ACTA CHEMICA SCANDINAVICA 27 (1973) 1653–1666

The Crystal Structure of Barium Telluropentathionate Trihydrate

KARL GJERRESTAD and KJARTAN MARØY

Chemical Institute, University of Bergen, N-5000 Bergen, Norway

The crystal structure of barium telluropentathionate trihydrate, $BaTe(S_2O_3)_2.3H_2O$, has been determined by X-ray methods. The salt crystallizes in the monoclinic space group $P2_1/c$ (No. 14) with four formula units in a unit cell of dimensions $a = 11.139(3)$ Å, $b = 5.243(2)$ Å, $c = 21.306(6)$ Å, $\beta = 106.94(4)°$. The refinement was carried out by a full-matrix least squares program using 2389 non-zero reflections, recorded by means of a single-crystal diffractometer. The R value was 0.024.

The telluropentathionate ion has the *trans* form, the sulphonate groups being rotated out of the plane of the three middle atoms to different sides of the plane. The dimensions of the S–S–Te–S–S chain, from one end of the chain to the other, are S(1)–S(2) = 2.102(2) Å, S(2)–Te = 2.384(2) Å, Te–S(4) = 2.392(2) Å, S(4)–S(5) = 2.090(2) Å, ∠S(1)–S(2)–Te = 103.08(5)°, ∠S(2)–Te–S(4) = 96.02(4)°, ∠Te–S(4)–S(5) = 102.59(5)°. The SSTe/STeS dihedral angles are 87.7° and 98.7°.

The crystal structures of two barium pentathionate dihydrates,[1,2] of barium selenopentathionate dihydrate [3,4] and trihydrate,[5] and of barium telluropentathionate dihydrate [6,7] and trihydrate [8] have been reported. The latter structure was solved and refined by means of film data. The results of the refinement were not quite satisfactory, the standard deviations being high, compared to those of the barium selenopentathionate hydrates.[4,5] The present work is a more detailed description of this structure analysis, including least squares refinement of diffractometer data.

The pentathionate, selenopentathionate, and telluropentathionate ions have been found to occur in two rotational-isomeric forms, and crystallize in the *cis* form in all of their barium salts, except in barium telluropentathionate trihydrate. The telluropentathionate ion has the *trans* form in the trihydrate, the sulphonate groups being located on opposite sides of the plane through the three middle atoms. The *trans* form of this ion was also found in the crystals of ammonium telluropentathionate [9] and rubidium telluropentathionate hemitrihydrate.[10]

EXPERIMENTAL

Barium telluropentathionate trihydrate, $BaTe(S_2O_3)_2.3H_2O$, was obtained by crystallization of crude barium telluropentathionate from dilute hydrochloric acid.[11] The crystals are light yellowish-green, flat prisms.

The intensity data used for the solution and first refinement of the structure were collected by the multiple-film technique. Integrated zero-layer and equi-inclination Weissenberg photographs were taken with Cu$K\alpha$ radiation (Ni-filtered) for the $h0l$, $h1l$, $h2l$, and $0kl$ reflections. The intensities of the 1106 independent, observed reflections were measured visually.

The intensity data used for a more accurate refinement of the structure were measured on a Siemens automatic single-crystal diffractometer using Mo$K\alpha$ radiation (Nb-filtered) and a scintillation counter.

The crystal was mounted with the b axis approximately parallel to the ϕ axis of the diffractometer, and the orientation of the crystal and preliminary unit cell dimensions were determined from the θ, χ, and ϕ angles of 10 non-coplanar reciprocal vectors.

The $\theta-2\theta$ scan technique and five-value procedure were used. The scan width was 0.70° for all reflections, and the maximum scan time per degree was 24 sec. For strong reflections the diffractometer automatically selects higher scan speed, and inserts a proper attenuation filter into the primary beam, if needed to avoid counting losses.

Two reflections, 700 and 0010, were used as reference, and measured two times each at intervals of 50 reflections. The intensities of the reference reflections decreased by 7 % during the data collection, and were used to bring the net intensities to a common scale.

Out of 2877 reflections attainable within $\theta = 28°$, 488 were found to have net intensities below three times its standard deviation. These reflections were assigned an intensity equal to this limit, and labelled as unobserved.

Lorentz and polarization corrections were applied, and absorption corrections were carried out using a modified version of the Gaussian integration method described by Coppens *et al.*[12] The linear absorption coefficients for Cu$K\alpha$ and Mo$K\alpha$ radiations are 526 cm^{-1} and 66.2 cm^{-1}, respectively. The crystals used were prisms extended along the b axes and bounded by (100) and (001). The distances between the (100), between the (010), and between the (001) boundary faces were 0.036, 0.102, and 0.066 mm, respectively, for the crystal used to collect the $h0l-h2l$ film data, 0.014, 0.080, and 0.072 mm, respectively, for the crystal used to collect the $0kl$ film data, and 0.033, 0.167, and 0.110 mm, respectively, for the crystal used to collect the diffractometer data.

The film data were eventually also corrected for secondary extinction, using the formula $F_{corr} = KF_o(1+\beta CI_o)$.[13] Here $\beta = 2(1+\cos^4 2\theta)/(1+\cos^2 2\theta)^2$, and C was calculated to 1.34×10^{-7}.

The scattering factor curves used were those given in *International Tables for X-Ray Crystallography*,[14] Table 3.3 1B for tellurium, Table 3.3. 1A for sulphur and oxygen, and the one given by Thomas and Umeda [15] for barium ion. The curves for barium, tellurium and sulphur were corrected for anomalous dispersion using the $\Delta f'$ and $\Delta f''$ values given by Cromer,[16] and taking the amplitude of f as the corrected value.

Least squares refinement was carried out with a program minimizing the function

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

For the film data $W = [(3K)^2 + (2F_o)^2/4W_o + (0.07\ F_o)^6]^{-1}$, where W_o is a weight factor based on the estimated reliability of the individual intensities. For the diffractometer data $W = 4(I_t - I_b)^2/F_o^2[I_t + I_b + k^2(I_t - I_b)^2]$ 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. Unobserved reflections were included with $|F_o|$ equal to the observable limit when $|F_c|$ exceeded this limit.

The programs used for calculations of setting angles and preparation of input tape data for the diffractometer, conversion of diffractometer output tape data to the computer, calculation of atomic distances and angles, and for secondary extinction corrections of the film data are written by K. Maartmann-Moe of this institute. The programs used for calculation of unit cell dimensions, film data processing, absorption corrections, two-dimensional Fourier summations, and least squares refinement were made available

by the Chemical Department of X-Ray Crystallography, Weizmann Institute of Science, Rehovoth, Israel. The programs used for diffractometer data processing and three-dimensional Fourier summations are written by K. Åse of this institute. The program used for drawing of illustrations is written by C. K. Johnson, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA. The calculations were carried out on an IBM 360/50H computer.

The unit cell dimensions, calculated by means of a least squares program using the θ angles ($\theta = 18-22°$) of 10 reflections measured on the diffractometer are, $a = 11.139(3)$ Å, $b = 5.243(2)$ Å, $c = 21.306(6)$ Å, $\beta = 106.94(4)°$. The space group is $P2_1/c$ (No. 14) with four $BaTe(S_2O_3)_2.3H_2O$ formula units per unit cell.[11]

THE STRUCTURE ANALYSIS

Two-dimensional Patterson maps, calculated on the basis of the *h*0*l* and 0*kl* film data, revealed the positions of the two heavy atoms. The subsequent electron density maps allowed the location of the four sulphur atoms, and since two sulphur atoms are coordinated to the tellurium atom, it was possible to distinguish the tellurium atom from the barium ion. The sulphonate and water oxygen atoms were located in additional electron density maps.

Least squares refinement based on the 1106 independent, observed *h*0*l*, *h*1*l*, *h*2*l* and 0*kl* reflections was then carried out. With individual isotropic thermal parameters for all atoms the R value ($\sum||F_o| - |F_c||/\sum|F_o|$) converged at 0.120. Introduction of anisotropic thermal parameters for barium, tellurium and sulphur, followed by secondary extiction corrections, reduced the R value to 0.106 only.

None of the thermal parameters were unusually high, and the atomic distances and angles were not much different from those found in the rubidium salt of telluropentathionic acid.[10] However, the standard deviations were rather high, the agreements between $|F_o|$ and $|F_o|$ for many of the strong

Table 1. Atomic coordinates for barium telluropentathionate trihydrate. Origin at a centre of symmetry. Standard deviations are given in parentheses.

	x	y	z
Ba	0.86098(2)	0.83134(6)	0.09725(1)
S(1)	0.16922(9)	0.62221(21)	0.04248(5)
S(2)	0.32916(10)	0.80347(23)	0.10351(5)
Te	0.40372(2)	0.50579(6)	0.19076(1)
S(4)	0.53083(10)	0.26496(23)	0.13903(5)
S(5)	0.70999(9)	0.41366(21)	0.18220(5)
O(1)	0.07601(31)	0.62342(91)	0.07634(18)
O(2)	0.13999(41)	0.77857(93)	−0.01489(18)
O(3)	0.20295(39)	0.36689(81)	0.03066(21)
O(4)	0.74671(29)	0.33338(69)	0.25033(14)
O(5)	0.78286(30)	0.29377(73)	0.14358(16)
O(6)	0.70578(31)	0.68819(64)	0.17507(16)
$H_2O(1)$	0.07150(32)	0.13818(69)	0.14962(17)
$H_2O(2)$	0.01078(33)	0.59785(79)	0.21127(17)
$H_2O(3)$	0.59990(38)	0.80036(106)	0.03228(19)

reflectrons were not good, and two-dimensional difference election density maps showed unexpected high peaks.

The new set of data, recorded by means of a single-crystal diffractometer, was used for the further refinement of the structure. With atomic coordinates and thermal parameters as derived from the film data, the R value was 0.079. Refinement of the same parameters as in the film data set reduced the reliability index to 0.036, and by using anisotropic thermal parameters for all atoms, the refinement converged at $R = 0.024$. Unobserved reflections are included when $|F_o|$ exceeds the observable limit. The final maximum shift of a parameter was about one fifth of its standard deviation.

A three-dimensional difference electron density map showed no peaks higher than 0.6 e/Å^3. The regions of positive electron density near the water oxygen atoms were too diffuse for location of the hydrogen atoms.

Tables 1 and 2 give the final atomic parameters with standard deviations from least squares. The structure factors, calculated on the basis of these parameters, and the observed ones, from the diffractometer data, are given in Table 3.

Table 2. 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	247(1)	287(1)	302(1)	26(1)	64(1)	113(1)
S(1)	179(5)	201(5)	184(5)	−13(4)	0(4)	41(4)
S(2)	221(5)	240(6)	314(6)	−62(5)	18(5)	6(4)
Te	180(1)	308(2)	224(1)	3(1)	−28(1)	49(1)
S(4)	167(5)	295(6)	261(5)	−13(4)	−92(4)	43(4)
S(5)	152(5)	225(5)	206(4)	−10(4)	2(4)	58(4)
O(1)	262(19)	824(33)	467(22)	−159(21)	−225(22)	197(17)
O(2)	663(30)	755(33)	394(22)	−380(26)	376(23)	−207(20)
O(3)	523(27)	394(25)	740(30)	149(21)	−337(22)	−139(23)
O(4)	264(17)	400(20)	235(16)	−59(17)	70(15)	−7(13)
O(5)	252(17)	442(22)	447(20)	0(17)	−135(17)	180(16)
O(6)	355(20)	241(18)	443(20)	0(16)	39(16)	154(16)
$H_2O(1)$	362(20)	285(20)	458(21)	23(17)	58(17)	55(16)
$H_2O(2)$	345(21)	504(25)	397(20)	−82(18)	23(18)	58(16)
$H_2O(3)$	419(24)	1039(40)	417(23)	72(27)	60(25)	50(19)

RESULTS

The dimensions of the telluropentathionate ion, calculated from the atomic coordinates of Table 1, are listed in Table 4. The standard deviations given include estimated uncertainties in unit cell dimensions.

Fig. 1 is a view of the ion, as seen along a line through Te and the coordinate midpoint of S(2) and S(4), with principal bond lengths and angles. The largest differences between these values and those arrived at by the refinement based

Table 3. Observed and calculated structure factors (× 10) for barium telluropentathionate trihydrate. A minus sign on $F(O)$ indicates an unobserved reflection.

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	0	2	501	-461	4	0-22	447	-443	8	0-26	321	-303	12	0	4	416	-422	1	1 19	1009	-1003			
0	0	4	1755	-1758	4	0-20	416	-414	8	0-24	738	-722	12	0	6	591	591	1	1 20	533	-520			
0	0	6	251	211	4	0-18	407	-411	8	0-22	359	375	12	0	8	-132	-104	1	1 21	805	818			
0	0	8	1210	-1226	4	0-16	817	814	8	0-20	-111	-96	13	0-19		499	-486	1	1 22	-121	46			
0	0	10	2115	2165	4	0-14	2623	2631	8	0-18	315	318	13	0-16		547	-535	1	1 23	169	-159			
0	0	12	-167	138	4	0-12	1173	-1166	8	0-16	376	317	13	0-14		-124	-123	1	1 24	425	421			
0	0	14	1736	-1746	4	0-10	1599	-1621	8	0-14	1766	-1796	13	0-12		1393	1415	1	1 25	311	-314			
0	0	16	240	-108	4	0 -8	-159	67	8	0-12	-99	-27	13	0-10		523	-524	1	1 26	227	213			
0	0	18	1111	-1111	4	0 -6	1439	-1415	8	0-10	1021	1023	13	0 -8		652	-654	2	1-27	522	535			
0	0	20	1127	1154	4	0 -4	2591	2602	8	0 -8	1226	1191	13	0 -6		347	359	2	1-26	478	480			
0	0	22	591	574	4	0 -2	441	-450	8	0 -6	242	228	13	0 -4		567	-578	2	1-25	642	-627			
0	0	24	626	-657	4	0 0	2254	-2379	8	0 -4	1737	-1788	13	0 -2		1276	1264	2	1-24	632	649			
0	0	26	-158	-21	4	0 2	1267	-1200	8	0 -2	-111	-93	13	0 0		467	474	2	1-23	332	308			
1	0	0	386	-349	4	0 4	731	-712	8	0 0	560	498	13	0 2		1082	-1039	2	1-22	222	-208			
1	0	24	207	-205	4	0 6	2728	2710	8	0 2	-113	-37	13	0 4		-119	14	2	1-21	117	-113			
1	0	22	-124	-66	4	0 8	1495	1463	8	0 4	1038	1044	14	0-16		637	-681	2	1-20	872	-861			
1	0	20	130	126	4	0 10	2624	-2600	8	0 6	1378	-1406	14	0-14		255	257	2	1-19	195	-195			
1	0	18	1065	1074	4	0 12	484	467	8	0 8	421	-397	14	0-12		-130	113	2	1-18	352	-352			
1	0	16	1282	-1265	4	0 14	-109	25	8	0 10	610	601	14	0-10		753	753	2	1-17	1489	1496			
1	0	14	1114	-1118	4	0 16	187	173	8	0 12	518	516	14	0 -8		158	151	2	1-16	632	625			
1	0	12	413	415	4	0 18	809	801	8	0 14	923	922	14	0 -6		815	-797	2	1-15	895	-909			
1	0	10	149	165	4	0 20	1149	-1167	8	0 16	634	-640	14	0 -4		315	303	2	1-14	753	752			
1	0	-8	1627	1716	4	0 22	342	-326	8	0 18	368	-370	14	0 -2		-131	71	2	1-13	441	-446			
1	0	-6	619	-556	5	0-28	708	-704	9	0-26	312	-299	14	0 0		-159	52	2	1-12	674	-689			
1	0	-4	811	-795	5	0-26	829	811	9	0-24	167	-148	0	1 1		646	-633	2	1-11	197	-125			
1	0	-2	1101	1143	5	0-24	137	148	9	0-22	1333	-1332	0	1 2		1606	1553	2	1-10	1438	-1446			
1	0	0	126	-169	5	0-22	400	383	9	0-20	709	720	0	1 3		1625	1592	2	1 -9	1184	-1160			
1	0	2	2586	2677	5	0-20	159	154	9	0-18	1216	1195	0	1 4		1996	1975	2	1 -8	633	-618			
1	0	4	137	56	5	0-18	1349	-1346	9	0-16	829	-845	0	1 5		3113	-3193	2	1 -7	2358	2329			
1	0	6	3363	-3443	5	0-16	815	824	9	0-14	470	448	0	1 6		-91	-9	2	1 -6	639	673			
1	0	8	440	437	5	0-14	875	886	9	0-12	565	-955	0	1 7		982	916	2	1 -5	858	-823			
1	0	10	275	-261	5	0-12	105	-84	9	0-10	-105	56	0	1 8		2222	-2183	2	1 -4	2349	2369			
1	0	12	693	690	5	0-10	3158	-3330	9	0 -8	2141	2194	0	1 9		1295	1287	2	1 -3	1436	-1439			
1	0	14	1336	1329	5	0 -8	2962	-2938	9	0 -6	434	-407	0	1 10		462	-458	2	1 -2	867	820			
1	0	16	1547	-1569	5	0 -6	819	775	9	0 -4	632	-631	0	1 11		419	-451	2	1 -1	700	664			
1	0	18	543	547	5	0 -4	2159	2132	9	0 -2	1285	-1234	0	1 12		1465	1465	2	1 0	1413	-1340			
1	0	20	207	258	5	0 -2	153	145	9	0 0	351	-340	0	1 13		1396	1384	2	1 1	570	-549			
1	0	22	-111	-83	5	0 0	455	505	9	0 2	1908	1931	0	1 14		743	713	2	1 2	564	-579			
1	0	24	1058	1063	5	0 2	1369	-1447	9	0 4	189	-196	0	1 15		1090	-1114	2	1 3	2329	2301			
1	0	26	509	-601	5	0 4	667	616	9	0 6	751	-762	0	1 16		907	-921	2	1 4	1815	1720			
2	0	28	409	419	5	0 6	1265	1235	9	0 8	232	243	0	1 17		329	-333	2	1 5	853	825			
2	0	26	293	-304	5	0 8	-103	101	9	0 10	234	-241	0	1 18		1138	-1146	2	1 6	2158	2070			
2	0	22	1461	-1481	5	0 10	604	558	9	0 12	834	862	0	1 19		1011	1015	2	1 7	957	-995			
2	0	20	458	446	5	0 12	1617	-1611	9	0 14	416	398	0	1 20		-139	-55	2	1 8	354	-328			
2	0	18	-101	89	5	0 14	854	-838	9	0 16	230	-247	0	1 21		451	-464	2	1 9	144	140			
2	0	16	290	301	5	0 16	556	545	10	0-24	458	-462	0	1 22		283	265	2	1 10	1455	-1470			
2	0	14	844	828	5	0 18	286	-291	10	0-22	-113	-37	0	1 23		179	186	2	1 11	517	-503			
2	0	12	3113	-3173	5	0 20	135	79	10	0-20	461	-448	0	1 24		243	222	2	1 12	550	-571			
2	0	10	557	551	5	0 22	338	-326	10	0-18	-116	125	0	1 25		248	-264	2	1 13	652	646			
3	0	-8	2494	2552	6	0-26	587	-575	10	0-16	1557	1531	0	1 26		-123	43	2	1 14	496	483			
3	0	-6	1111	1108	6	0-24	865	880	10	0-14	623	-635	1	1-27		159	-139	2	1 15	253	247			
3	0	-4	348	344	6	0-22	1110	554	10	0-12	472	-478	1	1-26		276	303	2	1 16	710	718			
3	0	-2	2812	-2552	6	0-20	466	-472	10	0-10	175	183	1	1-25		-114	-12	2	1 17	1038	-1030			
3	0	0	519	-632	6	0-18	627	615	10	0 -8	1009	-1025	1	1-24		308	-297	2	1 18	321	304			
3	0	2	1613	1650	6	0-16	1625	-1621	10	0 -6	1550	1562	1	1-23		675	-684	2	1 19	121	143			
3	0	4	565	-569	6	0-14	-55	5	10	0 -4	307	-338	1	1-22		332	-292	2	1 20	475	-474			
3	0	6	-53	-14	6	0-12	1530	1563	10	0 -2	1126	-1137	1	1-21		711	712	2	1 21	179	-179			
3	0	8	2716	-2742	6	0-10	688	-685	10	0 0	-190	276	1	1-20		153	159	2	1 22	437	-454			
3	0	10	698	-703	6	0 -8	313	296	10	0 2	850	-860	1	1-19		253	267	2	1 23	175	185			
3	0	12	1223	1218	6	0 -6	1196	-1237	10	0 4	1279	1257	1	1-18		444	424	2	1 24	251	269			
3	0	14	1265	1260	6	0 -4	1118	-1129	10	0 6	1357	1341	1	1-17		-131	11	2	1 25	498	484			
3	0	16	346	317	6	0 -2	3450	3740	10	0 8	1128	-1142	1	1-16		696	689	3	1-27	151	-163			
3	0	18	777	-715	6	0 0	-140	-42	10	0 10	250	295	1	1-15		495	474	3	1-26	291	305			
3	0	20	467	-446	6	0 2	714	-711	10	0 12	332	-309	1	1-14		-43	27	3	1-25	804	820			
3	0	22	1059	1084	6	0 4	364	-372	10	0 14	171	181	1	1-13		1087	-1101	3	1-24	399	393			
3	0	24	-112	6	6	0 6	1251	-1252	11	0-24	571	549	1	1-12		534	-532	3	1-23	434	-442			
3	0	26	361	324	6	0 8	1568	1585	11	0-22	-151	-120	1	1-11		557	563	3	1-22	-134	46			
3	0	28	267	261	6	0 10	412	404	11	0-20	681	-677	1	1-10		796	-784	3	1-21	394	-390			
3	0	24	617	-565	6	0 12	1102	-1106	11	0-18	376	367	1	1 -9		815	831	3	1-20	718	-736			
3	0	22	186	-179	6	0 14	182	-188	11	0-16	262	310	1	1 -8		1118	1089	3	1-19	705	746			
3	0	20	1283	-1288	6	0 16	1069	-1051	11	0-14	695	758	1	1 -7		751	-762	3	1-18	636	-629			
3	0	18	1135	1136	6	0 18	756	751	11	0-12	-112	-8	1	1 -6		1207	1251	3	1-17	838	-828			
3	0	16	1572	1618	6	0 20	737	719	11	0-10	1654	-1679	1	1 -5		132	195	3	1-16	-59	-91			
3	0	14	1317	-1256	7	0-26	-115	-106	11	0 -8	-111	-52	1	1 -4		225	151	3	1-15	1034	993			
3	0	12	411	415	7	0-24	270	-253	11	0 -6	535	538	1	1 -3		2581	-2593	3	1-14	1022	1032			
3	0	10	1359	-1365	7	0-22	273	253	11	0 -4	522	506	1	1 -2		1645	-1679	3	1-13	456	-495			
3	0	-8	746	-706	7	0-20	1299	1290	11	0 -2	150	-133	1	1 -1		-97	-19	3	1-12	438	432			
3	0	-6	2757	2848	7	0-18	1074	-1055	11	0 0	1265	-1256	1	1 0		-116	6	3	1-11	2018	-2025			
3	0	-4	2234	-2204	7	0-16	1044	-1047	11	0 2	533	513	1	1 1		1479	1428	3	1-10	950	-949			
3	0	-2	1678	-1653	7	0-14	503	-457	11	0 4	604	592	1	1 2		738	728	3	1 -9	1471	1457			
3	0	0	1166	-1225	7	0-12	-68	77	11	0 6	-118	60	1	1 3		1093	-1163	3	1 -8	1396	-1360			
3	0	2	2685	-2659	7	0-10	2599	2625	11	0 8	620	632	1	1 4		1198	1173	3	1 -7	339	-353			
3	0	4	3500	3556	7	0 -8	986	-964	11	0 10	944	-985	1	1 5		1304	1304	3	1 -6	621	630			
3	0	6	449	-411	7	0 -6	873	-885	12	0-22	263	-285	1	1 6		-92	104	3	1 -5	149	204			
3	0	8	1234	-1223	7	0 -4	1429	1424	12	0-20	201	213	1	1 7		-89	-15	3	1 -4	1431	1415			
3	0	10	1344	1312	7	0 -2	666	-660	12	0-18	858	-884	1	1 8		765	-778	3	1 -3	1631	1569			
3	0	12	624	-612	7	0 0	1960	1934	12	0-16	-126	101	1	1 9		780	-770	3	1 -2	331	376			
3	0	14	1255	1245	7	0 2	118	172	12	0-14	728	729	1	1 10		947	-960	3	1 -1	2490	-2566			
3	0	16	434	421	7	0 4	1563	-2602	12	0-12	547	-553	1	1 11		2122	2095	3	1 0	933	-906			
3	0	18	665	-658	7	0 6	149	132	12	0-10	353	366	1	1 12		310	-296	3	1 1	1811	1824			
3	0	20	-114	2	7	0 8	553	-540	12	0 -8	712	-701	1	1 13		653	-627	3	1 2	292	-315			
3	0	22	731	-716	7	0 10	726	706	12	0 -6	733	-722	1	1 14		358	367	3	1 3	729	704			
3	0	24	241	240	7	0 12	457	485	12	0 -4	1408	1386	1	1 15		149	139	3	1 4	447	-406			
4	0	28	228	-235	7	0 14	1459	-1472	12	0 -2	137	171	1	1 16		723	711	3	1 5	403	-367			
4	0	26	146	-174	7	0 16	456	531	12	0 0	-160	115	1	1 17		-101	3	3	1 6	605	625			
4	0	24	854	864	7	0 18	338	380	12	0 2	332	-309	1	1 18		452	-469	3	1 7	1441	1419			

Table 3. 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	1	8	657	675	5	1	9	148	-155	7	1	15	-115	-28	10	1-12	517	497	13	1	-6	693	-684
3	1	9	1566	-1586	5	1	10	660	655	7	1	16	312	-341	10	1-11	1338	-1339	13	1	-5	-123	81
3	1	10	238	188	5	1	11	615	-595	7	1	17	729	-751	10	1-10	322	-301	13	1	-4	694	-684
3	1	11	355	-335	5	1	12	145	148	7	1	18	554	-543	10	1 -9	455	451	13	1	-3	530	513
3	1	12	685	-677	5	1	13	514	511	7	1	19	532	545	10	1 -8	579	-593	13	1	-2	181	194
3	1	13	684	689	5	1	14	358	-352	8	1-26		481	494	10	1 -7	591	617	13	1	-1	536	-536
3	1	14	165	154	5	1	15	265	-269	8	1-25		214	214	10	1 -6	-113	33	13	1	0	718	694
3	1	15	345	-357	5	1	16	128	-106	8	1-24		-111	-6	10	1 -5	354	-354	13	1	1	529	522
3	1	16	772	795	5	1	17	523	521	8	1-23		277	-284	10	1 -4	752	749	13	1	2	242	221
3	1	17	735	722	5	1	18	121	-72	8	1-22		517	-504	10	1 -3	1156	1152	13	1	3	442	-454
3	1	18	510	467	5	1	19	392	373	8	1-21		-104	36	10	1 -2	353	337	13	1	4	176	-192
3	1	19	434	-495	5	1	20	153	106	8	1-20		273	-264	10	1 -1	1039	-1026	14	1-15		332	-340
3	1	20	-110	-52	5	1	21	523	-545	8	1-19		950	941	10	1 0	594	-574	14	1-14		431	-444
3	1	21	260	-255	5	1	22	140	123	8	1-18		566	586	10	1 1	181	-185	14	1-13		-126	-82
3	1	22	187	-161	6	1-27		-118	-106	8	1-17		336	-356	10	1 2	690	-689	14	1-12		181	-191
3	1	23	564	551	6	1-26		253	-276	8	1-16		614	618	10	1 3	892	879	14	1-11		480	494
3	1	24	147	-131	6	1-25		158	162	8	1-15		-101	13	10	1 4	161	-156	14	1-10		-126	106
4	1-27		485	454	6	1-24		339	-319	8	1-14		456	-438	10	1 5	778	-815	14	1 -9		453	-431
4	1-26		360	-375	6	1-23		579	-564	8	1-13		228	-217	10	1 6	354	354	14	1 -8		346	334
4	1-25		-112	67	6	1-22		133	-116	8	1-12		764	-754	10	1 7	424	449	14	1 -7		-122	108
4	1-24		287	275	6	1-21		944	953	8	1-11		534	-527	10	1 8	453	463	14	1 -6		242	230
4	1-23		170	157	6	1-20		596	603	8	1-10		353	-390	10	1 9	306	-324	14	1 -5		235	-225
4	1-22		424	413	6	1-19		452	-453	8	1 -9		578	570	10	1 10	-131	149	14	1 -4		239	-167
4	1-21		166	151	6	1-18		935	947	8	1 -8		-104	71	10	1 11	637	-643	14	1 -3		348	-363
4	1-20		427	-434	6	1-17		302	-301	8	1 -7		572	-630	10	1 12	351	-325	14	1 -2		293	-186
4	1-19		1185	-1232	6	1-16		229	-225	8	1 -6		942	944	10	1 13	720	733	14	1 -1		674	671
4	1-18		654	-655	6	1-15		1067	1056	8	1 -5		357	-310	11	1-23	373	-377	0	2	0	667	-611
4	1-17		531	497	6	1-14		841	-839	8	1 -4		568	891	11	1-22	630	627	0	2	1	895	923
4	1-16		572	-573	6	1-13		577	-571	8	1 -3		-108	81	11	1-21	-115	-52	0	2	2	1714	-1678
4	1-15		-35	70	6	1-12		-56	-5	8	1 -2		753	-726	11	1-20	193	-185	0	2	3	1203	1214
4	1-14		-52	-31	6	1-11		1251	1304	8	1 -1		558	-619	11	1-19	446	-451	0	2	4	1216	1246
4	1-13		124	-146	6	1-10		955	985	8	1 0		866	-849	11	1-18	663	-663	0	2	5	-93	-123
4	1-12		1221	1248	6	1 -9		591	573	8	1 1		1451	1476	11	1-17	-115	-39	0	2	6	1383	1404
4	1-11		763	762	6	1 -8		638	668	8	1 2		256	303	11	1-16	179	-177	0	2	7	1503	-1534
4	1-10		1148	1132	6	1 -7		2134	-2115	8	1 3		156	176	11	1-15	786	777	0	2	8	2043	-1982
4	1 -9		1662	-1702	6	1 -6		722	-736	8	1 4		1154	1167	11	1-14	755	749	0	2	9	668	-665
4	1 -8		564	-555	6	1 -5		659	643	8	1 5		553	-548	11	1-13	387	-378	0	2	10	635	626
4	1 -7		654	664	6	1 -4		1226	-1238	8	1 6		252	264	11	1-12	705	724	0	2	11	607	608
4	1 -6		1580	-2005	6	1 -3		344	-337	8	1 7		274	278	11	1-11	-111	45	0	2	12	529	-533
4	1 -5		1180	1220	6	1 -2		672	-668	8	1 8		647	-658	11	1-10	-115	-86	0	2	13	1314	1320
4	1 -4		527	670	6	1 -1		154	-85	8	1 9		646	-641	11	1 -9	271	-253	0	2	14	226	-229
4	1 -3		406	-432	6	1 0		549	547	8	1 10		465	-468	11	1 -8	643	-642	0	2	15	-130	-16
4	1 -2		2258	2343	6	1 1		1078	1065	8	1 11		703	719	11	1 -7	-117	-107	0	2	16	1386	1384
4	1 -1		1123	1171	6	1 2		984	993	8	1 12		-119	73	11	1 -6	328	-311	0	2	17	344	-347
4	1 0		320	335	6	1 3		1186	-1188	8	1 13		-113	27	11	1 -5	1079	1073	0	2	18	476	-479
4	1 1		1554	-1564	6	1 4		201	-181	8	1 14		252	231	11	1 -4	-114	15	0	2	19	368	-376
4	1 2		1476	-1498	6	1 5		234	217	8	1 15		559	-511	11	1 -3	336	-291	0	2	20	253	-218
4	1 3		425	-423	6	1 6		1214	-1195	8	1 16		328	325	11	1 -2	574	568	0	2	21	196	196
4	1 4		1358	-1350	6	1 7		553	549	8	1 17		181	183	11	1 -1	328	-319	0	2	22	-108	-91
4	1 5		1574	1560	6	1 8		649	-650	9	1-26		380	363	11	1 0	-113	82	0	2	23	560	555
4	1 6		165	-169	6	1 9		162	-165	9	1-25		320	-355	11	1 1	-119	-113	0	2	24	232	-220
4	1 7		1339	-1293	6	1 10		658	652	9	1-24		227	222	11	1 2	917	-937	0	2	25	-129	53
4	1 8		656	670	6	1 11		1259	1241	9	1-23		288	-287	11	1 3	663	-679	1	2-26		293	-268
4	1 9		130	124	6	1 12		759	757	9	1-22		430	-441	11	1 4	551	-545	1	2-25		180	192
4	1 10		580	591	6	1 13		677	-685	9	1-21		460	487	11	1 5	772	775	1	2-24		434	403
4	1 11		528	-520	6	1 14		121	-115	9	1-20		658	-675	11	1 6	586	633	1	2-23		520	-515
4	1 12		276	-252	6	1 15		191	-191	9	1-19		455	-507	11	1 7	-123	-122	1	2-22		190	213
4	1 13		1332	-1315	6	1 16		832	-838	9	1-18		254	-241	11	1 8	542	536	1	2-21		719	-736
4	1 14		830	-675	6	1 17		571	572	9	1-17		1047	1047	11	1 9	340	-337	1	2-20		847	-834
4	1 15		1331	1387	6	1 18		303	-339	9	1-16		706	734	11	1 10	-129	91	1	2-19		149	135
4	1 16		-109	8	6	1 19		322	-311	9	1-15		270	-280	11	1 11	296	311	1	2-18		363	366
4	1 17		-105	-56	6	1 20		264	275	9	1-14		1166	1188	12	1-21	293	-285	1	2-17		498	514
4	1 18		154	147	7	1-27		158	-164	9	1-13		1275	-1261	12	1-20	476	479	1	2-16		135	-120
4	1 19		-114	23	7	1-26		-116	-71	9	1-12		761	-772	12	1-19	473	-467	1	2-15		496	500
4	1 20		528	503	7	1-25		680	-667	9	1-11		729	725	12	1-18	-115	-41	1	2-14		603	604
4	1 21		283	284	7	1-24		523	-531	9	1-10		1313	-1329	12	1-17	528	515	1	2-13		376	-387
4	1 22		353	-377	7	1-23		579	583	9	1 -9		506	-505	12	1-16	534	-532	1	2-12		504	503
4	1 23		632	-620	7	1-22		112	-56	9	1 -8		641	624	12	1-15	335	-396	1	2-11		748	-759
5	1-27		256	-320	7	1-21		-107	-24	9	1 -7		465	462	12	1-14	152	-144	1	2-10		1643	-1639
5	1-26		457	-516	7	1-20		554	570	9	1 -6		1152	1155	12	1-13	727	725	1	2 -9		551	563
5	1-25		-112	83	7	1-19		159	154	9	1 -5		660	662	12	1-12	448	458	1	2 -8		1011	998
5	1-24		268	-214	7	1-18		854	897	9	1 -4		776	787	12	1-11	212	222	1	2 -7		1390	1343
5	1-23		754	761	7	1-17		388	367	9	1 -3		1265	-1271	12	1-10	394	385	1	2 -6		165	153
5	1-22		628	568	7	1-16		162	-171	9	1 -2		367	-354	12	1 -9	838	-841	1	2 -5		768	779
5	1-21		833	-822	7	1-15		1133	-1119	9	1 -1		749	724	12	1 -8	399	-405	1	2 -4		642	-622
5	1-20		645	649	7	1-14		763	-755	9	1 0		536	-527	12	1 -7	593	582	1	2 -3		-92	58
5	1-19		238	-245	7	1-13		966	952	9	1 1		234	217	12	1 -6	639	-632	1	2 -2		1854	1851
5	1-18		650	-656	7	1-12		855	-841	9	1 2		256	-264	12	1 -5	236	-234	1	2 -1		1147	-1184
5	1-17		200	-193	7	1-11		582	571	9	1 3		-111	52	12	1 -4	-120	-92	1	2 0		1175	-1248
5	1-16		662	-661	7	1-10		-57	33	9	1 4		353	378	12	1 -3	-117	83	1	2 1		1249	-1207
5	1-15		425	-429	7	1 -9		549	-521	9	1 5		575	575	12	1 -2	125	-3	1	2 2		532	-520
5	1-14		333	324	7	1 -8		844	826	9	1 6		494	496	12	1 -1	324	341	1	2 3		987	985
5	1-13		1559	1583	7	1 -7		728	705	9	1 7		1005	-1037	12	1 0	338	321	1	2 4		372	352
5	1-12		582	1005	7	1 -6		449	429	9	1 8		145	-144	12	1 1	846	-850	1	2 5		548	548
5	1-11		585	-585	7	1 -5		2141	-2147	9	1 9		-119	-78	12	1 2	301	324	1	2 6		651	-673
5	1-10		447	463	7	1 -4		1057	-1053	9	1 10		821	-842	12	1 3	148	121	1	2 7		269	-276
5	1 -9		124	-134	7	1 -3		440	432	9	1 11		336	315	12	1 4	212	-211	1	2 8		1368	1397
5	1 -8		405	-405	7	1 -2		776	-782	9	1 12		-121	-91	12	1 5	-118	-15	1	2 9		613	-630
5	1 -7		272	284	7	1 -1		1221	1192	9	1 13		335	-343	12	1 6	237	-244	1	2 10		1002	-976
5	1 -6		1551	-1617	7	1 0		757	781	9	1 14		463	483	12	1 7	-120	67	1	2 11		243	-253
5	1 -5		834	-831	7	1 1		856	-925	9	1 15		358	392	12	1 8	197	185	1	2 12		825	-844
5	1 -4		565	-586	7	1 2		1427	1404	10	1-25		318	302	13	1-19	266	282	1	2 13		951	972
5	1 -3		1670	1726	7	1 3		944	923	10	1-24		314	308	13	1-18	174	165	1	2 14		713	709
5	1 -2		178	203	7	1 4		-111	-18	10	1-23		-112	33	13	1-17	738	-744	1	2 15		552	544
5	1 -1		427	-397	7	1 5		673	-677	10	1-22		-116	-138	13	1-16	318	-329	1	2 16		757	-765
5	1 0		1135	1184	7	1 6		508	-505	10	1-21		829	-813	13	1-15	539	525	1	2 17		-102	3
5	1 1		1257	-1267	7	1 7		374	-364	10	1-20		358	-404	13	1-14	533	-552	1	2 18		521	512
5	1 2		477	-466	7	1 8		318	-331	10	1-19		508	522	13	1-13	204	193	1	2 19		251	-289
5	1 3		283	286	7	1 9		1464	1490	10	1-18		259	-279	13	1-12	-125	-133	1	2 20		152	152
5	1 4		1358	-1414	7	1 10		-112	51	10	1-17		148	-139	13	1-11	-131	-134	1	2 21		431	-414
5	1 5		1007	-990	7	1 11		573	-559	10	1-16		-105	-53	13	1-10	565	554	1	2 22		536	-537
5	1 6		382	-361	7	1 12		-112	9	10	1-15		118	-113	13	1 -9	530	538	1	2 23		-112	57
5	1 7		553	548	7	1 13		233	214	10	1-14		561	576	13	1 -8	472	468	1	2 24		295	310
5	1 8		916	887	7	1 14		247	249	10	1-13		459	470	13	1 -7	1074	-1078	1	2 25		238	229

Table 3. Continued.

H	K	L	F(O)	F(C)
2	2-24	211	204
2	2-25	158	135
2	2-24	331	352
2	2-23	-112	103
2	2-22	235	-252
2	2-21	481	-474
2	2-20	763	777
2	2-19	725	-740
2	2-18	776	-779
2	2-17	640	636
2	2-16	393	-403
2	2-15	1019	1019
2	2-14	935	926
2	2-13	458	-456
2	2-12	-63	-57
2	2-11	536	-511
2	2-10	1151	1066
2	2-9	1065	-1064
2	2-8	1214	-1214
2	2-7	338	347
2	2-6	1537	-1564
2	2-5	1754	1748
2	2-4	2037	2089
2	2-3	427	428
2	2-2	435	-367
2	2-1	537	-563
2	2 0	560	514
2	2 1	2311	-2263
2	2 2	337	-339
2	2 3	372	327
2	2 4	1730	-1781
2	2 5	1744	1733
2	2 6	1224	1159
2	2 7	610	643
2	2 8	331	327
2	2 9	356	-345
2	2 10	215	196
2	2 11	592	-567
2	2 12	249	260
2	2 13	317	-288
2	2 14	1567	-1584
2	2 15	635	672
2	2 16	434	501
2	2 17	351	359
2	2 18	505	521
2	2 19	468	-501
2	2 20	263	-254
2	2 21	572	-562
2	2 22	-115	107
2	2 23	205	-164
2	2 24	458	-503
2	2-26	310	-325
3	2-25	273	266
3	2-24	257	-276
3	2-23	347	341
3	2-22	1783	1672
3	2-21	-139	16
3	2-20	58	-58
3	2-19	476	-467
3	2-18	390	-367
3	2-17	-136	52
3	2-16	247	224
3	2-15	1525	1523
3	2-14	436	-464
3	2-13	507	517
3	2-12	1458	1459
3	2-11	-62	-56
3	2-10	111	-55
3	2-9	550	-584
3	2-8	547	-561
3	2-7	628	-629
3	2-6	1041	1016
3	2-5	531	523
3	2-4	1471	-1488
3	2-3	697	651
3	2-2	1257	1323
3	2-1	333	-287
3	2 1	1416	-1429
3	2 2	1528	-1528
3	2 3	436	-454
3	2 4	561	548
3	2 5	676	655
3	2 6	758	-755
3	2 7	1277	1259
3	2 8	234	215
3	2 9	205	217
3	2 10	399	367
3	2 11	430	-405
3	2 12	1504	-1555
3	2 13	442	-454
3	2 14	605	595
3	2 15	158	-156
3	2 16	295	-277
3	2 17	450	464
3	2 18	576	-571
3	2 19	-113	33
3	2 20	861	857
3	2 21	269	-325
3	2 22	223	-217
3	2 23	128	-142
4	2-26	254	-252
4	2-25	115	111
4	2-24	197	158
4	2-23	438	461
4	2-22	632	-632
4	2-21	634	653
4	2-20	666	651
4	2-19	-105	19
4	2-18	646	657
4	2-17	967	-980
4	2-16	1343	-1355
4	2-15	-132	-76
4	2-14	176	181
4	2-13	374	376
4	2-12	374	-378
4	2-11	612	625
4	2-10	572	558
4	2-9	563	-564
4	2-8	1022	1119
4	2-7	1369	-1375
4	2-6	1464	-1438
4	2-5	612	-608
4	2-4	365	375
4	2-3	1168	1178
4	2-2	231	-214
4	2-1	671	658
4	2 0	328	-316
4	2 1	170	157
4	2 2	2533	2556
4	2 3	386	-381
4	2 4	502	-494
4	2 5	596	-584
4	2 6	849	-835
4	2 7	908	905
4	2 8	457	435
4	2 9	1022	1123
4	2 10	-132	-13
4	2 11	478	-476
4	2 12	1156	1185
4	2 13	851	-838
4	2 14	466	-469
4	2 15	722	-716
4	2 16	715	-699
4	2 17	443	446
4	2 18	544	551
4	2 19	459	459
4	2 20	442	-465
4	2 21	-117	32
4	2 22	461	443
5	2-26	153	158
5	2-25	128	-129
5	2-24	728	-698
5	2-23	500	510
5	2-22	205	222
5	2-21	480	477
5	2-20	453	446
5	2-19	186	174
5	2-18	363	-367
5	2-17	642	-654
5	2-16	819	758
5	2-15	1269	-1269
5	2-14	572	-574
5	2-13	-59	45
5	2-12	642	-628
5	2-11	911	907
5	2-10	1427	1399
5	2-9	138	-116
5	2-8	341	-364
5	2-7	746	-745
5	2-6	431	435
5	2-5	951	-957
5	2-4	901	-901
5	2-3	463	494
5	2-2	851	-926
5	2-1	1209	1311
5	2 0	1581	1561
5	2 1	412	395
5	2 2	751	-752
5	2 3	-105	-18
5	2 4	277	295
5	2 5	745	-754
5	2 6	442	429
5	2 7	289	-273
5	2 8	1154	-1132
5	2 9	758	907
5	2 10	714	721
5	2 11	-110	41
5	2 12	134	175
5	2 13	512	-500
5	2 14	-110	82
5	2 15	312	-301
5	2 16	328	324
5	2 17	132	-78
5	2 18	644	-646
5	2 19	422	436
5	2 20	371	385
5	2 21	377	384
6	2-26	255	-279
6	2-25	348	-341
6	2-24	160	166
6	2-23	301	-305
6	2-22	296	-293
6	2-21	281	292
6	2-20	541	-501
6	2-19	214	206
6	2-18	1064	1045
6	2-17	-102	-73
6	2-16	317	-341
6	2-15	932	-940
6	2-14	143	-141
6	2-13	868	-841
6	2-12	326	300
6	2-11	689	686
6	2-10	1574	-1564
6	2 -9	1231	1215
6	2 -8	1054	1059
6	2 -7	375	365
6	2 -6	601	597
6	2 -5	320	-315
6	2 -4	441	-420
6	2 -3	1911	-1038
6	2 -2	263	241
6	2 -1	393	384
6	2 0	1508	-1521
6	2 1	561	958
6	2 2	722	697
6	2 3	327	353
6	2 4	1258	1255
6	2 5	1009	-1020
6	2 6	582	-567
6	2 7	550	-538
6	2 8	466	430
6	2 9	175	-166
6	2 10	752	-720
6	2 11	742	749
6	2 12	244	-212
6	2 13	213	234
6	2 14	930	913
6	2 15	200	-210
6	2 16	274	-274
6	2 17	162	-174
6	2 18	-161	92
6	2 19	-116	17
6	2 20	234	-227
7	2-26	531	516
7	2-25	256	-251
7	2-24	-116	61
7	2-23	726	-748
7	2-22	560	-577
7	2-21	113	-55
7	2-20	244	242
7	2-19	451	442
7	2-18	411	-431
7	2-17	321	314
7	2-16	358	351
7	2-15	274	-274
7	2-14	575	585
7	2-13	869	-895
7	2-12	1615	-1631
7	2-11	343	344
7	2-10	385	377
7	2 -9	1167	1172
7	2 -8	-102	-56
7	2 -7	763	772
7	2 -6	-101	18
7	2 -5	222	-228
7	2 -4	637	842
7	2 -3	1042	-1149
7	2 -2	1358	-1393
7	2 -1	512	-517
7	2 0	158	140
7	2 1	638	635
7	2 2	-110	-44
7	2 3	475	510
7	2 4	402	-389
7	2 5	428	-434
7	2 6	1346	1352
7	2 7	658	-658
7	2 8	860	-861
7	2 9	351	-348
7	2 10	521	-518
7	2 11	455	453
7	2 12	923	620
7	2 13	621	625
7	2 14	388	-346
7	2 15	-115	-74
7	2 16	463	429
7	2 17	166	-184
7	2 18	-127	-96
8	2-25	-118	92
8	2-24	182	-202
8	2-23	303	-317
8	2-22	415	423
8	2-21	570	-577
8	2-20	535	-533
8	2-19	256	295
8	2-18	-105	-38
8	2-17	550	566
8	2-16	166	177
8	2-15	558	595
8	2-14	176	-161
8	2-13	-103	70
8	2-12	1127	1134
8	2-11	599	-586
8	2-10	743	-740
8	2 -9	-103	-53
8	2 -8	936	-916
8	2 -7	937	965
8	2 -6	1100	1109
8	2 -5	-112	24
8	2 -4	301	-297
8	2 -3	550	-587
8	2 -2	605	595
8	2 -1	1123	-1117
8	2 0	220	-194
8	2 1	374	-381
8	2 2	908	-909
8	2 3	694	719
8	2 4	481	473
8	2 5	372	394
8	2 6	391	-396
8	2 7	-114	-39
8	2 8	459	464
8	2 9	215	-225
8	2 10	330	332
8	2 11	377	-392
8	2 12	1148	-1156
8	2 13	624	593
8	2 14	271	289
8	2 15	453	459
8	2 16	190	183
9	2-24	886	893
9	2-23	-115	1
9	2-22	259	-267
9	2-21	406	-396
9	2-20	146	-127
9	2-19	256	-262
9	2-18	130	-122
9	2-17	690	653
9	2-16	557	-549
9	2-15	723	715
9	2-14	1048	1045
9	2-13	136	134
9	2-12	154	-155
9	2-11	525	-541
9	2-10	193	-181
9	2 -9	945	-959
9	2 -8	211	214
9	2 -7	276	266
9	2 -6	1158	-1213
9	2 -5	741	739
9	2 -4	1031	1025
9	2 -3	313	-302
9	2 -2	723	723
9	2 -1	636	-577
9	2 0	796	-768
9	2 1	430	-439
9	2 2	230	203
9	2 3	452	455
9	2 4	531	-546
9	2 5	878	877
9	2 6	435	427
9	2 7	146	179
9	2 8	529	533
9	2 9	320	-344
9	2 10	665	-689
9	2 11	226	-222
9	2 12	328	335
9	2 13	-123	-11
9	2 14	219	-223
10	2-23	352	364
10	2-22	539	543
10	2-21	-115	102
10	2-20	319	395
10	2-19	491	-493
10	2-18	657	-649
10	2-17	124	-91
10	2-16	351	349
10	2-15	351	404
10	2-14	449	-444
10	2-13	299	305
10	2-12	410	425
10	2-11	238	-219
10	2-10	677	684
10	2 -9	856	-859
10	2 -8	895	-872
10	2 -7	530	-594
10	2 -6	421	435
10	2 -5	443	426
10	2 -4	350	-364
10	2 -3	578	494
10	2 -2	366	-375
10	2 -1	347	336
10	2 0	1237	1215
10	2 1	215	-195
10	2 2	543	-559
10	2 3	227	-233
10	2 4	140	-107
10	2 5	297	283
10	2 6	-123	-101
10	2 7	624	652
10	2 8	317	-349
10	2 9	-120	-42
10	2 10	892	891
10	2 11	347	-343
10	2 12	213	-233
11	2-22	222	233
11	2-21	204	201
11	2-20	-115	-73
11	2-19	289	-295
11	2-18	518	503
11	2-17	840	-925
11	2-16	659	-663
11	2-15	-114	17
11	2-14	231	-303
11	2-13	550	541
11	2-12	405	405
11	2-11	172	159
11	2-10	-112	19
11	2 -9	351	-366
11	2 -8	695	714
11	2 -7	637	-658
11	2 -6	767	-773
11	2 -5	-116	58
11	2 -4	590	-588
11	2 -3	1054	1060
11	2 -2	964	970
11	2 -1	499	488
11	2 0	195	-187
11	2 1	180	-187
11	2 2	311	287
11	2 3	406	-412
11	2 4	-117	-10
11	2 5	281	-278
11	2 6	596	-593
11	2 7	370	392
11	2 8	411	440
11	2 9	152	122
11	2 10	-124	-91
12	2-20	755	747
12	2-19	167	-153
12	2-18	297	-306
12	2-17	425	-410
12	2-16	-118	-70
12	2-15	421	-425
12	2-14	244	242
12	2-13	174	176
12	2-12	710	-688
12	2-11	508	510
12	2-10	454	456
12	2 -9	-123	80
12	2 -8	-117	-16
12	2 -7	-112	46
12	2 -6	-118	23
12	2 -5	380	-391
12	2 -4	263	245
12	2 -3	156	147
12	2 -2	911	-914
12	2 -1	668	687
12	2 0	417	410
12	2 1	-117	27
12	2 2	455	468
12	2 3	434	-404
12	2 4	414	-425
12	2 5	374	-384
12	2 6	351	353
13	2-17	-122	-50
13	2-16	391	386
13	2-15	416	-404
13	2-14	776	-799
13	2-13	-126	-137
13	2-12	186	205
13	2-11	545	557
13	2-10	225	-223
13	2 -9	538	513
13	2 -8	202	170
13	2 -7	-116	29
13	2 -6	631	636
13	2 -5	446	-431
13	2 -4	630	-631
13	2 -3	439	-436
13	2 -2	141	130
13	2 -1	209	230
13	2 0	233	-203
13	2 1	285	289
13	2 2	152	-178
14	2-11	-126	-13
14	2-10	249	-240
14	2 -9	421	441
14	2 -8	342	343
14	2 -7	-121	65
14	2 -6	219	-228
14	2 -5	184	-186
0	3 1	1128	-1123
0	3 2	115	126
0	3 3	1412	1412
0	3 4	114	117
0	3 5	433	433
0	3 6	-95	41
0	3 7	931	949
0	3 8	268	271
0	3 9	991	-983
0	3 10	495	458
0	3 11	1960	-1957
0	3 12	495	-490
0	3 13	787	793
0	3 14	242	-235
0	3 15	390	367
0	3 16	234	235
0	3 17	347	343
0	3 18	170	-179
0	3 19	-112	-119
0	3 20	-117	-83
0	3 21	949	-988
0	3 22	-110	21
0	3 23	534	540
0	3 24	-117	-26
1	3-24	235	183
1	3-23	228	-221
1	3-22	424	413

Table 3. 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)
1	3-21	-108	51	3	3-14	-104	-116	5	3 -4	535	533	7	3 12	-115	-72	10	3 5	827	-844
1	3-20	319	-322	3	3-13	937	935	5	3 -3	-109	33	7	3 13	323	325	10	3 6	-119	-9
1	3-19	685	-674	3	3-12	117	106	5	3 -2	431	-444	7	3 14	-127	-135	10	3 7	444	464
1	3-18	-104	-2	3	3-11	485	490	5	3 -1	670	-674	7	3 15	615	591	10	3 8	-122	-38
1	3-17	639	-641	3	3-10	227	215	5	3 0	156	-152	7	3 16	-122	-67	10	3 9	436	403
1	3-16	466	464	3	3 -9	1156	1150	5	3 1	1031	986	8	3-23	-115	9	10	3 10	-130	-110
1	3-15	1227	1247	3	3 -8	380	395	5	3 2	194	203	8	3-22	284	290	11	3-19	249	228
1	3-14	349	-378	3	3 -7	1744	-1758	5	3 3	1556	1578	8	3-21	374	-379	11	3-18	290	312
1	3-13	430	-415	3	3 -6	347	-337	5	3 4	232	-251	8	3-20	-110	-13	11	3-17	377	-379
1	3-12	214	-227	3	3 -5	460	-470	5	3 5	1142	-1134	8	3-19	219	-213	11	3-16	-119	113
1	3-11	153	156	3	3 -4	179	187	5	3 6	274	259	8	3-16	314	-333	11	3-15	171	-174
1	3-10	-96	-12	3	3 -3	673	673	5	3 7	124	-128	8	3-17	801	-795	11	3-14	273	-282
1	3 -5	556	-565	3	3 -2	829	801	5	3 8	-110	-79	8	3-16	128	95	11	3-13	687	-679
1	3 -8	511	-513	3	3 -1	171	-173	5	3 9	138	147	8	3-15	1013	1023	11	3-12	311	311
1	3 -7	1288	-1284	3	3 0	-114	-131	5	3 10	135	129	8	3-14	231	-224	11	3-11	831	835
1	3 -6	252	-264	3	3 1	761	766	5	3 11	255	-232	8	3-13	443	483	11	3-10	173	152
1	3 -5	2307	2303	3	3 2	451	-465	5	3 12	466	444	8	3-12	296	-273	11	3 -9	646	626
1	3 -4	-95	-66	3	3 3	1346	-1045	5	3 13	1017	1014	8	3-11	620	-613	11	3 -8	209	-192
1	3 -3	960	956	3	3 4	209	186	5	3 14	315	-313	8	3-10	-106	-35	11	3 -7	833	-842
1	3 -2	113	-95	3	3 5	1372	-1374	5	3 15	614	-643	8	3 -9	258	269	11	3 -6	147	143
1	3 -1	644	-631	3	3 6	173	-147	5	3 16	135	-151	8	3 -8	-112	-97	11	3 -5	-123	-82
1	3 0	266	295	3	3 7	1049	1030	5	3 17	423	-432	8	3 -7	869	-861	11	3 -4	192	-187
1	3 1	354	327	3	3 8	443	-439	5	3 18	221	219	8	3 -6	346	349	11	3 -3	643	-664
1	3 2	261	-258	3	3 9	-109	69	6	3 17	-117	65	8	3 -5	639	651	11	3 -2	332	-295
1	3 3	1726	-1742	3	3 10	-104	-15	6	3-25	424	422	8	3 -4	-114	-20	11	3 -1	579	581
1	3 4	442	418	3	3 11	1065	1052	6	3-24	-119	-25	8	3 -3	1197	1202	11	3 0	-120	9
1	3 5	659	664	3	3 12	124	-70	6	3-23	771	-754	8	3 -2	270	-257	11	3 1	1045	1033
1	3 6	558	565	3	3 13	-103	-43	6	3-22	-118	12	8	3 -1	911	-995	11	3 2	143	-103
1	3 7	404	421	3	3 14	167	165	6	3-21	-108	11	8	3 0	825	821	11	3 3	534	-500
1	3 8	645	-658	3	3 15	952	-943	6	3-20	166	158	8	3 1	303	-311	11	3 4	222	228
1	3 9	706	-706	3	3 16	-112	72	6	3-19	-106	46	8	3 2	-117	5	11	3 5	-124	-109
1	3 10	-99	11	3	3 17	537	545	6	3-18	135	119	8	3 3	954	-979	11	3 6	-116	34
1	3 11	-100	-73	3	3 18	-115	14	6	3-17	328	326	8	3 4	443	-453	11	3 7	243	-212
1	3 12	271	282	3	3 19	-113	71	6	3-16	-105	-53	8	3 5	-116	33	12	3-17	405	392
1	3 13	1155	-1153	3	3 20	200	190	6	3-15	750	744	8	3 6	166	173	12	3-16	-133	165
1	3 14	391	-377	3	3 21	-121	23	6	3-14	428	424	8	3 7	1217	1239	12	3-15	780	-789
1	3 15	185	182	3	3 22	206	-191	6	3-13	1418	-1401	8	3 8	152	-153	12	3-14	232	213
1	3 16	-107	-73	4	3-25	736	-732	6	3-12	-106	-44	8	3 9	597	-583	12	3-13	291	-218
1	3 17	1073	1064	4	3-24	156	-102	6	3-11	688	-678	8	3 10	-122	-55	12	3-12	331	-335
1	3 18	154	-147	4	3-23	248	-248	6	3-10	470	-468	8	3 11	225	-249	12	3-11	-123	-27
1	3 19	238	-211	4	3-22	-153	21	6	3 -9	192	172	8	3 12	-120	33	12	3-10	-119	73
1	3 20	122	76	4	3-21	659	660	6	3 -8	-104	-48	8	3 13	-123	56	12	3 -9	-129	113
1	3 21	183	185	4	3-20	221	-232	6	3 -7	362	368	8	3 14	146	-136	12	3 -8	-124	30
1	3 22	225	217	4	3-19	119	27	6	3 -6	349	-346	9	3-22	186	-174	12	3 -7	716	725
1	3 23	491	-350	4	3-18	-104	64	6	3 -5	1676	1686	9	3-21	451	435	12	3 -6	307	-323
2	3-25	269	-302	4	3-17	600	610	6	3 -4	-117	-105	9	3-20	-119	81	12	3 -5	695	-673
2	3-24	-114	25	4	3-16	-100	-46	6	3 -3	1019	-1040	9	3-19	587	-593	12	3 -4	-120	27
2	3-23	849	865	4	3-15	660	-616	6	3 -2	132	138	9	3-18	-114	-53	12	3 -3	175	-173
2	3-22	-107	47	4	3-14	139	99	6	3 -1	825	-818	9	3-17	264	-253	12	3 -2	-120	-43
2	3-21	-117	33	4	3-13	1146	-1159	6	3 0	-116	-57	9	3-16	352	-373	12	3 -1	293	277
2	3-20	346	343	4	3-12	541	547	6	3 1	736	712	9	3-15	324	309	12	3 0	-126	115
2	3-19	715	-706	4	3-11	1479	1470	6	3 2	-117	108	9	3-14	-110	46	12	3 1	149	-148
2	3-18	810	-154	4	3-10	239	-246	6	3 3	-123	65	9	3-13	592	589	12	3 2	-122	9
2	3-17	163	-184	4	3 -9	243	256	6	3 4	-116	-41	9	3-12	-114	83	12	3 3	814	819
2	3-16	412	-389	4	3 -8	126	171	6	3 5	1302	1293	9	3-11	912	916	13	3-12	-125	-56
2	3-15	767	-746	4	3 -7	-99	74	6	3 6	163	106	9	3-10	206	214	13	3-11	691	-688
2	3-14	162	176	4	3 -6	777	778	6	3 7	493	-485	9	3 -9	1267	-1247	13	3-10	228	-230
2	3-13	1455	1457	4	3 -5	683	-680	6	3 8	669	652	9	3 -8	-116	62	13	3 -9	697	708
2	3-12	366	-352	4	3 -4	141	-153	6	3 9	1610	-1593	9	3 -7	336	-333	13	3 -8	-125	-82
2	3-11	1117	1114	4	3 -3	2158	-2144	6	3 10	-117	95	9	3 -6	157	-180	13	3 -7	329	306
2	3-10	-95	32	4	3 -2	405	-416	6	3 11	262	267	9	3 -5	318	318	13	3 -6	-119	9
2	3 -9	1112	-1107	4	3 -1	1431	1334	6	3 12	414	-435	9	3 -4	505	503	13	3 -5	236	267
2	3 -8	221	216	4	3 0	192	161	6	3 13	-114	-54	9	3 -3	-118	17	13	3 -4	165	164
2	3 -7	211	-222	4	3 1	1169	1156	6	3 14	-119	113	9	3 -2	-117	56	13	3 -3	174	-193
2	3 -6	535	-523	4	3 2	209	-205	6	3 15	586	555	9	3 -1	856	855	0	4 0	-115	79
2	3 -5	864	-850	4	3 3	187	-185	6	3 16	-114	-49	9	3 0	349	-367	0	4 1	716	-725
2	3 -4	200	236	4	3 4	-104	-65	6	3 17	-120	5	9	3 1	913	-912	0	4 2	894	-886
2	3 -3	1345	1345	4	3 5	-130	60	6	3 18	157	-126	9	3 2	-125	133	0	4 3	1126	-1110
2	3 -2	247	-231	4	3 6	-104	-15	7	3-24	331	362	9	3 3	844	-885	0	4 4	-120	49
2	3 -1	1752	1814	4	3 7	1243	-1234	7	3-23	227	227	9	3 4	173	-181	0	4 5	218	-210
2	3 0	-110	19	4	3 8	125	-121	7	3-22	-115	-67	9	3 5	650	663	0	4 6	873	862
2	3 1	2022	-2026	4	3 9	947	945	7	3-21	765	-784	9	3 6	278	-296	0	4 7	1124	1127
2	3 2	846	826	4	3 10	184	182	7	3-20	245	-222	9	3 7	-119	7	0	4 8	479	-486
2	3 3	759	-760	4	3 11	1137	1138	7	3-19	452	-468	9	3 8	-121	40	0	4 9	418	397
2	3 4	625	-620	4	3 12	152	-175	7	3-18	379	387	9	3 9	736	751	0	4 10	343	339
2	3 5	683	-675	4	3 13	207	-177	7	3-17	1065	1045	9	3 10	-122	-73	0	4 11	460	-455
2	3 6	526	-513	4	3 14	281	276	7	3-16	-106	-24	9	3 11	147	-207	0	4 12	177	-186
2	3 7	120	157	4	3 15	-155	-16	7	3-15	189	-221	9	3 12	-125	2	0	4 13	548	-547
2	3 8	-112	44	4	3 16	396	407	7	3-14	167	-150	10	3-21	-114	-36	0	4 14	285	297
2	3 9	2117	2099	4	3 17	1092	-1060	7	3-13	165	166	10	3-20	-110	-88	0	4 15	156	-171
2	3 10	304	-285	4	3 18	313	-308	7	3-12	-103	-42	10	3-19	481	481	0	4 16	775	759
2	3 11	187	-176	4	3 19	-113	-27	7	3-11	630	-627	10	3-18	-109	-15	0	4 17	448	401
2	3 12	-104	62	4	3 20	201	-183	7	3-10	434	-433	10	3-17	471	-459	0	4 18	695	-689
2	3 13	684	-675	5	3-25	404	-392	7	3 -9	1075	-1053	10	3-16	-115	-75	0	4 19	629	599
2	3 14	-103	41	5	3-24	230	-239	7	3 -8	213	-212	10	3-15	538	-525	0	4 20	-116	-35
2	3 15	277	285	5	3-23	142	-138	7	3 -7	1548	1541	10	3-14	292	303	0	4 21	-124	-158
2	3 16	155	-133	5	3-22	249	-244	7	3 -6	-116	-123	10	3-13	887	932	0	4 22	-114	-13
2	3 17	-104	32	5	3-21	284	-281	7	3 -5	626	633	10	3-12	-114	19	1	4-22	-120	137
2	3 18	164	202	5	3-20	-129	45	7	3 -4	-114	68	10	3-11	116	65	1	4-21	208	207
2	3 19	1053	1044	5	3-19	1417	1415	7	3 -3	189	-187	10	3-10	-114	-82	1	4-20	571	-563
2	3 20	-113	19	5	3-18	132	141	7	3 -2	270	261	10	3 -9	403	392	1	4-19	-108	0
2	3 21	254	-254	5	3-17	139	137	7	3 -1	288	-288	10	3 -8	424	456	1	4-18	588	583
2	3 22	-125	138	5	3-16	411	403	7	3 0	176	-169	10	3 -7	376	-367	1	4-17	757	-775
2	3-25	178	161	5	3-15	893	-909	7	3 1	1409	-1368	10	3 -6	-130	164	1	4-16	182	-219
2	3-24	179	200	5	3-14	-102	-65	7	3 2	-113	-39	10	3 -5	1174	-1197	1	4-15	-107	-80
2	3-23	-109	3	5	3-13	-93	-40	7	3 3	1010	1033	10	3 -4	195	-183	1	4-14	-107	106
2	3-22	-106	16	5	3-12	128	-146	7	3 4	508	507	10	3 -3	601	593	1	4-13	628	630
2	3-21	258	248	5	3-11	816	-819	7	3 5	466	439	10	3 -2	-119	-76	1	4-12	1064	1052
2	3-20	165	-158	5	3-10	802	811	7	3 6	-116	-26	10	3 -1	222	241	1	4-11	136	142
2	3-19	525	507	5	3 -9	548	542	7	3 7	417	-423	10	3 0	192	-179	1	4-10	1017	-1018
2	3-18	-104	-55	5	3 -8	118	-57	7	3 8	211	-222	10	3 1	143	132	1	4 -9	-102	30
2	3-17	1147	-1140	5	3 -7	947	941	7	3 9	-114	-70	10	3 2	175	-189	1	4 -8	225	-217
2	3-16	315	-310	5	3 -6	448	-441	7	3 10	203	216	10	3 3	-119	104	1	4 -7	501	-516
2	3-15	-106	-25	5	3 -5	1527	-1529	7	3 11	844	-834	10	3 4	-113	-12	1	4 -6	248	-261

Table 3. 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)
1	4	-5	613	-623	3	4	12	646	-684	6	4	-8	566	590	9	4	-8	-117	-16	1	5	3	619	-595
1	4	-4	249	-265	3	4	14	334	306	6	4	-7	221	-222	9	4	-7	322	-324	1	5	4	784	-768
1	4	-3	427	425	3	4	14	152	-157	6	4	-6	-108	-25	9	4	-6	506	-573	1	5	5	130	122
1	4	-2	519	508	3	4	15	207	-227	6	4	-5	742	757	9	4	-5	611	-529	1	5	6	186	-182
1	4	-1	462	466	3	4	16	169	-178	6	4	-4	625	-637	9	4	-4	695	690	1	5	7	172	-154
1	4	0	1439	-1520	3	4	17	217	-192	6	4	-3	559	614	9	4	-3	261	-262	1	5	8	436	404
1	4	1	-111	72	3	4	18	-113	63	6	4	-2	161	171	9	4	-2	210	218	1	5	9	633	-685
1	4	2	161	-153	3	4	19	214	-203	6	4	-1	208	-118	9	4	-1	767	744	1	5	10	601	610
1	4	3	264	-222	4	4	-23	479	-482	6	4	0	783	-782	9	4	0	-125	-92	1	5	11	531	514
1	4	4	674	657	4	4	-22	211	-232	6	4	1	579	-596	9	4	1	371	359	1	5	12	224	-229
1	4	5	831	-692	4	4	-21	179	-171	6	4	2	301	310	9	4	2	469	457	1	5	13	-117	-91
1	4	6	226	-233	4	4	-20	222	222	6	4	3	567	-571	9	4	3	412	-416	1	5	14	360	-349
1	4	7	231	248	4	4	-19	274	283	6	4	4	293	289	9	4	4	690	-711	1	5	15	-118	85
1	4	8	1134	1123	4	4	-18	200	215	6	4	5	655	649	9	4	5	239	-277	1	5	16	-115	35
1	4	9	795	783	4	4	-17	415	483	6	4	6	400	-401	9	4	6	184	187	1	5	17	123	162
1	4	10	-106	3	4	4	-16	871	-873	6	4	7	667	672	9	4	7	-134	-125	1	5	18	-125	129
1	4	11	-105	-11	4	4	-15	299	335	6	4	8	457	436	9	4	8	363	381	2	5	-19	-115	45
1	4	12	499	-506	4	4	-14	273	304	6	4	9	185	-173	9	4	9	231	267	2	5	-18	124	134
1	4	13	-105	-91	4	4	-13	699	-708	6	4	10	416	-413	10	4	-17	131	127	2	5	-17	508	528
1	4	14	361	407	4	4	-12	353	-368	6	4	11	401	-384	10	4	-16	164	181	2	5	-16	275	-273
1	4	15	340	-368	4	4	-11	747	-754	6	4	12	350	417	10	4	-15	253	-249	2	5	-15	493	-491
1	4	16	141	-159	4	4	-10	-112	58	6	4	13	233	-232	10	4	-14	413	-401	2	5	-14	238	-244
1	4	17	139	-139	4	4	-9	523	531	6	4	14	662	637	10	4	-13	479	-471	2	5	-13	-107	37
1	4	18	313	300	4	4	-8	1241	1236	6	4	15	-109	109	10	4	-12	-116	24	2	5	-12	-107	18
1	4	19	365	376	4	4	-7	493	500	7	4	-21	-123	131	10	4	-11	157	179	2	5	-11	-115	-124
1	4	20	222	-233	4	4	-6	758	-755	7	4	-20	325	344	10	4	-10	561	552	2	5	-10	675	675
1	4	21	153	144	4	4	-5	330	378	7	4	-19	619	-623	10	4	-9	317	317	2	5	-9	166	-144
2	4	-22	-114	110	4	4	-4	-112	3	7	4	-18	256	-246	10	4	-8	433	-465	2	5	-8	419	410
2	4	-21	271	267	4	4	-3	411	-421	7	4	-17	373	-364	10	4	-7	225	215	2	5	-7	1203	1216
2	4	-20	581	575	4	4	-2	514	510	7	4	-16	239	246	10	4	-6	-124	42	2	5	-6	728	-708
2	4	-19	341	379	4	4	-1	1196	-1113	7	4	-15	577	583	10	4	-5	-125	-117	2	5	-5	198	-172
2	4	-18	409	-425	4	4	0	152	-158	7	4	-14	759	761	10	4	-4	131	133	2	5	-4	459	-451
2	4	-17	-110	51	4	4	1	-119	15	7	4	-13	504	495	10	4	-3	400	-419	2	5	-3	432	-421
2	4	-16	-109	63	4	4	2	814	815	7	4	-12	511	-511	10	4	-2	179	192	2	5	-2	144	104
2	4	-15	813	-804	4	4	3	1103	1088	7	4	-11	132	88	10	4	-1	138	-162	2	5	-1	-119	-66
2	4	-14	437	422	4	4	4	1137	-1026	7	4	-10	-108	21	10	4	0	531	534	2	5	0	354	358
2	4	-13	322	-305	4	4	5	371	360	7	4	-9	563	-563	10	4	1	418	411	2	5	1	698	-679
2	4	-12	564	-583	4	4	6	421	-424	7	4	-8	318	-309	10	4	2	661	-659	2	5	2	351	347
2	4	-11	934	954	4	4	7	315	-311	7	4	-7	553	-556	10	4	3	291	265	2	5	3	942	964
2	4	-10	354	402	4	4	8	217	205	7	4	-6	-115	-96	10	4	4	149	-142	2	5	4	447	-451
2	4	-9	367	376	4	4	9	552	-936	7	4	-5	462	467	10	4	5	146	-87	2	5	5	-111	-94
2	4	-8	724	-702	4	4	10	692	-657	7	4	-4	746	763	10	4	6	-133	145	2	5	6	435	-411
2	4	-7	-105	57	4	4	11	-113	-55	7	4	-3	573	574	11	4	-15	-127	77	2	5	7	935	-947
2	4	-6	612	-661	4	4	12	445	431	7	4	-2	917	-912	11	4	-14	-123	-43	2	5	8	191	206
2	4	-5	1040	-1063	4	4	13	735	741	7	4	-1	-121	-11	11	4	-13	457	-473	2	5	9	193	183
2	4	-4	831	823	4	4	14	-115	-34	7	4	0	209	-180	11	4	-12	439	443	2	5	10	338	339
2	4	-3	944	-936	4	4	15	241	225	7	4	1	332	-352	11	4	-11	475	-472	2	5	11	331	-367
2	4	-2	538	-524	4	4	16	359	-373	7	4	2	447	454	11	4	-10	373	-315	2	5	12	473	474
2	4	-1	595	624	4	4	17	277	-287	7	4	3	494	-535	11	4	-9	555	553	2	5	13	608	624
2	4	0	714	715	4	4	18	423	424	7	4	4	160	-119	11	4	-8	638	659	2	5	14	192	-144
2	4	1	763	758	5	4	-22	148	-133	7	4	5	-122	26	11	4	-7	475	486	2	5	15	499	493
2	4	2	232	230	5	4	-21	523	-534	7	4	6	769	774	11	4	-6	-127	-69	2	5	16	588	-594
2	4	3	303	-292	5	4	-20	-117	126	7	4	7	622	618	11	4	-5	-125	-103	2	5	17	529	-525
2	4	4	341	-329	5	4	-19	-109	20	7	4	8	138	-122	11	4	-4	435	-454	3	5	-19	344	358
2	4	5	560	-567	5	4	-18	171	-182	7	4	9	155	141	11	4	-3	341	-327	3	5	-18	329	329
2	4	6	1284	1288	5	4	-17	559	567	7	4	10	-124	-119	11	4	-2	445	433	3	5	-17	-112	-51
2	4	7	910	-941	5	4	-16	473	489	7	4	11	271	-256	11	4	-1	413	-423	3	5	-16	-119	-38
2	4	8	137	158	5	4	-15	227	230	7	4	12	251	251	11	4	0	329	-329	3	5	-15	367	360
2	4	9	575	546	5	4	-14	713	-727	7	4	13	199	-203	11	4	1	338	334	3	5	-14	334	-344
2	4	10	293	-285	5	4	-13	-105	-66	7	4	14	278	-240	11	4	2	189	232	3	5	-13	134	-148
2	4	11	886	882	5	4	-12	131	116	8	4	-21	610	-613	12	4	-8	-127	27	3	5	-12	144	-146
2	4	12	222	215	5	4	-11	769	-781	8	4	-19	148	156	12	4	-7	389	349	3	5	-11	515	-520
2	4	13	-112	-81	5	4	-10	795	797	8	4	-18	-114	82	12	4	-6	240	-229	3	5	-10	-113	113
2	4	14	514	-518	5	4	-9	251	-271	8	4	-17	469	-453	12	4	-5	311	329	3	5	-9	547	559
2	4	15	462	-462	5	4	-8	347	-357	8	4	-16	468	492	0	5	1	422	441	3	5	-8	425	422
2	4	16	364	373	5	4	-7	1157	1180	8	4	-15	442	-428	0	5	2	751	-751	3	5	-7	-102	-25
2	4	17	419	-400	5	4	-6	1159	1051	8	4	-14	259	-238	0	5	3	534	559	3	5	-6	-126	73
2	4	18	-112	-2	5	4	-5	343	314	8	4	-13	575	575	0	5	4	457	-467	3	5	-5	118	99
2	4	19	-112	23	5	4	-4	253	-254	8	4	-12	417	408	0	5	5	893	-891	3	5	-4	675	-689
2	4	20	329	-319	5	4	-3	206	-201	8	4	-11	327	298	0	5	6	398	391	3	5	-3	-116	-97
3	4	-22	580	573	5	4	-2	1113	-1130	8	4	-10	767	-796	0	5	7	135	-125	3	5	-2	629	-627
3	4	-21	324	333	5	4	-1	243	-232	8	4	-9	154	156	0	5	8	384	377	3	5	-1	851	-875
3	4	-20	-106	21	5	4	0	771	786	8	4	-8	457	-449	0	5	9	331	349	3	5	0	450	484
3	4	-19	452	433	5	4	1	512	-528	8	4	-7	483	-436	0	5	10	-113	-57	3	5	1	336	329
3	4	-18	129	93	5	4	2	274	-255	8	4	-6	494	493	0	5	11	134	93	3	5	2	532	565
3	4	-17	-107	73	5	4	3	566	560	8	4	-5	714	-721	0	5	12	327	-335	3	5	3	235	-220
3	4	-16	213	-225	5	4	4	-112	-16	8	4	-4	555	-585	0	5	13	213	223	3	5	4	-110	58
3	4	-15	463	-444	5	4	5	539	526	8	4	-3	443	459	0	5	14	264	-267	3	5	5	-119	-37
3	4	-14	1011	-1022	5	4	6	251	-241	8	4	-2	718	731	0	5	15	745	-772	3	5	6	427	-414
3	4	-13	540	-523	5	4	7	287	-300	8	4	-1	590	577	0	5	16	239	189	3	5	7	518	491
3	4	-12	747	757	5	4	8	995	-1006	8	4	0	-117	12	0	5	17	152	-143	3	5	8	163	-116
3	4	-11	297	306	5	4	9	219	-157	8	4	1	-124	-79	0	5	18	398	391	3	5	9	392	-399
3	4	-10	-111	81	5	4	10	811	781	8	4	2	666	-686	1	5	-19	-113	-25	3	5	10	239	264
3	4	-9	527	526	5	4	11	414	-383	8	4	3	-122	-8	1	5	-18	224	-209	3	5	11	123	135
3	4	-8	626	-633	5	4	12	143	134	8	4	4	895	923	1	5	-17	488	-474	3	5	12	255	262
3	4	-7	-106	113	5	4	13	-113	74	8	4	5	613	-627	1	5	-16	453	-454	3	5	13	218	227
3	4	-6	177	182	5	4	14	-117	-79	8	4	6	-129	149	1	5	-15	258	269	3	5	14	-117	49
3	4	-5	312	-311	5	4	15	513	514	8	4	7	-123	-16	1	5	-14	133	-87	3	5	15	-115	-21
3	4	-4	526	-544	5	4	16	511	525	8	4	8	-122	-68	1	5	-13	623	-633	3	5	16	174	-167
3	4	-3	772	-767	5	4	17	-124	-38	8	4	9	591	599	1	5	-12	712	731	4	5	-19	498	-476
3	4	-2	615	667	6	4	-22	161	-183	8	4	10	-128	94	1	5	-11	218	229	4	5	-18	539	517
3	4	-1	-120	-80	6	4	-21	157	-216	8	4	11	165	174	1	5	-10	397	364	4	5	-17	304	328
3	4	0	518	522	6	4	-20	514	-500	8	4	12	511	-541	1	5	-9	710	719	4	5	-16	316	313
3	4	1	661	682	6	4	-19	442	-436	9	4	-19	-116	72	1	5	-8	452	-444	4	5	-15	402	411
3	4	2	230	-172	6	4	-18	528	540	9	4	-18	156	-175	1	5	-7	565	-557	4	5	-14	376	-330
3	4	3	357	362	6	4	-17	-113	-21	9	4	-17	229	-219	1	5	-6	117	-79	4	5	-13	120	-105
3	4	4	430	466	6	4	-16	-112	116	9	4	-16	631	-623	1	5	-5	525	512	4	5	-12	472	-482
3	4	5	448	-439	6	4	-15	503	506	9	4	-15	535	-526	1	5	-4	168	-153	4	5	-11	412	421
3	4	6	515	-485	6	4	-14	-110	102	9	4	-14	533	525	1	5	-3	311	-315	4	5	-10	279	-261
3	4	7	373	-362	6	4	-13	302	290	9	4	-13	-115	-93	1	5	-2	286	274	4	5	-9	943	-945
3	4	8	150	163	6	4	-12	153	182	9	4	-12	-118	-85	1	5	-1	-111	39	4	5	-8	352	359
3	4	9	216	-212	6	4	-11	-102	-1	9	4	-11	660	664	1	5	0	549	568	4	5	-7	275	-283
3	4	10	623	624	6	4	-10	549	-536	9	4	-10	280	-311	1	5	1	887	864	4	5	-6	353	340
3	4	11	264	282	6	4	-9	784	-778	9	4	-9	184	193	1	5	2	282	-250	4	5	-5	826	822

Table 3. Continued.

H	K	L	F(O)	F(C)
4	5	-4	313	-335
4	5	-3	376	-356
4	5	-2	337	-345
4	5	-1	-121	80
4	5	0	167	-209
4	5	1	618	-624
4	5	2	323	259
4	5	3	342	-374
4	5	4	740	743
4	5	5	534	534
4	5	6	-116	-29
4	5	7	-116	17
4	5	8	582	-581
4	5	9	277	274
4	5	10	-122	-154
4	5	11	-121	-112
4	5	12	254	255
4	5	13	572	-559
4	5	14	246	241
5	5	15	173	146
5	5	16	130	-115
5	5	17	-112	-41
5	5	16	335	322
5	5	15	147	129
5	5	14	296	283
5	5	13	640	644
5	5	12	554	-624
5	5	11	751	-809
5	5	10	491	-476
5	5	9	-115	-115
5	5	8	-106	35
5	5	7	-112	-29
5	5	6	644	642
5	5	5	398	-389
5	5	4	377	339
5	5	3	666	682
5	5	2	478	-511
5	5	1	242	-222
5	5	0	281	-267
5	5	1	398	-352
5	5	2	254	239
5	5	3	462	479
5	5	4	-125	136
5	5	5	333	-336
5	5	6	420	412
5	5	7	646	654
5	5	8	240	-257
5	5	9	-125	89
5	5	10	578	-561
5	5	11	533	-557
5	5	12	-124	-121
5	5	13	256	278
6	5	16	155	-153
6	5	17	376	-381
6	5	16	134	131
6	5	15	149	136
6	5	14	248	239
6	5	13	217	-204
6	5	12	-114	76
6	5	11	352	414
6	5	10	324	-324
6	5	9	-111	12
6	5	8	212	-158
6	5	7	670	-666
6	5	-6	242	236
6	5	-5	239	258
6	5	-4	574	568
6	5	-3	138	-130
6	5	-2	362	326
6	5	-1	534	539
6	5	0	515	-526
6	5	1	505	533
6	5	2	504	-468
6	5	3	666	-665
6	5	4	296	309
6	5	5	-129	42
6	5	6	223	250
6	5	7	144	-143
6	5	8	-121	-55
6	5	9	-139	121
6	5	10	237	-250
6	5	11	421	416
7	5	-17	-116	12
7	5	-16	153	-162
7	5	-15	533	-559
7	5	-14	527	543
7	5	-13	191	215
7	5	-12	424	453
7	5	-11	461	462
7	5	-10	214	-215
7	5	-9	235	-235
7	5	-8	176	-165
7	5	-7	326	301
7	5	-6	-121	-72
7	5	-5	417	-428
7	5	-4	257	252
7	5	-3	-131	100
7	5	-2	403	385
7	5	-1	809	801
7	5	0	-139	-53
7	5	1	339	-301
7	5	2	539	-567
7	5	3	-126	-56
7	5	4	238	-280
7	5	5	231	-236
7	5	6	269	232
7	5	7	304	-258
7	5	8	451	425
7	5	9	349	354
8	5	-16	-122	-84
8	5	-15	156	144
8	5	-14	-142	-45
8	5	-13	136	-125
8	5	-12	470	466
8	5	-11	252	-248
8	5	-10	505	523
8	5	-9	812	805
8	5	-8	456	-444
8	5	-7	129	-136
8	5	-6	353	-404
8	5	-5	-131	106
8	5	-4	-129	48
8	5	-3	-126	-51
8	5	-2	205	210
8	5	-1	708	-710
8	5	0	202	190
8	5	1	712	700
8	5	2	318	-285
8	5	3	-128	75
8	5	4	283	-266
8	5	5	419	-414
8	5	6	-129	62
8	5	7	-131	92
9	5	-13	434	-421
9	5	-12	-124	65
9	5	-11	351	385
9	5	-10	292	288
9	5	-9	-121	75
9	5	-8	161	166
9	5	-7	416	346
9	5	-6	514	-516
9	5	-5	-130	-79
9	5	-4	527	-519
9	5	-3	723	-715
9	5	-2	223	222
9	5	-1	361	378
9	5	0	348	357
9	5	1	163	-185
9	5	2	158	175
9	5	3	171	156
10	5	-2	-124	-44
10	5	-8	139	130
10	5	-7	206	212
10	5	-6	193	-205
10	5	-5	173	-184
10	5	-4	267	-210
10	5	-3	178	200
10	5	-2	-125	-133
0	6	0	816	824
0	6	1	-120	138
0	6	2	-112	-55
0	6	3	351	360
0	6	4	316	-305
0	6	5	152	116
0	6	6	362	-371
0	6	7	150	-157
0	6	8	176	-212
0	6	9	126	150
0	6	10	766	758
0	6	11	-119	-5
0	6	12	-124	141
0	6	13	-117	-95
1	6	-13	173	-174
1	6	-12	211	240
1	6	-11	-114	3
1	6	-10	234	-215
1	6	-9	-118	94
1	6	-8	739	732
1	6	-7	215	-229
1	6	-6	-109	19
1	6	-5	153	-145
1	6	-4	945	-905
1	6	-3	-114	97
1	6	-2	274	289
1	6	-1	-120	81
1	6	0	-134	69
1	6	1	236	221
1	6	2	355	382
1	6	3	-113	17
1	6	4	227	207
1	6	5	-111	14
1	6	6	769	-752
1	6	7	208	194
1	6	8	-115	95
1	6	9	-118	-101
1	6	10	-114	33
1	6	11	135	-137
1	6	12	145	152
2	6	-14	-121	-94
2	6	-13	130	-98
2	6	-12	738	-744
2	6	-11	121	-135
2	6	-10	308	403
2	6	-9	215	-232
2	6	-8	218	204
2	6	-7	-111	29
2	6	-6	254	226
2	6	-5	312	324
2	6	-4	291	274
2	6	-3	137	115
2	6	-2	1010	-1010
2	6	-1	-127	67
2	6	0	-134	4
2	6	1	-126	54
2	6	2	714	693
2	6	3	-120	-63
2	6	4	-117	31
2	6	5	-119	64
2	6	6	244	289
2	6	7	-115	41
2	6	8	939	-937
2	6	9	-122	-104
2	6	11	-124	-123
2	6	11	138	-233
3	6	-14	177	-153
3	6	-13	-113	-15
3	6	-12	229	-213
3	6	-11	219	-225
3	6	-10	439	-441
3	6	-9	152	137
3	6	-8	212	209
3	6	-7	279	312
3	6	-6	702	717
3	6	-5	-110	5
3	6	-4	237	-293
3	6	-3	135	154
3	6	-2	-134	-113
3	6	-1	-132	34
3	6	0	254	-261
3	6	1	-121	-92
3	6	2	294	-173
3	6	3	-123	51
3	6	4	723	703
3	6	5	166	-155
3	6	6	-118	33
3	6	7	160	-155
3	6	8	214	-197
3	6	9	-122	-33
3	6	10	275	-261
4	6	-13	-121	123
4	6	-12	-115	-32
4	6	-11	151	189
4	6	-10	657	-654
4	6	-9	-119	81
4	6	-8	-116	71
4	6	-7	-114	39
4	6	-6	144	-142
4	6	-5	-119	64
4	6	-4	717	743
4	6	-3	198	-147
4	6	-2	189	157
4	6	-1	-136	82
4	6	0	859	-877
4	6	1	161	139
4	6	2	-128	78
4	6	3	385	-392
4	6	4	-124	76
4	6	5	633	-635
4	6	6	298	276
4	6	7	-123	58
4	6	8	378	364
4	6	9	137	133
5	6	-12	156	137
5	6	-11	158	187
5	6	-10	118	24
5	6	-9	159	-131
5	6	-8	816	-796
5	6	-7	-123	-117
5	6	-6	248	277
5	6	-5	-123	-72
5	6	-4	255	272
5	6	-3	-124	-10
5	6	-2	-138	97
5	6	-1	-136	-107
5	6	0	327	307
5	6	1	245	-246
5	6	2	851	-892
5	6	3	-129	-31
5	6	4	-127	-20
5	6	5	136	131
5	6	6	596	618
5	6	7	-128	23
6	6	-11	188	-212
6	6	-10	-122	-81
6	6	-9	-119	86
6	6	-8	128	-114
6	6	-7	-121	-63
6	6	-6	472	-456
6	6	-5	193	-211
6	6	-4	-126	-46
6	6	-3	193	-159
6	6	-2	675	645
6	6	-1	183	-198
6	6	0	-141	-150
6	6	1	165	171
6	6	2	-132	63
6	6	3	139	207
6	6	4	378	-386
7	6	-8	-127	37
7	6	-7	134	-123
7	6	-6	771	-734
7	6	-5	144	-124
7	6	-4	-130	43
7	6	-3	-131	-19
7	6	-2	-129	71
7	6	-1	225	250
7	6	0	442	433

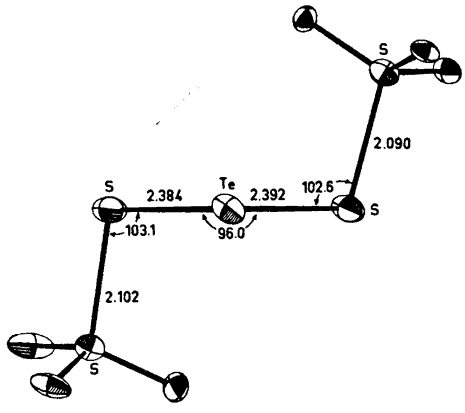

Fig. 1. The *trans* form of the telluropentathionate ion in $BaTe(S_2O_3)_2.3H_2O$ as seen along the *b* axis. The ellipsoids represent 50 % probability; the thermal parameters of the oxygen atoms are halved in size relative to those of the tellurium and sulphur atoms.

Table 4. Dimensions of the telluropentathionate ion. Standard deviations, including estimated uncertainties in unit cell dimensions, are given in parentheses.

Bond lengths and angles	
S(1) – S(2) = 2.1020(16) Å	S(4) – S(5) = 2.0898(16) Å
S(2) – Te = 2.3835(15)	Te – S(4) = 2.3924(16)
∠S(1) – S(2) – Te = 103.08(5)°	∠Te – S(4) – S(5) = 102.59(5)°
∠S(2) – Te – S(4) = 96.02(4)°	
S(1) – O(1) = 1.427(4) Å	S(5) – O(4) = 1.451(3) Å
S(1) – O(2) = 1.428(4)	S(5) – O(5) = 1.456(4)
S(1) – O(3) = 1.432(4)	S(5) – O(6) = 1.447(4)
∠S(2) – S(1) – O(1) = 107.2(2)°	∠S(4) – S(5) – O(4) = 106.7(2)°
∠S(2) – S(1) – O(2) = 102.2(2)°	∠S(4) – S(5) – O(5) = 102.0(2)°
∠S(2) – S(1) – O(3) = 108.2(2)°	∠S(4) – S(5) – O(6) = 109.1(2)°
∠O(1) – S(1) – O(2) = 114.3(3)°	∠O(4) – S(5) – O(4) = 113.5(2)°
∠O(1) – S(1) – O(3) = 111.1(3)°	∠O(4) – S(5) – O(6) = 112.5(2)°
∠O(2) – S(1) – O(3) = 113.1(3)°	∠O(5) – S(6) – O(6) = 112.1(2)°
Dihedral angles	
S(1)S(2)Te/S(2)TeS(4) = 87.7°	S(2)TeS(4)/TeS(4)S(5) = 98.7°
TeS(2)S(1)/S(2)S(1)O(1) = 70.0°	TeS(4)S(5)/S(4)S(5)O(4) = 68.8°
TeS(2)S(1)/S(2)S(1)O(2) = 169.5°	TeS(4)S(5)/S(4)S(5)O(5) = 171.9°
TeS(2)S(1)/S(2)S(1)O(3) = 50.0°	TeS(4)S(5)/S(4)S(5)O(6) = 53.1°
S(2)S(1)O(1)/S(2)S(1)O(2) = 120.5°	S(4)S(5)O(4)/S(4)S(5)O(5) = 119.3°
S(2)S(1)O(1)/S(2)S(1)O(3) = 119.9°	S(4)S(5)O(4)/S(4)S(5)O(6) = 121.9°
S(2)S(1)O(2)/S(2)S(1)O(3) = 119.6°	S(4)S(5)O(5)/S(4)S(5)O(6) = 118.8°
Non-bonded distances	
S(1) – Te = 3.5168(17) Å	Te – S(5) = 3.5028(18) Å
S(1) – S(4) = 4.3747(22)	S(2) – S(5) = 4.5652(23)
S(2) – S(4) = 3.5497(21)	S(1) – S(5) = 5.9914(27)

on film data [8] are about 1.5 times the standard deviations estimated for the film data values.

The non-planar S – S – Te – S – S chain in the *trans* form possesses the symmetry of a twofold axis, when the two halves of the chain are identical. This is the case in the crystals of tellurium dibenzenethiosulphonate,[17] where a twofold axis is crystallographically required.

In the present salt the crystal symmetry does not impose a twofold axis, but the dimensions are, except for the dihedral angles, nearly the same in the two halves of the telluropentathionate ion. The S – S and S – Te bond lengths, and the S – S – Te bond angles differ by only 0.0122 Å, 0.0089 Å, and 0.49°, respectively, and thus correspond nearly to the symmetry of a twofold axis. The dihedral angles between the S – S – Te and S – Te – S planes, however, differ by 11.0°. This difference in the degrees of rotation about the S – Te bonds is also seen from the non-bonded S(1) – S(4) and S(2) – S(5) distances which differ by 0.1905 Å. The dimensions of the two distorted tetrahedrally shaped thiosulphate groups are also nearly the same, and as seen from the

dihedral angles of Table 4, there is only a small difference in the degrees of rotation of the sulphonate groups about the S – S bonds.

The oxygen atoms are numbered in the same order as in the description of the structure of barium telluropentathionate dihydrate.[7] The dihedral angles thus show that the degrees of rotation of the sulphonate groups about the S – S bonds are different by about 21° in the two structures.

Table 5 gives the dimensions of the *trans* form of the S – S – Te – S – S chain in three compounds. The greatest variations are again found in the

Table 5. Bond lengths (Å), bond angles (°) and dihedral angles (°) of the S – S – Te – S – S chain in the *trans* form. Standard deviations are given in parentheses.

	$BaTe(S_2O_3)_2.3H_2O$	$Rb_2Te(S_2O_3)_2.1\frac{1}{2}H_2O$[10]	$Te(S_2O_2C_6H_5)_2$[17]
S – S	2.102(2), 2.090(2)	2.116(11), 2.126(9)	2.080(2)
S – Te	2.384(2), 2.392(2)	2.364(9), 2.370(7)	2.380(2)
∠S – S – Te	103.08(5), 102.59(5)	103.3(4), 102.8(3)	103.46(7)
∠S – Te – S	96.02(4)	100.1(3)	97.71(6)
∠SSTe/STeS	87.7, 98.7	77.7, 89.2	97.4

SSTe/STeS diredral angles. In each of the two salts, the two angles within a chain differ by about 11°, and the average values in the two salts differ by about 10°. The larger dihedral angles in tellurium dibenzenethiosulphonate might be due to the space requirement of the benzenesulphonate groups. The variations in the two salts, however, show that the dihedral angles are also influenced by the cation-oxygen coordination or by other packing effects. The variations in S – S and S – Te bond lengths, and in S – S – Te bond angles are small, though significant. The S – Te – S bond angles differ from 96.02(4)° in the barium salt to 100.1(3)° in the rubidium salt.

Among the barium salts of penta-, selenopenta- and telluropentathionic acids, $BaTe(S_2O_3).3H_2O$ is the only example where the anion occurs in the *trans* form. In the crystals where the *cis* form is found, each barium ion is in close contact with nine oxygen atoms, of which three are from the water molecules and the remaining six are from the anions. Two of the latter contacts are from different sulphonate groups of the same anion. All the oxygen atoms, except that of one of the water molecules in $BaSe(S_2O_3)_2.3H_2O$,[5] are involved in the Ba – O coordination. The Ba – O distances are in the range 2.75 – 2.94 Å.[4,5,7]

In the present structure the barium ions are each surrounded by eight oxygen atoms in the range 2.69 – 2.85 Å. All the water and sulphonate oxygen atoms, except O(4), take part once in these approaches. In addition there is one Ba – O distance of 3.19 Å, this oxygen atom being from the same sulphonate group as one of those involved in the closer contacts. The individual distances and related angles are listed in Table 6. Fig. 2 is a stereoscopic view as seen normal to the *b* crystal plane, showing the content of two

Table 6. Distances (Å), and angles (°) between directions, from barium ion to oxygen atoms. Standard deviations of the distances and angles are 0.003–0.005 Å and 0.1°, respectively.

				I	II	III	IV	V	VI	VII	VIII
I	$H_2O(1)$	$(1+x,1+y,z)$	2.794								
II	$H_2O(2)$	$(1+x,y,z)$	2.797	71.7							
III	$H_2O(3)$	(x,y,z)	2.838	148.1	131.7						
IV	O(1)	$(1+x,y,z)$	2.783	68.1	69.2	135.0					
V	O(2)	$(1-x,2-y,\bar{z})$	2.693	70.5	141.9	85.2	91.9				
VI	O(3)	$(1-x,1-y,\bar{z})$	2.808	123.1	126.8	64.6	71.7	72.4			
VII	O(5)	(x,y,z)	3.190	131.1	59.5	76.5	91.6	157.4	87.6		
VIII	O(5)	$(x,1+y,z)$	2.848	71.2	103.7	81.1	138.9	68.6	129.4	120.4	
IX	O(6)	(x,y,z)	2.824	120.3	71.7	63.6	133.8	134.2	116.5	46.7	73.8

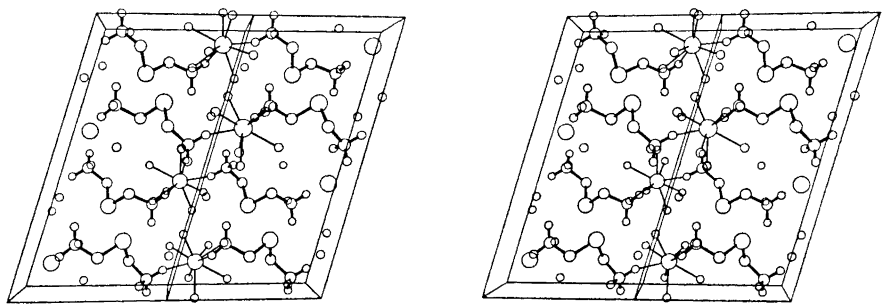

Fig. 2. A stereoscopic view as seen normal to the *b* crystal plane. The Ba–O coordination is indicated by the thin lines.

unit cells along the *a* axis. The Ba–O contacts are indicated by thin lines, whereas the bonds within the telluropentathionate ions are indicated by thick lines. The sulphonate oxygen atoms coordinated to the two barium ions in the middle of the figure are from the four nearest telluropentathionate ions shown, or from ions generated from the latter by addition or substraction of whole *b* units. The Ba–O coordination thus forms layers parallel to the *c* crystal plane, with thickness half the *c* spacing. The relation between neighbour layers is through twofold screw axes at $z=\frac{1}{4}$ and $\frac{3}{4}$. There are no Ba–O coordination contacts across the interfaces between the layers. This is very similar to the situation found for $BaTe(S_2O_3)_2.2H_2O$,[7] and the other barium salts with anions in the *cis* form, and where the crystals show perfect cleavage along the *c* crystal planes.[18] There is no such tendency of cleavage in the present crystals, and this might be due to the closer packing of the layers, to hydrogen bonds or other interionic contacts between the layers.

The most probable hydrogen bonds are; from $H_2O(1)$ to O(1) at (x,y,z) and $(x,y-1,z)$ with distances 2.993(6) Å and 3.126(6) Å and angle 117.9(2)°, from $H_2O(2)$ to $H_2O(1)$ at (x,y,z) and O(4) at $(1-x,\frac{1}{2}+y,\frac{1}{2}-z)$ with distances

2.917(6) Å and 2.864(5) Å and angle 99.3(2)°, and from $H_2O(3)$ to O(6) at (x,y,z) and O(3) at $(1-x,1-y,z)$ with distances 2.984(5) Å and 3.018(7) Å and angle 105.9(2)°. Only one of these assumed hydrogen bonds, $H_2O(2)-O(4)$, is across the interface between barium-oxygen coordination layers.

The closest interionic Te···Te approaches are between the tellurium atom at (x,y,z) and those at $(1-x,\frac{1}{2}+y,\frac{1}{2}-z)$ and $(1-x,-\frac{1}{2}+y,\frac{1}{2}-z)$. The distances are 3.833(1) Å and the Te···Te···Te angle is 86.31(3)°. The oxygen atom O(4), not involved in the Ba – O coordination, at $(1-x,\frac{1}{2}+y,\frac{1}{2}-z)$, is at a distance of 2.926(4) Å from tellurium. This oxygen atom and the tellurium at $(1-x,-\frac{1}{2}+y,\frac{1}{2}-z)$ are located only 0.11 Å and 0.40 Å, respectively, out of the S(2) – Te – S(4) plane. The angles between directions from tellurium to its four neighbours in this plane are: $\angle S(2)-Te-S(4)=96.02(4)°$, $\angle S(4)-Te\cdots Te=69.49(4)°$, $\angle Te\cdots Te\cdots O(4)=113.55(6)°$, $\angle O(4)\cdots Te-S(2)=80.63(7)°$, $\angle S(2)-Te\cdots Te=164.25(4)°$, and $\angle S(4)-Te\cdots O(4)=175.86(8)°$. There are thus two approximately linear systems, S(2) – Te···Te and S(4) – Te···O(4), at nearly right angles. The Te···Te and Te···O approaches are 0.29 Å and 0.65 Å, respectively, shorter than the sum of the van der Waals radii of the atoms involved.[19] The Te···Te and Te···O contacts are across the interfaces between the layers mentioned earlier.

REFERENCES

1. Foss, O. and Zachariasen, H. *Acta Chem. Scand.* **8** (1954) 473.
2. Foss, O. and Tjomsland, O. *Acta Chem. Scand.* **10** (1956) 288.
3. Foss, O. and Tjomsland, O. *Acta Chem. Scand.* **8** (1954) 1701.
4. Marøy, K. *Acta Chem. Scand.* **26** (1972) 36.
5. Marøy, K. *Acta Chem. Scand.* **26** (1972) 45.
6. Foss, O. and Tjomsland, O. *Acta Chem. Scand.* **12** (1958) 52.
7. Marøy, K. *Acta Chem. Scand.* **27** (1973) 1695.
8. Gjerrestad, K. and Marøy, K. *Acta Chem. Scand.* **24** (1970) 3402.
9. Foss, O. and Larssen, P. A. *Acta Chem. Scand.* **8** (1954) 1042.
10. Marøy, K. *Acta Chem. Scand.* **25** (1971) 2557.
11. Foss, O. and Tjomsland, O. *Acta Chem. Scand.* **10** (1956) 416.
12. Coppens, P., Leiserowitz, L. and Rabinovich, D. *Acta Cryst.* **18** (1965) 1035.
13. Zachariasen, W. H. *Acta Cryst.* **16** (1963) 1139.
14. *International Tables for X-Ray Crystallography*, Kynoch Press, Birmingham 1962, Vol. III.
15. Thomas, L. H. and Umeda, K. *J. Phys. Chem.* **26** (1957) 293.
16. Cromer, D. T. *Acta Cryst.* **18** (1965) 17.
17. Åse, K. *Acta Chem. Scand.* **25** (1971) 838.
18. Foss, O. *Advan. Inorg. Chem. Radiochem.* **2** (1960) 237.
19. Bondi, A. *J. Phys. Chem.* **68** (1964) 441.

Received December 27, 1972.