

crystallographically symmetry related. This is not the case in the present compound, which also shows an apparent difference between the two hydrogen-bridged formate groups. As mentioned previously, the distances C(2)-O(3) and C(2)-O(4) differ significantly in contrast to C(1)-O(1) and C(1)-O(2) which are of about the same length (*cf.* Table 4). Furthermore, the number of ionic contacts to potassium is different: one formate group has 4+1 whereas the other has 3+0 potassium-oxygen contacts.

According to the facts given above there may be a tendency towards less ionization in one of the groups than in the other. This has important bearings on the symmetry character of the hydrogen bond in the dimer.

As mentioned earlier the positions of the hydrogen atoms have not been located experimentally. Naturally nothing definite can be said about the character of the hydrogen bond from the X-ray data. Attempts will be made to attack this problem with other methods.

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The Crystal Structure of $\text{La}_2\text{Be}_2\text{O}_5^*$

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The crystal structure of $\text{La}_2\text{Be}_2\text{O}_5$ has been derived and refined from Mo $K\alpha$ X-ray diffraction data. The C-centered monoclinic unit cell with $a_0 = 7.536$, $b_0 = 7.348$, $c_0 = 7.439 \text{ \AA}$, $\beta = 91^\circ 33'$ contains four formula weights. The atomic arrangement in this equilibrium phase consists of a three-dimensional framework of cornersharing beryllium-oxygen tetrahedra with lanthanum atoms irregularly coordinated to ten oxygen atoms. The structure is compared with those of other oxide compounds containing beryllium and, in particular, with the structures of the recently reported nonequilibrium phases $\text{Ca}_{12}\text{Be}_{17}\text{O}_{29}$ and Y_2BeO_4 .

Introduction

The work described in this paper is part of a continuing study of binary oxide compounds that contain beryllia as a member. We have previously reported the crystal

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structures of the compounds $\text{Ca}_{12}\text{Be}_{17}\text{O}_{29}$ and Y_2BeO_4 (Harris & Yakel, 1966, 1967). Unusual trigonal beryllium-oxygen coordinations appeared in these probably metastable crystals which we could form only by quenching from the liquid state.

In both $\text{Ca}_{12}\text{Be}_{17}\text{O}_{29}$ and Y_2BeO_4 , the heavy cations have a large radius (0.99 and 0.97 Å, respectively) relative to those in the known equilibrium compounds

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of BeO with Al_2O_3 , SiO_2 , and Cr_2O_3 ($R_{\text{cat}}=0.51$, 0.42, and 0.69 Å, respectively) where regular, or nearly regular, tetrahedral beryllium–oxygen coordinations are found. We were thus prompted to investigate the crystal structure of an apparent equilibrium phase at the 1:2 composition of the La_2O_3 –BeO system in which the heavy cation radius is still larger (1.14 Å).

The compound $\text{La}_2\text{Be}_2\text{O}_5$ was first reported by Weir & Van Valkenburg (1960) who established its formula on the basis of solid-state synthesis and listed optical and powder-pattern X-ray diffraction data. An equilibrium phase diagram for the La_2O_3 –BeO system presented by Levin, Robbins & McMurdie (1961) shows a low-melting eutectic near the 1:2 composition and suggests that the $\text{La}_2\text{Be}_2\text{O}_5$ phase itself may form peritectically just to the BeO-rich side of the eutectic. A 1:2 phase was also observed in this system by Kuo & Yen (1964). They postulated an orthorhombic unit cell for their compound, with $a_0=3.81$, $b_0=9.95$, $c_0=11.07$ Å, $Z=4$ formula weights per cell, and gave refractive indices $n_x=1.980$ and $n_y=2.035$. Bragg spacings computed from these cell parameters are not in good agreement with the powder pattern for $\text{La}_2\text{Be}_2\text{O}_5$ listed by Weir & Van Valkenburg (1960) although the optical data show fair correspondence with the earlier results.

Experimental

We grew lath-like crystals of $\text{La}_2\text{Be}_2\text{O}_5$ by cooling melts near the eutectic of the La_2O_3 –BeO system. Our experiments confirmed the equilibrium nature of this

phase. Powder patterns from crushed crystals were in excellent agreement with the $\text{La}_2\text{Be}_2\text{O}_5$ pattern reported by Weir & Van Valkenburg (1960). The crystal selected for the X-ray diffraction investigation had a shape roughly approximating a right triangular prism with an altitude of 0.17 mm, a base width of 0.08 mm, and a uniform thickness of 0.03 mm. Later results showed that the triangular faces were parallel to {101} planes; smaller faces seemed to be parallel to {111} planes, but most were too uneven for positive identification. The \mathbf{b} axis was approximately parallel to the long triangular edge of the crystal.

Preliminary diffraction film data provided estimates of crystal orientation and lattice parameters. The crystal system was monoclinic and systematic reflection absences occurred consistent with space groups $C2/c$ or Cc . The crystal was transferred to a computer-controlled four-circle diffractometer (Busing, Ellison & Levy, 1964, 1965) for refinement of lattice parameters and collection of intensity data. The \mathbf{b} axis was offset about 5° from the φ axis of the diffractometer and zirconium- or niobium-filtered Mo $K\alpha$ X-radiation ($\lambda K\alpha_1=0.70926$ Å) was used for all experiments. A least-squares fit to measurements of scattering angles of 12 high-angle reflections gave the following lattice parameters:

$$\begin{aligned} a_0 &= 7.5356 \pm 0.0006 \text{ \AA} & \beta &= 91^\circ 33' \pm 1' \\ b_0 &= 7.3476 \pm 0.0017 & U &= 411.7 \pm 0.2 \text{ \AA}^3 \\ c_0 &= 7.4387 \pm 0.0006 & \rho_x &= 6.061 \pm 0.003 \text{ g.cm}^{-3}, \\ &&& \text{assuming } Z=4 \text{ formula} \\ &&& \text{weights per cell.} \end{aligned}$$

Table 1. *Atomic parameters for $\text{La}_2\text{Be}_2\text{O}_5$*

Least-squares standard errors in the last significant figure are given in parentheses.
Fractional position parameters.

Positions	Atom	<i>x</i>	<i>y</i>	<i>z</i>
8(f)	La	0.23777 (2)	0.03494 (2)	0.19645 (2)
8(f)	Be	0.4693 (5)	0.2183 (5)	-0.4697 (5)
8(f)	O(1)	0.0987 (3)	0.1569 (3)	-0.0845 (2)
4(d)	O(2)	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{2}$
4(e)	O(3)	0	0.2493 (4)	$\frac{1}{4}$
4(b)	O(4)	0	$\frac{1}{2}$	0

Thermal vibration parameters*.

B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
0.00214 (1)	0.00179 (1)	0.00171 (1)	0.00052 (1)	0.00052 (1)	0.00011 (1)
0.0021 (4)	0.0017 (4)	0.0018 (3)	-0.0002 (3)	-0.0000 (3)	-0.0002 (3)
0.0030 (2)	0.0029 (2)	0.0019 (2)	0.0011 (2)	0.0005 (1)	-0.0003 (1)
0.0010 (2)	0.0031 (3)	0.0033 (3)	-0.0004 (2)	-0.0003 (2)	0.0005 (2)
0.0019 (2)	0.0029 (3)	0.0011 (2)	0	-0.0002 (2)	0
0.0033 (3)	0.0015 (2)	0.0055 (4)	0.0001 (2)	0.0021 (3)	0.0010 (3)

R.M.S. thermal displacements (Å) along principal axes.

Positions	Atom	Axis 1	Axis 2	Axis 3
8(f)	La	0.0598 (3)	0.0673 (3)	0.0876 (3)
8(f)	Be	0.064 (8)	0.073 (7)	0.079 (7)
8(f)	O(1)	0.060 (4)	0.081 (3)	0.107 (3)
4(d)	O(2)	0.051 (6)	0.086 (4)	0.103 (4)
4(e)	O(3)	0.054 (5)	0.075 (5)	0.089 (4)
4(b)	O(4)	0.056 (6)	0.079 (5)	0.138 (4)

* Coefficients in the expression $B_{11}h^2 + B_{22}k^2 + B_{33}l^2 + 2B_{12}hk + 2B_{13}hl + 2B_{23}kl$.

We can find no relationship between this unit cell and that reported by Kuo & Yen (1964).

$\theta-2\theta$ scans were used to measure intensities of reflections from $2\theta=28^\circ$ to 130° ; low-angle data were observed in an ω -scanning mode. A total of 3605 independent reflections allowed by the possible space groups were examined. Replicate measurements brought the total number of observations, not including standards, to 3974.

The observed data were corrected for Lorentz-polarization and absorption effects. The latter corrections were made by approximating the crystal shape with six bounding planes and using the ORABS computer program of Wehe, Busing & Levy (1962). Replicate measurements were then averaged and relative F^2 values placed on an approximate absolute scale by Wilson's (1942) method. Statistical tests suggested a centrosymmetric intensity distribution. After a satisfactory trial structure had been derived, secondary extinction corrections were applied to all data following the procedure of Zachariasen (1963).

Results

Peaks on the Harker sections of a three-dimensional Patterson function synthesized from the 3605 corrected and scaled independent F^2 values gave initial parameters for lanthanum atoms in the 8(f) general positions of the space group $C2/c$. Tentative parameters for sixteen oxygen atoms, eight in 8(f), four in 4(e), and four in 4(d), were also deduced. Standard Fourier methods confirmed these tentative locations and showed the remaining four oxygen atoms [in 4(b) positions] and eight beryllium atoms [in 8(f) positions].

Iterative structure-factor, least-squares calculations (Busing, Martin & Levy, 1962) were employed to refine the trial structure. The least-squares procedure minimized residuals in weighted F^2 . We assumed the X-ray

scattering factors for La^{3+} and Be^{2+} given by Cromer & Waber (1965) and those for O^{-1} given in *International Tables for X-ray Crystallography* (1962). Anomalous dispersion corrections for the scattering of Mo $K\alpha$ X-rays by lanthanum atoms were also taken from the latter source. The real part of this correction was applied by drawing a smooth curve through the given values of Af' as a function of $\sin \theta/\lambda$ and making an appropriate adjustment in each entry of the La^{3+} scattering-factor table used by the least-squares program. An average value of +2.8 electrons was assumed for the imaginary part of the dispersion correction. The observations were weighted in inverse proportion to a variance defined as

$$\sigma^2(F^2) = s(A^{-1} Lp)^2 [\sigma_{st}^2 + (0.04N)^2] + [0.10(F_{\text{corr}}^2 - F_{\text{uncorr}}^2)]^2,$$

where s is a scale factor, A^{-1} is an absorption correction, Lp is a Lorentz-polarization correction, σ_{st}^2 is the statistical variance of N (the net count), and F_{uncorr}^2 and F_{corr}^2 are the observed values of F^2 before and after correction for secondary extinction. The final term in the above equation is an attempt to allow for uncertainties in determining the constants governing the secondary extinction corrections.

Four least-squares cycles, the last three with anisotropic thermal vibration parameters, produced the following measures of agreement between observed and calculated $|F|$ and F^2 values:

$$\begin{aligned} R_1 &[\equiv \sum(|F|_o - s|F|_c)/\sum|F|_o] = 0.066 \\ R_2 &[\equiv \sum(|F_o^2 - sF_c^2|)/\sum F_o^2] = 0.056 \\ \sigma_1 &[\equiv \sqrt{\sum w(F_o^2 - sF_c^2)^2}/\sqrt{n-m}] = 1.106, \end{aligned}$$

where w is a weight [$\equiv 1/\sigma^2(F_o^2)$], n is the number of observations, and m is the number of variable parameters. The sums and averages were taken over all 3605 independent reflections.

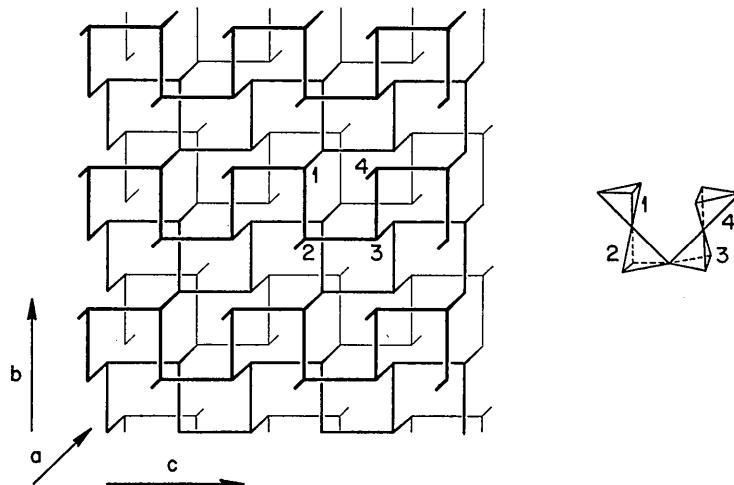


Fig. 1. A schematic representation of the tetrahedral framework in $\text{La}_2\text{Be}_2\text{O}_5$. Tetrahedra have been replaced by sets of three orthogonal Be-O vectors, as described in the text. Unit-cell vectors are shown at the lower left, and two units of a 'square-wave' string of tetrahedra are shown at the right.

Table 2. Comparison of observed and calculated $|F|$ values

$FC = 10 \cdot |F|_{\text{calc}}$, with the sign of A_{calc} . $FO = 10 \cdot |F|_{\text{obs}}$. $SIG = 10 \cdot \sigma(|F|_{\text{obs}})$, where $\sigma(|F|_{\text{obs}})$ is defined as $\sigma(F^2_{\text{obs}})/2|F|_{\text{obs}}$ unless F^2_{obs} is less than 1 (indicated by a W to the right of the entry for SIG in the table), in which case $SIG = \sigma(F^2_{\text{obs}})$. All F^2_{obs} have been scaled with the least-squares scale factor; all $|F|_{\text{obs}}$ have been scaled with the square root of that factor.

L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG
*** 0 O L ***	*** 10 O L ***	*** 1 I 1 L ***	*** 5 I 1 L ***	*** 11 I 1 L ***	*** 19 I 1 L ***	*** 4 2 L ***	*** 10 2 L ***	*** 16 2 L ***															
2 -2379 2461 51	-16 79 0 278 W	1 -389 407 11	17 -13 24 183	1 222 251 19	-3 -41 0 198 W	7 -589 579 16	-11 -411 475 31	-6 -498 498 28															
4 1149 1160 24	-14 -625 612 30	2 -2524 2542 49	18 -113 118 27	2 1354 1346 29	-2 407 369 30	8 -1715 1669 34	-10 -775 782 25	-5 -308 263 52															
6 1034 1056 22	-12 1113 1098 26	3 1309 1138 27	4 2831 2799 53	*** 7 I 1 L ***	4 -1047 399 24	9 766 763 19	-9 429 411 32	-4 -694 691 27															
8 -1741 1725 36	-10 -1035 1001 26	5 -494 499 12	5 164 202 25	0 -547 549 16	10 1178 1169 26	-8 -490 509 27	-3 -308 261 52																
10 1723 1704 35	-8 416 475 24	6 -2323 2280 43	-17 -186 208 25	6 234 252 23	2 426 438 16	11 -370 362 20	-7 9 0 215 W	-2 -598 608 28															
12 -673 649 22	-6 265 313 32	7 414 430 40	-16 -808 836 21	7 27 103 44	12 -421 419 18	13 -26 69 79	-5 -425 429 25	-1 -276 242 55															
14 5 0 165 W	-4 -176 1390 24	15 416 430 40	-16 -808 836 21	7 27 103 44	16 -425 429 25	17 -21 221 27	-1 -31 42 151																
16 568 563 22	-2 1585 1586 33	8 595 584 16	-15 135 117 48	8 320 327 22	*** 0 2 L ***	17 -25 218 32	-4 -1057 1060 25																
18 -787 782 20	0 -1052 1034 22	9 -199 158 28	-16 856 854 22	9 -237 254 23	15 178 203 27	-3 539 520 22	2 283 301 23																
*** 2 O L ***	4 744 758 19	11 -21 253 20	-12 -1053 1035 24	11 -13 0 98 W	0 2910 3135 71	16 529 530 18	-2 1638 1647 34	3 -218 243 25															
-18 629 630 19	6 -1312 1294 28	13 205 209 40	-10 -513 501 17	13 -195 157 35	3 1145 1158 24	17 -271 290 21	-1 -698 700 21	4 -585 590 19															
-16 -509 500 22	10 -503 520 20	14 1073 1106 26	-9 183 141 33	14 -376 390 16	5 426 440 14	18 -545 547 17	0 -997 981 21	5 -237 251 23															
-14 -321 255 31	12 26 0 100 W	15 -91 122 63	-8 1275 1270 27	15 77 146 21	5 266 275 10	19 -107 1105 25	1 -356 348 16	6 -577 584 18	*** 6 2 L ***	2 306 344 17	7 -245 280 18												
-12 1039 1048 24	14 428 411 19	16 -632 656 19	-7 -558 578 16	16 1114 1127 23	6 544 571 16	20 -707 683 19	9 -137 153 28																
-10 -1694 1684 34	-8 1661 1686 34	17 105 0 136 W	-6 -1873 1888 37	17 105 0 136 W	8 -1729 1731 27	-17 -179 188 26	5 -407 428 17																
-8 1861 1868 37	*** 12 O L ***	18 75 133 35	-5 -390 394 13	8 -1729 1731 27	8 -1729 1730 34	-17 -179 188 26	6 -936 965 22	*** 18 2 L ***															
-6 -899 917 19	-4 -999 917 19	-6 -1236 1276 26	-14 613 658 20	*** 3 1 L ***	-4 -154 154 30	-15 686 683 17	-15 0 116 W	7 -441 441 18															
-2 2733 3056 65	-12 -801 795 23	-6 -1284 1294 28	-12 -1053 1035 24	-11 -105 0 98 W	10 1509 1496 31	-16 -321 330 20	8 922 915 22	-6 -551 553 26															
-10 -374 3537 86	-10 -853 844 24	-18 326 339 20	-11 -152 155 18	-11 -12 0 202 W	11 -564 575 18	-13 415 413 19	9 -414 422 18	-5 -285 115 107															
-2 2802 2760 53	-8 -91 92 108	-17 -77 145 37	-6 -1264 1256 25	-10 -632 633 23	13 -228 227 26	-11 -559 557 19	11 -90 60 87	-3 -265 0 267 W															
4 250 267 18	-6 -577 583 23	-16 -838 859 21	1 361 385 13	-9 -158 187 55	14 53 161 33	-10 -1076 1068 24	12 -114 0 112 W	-2 513 413 36															
-6 -1498 1468 26	-11 1176 1203 27	-15 168 177 35	2 1811 1786 35	-8 -983 996 25	15 197 70 105	12 -114 0 112 W	13 -142 130 38	-1 -239 0 239 W															
8 1869 1821 36	-2 -317 1309 29	-14 999 982 24	-3 -435 435 15	-7 -246 238 16	16 491 501 21	-8 1071 1097 24	14 454 478 16	0 -63 135 29															
10 -1642 1613 33	0 928 918 21	-13 -252 266 22	-4 -1939 1867 37	-6 -882 924 24	17 -266 275 23	-7 -393 404 14	15 -174 159 30	1 13 126 34															
12 707 708 20	2 131 115 47	-12 -858 873 21	5 117 95 42	-5 -42 93 111	18 -574 586 18	-6 -248 228 17	-2 -166 152 37	3 168 158 33	*** 12 2 L ***	3 168 158 33	4 510 524 17												
14 151 154 43	-4 -567 559 19	-11 -54 51 87	6 887 867 20	-4 -337 410 30	-3 -39 0 202 W	*** 12 2 L ***	-15 154 0 197 W	5 -251 266 19															
16 -586 577 20	6 1014 1041 24	-10 -5 77 W	7 -145 123 36	-3 -39 0 202 W	8 -938 962 20	-15 154 0 197 W	5 -251 266 19																
18 605 627 17	8 -735 738 20	-9 161 189 18	8 136 161 26	-2 -335 461 26	9 -18 694 680 19	-16 608 577 26	-13 -373 305 45	*** 1 3 L ***															
10 325 331 19	-8 -1268 1280 26	-9 -198 194 24	-1 209 292 36	-18 -694 680 19	-1 -926 943 20	-13 -373 305 45	-1 -26 414 18																
*** 4 O L ***	12 273 262 25	-7 -394 412 13	-10 -817 813 21	-11 -217 198 34	0 -183 1865 35	-13 -356 215 69	-18 -146 198 28																
14 -384 400 15	-6 -2368 2394 45	-11 250 239 27	-1 254 273 25	-16 -362 369 21	-10 -183 1865 35	-13 -356 215 69	-18 -146 198 28																
-18 -612 622 18	-12 -801 795 23	-5 -881 904 19	12 922 915 22	-2 -1060 1067 26	-15 60 127 40	1 711 702 17	-11 356 215 69																
16 -377 376 21	*** 14 O L ***	-4 -291 2394 45	-13 266 224 31	-3 331 351 18	-14 -23 92 56	2 1162 1138 24	-10 709 702 29	-17 247 274 23															
-14 -243 267 22	-3 -606 635 16	-14 -725 720 20	-15 -1801 1913 26	-15 80 0 116 W	-5 -95 87 61	-12 952 956 23	-6 -242 416 26	-15 -578 570 20															
-12 -1122 1129 25	-12 756 757 24	-13 -1801 1913 26	-15 -251 266 22	-13 68 103 37	-4 -792 803 19	-5 -553 551 15	-7 33 100 122	-14 -874 893 22															
-10 -1606 1606 33	-10 -587 594 26	-1 -52 87 29	16 209 205 27	-6 -124 76 74	-11 -666 661 18	-6 -246 1218 26	-6 -422 418 32	-13 -556 557 19															
-6 -169 1672 25	-8 -117 0 273 W	-1 -52 87 29	17 -112 0 104 W	7 126 156 36	-9 -761 787 19	7 677 690 17	-6 -408 450 28	-12 -210 0 288 W															
-6 -515 528 14	-6 -568 560 29	-1 -313 325 16	1 -313 181 29	-5 -107 518 20	-9 -1547 1562 31	8 1333 1316 28	-6 -404 454 13	-9 -482 472 17															
-2 -2951 3096 61	-2 -813 803 21	-3 -687 683 19	-3 -160 161 26	-3 -156 134 26	-9 -156 134 26	-10 -1209 1220 27	-8 -780 771 31	-9 -838 814 20															
2 -1354 1314 28	2 -243 266 23	5 -391 406 24	-16 -761 759 20	-13 -167 122 26	-10 -1601 1611 22	-11 350 355 19	-8 -729 713 31	-9 -826 815 37															
4 459 464 13	4 739 749 20	6 168 1673 33	-15 -251 266 22	-13 68 103 37	-4 -792 803 19	-13 43 54 97	-1 -248 252 24	-6 -1838 1858 36															
6 -642 847 21	-6 -182 179 21	-16 -689 681 19	-2 -179 173 34	-1 791 797 22	-14 230 265 23	-12 710 714 25	-12 -963 969 23																
6 -182 209 31	-5 -188 218 28	4 1282 1259 27	-3 -189 243 24	-5 -145 153 40	-16 -560 565 19	-11 -137 149 25	-13 -344 301 44	-13 723 729 21															
-12 -379 380 20	12 -208 238 18	-10 -754 762 20	-11 -53 189 23	-12 133 0 172 W	-13 1167 1127 31	-1 1060 1011 22	-10 -709 702 29	-11 -90 46 105															
14 -287 239 29	11 -109 181 29	-10 -517 510 18	-11 -167 122 27	-4 -157 213 21	-5 -126 592 25	-2 2371 2297 44	-10 -131 130 28	-12 -276 340 33															
16 762 767 21	*** 16 O L ***	12 1069 1065 25	-9 -74 183 23	-10 -168 173 27	-12 -28 82 38	-3 -22 0 230 W	-10 -162 1156 25	-13 -312 372 19															
-18 -628 637 18	-13 -210 210 31	*** 5 1 L ***	-13 -347 355 15	-2 -378 447 29	-10 -123 244 47	-11 398 408 18	-10 -604 627 19	-11 339 341 18															
-10 -1662 1657 33	-4 -532 560 20	-10 -104 129 32	-8 -307 292 20	8 -83 54 101	-9 -106 95 35	-10 -1209 1222 27	-10 -358 408 30	-17 -350 333 22															
-8 -1075 1079 23	6 -692 702 19	-18 -395 387 18	-1 -153 138 27	-2 -100 157 36	-13 -131 138 44	-12 -132 139 27	-11 30 142 35	-16 -627 647 20															
-6 -14 39 32	8 -313 304 21	-17 -197 226 22	-3 -161 156 22	-2 -104 151 33	-1 305 322 W	-1 -621 614 18	-13 300																

Table 2 (cont.)

L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG												
***	3	3	L ***	***	9	3	L ***	***	13	3	L ***	***	2	4	L ***	***	8	4	L ***	***	12	4	L ***	***	1	5	L ***	***	7	5	L ***	***	11	5	L ***				
4	-2277	2203	42	-15	-466	475	19	13	267	270	17	2	989	955	23	-17	245	0	164 W	11	-40	127	37	8	191	149	31	-12	-153	166	34	14	-151	134	33				
5	1627	1636	33	-16	-625	649	19	3	-928	903	19	-16	51	0	137 W	12	190	173	31	9	-17	31	143	-11	-101	0	118 W	-10	-224	251	20	***	13	5	L ***				
6	1272	1265	26	-13	285	296	23	***	15	3	L ***	4	-10	96	26	-15	178	223	24	13	-209	186	27	10	192	167	20	-10	-224	251	20	***	13	5	L ***				
7	-592	579	16	-12	62	104	56	5	-628	611	16	-14	316	313	22	-13	-666	644	21	***	14	4	L ***	11	-550	538	18	-9	762	755	20	-13	233	0	236 W				
8	-227	235	19	-11	112	143	40	-11	-182	0	242 W	6	-803	807	19	-12	-603	602	19	***	14	4	L ***	12	-450	447	19	-6	-559	577	17	-13	233	0	236 W				
9	79	72	69	-10	402	412	18	-10	-498	430	34	7	1101	1098	23	-12	-603	602	19	13	907	903	23	-7	-1388	1345	20	-12	-111	0	263 W								
10	-455	453	18	-9	-622	632	19	-9	461	464	37	8	1276	1223	21	-11	811	804	21	-1	511	521	22	14	464	445	21	-6	-760	762	19	-11	323	185	75				
11	590	625	18	-8	-990	1023	23	-8	590	513	34	9	-1283	1272	27	-10	778	797	20	-11	-510	523	22	15	-729	757	20	-5	1522	1533	31	-10	281	246	48				
12	857	834	22	-7	878	888	21	-7	-117	367	37	10	-696	882	20	-9	-818	839	20	-10	-358	392	24	16	-251	235	29	-4	560	560	16	-9	-649	679	23				
13	-562	562	20	-6	1174	1193	26	-6	-600	543	29	11	815	834	21	-8	-257	239	24	9	291	353	20	17	253	257	24	-3	-917	926	21	-8	-435	476	25				
14	-828	822	24	-5	-993	1011	23	-5	328	323	36	12	374	371	20	-7	280	302	17	-8	-25	303	53	18	28	0	95 W	-2	-89	84	38	-7	794	841	23				
15	466	472	20	-4	-881	907	21	-4	45	0	218 W	13	-164	116	54	-6	-179	177	24	-7	161	194	47	1	-396	406	14	-6	357	392	27	-1	-396	406	14				
16	312	296	24	-3	305	331	18	-3	173	173	59	14	-19	83	72	-5	706	714	18	-6	306	376	26	***	3	5	L ***	0	-584	591	14	-5	-592	604	24				
17	-87	89	56	-2	-245	240	18	-2	338	371	34	15	-248	340	20	-4	949	971	21	-6	-633	657	22	10	1107	1097	24	-1	-119	194	52								
18	-11	32	147	-1	165	171	24	-1	-372	410	17	16	-401	400	20	-3	-1199	1216	26	-4	-588	629	22	-18	145	157	30	2	688	681	18	-3	33	189	49				
***	5	3	L ***	1	-920	916	21	1	583	615	21	18	381	369	19	-1	1382	1393	20	-2	534	592	22	-16	-347	340	20	4	-835	843	20	-1	691	695	23				
-18	-389	394	18	3	815	805	20	3	-448	457	21	***	4	4	L ***	-1	-878	849	20	0	-277	252	25	-14	442	433	20	6	240	241	22	1	-799	805	22				
-17	364	361	20	4	1136	1131	25	4	-108	394	21	-18	-430	438	17	-3	-14	113	133	21	-2	-231	166	45	-12	-347	325	22	8	50	112	36	3	900	922	23			
-16	605	594	20	5	633	675	18	5	221	244	24	-17	344	344	19	-4	-170	198	23	-3	358	389	21	-11	406	365	20	9	-540	541	18	4	256	313	20				
-14	-770	765	21	7	-311	109	40	7	116	134	38	-16	256	268	25	5	830	812	20	4	408	422	22	-10	-3	96	44	44	10	-415	385	21	5	-396	416	20			
-13	470	439	21	8	-259	243	25	8	316	308	22	-15	73	95	57	6	905	888	21	-5	-556	566	19	-9	545	536	16	11	708	721	20	6	-9	0	122 W				
-12	513	533	18	9	331	343	21	-9	-245	228	27	-14	239	234	31	-7	-941	959	20	-6	-575	593	18	-9	519	545	15	12	382	410	19	7	-80	198	22				
-11	-162	179	27	10	573	585	19	-10	-408	434	16	-13	-530	512	19	-8	-686	646	19	7	533	534	19	-7	-1605	1620	33	13	-833	817	21	8	-249	248	24				
-10	183	171	26	11	-579	564	19	11	300	293	19	-12	-540	550	18	9	787	720	20	8	361	349	20	-6	-564	665	21	14	-304	314	20	9	467	474	18				
-9	618	632	17	12	-691	697	19	12	-100	110	25	11	-358	364	20	-10	-90	132	35	4	820	835	18	16	62	79	56	11	-438	438	18	12	-248	271	18				
-8	-1193	1196	25	13	473	462	19	***	17	3	L ***	10	-941	942	22	-10	-1061	1054	23	12	94	161	30	11	-7	0	84 W	-3	-170	1772	34	***	9	5	L ***				
-7	1029	1033	22	14	420	435	17	-9	-673	713	19	13	-157	156	40	-12	-122	122	94	12	-674	675	15	***	15	5	L ***												
-6	1404	1414	29	15	-250	237	23	-8	-517	582	37	-7	743	757	18	14	-253	266	23	-1	450	467	12	-2	-674	675	15	***	15	5	L ***								
-5	-1528	1518	30	16	-47	97	38	-7	382	317	43	-6	133	176	17	15	379	395	18	***	16	4	L ***	-10	-151	150	24	-1	-358	377	39	1	-358	377	39				
-4	-1697	1710	33	-3	-849	860	19	-5	-231	0	302 W	-5	-280	284	12	-6	-280	284	12	***	10	4	L ***	-10	-254	149	64	-16	312	325	19	1	-358	277	39				
-3	570	581	13	-1	-258	250	11	-3	-90	0	324 W	-7	-281	287	17	-1	-281	287	17	-10	1224	1204	24	-15	-652	617	20	-11	-358	277	39								
-2	-258	250	11	-15	458	473	28	-3	-90	0	324 W	-2	-1493	1519	30	***	10	4	L ***	-9	-138	0	200 W	-3	-1949	1857	37	-13	473	491	19	-9	670	596	28				
-1	-1066	1069	22	-12	-13	-219	308	44	-1	294	0	316 W	-2	-1272	1299	26	-2	-172	172	26	-4	-152	152	40	-11	27	86	62	-7	-728	674	28							
-2	-1673	1629	32	-12	-105	214	64	0	530	519	18	-1	2116	2153	41	-15	-212	183	68	-7	-205	206	199	-5	1501	1512	40	-11	27	86	62	-7	-335	277	47				
3	1159	1122	24	-11	-67	107	128	1	-2	29	429	163	43	-1	1435	1399	28	-16	-249	240	36	-2	-378	372	26	-1	-299	992	22	-9	-758	758	20	-5	359	285	53		
4	1625	1552	31	-10	-579	582	18	6	852	852	19	-1	270	272	26	-16	-602	608	27	-2	-554	568	23	8	-221	199	26	-8	-572	566	18	4	25	0	300 W				
5	-1139	1131	24	-9	572	558	30	3	234	230	29	6	615	616	16	-1	-367	384	24	-3	-637	605	30	9	-292	326	17	-3	-1211	1241	27	-4	-48	504	14	-4	163	129	49
6	-1126	1126	24	-11	-283	277	20	9	1345	1338	28	-13	-534	533	20	-12	-75	0	115 W	2	-237	237	20	10	-128	1234	27	5	176	127	50	-2	-749	751	20	6	-61	145	33
7	-1045	1047	22	-11	-266	215	40	-14	-124	124	42	1	-805	802	23	-11	-218	217	42	-16	-420	443	20	8	-229	232	25	***	17	5	L ***								
8	-728	742	19	8	365	381	18	4	-859	868	18	-6	-718	717	20	-5	-345	348	33	-13	-746	733	21	-14	-603	624	22	-7	-553	527	26	1	-595	598	20				
9	-1563	1631	27	-9	-285	297	36	-12	599	582	20	-1	-1758	1735	27	-8	-674	688	25	-3	-117	235	21	-11	-661	694	19	-6	138	0	249 W								
10	-172	217	22	0	719	711	19	-11	-921	922	22	-1	-1758	1735	27	-																							

Table 2 (*cont.*)

L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG					
***	2	6	L	***	6	6	L	***	12	6	L	***	***	1	7	L	***	***	7	7	L	***	***	13	7	L	***					
-17	-541	546	18	3	-196	297	18	-2	-251	313	31	4	81	88	40	-12	-61	128	41	-12	-80	0	261	W	-4	179	175	22				
-16	-151	197	25	4	192	121	43	-1	-924	903	24	5	-1805	1800	36	-11	-124	198	27	-11	-297	0	292	W	-3	-1276	1254	27				
-15	166	0	146 W	5	-827	801	20	0	86	123	45	6	-311	166	24	-10	-188	202	32	-10	70	0	291	W	-2	-356	379	14				
-14	15	0	138 W	6	-144	184	38	1	-369	392	21	7	999	984	23	-9	-733	750	20	-9	-817	827	26	-1	-1025	2032	39	-12	-221	230	30	
-13	515	546	18	7	1302	1269	28	2	180	159	46	8	-116	129	34	-8	-70	73	68	-8	-38	0	286	W	0	448	457	12				
-11	-157	118	26	8	-406	411	18	3	-383	377	21	9	-77	94	53	-7	-1320	1334	28	7	892	864	27	1	1668	1610	33	-10	-178	173	21	
-10	-133	165	29	10	-89	157	28	1	719	714	21	11	-815	816	21	-5	-1340	1338	28	-6	-60	0	303	W	2	-34	352	18				
-9	1381	1395	29	11	535	525	19	6	-227	204	33	12	-41	22	313	-4	-19	153	27	-4	-34	0	307	W	4	124	107	44				
-8	468	486	16	12	-570	170	28	7	-839	850	22	13	982	997	24	-3	-639	609	18	-3	-27	0	317	W	5	-384	362	19				
-7	-153	152	25	13	115	99	46	8	-255	273	25	14	-35	161	32	-2	-52	0	78	W	-1	-197	190	19	6	-72	102	46				
-6	29	88	33	14	151	125	46	9	503	491	20	15	-777	756	22	-1	-264	306	16	0	497	460	39	7	1202	1194	26	-1	21	90	66	
-5	-193	206	15	15	-442	463	17	10	-3	97	97	W	16	-34	0	105	W	0	22	52	121	8	-186	144	44	-3	-1260	1270	27			
-4	-301	303	13	16	-162	203	21	11	-59	0	97	W	17	357	363	16	1	1411	1397	29	-1	-952	934	24	10	177	153	41				
-3	1415	1436	29	12	48	0	89	W	13	-10	59	10	-18	149	27	2	-21	73	92	1	-1465	1486	31	8	133	134	40					
-2	669	693	16	13	-2324	2347	44	14	-8	19	263	20	***	3	7	L	***	3	-1572	1538	22	3	712	742	21	11	696	682	21			
-1	0	-847	812	12	-16	-9	86	51	***	14	6	L	***	-17	-498	508	17	5	1171	1166	26	4	-533	534	23	13	-226	189	38			
1	2109	2011	39	15	-236	265	14	-16	-86	136	38	6	11	0	105	W	6	69	0	125	W	14	-33	0	115	W	3	-31	0	118	W	
2	777	773	19	14	-28	261	23	-11	-591	630	19	15	-921	909	23	7	-340	353	22	-7	-192	175	34	15	-356	333	23	4	135	141	42	
3	-892	886	20	13	-734	735	20	-10	-16	111	67	14	-69	113	49	8	155	170	35	8	-106	70	75	16	97	113	48	5	773	780	21	
4	131	109	35	12	-254	236	27	-2	-327	334	28	13	-899	909	23	-1	-341	351	20	9	503	520	18	17	606	622	17	6	-107	151	37	
5	-517	518	15	11	1045	1013	24	-8	26	52	196	-10	-166	172	31	10	-30	120	37	10	23	0	91	W	***	4	8	B	L	***		
6	-181	187	20	12	-266	277	22	-7	-222	196	52	11	-411	421	19	11	841	828	22	11	-621	617	17	8	298	304	24	-1	1455	1468	31	
7	1396	1367	29	-9	-888	912	22	-6	-325	356	27	10	-35	0	95	W	12	18	86	57	4	-59	184	33	1	-651	654	19	9	-266	277	19
8	333	350	17	-8	-219	251	20	-5	-714	699	24	13	-455	448	18	13	-665	687	20	***	15	7	L	***	-16	9	95	51	10	-154	152	46
9	-1366	1339	29	-7	264	271	20	-4	-201	214	51	8	-43	66	64	14	-34	0	111	W	-15	19	69	83	24	11	-271	271	24			
10	-233	165	30	-6	-80	151	27	3	-876	881	25	-7	-184	1825	27	15	394	408	18	9	646	556	28	-14	-37	0	115	W	12	140	142	43
11	976	978	24	-5	703	712	18	-2	-244	293	35	-6	-108	132	27	16	-57	93	42	8	15	0	269	W	13	-575	544	21				
12	156	43	61	-3	-369	405	15	-1	-600	633	28	-5	-1913	1938	38	-7	-657	583	31	12	251	253	26	14	19	0	95	W	2	71	100	35
13	-147	75	87	-3	-1490	1505	31	0	-37	0	125	W	***	9	7	L	***	6	-26	0	301	W	11	-1016	1026	24	15	449	430	16		
14	210	225	28	-2	-256	236	19	1	-156	96	81	-3	-1289	1293	27	9	-409	428	59	-9	-210	202	26	***	10	8	B	L	***			
15	-367	351	22	1	1455	1438	30	2	18	142	36	-2	-137	140	20	-15	-716	700	19	-14	-114	0	315	W	6	-307	315	48				
16	-128	136	38	0	260	264	14	3	363	380	22	-1	161	190	15	-14	21	0	111	W	-15	19	69	83	24	11	-271	271	24			
17	5794	604	18	2	-62	75	66	5	-718	745	21	1	1202	1182	25	-2	-18	0	122	W	-16	-57	44	31	-1	-17	122	24				
18	4	-377	386	18	7	606	628	19	8	-98	100	12	-10	-115	104	54	-1	-544	471	39	-6	-36	17	23	13	156	677	24				
19	5	870	867	21	9	108	98	6	-273	300	21	0	-100	141	14	-13	-387	381	22	-2	-16	0	322	W	-15	-374	354	21				
20	-106	107	22	23	-127	139	37	-6	-247	277	36	-1	-165	174	28	-2	-147	166	41	-6	-349	382	16	-1	-177	172	24					
21	-106	107	27	6	-127	139	37	-6	-247	277	36	-1	-165	174	28	-2	-147	166	41	-6	-349	382	16	-1	-177	172	24					
22	-127	139	37	7	-127	139	37	-6	-247	277	36	-1	-165	174	28	-2	-147	166	41	-6	-349	382	16	-1	-177	172	24					
23	-112	125	29	-9	-126	127	28	-10	-126	127	28	-9	-126	127	28	-10	-126	127	28	-9	-126	127	28	-1	-127	127	28					
24	-125	127	28	11	-197	230	23	-14	-81	0	138	W	6	118	144	31	-1	-612	587	29	-16	-12	155	30	1	-1027	1007	24				
25	-166	167	21	10	-46	0	112	W	-15	-88	84	22	-6	118	120	38	-13	-331	296	41	4	101	115	24	-11	-1027	1007	24				
26	-161	176	33	10	-56	54	22	-2	-174	206	22	-5	-1765	1765	35	-12	-54	0	266	W	4	101	130	32	-10	-185	190	32				
27	-153	161	20	11	-308	318	19	-4	-51	0	71	W	-11	-204	264	52	-6	-66	150	23	-9	-955	960	23	-8	-418	408	35				
28	-114	121	25	12	-226	224	14	-7	-214	218	27	14	-25	0	93	W	0	-12	109	111	-7	-641	671	21	6	-1065	1074	27				
29	-173	174	28	8	-73	0	91	W	-10	-71	106	46	-9	-707	795	20	***	11	-173	174	31	-15	-67	178	29	13	-265	267	21			
30	-246	255	41	-9	-295	319	17	-8	-707	795	20	***	11	7	L	***	-1	-1051	1056	36	-14	-13	0	113	W	***	12	8	L	***		
31	8	189	172	36	-17	384	388	17	-7	-1379	1395	29	-14	-33	0	210	W	3	1101	1115	24	-12	-122	158	34	-12	-215	211	27			
32	-1574	1542	32	-4	-187	130	120	13	-328	329	29	-2	-343	362	17	-2	-254	165	31	-12	-1027	1007	24	-11	-666	643	26	12	249	277	26	
33	-5157	4942	30	-5	-145	150	87	-14	-15	163	29	-1	-1456	1459	30	-17	-687	797	27	-12	-1027	1007	24	-11	-708	782	27	-1	-227	250	21	
34	-1567	1543	30	-2	-30	0	268	W	15	-309	317	23	-1	-1176	1144	26	-1	-288	345	22	-11	-207	210	31	-1	-575	564	12	-1	-207	210	31
35	-1574	1542	30	-2	-30	0	268	W	15	-309	317	23	-1	-1176	1144	26	-1	-288	345	22	-11	-207	210	31	-1	-575	564	12	-1	-207	210	31

Table 2 (cont.)

L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG																	
***	3	9	L	***	***	9	9	L	***	***	0	10	L	***	***	6	10	L	***	***	12	10	L	***	***	3	11	L	***															
7	-570	587	19	1	-930	938	24	8	635	614	20	0	880	860	19	8	372	371	19	13	-408	416	19	-11	-148	0	244	W	8	-853	824	23												
8	145	200	26	2	389	384	23	9	989	976	24	1	678	672	20	9	291	284	20	14	483	516	17	-10	-245	187	76	9	-468	486	21	-10	-580	562	26									
9	-202	247	23	3	1127	1123	26	10	-620	630	19	2	-186	211	31	10	-168	202	22	15	326	320	19	-9	-403	376	42	10	670	667	21	-9	154	0	259	W								
10	161	134	48	4	-425	461	18	11	-650	627	21	3	-177	118	51	-	-	-	-	-6	-594	599	30	11	285	233	33	-6	-243	0	256	W												
11	658	608	21	5	-656	648	21	12	253	184	42	4	-45	100	59	***	14	10	L	***	***	5	11	L	***	-7	-548	572	31	12	-307	261	32	-7	72	0	245	W						
12	-311	200	25	6	230	197	32	13	204	247	37	5	-552	537	20	-	-	-	-	-6	574	561	32	13	-25	0	117	W	-6	-232	0	268	W											
13	-846	835	22	7	87	124	46	14	-26	0	127	W	6	549	522	20	-8	-105	93	18	-14	495	483	18	-5	-375	459	34	14	-57	0	101	W	-5	-286	137	100							
14	266	286	21	8	-51	99	69	15	186	235	24	7	848	833	22	-7	23	212	42	-13	300	309	21	-4	-436	497	30	-4	640	601	29	-3	494	462	34									
15	585	535	18	9	427	447	20	16	-239	237	22	8	-603	588	20	-6	-144	179	49	-12	-352	308	24	-3	93	72	210	***	4	12	L	***	-2	-783	785	26								
16	-215	195	27	10	-272	257	30	-	-	-	-	9	-710	700	21	-5	-527	503	25	-11	-57	0	127	W	-2	-111	187	80	-1	-332	238	66	-1	671	661	21								
17	-558	590	18	***	2	10	L	***	10	526	519	19	-	430	410	29	-10	-145	177	34	-1	-299	332	46	-14	-187	152	37	-1	-32	238	66	-1	96	160	47								
18	12	210	184	15	13	531	540	17	-16	219	173	34	12	-100	167	30	-3	-324	286	57	-8	504	499	19	1	655	670	23	-2	622	616	20	1	96	160	47								
19	-292	279	21	-	-	15	113	36	158	13	119	119	46	-4	-171	307	37	-7	754	726	21	-2	666	621	21	-11	448	443	21	-2	-160	200	37	-	-	-	-							
20	-163	684	19	***	11	9	L	***	-14	166	162	41	14	-40	0	101	W	0	324	319	23	-6	-639	613	23	3	-530	540	21	-10	-754	748	21	3	161	125	64							
21	317	340	18	-	-	13	345	323	25	***	8	10	L	***	1	29	0	132	W	-5	-662	658	21	4	521	566	20	-9	-374	357	23	4	-320	346	23									
22	669	667	21	-12	28	216	50	-12	-418	386	24	***	8	10	L	***	2	46	79	72	-4	749	738	20	5	263	315	20	-6	800	805	21	5	-342	358	23								
23	-150	77	91	-11	-267	201	57	-12	-418	386	24	***	8	10	L	***	3	326	364	20	-3	410	419	17	6	-215	268	25	-7	224	260	23	6	510	513	20								
24	-119	205	29	-10	84	0	241	W	-10	656	666	20	-18	-234	248	23	-4	-251	283	21	-2	-342	340	20	7	113	111	51	-6	-64	0	120	W	7	371	389	20							
25	-907	535	18	-8	-161	119	44	-8	-619	619	19	-12	411	410	20	6	391	394	19	0	-336	306	20	9	-241	252	24	-4	-192	379	21	9	-167	177	32									
26	8	305	346	19	-7	-903	909	27	-11	697	684	21	7	399	395	18	-1	-554	573	20	10	350	370	18	-3	-483	501	18	10	285	301	18	-	-	-	-								
27	-1101	1087	25	-6	420	425	37	-6	399	428	16	-10	-451	485	18	-	-	-	-	2	798	794	23	-2	979	984	23	-1	640	678	18	***	12	12	L	***	-	-	-					
28	-650	654	19	-5	642	663	27	-5	-136	134	35	-	-572	584	19	***	16	10	L	***	3	815	805	23	***	13	11	L	***	0	-994	975	22	-	-	-	-							
29	-1182	1183	26	-4	-220	290	42	-4	459	460	17	-	355	395	18	-	4	916	904	23	-4	-561	566	20	-9	-378	390	25	-8	266	273	43	-	-	-	-								
30	-1182	1183	26	-4	-220	290	42	-4	459	460	17	-	355	395	18	-	4	916	904	23	-4	-561	566	20	-9	-378	390	25	-8	-166	293	38	-	-	-	-								
31	1419	1408	30	4	317	324	23	4	115	116	86	-	7	105	105	61	-3	-473	367	35	5	609	626	21	-8	-477	357	39	1	378	390	25	-6	-561	579	20	-3	-358	443	32	-	-	-	-
32	-714	715	20	5	383	326	25	5	-343	358	19	-	1	-588	601	21	***	1	11	L	***	12	511	532	18	-1	-360	267	65	8	874	862	23	-1	291	285	49	-	-	-	-			
33	-5111	1111	26	6	-175	215	25	6	585	561	21	2	-367	408	22	-15	-397	394	18	14	-459	450	17	1	-448	452	22	10	-669	665	20	1	4	100	64	-	-	-	-					
34	621	179	39	7	-105	108	50	8	-553	561	19	4	-518	510	21	-15	-452	489	21	12	-505	502	21	11	-213	212	28	2	101	59	114	-	-	-	-									
35	734	518	20	8	-186	213	29	9	-535	545	19	5	597	589	20	-12	-511	527	20	3	-356	392	21	12	-289	237	29	3	-226	232	29	-	-	-	-									
36	8	-186	213	29	9	-535	545	19	5	598	581	20	5	597	589	20	-12	-511	527	20	4	-434	423	21	13	-26	42	114	4	437	424	21	-	-	-	-								
37	939	387	19	10	161	146	42	10	705	701	21	6	-241	448	20	-11	-772	339	35	-	-	5139	415	19	5	-139	145	49	5	308	354	19	-	-	-	-								
38	10	-182	178	36	11	-548	537	18	11	625	650	20	7	-746	750	22	-10	-58	183	29	-2	-203	226	32	6	124	62	90	***	6	528	497	20	7	-279	296	21	-	-	-	-			
39	12	-277	250	23	12	-203	274	28	8	451	459	21	-9	-230	237	28	-11	-20	0	115	W	7	-223	232	22	-1	-552	571	19	3	244	196	32	-	-	-	-							
40	146	183	18	1	-781	773	23	-6	-157	112	48	-5	-562	531	20	7	-400	408	20	5	647	649	21	-10	-1016	1012	24	2	-549	494	27	***	1	13	L	***	-	-	-					
41	-525	531	17	4	-334	357	21	-3	-1023	1004	23	-5	-557	527	29	-10	-220	251	27	8	-7	101	53	2	511	524	21	-12	-167	178	31	-5	-273	230	32	-	-	-	-					
42	-627	619	19	5	-242	248	28	-2	954	956	22	-7	-751	743	24	-11	-198	408	23	9	-249	222	34	-2	-179	243	20	-5	570	496	30	-	-	-	-									
43	63	150	26	6	88	78	72	-1	1194	1165	26	0	474	484	19	12	470	435	22	10	362	371	20	5	30	113	W	7	429	445	21	-10	138	0	150	W	-	-	-	-				
44	-162	285	20	7	-92	130	39	0	-824	813	23	1	273	250	38	13	513	509	19	11	-395	420	19	6	-457	469	19	8	-709	669	23	-9	-78	66	25	-	-	-	-					
45	9	178	197	18	8	63	74	62	1	-958	939	23	-2	-78	163	39	14	-572	552	19	12	-480	478	18	7	-396	373	24	-9	-388	394	21	-8	438	419	22	-	-	-	-				
46	248	280	20	-10	-172	185	23	3	-274	290	23	-6	-141	262	21	11	-372	378	18	13	-372	378	18	8	887	880	23	10	493	504	19	-7	190	216	27	-	-	-	-					
47	473	481	20	***	15	9	L	***	5	-648	655	20	***</																															

Table 2 (cont.)

L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG	L	FC	FO	SIG														
***	3	13	L	***	***	7	13	L	***	***	0	14	L	***	***	4	14	L	***	***	10	14	L	***	***	3	15	L	***												
-5	282	292	24	4	763	760	23	0	-1037	1060	26	10	-591	567	20	4	-335	338	25	10	306	286	23	-3	133	129	72	-8	-325	342	20										
-4	-1036	1064	25	5	69	172	32	1	-39	0	147 W	11	11	74	66	5	-97	0	123 W	-1	-143	247	39	-7	142	162	35	2	-544	608	21										
-3	-284	260	27	6	-481	488	21	2	912	904	23	6	651	651	19	***	5	15	L	***	-1	-54	158	60	-6	-61	133	41	3	387	350	30									
-2	364	353	22	7	24	85	75	3	92	0	150 W	***	6	14	L	***	7	20	0	101 W	0	445	452	18	-5	51	100	60	4	554	573	20									
-1	-38	70	82	8	-25	0	139 W	4	-234	213	25	***	12	14	L	***	-10	-114	63	94	1	20	0	129 W	-4	463	475	20	5	-427	388	24									
0	164	188	25	9	-195	214	27	5	48	76	95	-11	-41	0	119 W	***	12	14	L	***	-9	-50	0	112 W	2	-659	700	20	-3	-195	182	38	6	-440	462	18					
1	118	121	74	10	417	381	21	6	-379	381	23	-10	750	748	20	-8	525	547	19	3	163	199	26	-2	-723	722	21	7	215	233	26										
2	-786	789	25	11	218	143	43	7	-84	65	104	-9	-13	0	123 W	-4	-636	580	24	-7	93	0	139 W	-1	280	278	26	0	680	678	19	***	3	17	L	***					
3	-316	306	29	8	744	758	21	-8	-79	472	20	-3	61	168	71	-6	-662	894	22	***	0	16	L	***	0	-254	286	36	1	-263	320	26	-6	-607	610	18					
4	1031	126	26	***	9	13	L	***	9	13	108	56	-7	18	49	122	-4	651	580	24	5	132	0	146 W	0	-802	801	24	3	97	140	52	-5	382	409	19					
5	220	198	44	6	-727	732	21	-6	81	143	40	-1	-58	83	131	-4	635	644	20	2	610	582	22	4	-177	228	29	-4	429	390	23										
7	-63	113	59	-9	-142	213	59	12	406	414	17	4	610	608	21	1	67	99	58	-2	-260	250	31	3	-176	146	52	5	75	114	57	-3	-325	272	30						
8	128	174	38	-6	-603	589	28	-3	120	188	30	2	18	0	127 W	-1	47	112	58	3	-195	167	38	-1	34	0	141 W	0	-264	301	21										
9	-105	158	38	-7	239	290	42	***	2	14	L	***	-2	-830	858	22	-3	-114	112	51	0	-339	354	21	4	-85	0	161 W	6	440	428	21									
11	207	223	28	-6	-837	840	24	-1	-17	126	45	4	347	358	20	2	740	738	24	6	-260	282	21	2	507	490	25	-1	-154	178	38										
12	-614	624	19	-4	512	483	32	-11	-79	150	36	1	-25	26	386	***	1	15	L	***	3	-188	224	36	7	179	196	31	3	-303	250	39									
13	-217	245	20	-3	-49	131	102	-2	847	828	21	-2	-294	287	34	-1	-62	118	56	3	32	0	154 W	-11	-839	835	24	8	683	680	21	-6	-51	0	121 W	4	-578	588	20		
***	5	13	L	***	-1	205	277	W	-8	-688	694	20	4	-138	139	57	-10	63	131	41	6	454	468	21	-3	216	197	36	2	365	345	25	-2	289	302	23					
-12	-403	419	18	0	-504	492	19	-7	12	88	75	5	-154	129	55	-9	33	0	131 W	-7	-137	152	41	***	2	16	L	***	-4	-452	459	18	5	365	345	25					
-11	-22	0	122 W	2	742	743	24	-5	17	0	131 W	7	72	136	47	-7	-45	123	49	9	67	0	120 W	-9	-227	251	25	-2	655	655	19	-7	172	166	39	0	-659	470	17		
-10	-161	174	35	3	273	303	25	-4	400	420	20	8	-682	657	21	-6	-797	785	23	10	-360	381	18	-7	172	166	39	0	-269	278	26	***	7	17	L	***					
-9	-126	150	42	4	-772	787	22	-3	35	94	66	9	14	0	113 W	-5	107	0	151 W	-8	-544	541	19	-1	211	182	52	-4	-410	387	21	-2	189	207	39	-3	166	189	31		
-8	641	651	20	5	-82	147	W	-2	-792	809	22	10	566	539	20	-4	864	873	22	***	7	15	L	***	-6	206	164	46	4	21	173	31	-5	184	174	43	-2	343	350	24	
-7	220	196	35	6	262	283	25	-1	-139	90	69	11	-12	0	88 W	-3	-133	155	40	-2	-552	576	22	-9	-44	0	109 W	-4	359	341	23	-3	-92	135	49	-2	6	135	40		
-6	-914	927	22	7	-39	115	47	0	1126	1102	24	-1	-38	0	126 W	-1	-603	583	19	-3	-184	174	43	-2	-690	698	22	5	-90	133	42	0	317	304	21	1	-310	347	25		
-5	-236	232	29	8	113	165	30	1	7	0	191 W	***	8	14	L	***	1	-639	669	19	1	41	0	164 W	2	784	796	20	***	10	16	L	***	2	-526	525	23	3	352	367	22
-4	-819	801	21	9	162	147	39	-2	-551	550	24	3	-28	186	39	-10	-639	667	19	2	-584	323	3	-138	208	37	1	-281	305	35	0	388	363	22	***	0	18	L	***		
-3	110	155	31	10	-418	420	17	4	147	183	45	-9	34	276	22	-8	-582	574	23	-3	-144	188	59	1	-212	214	51	-1	260	0	270 W	0	388	363	22						
-2	-396	388	20	-1	134	142	42	5	-10	147	183	45	-8	34	276	22	-8	-582	574	23	3	-144	188	59	1	-212	214	51	-5	-72	159	40									
-1	0	488	477	17	6	-232	284	53	***	4	14	L	***	1	84	42	204	2	255	251	34	***	3	15	L	***	5	-119	137	47	-5	-119	137	47	0	-458	499	20			
1	-277	221	48	-8	-646	629	21	7	111	148	48	-6	-149	203	28	5	161	161	50	-2	38	0	327 W	3	147	159	176	0	388	363	22	***	0	18	L	***					
2	784	768	25	-7	-222	281	35	-8	-784	787	23	-5	58	153	31	6	724	709	22	-1	10	0	343 W	4	21	73	116	5	32	32	135	53	***	1	17	L	***	0	-456	467	25
3	341	343	29	-6	607	597	21	9	-67	62	104	-4	-627	659	20	7	-164	138	54	0	392	401	24	5	32	32	135	53	***	1	17	L	***	1	458	499	20				
4	-962	969	24	-5	104	131	50	10	750	740	21	-3	-109	62	109	8	-279	250	36	1	55	161	48	6	397	411	23	2	424	415	24	-3	-307	325	38						
5	-212	255	30	-4	-246	357	40	11	-28	0	122 W	-2	-886	890	23	9	-7	0	139 W	2	-738	761	24	-7	-198	179	41	-8	-244	211	32	-3	-313	329	29	-1	527	524	20		
6	619	626	21	-3	13	0	279 W	12	-321	294	22	-1	56	186	31	3	-230	217	29	3	114	166	42	8	-658	551	20	-7	-557	524	22	4	-100	26	280						
7	104	146	48	-2	-110	140	59	-6	-210	212	29	0	-723	732	19	11	-45	0	117 W	4	699	704	22	9	237	260	25	-5	414	410	21	5	-72	159	40						
8	-86	0	147 W	-1	-232	284	53	***	4	14	L	***	1	84	42	204	-5	-119	137	47	6	-390	398	20	***	4	16	L	***	-3	-333	381	33	***	2	18	L	***			
-12	220	0	247 W	7	110	0	111 W	-6	-93	187	30	9	-21	0	102 W	-6	772	746	21	-6	-664	583	26	-2	-311	328	22	3	-343	329	29	-1	527	524	20						
-11	-64	0	270	22	-2	88	0	249 W	-5	99	110	57	-5	-78	108	60	-5	71	131	79	-3	191	178	41	4	-633	601	21	0	515	512	18	-2	462	446	21					
-10	158	0	286 W	-9	-187	33	419	-4	-518	510	28	***	10	14	L	***	-4	-817	840	22	-4	403	430	28	8	-786	816	21	5	382	374	25	-1	-431	428	28					
-9	187	33	419	***	13	13	L	***	-3	-45	104	50	-3	-104	0	135 W	-3	-817	840	22	-1	-307	293																		

Atomic position and thermal vibration parameters from the final least-squares cycle are listed in Table 1. A comparison of observed and computed $|F|$ values is given in Table 2. A final difference Fourier synthesis with all atoms removed showed no positive or negative peak containing more than 0.5 electron. The largest excursions on this map were associated with the subtracted lanthanum atom.

Description of the structure

The ORFFE program of Busing, Martin & Levy (1964) was used with the parameters of Table 1 to compute interatomic distances and angles. A selection of the more important of these appears in Table 3. Several drawings of the structure were prepared with the ORTEP program written by Johnson (1965).

Table 3. Interatomic distances and angles in $\text{La}_2\text{Be}_2\text{O}_5$

Distances	Standard deviation	
Be–O(1)	1.602 Å	0.004 Å
Be–O(2)	1.637	0.004
Be–O(3)	1.661	0.003
Be–O(4)	1.678	0.004
La–O(1)	2.415	0.002
La–O(3)	2.426	0.002
La–O(1)	2.480	0.002
La–O(4)	2.502 ₃	0.002 ₂
La–O(2)	2.556 ₃	0.0004
La–O(1)	2.719	0.002
La–O(2)	2.755 ₅	0.000 ₃
La–O(3)	2.903	0.002
La–O(4)	2.971 ₄	0.000 ₃
La–O(1)	2.999	0.002
Angles	Standard deviation	
O(1)–Be–O(4)	113.4°	0.2
O(1)–Be–O(3)	111.8	0.2
O(1)–Be–O(2)	117.4	0.2
O(2)–Be–O(4)	105.1	0.2
O(2)–Be–O(3)	102.9	0.2
O(3)–Be–O(4)	105.0	0.2

From the results listed in Table 3, we see at once that the beryllium–oxygen coordination polyhedron in $\text{La}_2\text{Be}_2\text{O}_5$ closely approximates a regular tetrahedron with interatomic distances comparable to those found in BeO (Smith, Newkirk & Kahn, 1964) and chrysocobalt, Al_2BeO_4 (Farrell, Fang & Newnham, 1963). Further consideration shows that each beryllium–oxygen tetrahedron shares three of its four corners with three other beryllium–oxygen tetrahedra. The linked tetrahedra form a space-filling framework* that is an important feature of the structure.

To describe the inter-tetrahedral linkages, we note that each tetrahedron is oriented so that three of its

Be–O vectors are roughly parallel to the unit-cell axes. The oxygen atoms at the ends of these vectors are the ones shared with adjacent tetrahedra. In an idealized representation, we may neglect the departures of the monoclinic angle and of the O–Be–O angles from 90° and replace each tetrahedron by three orthogonal vectors based at the central beryllium atom and directed along the idealized bonds to the shared oxygen atoms. The result of doing this is shown in Fig. 1.

Depending on the direction of view, one may reconstruct the three-dimensional pattern by considering strings of corner-sharing tetrahedra to be extended through the structure, repeated by axial translations into two-dimensional arrays, and cross-linked by corner-sharing with tetrahedra in adjacent related arrays. Viewed in the a direction, one may see strings with a ‘squarewave’ appearance (Fig. 1) resembling those found in petalite, $\text{LiAlSi}_4\text{O}_{10}$ (Liebau, 1961c), extending in [001] directions. Arrays on 200 planes are formed by the b lattice repetition and arrays on adjacent 200 planes are related by the C -centering operation. Viewed in the c direction, one may see strings resembling those found in diopside, $\text{CaMg}(\text{SiO}_3)_2$ (Warren & Bragg, 1928), extending in [110] or [−110] directions. Arrays on 002 planes are formed by the a (or b) lattice repetition and arrays on adjacent 002 planes are related by the two-fold axes half-way between them. Viewed in the b direction, one may see (Fig. 2) strings that are a variation of those found in wollastonite, CaSiO_3 (Mamedov & Belov, 1956), extending in [101] directions. Arrays on 020 planes are formed by the c (or a) lattice repetition and arrays on adjacent 020 planes are related by the c -glide operation.

The consequence of this linking together of tetrahedral strings is the formation of cube-like cages of tetrahedra whose outline is easily seen in Figs. 1 and 2. We note that six edges of a cage follow Be–O–Be bonds while the remaining six are only suggested by opposed tetrahedra faces. Each cage provides a location for a lanthanum atom, but the lanthanum–oxygen coordination polyhedron is rather irregular with five close La–O contacts, two longer contacts, and three still longer contacts in which interactions must be relatively weak (see Table 3). A detailed view of such a lanthanum atom environment is given in Fig. 3.

A few additional points are noteworthy. As shown in Fig. 3, the thermal motion ellipsoids of the oxygen atoms have principal axes normal and parallel to Be–O bonds – a further evidence of the structural importance of the tetrahedral framework. The thermal vibration of the O(4) atom is unusual in that it is large and directed along the line of two long (2.97 Å) contacts with lanthanum atoms. One might imagine that this reflects a static displacement of the O(4) atom favored by the resultant shortening of one of the 2.97 Å lanthanum contacts. Such a displacement would also produce a nonlinear Be–O–Be sequence which might be energetically favored, in analogy with the behavior of corner-sharing (SiO_4) tetrahedra (Liebau, 1961d). To

* We used the word ‘framework’ for want of a better term. It does not conform to the framework concept used in silicate structures since only three of the four corners of each tetrahedron are shared. The name ‘interrupted framework’ might be a more correct description.

this point, note that the Be–O(3)–Be angle is $163.5 \pm 0.3^\circ$, but that the Be–O(2)–Be angle is required to be 180° and the thermal vibration parameters of the O(2) atom do not appear abnormal. We did not test structure models in which either the center of symmetry was removed or a pair of partial atoms replaced the O(4) atom.

Finally, the Be–O(1) bond is significantly shorter than the other three beryllium–oxygen bonds, and O(1) is the oxygen atom not shared with an adjacent tetrahedron.* A similar reduction in bond length with decreasing degree of oxygen association between tetrahedra has been reported in structures containing connected PO_4 , SiO_4 and BO_4 tetrahedra (de Decker, 1941; Grund, 1954; Prewitt & Shannon, 1967, respectively).

Discussion

Beryllium oxide (Smith, Newkirk & Kahn, 1964), Al_2BeO_4 (Bragg & Brown, 1926), and Cr_2BeO_4 (Weir & Van Valkenburg, 1960) have structures which are described in terms of close-packed layers of oxygen atoms with small metal atoms regularly occupying certain interstitial sites. The structure of beryl, $\text{Be}_3\text{Al}_2\text{Si}_6\text{O}_{18}$, is usually classified as a ring silicate in which beryllium atoms act as an inter-ring link while preserving their tetrahedral environment (Bragg & West, 1926). Phenakite, Be_2SiO_4 , has a three-dimensional arrangement of corner-sharing (BeO_4) and (SiO_4) tetrahedra in which each oxygen atom is bonded to two beryllium atoms and one silicon atom (Bragg & Zachariasen, 1930).

In $\text{La}_2\text{Be}_2\text{O}_5$, we see a structure that must be described as a three-dimensional framework formed exclusively of linked (BeO_4) tetrahedra. Although close contacts occur between oxygen atoms of a given BeO_4

tetrahedron, there are no extensive parts of this framework in which the oxygen or oxygen–lanthanum atom arrangement is close-packed. The structure of $\text{La}_2\text{Be}_2\text{O}_5$ may in this sense be compared with silicate structures; some associations with known silicate string configurations were made in the preceding section.

Silicates of general formula $\text{A}_2\text{Si}_2\text{O}_5$ are known and structures for compounds with $\text{A} = \text{Li}$, Na , and (0.25 Li, 0.25 Al, 0.5 vacancy) have been reported (Liebau, 1961*a, b, c*; Grund, 1954). In all studied to date, the silicate tetrahedra combine into sheets with A cations lying between the sheets. Structures of alkali titanates of general formula $\text{A}_2\text{Ti}_2\text{O}_5$ have also been given (Barblan, 1943; Andersson & Wadsley, 1961). Here too, sheet-like combinations of TiO_4 tetrahedra* are found. The structures of V_2O_5^* and the stable orthorhombic forms of P_2O_5 contain corner-sharing XO_4 tetrahedra; V_2O_5^* (Ketelaar, 1936) and the so-called third form of P_2O_5 (MacGillavry, de Decker & Nyland, 1949) have sheet-like configurations, but the second form of P_2O_5 has a three-dimensional framework with spirals of PO_4 tetrahedra about 2_1 screw axes (de Decker, 1941).

The BeO_4 tetrahedra in $\text{La}_2\text{Be}_2\text{O}_5$ do not join to form sheets, perhaps because of the high surface charge that a sheet of net composition Be_2O_5 would have. Rather, they form a unique three-dimensional framework of corner-sharing tetrahedra with cage-like sites for the large lanthanum cations. The second form of P_2O_5 is the only other example of an X_2O_5 framework, but the motifs are not alike and the effect of charge neutralization is absent in P_2O_5 .

It is important to contrast the $\text{La}_2\text{Be}_2\text{O}_5$ structure with the metastable $\text{Ca}_{12}\text{Be}_{17}\text{O}_{29}$ and Y_2BeO_4 structures (Harris & Yakel, 1966, 1967). In the latter, linear or

* All oxygen atoms have four lanthanum atom near neighbours at distances from 2.415 to 2.999 Å.

* The situation is complicated in these structures owing to the approach of a fifth oxygen atom to the XO_4 tetrahedra to give trigonal bipyramidal coordination (see also Byström, Wilhelmi & Brotzen, 1950).

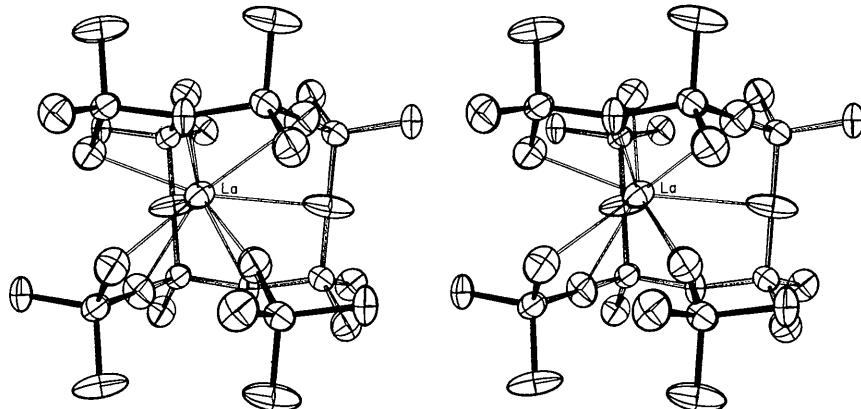


Fig. 3. Stereoscopic drawings of the lanthanum atom environment in $\text{La}_2\text{Be}_2\text{O}_5$. The unit-cell origin is half-way between the O(4) atoms (elongated ellipsoids) at the left of the drawing. The $+b$ axis is vertical and directed upward in the drawing plane. The $+c$ axis emerges up and to the right from the paper at an angle of 25° to the drawing plane, and the $+a$ axis emerges behind the paper in a right-handed relation to b and c . Atoms are represented by thermal displacement ellipsoids including 99.9% probability ($4 \times \text{r.m.s. displacement}$). Bounding and principal ellipses only are shown for lanthanum and beryllium atoms; forward principal axes are added for oxygen atoms. Thin bonds between lanthanum and oxygen atoms indicate important short contacts.

planar groupings of relatively normal calcium-oxygen and yttrium-oxygen coordination polyhedra were found, but beryllium atoms were not normally coordinated. Oxygen environments about beryllium atoms ranging from tetrahedral to trigonal were reported in $\text{Ca}_{12}\text{Be}_{17}\text{O}_{29}$ and trigonal environments exclusively were reported in Y_2BeO_4 . The principle underlying both structures seems to be the maintenance of normal heavy cation-oxygen coordination, albeit in a metastable phase, with beryllium atoms fitting in where best they can. The situation is reversed in $\text{La}_2\text{Be}_2\text{O}_5$. Here the principle underlying the structure seems to be the maintenance of a framework of normal BeO_4 tetrahedra with lanthanum atoms fitting in where best they can.

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