The Crystal Structure of Barium Selenopenta-
thionate Trihydrate

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The crystal structure of barium selenopentathionate trihydrate, $BaSe(S_2O_3)_2.3H_2O$, has been determined from three-dimensional X-ray data. The salt crystallizes in the monoclinic space group $P2_1/c$ (No. 14) with four formula units in a unit cell of dimensions $a=10.502(3)$ Å, $b=4.992(2)$ Å, $c=23.987(6)$ Å, $\beta=110.85(4)°$. Least squares refinement was carried out using 2519 non-zero reflections, recorded by means of a single-crystal diffractometer and $MoK\alpha$ radiation (Nb-filtered).

The selenopentathionate ion has the *cis* form, the sulphonate groups being rotated out of the plane through the three middle atoms to the same side of the plane. The dimensions of the $S-S-Se-S-S$ chain, from one end of the chain to the other, are $S(1)-S(2)=2.1038$ (17) Å, $S(2)-Se=2.1810(19)$ Å, $Se-S(4)=2.1783(19)$ Å, $S(4)-S(5)=2.0933(21)$ Å, $\angle S(1)-S(2)-Se=104.07(7)°$, $\angle S(2)-Se-S(4)=104.00$ (8)°, $\angle Se-S(4)-S(5)=103.42(7)°$. The SSSe/SSeS dihedral angles are 106.7° and 105.9°.

The pentathionate, selenopentathionate, and telluropentathionate ions have been found to occur in two rotational-isomeric forms. The *cis* form of the selenopentathionate ion was found in the crystals of barium selenopentathionate dihydrate,[1,2] and the *trans* form was found in the crystals of ammonium selenopentathionate hemitrihydrate.[3] The telluropentathionate ion occurs in the *cis* form in the crystals of barium telluropentathionate dihydrate,[4,5] whereas the *trans* form was found in the crystals of barium telluropentathionate trihydrate,[6] and also in ammonium telluropentathionate [7] and rubidium telluropentathionate hemitrihydrate.[8] The telluropentathionate ion thus occurs in two rotational-isomeric forms in its barium salts, the *cis* form in a dihydrate and the *trans* form in a trihydrate. The selenopentathionate ion has now been found to have the *cis* form in the trihydrate as well as in the dihydrate [1,2] of its barium salt. The crystal structure of barium selenopentathionate trihydrate, described here, has been briefly reported earlier.[9]

EXPERIMENTAL

Barium selenopentathionate trihydrate, $BaSe(S_2O_3)_2.3H_2O$, was obtained by recrystallization of crude barium selenopentathionate from dilute hydrochloric acid.[4] The crystals were light yellow prisms, extended along the b axis, and of varying thickness.

The intensity data were measured on a Siemens automatic single-crystal diffractometer using (Nb-filtered) MoKα radiation and a scintillation counter. A crystal bounded by (100) and (001), with distances between parallel boundary faces of about 0.10 mm, and with a length of about 0.30 mm, was mounted with the b axis parallel to the ϕ axis of the diffractometer.

The procedure followed was similar to that described in a preceding paper,[2] using the $\theta - 2\theta$ scan technique and the method of five-value measurements. The scan width was $1.0°$ for all reflections. Three reflections were used as reference, and measured at intervals of 50 reflections.

The crystal slowly decomposed, with liberation of selenium, during the data collection. The crystal became red and the net counts of the reference reflections decreased by about 20 %.

Out of 2866 reflections attainable within $\theta = 28°$, 347 were found to have net intensity below twice its standard deviation, and were assigned an intensity equal to this limit. These reflections were labelled as unobserved.

The net intensities were scaled by means of the reference reflections, and Lorentz and polarization corrections were applied. Absorption corrections and, eventually, secondary extinction corrections were applied. The absorption corrections were done by means of the Gaussian integration method as described by Coppens et al.[10] The number of grid points used along the a, b, and c axis were 6, 12, and 6, respectively. The linear absorption coefficient for MoKα radiation is 75.1 cm^{-1}. Secondary extinction corrections were carried out later, according to Zachariasen.[11] The formula used was $F_{corr} = KF_o(1 + \beta CI_o)$, where $\beta = 2(1 + \cos^4 2\theta)/(1 + \cos^2 2\theta)^2$, and C was found to be 1.04×10^{-7}.

The scattering curves used were those given in *International Tables for X-Ray Crystallography*,[12] Table 3.3.1A, for selenium, sulphur, and oxygen atoms, and the one given by Thomas and Umeda[13] for barium ion. The scattering curves for barium and selenium were corrected for anomalous dispersion using the $\Delta f'$ and $\Delta f''$ values given by Cromer,[14] and taking the amplitude of f as the corrected value.

The structure was refined by means of a full-matrix least squares program minimizing the function

$$r = \sum W(|F_o| - K|F_c|)^2$$

Here $W = 4(I_t - I_b)^2/F_o^2[I_t + I_b + k^2(I_t - I_b)^2]$, where I_t is the total intensity of a reflection, I_b is the background intensity, and k is the relative standard deviation in the scaling curve based on the reference reflections. The value of k was put equal to 0.014. Unobserved reflections were included with $|F_o|$ equal to the observable limit when $|F_c|$ exceeded this limit.

The calculations were carried out on an IBM 360/50H computer. The programs used for preparation of input tape data for the diffractometer, and conversion of diffractometer output tape data to the IBM computer, were written by Mr. K. Maartmann-Moe, and the programs used for data processing, secondary extinction corrections and Fourier summations were written by Mr. K. Åse, both of this Institute. The programs used for least squares refinement and absorption corrections were made available by the Chemical Department of X-Ray Crystallography, Weizmann Institute of Science, Rehovoth, Israel. The latter program was modified by Mr. K. Åse.

The unit cell dimensions, calculated by means of a least squares program using the θ angles ($\theta = 20 - 24°$) of 22 reflections measured on the diffractometer, are $a = 10.502(3)$ Å, $b = 4.992(2)$ Å, $c = 23.987(6)$ Å, and $\beta = 110.85(4)°$. From systematic absences, $0k0$: $k = 2n + 1$, $h0l$: $l = 2n + 1$, the space group is $P2_1/c$ (No. 14), and there are four formula units per unit cell. The calculated density is 2.79 g/cm³, and the density observed by flotation was 2.76 g/cm³.

THE STRUCTURE ANALYSIS

The coordinates for the barium ion and the selenium atom were derived from a three-dimensional Patterson map, calculated on the basis of the 2519 observed reflections. An electron density map, with signs based on the barium and selenium contributions, allowed the location of the four sulphur atoms of the asymmetric unit. In the next Fourier map, the six sulphonate oxygen atoms could be placed in peaks of electron density $10-13$ $e/Å^3$. This map showed, in addition, three peaks of density 11.0, 5.3 and 3.4 $e/Å^3$. The two highest peaks were at distances of about 2.8 Å from the barium ion, and water oxygen atoms were placed in these two positions.

Least squares refinement was then carried out, using isotropic thermal parameters for all atoms. The R value $(= \sum ||F_o| - |F_c||/\sum |F_c|)$, being 0.119 at this stage, was reduced to 0.048 by introduction of anisotropic thermal parameters for barium, selenium, and sulphur. Using anisotropic thermal parameters also for the sulphonate oxygen atoms, the R value became 0.043. The thermal parameter for $H_2O(2)$, the water oxygen atom situated at low electron density in the Fourier map, was high, but the occupancy factor was not reduced on refinement.

The observed structure factors were then corrected for secondary extinction, and anisotropic thermal parameters were applied for all atoms. The R value was reduced to 0.040.

A difference electron density map, calculated at this stage, showed a peak of 3.1 $e/Å^3$ in the same position as the peak of 3.4 $e/Å^3$ in the latest electron density map. The $H_2O(3)$ oxygen atom was placed in this position. On refinement, the occupancy factor of this atom was reduced from 1.00 to 0.54.

All the parameters (136), except the occupancy factors, were refined simultaneously in the last cycles. The final R value was 0.034, with unobserved reflections included when $|F_c|$ exceeds the observable limit. The final maximum shift of a parameter was about one tenth of its standard deviation.

Table 1. Atomic coordinates, in fraction of cell edges, for barium selenopentathionate trihydrate. Origin at a centre of symmetry. Standard deviations from least squares are given in parentheses.

	x	y	z
Ba	$-0.292726(27)$	0.772863(55)	$-0.049768(12)$
S(1)	$-0.40889(11)$	0.69509(24)	0.09452(6)
S(2)	$-0.26049(14)$	0.71687(40)	0.18077(6)
Se	$-0.10094(6)$	0.44414(15)	0.17764(3)
S(4)	0.06295(15)	0.70869(41)	0.17635(6)
S(5)	0.05472(12)	0.68511(25)	0.08800(5)
O(1)	$-0.43461(39)$	0.41562(75)	0.08077(19)
O(2)	$-0.52114(40)$	0.82955(89)	0.10513(19)
O(3)	$-0.35852(41)$	0.83126(78)	0.05363(17)
O(4)	0.05315(41)	0.40669(77)	0.07285(18)
O(5)	0.18262(37)	0.81348(90)	0.09402(19)
O(6)	$-0.06528(36)$	0.82741(76)	0.05136(17)
$H_2O(1)$	$-0.24680(37)$	0.28487(65)	0.01497(16)
$H_2O(2)$	$-0.36479(83)$	0.69728(169)	$-0.17284(28)$
$H_2O(3)$	$-0.58965(113)$	0.72515(271)	$-0.26657(59)$

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Table 2. Anisotropic thermal parameters expressed in the form $\exp[-2\pi^2(h^2a^{-2}U_{11}+\cdots +2hka^{-1}b^{-1}U_{12}+\cdots)]$. All values have been multiplied by 10^4. Standard deviations are given in parentheses.

	U_{11}	U_{22}	U_{33}	U_{12}	U_{23}	U_{13}
Ba	256(1)	253(2)	330(3)	4(1)	36(1)	107(1)
S(1)	194(5)	253(6)	366(6)	3(4)	36(5)	109(5)
S(2)	326(7)	899(14)	364(7)	62(8)	−107(8)	135(6)
Se	344(3)	754(5)	442(3)	87(3)	252(3)	178(2)
S(4)	319(7)	989(14)	308(7)	−152(8)	−130(8)	133(5)
S(5)	224(5)	277(6)	315(6)	5(5)	18(5)	135(5)
O(1)	395(21)	271(21)	686(27)	−92(17)	−13(19)	153(20)
O(2)	369(20)	545(26)	678(27)	219(19)	186(21)	317(20)
O(3)	550(24)	348(21)	479(22)	8(18)	63(17)	327(19)
O(4)	508(23)	306(21)	588(25)	65(18)	−46(19)	273(20)
O(5)	276(18)	612(28)	599(25)	−75(18)	158(21)	200(18)
O(6)	304(18)	341(21)	467(21)	72(16)	14(17)	54(16)
$H_2O(1)$	431(20)	208(17)	413(19)	10(15)	27(15)	168(16)
$H_2O(2)$	1446(65)	1548(73)	592(35)	328(54)	−93(40)	179(38)
$H_2O(3)$ [a]	592(63)	1440(130)	1153(94)	−25(74)	297(84)	−106(61)

[a] Occupancy factor for $H_2O(3)$ oxygen atom, 0.54 instead of 1.00.

The highest peak in a final difference electron density map was about 0.9 e/$Å^3$. The map showed two peaks near $H_2O(1)$, about 1.0 Å from the water oxygen atom and in direction towards O(1) and O(4). The remaining four hydrogen atoms were not located; the regions of positive electron density near $H_2O(2)$ and $H_2O(3)$ had no distinct peaks at expected distances and angles.

Tables 1 and 2 give the final atomic parameters and their standard deviations from least squares. The observed structure factors, and the ones calculated on the basis of the parameters of Tables 1 and 2, are listed in Table 4.

Table 3. Orthogonal coordinates (Å) for barium selenopentathionate trihydrate $(P2_1/c)$ and barium selenopentathionate dihydrate $(Pnma)$. Standard deviations are given in parentheses. The $H_2O(3)$ oxygen atom of the trihydrate is not included.

	x'		y'		z'	
	$P2_1/c$	$Pnma$	$P2_1/c$	$Pnma$	$P2_1/c$	$Pnma$
Ba	3.858(0)	3.922(1)	2.649(0)	2.609	−1.116(0)	−1.088(1)
S(1)	3.470(1)	3.501(2)	5.101(1)	5.060(2)	2.119(1)	2.071(2)
S(2)	3.579(2)	3.533(3)	4.279(2)	4.316(2)	4.052(2)	4.029(2)
Se	2.217(1)	2.178(2)	2.577(1)	2.609	3.982(1)	3.965(2)
S(4)	3.538(2)	3.533(3)	0.845(2)	0.901(2)	3.953(2)	4.029(2)
S(5)	3.420(1)	3.501(2)	0.177(1)	0.157(2)	1.973(1)	2.071(2)
O(1)	2.075(4)	2.127(5)	5.254(4)	5.218(5)	1.811(4)	1.700(6)
O(2)	4.144(4)	4.176(6)	6.371(4)	6.314(6)	2.357(5)	2.293(6)
O(3)	4.150(4)	4.211(5)	4.223(5)	4.138(5)	1.202(4)	1.215(6)
O(4)	2.030(4)	2.127(5)	0.064(4)	−0.001(5)	1.633(4)	1.700(6)
O(5)	4.061(4)	4.176(6)	−1.115(4)	−1.097(6)	2.107(4)	2.293(6)
O(6)	4.130(4)	4.211(5)	1.124(4)	1.079(5)	1.151(4)	1.215(6)
$H_2O(1)$	1.422(3)	1.444(7)	2.720(4)	2.609	0.335(4)	0.327(9)
$H_2O(2)$	3.481(8)	3.333(17)	2.357(9)	2.609	−3.869(7)	−3.855(18)

Table 4. Observed and calculated structure factors for barium selenopentathionate trihydrate. A minus sign on $F(O)$ indicates an unobserved reflection.

H	K	L	F(O)	F(C)
0	0	2	200	144
0	0	4	88	-89
0	0	6	48	-30
0	0	8	349	-366
0	0	10	54	-58
0	0	12	39	61
0	0	14	174	-175
0	0	16	49	48
0	0	18	88	85
0	0	20	21	27
0	0	22	145	142
0	0	24	22	20
0	0	26	62	-61
0	0	28	16	-16
1	0	-30	10	-11
1	0	-28	52	49
1	0	-26	52	50
1	0	-24	29	31
1	0	-22	56	54
1	0	-20	74	-74
1	0	-18	114	-114
1	0	-16	36	-37
1	0	-14	138	-139
1	0	-12	35	-34
1	0	-10	80	85
1	0	-8	65	-64
1	0	-6	216	229
1	0	-4	212	207
1	0	-2	63	-66
1	0	0	67	68
1	0	2	155	-136
1	0	4	256	-261
1	0	6	33	30
1	0	8	121	-125
1	0	10	10	-12
1	0	12	206	209
1	0	14	57	55
1	0	16	93	93
1	0	18	72	73
1	0	20	78	-77
1	0	22	10	-11
1	0	24	19	-17
1	0	26	67	-65
1	0	28	-9	1
2	0	-30	14	14
2	0	-28	12	10
2	0	-26	-8	-3
2	0	-24	33	-30
2	0	-22	41	-40
2	0	-20	97	-96
2	0	-18	100	-98
2	0	-16	64	63
2	0	-14	124	126
2	0	-12	174	175
2	0	-10	154	157
2	0	-8	119	-121
2	0	-6	207	-201
2	0	-4	34	-31
2	0	-2	149	-131
2	0	0	55	-47
2	0	2	109	-102
2	0	4	235	-221
2	0	6	93	89
2	0	8	211	215
2	0	10	132	126
2	0	12	97	100
2	0	14	67	-67
2	0	16	132	-132
2	0	18	36	-35
2	0	20	49	-49
2	0	22	20	-18
2	0	24	23	20
2	0	26	9	7
3	0	-30	34	-31
3	0	-28	45	-43
3	0	-26	47	-48
3	0	-24	29	-30
3	0	-22	16	14
3	0	-20	72	69
3	0	-18	121	121
3	0	-16	141	143
3	0	-14	94	93
3	0	-12	21	-23
3	0	-10	130	-131
3	0	-8	209	-216
3	0	-6	155	-162
3	0	-4	100	-90
3	0	-2	36	30
3	0	0	165	162
3	0	2	212	217
3	0	4	193	184
3	0	6	59	60
3	0	8	56	-52
3	0	10	130	-129
3	0	12	100	-103
3	0	14	95	-90
3	0	16	61	-63

H	K	L	F(O)	F(C)
3	0	18	13	-10
3	0	20	44	45
3	0	22	67	67
3	0	24	54	51
3	0	26	12	14
4	0	-30	33	-31
4	0	-28	-8	-1
4	0	-26	84	81
4	0	-24	63	61
4	0	-22	23	24
4	0	-20	29	28
4	0	-18	58	-59
4	0	-16	28	-29
4	0	-14	16	-15
4	0	-12	149	-156
4	0	-10	84	-87
4	0	-8	-9	19
4	0	-6	62	61
4	0	-4	250	270
4	0	-2	226	233
4	0	0	-10	18
4	0	2	15	-13
4	0	4	140	-138
4	0	6	119	-121
4	0	8	10	-12
4	0	10	22	-21
4	0	12	-8	-18
4	0	14	42	44
4	0	16	50	48
4	0	18	66	64
4	0	20	48	47
4	0	22	10	-8
4	0	24	35	-36
5	0	-30	60	56
5	0	-28	-8	2
5	0	-26	51	50
5	0	-24	-7	-1
5	0	-22	97	-96
5	0	-20	25	-24
5	0	-18	126	-130
5	0	-16	125	-127
5	0	-14	98	100
5	0	-12	35	36
5	0	-10	122	123
5	0	-8	191	197
5	0	-6	75	-76
5	0	-4	22	19
5	0	-2	15	-9
5	0	0	202	-208
5	0	2	82	-80
5	0	4	81	-80
5	0	6	86	-84
5	0	8	161	161
5	0	10	123	123
5	0	12	74	74
5	0	14	76	74
5	0	16	47	-45
5	0	18	50	-50
5	0	20	12	-11
6	0	-30	32	30
6	0	-28	55	-51
6	0	-26	29	-27
6	0	-24	23	-24
6	0	-22	151	-150
6	0	-20	24	24
6	0	-18	118	121
6	0	-16	60	59
6	0	-14	221	230
6	0	-12	23	21
6	0	-10	165	-168
6	0	-8	20	20
6	0	-6	170	-174
6	0	-4	167	-171
6	0	-2	44	47
6	0	0	153	-157
6	0	2	32	34
6	0	4	192	193
6	0	6	42	40
6	0	8	123	123
6	0	10	33	34
6	0	12	141	-139
6	0	14	42	-41
6	0	16	96	-55
6	0	18	55	-55
6	0	20	38	38
7	0	-30	16	-14
7	0	-26	-8	-2
7	0	-22	95	94
7	0	-20	34	34
7	0	-20	53	54
7	0	-18	75	75
7	0	-16	65	-67
7	0	-14	24	15
7	0	-12	15	-16
7	0	-10	203	-208

H	K	L	F(O)	F(C)
7	0	-8	33	-32
7	0	-6	7	1
7	0	-4	41	40
7	0	-2	240	244
7	0	0	62	56
7	0	2	51	-53
7	0	4	45	46
7	0	6	89	-89
7	0	8	46	-46
7	0	10	-7	0
7	0	12	114	-112
7	0	14	16	-16
7	0	16	43	42
7	0	18	19	20
8	0	-30	35	33
8	0	-28	63	62
8	0	-26	46	47
8	0	-24	27	26
8	0	-22	35	-34
8	0	-20	51	-53
8	0	-18	9	-7
8	0	-16	67	-70
8	0	-14	92	-93
8	0	-12	33	-32
8	0	-10	9	4
8	0	-8	151	155
8	0	-6	210	217
8	0	-4	52	51
8	0	-2	-7	-6
8	0	0	82	-79
8	0	2	128	-131
8	0	4	32	-31
8	0	6	29	-31
8	0	8	22	-26
8	0	10	51	51
8	0	12	44	44
8	0	14	47	48
8	0	16	54	54
9	0	-28	14	8
9	0	-26	23	-22
9	0	-24	54	-55
9	0	-22	82	-80
9	0	-20	72	-71
9	0	-18	-9	-6
9	0	-16	64	64
9	0	-14	91	91
9	0	-12	87	88
9	0	-10	23	22
9	0	-8	19	-17
9	0	-6	10	-13
9	0	-4	57	-56
9	0	-2	91	-92
9	0	0	88	-90
9	0	2	54	-52
9	0	4	45	44
9	0	6	111	112
9	0	8	82	82
9	0	10	34	35
9	0	12	10	-11
9	0	14	31	-29
10	0	-28	15	-16
10	0	-26	47	-45
10	0	-24	26	-27
10	0	-22	42	40
10	0	-20	63	66
10	0	-18	95	94
10	0	-16	47	49
10	0	-14	58	-58
10	0	-12	60	-60
10	0	-10	48	-48
10	0	-8	54	-54
10	0	-6	23	-22
10	0	-4	35	-36
10	0	-2	72	71
10	0	0	72	77
10	0	2	74	77
10	0	4	50	49
10	0	6	10	8
10	0	8	38	-39
10	0	10	50	-50
10	0	12	35	-32
11	0	-26	38	38
11	0	-24	15	17
11	0	-22	69	66
11	0	-20	-8	-2
11	0	-18	23	-22
11	0	-16	-8	-3
11	0	-14	113	-112
11	0	-12	74	-73
11	0	-10	-8	5
11	0	-8	1	1
11	0	-6	116	117
11	0	-4	111	107
11	0	-2	-8	4
11	0	0	12	12
11	0	2	36	-35
11	0	4	62	-59

H	K	L	F(O)	F(C)
11	0	6	13	-14
11	0	8	47	-48
12	0	-24	60	-58
12	0	-22	-9	-1
12	0	-20	35	-37
12	0	-18	85	-82
12	0	-16	21	20
12	0	-14	9	-6
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1	1	4	-9	75
1	1	5	41	-39
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Table 4. Continued.

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0	2	15	-7	-2
0	2	16	11	11
0	2	17	12	14
0	2	18	60	-61
0	2	19	51	52
0	2	20	81	-83
0	2	21	-9	6
0	2	22	65	-65
0	2	23	17	-19
0	2	24	23	-23
0	2	25	11	-12
0	2	26	28	30
0	2	27	20	-19
0	2	28	40	40
1	2	-29	-9	6
1	2	-28	19	-19
1	2	-27	18	18
1	2	-26	45	-45
1	2	-25	-9	-9
1	2	-24	61	-61
1	2	-23	31	-30
1	2	-22	9	3
1	2	-21	7	-7
1	2	-20	29	28
1	2	-19	27	-27
1	2	-18	65	63
1	2	-17	17	-18
1	2	-16	118	119
1	2	-15	32	33
1	2	-14	51	49
1	2	-13	15	15
1	2	-12	39	38
1	2	-11	32	-30
1	2	-10	17	14
1	2	-9	68	67
1	2	-8	109	-113
1	2	-7	33	-32
1	2	-6	109	-112
1	2	-5	32	-32
1	2	-4	94	-97
1	2	-3	30	-28
1	2	-2	104	-104
1	2	-1	79	-82
1	2	0	86	82
1	2	1	52	-50
1	2	2	104	104
1	2	3	32	-30
1	2	4	107	106

Table 4. Continued.

H	K	L	F(O)	F(C)
1	2	5	32	-34
1	2	6	132	133
1	2	7	58	60
1	2	8	24	25
1	2	9	75	72
1	2	10	43	-43
1	2	11	17	16
1	2	12	76	-74
1	2	13	21	22
1	2	14	116	-119
1	2	15	14	-16
1	2	16	67	-66
1	2	17	40	-41
1	2	18	13	-14
1	2	19	-7	-3
1	2	20	9	8
1	2	21	-8	-7
1	2	22	35	36
1	2	23	14	-15
1	2	24	31	31
1	2	25	-9	6
1	2	26	25	27
1	2	27	-9	0
2	2	-29	24	-23
2	2	-28	-8	1
2	2	-27	-8	2
2	2	-26	24	24
2	2	-25	21	18
2	2	-24	12	-11
2	2	-23	34	-31
2	2	-22	68	68
2	2	-21	-8	3
2	2	-20	75	75
2	2	-19	15	16
2	2	-18	19	15
2	2	-17	-7	2
2	2	-16	41	42
2	2	-15	100	101
2	2	-14	106	-107
2	2	-13	35	35
2	2	-12	174	-179
2	2	-11	64	-65
2	2	-10	39	-34
2	2	-9	-6	0
2	2	-8	62	-65
2	2	-7	77	-78
2	2	-6	80	78
2	2	-5	70	-69
2	2	-4	174	179
2	2	-3	64	66
2	2	-2	56	51
2	2	-1	43	-43
2	2	0	149	149
2	2	1	15	11
2	2	2	136	135
2	2	3	113	113
2	2	4	42	-44
2	2	5	-6	0
2	2	6	37	-35
2	2	7	33	33
2	2	8	145	-145
2	2	9	23	23
2	2	10	157	-156
2	2	11	86	-88
2	2	12	21	19
2	2	13	34	-33
2	2	14	32	31
2	2	15	-7	-6
2	2	16	60	60
2	2	17	25	-25
2	2	18	79	81
2	2	19	27	27
2	2	20	13	11
2	2	21	9	9
2	2	22	13	13
2	2	23	17	-15
2	2	24	12	10
2	2	25	13	16
2	2	26	30	-30
3	2	-29	-8	-2
3	2	-28	28	28
3	2	-27	-8	-1
3	2	-26	69	69
3	2	-25	33	32
3	2	-24	11	-12
3	2	-23	12	-11
3	2	-22	-7	-7
3	2	-21	-7	2
3	2	-20	18	-16
3	2	-19	29	27
3	2	-18	157	-158
3	2	-17	52	-51
3	2	-16	64	-63
3	2	-15	-6	1
3	2	-14	38	-37
3	2	-13	31	29
3	2	-12	68	-70
3	2	-11	57	-58
3	2	-10	168	171
3	2	-9	28	26
3	2	-8	127	130
3	2	-7	7	2
3	2	-6	50	47
3	2	-5	38	-37
3	2	-4	175	180
3	2	-3	116	117

H	K	L	F(O)	F(C)
3	2	-2	84	-85
3	2	-1	33	32
3	2	0	151	-150
3	2	1	54	-52
3	2	2	52	-50
3	2	3	31	33
3	2	4	212	-210
3	2	5	37	-37
3	2	6	34	-33
3	2	7	8	-7
3	2	8	89	88
3	2	9	54	54
3	2	10	13	10
3	2	11	56	-56
3	2	12	126	125
3	2	13	24	-23
3	2	14	98	98
3	2	15	25	25
3	2	16	-8	2
3	2	17	8	-6
3	2	18	40	40
3	2	19	36	37
3	2	20	44	-45
3	2	21	21	22
3	2	22	74	-75
3	2	23	23	-24
3	2	24	17	-17
3	2	25	-9	-4
4	2	-30	30	29
4	2	-29	23	21
4	2	-28	21	-19
4	2	-27	14	17
4	2	-26	27	-25
4	2	-25	30	30
4	2	-24	74	-74
4	2	-23	33	-32
4	2	-22	64	-64
4	2	-21	60	-60
4	2	-20	25	27
4	2	-19	-7	-2
4	2	-18	-7	-1
4	2	-17	26	-27
4	2	-16	46	46
4	2	-15	-6	0
4	2	-14	112	114
4	2	-13	34	35
4	2	-12	19	19
4	2	-11	52	-53
4	2	-10	80	81
4	2	-9	28	28
4	2	-8	21	20
4	2	-7	114	116
4	2	-6	164	-168
4	2	-5	8	3
4	2	-4	86	-87
4	2	-3	12	10
4	2	-2	132	-135
4	2	-1	44	-42
4	2	0	117	-116
4	2	1	123	-124
4	2	2	93	92
4	2	3	18	17
4	2	4	42	41
4	2	5	13	14
4	2	6	45	48
4	2	7	36	-36
4	2	8	126	125
4	2	9	37	39
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4	2	11	13	12
4	2	12	-9	9
4	2	13	14	15
4	2	14	-8	-1
4	2	15	61	63
4	2	16	102	-101
4	2	17	-9	-3
4	2	18	44	-44
4	2	19	21	-21
4	2	20	16	-17
4	2	21	-9	-10
4	2	22	18	-15
4	2	23	30	-30
5	2	-30	29	-28
5	2	-29	-9	2
5	2	-28	41	-40
5	2	-27	17	-16
5	2	-26	21	-21
5	2	-25	-8	-7
5	2	-24	16	13
5	2	-23	24	-25
5	2	-22	30	28
5	2	-21	22	-22
5	2	-20	85	86
5	2	-19	28	27
5	2	-18	91	92
5	2	-17	21	22
5	2	-16	44	44
5	2	-15	23	23
5	2	-14	18	16
5	2	-13	48	47
5	2	-12	92	-93
5	2	-11	12	-11
5	2	-10	125	-127
5	2	-9	28	-28
5	2	-8	61	-58
5	2	-7	8	-5

H	K	L	F(O)	F(C)
5	2	-6	59	-60
5	2	-5	46	-48
5	2	-4	18	17
5	2	-3	27	-28
5	2	-2	88	90
5	2	-1	7	-4
5	2	0	60	59
5	2	1	47	-44
5	2	2	134	133
5	2	3	11	6
5	2	4	83	82
5	2	5	59	58
5	2	6	27	-26
5	2	7	24	22
5	2	8	54	-56
5	2	9	23	24
5	2	10	114	-113
5	2	11	10	-6
5	2	12	94	-94
5	2	13	42	-43
5	2	14	-8	-4
5	2	15	-8	-3
5	2	16	-8	4
5	2	17	-8	4
5	2	18	28	30
5	2	19	9	-10
5	2	20	41	39
5	2	21	-9	0
5	2	22	12	14
6	2	-30	10	6
6	2	-29	15	13
6	2	-28	18	17
6	2	-27	-8	-6
6	2	-26	26	24
6	2	-25	-8	0
6	2	-24	52	52
6	2	-23	-8	-1
6	2	-22	54	53
6	2	-21	-7	-1
6	2	-20	13	13
6	2	-19	45	44
6	2	-18	49	-48
6	2	-17	33	33
6	2	-16	111	-114
6	2	-15	21	-19
6	2	-14	105	-107
6	2	-13	24	-24
6	2	-12	42	-43
6	2	-11	35	-35
6	2	-10	23	24
6	2	-9	20	-22
6	2	-8	94	93
6	2	-7	35	35
6	2	-6	104	103
6	2	-5	14	12
6	2	-4	108	108
6	2	-3	28	-25
6	2	-2	83	83
6	2	-1	21	22
6	2	0	17	17
6	2	1	33	32
6	2	2	50	-49
6	2	3	21	21
6	2	4	96	-96
6	2	5	20	17
6	2	6	108	-107
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6	2	9	48	-48
6	2	10	13	10
6	2	11	-8	-1
6	2	12	50	52
6	2	13	-8	0
6	2	14	65	64
6	2	15	-8	0
6	2	16	39	39
6	2	17	14	11
6	2	18	21	22
6	2	19	-9	-5
6	2	20	-9	1
7	2	-29	22	22
7	2	-28	20	21
7	2	-27	11	11
7	2	-26	20	-17
7	2	-25	-8	3
7	2	-24	30	-30
7	2	-23	19	18
7	2	-22	65	-64
7	2	-21	13	-13
7	2	-20	58	-58
7	2	-19	9	-10
7	2	-18	16	-14
7	2	-17	-7	-1
7	2	-16	19	-20
7	2	-15	50	-52
7	2	-14	24	24
7	2	-13	26	-28
7	2	-12	74	74
7	2	-11	13	12
7	2	-10	10	78
7	2	-9	-7	2
7	2	-8	89	88
7	2	-7	56	56
7	2	-6	12	9
7	2	-5	44	44
7	2	-4	101	-102

H	K	L	F(O)	F(C)
7	2	-3	12	8
7	2	-2	106	-103
7	2	-1	11	9
7	2	0	85	-85
7	2	1	18	-18
7	2	2	23	-21
7	2	3	48	-50
7	2	4	31	32
7	2	5	-7	-4
7	2	6	29	28
7	2	7	-8	-4
7	2	8	43	43
7	2	9	24	-24
7	2	10	57	56
7	2	11	-8	8
7	2	12	48	48
7	2	13	16	15
7	2	14	23	23
7	2	15	17	19
7	2	16	20	-22
7	2	17	31	31
7	2	18	46	-47
8	2	-29	17	13
8	2	-28	44	-43
8	2	-27	-8	-4
8	2	-26	74	-72
8	2	-25	48	-46
8	2	-24	-8	4
8	2	-23	-8	-4
8	2	-22	17	16
8	2	-21	-7	-2
8	2	-20	15	16
8	2	-19	22	-22
8	2	-18	80	80
8	2	-17	32	32
8	2	-16	30	31
8	2	-15	-7	-3
8	2	-14	42	43
8	2	-13	11	-10
8	2	-12	68	68
8	2	-11	55	55
8	2	-10	77	-77
8	2	-9	11	-4
8	2	-8	100	-99
8	2	-7	17	-13
8	2	-6	89	-94
8	2	-5	18	17
8	2	-4	107	-106
8	2	-3	53	-55
8	2	-2	33	33
8	2	-1	21	-19
8	2	0	67	66
8	2	1	23	22
8	2	2	36	37
8	2	3	24	-25
8	2	4	83	82
8	2	5	9	11
8	2	6	32	31
8	2	7	18	20
8	2	8	9	-4
8	2	9	-8	-6
8	2	10	-8	-8
8	2	11	27	29
8	2	12	60	-62
8	2	13	19	16
8	2	14	53	-54
8	2	15	15	-15
8	2	16	18	-20
9	2	-28	16	13
9	2	-27	10	-9
9	2	-26	11	-9
9	2	-25	30	-30
9	2	-24	60	60
9	2	-23	-8	-3
9	2	-22	84	83
9	2	-21	32	30
9	2	-20	14	13
9	2	-19	-7	1
9	2	-18	38	40
9	2	-17	40	41
9	2	-16	46	-46
9	2	-15	15	14
9	2	-14	114	-117
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9	2	-12	18	-17
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9	2	-9	14	-12
9	2	-8	21	-21
9	2	-7	33	-35
9	2	-6	78	79
9	2	-5	25	25
9	2	-4	15	12
9	2	-3	28	-27
9	2	-2	74	74
9	2	-1	26	-22
9	2	0	109	109
9	2	1	47	48
9	2	2	18	-16
9	2	3	10	10
9	2	4	19	-21
9	2	5	17	17
9	2	6	65	-65
9	2	7	22	18
9	2	8	98	-100
9	2	9	43	-42

H	K	L	F(O)	F(C)
9	2	10	10	-6
9	2	11	16	-16
9	2	12	-9	9
9	2	13	-9	5
10	2	-26	17	19
10	2	-25	-8	2
10	2	-24	10	12
10	2	-23	19	19
10	2	-22	-8	4
10	2	-21	41	41
10	2	-20	85	-85
10	2	-19	13	-9
10	2	-18	65	-64
10	2	-17	14	-14
10	2	-16	15	-17
10	2	-15	9	-6
10	2	-14	25	-25
10	2	-13	46	-47
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10	2	-11	11	-10
10	2	-10	66	65
10	2	-8	17	17
10	2	-6	85	83
10	2	-5	40	40
10	2	-4	13	14
10	2	-3	32	33
10	2	-2	41	-39
10	2	-1	-8	-3
10	2	0	19	-22
10	2	1	24	24
10	2	2	89	-89
10	2	3	15	-11
10	2	4	45	-46
10	2	5	32	-33
10	2	6	30	29
10	2	7	-9	-6
10	2	8	-9	6
10	2	9	21	-21
10	2	10	44	43
11	2	-24	43	-44
11	2	-23	18	-19
11	2	-22	20	-19
11	2	-21	-8	7
11	2	-20	16	-15
11	2	-19	-8	0
11	2	-18	-8	2
11	2	-17	13	-10
11	2	-16	50	51
11	2	-15	9	-8
11	2	-14	51	51
11	2	-13	16	-14
11	2	-12	59	58
11	2	-11	20	20
11	2	-10	33	34
11	2	-9	50	50
11	2	-8	49	-51
11	2	-7	11	12
11	2	-6	66	-67
11	2	-5	15	-13
11	2	-4	65	-64
11	2	-3	18	-17
11	2	-2	52	-50
11	2	-1	23	-22
11	2	0	20	19
11	2	1	11	7
11	2	2	25	24
11	2	3	14	13
11	2	4	24	24
11	2	5	14	-15
11	2	6	49	48
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12	2	-18	33	33
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12	2	-10	57	-58
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12	2	-8	44	-45
12	2	-7	18	-16
12	2	-6	11	-11
12	2	-5	20	-21
12	2	-4	24	22
12	2	-3	-8	-4
12	2	-2	37	37
12	2	-1	-9	-2
12	2	0	42	43
12	2	1	-9	0
12	2	2	33	34
13	2	-15	18	-20
13	2	-13	-9	-14
13	2	-12	-9	-6
13	2	-11	9	-8
13	2	-10	21	18
13	2	-9	-9	2
13	2	-8	26	25
13	2	-7	9	-11
13	2	-6	34	33

Table 4. Continued.

H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)
0	3	1	38	-36	2	3	0	65	-61	4	3	1	54	-53	6	3	9	20	-20	9	3-13		35	-34	0	4	0	93	91
0	3	2	40	-36	2	3	1	12	-7	4	3	2	99	94	6	3	10	22	22	9	3-12		-8	6	0	4	1	77	74
0	3	3	39	-40	2	3	2	176	-172	4	3	3	42	-39	6	3	11	13	-9	9	3-11		65	-67	0	4	2	52	50
0	3	4	134	134	2	3	3	20	-16	4	3	4	73	71	6	3	12	56	58	9	3-10		37	36	0	4	3	67	65
0	3	5	31	-28	2	3	4	115	-112	4	3	5	61	59	6	3	13	9	7	9	3	-9	11	-8	0	4	4	32	32
0	3	6	90	86	2	3	5	57	-57	4	3	6	54	55	6	3	14	33	34	9	3	-8	79	79	0	4	5	28	27
0	3	7	24	24	2	3	6	19	-19	4	3	7	40	41	6	3	15	30	32	9	3	-7	11	-6	0	4	6	-7	2
0	3	8	73	70	2	3	7	61	-61	4	3	8	27	-26	6	3	16	37	-37	9	3	-6	61	63	0	4	7	44	45
0	3	9	67	65	2	3	8	16	-14	4	3	9	52	52	6	3	17	31	31	9	3	-5	43	41	0	4	8	66	-62
0	3	10	91	90	2	3	9	17	15	4	3	10	84	-84	6	3	18	25	-26	9	3	-4	19	15	0	4	9	48	-49
0	3	11	87	88	2	3	10	43	44	4	3	11	19	18	7	3-27		13	10	9	3	-3	69	69	0	4	10	50	-52
0	3	12	85	-85	2	3	11	17	-17	4	3	12	62	-62	7	3-26		18	-19	9	3	-2	23	-21	0	4	11	28	-28
0	3	13	56	59	2	3	12	67	66	4	3	13	52	-52	7	3-25		-8	-4	9	3	-1	-8	-2	0	4	12	45	-46
0	3	14	101	-103	2	3	13	24	-24	4	3	14	38	-42	7	3-24		43	-43	9	3	0	60	-60					
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1	3	8	158	-158	3	3	8	92	89	5	3	13	30	-37	8	3-19		34	34	11	3-15		31	33					
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2	3-15		41	-41	4	3-14		19	-20	6	3	-5	93	92	8	3	11	26	-24	12	3	-5	11	-3					
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2	3-13		32	32	4	3-12		68	-69	6	3	-3	57	57	8	3	13	-9	-10										
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2	3	-8	76	76	4	3	-7	36	-35	6	3	2	-7	-5	9	3-21		13	10										
2	3	-7	23	-21	4	3	-6	36	-35	6	3	3	50	-48	9	3-20		32	-32										
2	3	-6	171	173	4	3	-5	14	14	6	3	4	33	-30	9	3-19		15	12										
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2	3	-4	111	108	4	3	-3	10	-7	6	3	6	18	17	9	3-17		20	-19										
2	3	-3	70	71	4	3	-2	-6	-4	6	3	7	14	-15	9	3-16		54	-54										
2	3	-2	9	6	4	3	-1	32	31	6	3	8	78	80	9	3-15		10	10										
2	3	-1	104	106	4	3	0	74	74						9	3-14		24	-25										

Table 4. Continued.

H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)
0	4	13	27	28	3	4	-23	27	-27	5	4	-7	67	68	8	4	-17	20	17	1	5	-14	17	18	3	5	-20	14	14
0	4	14	34	-33	3	4	-22	-8	-3	5	4	-6	24	24	8	4	-16	37	-39	1	5	-13	11	-11	3	5	-19	11	-16
0	4	15	34	-34	3	4	-21	15	-16	5	4	-5	14	17	8	4	-15	-8	2	1	5	-12	50	50	3	5	-18	12	10
0	4	16	24	25	3	4	-20	39	40	5	4	-4	12	-10	8	4	-14	31	-34	1	5	-11	11	9	3	5	-17	32	32
0	4	17	25	-23	3	4	-19	-8	3	5	4	-3	22	22	8	4	-13	24	-23	1	5	-10	31	31	3	5	-16	-9	-2
0	4	18	30	33	3	4	-18	59	58	5	4	-2	48	-47	8	4	-12	-8	4	1	5	-9	21	21	3	5	-15	31	31
0	4	19	16	-18	3	4	-17	-8	4	5	4	-1	56	57	8	4	-11	27	-28	1	5	-8	28	28	3	5	-14	54	-53
0	4	20	34	37	3	4	-16	37	37	5	4	0	68	-67	8	4	-10	31	31	1	5	-7	44	42	3	5	-13	13	-10
0	4	21	31	-34	3	4	-15	32	32	5	4	1	-8	-5	8	4	-9	46	-47	1	5	-6	19	19	3	5	-12	45	-47
0	4	22	39	39	3	4	-14	29	29	5	4	2	50	-49	8	4	-8	45	49	1	5	-5	44	43	3	5	-11	29	-29
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1	4	-21	41	42	3	4	-9	25	24	5	4	7	74	-75	8	4	-3	39	40	1	5	0	41	-40	3	5	-6	43	40
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1	4	-17	10	-8	3	4	-5	50	-49	5	4	11	17	18	8	4	1	17	13	1	5	4	12	10	3	5	-2	35	38
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1	4	-7	40	-40	3	4	5	28	27	6	4	-21	50	-49	9	4	-20	25	-25	1	5	14	-9	-5	3	5	8	57	-57
1	4	-6	83	64	3	4	6	33	32	6	4	-20	-8	-2	9	4	-19	40	-39	1	5	15	22	23	3	5	9	17	-16
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1	4	-4	76	76	3	4	8	22	-22	6	4	-18	31	31	9	4	-17	28	-30	1	5	17	19	19	3	5	11	50	-50
1	4	-3	82	84	3	4	9	21	18	6	4	-17	10	-11	9	4	-16	22	22	1	5	18	29	-33	3	5	12	-9	7
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1	4	1	70	70	3	4	13	10	10	6	4	-13	72	72	9	4	-12	42	41	2	5	-17	20	27					
1	4	2	68	-66	3	4	14	54	-55	6	4	-12	36	36	9	4	-11	36	35	2	5	-16	44	44					
1	4	3	54	52	3	4	15	9	8	6	4	-11	52	55	9	4	-10	35	35	2	5	-15	24	23					
1	4	4	66	-86	3	4	16	15	-15	6	4	-10	15	-14	9	4	-9	21	21	2	5	-14	16	16					
1	4	5	33	-31	3	4	17	32	-30	6	4	-9	32	-32	9	4	-8	-8	3	2	5	-13	10	11					
1	4	6	48	-48	3	4	18	-9	9	6	4	-8	30	-30	9	4	-7	-8	4	2	5	-12	16	11					
1	4	7	-8	-4	3	4	19	31	-31	6	4	-7	-8	2	9	4	-6	31	-31	2	5	-11	28	28					
1	4	8	31	-31	3	4	20	13	15	6	4	-6	-8	-68	9	4	-5	20	19	2	5	-10	36	-36					
1	4	9	57	-57	4	4	-25	-9	3	6	4	-5	16	-14	9	4	-4	45	-45	2	5	-9	32	31					
1	4	10	25	23	4	4	-24	44	43	6	4	-4	67	-67	9	4	-3	17	17	2	5	-8	62	-60					
1	4	11	77	-76	4	4	-23	26	26	6	4	-3	16	-15	9	4	-2	42	-41	2	5	-7	21	21					
1	4	12	60	61	4	4	-22	32	34	6	4	-2	30	-30	9	4	-1	-9	2	2	5	-6	24	-26					
1	4	13	11	10	4	4	-21	33	34	6	4	-1	33	31	9	4	0	29	-30	2	5	-5	-8	-3					
1	4	14	45	48	4	4	-20	24	26	6	4	0	15	-14	9	4	1	-9	2	2	5	-4	53	-52					
1	4	15	-8	7	4	4	-19	40	40	6	4	1	50	-50	9	4	2	-9	-1	2	5	-3	-9	-5					
1	4	16	52	52	4	4	-18	-8	-5	6	4	2	45	42	9	4	3	41	-42	2	5	-2	9	-5					
1	4	17	20	21	4	4	-17	-8	-6	6	4	3	59	-61	9	4	4	26	25	2	5	-1	64	-62					
1	4	18	18	19	4	4	-16	50	-50	6	4	4	63	62	9	4	5	33	-33	2	5	0	34	31					
1	4	19	46	47	4	4	-15	-8	1	6	4	5	11	11	9	4	6	29	30	2	5	1	20	-18					
1	4	20	20	-19	4	4	-14	54	-55	6	4	6	36	37	10	4	-18	30	31	2	5	2	20	20					
1	4	21	-9	0	4	4	-13	40	42	6	4	7	-8	2	10	4	-17	23	26	2	5	3	19	18					
1	4	22	17	-18	4	4	-12	50	-51	6	4	8	28	26	10	4	-16	27	28	2	5	4	40	40					
2	4	-24	22	-24	4	4	-11	-7	-1	6	4	9	48	49	10	4	-15	43	43	2	5	5	34	32					
2	4	-23	-9	2	4	4	-10	33	-33	6	4	10	16	-11	10	4	-14	12	11	2	5	6	52	52					
2	4	-22	42	-41	4	4	-9	39	-40	6	4	11	48	50	10	4	-13	12	13	2	5	7	36	36					
2	4	-21	16	16	4	4	-8	15	15	6	4	12	29	-31	10	4	-12	20	-20	2	5	8	-9	1					
2	4	-20	25	-24	4	4	-7	76	-78	6	4	13	11	-12	10	4	-11	-9	-8	2	5	9	21	20					
2	4	-19	16	-17	4	4	-6	58	57	6	4	14	18	-21	10	4	-10	41	-41	2	5	10	14	-14					
2	4	-18	27	-29	4	4	-5	92	-92	6	4	15	-9	0	10	4	-9	-9	2	2	5	11	14	15					
2	4	-17	69	-71	4	4	-4	76	76	7	4	-23	-9	6	10	4	-8	46	-47	2	5	12	37	-39					
2	4	-16	-8	1	4	4	-3	23	22	7	4	-22	38	38	10	4	-7	19	-18	2	5	13	27	25					
2	4	-15	54	-56	4	4	-2	67	67	7	4	-21	-8	-1	10	4	-6	39	-40	2	5	14	48	-48					
2	4	-14	51	51	4	4	-1	101	99	7	4	-20	34	36	10	4	-5	13	-12	2	5	15	-9	2					
2	4	-13	24	-24	4	4	0	42	40	7	4	-19	11	9	10	4	-4	12	-10	2	5	16	-9	-8					
2	4	-12	58	57	4	4	1	71	72	7	4	-18	39	39	10	4	-3	22	-23	2	5	17	25	-25					
2	4	-11	34	34	4	4	2	-8	-5	7	4	-17	45	45	10	4	-2	26	26										
2	4	-10	63	64	4	4	3	43	43	7	4	-16	-8	-3	10	4	-1	35	-35										
2	4	-9	94	92	4	4	4	43	-43	7	4	-15	15	16	10	4	0	37	37										
2	4	-8	38	39	4	4	5	15	-14	7	4	-14	30	-31	10	4	1	9	-8										
2	4	-7	33	33	4	4	6	47	-48	7	4	-13	26	25	10	4	2	36	37										
2	4	-6	29	-25	4	4	7	38	-39	7	4	-12	42	-40	11	4	-11	33	-34										
2	4	-5	14	-15	4	4	8	61	-61	7	4	-11	27	28	11	4	-10	-9	-6										
2	4	-4	64	-44	4	4	9	10	-1	7	4	-10	62	-61	11	4	-9	32	-33										
2	4	-3	7	3	4	4	10	35	-36	7	4	-9	48	-48	11	4	-8	14	14										
2	4	-2	94	-95	4	4	11	16	-17	7	4	-8	29	-29	11	4	-7	40	-40										
2	4	-1	12	-10	4	4	12	15	15	7	4	-7	46	-47	11	4	-6	32	30										
2	4	0	86	-85	4	4	13	39	-39	7	4	-6	-8	-1	0	5	1	32	30										
2	4	1	9	7	4	4	14	28	30	7	4	-5	48	-47	0	5	2	61	-62										
2	4	2	40	-38	4	4	15	22	-24	7	4	-4	26	24	0	5	3	39	36										
2	4	3	-8	-5	4	4	16	44	45	7	4	-3	61	-61	0	5	4	59	-60										
2	4	4	17	19	4	4	17	16	-17	7	4	-2	71	69	0	5	5	12	9										
2	4	5	83	-81	4	4	18	39	41	7	4	-1	27	24	0	5	6	58	-59										
2	4	6	67	66	5	4	-25	26	25	7	4	0	54	55	0	5	7	19	-18										
2	4	7	55	-54	5	4	-24	-9	2	7	4	1	40	40	0	5	8	26	-23										
2	4	8	64	62	5	4	-23	31	31	7	4	2	32	31	0	5	9	58	-58										
2	4	9	11	7	5	4	-22	32	-33	7	4	3	14	15	0	5	10	19	19										
2	4	10	48	49	5	4	-21	12	-11	7	4	4	-9	6	0	5	11	67	-68										
2	4	11	31	32	5	4	-20	39	-39	7	4	5	41	39	0	5	12	18	16										
2	4	12	20	19	5	4	-19	9	8	7	4	6	42	-42	0	5	13	20	-22										
2	4	13	72	75	5	4	-18	44	-45	7	4	7	9	3	0	5	14	34	34										
2	4	14	24	-25	5	4	-17	25	-24	7	4	8	39	-41	0	5	15	-9	6										
2	4	15	42	43	5	4	-16	43	-43	7	4	9	-9	-5	0	5	16	37	37										
2	4	16	29	-29	5	4	-15	63	-63	7	4	10	35	-36	0	5	17	28	28										
2	4	17	10	-9	5	4	-14	-8	4	7	4	11	17	17	0	5	18	14	11										
2	4	18	31	-34	5	4	-13	8	-7	7	4	12	33	-33	0	5	19	31	32										
2	4	19	-9	-2	5	4	-12	37	37	8	4	-22	-9	7	1	5	-20	36	-38										
2	4	20	32	-35	5	4	-11	18	-17	8	4	-21	-8	6	1	5	-19	15	-12										
2	4	21	10	-12	5	4	-10	17	64	8	4	-20	29	-29	1	5	-18	12	-12										
3	4	-25	-9	-7	5	4	-9	9	1	8	4	-19	8	-6	1	5	-17	21	-21										
3	4	-24	-9	-9	5	4	-8	71	72	8	4	-18	40	-39	1	5	-16	-9	-2										
															1	5	-15	33	-34										

Table 4. Continued.

H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)
3	5	15	-9	-13	5	5	-4	29	-29	7	5	-12	24	-23	0	6	10	36	37	3	6	-13	22	-21
4	5	-20	23	-22	5	5	-3	22	-22	7	5	-11	35	-35	0	6	11	-10	10	3	6	-12	-9	4
4	5	-19	17	16	5	5	-2	46	-45	7	5	-10	-9	7	0	6	12	15	19	3	6	-11	32	-32
4	5	-18	31	-31	5	5	-1	43	-45	7	5	-9	14	-15	1	6	-13	25	21	3	6	-10	16	13
4	5	-17	13	-11	5	5	0	12	-13	7	5	-8	36	36	1	6	-12	15	15	3	6	-9	-9	-8
4	5	-16	10	-8	5	5	1	47	-47	7	5	-7	-8	-2	1	6	-11	29	29	3	6	-8	21	22
4	5	-15	41	-41	5	5	2	29	29	7	5	-5	-9	9	1	6	-10	-9	-6	3	6	-7	-9	10
4	5	-14	18	-17	5	5	3	21	-21	7	5	-4	34	34	1	6	-9	34	33	3	6	-6	21	21
4	5	-13	59	-60	5	5	4	27	29	7	5	-3	14	14	1	6	-8	21	-24	3	6	-5	21	21
4	5	-12	-8	6	5	5	5	-9	3	7	5	-2	-9	6	1	6	-7	9	6	3	6	-4	14	10
4	5	-11	26	-25	5	5	6	49	49	7	5	-1	27	26	1	6	-6	41	-41	3	6	-3	54	53
4	5	-10	49	49	5	5	7	9	4	7	5	0	26	-25	1	6	-5	21	-18	3	6	-2	-9	0
4	5	-9	22	21	5	5	8	34	35	7	5	1	36	34	1	6	-4	32	-32	3	6	-1	39	41
4	5	-8	33	35	5	5	9	16	15	7	5	2	21	-22	1	6	-3	35	-34	3	6	0	16	-10
4	5	-7	26	26	5	5	10	-10	-4	7	5	3	18	18	1	6	-2	-9	-7	3	6	1	15	13
4	5	-6	42	43	5	5	11	19	19	7	5	4	29	-29	1	6	-1	46	-46	3	6	2	30	-30
4	5	-5	22	20	5	5	12	-9	-9	7	5	5	-9	0	1	6	0	12	10	3	6	3	-10	-2
4	5	-4	24	25	6	5	-19	16	17	7	5	6	25	-25	1	6	1	31	-30	3	6	4	24	-24
4	5	-3	17	18	6	5	-18	26	27	8	5	-15	31	-31	1	6	2	29	28	3	6	5	35	-33
4	5	-2	40	-39	6	5	-17	14	16	8	5	-14	28	28	1	6	3	19	-17	3	6	6	11	-10
4	5	-1	16	14	6	5	-16	14	10	8	5	-13	-9	2	1	6	4	37	38	3	6	7	28	-27
4	5	0	38	-40	6	5	-15	22	22	8	5	-12	31	32	1	6	5	-9	-4	3	6	8	-10	-4
4	5	1	21	21	6	5	-14	14	-14	8	5	-11	12	15	1	6	6	18	21	4	6	-12	34	35
4	5	2	44	-44	6	5	-13	21	20	8	5	-10	35	35	1	6	7	26	24	4	6	-11	-9	2
4	5	3	-9	4	6	5	-12	46	-49	8	5	-9	21	20	1	6	8	-9	7	4	6	-10	-9	11
4	5	4	44	-41	6	5	-11	28	28	8	5	-8	29	30	1	6	9	34	33	4	6	-9	30	28
4	5	5	45	-45	6	5	-10	39	-39	8	5	-7	29	27	1	6	10	-9	-4	4	6	-8	12	-8
4	5	6	17	15	6	5	-9	-8	2	8	5	-6	18	-15	1	6	11	30	31	4	6	5	50	51
4	5	7	57	-56	6	5	-8	31	-30	8	5	-5	22	21	2	6	-13	16	19	4	6	-6	22	-23
4	5	8	20	19	6	5	-7	37	-39	8	5	-4	33	-35	2	6	-12	18	-19	4	6	-5	23	24
4	5	9	-9	-30	6	5	-6	21	-19	8	5	-3	13	12	2	6	-11	27	-26	4	6	-4	31	-33
4	5	10	10	15	6	5	-5	50	-50	8	5	-2	34	-37	2	6	-10	24	-26	4	6	-3	13	-6
4	5	11	10	-5	6	5	-4	22	22	8	5	-1	-9	0	2	6	-9	33	-33	4	6	-2	30	-29
4	5	12	33	33	6	5	-3	39	-38	8	5	0	39	-38	2	6	-8	17	-17	4	6	-1	40	-34
4	5	13	25	25	6	5	-2	31	30	8	5	1	26	-27	2	6	-7	37	-36	4	6	0	13	-10
4	5	14	13	11	6	5	-1	-9	5	8	5	2	-9	-5	2	6	-6	-9	-2	4	6	1	53	-52
5	5	-20	-9	-6	6	5	0	36	35	9	5	-9	18	19	2	6	-5	17	-18	4	6	2	-10	-3
5	5	-19	27	-27	6	5	1	30	31	9	5	-8	18	-20	2	6	-4	22	23	4	6	3	19	-18
5	5	-18	-9	2	6	5	2	42	43	9	5	-7	-9	-3	2	6	-3	-9	7	4	6	4	18	19
5	5	-17	14	-14	6	5	3	25	26	9	5	-6	28	-28	2	6	-2	43	47	4	6	5	-10	-2
5	5	-16	39	40	6	5	4	12	12	9	5	-5	33	-33	2	6	-1	-9	-3	5	6	-10	28	-29
5	5	-15	-9	2	6	5	5	29	28	0	6	0	25	-23	2	6	0	34	36	5	6	-9	17	-15
5	5	-14	40	42	6	5	6	-9	-8	0	6	1	20	-18	2	6	1	10	9	5	6	-8	34	-34
5	5	-13	12	10	6	5	7	13	18	0	6	2	20	-18	2	6	2	-9	6	5	6	-7	20	-24
5	5	-12	22	21	6	5	8	24	-24	0	6	3	49	-48	2	6	3	33	33	5	6	-6	16	-16
5	5	-11	31	33	6	5	9	14	16	0	6	4	13	-15	2	6	4	15	-13	5	6	-5	33	-32
5	5	-10	20	20	7	5	-18	25	-24	0	6	5	44	-41	2	6	5	33	34	5	6	-4	-9	4
5	5	-9	44	44	7	5	-17	-9	-1	0	6	6	-9	-6	2	6	6	25	-25	5	6	-3	27	-27
5	5	-8	18	-18	7	5	-16	30	-29	0	6	7	12	-12	2	6	7	33	31	5	6	-2	23	24
5	5	-7	39	39	7	5	-15	17	-18	0	6	8	25	25	2	6	8	24	-24	5	6	-1	18	-17
5	5	-6	38	-39	7	5	-14	21	-20	0	6	9	-9	1	2	6	9	-9	-3	5	6	0	32	32
5	5	-5	18	17	7	5	-13	36	-37						2	6	10	-10	-10	5	6	1	14	-13
																				5	6	2	21	19

Orthogonal coordinates, in Å, are given in Table 3 under the heading $P2_1/c$. The coordinates refer to the same origin as in Table 1, and to the a', b', and c' axes where a' is parallel to b, and b' is parallel to a. For comparison, the coordinates of barium selenopentathionate dihydrate, in Å, calculated from the fractional orthorhombic coordinates [2] and referred to a corresponding origin, are given in Table 3 under the heading *Pnma*.

THE SELENOPENTATHIONATE ION

The dimensions of the selenopentathionate ion, calculated from the atomic coordinates of Table 1, are listed in Table 5. Fig. 1 gives a view of the ion as seen along the b axis, with principal bond lengths and angles, and also a view as seen normal to the b axis, along an approximate mirror plane.

The selenopentathionate ion has the same rotational-isomeric form, the *cis* form, in this salt as in the crystals of barium selenopentathionate dihydrate.[1],[2] In the orthorhombic crystals of the dihydrate, the selenium atom of the selenopentathionate ion is situated in a crystallographic mirror plane, and the two halves of the ion are exactly equal. In the monoclinic crystals of the trihydrate, no mirror plane symmetry is crystallographically required. However, as seen from the transformed, orthogonal coordinates for the trihydrate,

Table 5. Dimensions of the selenopentathionate ion. Standard deviations are given in parentheses.

Bond lengths and angles

S(1) − S(2) = 2.1038(17) Å   S(4) − S(5) = 2.0933(21) Å
S(2) − Se   = 2.1810(19)   Se − S(4)   = 2.1783(19)
∠S(1) − S(2) − Se = 104.07(7)°   ∠Se − S(4) − S(5) = 103.42(7)°
                    ∠S(2) − Se − S(4) = 104.00(8)°

S(1) − O(1) = 1.437(4) Å   S(5) − O(4) = 1.435(4) Å
S(1) − O(2) = 1.456(5)   S(5) − O(5) = 1.448(4)
S(1) − O(3) = 1.440(5)   S(5) − O(6) = 1.441(4)
∠S(2) − S(1) − O(1) = 106.8(2)°   ∠S(4) − S(5) − O(4) = 107.7(2)°
∠S(2) − S(1) − O(2) = 99.6(2)°   ∠S(4) − S(5) − O(5) = 99.9(2)°
∠S(2) − S(1) − O(3) = 108.8(2)°   ∠S(4) − S(5) − O(6) = 107.6(2)°
∠O(1) − S(1) − O(2) = 113.0(3)°   ∠O(4) − S(5) − O(5) = 112.4(3)°
∠O(1) − S(1) − O(3) = 112.8(3)°   ∠O(4) − S(5) − O(6) = 113.2(2)°
∠O(2) − S(1) − O(3) = 114.7(3)°   ∠O(5) − S(5) − O(6) = 114.9(2)°

Dihedral angles

S(1)S(2)Se/S(2)SeS(4)   = 106.7°   S(2)SeS(4)/SeS(4)S(5)   = 105.9°

SeS(2)S(1)/S(2)S(1)O(1) = 49.7°   SeS(4)S(5)/S(4)S(5)O(4) = 50.3°
SeS(2)S(1)/S(2)S(1)O(2) = 167.4°   SeS(4)S(5)/S(4)S(5)O(5) = 167.7°
SeS(2)S(1)/S(2)S(1)O(3) = 72.3°   SeS(4)S(5)/S(4)S(5)O(6) = 72.1°
S(2)S(1)O(1)/S(2)S(1)O(2) = 117.7°   S(4)S(5)O(4)/S(4)S(5)O(5) = 117.5°
S(2)S(1)O(1)/S(2)S(1)O(3) = 122.0°   S(4)S(5)O(4)/S(4)S(5)O(6) = 122.3°
S(2)S(1)O(2)/S(2)S(1)O(3) = 120.3°   S(4)S(5)O(5)/S(4)S(5)O(6) = 120.2°

Non-bonded distances

S(1) − Se   = 3.3784(12) Å   Se − S(5)   = 3.3533(16) Å
S(1) − S(4) = 4.6354(18)   S(2) − S(5) = 4.6021(23)
S(2) − S(4) = 3.4361(23)   S(1) − S(5) = 4.9268(12)

in Å, listed in Table 3, and from bond lengths and angles, Table 5, and from Fig. 1, the selenopentathionate ion conforms approximately to mirror plane symmetry also in the trihydrate. Only the largest deviations from mirror plane symmetry are significant.

The transformed, orthogonal coordinates for the trihydrate (Table 3) agree closely with the coordinates for the dihydrate, listed in the same table. The average values of the dimensions in the two halves of the ion in the trihydrate, and the corresponding dimensions of the ion in the dihydrate,[2] are listed in Table 6. Except for the S(2) − Se − S(2′) bond angles, which differ by 0.94°, the dimensions of the selenopentathionate ion are within the errors the same in the two salts.

The average length of the terminal sulphur − sulphur bonds, 2.0986(13) Å, is significantly shorter than the average length of the corresponding bonds, 2.118(3) Å, in the crystals of ammonium selenopentathionate hemitrihydrate.[3] The bonds are all a little longer than twice the single covalent bond radius for sulphur, 2.08 Å.[15] The selenium − sulphur bonds, 2.1810(19) Å and 2.1783(19) Å, are of the same length as one of the corresponding bonds in the ammonium salt, where the observed bond lengths were 2.181(3) Å and 2.153(3) Å.[3] These bonds, between divalent atoms, are all a little shorter than the sum of the single covalent bond radii for selenium and sulphur, 2.21 Å.[15] The two

Table 6. Dimensions of the *cis* form of the selenopentathionate ion in barium seleno-pentathionate trihydrate (left column) and in barium selenopentathionate dihydrate (right column). Those for the trihydrate, where exact mirror plane symmetry is not required, are averages for the two slightly differing halves of the ion.

S(1)−S(2)	2.0986(13) Å	2.0957(30) Å
S(2)−Se	2.1797(14)	2.1804(28)
∠S(1)−S(2)−Se	103.75(5)°	103.96(11)°
∠S(2)−Se−S(2′)	104.00(8)°	103.06(11)°
∠S(1)S(2)Se/S(2)SeS(2′)	106.3°	106.0°
S(1)−O(1)	1.436(3) Å	1.432(5) Å
S(1)−O(2)	1.452(3)	1.441(6)
S(1)−O(3)	1.440(3)	1.444(6)
∠S(2)−S(1)−O(1)	107.2(2)°	107.1(3)°
∠S(2)−S(1)−O(2)	99.7(2)°	99.1(3)°
∠S(2)−S(1)−O(3)	108.2(2)°	108.6(3)°
∠O(1)−S(1)−O(2)	112.7(2)°	113.1(3)°
∠O(1)−S(1)−O(3)	113.0(2)°	112.9(3)°
∠O(2)−S(1)−O(3)	114.8(2)°	114.7(3)°
∠SeS(2)S(1)/S(2)S(1)O(1)	50.0°	50.6°
∠SeS(2)S(1)/S(2)S(1)O(2)	167.6°	168.3°
∠SeS(2)S(1)/S(2)S(1)O(3)	72.2°	71.7°
∠S(2)S(1)O(1)/S(2)S(1)O(2)	117.6°	117.7°
∠S(2)S(1)O(1)/S(2)S(1)O(3)	122.1°	122.3°
∠S(2)S(1)O(2)/S(2)S(1)O(3)	120.3°	120.0°

S−S−Se bond angles are 104.07(7)° and 103.42(7)°, and the S−Se−S bond angle is 104.00(8)°, compared to 104.0(2)° and 101.1(2)°, and 104.9(2)°, for the corresponding angles in the ammonium salt.[3]

The main difference between the S−S−Se−S−S chains in the barium selenopentathionate hydrates and in ammonium selenopentathionate hemitri-hydrate,[3] is that in the former salts the S−S bonds are rotated about 106°
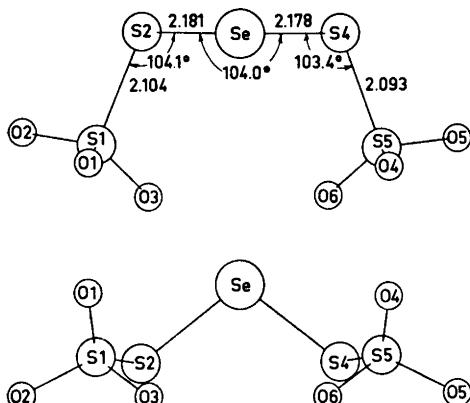
Fig. 1. The *cis* form of the selenopenta-thionate ion in BaSe(S₂O₃)₂.3H₂O, as seen along the *b* axis (above), and as seen normal to the *b* axis, along an approximate mirror plane (below).
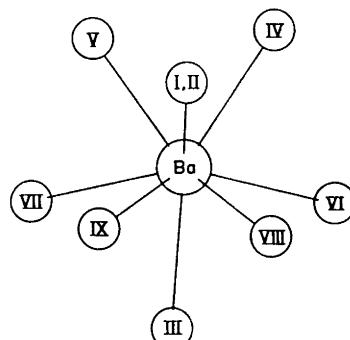
Fig. 2. A view of the barium-oxygen coordination in BaSe(S₂O₃)₂.3H₂O, as seen along the *b* axis. The oxygen atoms are marked I−IX in accordance with Table 7.

out of the plane through the three middle atoms, to the same side of the plane, *cis*, whereas in the latter salt the S − S bonds are rotated about 84° out of the plane, to opposite sides of the plane, *trans*.

The six S − O bond lengths are in the range 1.440 − 1.456 Å, with an average of 1.443 Å. The six O − S − O bond angles are in the range 112.4 − 114.9°, with an average of 113.5° and the six S − S − O bond angles are in the range 99.6 − 108.8° with an average of 105.1°. The average values of the bond lengths and bond angles of the sulphonate groups agree well with the dimensions of these groups in organic sulphonates *e.g.* ammonium acid *o*-carboxybenzene-sulphonate [16] and 1,5-endomethylenequinolizidinium *p*-toluenesulphonate.[17] In these compounds the average values of the S − O bond lengths O − S − O bond angles, and C − S − O bond angles are, respectively, 1.443 Å and 1.457 Å, 112.4° and 113.1°, and 106.4° and 105.5°; the individual values differ only slightly from the average values.

The S(2) − S(1) − O(2) and S(4) − S(5) − O(5) bond angles, one of each sulphonate group, are about 8° smaller than the other S − S − O bond angles. The S(1) − O(2) bond is rotated only 12.6° out of the plane through S(1), S(2), and Se, and is pointing in a direction opposite to the direction of the S(2) − Se bond. Similarly, the S(4) − O(5) bond is rotated 12.3° out of the plane through Se, S(4), and S(5), and is pointing in a direction opposite to the direction of the S(4) − Se bond. The distances from Se to these oxygen atoms, O(2) and O(5), are 4.554 Å and 4.532 Å, respectively, and the distances from Se to the other four oxygen atoms, O(1), O(3), O(4), and O(6), are 3.450 Å, 3.764 Å, 3.445 Å, and 3.712 Å, respectively.

THE IONIC ENVIRONMENT

The arrangement of oxygen atoms around the barium ions is the same as in the crystals of barium selenopentathionate dihydrate.[1,2] The barium ions are surrounded by nine oxygen atoms, with Ba − O distances ranging from 2.746(3) Å to 2.940(3) Å. The individual distances and related angles are listed in Table 7, and a view of the arrangement is given in Fig. 2. The six sulphonate oxygen atoms and the $H_2O(2)$ oxygen atom are included once in the barium-oxygen approaches, the $H_2O(1)$ oxygen atom is included twice, whereas the $H_2O(3)$ oxygen atom is not included.

Table 7. Distances (Å), and angles (°) between directions, from barium ions to oxygen atoms. Standard deviations of the bond lengths and angles are 0.003 − 0.006 Å and 0.1 − 0.2°, respectively.

				I	II	III	IV	V	VI	VII	VIII
I	$H_2O(1)$	(x,y,z)	2.836								
II	$H_2O(1)$	$(x,1+y,z)$	2.940	119.6							
III	$H_2O(2)$	(x,y,z)	2.800	113.0	127.3						
IV	O(3)	(x,y,z)	2.817	69.8	59.4	152.0					
V	O(6)	(x,y,z)	2.746	71.1	61.3	140.2	67.7				
VI	O(1)	$(\bar{x}-1,1-y,\bar{z})$	2.850	79.5	112.7	79.1	74.0	137.7			
VII	O(4)	$(\bar{x},1-y,\bar{z})$	2.904	81.3	112.3	71.6	134.5	70.1	134.9		
VIII	O(2)	$(\bar{x}-1,2-y,\bar{z})$	2.771	146.2	65.5	73.2	89.8	126.5	68.9	129.8	
IX	O(5)	$(\bar{x},2-y,\bar{z})$	2.757	147.3	62.6	71.8	122.0	85.1	131.8	69.4	66.4

The water molecule $H_2O(1)$, in close contact with two barium ions, forms hydrogen bonds to O(1) and O(4) at distances of 3.004(7) A and 3.018(5) Å, respectively; the $O(1) - H_2O(1) - O(4)$ angle is 119.2(2)°. Hydrogen atoms, in accordance with these hydrogen bonds, could be located in the final difference electron density map. The six angles between the directions from $H_2O(1)$ to the two barium ions and two oxygen atoms are in the range $91.4(1)° - 119.2(2)°$.

The water molecule $H_2O(2)$ is coordinated to one barium ion, but has no approach to a sulphonate oxygen atom closer than 3.26 Å. The shortest distance from $H_2O(3)$ to a barium ion is 3.40 Å, and the shortest distance from this water molecule to a sulphonate oxygen atom is 3.35 Å. The $H_2O(2)$ and $H_2O(3)$ hydrogen atoms were not located in the final difference electron density map. If hydrogen bonds are formed, they most likely occur between the two water molecules. The water molecules are situated near the twofold screw axis at $-\frac{1}{2}, y, -\frac{1}{4}$, and the shortest oxygen–oxygen distances between them are $H_2O(2) - H_2O(3) = 2.623(12)$ Å, $H_2O(2) - H_2O(3') = 2.725(16)$ Å, $H_2O(2) - H_2O(3'') = 2.968(16)$ Å, and $H_2O(3) - H_2O(3') = 3.057(18)$ Å. The related angles are $\angle H_2O(3) - H_2O(2) - H_2O(3') = 69.7(4)°$, $\angle H_2O(3) - H_2O(2) - H_2O(3'') = 67.0(4)°$, $\angle H_2O(3') - H_2O(2) - H_2O(3'') = \angle H_2O(2') - H_2O(3) - H_2O(2'') = 122.6(4)°$, $\angle H_2O(3') - H_2O(3) - H_2O(3'') = 109.6(4)°$, and $\angle H_2O(2) - H_2O(3) - H_2O(2') = 116.0(4)°$. Here, a prime denotes an atom at $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$ and a double-prime denotes an atom at $1 - x, -\frac{1}{2} + y, \frac{1}{2} - z$.

The closest interionic Se – Se and Se – S approaches are, $Se - Se' = 4.1877(9)$ Å, where Se' is at $\bar{x}, \frac{1}{2} + y, \frac{1}{2} - z$ relative to Se, and $Se - S(4') = 3.5796(17)$ Å, where S(4') is at $\bar{x}, -\frac{1}{2} + y, \frac{1}{2} - z$ relative to S(4). There is no interionic S – S distance shorter than 4.12 Å.

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