1/c$ (No. 14 of the *International Tables*), *i.e.* $h0l$ with $l=2n+1$, and $0k0$ with $k=2n+1$.

The cell constants were obtained from a Guinier powder photograph (Cu$K\alpha_1$ radiation). Refinement gave the following cell dimensions (based on comparison with the internal standard KCl; $a=6.2919$ Å [7]): $a=5.642 \pm 1$ Å, $b=8.601 \pm 2$ Å, $c=8.822 \pm 2$ Å, $\beta=123.76 \pm 0.02°$.

With a cell content of 2 formula units, the calculated density is 5.41 g/cm^3, in good agreement with the observed density, which is 5.37 g/cm^3.

A Patterson projection along [010] showed, as in many other mercury(I) compounds, a mercury doublet lying approximately parallel to the plane of projection. The mercury atoms were tentatively placed in the point position 4(e) of space group $P2_1/c$, *i.e.* $\pm(x,y,z)$, $\pm(x,\frac{1}{2}-y,\frac{1}{2}+z)$, with x and z parameters estimated from the Patterson projection. A Fourier projection with the structure factor signs thus obtained showed minor peaks. These could be interpreted as caused by the silicon and several of the other non-hydrogen atoms. Assuming the centre of an undistorted SiF_6 octahedron to be located $b/2$ above the mercury doublet with Si atoms in point position 2(a), (0,0,0), $(0,\frac{1}{2},\frac{1}{2})$, and the F atoms occupying 4(e) positions, y parameters for all "visible" atoms were roughly calculated. The minor peaks were thereby interpreted as being due to fluorine atoms. In the calculations, Hg – Hg and Si – F distances of 2.50 Å and 1.65 Å, respectively, were postulated. In this way, essentially two sets of parameters were obtained, corresponding to two possible ways of tilting the SiF_6 octahedron with respect to the mercury doublet. Both arrangements were tested by a three-dimensional least squares refinement. As a result, one model could be discarded.

The position of the water molecule came out very clearly when a three-dimensional difference Fourier map was calculated. The scale factors and parameters of all atoms were then refined, assuming isotropic thermal motion of all atoms. The R factor was then 0.085. As in all Hg(I) structures previously studied by the present author, the total difference Fourier after refinement showed a tendency towards anisotropic vibration of the mercury atoms. A refinement including anisotropic temperature factors for Hg was carried out, keeping the scale factors mutually fixed. The R factor came out slightly lower – 0.076 – and the standard deviations decreased by ~ 10 %. The improvement in accuracy is rather low in comparison with that obtained for other Hg(I) compounds. This may have two reasons: (1) the contribution of the non-metal atoms to the structure factors is comparatively large in the fluorosilicate, and (2) the orientation of the rotational axis with respect to the mercury doublet is unfavourable for anisotropic refinement.

Table 1. Final parameters obtained, refining with anisotropic temperature factors for Hg. The temperature factor expression used is $\exp - (\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + \beta_{12}hk + \beta_{13}hl + \beta_{23}kl)$.

	x	y	z	B Å^2
4(*e*) Hg	0.20340 ± 31	0.08321 ± 25	0.03073 ± 21	[a]
2(*a*) Si	0	1/2	0	1.55 ± 23
4(*e*) F_1	0.0446 ± 41	0.1317 ± 31	0.3732 ± 26	2.01 ± 39
4(*e*) F_2	0.1174 ± 46	0.3631 ± 32	0.1661 ± 30	2.45 ± 41
4(*e*) F_3	0.3347 ± 46	0.5662 ± 32	0.0919 ± 28	2.31 ± 40
4(*e*) O	0.4215 ± 62	0.6991 ± 43	0.4335 ± 35	2.63 ± 55

[a] $\beta_{ij} \times 10^4$ for Hg

ij=	11	22	33	12	13	23
	209 ± 7	68 ± 6	105 ± 3	−42 ± 9	176 ± 7	−10 ± 5

In all, 27 parameters were refined and 341 structure factors used. Parameters from the last cycle of refinement are listed in Table 1, and observed and calculated structure factors in Table 4. An attempt to refine the structure assuming the less symmetrical space group *Pc* gave no improvement.

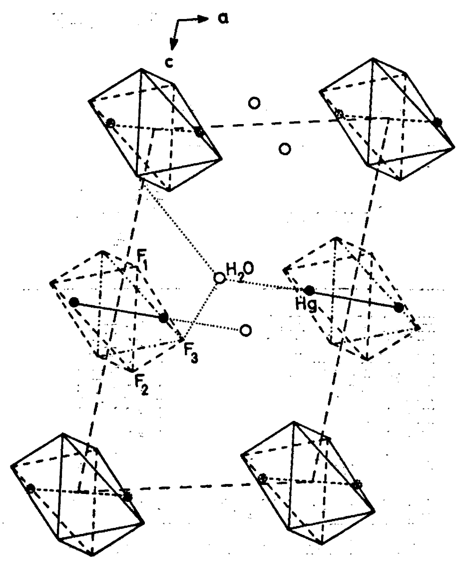

Fig. 1. One unit cell of $Hg_2SiF_6.2H_2O$. Mercury doublets and octahedra drawn with mainly full lines have their centres in the plane $b = 0.5$, those drawn with broken lines have their centres in the plane $b = 0$.

The resulting structure, illustrated in Fig. 1, consists of $H_2O-Hg-Hg-H_2O$ and SiF_6 groups. The bonding distance within the mercury doublet is 2.495 ± 3 Å, and the distance Hg – O is 2.20 ± 3 Å. The angle Hg – Hg – O is 170.9 ± 0.9°. The SiF_6 anion is undistorted, all Si – F distances are equal within one standard deviation, with a mean value of 1.70 ± 2 Å, and symmetry independent angles within the group very close to ideal values (*cf.* Table 2). The mercury atom

Table 2. Interatomic distances and angles calculated with parameters shown in Table 1.

Distances, Å

	Hg	H_2O	F_1	F_2	F_3
Hg	2.495 ± 3	2.199 ± 31	2.713 ± 25	2.847 ± 26 3.011 ± 22	2.874 ± 21
Si			1.706 ± 22	1.701 ± 25	1.688 ± 22
H_2O			2.583 ± 34 2.898 ± 38	> 3.00	2.651 ± 41 2.999 ± 35
F (within the SiF_6 group)			Mean distance value 2.40 ± 4		
F_1 (between SiF_6 groups)			> 3.40	2.883 ± 34	3.390 ± 29
F_2, F_3			> 3.40	> 3.40	> 3.40

Rmsd's for Hg (Å): r_1 0.138 ± 9, r_2 0.165 ± 30, r_3 0.172 ± 13.

Selected angles, degrees

Hg – Hg – O	170.9 ± 0.9
$F_1-H_2O-F_3$	110.2 ± 1.3
F_1-Si-F_2	91.4 88.6 ± 1.1
F_1-Si-F_3	90.3 89.7 ± 1.1
F_2-Si-F_3	91.3 88.7 ± 1.1

Table 3. Comparison of distances found in Hg(I) compounds with close Hg – O contacts.

Compound	Hg – Hg distance (Å)	Hg – O shortest distance (Å)	∠Hg – Hg – O degrees	Reference
$Hg_2(NO_3)_2.2H_2O$	2.54 ± 1	2.15 ± 10	~ 160	3
$Hg_2(ClO_4)_2.4H_2O$	2.50 ± 1	2.14 ± 10	180	2
$Hg_2SiF_6.2H_2O$	2.495 ± 3	2.20 ± 3	171 ± 1	
$Hg_2(BrO_3)_2$	2.507 ± 6	2.16 ± 3	174 ± 1	9
Hg_2SO_4	2.500 ± 3	2.24 ± 2	165 ± 1	10
Hg_2SeO_4	2.51 ± 1	2.21 ± 5	160 ± 1	10
Hg(I)-*o*-phthalate	2.519 ± 4	2.16 ± 5 2.08 ± 5	172 ± 2 174 ± 2	11
$Hg_2(I)(phen)(NO_3)_2$[a]	2.516 ± 7	2.22 ± 4	171 ± 1	12

[a] 1,10-Phenanthroline Hg(I)nitrate.

Table 4. hkl, F_{obs} and F_{calc} for $Hg_2SiF_6.2H_2O$.

h	k	l	F_{obs}	F_{calc}
-6	0	10	74	70
-4	0	8	107	92
-4	0	10	99	83
-3	0	8	54	53
-2	0	6	70	63
-2	0	8	104	87
-2	0	10	58	54
-1	C	4	151	180
-1	0	6	179	187
-1	0	8	117	114
0	0	2	231	280
0	0	4	100	112
0	0	6	64	59
1	0	-2	152	185
1	0	C	145	12C
1	0	2	54	48
1	0	4	73	71
1	0	6	55	57
1	0	8	48	49
2	0	-4	64	61
?	0	-2	129	118
2	0	0	166	152
2	0	2	162	162
2	0	4	108	112
2	0	6	63	66
3	0	-6	148	147
3	0	-4	202	227
3	0	-2	189	180
3	0	0	126	108
3	0	2	44	4C
4	0	-6	84	80
4	0	-4	26	26
4	0	0	57	51
4	0	2	79	77
4	0	4	64	66
5	0	-6	77	74
5	0	-4	110	113
5	0	-2	110	110
5	0	0	108	103
5	0	2	80	82
6	0	-8	92	94
6	0	-6	96	109
6	0	-4	87	94
6	0	-2	48	46
-6	1	9	64	59
-4	1	9	93	86
-3	1	7	128	111
-2	1	6	71	68
-1	1	4	69	68
-1	1	5	121	132
-1	1	7	80	89
-1	1	9	61	59
0	1	1	143	165
0	1	2	64	51
0	1	3	171	180
0	1	4	53	63
0	1	5	76	78
0	1	6	74	73
0	1	8	42	46
1	1	-3	131	143
1	1	-2	99	99
1	1	-1	62	44
1	1	0	145	129
1	1	2	90	83
1	1	4	54	56
1	1	5	84	84
1	1	7	79	77
2	1	-4	71	7C
2	1	-3	65	56
2	1	-2	120	108
2	1	-1	183	161
2	1	0	128	114
2	1	1	193	184
2	1	3	150	154
2	1	5	104	96
3	1	-7	117	111
3	1	-6	37	44
3	1	-5	139	145
3	1	-3	176	187
3	1	-1	190	182
3	1	0	49	48
3	1	1	116	108
3	1	2	86	80
3	1	4	49	51
4	1	-7	100	103
4	1	-6	48	53
4	1	-5	91	88
4	1	-4	100	90
4	1	-3	43	45
4	1	-2	68	65
4	1	0	53	51
4	1	1	62	51
4	1	3	50	51
5	1	-5	47	56
5	1	-3	91	94
5	1	-1	92	98
5	1	1	68	60
6	1	-7	71	80
6	1	-5	58	71
6	1	-3	53	50
6	1	-2	36	42
-5	2	9	88	84
-4	2	8	53	46
-4	2	9	29	25
-4	2	10	24	32
-3	2	7	77	71
-3	2	8	36	31
-3	2	9	85	74
-2	2	6	36	31
-2	2	7	103	100
-2	2	8	50	44
-2	2	9	51	49
-2	2	10	37	37
-1	2	4	106	129
-1	2	5	43	45
-1	2	6	82	82
-1	2	8	49	47
-1	2	9	31	30
0	2	1	56	58
0	2	2	118	131
0	2	3	137	143
0	2	4	74	76
0	2	5	110	118
0	2	6	37	32
0	2	7	67	71
1	2	-4	114	129
1	2	-3	121	148
1	2	-2	105	128
1	2	-1	178	202
1	2	0	79	57
1	2	1	20C	191
1	2	3	158	163
1	2	4	34	31
1	2	5	72	75
1	2	6	30	32
1	2	7	22	25
2	2	-5	144	170
2	2	-4	20	16
2	2	-3	168	203
2	2	-2	98	82
2	2	-1	125	104
2	2	0	105	91
2	2	1	65	55
2	2	2	66	61
2	2	3	29	26
2	2	4	42	39
2	2	5	32	31
2	2	6	22	21
3	2	-7	70	71
3	2	-6	65	61
3	2	-5	62	59
3	2	-4	80	74
3	2	-3	24	16
3	2	-2	74	64
3	2	-1	135	119
3	2	0	47	39
3	2	1	99	100
3	2	2	28	18
3	2	3	76	73
3	2	5	62	66
4	2	-7	89	83
4	2	-6	40	38
4	2	-5	99	96
4	2	-3	125	121
4	2	-1	128	129
4	2	0	40	39
4	2	1	76	75
4	2	2	45	43
4	2	3	37	37
5	2	-7	96	97
5	2	-6	51	50
5	2	-5	68	63
5	2	-4	64	62
5	2	-3	46	49
5	2	-2	66	62
5	2	0	49	51
5	2	1	16	16
6	2	-8	45	47
6	2	-6	42	47
6	2	-5	34	40
6	2	-4	38	41
6	2	-3	50	54
6	2	-2	30	30
6	2	-1	54	58
-5	3	10	67	67
-3	3	8	84	75
-3	3	10	63	64
-2	3	6	135	142
-2	3	8	93	92
-2	3	10	46	43
-1	3	4	82	87
-1	3	5	29	24
0	3	1	22	15
0	3	2	52	51
0	3	3	47	47
0	3	4	85	96
0	3	6	111	115
0	3	8	82	83
1	3	-4	84	87
1	3	-3	42	42
1	3	-2	128	158
1	3	-1	38	26
1	3	0	220	221
1	3	2	179	198
1	3	3	35	31
1	3	4	129	136
1	3	6	75	74
2	3	-5	36	33
2	3	-4	147	164
2	3	-3	48	44
2	3	-2	173	177
2	3	0	144	136
2	3	4	32	29
2	3	6	41	39
3	3	-6	64	58
3	3	-4	20	8
3	3	-2	40	29
3	3	0	96	85
3	3	2	120	123
3	3	4	89	92
4	3	-6	91	87
4	3	-4	140	150
4	3	-2	157	149
4	3	C	121	117
4	3	2	69	69
5	3	-8	85	87
5	3	-6	101	106
5	3	-4	86	85
6	3	-4	52	51
6	3	-2	68	71
-6	4	8	27	26
-5	4	9	71	72
-4	4	8	50	48
-3	4	7	63	63
-3	4	8	34	30
-3	4	9	65	63
-2	4	7	100	100
-2	4	8	29	28
-2	4	9	45	45
-1	4	4	30	34
-1	4	5	22	23
-1	4	6	60	60
-1	4	8	39	38
-1	4	9	24	26
0	4	1	40	44
0	4	2	64	65
0	4	3	84	89
0	4	4	27	23
0	4	5	79	91
0	4	6	22	22
0	4	7	65	72
1	4	-3	91	102
1	4	-2	50	52
1	4	-1	175	186
1	4	0	65	53
1	4	1	183	192
1	4	2	32	29
1	4	3	118	125
1	4	4	50	48
1	4	5	69	69
1	4	6	40	38
1	4	7	30	29
2	4	-5	132	154
2	4	-4	56	57
2	4	-3	138	156
2	4	-2	72	67
2	4	-1	114	104
2	4	0	86	73
2	4	1	35	30
2	4	2	85	85
2	4	3	20	14
2	4	4	60	61
2	4	5	26	25
2	4	6	38	38
3	4	-6	68	66
3	4	-5	3C	22
3	4	-4	101	102
3	4	-3	37	33
3	4	-2	96	88
3	4	-1	72	62
3	4	0	78	69
3	4	1	79	79
3	4	2	42	39
3	4	3	69	76
4	4	-7	61	57
4	4	-6	56	56
4	4	-5	102	107
4	4	-4	45	43
4	4	-3	117	119
4	4	-1	107	98
4	4	1	71	71
4	4	2	27	25
4	4	3	36	35
5	4	-7	77	79
5	4	-5	61	64
5	4	-4	40	35
5	4	-3	3C	30
5	4	-2	34	31
5	4	0	30	31
6	4	-6	36	38
6	4	-5	27	28
6	4	-4	34	35
6	4	-3	43	46
-5	5	8	44	46
-3	5	7	69	64
-2	5	6	58	53
-1	5	5	106	120
-1	5	7	78	82
0	5	1	129	144
0	5	3	131	138
C	5	5	75	79
1	5	-3	119	138
1	5	-2	59	60
1	5	-1	95	92
1	5	0	76	62
1	5	2	86	87
1	5	4	69	68
1	5	5	44	47
2	5	-4	73	75
2	5	-3	39	37
2	5	-2	70	63
2	5	-1	110	97
2	5	1	110	109
2	5	3	85	87
2	5	5	54	54
3	5	-5	88	85
3	5	-3	105	102
3	5	-1	102	99
3	5	0	69	60
3	5	1	73	64
3	5	2	43	45
3	5	4	32	37
4	5	-7	62	67
4	5	-5	56	56
4	5	-4	45	45
4	5	-2	78	74
4	5	0	54	55
4	5	1	54	51
5	5	-5	59	62
5	5	-3	86	86
5	5	-1	84	84

neighbours are, besides the closely associated water molecule, three fluorine atoms at 2.71 ± 3 Å, 2.85 ± 3 Å, and 2.87 ± 3 Å, from two SiF_6 groups. There are no other atoms closer than 3.0 Å. The distances $F_1 - H_2O$ and $F_3 - H_2O$ are 2.58 ± 4 Å, and 2.65 ± 4 Å, respectively, probably depending on hydrogen bonding. The angle $F_1 - H_2O - F_3$ is 110 ± 1°, close to the tetrahedral angle.

Table 5. Computer programs used for the crystallographic calculations. All programs written in FORTRAN IV.

No.	Program name and function. Computer.	Authors
1	DATAP2. Lp and absorption corrections. Preparative calculations for extinction correction according to Zachariasen's 1963-formula. IBM 360/751.	P. Coppens, L. Leiserowitz and D. Rabinovich, Rehovoth, Israel. Modified by O. Olofsson and M. Elfström, Uppsala, Sweden. Inclusion of calculations for extinction correction by B. G. Brandt and S. Åsbrink, Stockholm, Sweden. Further modifications by B. G. Brandt and A. G. Nord, Stockholm, Sweden.
2	DRF. Fourier summations and structure factor calculations. IBM 360/75.	A. Zalkin, Berkeley, USA. Modified by R. Liminga and J.-O. Lundgren, Uppsala, Sweden. Further modified by O. Lindgren, Göteborg, and by A. G. Nord and B. G. Brandt, Stockholm, Sweden.
3	LALS. Full matrix least squares refinement of positional and thermal parameters and of scale factors. IBM 360/75.	P. K. Gantzel, R. A. Sparks and K. N. Trueblood, Los Angeles, USA. Modified by A. Zalkin, Berkeley, USA, and by J.-O. Lundgren, R. Liminga and C.-I. Brändén, Uppsala, Sweden. Further modified by O. Lindgren, Göteborg, and by B. G. Brandt and A. G. Nord, Stockholm, Sweden.
4	DISTAN. Calculation of interatomic distances and bond angles with estimated standard deviations. IBM 360/75.	A. Zalkin, Berkeley, USA. Modified by A. G. Nord and B. G. Brandt, Stockholm, Sweden.
5	ORTEP. Thermal-ellipsoid plot. For crystal structure illustrations. IBM 360/75.	C. K. Johnson, Oak Ridge, USA. Modified by, I. Carlbom, Stockholm, Sweden.
6	PWF. Evaluation of intensities and indexing from film scanner output for Weissenberg and precession geometries. IBM 1800.	P.-E. Werner, Stockholm, Sweden.
7	ANP. Indexing refinement from film scanner output for Weissenberg and precession geometries. IBM 1800.	P.-E. Werner, Stockholm, Sweden.
8	SFALE. Film factors from common reflections. IBM 1800.	M. Leijonmarck, Stockholm, Sweden.
9	PIRUM. Indexing of powder photographs and least squares refinement of unit cell parameters. IBM 1800.	P.-E. Werner, Stockholm, Sweden.

Table 6. The first 25 lines in a Guinier powder photograph of $Hg_2SiF_6.2H_2O$ ($CuK\alpha_1$ radiation).

I	$h\ k\ l$	$\sin^2\theta_{obs} \times 10^5$	$\sin^2\theta_{calc} \times 10^5$
v st	0 1 1	1905	1904
m	{−1 1 1 { 1 0 0	2684	{2684 {2696
m	0 2 0	3203	3207
m	−1 0 2	3264	3274
st	1 1 0	3489	3498
w	−1 1 2	4069	4076
v w	0 2 1	4300	4310
st	0 0 2	4404	4411
st	−1 2 1	5096	5090
v w	0 1 2	5210	5213
m	−1 2 2	6479	6482
v w	−2 0 2	7532	7529
m	0 2 2	7614	7619
w	−1 1 3	7667	7674
m	{ 0 3 1 {−2 1 2	8325	{8320 {8331
st	−2 1 1	8843	8856
st	1 2 1	8914	8923
st	1 3 0	9905	9913
m	−1 2 3	10080	10080
m	−1 3 2	10492	10492
m	{ 0 1 3 {−2 2 2	10725	{10728 {10737
w	−2 2 1	11266	11261
w	2 1 0	11586	11586
v w	1 1 2	11746	11743
m	−2 2 3	12414	12418

F − F distances within the SiF_6 group are 2.40 ± 4 Å. The shortest distance between the groups is 2.88 ± 4 Å.

A comparison between bonding distances in the present structure and those investigated earlier (*cf.* Table 3) shows a good agreement in mercury-mercury bond length for compounds containing Hg − O contacts. The Hg − O distances and Hg − Hg − O angles found show that the size and shape of the nearly linear O − Hg − Hg − O group are independent of the character of the oxygen-containing ligand. Assuming the van der Waals radius of mercury to be 1.50 Å (half the shortest bonding distance in the metal) and that of fluorine to be 1.36 Å, the interaction between the mercury doublet and the SiF_6 anion is weak. On the other hand, the Hg − O bond distance, although not as short as in HgO,[8] is well below the sum of $r(Hg^{2+})$ and $r(O^{2-})$, which is 2.44 Å (if $r(Hg^{2+})$ is assumed to be 1.04 Å).

Thus, $Hg_2SiF_6.2H_2O$ and the other mercurous compounds containing crystal water should be looked upon as ionic structures with an $(HgH_2O)_2{}^{2+}$ cation.

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