

The $\text{Fe}^{2+}_3(\text{H}_2\text{O})_n[\text{PO}_4]_2$ Homologous Series. II. The Crystal Structure of $\text{Fe}^{2+}_3(\text{H}_2\text{O})[\text{PO}_4]_2$

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Abstract

The synthetic compound $\text{Fe}^{2+}_3(\text{H}_2\text{O})[\text{PO}_4]_2$ has a 9.431(1) Å, b 10.066(1) Å, c 8.040(1) Å, β 117.632(7)°, $P2_1/a$, $Z = 4$. Its structure, refined to $R(hkl) = 0.058$ for 2457 independent reflections, consists of complex open framework formed by edge- and corner-linking of distorted Fe(1) and Fe(3) octahedra, of distorted Fe(2) polyhedra of five-fold oxygen coordination, and of PO_4 tetrahedra. Average bond distances are Fe(1)-O, 2.16 Å; Fe(2)-O, 2.08 Å; Fe(3)-O, 2.15 Å; P(1)-O, 1.55 Å; and P(2)-O, 1.54 Å. Unusual features of the structure include a Fe(2)-P(2) O(6)-O(8) 2.41 Å shared edge, and a Fe(2)-Fe(2') O(4)-O(4') 2.63 Å shared edge. It is proposed that a bounded oxidative sequence may exist for the crystal, where $\text{Fe}(1)^{2+} \rightarrow \text{Fe}(1)^{3+}$ and $\text{H}_2\text{O} \rightarrow \text{OH}^-$. The limiting formula for a stable oxidized crystal would be $\text{Fe}^{2+}_3\text{Fe}^{3+}(\text{OH})[\text{PO}_4]_2$.

Introduction

The homologous series $\text{Fe}^{2+}_3(\text{H}_2\text{O})_n[\text{PO}_4]_2$ includes several compounds where all water molecules and all phosphate oxygens are also bound to the transition metal. Well-characterized natural compounds include vivianite and metavivianite ($n=8$), ludlamite ($n=4$), phosphoferrite ($n=3$), sarcopside and graf-tonite ($n=0$). In addition, several recently synthesized compounds have been brought to our attention, including the subject of this study, where $n=1$.

Experimental

Single crystals of $\text{Fe}^{2+}_3(\text{H}_2\text{O})[\text{PO}_4]_2$ were synthesized by Dr. E. Matfievich at 230°C and 400 bars pressure, using a hydrothermal technique with synthetic vivianite as starting material. Dr. Matfievich informs us that wet chemical analyses closely conform with the ideal formula and that Mössbauer resonance studies have been performed on the compound.

Preliminary single crystal Weissenberg and precession photographs establish the space group and cell parameters, the latter refined by twelve reflections on the PICKER four-circle automated diffractometer. The results are a 9.431(1) Å, b 10.066(1) Å, c 8.040(1) Å, β 117.632(7)°, space group $P2_1/a$, $Z = 4$. A powder pattern, indexed with the aid of the single crystal data, appears in Table 1.

A superior single crystal measuring 0.09 mm along

a , 0.11 mm along b , and 0.04 mm along c was selected for intensity measurements. The compound is pale green in color, with crystals tabular parallel to (001) and striated parallel to [100]. Figure 1 features an idealized sketch of typical development of the crystals.

Successive shells of reflections were gathered to $\sin \theta/\lambda = 0.8$ on the PICKER diffractometer with $\text{MoK}\alpha$ radiation and graphite monochromator. Full scans ranged from 2.4° at the lower levels to 2.8° at high angles with a scan speed of 2°/minute. Twenty-second background measurements were taken on each side of the peak. The data were processed to obtain $F(\text{obs})$ after applying an absorption correction by the Gaussian integral method described by Burnham (1966). All 2457 independent reflections were accepted for the ensuing study.

Structure Determination and Refinements

The Patterson synthesis, $P(uvw)$, revealed that all metals reside in general positions, requiring coordinate determination for Fe(1), Fe(2), Fe(3), P(1), and P(2). Several minimum functions provided unambiguous location of the metals which afforded sufficient scattering matter for a β -general synthesis as described by Ramachandran and Srinivasan (1970). The ensuing map revealed all non-hydrogen atom locations without difficulty.

Full-matrix least-squares refinement, including scale factor, non-hydrogen atomic coordinates and isotropic thermal vibration parameters with 2457 in-

TABLE 1. $Fe_2(H_2O)(PO_4)_2$ Powder Data*

l/T_0	$d(\text{obs})$	$d(\text{calc})$	hkl	l/T_0	$d(\text{obs})$	$d(\text{calc})$	hkl
70	5.810	5.814	011	20	2.611	2.616	230
20	4.146	4.155	121	5	2.571	2.573	213
40	4.097	4.100	111	40	2.512	2.517	040
20	3.723	3.730	112	5	2.469	2.471	122
10	3.551	3.561	002	20	2.435	2.437	320
100	3.351	3.357	012	5	2.378	2.384	313
35	3.020	3.035	021	30	2.324	2.328	123
20	2.984	2.992	311	10	2.039	2.045	410
15	2.903	2.911	211	20	2.003	2.006	204
10	2.722	2.729	112	10	1.834	1.836	121
15	2.680	2.687	121	10	1.833	1.835	324
45	2.655	2.659	321	10	1.801	1.805	224
				15	1.672	1.675	242

* Powder diffractogram, $10^\circ/\text{minute}$, CuK α radiation, Si ($d = 5.4301 \text{ \AA}$) internal. Indices are based on strong single crystal reflections and cell parameters stated in the text.

dependent reflections converged to $R(hkl) = \sum |F(\text{obs}) - F(\text{calc})| / \sum F(\text{obs}) = 0.068$. For the 1569 reflections exceeding three times the estimated background error, $R(hkl) = 0.039$. Estimated standard errors in distances are $Me-O \pm 0.004 \text{ \AA}$ and $O-O' \pm 0.006 \text{ \AA}$. Scattering curves for Fe^{2+} , P^{5+} , and O^{2-} derive from the tables of Cromer and Mann (1968).

Final atomic coordinate parameters appear in Table 2, and the structure factor data are presented in Table 3.¹

Description of the Structure

Topology and Geometry

The crystal structure of $Fe^{2+}_n(H_2O)_n(PO_4)_n$ is complex, and bears no obvious relationship with any

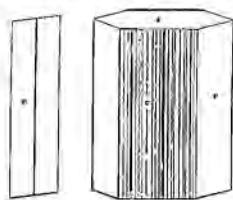


FIG. 1. Typical crystal of $Fe^{2+}_n(H_2O)_n(PO_4)_n$, showing the forms (010), (011) and (120). A. Plan; B. Clinographic projection.

¹ To receive a copy of Table 3, order document number AM-75-003-A from the Business office, Mineralogical Society of America, 1909 K Street, N.W., Washington, D.C. 20006. Please remit \$1.00 for the microfiche.

known structure. There are feeble resemblances to other members of the homologous series, and these relationships shall be emphasized.

To appreciate the problem more fully, we rewrite the formula as a cluster $M^{2+}_2S^{3+}_2\phi_n$, which consists of three divalent transition metals—two octahedrally coordinated ($= M$) and one five coordinated ($= S$)—and nine oxygen-ligand vertices, ϕ , per formula unit. Characteristic of the homologous series $Fe^{2+}_n(H_2O)_n(PO_4)_n$, all n -water molecules are aquated (are found as ligand groups) to the transition metal and all oxygens associated with the $[PO_4]^{3-}$ ligand ($= O_p$) are also bound to transition metals.

In a detailed study on this homologous series certain common characteristics among these structures were emphasized (Moore, 1971). As n decreases, the degree of octahedral condensation or polymerization increases: for $n = 8$ (vivianite), the octahedral com-

TABLE 2. Atomic Coordinate and Isotropic Thermal Vibration Parameters for $Fe_2(H_2O)(PO_4)_2$ *

Atom	x	y	z	$u(k^2)$
Fe(1)	0.0315(2)	0.1259(2)	0.9130(1)	0.43(1)
Fe(2)	-0.386(2)	-0.771(2)	-0.099(2)	.69(1)
Fe(3)	-0.911(2)	-1.241(2)	-0.278(1)	.54(1)
P(1)	-0.740(2)	-0.872(2)	-0.066(2)	.40(2)
P(2)	-1.172(2)	-0.829(2)	-0.262(2)	.55(2)
O(1)	-0.205(6)	-1.076(6)	-0.326(5)	.72(5)
O(2)	-0.215(6)	-0.029(6)	-0.572(5)	.67(5)
O(3)	-0.520(6)	-1.516(6)	-0.110(5)	.70(5)
O(4)	-0.593(6)	-0.308(6)	-1.197(5)	.71(5)
O(5)	-0.018(6)	-0.713(6)	-1.491(5)	.64(5)
O(6)	-0.231(6)	-0.097(6)	-1.113(5)	.71(5)
O(7)	-0.077(6)	-0.774(6)	-1.173(5)	.61(5)
O(8)	-0.237(6)	-0.326(6)	-0.055(5)	.61(5)
Ow	-0.015(9)	-0.825(9)	-0.690(5)	.98(5)

* Estimated standard errors refer to the last digit.

bination includes the edge-sharing dimer $M_2\phi_{1c}$ + the monomer $M\phi_{1c} = M_2\phi_{1a}$, which is equivalent to the expression $\phi_{1c} = (H_2O)_c + (Op)_c$. For $n = 4$ (jadlamite) the cluster formula is $M_4\phi_{1a}$ and the structure contains corner-linked chains of $M_2\phi_{1a}$ linear edge-sharing trimers bridged by the $[PO_4]$ tetrahedra. For $n = 3$ (phosphoferrite), these linear edge-sharing trimers $M_2\phi_{1a}$ fuse by further edge- and corner-sharing to form $M_3\phi_{1a}$ sheets. For $n = 0$, one of the dimorphs is sarcopside (cf Moore, 1972) which is an ordered derivative of the olivine structure type. With the cluster formula $M_2\phi_{1a}$, we observe the same linear edge-sharing trimers as the structural motif. Since $Fe^{2+}_3 (H_2O)[PO_4]_2$ is compositionally wedged in between, we had anticipated that it, too, would possess these linear edge-sharing trimers.

The $Fe_3(H_2O)[PO_4]_2$ structure not only reveals the absence of such linear trimers, but also provides two kinds of oxygen coordination about the transition metals: two distorted octahedra and one very distorted tetragonal pyramid! In addition, this awkward structure has resisted any obvious vehicle of description, and we despaired of finding a suitable projection until we selected a projection down $a' = a - c$, showing the plane $b \times c' \sin \beta'$, where $c' = a + c$. A slab of the structure, where the transition metal coordinates are bounded by $1/4 \leq x' \leq 1/2$, is provided in Figure 2. This projection, which features the transition metal polyhedra only, has advantages in that all three non-equivalent metals can be referred to a common level in x' . At $x' = 1/2$, the polyhedra are stippled, revealing a chain which runs parallel to $c' \sin \beta'$ with a crankshaft motif. Equivalent chains are further

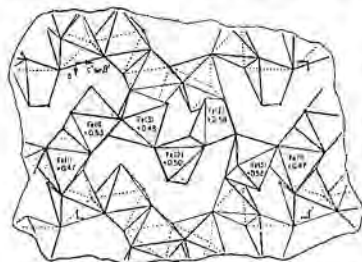


FIG. 2. Polyhedral diagram of the Fe-O arrangement between $1/4 \leq x' \leq 1/2$, where $a' = a - c$ and $c' = a + c$. The chain-like character is shown by stippling. Solid dots denote linkages of corners above and below this slab.

linked above and below to form a highly complex polyhedral framework. The $Fe(1)$ -O octahedron shares three of its edges; one with $Fe(1)$, namely OW^1-OW , and two with $Fe(3)$'s, namely $O(1)-O(3)^{II}$ and $O(2)^I-O(5)^I$. This immediate neighborhood is the $3_2(2)$ -cluster of Moore (1974a). The $Fe(3)$ -O octahedron shares two edges with $Fe(1)$ octahedra. Considering only the octahedra, this is the $2_2(2)$ configuration of Moore (1974a). The $Fe(2)$ -O distorted tetragonal pyramids share a mutual edge $O(4)-O(4)^I$ whose center is the center of inversion. In addition, an unanticipated feature, the edge $O(6)-O(8)$ is shared with the $P(2)O_4$ tetrahedron. We feel it necessary and desirable to point out the edge-sharing neighborhoods, for they have considerable implications in homonuclear electron transfer-absorption where the probability of transfer is increased as the distance between metal centers is decreased.

As yet, no theory predicts or explains *a priori* the existence of such an unusual structure. In many respects, the structure is reminiscent of the complex grastonite structure. Although sarcopside is a limiting hexagonal close-packed oxygen structure, the high-temperature dimorph grastonite bears no obvious relationship with it. This unusual structure, as shown by Calvo (1968), possesses three non-equivalent metal positions, two five-coordinated and one seven-coordinated. Despite attempts at several projections, no obvious relationship to $Fe_3(H_2O)[PO_4]_2$ could be found. Unlike $Fe_3(H_2O)[PO_4]_2$, no edges in grastonite are shared between the PO_4 tetrahedra and the five-coordinated polyhedra. It is possible that these unusual structures can be rationalized via some sphere-packing theory.

Bond Distances and Angles

Polyhedral interatomic distances are listed in Table 4. The averages for the Fe^{2+} -O octahedral and P-O tetrahedral distances are within the range reported for numerous well-refined structures. The polyhedral interatomic angles in Table 5 reveal rather severe distortions for the octahedra, ranging from $O(1)^{II}-Fe(3)-O(3)$ 76.9° to $O(2)^I-Fe(1)-O(3)^{II}$ 116.8° .

The $Fe(2)$ -O polyhedron possesses five vertices, but its angular distortions are so severe that distinction between tetragonal pyramidal and trigonal bipyramidal coordination is not possible. According to the interatomic angle distribution for these two kinds of polyhedra in Stephenson and Moore (1968), the $Fe(2)$ -O polyhedron resembles a trigonal bipyramid with the angle $O(4)-Fe(2)-O(8)$ 170.0° (deviating by 10° from the ideal 180° angle), but most

TABLE 4. Polyhedral Interatomic Distances for Fe₃(H₂O)₆(PO₄)₂

Fe(1)		Fe(2)		Fe(3)		P(1)					
Fe(1)	-0(5) ⁱ	2.070	Fe(2)	-0(7) ⁱⁱ	1.987	Fe(3)	-0(6) ⁱⁱⁱ	2.083	P(1)-O(1)	1.542	
"	-0(3) ⁱⁱ	2.092	"	-0(6)	2.036	"	-0(1) ⁱ	2.135	"	-0(3)	1.543
"	-0 ^{iv}	2.101	"	-0(9) ⁱ	2.052	"	-0(2) ⁱ	2.190	"	-0(2)	1.504
"	-0(1) ⁱ	2.152	"	-0(9) ⁱ	2.086	"	-0(9) ⁱⁱⁱ	2.145	"	-0(4)	1.561
"	-0(2) ⁱ	2.166	"	-0(8)	2.243	"	-0(5) ⁱ	2.206	"	average	1.548
"	-0 ^{iv}	2.383				"	-0(3)	2.211			
average		2.151	average		2.081	average		2.153	O(1)-O(4)	2.085	
O(1)	-0(3) ⁱⁱ	2.703*	Fe(2)	-P(2)	2.747	O(1) ⁱⁱ	-0(3) ⁱ	2.703*	O(2)-O(4)	2.517	
OW	-0(1) ⁱ	2.731*				O(2) ⁱ	-0(5) ⁱ	2.749*	O(3)-O(6)	2.536	
O(2) ⁱ	-0(5) ⁱ	2.749	O(6)	-0(8) ⁱ	2.413 [†]	O(1) ⁱⁱ	-0(8) ⁱⁱⁱ	2.935	O(2)-O(3)	2.540	
OW ⁱⁱ	-0(5) ⁱ	2.847	O(9) ⁱ	-0(9) ⁱ	2.627 ^v	O(6)	-0(9) ⁱⁱⁱ	2.997	O(1)-O(2)	2.593	
OW ⁱⁱ	-0(2) ⁱ	2.887	O(7) ⁱⁱ	-0(8) ⁱⁱ	2.981	O(6)	-0(5) ⁱ	2.975	average	2.526	
OW ⁱⁱ	-0(2) ⁱ	2.924	O(4)	-0(7) ⁱⁱ	3.069	O(1) ⁱⁱ	-0(2) ⁱ	3.031			
O(3) ⁱⁱ	-0(5) ⁱ	2.951*	O(9) ⁱ	-0(6)	3.167	O(9) ⁱⁱ	-0(3) ⁱ	3.084	P(2)		
OW ⁱⁱ	-0 ^{iv}	3.103	O(4) ⁱ	-0(6)	3.197	O(5) ⁱⁱ	-0(5) ⁱ	3.100			
OW ⁱⁱ	-0(1) ⁱ	3.143	O(4) ⁱ	-0(9)	3.364	O(2) ⁱ	-0(9) ⁱⁱⁱ	3.108	P(2)-O(7)	1.529	
OW ⁱⁱ	-0(3) ⁱⁱ	3.353	O(4) ⁱ	-0(7) ⁱⁱ	3.514	O(5) ⁱ	-0(8) ⁱⁱⁱ	3.108	"	-0(5)	1.539
O(1) ⁱ	-0(5) ⁱ	3.479	average		3.041	O(2) ⁱ	-0(3)	3.318	"	-0(6)	1.555
O(2) ⁱ	-0(3) ⁱⁱ	3.626				O(3)	-0(6)	3.391	"	-0(8)	1.556
average		3.041				average		3.037	average	1.542	
						Hydrogen Bonds			O(6)-O(8)	2.413 [†]	
						OW ... O(7) ⁱ	2.72		O(5)-O(7)	2.496	
						OW ... O(7) ⁱ	3.43		O(6)-O(7)	2.532	
									O(5)-O(9)	2.535	
									O(7)-O(8)	2.555	
									O(5)-O(6)	2.571	
									average	2.517	

ⁱ $i = -x, -y, -z$; ⁱⁱ $ii = 1/2+x, 1/2-y, z$; ⁱⁱⁱ $iii = 1/2-x, 1/2+y, -z$ applied to coordinates in Table 2.
 * Octahedral shared edges. † \dagger Fe(2)-P(2) shared edge. ^v v Fe(2)-Fe(2) shared edge.

of the remaining distances more closely resemble the tetragonal pyramid. The Fe(2)-O 2.08 Å average can be compared with the M(2)-O 2.14 and M(3)-O 2.05 Å averages reported by Calvo (1958) for the distorted tetragonal pyramid and trigonal bipyramid respectively in goethite. However, his material contains considerable Mn²⁺ which probably contribute to the longer averages through partial solutions.

TABLE 5. Polyhedral Interatomic Angles for Fe₃(H₂O)₆(PO₄)₂

Fe(1)		Fe(2)		Fe(3)		P(1)				
O(1)	-0(3) ⁱⁱ	79.11*	O(6)	-0(8)	68.47*	O(1) ⁱⁱ	-0(3) ⁱ	76.89*	O(1)-O(4)	106.40*
O(5) ⁱ	-0 ^{iv}	79.24	O(4)	-0(4)	78.85	O(2) ⁱ	-0(5) ⁱ	78.43	O(2)-O(4)	108.29
O(2) ⁱ	-0 ^{iv}	79.84	O(7) ⁱⁱ	-0(8) ⁱⁱ	89.40	O(1) ⁱⁱ	-0(8) ⁱⁱⁱ	86.60	O(3)-O(4)	109.58
O(1)	-0 ^{iv}	79.89	O(9) ⁱ	-0(7) ⁱⁱ	93.94	O(5) ⁱ	-0(6)	87.82	O(1)-O(3)	110.73
O(2) ⁱ	-0(5) ⁱ	80.89	O(4) ⁱ	-0(5)	101.57	O(6)	-0(6) ⁱⁱⁱ	88.40	O(2)-O(3)	110.73
O(2) ⁱ	-0 ^{iv}	85.12	O(4) ⁱ	-0(6)	101.75	O(3) ⁱⁱ	-0(9) ⁱⁱⁱ	90.15	O(2)-O(2)	110.98
OW	-0 ^{iv}	87.32	O(4) ⁱ	-0(6) ⁱⁱ	101.92	O(1) ⁱⁱ	-0(2) ⁱ	90.28		
O(1) ⁱ	-0 ^{iv}	87.62	O(9) ⁱ	-0(7) ⁱⁱ	119.30	O(2) ⁱ	-0(5) ⁱ	91.11	P(2)	
O(3) ⁱⁱ	-0(3) ⁱⁱ	90.32	O(6)	-0(7) ⁱⁱ	136.86	O(5) ⁱ	-0(6)	91.15		
O(3) ⁱⁱ	-0 ^{iv}	105.15	O(4) ⁱ	-0(6)	170.00	O(2) ⁱ	-0(6)	94.43	O(6)-O(8)	101.76*
O(1) ⁱ	-0(5) ⁱ	111.02				O(2) ⁱ	-0(3)	99.35	O(5)-O(7)	109.38*
O(2) ⁱ	-0(3) ⁱⁱ	116.77				O(3)	-0(6)	104.31	O(6)-O(7)	110.32
									O(5)-O(8)	110.46
									O(7)-O(8)	111.83
									O(5)-O(6)	112.88

Severe cation-cation repulsion across shared edges results in some very short distances; thus O(6)-O(8), the edge shared by Fe(2) and P(2), equals 2.41 Å, whereas O(4)-O(4)', which is shared by two Fe(2), equals 2.63 Å. These distances are the shortest for their polyhedra. Short distances between octahedral shared edges also occur, with the exception of OW-OW' 3.10 Å. This latter distance reflects the long Fe(1)-OW' 2.38 Å bond.

Hydrogen Bonds and Electrostatic Valence Balances

The OW molecule can donate two hydrogen bonds with the most likely acceptor being O(7), which coordinates to P(2) and Fe(2) only. Accepting $\xi = +1/6$ for the hydrogen bond strength as suggested by Baur (1970), a model can be found where O(7) accepts one strong and one weak hydrogen bond; OW...O(7) 2.72 Å and OW-O(7)' 3.43 Å with the angle O(7)-OW-O(7)' 100.1°. Two strong hydrogen bonds would result in a very nearly saturated O(7) anion, since $\Sigma = 5/4 + 2/5 + 1/6 + 1/6 = 1.98$. Since Fe(2)-O(7) and P(2)-O(7) are the shortest distances for their polyhedra, the presence of one feeble bond is more likely.

The remaining anions deviate only slightly from saturation by cations and accordingly show no systematic deviations in their Me-O bond distances. All oxide anions associated with Fe(1) are slightly un-

dersaturated with $\Delta\Sigma = -0.05$, adding further support to the likely preferential oxidation at the Fe(1) site discussed below.

A Proposed Oxidation Sequence for $\text{Fe}^{2+}_x(\text{H}_2\text{O})_x[\text{PO}_4]_3$

Moore (1971) has pointed out that only certain compositions in the homologous series $\text{Fe}^{2+}_x(\text{H}_2\text{O})_x[\text{PO}_4]_3$ are capable of continuous oxidation of the metals without destruction of the structure. The compositions are limited by the condition of maintenance of local electrostatic neutrality of cations about anions during oxidation. Permissible bonded units include H₂O-bridged ferrous ions (as in edge-sharing Fe²⁺ octahedra) where Fe²⁺(OH)₂Fe²⁺ can be continuously oxidized to hydroxide-bridged ferric ions—Fe³⁺(OH)₂Fe³⁺. On the other hand, hydroxide-bridged ferrous ions, Fe²⁺(OH)₂Fe²⁺, lead to extreme oxygen undersaturation. Analogously, such species as Fe²⁺(OH) or Fe²⁺(OH)₂Fe²⁺ also lead to local charge balance difficulties and are, accordingly, not observed. Of the homologous series, only $x = 3$ is capable of continuous oxidation to a stable ferric end-member since permissible end-member combinations are preserved. Thus, the series Fe²⁺₃(H₂O)₃[PO₄]₃ (phosphoferrite)—Fe²⁺₃(OH)₃[PO₄]₃ (kryzhanovskite) is observed in Nature; the others decompose to yield essentially amorphous ferric equivalents after progressive and complete oxidation (Moore, 1971). A more recent study on pure synthetic phosphoferrite and its ferric equivalent has established beyond doubt the existence of both ferrous and ferric end-member compositions belonging to the same structure type when the hydrogen atom positions are excluded (Moore, 1974b).

Since Fe²⁺(OH)₂Fe²⁺ ions occur in Fe²⁺₃(H₂O)₃[PO₄]₃, we propose that a bounded mixed valence composition can occur as a stable crystal. The mid-point of the OW-OW' edge shared between two Fe(1) atoms is an inversion center. This suggests that an upper bound for a stable oxidized equivalent would be Fe²⁺₂Fe³⁺(OH)₂[PO₄]₃ where Fe(1) is completely oxidized.

If such an oxidative sequence does indeed exist, then mixed-valence transfer and intense pleochroism should occur with maximum absorption along the Fe(1)²⁺—Fe(3)²⁺ direction. Unique Fe-Fe separations across the shared edges are Fe(1)—Fe(1) 3.25 Å, Fe(1)—Fe(3) 3.11 and 3.20 Å, and Fe(2)—Fe(2) 3.20 Å. We provide a skeleton of Fe-Fe' connections and distances across shared edges in Figure 3. These distances are similar to those found between the

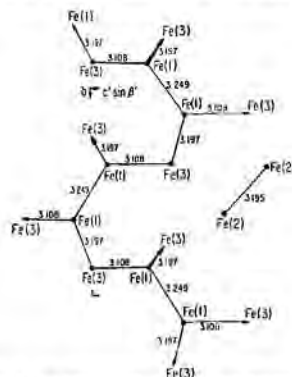


FIG. 3. The links between the Fe atoms where edges are shared. This diagram follows from Figure 2. Arrows, pointing in the plane and above or below, denote edge-links.

shared edge in vivianite, suggesting that mild oxidation of $\text{Fe}^{2+}_3(\text{H}_2\text{O})(\text{PO}_4)_2$ would result in intense pleochroism, similar to that observed for vivianite.

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Published in *The American Mineralogist*, Volume 60 (May-June, 1975).

TABLE 3. Calculated and Observed Structure Factors for $\text{Fe}_3(\text{H}_2\text{O})[\text{PO}_4]_2$

H	K	L	FO	FC	0	6	2	52.9	51.2
0	0	1	16.7	18.5	0	6	3	11.5	10.1
0	0	2	63.1	70.7	0	6	4	29.3	27.0
0	0	3	49.0	53.7	0	6	5	29.6	30.1
0	0	4	36.7	39.8	0	6	6	9.7	10.5
0	0	5	49.7	49.2	0	6	7	30.0	30.8
0	0	6	93.5	98.5	0	6	8	13.1	10.3
0	0	7	26.5	25.8	0	6	9	8.7	4.7
0	0	8	15.2	15.4	0	7	1	30.9	29.3
0	0	9	64.4	66.6	0	7	2	37.0	38.0
0	0	10	9.1	11.1	0	7	3	35.4	35.8
0	1	1	95.7	97.8	0	7	4	5.3	3.4
0	1	2	193.8	188.1	0	7	5	17.9	19.4
0	1	3	3.0	2.4	0	7	6	7.9	5.5
0	1	4	99.8	103.5	0	7	7	25.0	23.3
0	1	5	13.9	11.1	0	7	8	45.0	45.3
0	1	6	12.1	12.2	0	7	9	51.3	51.5
0	1	7	74.9	77.0	0	8	0	130.1	117.8
0	1	8	50.9	54.2	0	8	1	9.0	13.0
0	1	9	11.5	9.5	0	8	2	16.4	14.5
0	1	10	4.0	1.7	0	8	3	4.4	9.0
0	2	0	7.5	8.9	0	8	4	14.8	15.6
0	2	1	46.1	48.2	0	8	5	20.8	21.5
0	2	2	38.4	39.0	0	8	6	79.1	78.7
0	2	3	43.3	44.0	0	8	7	7.9	9.6
0	2	4	18.6	19.9	0	8	8	15.2	15.4
0	2	5	50.5	51.8	0	8	9	29.6	30.8
0	2	6	5.4	4.7	0	9	1	29.3	40.1
0	2	7	26.5	26.2	0	9	2	30.2	30.7
0	2	8	9.6	8.5	0	9	3	32.5	31.1
0	2	9	8.3	0.9	0	9	4	41.5	42.5
0	2	10	4.0	2.3	0	9	5	31.1	30.1
0	3	1	86.1	91.1	0	9	6	35.5	36.4
0	3	2	97.8	100.4	0	9	7	4.5	6.1
0	3	3	46.8	49.3	0	9	8	41.7	41.3
0	3	4	108.2	111.4	0	10	0	27.9	26.6
0	3	5	11.7	12.2	0	10	1	7.5	6.7
0	3	6	4.9	3.4	0	10	2	27.9	26.2
0	3	7	41.2	41.9	0	10	3	15.8	12.4
0	3	8	52.1	53.4	0	10	4	13.3	6.0
0	3	9	31.6	31.1	0	10	5	11.7	15.0
0	3	10	19.0	18.1	0	10	6	9.2	6.7
0	4	0	295.6	249.6	0	10	7	27.8	27.7
0	4	1	26.5	26.7	0	10	8	10.5	8.8
0	4	2	3.5	0.5	0	11	1	27.1	24.0
0	4	3	75.7	76.0	0	11	2	12.0	8.9
0	4	4	24.5	24.7	0	11	3	47.5	46.7
0	4	5	3.9	4.8	0	11	4	5.9	9.0
0	4	6	129.0	131.9	0	11	5	4.8	9.5
0	4	7	17.9	16.1	0	11	6	13.3	15.6
0	4	8	7.5	3.9	0	11	7	6.8	7.8
0	4	9	37.2	39.5	0	12	0	58.9	53.7
0	4	10	6.0	3.9	0	12	1	13.8	12.0
0	5	1	83.8	84.9	0	12	2	19.8	22.8
0	5	2	89.4	93.0	0	12	3	32.8	35.9
0	5	3	24.1	25.4	0	12	4	8.5	6.7
0	5	4	81.5	82.0	0	12	5	39.0	39.5
0	5	5	11.8	5.3	0	12	6	59.3	57.9
0	5	6	52.0	54.5	0	13	1	15.1	14.6
0	5	7	60.9	65.0	0	13	2	22.2	22.4
0	5	8	36.8	38.5	0	13	3	16.8	16.5
0	5	9	19.0	20.5	0	13	4	13.7	12.7
0	5	10	17.2	17.8	0	13	5	29.3	27.6
0	6	0	18.4	17.2	0	14	0	5.4	1.2
0	6	1	5.1	6.4	0	14	1	31.0	28.4
					0	14	2	5.3	5.9

(2)

(2)

					H	K	L	FO	FC
0	14	3	7.7	0.3					
0	14	4	21.3	21.0					
0	15	1	5.4	1.4					
1	15	-2	14.9	11.6	1	13	0	28.4	29.2
1	15	-1	20.8	17.9	1	13	1	60.6	57.8
1	15	0	8.4	6.8	1	13	2	5.6	5.0
1	15	1	58.8	57.1	1	13	3	11.0	6.3
1	14	3	69.2	66.6	1	13	4	25.2	20.2
1	14	2	28.9	24.2	1	13	5	5.3	3.1
1	14	1	14.6	17.0	1	12	6	5.1	3.2
1	14	0	30.9	30.7	1	12	5	24.6	21.4
1	14	-1	45.7	47.1	1	12	4	24.4	23.3
1	14	-2	32.3	32.3	1	12	3	29.3	29.3
1	14	-3	35.2	37.0	1	12	2	9.8	10.8
1	14	-4	9.5	10.6	1	12	1	5.1	7.9
1	13	-5	35.2	31.5	1	12	0	13.5	12.2
1	13	-4	5.9	6.2	1	12	-1	10.3	8.6
1	13	-3	13.0	10.5	1	12	-2	24.5	26.0
1	13	-2	17.4	13.9	1	12	-3	5.6	4.8
1	13	-1	5.1	1.5	1	12	-4	5.8	6.8
					1	12	-5	21.7	17.8
					1	12	-6	11.7	5.8
					1	11	-7	7.4	9.8
					1	11	-6	5.5	4.8
					1	11	-5	51.5	49.5
					1	11	-4	28.8	28.6
					1	11	-3	5.3	1.1
					1	11	-2	22.5	22.8
					1	11	-1	4.7	2.5
					1	11	0	10.6	10.0
					1	11	1	104.0	104.6
					1	11	2	17.6	21.2
					1	11	3	26.7	28.0
					1	11	4	35.3	34.6
					1	11	5	28.8	29.5
					1	11	6	12.2	9.7
					1	11	7	54.2	54.9
					1	10	7	12.0	12.3
					1	10	6	15.3	2.9
					1	10	5	41.4	44.3
					1	10	4	59.5	59.2
					1	10	3	111.4	110.7
					1	10	2	14.5	13.7
					1	10	1	4.9	8.1
					1	10	0	70.3	71.9
					1	10	-1	56.5	56.6
					1	10	-2	5.0	3.4
					1	10	-3	71.0	47.4
					1	10	-4	18.6	15.7
					1	10	-5	5.3	8.6
					1	10	-6	38.8	37.7
					1	10	-7	35.9	32.7
					1	10	-8	42.5	38.6
					1	9	-9	5.0	1.4
					1	9	-8	15.5	10.3
					1	9	-7	12.5	4.6
					1	9	-6	6.9	4.6
					1	9	-5	48.0	46.6
					1	9	-4	17.2	15.8
					1	9	-3	58.2	61.8
					1	9	-2	31.4	31.0
					1	9	-1	6.2	11.4
					1	9	0	32.0	33.3
					1	9	1	82.0	83.6
					1	9	2	24.3	24.7
					1	9	3	4.8	4.8
					1	9	4	22.5	20.9

(3)

1	9	5	6.2	3.6
1	9	6	26.3	27.3
1	9	7	37.8	40.5
1	9	8	4.6	4.2
1	8	8	10.8	12.6
1	8	7	31.7	36.0
1	8	6	15.8	12.1
1	8	5	9.8	13.0
1	8	4	45.3	44.7
1	8	3	4.7	3.8
1	8	2	40.5	41.5
1	8	1	35.6	34.7
1	8	0	10.6	0.8
1	8	-1	74.7	75.8
1	8	-2	28.3	31.2
1	8	-3	23.3	24.7
1	8	-4	10.6	11.5
1	8	-5	14.3	18.6
1	8	-6	5.0	4.7
1	8	-7	9.5	4.4
1	8	-8	11.9	9.5
1	8	-9	10.8	7.2
1	7	-9	12.0	14.8
1	7	-8	36.7	36.0
1	7	-7	7.1	6.2
1	7	-6	4.9	6.1
1	7	-5	92.7	91.1
1	7	-4	5.1	3.1
1	7	-3	10.0	3.8
1	7	-2	20.4	15.5
1	7	-1	4.2	2.5
1	7	0	10.2	9.4
1	7	1	113.2	115.0
1	7	2	60.6	63.0
1	7	3	4.7	3.0
1	7	4	35.4	37.2
1	7	5	26.3	26.7
1	7	6	12.4	14.1
1	7	7	59.5	60.0
1	7	8	4.7	2.6
1	7	9	9.4	9.7
1	6	9	46.2	51.2
1	6	8	33.6	35.7
1	6	7	35.6	38.0
1	6	6	17.4	16.6
1	6	5	22.5	24.2
1	6	4	10.9	12.1
1	6	3	93.6	96.5
1	6	2	50.2	50.8
1	6	1	48.5	49.9
1	6	0	63.1	63.5
1	6	-1	79.2	83.2
1	6	-2	129.6	129.4
1	6	-3	108.3	109.2
1	6	-4	31.4	29.5
1	6	-5	11.5	14.9
1	6	-6	52.6	49.9
1	6	-7	45.6	45.9
1	6	-8	14.3	15.8
1	6	-9	29.2	31.1
1	6	-10	4.8	3.0
1	5	-10	4.8	7.3
1	5	-9	7.6	3.1
1	5	-8	9.5	2.2
1	5	-7	10.3	7.7
1	5	-6	6.8	10.9

1	5	-5	64.0	65.6
1	5	-4	8.4	0.9
1	5	-3	59.9	62.7
1	5	-2	9.4	10.8
1	5	-1	24.4	25.6
1	5	0	35.3	36.3
1	5	1	103.5	106.8
1	5	2	41.9	41.2
1	5	3	15.3	14.5
1	5	4	14.8	15.3
1	5	5	18.6	20.4
1	5	6	48.3	48.6
1	5	7	63.8	68.0
1	5	8	10.4	8.8
1	5	9	27.9	27.8
1	4	9	12.5	12.5
1	4	8	4.5	6.1
1	4	7	26.5	27.7
1	4	6	21.5	18.8
1	4	5	20.5	23.5

(4)

4

H	K	L	FO	FC	I	J	K	L	M	N
1	4	4	56.7	56.6	1	1	-5	126.9	129.2	
1	4	3	8.7	4.5	1	1	-4	41.3	40.7	
1	4	2	60.4	62.4	1	1	-3	3.4	7.5	
1	4	1	41.9	41.1	1	1	-2	72.6	77.3	
1	4	0	10.5	8.8	1	1	-1	21.7	20.2	
1	4	-1	14.8	16.6	1	1	0	3.5	7.0	
1	4	-2	20.2	22.0	1	1	1	119.6	116.0	
1	4	-3	11.0	12.4	1	1	2	63.0	62.4	
1	4	-4	32.7	31.1	1	1	3	26.3	26.1	
1	4	-5	21.8	21.9	1	1	4	37.6	37.6	
1	4	-6	9.9	9.9	1	1	5	37.9	37.2	
1	4	-7	11.6	6.4	1	1	6	52.8	55.8	
1	4	-8	16.0	14.8	1	1	7	56.6	59.3	
1	4	-9	12.7	12.0	1	1	8	4.3	3.2	
1	4	-10	4.8	10.4	1	1	9	8.0	3.9	
1	3	-10	10.4	6.2	2	0	-11	4.4	2.3	
1	3	-9	16.3	17.6	2	0	-10	47.6	49.1	
1	3	-8	39.7	41.9	2	0	-9	30.5	33.3	
1	3	-7	60.8	60.4	2	0	-8	40.2	43.1	
1	3	-6	36.4	39.9	2	0	-7	26.8	27.4	
1	3	-5	142.7	142.5	2	0	-6	23.8	21.2	
1	3	-4	20.9	22.6	2	0	-5	7.7	10.5	
1	3	-3	60.9	59.2	2	0	-4	272.1	244.3	
1	3	-2	49.9	52.5	2	0	-3	9.0	8.5	
1	3	-1	26.8	30.7	2	0	-2	31.0	31.6	
1	3	0	61.6	61.7	2	0	-1	19.8	24.4	
1	3	1	103.0	105.2	2	0	0	16.2	12.5	
1	3	2	29.7	26.2	2	0	1	8.8	11.6	
1	3	3	19.4	20.4	2	0	2	93.9	102.0	
1	3	4	49.5	51.2	2	0	3	69.7	70.0	
1	3	5	21.0	19.5	2	0	4	17.5	17.5	
1	3	6	17.3	14.4	2	0	5	64.8	68.2	
1	3	7	43.9	45.7	2	0	6	63.4	66.4	
1	3	8	26.9	25.2	2	0	7	21.2	19.7	
1	3	9	16.0	14.2	2	0	8	115.7	119.2	
1	3	10	13.3	11.5	2	0	9	7.9	13.4	
1	2	10	23.6	27.6	2	1	9	26.5	25.6	
1	2	9	50.5	53.9	2	1	8	14.8	5.2	
1	2	8	13.0	6.6	2	1	7	21.0	20.5	
1	2	7	15.7	11.4	2	1	6	41.8	44.2	
1	2	6	26.5	27.9	2	1	5	47.1	50.2	
1	2	5	10.0	6.2	2	1	4	137.4	143.2	
1	2	4	78.1	79.8	2	1	3	44.7	45.6	
1	2	3	102.3	106.6	2	1	2	21.2	21.8	
1	2	2	69.9	71.9	2	1	1	97.9	98.2	
1	2	1	31.2	30.1	2	1	0	11.5	9.8	
1	2	0	19.5	24.6	2	1	-1	9.8	4.5	
1	2	-1	83.8	84.3	2	1	-2	64.9	65.8	
1	2	-2	177.3	165.8	2	1	-3	67.3	67.6	
1	2	-3	160.1	154.7	2	1	-4	26.9	25.9	
1	2	-4	119.4	115.5	2	1	-5	23.4	23.9	
1	2	-5	79.3	81.0	2	1	-6	34.6	34.8	
1	2	-6	26.4	25.4	2	1	-7	36.9	36.5	
1	2	-7	76.2	79.5	2	1	-8	39.0	41.8	
1	2	-8	18.2	19.1	2	1	-9	19.7	22.9	
1	2	-9	56.3	56.2	2	1	-10	33.9	35.3	
1	2	-10	14.0	13.5	2	1	-11	4.6	10.4	
1	2	-11	36.7	39.8	2	2	-11	4.5	0.4	
1	1	-11	44.0	44.9	2	2	-10	25.4	23.6	
1	1	-10	11.1	9.0	2	2	-9	4.4	1.9	
1	1	-9	34.3	33.8	2	2	-8	16.4	19.2	
1	1	-8	4.4	8.7	2	2	-7	13.1	15.8	
1	1	-7	46.3	46.5	2	2	-6	13.7	16.9	
1	1	-6	19.5	18.2	2	2	-5	4.0	1.8	
1	1	-5	19.5	18.2	2	2	-4	6.2	5.8	

5

7 3 5 8.9 14.7

					H	K	L	FO	FC
2	2	-3	57.5	57.4					
2	2	-2	26.5	28.1	2	3	2	26.3	37.1
2	2	-1	43.8	46.4	2	3	1	26.3	29.4
2	2	0	29.0	29.6	2	3	0	139.7	135.9
2	2	1	40.8	41.1	2	3	-1	46.0	46.9
2	2	2	10.5	9.7	2	3	-2	16.4	19.6
2	2	3	35.8	34.7	2	3	-3	51.6	49.5
2	2	4	28.7	30.8	2	3	-4	8.9	8.1
2	2	5	24.0	26.0	2	3	-5	67.5	67.5
2	2	6	5.9	3.4	2	3	-6	4.6	8.8
2	2	7	19.8	22.1	2	3	-7	45.0	46.8
2	2	8	4.5	2.2	2	3	-8	61.2	43.6
2	2	9	9.8	4.2	2	3	-9	4.5	6.1
2	2	9	28.4	30.6	2	3	-10	34.1	36.8
2	3	8	4.4	6.5	2	3	-11	10.1	11.5
2	3	7	4.3	4.0	2	4	-11	10.6	7.0
2	3	6	4.2	5.6	2	4	-10	68.4	71.2
2	3	5	15.3	12.4	2	4	-9	25.1	26.5
2	3	4	121.2	126.1	2	4	-8	23.7	27.0
2	3	3	59.8	61.7	2	4	-7	11.8	13.0
					2	4	-6	9.2	2.8
					2	4	-5	4.5	0.3
					2	4	-4	136.9	138.6
					2	4	-3	25.5	23.9
					2	4	-2	66.0	67.6
					2	4	-1	42.5	41.8
					2	4	0	102.5	99.2
					2	4	1	47.6	47.3
					2	4	2	215.5	215.5
					2	4	3	42.2	43.4
					2	4	4	30.4	30.3
					2	4	5	33.9	36.6
					2	4	6	37.3	39.0
					2	4	7	7.5	4.8
					2	4	8	64.9	66.4
					2	4	9	10.2	6.8
					2	5	9	9.2	11.0
					2	5	8	4.5	3.3
					2	5	7	11.9	6.0
					2	5	6	9.4	12.6
					2	5	5	30.2	32.0
					2	5	4	102.0	105.8
					2	5	3	33.3	34.7
					2	5	2	50.3	52.8
					2	5	1	20.4	19.2
					2	5	0	3.6	2.5
					2	5	-1	3.5	1.5
					2	5	-2	115.6	117.0
					2	5	-3	108.4	108.6
					2	5	-4	39.9	40.1
					2	5	-5	13.9	12.8
					2	5	-6	58.5	61.3
					2	5	-7	33.0	33.4
					2	5	-8	67.9	68.5
					2	5	-9	12.5	13.7
					2	5	-10	29.3	29.1
					2	6	-10	39.0	39.5
					2	6	-9	4.8	6.4
					2	6	-8	31.3	30.7
					2	6	-7	48.6	48.0
					2	6	-6	27.3	27.7
					2	6	-5	76.8	77.2
					2	6	-4	4.7	3.6
					2	6	-3	16.8	13.4
					2	6	-2	36.4	38.6

6

2	6	-1	12.3	15.4
2	6	0	38.4	39.3
2	6	1	18.5	20.3
2	6	2	5.5	6.5
2	6	3	5.5	6.7
2	6	4	42.4	46.0
2	6	5	7.8	1.9
2	6	6	17.2	17.5
2	6	7	22.1	20.2
2	6	8	4.5	6.4
2	7	8	4.6	2.6
2	7	7	4.7	0.3
2	7	6	11.8	14.8
2	7	5	20.7	20.2
2	7	4	65.0	65.3
2	7	3	50.8	52.1
2	7	2	29.9	28.9
2	7	1	29.9	32.8
2	7	0	50.9	53.1
2	7	-1	81.6	83.2
2	7	-2	100.6	99.8
2	7	-3	39.7	41.4
2	7	-4	35.9	37.9
2	7	-5	46.1	45.8
2	7	-6	6.9	6.4
2	7	-7	38.1	41.3
2	7	-8	8.9	2.1
2	7	-9	4.9	2.9
2	7	-10	15.7	13.5
2	8	-9	22.4	14.8
2	8	-8	26.4	27.2
2	8	-7	10.1	14.4
2	8	-6	39.4	40.4
2	8	-5	11.3	13.9
2	8	-4	150.3	149.5
2	8	-3	19.9	22.8
2	8	-2	38.3	39.1
2	8	-1	20.4	18.2
2	8	0	49.6	49.8
2	8	1	23.9	23.8
2	8	2	108.0	108.4
2	8	3	4.6	6.0
2	8	4	31.8	31.8
2	8	5	56.4	56.6
2	8	6	4.6	8.0
2	8	7	12.4	15.3
2	8	8	31.9	33.5
2	9	7	11.0	10.4
2	9	6	9.3	2.1
2	9	5	32.2	32.4
2	9	4	57.2	59.0
2	9	3	35.5	34.8
2	9	2	26.2	27.9
2	9	1	30.9	30.9
2	9	0	13.9	13.1
2	9	-1	4.3	8.7
2	9	-2	92.3	92.9
2	9	-3	81.1	81.8
2	9	-4	44.9	46.2
2	9	-5	46.5	47.4
2	9	-6	36.7	36.0
2	9	-7	18.7	17.9
2	9	-8	58.9	57.2
2	9	-9	26.5	25.6
2	10	-8	11.2	14.5
2	10	-7	22.8	22.3

2	10	-6	20.3	23.4
2	10	-5	56.8	54.7
2	10	-4	23.7	25.0
2	10	-3	14.3	17.2
2	10	-2	4.6	7.7
2	10	-1	33.7	34.9
2	10	0	24.7	26.4
2	10	1	48.5	49.5
2	10	2	9.0	2.9
2	10	3	4.8	2.9
2	10	4	19.3	19.6
2	10	5	14.8	18.9
2	10	6	22.8	17.8
2	10	7	4.7	3.8
2	11	6	16.3	11.7
2	11	5	34.0	34.7
2	11	4	12.0	14.4
2	11	3	7.8	1.8
2	11	2	25.7	25.7
2	11	1	10.8	14.3

7

H	K	L	FD	FC	3	12	1	4.9	2.3
2	11	0	17.6	20.4	3	12	0	13.3	14.7
2	11	-1	78.4	77.1	3	12	-1	4.9	12.6
2	11	-2	40.9	41.6	3	12	-2	20.8	18.1
2	11	-3	14.3	7.6	3	12	-3	23.9	22.6
2	11	-4	18.1	23.4	3	12	-4	12.7	12.4
2	11	-5	45.8	40.3	3	12	-5	13.3	13.6
2	11	-6	5.5	1.2	3	12	-6	8.9	9.8
2	11	-7	31.9	32.2	3	12	-7	11.5	5.4
2	11	-8	15.9	16.9	3	11	-8	15.1	10.9
2	12	-7	14.6	7.0	3	11	-7	49.5	48.1
2	12	-6	32.1	30.8	3	11	-6	12.3	12.5
2	12	-5	5.6	2.6	3	11	-5	12.1	10.0
2	12	-4	89.3	86.1	3	11	-4	14.1	11.8
2	12	-3	15.2	21.3	3	11	-3	31.2	31.1
2	12	-2	39.0	38.7	3	11	-2	8.8	5.0
2	12	-1	13.7	13.2	3	11	-1	12.5	8.2
2	12	0	13.9	17.5	3	11	0	30.7	30.8
2	12	1	32.6	32.7	3	11	1	4.6	2.2
2	12	2	49.8	53.3	3	11	2	4.8	4.6
2	12	3	27.9	26.0	3	11	3	33.4	33.8
2	12	4	17.4	12.0	3	11	4	23.1	22.7
2	12	5	55.1	50.8	3	11	5	22.7	22.5
2	13	4	26.1	25.0	3	10	6	5.0	3.2
2	13	3	48.6	45.4	3	10	5	55.9	59.3
2	13	2	5.3	4.9	3	10	4	27.5	29.3
2	13	1	28.0	25.4	3	10	3	9.0	5.8
2	13	0	13.9	14.7	3	10	2	24.0	26.4
2	13	-1	24.1	22.3	3	10	1	10.9	9.6
2	13	-2	66.4	66.7	3	10	0	70.0	70.2
2	13	-3	30.1	30.2	3	10	-1	68.1	68.3
2	13	-4	40.4	40.7	3	10	-2	28.9	26.9
2	13	-5	24.5	25.3	3	10	-3	4.6	2.6
2	13	-6	16.8	11.9	3	10	-4	10.2	8.9
2	14	-4	12.7	15.6	3	10	-5	22.0	21.7
2	14	-3	10.6	9.0	3	10	-6	48.1	48.2
2	14	-2	5.2	2.0	3	10	-7	54.1	52.0
2	14	-1	20.5	17.1	3	10	-8	11.6	10.1
2	14	0	25.7	27.7	3	9	-9	54.3	51.6
2	14	1	26.9	25.9	3	9	-8	6.9	5.0
2	14	2	25.5	20.4	3	9	-7	24.1	25.2
2	14	3	9.5	11.3	3	9	-6	11.1	1.6
2	15	0	15.4	13.4	3	9	-5	4.9	7.0
2	15	-1	44.9	41.6	3	9	-4	12.7	15.9
3	14	2	30.6	32.6	3	9	-3	82.3	82.0
3	14	1	9.6	4.0	3	9	-2	29.8	31.9
3	14	0	13.7	11.4	3	9	-1	6.2	2.8
3	14	-1	24.3	24.6	3	9	0	47.9	46.6
3	14	-2	13.6	16.0	3	9	1	11.4	7.0
3	14	-3	14.0	4.1	3	9	2	28.0	26.2
3	14	-4	13.8	11.8	3	9	3	21.5	27.8
3	13	-6	20.2	18.4	3	9	4	19.8	20.7
3	13	-5	11.4	3.1	3	9	5	41.4	40.6
3	13	-4	50.6	48.8	3	9	6	6.7	1.6
3	13	-3	30.9	27.7	3	9	7	20.4	23.5
3	13	-2	8.5	9.3	3	8	7	25.0	23.2
3	13	-1	5.1	4.0	3	8	6	28.6	25.3
3	13	0	5.0	3.6	3	8	5	21.2	21.2
3	13	1	19.1	19.2	3	8	4	8.0	14.0
3	13	2	23.6	19.2	3	8	3	4.5	6.3
3	13	3	38.5	40.0	3	8	2	18.9	12.6
3	12	5	5.2	4.2	3	8	1	4.2	4.8
3	12	4	18.6	15.5	3	8	0	4.3	8.1
3	12	3	5.1	4.8	3	8	-1	17.5	18.2
3	12	2	9.0	6.2	3	8	-2	22.7	23.2
3	12	1			3	8	-3	4.4	7.4

8

					H	K	L	FO	FC
3	8	-4	12.8	14.9					
3	8	-5	25.6	21.8					
3	8	-6	12.1	14.2					
3	8	-7	20.2	18.6					
3	8	-8	20.0	19.1					
3	8	-9	16.4	8.4					
3	8	-10	28.5	28.7					
3	7	-10	14.1	20.7					
3	7	-9	34.3	32.9					
3	7	-8	12.7	11.9					
3	7	-7	53.3	55.1					
3	7	-6	16.7	13.6					
3	7	-5	20.8	20.8					
3	7	-4	34.9	35.3					
3	7	-3	52.4	53.5					
3	7	-2	11.9	11.2					
3	7	-1	37.2	38.4					
3	7	0	17.3	17.7					
3	7	1	30.1	32.4					
3	7	2	36.8	36.2					
					3	7	3	92.0	93.6
					3	7	4	12.6	16.8
					3	7	5	4.5	2.6
					3	7	6	28.8	33.5
					3	7	7	23.5	23.9
					3	7	8	9.5	2.3
					3	6	8	12.1	14.1
					3	6	7	14.9	12.5
					3	6	6	55.2	55.8
					3	6	5	83.8	86.9
					3	6	4	21.1	23.2
					3	6	3	4.2	3.2
					3	6	2	4.2	3.6
					3	6	1	14.6	13.4
					3	6	0	49.0	47.2
					3	6	-1	141.9	141.5
					3	6	-2	57.0	59.2
					3	6	-3	82.9	83.9
					3	6	-4	18.8	14.9
					3	6	-5	38.9	38.8
					3	6	-6	79.5	81.1
					3	6	-7	75.3	75.7
					3	6	-8	39.9	39.8
					3	6	-9	21.0	24.3
					3	6	-10	28.6	27.5
					3	5	-11	4.8	9.2
					3	5	-10	4.8	7.3
					3	5	-9	59.1	58.1
					3	5	-8	14.5	14.8
					3	5	-7	32.4	32.9
					3	5	-6	4.5	3.1
					3	5	-5	55.2	57.8
					3	5	-4	18.9	17.5
					3	5	-3	131.7	131.8
					3	5	-2	21.6	22.8
					3	5	-1	79.1	78.6
					3	5	0	93.6	95.0
					3	5	1	30.7	32.3
					3	5	2	42.2	41.1
					3	5	3	43.0	46.7
					3	5	4	16.0	14.8
					3	5	5	37.5	39.6
					3	5	6	26.7	28.1
					3	5	7	16.6	15.5
					3	5	8	48.3	47.8
					3	4	8	4.5	5.9
					3	4	7	21.5	20.1
					3	4	6	23.1	18.7
					3	4	5	25.2	26.4
					3	4	4	13.1	13.4
					3	4	3	39.1	37.2
					3	4	2	32.3	31.8
					3	4	1	60.3	58.3
					3	4	0	29.0	30.1
					3	4	-1	23.9	26.2
					3	4	-2	46.4	46.3
					3	4	-3	22.6	23.1
					3	4	-4	17.3	19.2
					3	4	-5	29.5	29.7
					3	4	-6	4.5	1.1
					3	4	-7	48.9	48.8
					3	4	-8	12.6	14.9
					3	4	-9	13.3	18.3
					3	4	-10	35.9	33.1

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3	4	-11	8.0	4.8
3	3	-11	6.1	1.5
3	3	-10	4.7	3.8
3	3	-9	35.9	37.1
3	3	-8	6.7	7.6
3	3	-7	61.3	61.5
3	3	-6	6.4	4.7
3	3	-5	4.1	3.7
3	3	-4	16.1	16.1
3	3	-3	103.6	104.3
3	3	-2	3.2	1.4
3	3	-1	28.7	33.2
3	3	0	11.4	11.7
3	3	1	88.1	91.6
3	3	2	87.8	87.8
3	3	3	122.0	124.1
3	3	4	7.5	7.7
3	3	5	4.2	1.6
3	3	6	48.1	49.5
3	3	7	6.1	4.6
3	3	8	12.4	9.3
3	3	9	16.5	17.0
3	2	9	33.3	33.6
3	2	8	33.3	34.7
3	2	7	4.3	3.5
3	2	6	57.2	58.0
3	2	5	76.9	80.1
3	2	4	59.2	62.1
3	2	3	41.6	42.3
3	2	2	9.0	12.8
3	2	1	10.3	10.0
3	2	0	103.0	103.5
3	2	-1	261.3	237.9
3	2	-2	14.1	17.8
3	2	-3	84.2	87.2
3	2	-4	94.5	97.4
3	2	-5	3.8	4.3
3	2	-6	16.1	17.6
3	2	-7	70.9	71.1
3	2	-8	55.9	53.5
3	2	-9	23.4	23.0
3	2	-10	39.4	42.0
3	2	-11	33.3	33.3
3	1	-11	6.4	7.4
3	1	-10	6.4	4.4
3	1	-9	57.3	59.0
3	1	-8	28.1	28.8
3	1	-7	28.6	28.9
3	1	-6	27.7	30.7
3	1	-5	45.8	48.0
3	1	-4	18.8	16.7
3	1	-3	108.5	108.8
3	1	-2	41.0	42.3
3	1	-1	141.2	137.2
3	1	0	82.0	84.0
3	1	1	25.9	28.8
3	1	2	57.1	57.1
3	1	3	85.6	88.8
3	1	4	36.1	37.9
3	1	5	17.7	18.6
3	1	6	54.7	57.4
3	1	7	18.6	16.0
3	1	8	24.1	23.8
3	1	9	10.5	8.3
4	0	-11	25.0	22.8
4	0	-10	35.5	37.3

4	0	-9	6.9	2.4
4	0	-8	106.7	108.1
4	0	-7	9.3	8.2
4	0	-6	135.9	136.2
4	0	-5	7.6	7.9
4	0	-4	152.8	146.0
4	0	-3	80.1	84.1
4	0	-2	69.8	72.4
4	0	-1	14.8	15.7
4	0	0	112.1	111.5
4	0	1	113.3	115.7
4	0	2	41.9	45.6
4	0	3	29.6	29.6
4	0	4	90.3	91.6
4	0	5	32.5	33.2
4	0	6	27.5	27.1
4	0	7	40.7	44.9
4	0	8	31.3	35.7
4	1	8	28.0	30.0
4	1	7	11.2	14.4

10

4	1	6	43.6	47.0
4	1	5	34.7	35.3
4	1	4	4.1	1.2
4	1	3	43.0	44.8
4	1	2	13.0	10.9
4	1	1	79.2	80.3
4	1	0	161.0	156.4
4	1	-1	81.8	81.8
4	1	-2	55.7	55.3
4	1	-3	13.4	14.5
4	1	-4	17.4	16.7
4	1	-5	63.8	67.2
4	1	-6	107.1	109.3
4	1	-7	16.2	15.3
4	1	-8	83.8	88.1
4	1	-9	34.1	37.6
4	1	-10	12.7	15.9
4	1	-11	13.2	10.4
4	2	-11	4.7	6.4
4	2	-10	4.8	5.6
4	2	-9	10.6	11.7
4	2	-8	4.4	2.8
4	2	-7	4.2	8.7
4	2	-6	11.5	5.9
4	2	-5	20.1	22.4
4	2	-4	25.1	25.7
4	2	-3	65.6	62.5
4	2	-2	62.8	62.7
4	2	-1	28.0	27.8
4	2	0	12.6	10.4
4	2	1	41.4	42.2
4	2	2	14.2	17.7
4	2	3	13.2	11.0
4	2	4	5.9	8.3
4	2	5	21.7	24.0
4	2	6	16.2	19.7
4	2	7	4.5	12.3
4	2	8	14.4	13.5
4	3	8	23.1	18.6
4	3	7	4.7	6.8
4	3	6	51.3	55.2
4	3	5	9.1	7.6
4	3	4	13.1	11.8
4	3	3	32.9	33.3
4	3	2	51.0	49.9
4	3	1	61.3	63.0
4	3	0	101.6	103.9
4	3	-1	17.5	17.6
4	3	-2	24.3	24.1
4	3	-3	11.6	12.6
4	3	-4	32.6	36.1
4	3	-5	89.7	91.6
4	3	-6	24.1	23.2
4	3	-7	38.8	37.5
4	3	-8	63.4	64.0
4	3	-9	11.2	9.7
4	3	-10	4.7	7.7
4	3	-11	16.9	21.3
4	4	-11	4.6	2.4
4	4	-10	26.5	28.2
4	4	-9	8.4	9.1
4	4	-8	49.1	51.4
4	4	-7	5.6	1.3
4	4	-6	109.8	112.0

4	4	-4	101.8	101.2
4	4	-3	94.0	97.4
4	4	-2	175.1	169.7
4	4	-1	25.8	27.3
4	4	0	70.2	71.9
4	4	1	51.4	52.4
4	4	2	11.7	16.0
4	4	3	31.6	31.2
4	4	4	43.8	44.8
4	4	5	11.4	6.7
4	4	6	7.0	10.6
4	4	7	53.1	56.6
4	4	8	34.6	38.2
4	5	8	32.5	34.1
4	5	7	16.6	17.8
4	5	6	49.5	51.9
4	5	5	33.5	35.6
4	5	4	28.4	28.8
4	5	3	39.0	40.5
4	5	2	4.1	3.8
4	5	1	52.2	54.6
4	5	0	131.0	131.8
4	5	-1	87.0	86.8
4	5	-2	37.7	40.3
4	5	-3	19.4	19.1
4	5	-4	11.3	13.2
4	5	-5	4.3	7.9
4	5	-6	90.2	90.7
4	5	-7	41.8	41.5
4	5	-8	49.8	50.5
4	5	-9	36.0	37.4
4	5	-10	13.4	11.9
4	5	-11	8.3	3.9
4	6	-11	4.9	3.1
4	6	-10	4.9	1.4
4	6	-9	26.2	28.4
4	6	-8	4.8	6.5
4	6	-7	37.7	40.6
4	6	-6	10.3	5.4
4	6	-5	16.1	17.0
4	6	-4	57.2	59.4
4	6	-3	22.4	22.2
4	6	-2	90.9	89.5
4	6	-1	24.9	26.0
4	6	0	4.0	0.8
4	6	1	103.1	104.0
4	6	2	35.3	36.5
4	6	3	60.9	59.2
4	6	4	26.2	22.3
4	6	5	7.0	11.9
4	6	6	28.2	31.8
4	6	7	15.4	17.7
4	7	7	22.2	23.1
4	7	6	53.8	54.8
4	7	5	43.6	43.5
4	7	4	14.0	12.8
4	7	3	20.2	20.8
4	7	2	4.1	5.9
4	7	1	74.3	72.7
4	7	0	36.5	37.3
4	7	-1	8.9	0.4
4	7	-2	17.5	19.2
4	7	-3	33.9	35.3
4	7	-4	41.2	42.9
4	7	-5	53.5	54.4

11

4	7	-6	21.9	19.6
4	7	-7	20.7	21.7
4	7	-8	24.3	28.3
4	7	-9	9.0	9.3
4	7	-10	5.0	2.5
4	8	-10	5.1	10.6
4	8	-9	11.2	9.4
4	8	-8	62.8	62.0
4	8	-7	13.9	17.3
4	8	-6	45.2	45.3
4	8	-5	23.3	25.0
4	8	-4	12.5	14.5
4	8	-3	21.7	22.4
4	8	-2	63.4	63.5
4	8	-1	23.9	26.8
4	8	0	78.0	77.0
4	8	1	40.5	40.3
4	8	2	49.1	49.2
4	8	3	60.7	59.3
4	8	4	52.8	55.6

H	K	L	FU	FL
4	8	5	14.8	16.0
4	8	6	12.8	7.1
4	8	7	32.2	35.1
4	9	6	41.4	42.3
4	9	5	34.6	33.8
4	9	4	34.7	33.0
4	9	3	23.6	23.9
4	9	2	20.8	21.1
4	9	1	26.2	25.2
4	9	0	88.1	88.3
4	9	-1	46.4	45.9
4	9	-2	47.9	48.3
4	9	-3	4.5	7.5
4	9	-4	11.2	3.9
4	9	-5	8.5	5.1
4	9	-6	52.5	52.8
4	9	-7	25.6	23.5
4	9	-8	18.2	18.9
4	9	-9	37.0	37.4
4	10	-9	12.5	11.3
4	10	-8	15.1	13.0
4	10	-7	12.3	6.9
4	10	-6	5.1	6.8
4	10	-5	4.8	3.3
4	10	-4	38.4	35.8
4	10	-3	29.5	27.1
4	10	-2	16.8	17.2
4	10	-1	4.4	2.2
4	10	0	20.9	22.3
4	10	1	40.5	42.3
4	10	2	28.1	27.8
4	10	3	33.0	31.0
4	10	4	5.0	11.0
4	10	5	12.8	6.2
4	11	5	18.8	13.2
4	11	4	5.1	4.3
4	11	3	9.6	17.1
4	11	2	16.4	14.6
4	11	1	33.3	31.4
4	11	0	41.3	41.8
4	11	-1	11.4	3.9
4	11	-2	4.6	1.2
4	11	-3	25.6	21.6
4	11	-4	4.8	4.5
4	11	-5	23.3	23.2
4	11	-6	9.3	8.7
4	11	-7	10.9	8.3
4	11	-8	14.3	9.5
4	12	-7	5.5	2.1
4	12	-6	19.3	20.1
4	12	-5	10.7	4.4
4	12	-4	12.7	10.3
4	12	-3	5.0	6.4
4	12	-2	45.0	44.9
4	12	-1	35.5	36.0
4	12	0	66.7	63.4
4	12	1	32.6	31.5
4	12	2	48.4	48.2
4	12	3	41.5	38.0
4	12	4	34.1	34.8
4	13	3	11.7	4.9
4	13	2	12.9	17.7
4	13	1	13.2	11.2
4	13	0	46.9	46.1

12

2

4	13	-2	27.1	25.3
4	13	-3	10.6	13.8
4	13	-4	9.1	9.1
4	13	-5	5.3	6.1
4	13	-6	37.2	33.8
4	14	-4	5.5	11.2
4	14	-3	20.6	24.6
4	14	-2	13.4	8.5
4	14	-1	5.1	5.0
4	14	0	18.3	15.6
4	14	1	5.1	1.6
5	14	-1	24.7	21.2
5	14	-2	17.4	11.8
5	14	-3	48.9	48.7
5	13	-6	5.3	5.3
5	13	-5	44.9	44.7
5	13	-4	8.4	4.7
5	13	-3	14.6	10.6
5	13	-2	44.1	39.1
5	13	-1	28.0	28.6
5	13	0	18.1	18.1
5	13	1	11.0	12.2
5	13	2	5.0	1.1
5	12	3	8.2	11.5
5	12	2	5.0	1.7
5	12	1	4.9	8.2
5	12	0	10.3	6.1
5	12	-1	13.9	7.6
5	12	-2	18.3	12.4
5	12	-3	5.0	1.1
5	12	-4	5.0	2.7
5	12	-5	10.8	11.4
5	12	-6	5.3	10.4
5	12	-7	17.8	15.6
5	11	-8	18.1	9.2
5	11	-7	7.3	6.5
5	11	-6	11.9	7.2
5	11	-5	63.3	60.7
5	11	-4	23.6	22.7
5	11	-3	38.0	37.8
5	11	-2	41.9	44.1
5	11	-1	27.5	25.3
5	11	0	17.1	18.4
5	11	1	36.6	39.9
5	11	2	4.9	10.5
5	11	3	20.4	17.6
5	11	4	38.9	36.6
5	10	5	30.4	27.7
5	10	4	29.5	24.7
5	10	3	4.7	2.7
5	10	2	38.0	35.3
5	10	1	64.9	63.8
5	10	0	9.8	7.9
5	10	-1	42.7	43.3
5	10	-2	18.3	18.9
5	10	-3	57.2	57.5
5	10	-4	71.5	72.6
5	10	-5	66.7	65.7
5	10	-6	23.6	20.6
5	10	-7	38.3	37.0
5	10	-8	19.9	20.4
5	10	-9	20.9	17.9
5	9	-9	18.6	17.8
5	9	-8	7.1	8.5
5	9	-7	13.4	7.3

5	9	-6	36.5	35.3
5	9	-5	48.9	48.4
5	9	-4	14.2	15.3
5	9	-3	34.0	35.7
5	9	-2	56.4	53.3
5	9	-1	55.6	57.8
5	9	0	9.1	10.1
5	9	1	19.7	19.4
5	9	2	21.6	26.0
5	9	3	22.0	21.5
5	9	4	38.5	35.8
5	9	5	33.1	33.8
5	8	6	20.6	20.1
5	8	5	6.2	5.2
5	8	4	18.5	19.1
5	8	3	11.6	14.0
5	8	2	15.6	11.8
5	8	1	26.9	29.0
5	8	0	13.1	9.0
5	8	-1	8.5	7.1

13

H	K	L	FQ	FC					
					5	4	7	7.0	2.6
					5	4	6	18.2	18.2
					5	4	5	6.0	7.4
					5	4	4	11.2	10.4
					5	4	3	31.6	35.2
					5	4	2	5.0	3.2
					5	4	1	65.2	70.2
					5	4	0	14.2	11.3
					5	4	-1	41.4	42.9
					5	4	-2	60.2	61.0
					5	4	-3	30.7	29.4
					5	4	-4	29.0	28.1
					5	4	-5	7.1	6.5
					5	4	-6	38.1	37.7
					5	4	-7	40.8	41.8
					5	4	-8	24.1	24.3
					5	4	-9	7.3	5.5
					5	4	-10	4.9	4.1
					5	4	-11	19.7	19.7
					5	3	-11	69.9	69.4
					5	3	-10	4.8	7.4
					5	3	-9	36.3	36.6
					5	3	-8	16.2	15.5
					5	3	-7	59.8	60.6
					5	3	-6	31.4	30.5
					5	3	-5	40.4	39.6
					5	3	-4	73.8	72.8
					5	3	-3	17.2	19.3
					5	3	-2	43.3	45.8
					5	3	-1	20.8	21.0
					5	3	0	10.2	9.4
					5	3	1	75.9	78.7
					5	3	2	43.7	46.2
					5	3	3	22.5	26.6
					5	3	4	45.2	47.1
					5	3	5	13.1	10.2
					5	3	6	4.7	10.4
					5	3	7	21.7	22.5
					5	2	8	44.5	45.2
					5	2	7	71.7	72.7
					5	2	6	14.1	11.2
					5	2	5	24.8	28.9
					5	2	4	19.2	18.6
					5	2	3	71.9	74.3
					5	2	2	28.6	27.7
					5	2	1	104.9	106.6
					5	2	0	72.3	76.4
					5	2	-1	65.7	66.7
					5	2	-2	21.6	22.2
					5	2	-3	20.2	20.7
					5	2	-4	100.3	100.3
					5	2	-5	134.1	133.9
					5	2	-6	4.0	6.3
					5	2	-7	29.2	31.0
					5	2	-8	27.5	30.0
					5	2	-9	15.6	11.4
					5	2	-10	49.6	54.4
					5	2	-11	32.5	32.5
					5	1	-12	9.3	4.6
					5	1	-11	33.0	33.4
					5	1	-10	27.1	28.8
					5	1	-9	11.9	8.6
					5	1	-8	46.4	48.7
					5	1	-7	64.6	64.7
					5	1	-6	3.9	1.6
					5	1	-5	60.2	61.0

14

					H	K	L	FD	FC
5	1	-4	53.5	52.9					
5	1	-3	25.9	28.0	6	0	-5	20.1	17.9
5	1	-2	54.9	55.4	6	0	-4	190.5	185.7
5	1	-1	57.8	57.3	6	0	-3	96.1	97.5
5	1	0	10.6	12.1	6	0	-2	82.8	82.5
5	1	1	55.8	58.4	6	0	-1	132.3	133.2
5	1	2	33.0	35.5	6	0	0	51.6	52.4
5	1	3	83.4	87.6	6	0	1	14.5	16.7
5	1	4	31.3	33.0	6	0	2	82.4	84.6
5	1	5	14.4	12.5	6	0	3	13.4	16.0
5	1	6	4.6	1.3	6	0	4	43.3	43.8
5	1	7	33.3	34.4	6	0	5	100.8	102.5
5	1	8	23.8	24.8	6	0	6	11.6	9.3
6	0	-12	61.4	59.4	6	0	7	23.1	24.4
6	0	-11	17.5	14.6	6	1	7	8.5	12.8
6	0	-10	51.8	52.7	6	1	6	4.6	1.1
6	0	-9	49.1	48.9	6	1	5	13.3	8.4
6	0	-8	42.6	43.7	6	1	4	39.2	42.2
6	0	-7	3.9	2.5	6	1	3	53.6	56.1
6	0	-6	3.8	6.2	6	1	2	67.3	68.9
					6	1	1	44.6	44.5
					6	1	0	61.2	62.3
					6	1	-1	24.3	24.9
					6	1	-2	67.5	91.5
					6	1	-3	62.8	62.3
					6	1	-4	50.5	50.3
					6	1	-5	71.7	72.5
					6	1	-6	27.7	28.1
					6	1	-7	19.8	19.1
					6	1	-8	37.0	35.7
					6	1	-9	39.3	40.7
					6	1	-10	43.8	45.5
					6	1	-11	18.4	17.5
					6	1	-12	33.8	38.3
					6	2	-12	7.4	0.3
					6	2	-11	26.1	24.1
					6	2	-10	7.0	2.3
					6	2	-9	10.6	12.5
					6	2	-8	15.4	16.1
					6	2	-7	4.0	7.7
					6	2	-6	22.9	22.9
					6	2	-5	39.0	39.7
					6	2	-4	6.9	11.4
					6	2	-3	30.4	30.0
					6	2	-2	5.1	4.6
					6	2	-1	3.5	3.7
					6	2	0	12.3	14.3
					6	2	1	3.8	5.9
					6	2	2	3.9	8.7
					6	2	3	5.4	7.4
					6	2	4	18.0	17.4
					6	2	5	12.3	10.5
					6	2	6	12.0	13.8
					6	2	7	12.2	7.0
					6	3	7	22.5	23.9
					6	3	6	11.9	8.4
					6	3	5	4.5	8.5
					6	3	4	23.0	21.4
					6	3	3	67.7	69.5
					6	3	2	41.0	45.1
					6	3	1	26.4	25.1
					6	3	0	41.7	41.7
					6	3	-1	28.5	29.6
					6	3	-2	88.7	88.6
					6	3	-3	68.3	65.4

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6	3	-4	112.0	115.1
6	3	-5	32.2	30.5
6	3	-6	48.6	51.7
6	3	-7	4.0	3.6
6	3	-8	24.9	26.5
6	3	-9	14.5	13.7
6	3	-10	27.0	27.0
6	3	-11	37.9	35.7
6	4	-11	4.9	3.6
6	4	-10	60.8	60.6
6	4	-9	39.7	37.6
6	4	-8	50.8	50.9
6	4	-7	33.1	34.5
6	4	-6	61.3	63.3
6	4	-5	4.0	3.6
6	4	-4	143.7	143.0
6	4	-3	40.8	42.8
6	4	-2	44.1	43.5
6	4	-1	61.6	62.9
6	4	0	20.6	20.0
6	4	1	9.6	9.1
6	4	2	64.8	67.1
6	4	3	55.1	58.2
6	4	4	47.7	48.6
6	4	5	79.6	81.1
6	4	6	22.4	21.3
6	5	6	4.7	5.7
6	5	5	41.1	42.8
6	5	4	30.5	32.1
6	5	3	35.1	36.7
6	5	2	84.2	82.5
6	5	1	3.9	9.1
6	5	0	62.3	63.1
6	5	-1	23.7	21.7
6	5	-2	79.4	80.8
6	5	-3	30.0	30.3
6	5	-4	31.0	31.1
6	5	-5	34.7	36.3
6	5	-6	25.0	23.2
6	5	-7	4.2	1.6
6	5	-8	38.4	36.6
6	5	-9	25.7	25.6
6	5	-10	26.9	28.6
6	5	-11	18.6	16.3
6	6	-11	35.2	34.2
6	6	-10	4.9	2.5
6	6	-9	13.8	16.1
6	6	-8	26.5	27.8
6	6	-7	8.0	6.6
6	6	-6	19.6	19.8
6	6	-5	7.3	7.5
6	6	-4	4.1	0.8
6	6	-3	12.5	10.8
6	6	-2	9.2	9.4
6	6	-1	43.3	39.7
6	6	0	4.0	10.3
6	6	1	21.9	23.0
6	6	2	18.9	18.8
6	6	3	4.2	1.1
6	6	4	34.3	31.5
6	6	5	4.8	4.6
6	6	6	22.4	18.0
6	7	6	7.4	9.1
6	7	5	9.0	6.0
6	7	4	49.9	47.0
6	7	3	15.3	14.2

6	7	2	16.7	19.9
6	7	1	8.4	7.8
6	7	0	5.4	1.7
6	7	-1	32.2	33.0
6	7	-2	16.0	15.2
6	7	-3	68.9	69.4
6	7	-4	70.5	70.9
6	7	-5	6.7	3.9
6	7	-6	36.6	35.9
6	7	-7	49.4	50.8
6	7	-8	33.3	31.3
6	7	-9	6.8	3.5
6	7	-10	39.8	40.9
6	8	-10	64.4	62.1
6	8	-9	10.5	9.3
6	8	-8	26.0	27.6
6	8	-7	44.4	45.3
6	8	-6	37.5	38.6
6	8	-5	24.6	26.7
6	8	-4	77.5	77.5

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H	M	L	FO	FC	H	M	L	FO	FC
6	8	-3	26.3	25.9	6	13	-4	37.1	36.9
6	8	-2	48.0	47.7	6	13	-5	7.6	2.0
6	8	-1	50.1	50.4	7	13	-4	5.0	7.3
6	8	0	34.6	34.6	7	13	-3	15.7	14.5
6	8	1	6.4	1.5	7	13	-2	10.4	15.9
6	8	2	27.2	28.2	7	13	-1	17.9	20.0
6	8	3	51.4	52.5	7	12	1	14.2	12.6
6	8	4	23.4	26.9	7	12	0	29.0	25.9
6	8	5	30.9	31.5	7	12	-1	26.0	28.2
6	9	5	24.7	26.8	7	12	-2	13.1	10.2
6	9	4	30.9	33.0	7	12	-3	14.9	18.7
6	9	3	8.0	9.2	7	12	-4	17.9	17.1
6	9	2	67.8	67.2	7	12	-5	14.6	6.8
6	9	1	28.0	28.7	7	12	-6	23.9	25.6
6	9	0	24.1	20.4	7	11	-8	31.5	27.3
6	9	-1	4.4	2.5	7	11	-7	24.2	25.3
6	9	-2	16.1	14.6	7	11	-6	5.0	8.3
6	9	-3	28.1	27.4	7	11	-5	19.0	17.2
6	9	-4	52.3	51.3	7	11	-4	20.7	22.4
6	9	-5	12.9	11.2	7	11	-3	55.0	54.5
6	9	-6	22.6	21.9	7	11	-2	53.4	51.1
6	9	-7	9.0	2.2	7	11	-1	19.8	19.3
6	9	-8	26.6	26.0	7	11	0	43.5	41.6
6	9	-9	27.6	27.7	7	11	1	24.7	25.2
6	10	-9	16.0	20.0	7	11	2	21.1	19.5
6	10	-8	5.1	7.1	7	10	3	34.1	34.6
6	10	-7	12.1	11.2	7	10	2	25.8	23.7
6	10	-6	11.5	9.3	7	10	1	4.7	9.6
6	10	-5	4.8	2.6	7	10	0	15.7	17.2
6	10	-4	4.7	5.8	7	10	-1	69.6	68.6
6	10	-3	21.1	19.9	7	10	-2	13.4	7.9
6	10	-2	24.4	22.9	7	10	-3	30.1	29.3
6	10	-1	18.3	17.5	7	10	-4	29.5	29.5
6	10	0	15.3	10.3	7	10	-5	31.6	32.1
6	10	1	9.7	8.2	7	10	-6	4.9	7.7
6	10	2	18.7	19.8	7	10	-7	31.2	30.3
6	10	3	16.4	16.0	7	10	-8	53.2	51.7
6	10	4	27.7	26.0	7	9	-9	31.7	32.8
6	11	3	13.0	7.0	7	9	-8	4.9	0.8
6	11	2	33.6	32.0	7	9	-7	17.9	19.8
6	11	1	6.8	3.1	7	9	-6	50.3	50.1
6	11	0	27.6	25.3	7	9	-5	28.6	25.0
6	11	-1	17.4	18.4	7	9	-4	13.8	11.9
6	11	-2	9.3	2.5	7	9	-3	33.4	30.4
6	11	-3	39.6	39.5	7	9	-2	14.2	15.6
6	11	-4	44.4	45.8	7	9	-1	9.1	6.8
6	11	-5	30.9	28.7	7	9	0	29.0	27.7
6	11	-6	15.9	14.1	7	9	1	4.5	3.0
6	11	-7	32.8	34.6	7	9	2	27.5	26.6
6	11	-8	23.2	23.4	7	9	3	21.3	25.1
6	12	-7	56.1	55.6	7	9	4	8.5	2.2
6	12	-6	30.8	30.8	7	8	4	33.0	32.5
6	12	-5	15.6	11.5	7	8	3	21.6	23.4
6	12	-4	21.1	21.0	7	8	2	4.4	0.9
6	12	-3	11.6	12.3	7	8	1	4.3	4.7
6	12	-2	15.9	20.7	7	8	0	40.0	40.6
6	12	-1	44.1	40.6	7	8	-1	4.2	2.3
6	12	0	42.7	42.9	7	8	-2	18.3	19.0
6	12	1	11.2	10.4	7	8	-3	22.9	20.0
6	12	2	6.9	5.6	7	8	-4	13.9	10.3
6	13	0	11.1	5.0	7	8	-5	43.0	44.6
6	13	-1	16.5	16.6	7	8	-6	11.2	7.0
6	13	-2	8.6	7.5	7	8	-7	30.9	30.3
6	13	-3	40.4	40.6	7	8	-8	23.5	24.6
					7	8	-9	5.0	5.9
					7	8	-10	24.8	23.2

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					H	K	L	FD	FC
7	7	-10	14.5	11.2					
7	7	-9	50.6	48.7	7	6	1	20.6	22.4
7	7	-8	20.8	21.5	7	6	0	6.7	4.9
7	7	-7	21.6	21.4	7	6	-1	82.4	82.7
7	7	-6	13.7	12.3	7	6	-2	75.0	74.8
7	7	-5	18.2	18.4	7	6	-3	67.3	67.1
7	7	-4	16.3	15.9	7	6	-4	21.3	22.3
7	7	-3	80.9	80.8	7	6	-5	30.3	28.8
7	7	-2	32.7	32.2	7	6	-6	23.7	25.0
7	7	-1	50.5	52.2	7	6	-7	71.1	70.1
7	7	0	73.6	76.9	7	6	-8	39.1	38.4
7	7	1	22.8	21.7	7	6	-9	37.9	38.9
7	7	2	11.1	10.6	7	6	-10	10.7	4.1
7	7	3	31.2	33.1	7	6	-11	38.2	39.3
7	7	4	16.7	21.2	7	5	-11	6.5	10.2
7	7	5	4.6	2.2	7	5	-10	7.6	5.3
7	6	5	30.0	31.3	7	5	-9	55.0	54.1
7	6	4	21.6	21.7	7	5	-8	7.1	11.1
7	6	3	44.1	44.9	7	5	-7	4.2	5.5
7	6	2	18.2	15.0	7	5	-6	73.7	72.7
					7	5	-5	5.8	1.9
					7	5	-4	3.9	1.6
					7	5	-3	21.2	21.6
					7	5	-2	3.9	6.6
					7	5	-1	10.1	14.0
					7	5	0	47.6	44.9
					7	5	1	10.1	8.3
					7	5	2	35.5	34.7
					7	5	3	33.3	32.6
					7	5	4	7.1	4.8
					7	5	5	36.9	37.3
					7	4	6	4.7	3.7
					7	4	5	8.0	4.1
					7	4	4	16.2	14.1
					7	4	3	10.4	12.0
					7	4	2	11.8	12.0
					7	4	1	23.9	24.9
					7	4	0	22.5	22.5
					7	4	-1	14.0	15.2
					7	4	-2	7.7	10.8
					7	4	-3	17.2	17.5
					7	4	-4	17.2	19.5
					7	4	-5	30.2	30.7
					7	4	-6	12.2	15.2
					7	4	-7	6.2	10.8
					7	4	-8	25.5	28.1
					7	4	-9	4.4	4.8
					7	4	-10	16.4	15.4
					7	4	-11	9.1	14.8
					7	3	-11	6.4	1.8
					7	3	-10	12.2	11.3
					7	3	-9	46.9	47.3
					7	3	-8	8.7	4.3
					7	3	-7	14.9	13.0
					7	3	-6	63.6	64.6
					7	3	-5	3.9	1.1
					7	3	-4	29.8	31.0
					7	3	-3	88.1	87.7
					7	3	-2	5.2	5.0
					7	3	-1	56.8	54.6
					7	3	0	86.9	86.9
					7	3	1	37.2	35.7
					7	3	2	19.1	19.8
					7	3	3	6.1	5.8
					7	3	4	34.4	35.8

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7	3	5	8.9	14.7
7	3	6	11.5	13.4
7	2	6	26.6	30.1
7	2	5	9.0	15.5
7	2	4	28.4	29.9
7	2	3	88.5	89.8
7	2	2	30.6	29.2
7	2	1	29.2	28.7
7	2	0	3.8	0.8
7	2	-1	45.5	48.6
7	2	-2	63.0	63.2
7	2	-3	75.1	76.9
7	2	-4	38.5	38.4
7	2	-5	42.5	41.2
7	2	-6	65.8	69.2
7	2	-7	95.5	95.3
7	2	-8	58.1	57.4
7	2	-9	4.3	3.8
7	2	-10	12.1	7.7
7	2	-11	19.8	16.6
7	2	-12	4.9	1.8
7	1	-12	15.0	17.4
7	1	-11	15.9	18.0
7	1	-10	4.5	3.9
7	1	-9	75.3	73.7
7	1	-8	22.9	19.7
7	1	-7	14.5	16.5
7	1	-6	59.9	61.3
7	1	-5	8.5	6.9
7	1	-4	14.1	13.3
7	1	-3	23.3	20.0
7	1	-2	22.8	23.2
7	1	-1	44.6	46.6
7	1	0	77.8	78.9
7	1	1	42.3	42.4
7	1	2	13.7	13.0
7	1	3	6.3	3.7
7	1	4	29.0	32.8
7	1	5	18.8	19.6
7	1	6	21.8	24.4
8	0	-12	10.5	7.4
8	0	-11	13.0	13.3
8	0	-10	11.8	4.7
8	0	-9	47.5	50.6
8	0	-8	108.6	106.9
8	0	-7	18.7	18.6
8	0	-6	78.0	78.1
8	0	-5	80.4	81.3
8	0	-4	59.3	60.2
8	0	-3	8.6	8.9
8	0	-2	72.4	71.8
8	0	-1	98.0	101.3
8	0	0	32.7	31.0
8	0	1	52.1	54.2
8	0	2	63.3	67.0
8	0	3	38.4	38.1
8	0	4	41.3	44.0
8	0	5	25.0	27.9
8	1	5	23.3	24.9
8	1	4	9.2	7.9
8	1	3	4.1	3.2
8	1	2	15.2	16.0
8	1	1	31.2	32.4
8	1	0	82.1	83.5
8	1	-1	43.8	44.3
8	1	-2	63.5	63.1

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8	1	-3	3.7	2.3
8	1	-4	43.7	43.8
8	1	-5	23.0	23.4
8	1	-6	41.0	40.8
8	1	-7	31.8	29.7
8	1	-8	48.5	47.1
8	1	-9	13.0	6.8
8	1	-10	25.6	25.7
8	1	-11	30.9	33.7
8	1	-12	49.0	42.8
8	2	-11	4.7	3.7
8	2	-10	14.0	7.2
8	2	-9	4.3	0.5
8	2	-8	15.9	16.4
8	2	-7	12.7	10.7
8	2	-6	17.5	17.9
8	2	-5	35.6	36.0
8	2	-4	11.6	8.1
8	2	-3	51.0	51.0
8	2	-2	3.7	6.7

H	K	L	FO	FC						
8	2	-1	17.9	17.7	8	6	-5	27.3	28.1	
8	2	0	3.8	6.1	8	6	-4	11.7	13.0	
8	2	1	15.9	15.1	8	6	-3	43.0	42.7	
8	2	2	4.0	3.3	8	6	-2	12.9	13.2	
8	2	3	20.5	18.8	8	6	-1	4.1	6.6	
8	2	4	11.7	7.0	8	6	0	34.0	34.5	
8	2	5	4.7	1.9	8	6	1	8.2	5.1	
8	3	5	18.9	23.0	8	6	2	12.2	9.6	
8	3	4	19.7	17.1	8	6	3	4.7	7.9	
8	3	3	19.0	20.0	8	6	4	11.4	12.8	
8	3	2	9.0	13.4	8	7	4	38.3	38.8	
8	3	1	27.7	29.1	8	7	3	38.3	33.7	
8	3	0	49.3	51.1	8	7	2	17.5	16.9	
8	3	-1	45.5	45.5	8	7	1	24.0	22.1	
8	3	-2	48.4	48.7	8	7	0	58.9	58.8	
8	3	-3	7.5	9.3	8	7	-1	6.1	9.2	
8	3	-4	30.2	31.6	8	7	-2	52.6	53.8	
8	3	-5	14.5	15.9	8	7	-3	32.1	28.8	
8	3	-6	50.7	49.2	8	7	-4	26.9	24.8	
8	3	-7	7.1	2.2	8	7	-5	18.4	17.8	
8	3	-8	50.1	52.2	8	7	-6	28.1	28.0	
8	3	-9	6.6	5.8	8	7	-7	14.3	11.9	
8	3	-10	12.0	7.0	8	7	-8	10.5	10.2	
8	3	-11	30.2	32.4	8	7	-9	9.1	10.8	
8	4	-11	33.8	34.5	8	7	-10	25.6	24.3	
8	4	-10	17.7	21.4	8	8	-10	4.9	0.8	
8	4	-9	16.4	18.3	8	8	-9	5.0	2.4	
8	4	-8	88.3	84.4	8	8	-8	59.4	58.9	
8	4	-7	4.1	1.5	8	8	-7	14.9	11.7	
8	4	-6	37.2	35.6	8	8	-6	8.6	7.2	
8	4	-5	64.3	62.3	8	8	-5	69.1	65.7	
8	4	-4	15.3	15.3	8	8	-4	19.4	18.0	
8	4	-3	7.4	3.3	8	8	-3	16.6	17.4	
8	4	-2	68.6	69.5	8	8	-2	47.8	48.2	
8	4	-1	69.5	72.4	8	8	-1	4.4	5.7	
8	4	0	54.6	53.7	8	8	0	24.2	25.4	
8	4	1	82.4	83.1	8	8	1	78.8	76.4	
8	4	2	5.8	12.6	8	8	2	4.6	4.9	
8	4	3	13.4	10.3	8	8	3	4.8	7.0	
8	4	4	37.7	37.5	8	9	3	29.3	29.5	
8	4	5	6.4	2.7	8	9	2	4.5	1.2	
8	5	5	4.8	1.8	8	9	1	8.9	4.6	
8	5	4	4.6	6.0	8	9	0	40.0	39.6	
8	5	3	6.6	7.9	8	9	-1	33.8	33.5	
8	5	2	4.3	0.4	8	9	-2	14.7	7.5	
8	5	1	23.7	26.2	8	9	-3	33.7	32.2	
8	5	0	52.0	53.8	8	9	-4	12.1	9.2	
8	5	-1	51.7	51.1	8	9	-5	7.6	2.4	
8	5	-2	51.9	50.3	8	9	-6	67.6	64.7	
8	5	-3	28.7	30.7	8	9	-7	51.1	49.5	
8	5	-4	27.0	27.7	8	9	-8	4.8	1.6	
8	5	-5	21.3	20.4	8	9	-9	13.9	8.7	
8	5	-6	56.7	55.5	8	10	-8	28.5	27.8	
8	5	-7	78.1	76.5	8	10	-7	11.7	8.1	
8	5	-8	28.7	31.4	8	10	-6	4.8	0.8	
8	5	-9	4.6	6.6	8	10	-5	21.5	19.5	
8	5	-10	35.3	35.7	8	10	-4	22.3	21.3	
8	5	-11	4.9	12.6	8	10	-3	31.5	30.9	
8	6	-11	4.9	2.5	8	10	-2	7.3	4.4	
8	6	-10	19.0	18.8	8	10	-1	11.3	8.3	
8	6	-9	20.5	23.0	8	10	0	26.1	29.1	
8	6	-8	32.9	30.3	8	10	1	7.8	3.8	
8	6	-7	4.3	6.3	8	10	2	4.8	13.3	
8	6	-6	16.1	17.5	8	11	1	27.6	19.0	
					8	11	0	10.3	19.5	
					8	11	-1	4.8	8.1	

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				H	K	L	FO	FC	
8	11	-2	34.3	34.8					
8	11	-3	25.9	22.7					
8	11	-4	8.1	6.5					
8	11	-5	32.9	34.3					
8	11	-6	26.5	26.7					
8	11	-7	11.4	6.7					
8	12	-5	37.0	35.3					
8	12	-4	27.8	25.9					
8	12	-3	34.4	32.2					
8	12	-2	33.4	32.7					
8	12	-1	25.4	21.4					
9	11	-6	4.9	8.0					
9	11	-5	22.6	20.7					
9	11	-4	36.0	34.1					
9	11	-3	4.7	1.4					
9	11	-2	7.6	6.7					
9	11	-1	21.8	19.6					
9	10	0	44.0	45.0					
9	10	-1	63.7	62.5					
9	10	-2	32.7	30.3					
9	10	-3			9	10	-3	7.1	9.3
9	10	-4			9	10	-4	24.8	24.0
9	10	-5			9	10	-5	49.2	48.7
9	10	-6			9	10	-6	4.8	13.0
9	10	-7			9	10	-7	17.6	14.8
9	10	-8			9	10	-8	9.7	11.9
9	9	-8			9	9	-8	33.0	30.9
9	9	-7			9	9	-7	46.9	45.3
9	9	-6			9	9	-6	10.3	6.4
9	9	-5			9	9	-5	26.6	26.1
9	9	-4			9	9	-4	56.8	55.9
9	9	-3			9	9	-3	16.9	16.8
9	9	-2			9	9	-2	4.6	1.9
9	9	-1			9	9	-1	4.5	4.3
9	9	0			9	9	0	5.7	3.5
9	9	1			9	9	1	26.2	23.9
9	8	2			9	8	2	4.7	6.9
9	8	1			9	8	1	36.5	36.5
9	8	0			9	8	0	8.9	8.3
9	8	-1			9	8	-1	17.6	18.5
9	8	-2			9	8	-2	31.4	27.8
9	8	-3			9	8	-3	13.4	11.8
9	8	-4			9	8	-4	4.4	7.6
9	8	-5			9	8	-5	29.4	27.5
9	8	-6			9	8	-6	4.5	5.6
9	8	-7			9	8	-7	4.6	1.7
9	8	-8			9	8	-8	4.9	10.2
9	8	-9			9	8	-9	6.5	6.2
9	7	-10			9	7	-10	29.3	28.2
9	7	-9			9	7	-9	4.8	8.4
9	7	-8			9	7	-8	4.6	6.8
9	7	-7			9	7	-7	10.3	9.9
9	7	-6			9	7	-6	8.5	12.2
9	7	-5			9	7	-5	15.6	13.8
9	7	-4			9	7	-4	44.3	44.7
9	7	-3			9	7	-3	13.8	15.1
9	7	-2			9	7	-2	24.2	25.3
9	7	-1			9	7	-1	35.5	37.2
9	7	0			9	7	0	12.6	10.1
9	7	1			9	7	1	27.4	27.7
9	7	2			9	7	2	32.9	34.3
9	7	3			9	7	3	16.5	15.1
9	6	3			9	6	3	8.1	3.9
9	6	2			9	6	2	11.5	8.2
9	6	1			9	6	1	33.4	36.0
9	6	0			9	6	0	22.7	21.9
9	6	-1			9	6	-1	39.2	36.9
9	6	-2			9	6	-2	34.8	31.9
9	6	-3			9	6	-3	4.1	5.7
9	6	-4			9	6	-4	7.5	7.3
9	6	-5			9	6	-5	70.5	70.9
9	6	-6			9	6	-6	49.6	48.9
9	6	-7			9	6	-7	30.5	29.0
9	6	-8			9	6	-8	14.4	17.6
9	6	-9			9	6	-9	4.6	1.6
9	6	-10			9	6	-10	18.1	21.4
9	5	-11			9	5	-11	4.6	1.9
9	5	-10			9	5	-10	18.5	17.7
9	5	-9			9	5	-9	27.1	26.4
9	5	-8			9	5	-8	11.1	10.4
9	5	-7			9	5	-7	57.4	59.0
9	5	-6			9	5	-6	4.1	6.3
9	5	-5			9	5	-5	23.0	22.2
9	5	-4			9	5	-4	77.3	76.1

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9	5	-3	8.1	7.0
9	5	-2	19.7	16.6
9	5	-1	21.0	22.4
9	5	0	12.6	11.7
9	5	1	9.9	9.3
9	5	2	49.1	48.8
9	5	3	4.5	1.1
9	5	4	16.7	15.5
9	4	4	19.4	22.3
9	4	3	20.1	18.4
9	4	2	9.4	2.1
9	4	1	19.5	22.1
9	4	0	4.0	4.8
9	4	-1	7.5	2.9
9	4	-2	37.5	36.4
9	4	-3	3.9	0.4
9	4	-4	21.7	18.5
9	4	-5	17.6	18.7
9	4	-6	4.0	3.4
9	4	-7	4.2	5.3
9	4	-8	7.9	5.3
9	4	-9	16.9	19.9
9	4	-10	12.2	8.5
9	4	-11	4.7	9.5
9	3	-11	9.4	10.5
9	3	-10	55.8	54.8
9	3	-9	4.3	1.0
9	3	-8	19.7	18.5
9	3	-7	33.7	32.9
9	3	-6	40.6	40.8
9	3	-5	13.1	13.6
9	3	-4	52.1	52.9
9	3	-3	30.7	31.1
9	3	-2	9.4	8.7
9	3	-1	37.1	37.1
9	3	0	8.7	12.0
9	3	1	18.9	20.4
9	3	2	52.0	54.6
9	3	3	26.3	29.5
9	3	4	15.0	13.7
9	2	4	65.0	64.0
9	2	3	8.6	5.1
9	2	2	26.0	23.1
9	2	1	66.0	69.3
9	2	0	31.9	32.3
9	2	-1	3.8	3.4
9	2	-2	60.7	60.9
9	2	-3	33.6	34.2
9	2	-4	8.8	11.2
9	2	-5	118.1	117.2
9	2	-6	58.9	56.4
9	2	-7	18.3	17.7
9	2	-8	12.0	10.4
9	2	-9	36.2	35.9
9	2	-10	6.8	13.4
9	2	-11	57.7	58.3
9	1	-11	20.4	22.1
9	1	-10	33.6	33.2
9	1	-9	11.8	5.0
9	1	-8	15.8	14.4
9	1	-7	47.4	46.8
9	1	-6	3.7	1.6
9	1	-5	3.7	0.8
9	1	-4	30.6	79.3
9	1	-3	54.8	55.2
9	1	-2	26.5	26.1

9	1	-1	42.5	42.9
9	1	0	9.7	8.8
9	1	1	7.6	9.4
9	1	2	54.7	56.5
9	1	3	19.2	18.5
9	1	4	19.6	16.5
10	0	-11	9.4	7.4
10	0	-10	27.3	29.3
10	0	-9	77.4	75.1
10	0	-8	30.2	27.8
10	0	-7	51.1	55.1
10	0	-6	42.0	40.1
10	0	-5	27.7	27.7
10	0	-4	11.2	9.2
10	0	-3	60.4	61.1
10	0	-2	48.6	50.7
10	0	-1	28.6	28.3
10	0	0	38.4	38.0
10	0	1	8.5	5.5
10	0	2	63.4	62.1

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H	K	L	FD	FC					
10	0	3	65.1	66.8	10	5	-1	53.3	54.4
10	1	3	22.9	25.8	10	5	-2	9.3	6.6
10	1	2	20.8	20.9	10	5	-3	4.1	4.1
10	1	1	21.4	22.6	10	5	-4	84.2	82.6
10	1	0	38.6	36.0	10	5	-5	17.1	15.4
10	1	-1	54.1	53.7	10	5	-6	9.4	8.8
10	1	-2	21.4	19.9	10	5	-7	4.2	2.7
10	1	-3	49.5	47.5	10	5	-8	8.1	4.0
10	1	-4	86.9	86.0	10	5	-9	19.2	16.6
10	1	-5	3.8	6.7	10	5	-10	50.4	47.4
10	1	-6	3.9	1.6	10	6	-10	11.3	3.0
10	1	-7	30.0	29.9	10	6	-9	16.9	19.8
10	1	-8	16.3	16.6	10	6	-8	36.8	35.4
10	1	-9	6.1	5.3	10	6	-7	18.1	19.6
10	1	-10	38.1	38.1	10	6	-6	37.3	36.7
10	1	-11	30.8	28.7	10	6	-5	4.2	3.8
10	2	-11	15.3	10.4	10	6	-4	19.8	19.4
10	2	-10	10.6	5.2	10	6	-3	33.7	34.3
10	2	-9	4.3	5.4	10	6	-2	32.1	31.5
10	2	-8	16.5	17.0	10	6	-1	17.8	21.1
10	2	-7	23.8	24.6	10	6	0	14.2	9.5
10	2	-6	13.0	11.1	10	6	1	17.1	16.8
10	2	-5	18.2	16.0	10	6	2	4.5	6.2
10	2	-4	14.8	14.0	10	7	1	12.1	6.7
10	2	-3	3.9	3.5	10	7	0	27.7	26.3
10	2	-2	15.1	15.6	10	7	-1	4.4	2.9
10	2	-1	6.0	5.5	10	7	-2	19.4	18.6
10	2	0	4.1	2.9	10	7	-3	11.5	9.1
10	2	1	17.9	15.7	10	7	-4	11.0	17.1
10	2	2	13.0	9.0	10	7	-5	4.4	3.3
10	2	3	21.6	20.8	10	7	-6	46.9	49.3
10	3	3	10.0	14.5	10	7	-7	31.8	31.6
10	3	2	50.9	50.6	10	7	-8	12.5	8.9
10	3	1	18.6	18.8	10	7	-9	30.5	28.7
10	3	0	38.5	38.8	10	8	-9	39.4	37.4
10	3	-1	24.8	24.8	10	8	-8	10.0	12.7
10	3	-2	10.0	8.9	10	8	-7	11.2	13.3
10	3	-3	24.7	24.3	10	8	-6	40.6	37.3
10	3	-4	30.3	31.4	10	8	-5	21.2	20.1
10	3	-5	15.8	14.9	10	8	-4	4.5	4.2
10	3	-6	23.0	22.6	10	8	-3	62.1	59.4
10	3	-7	29.5	29.1	10	8	-2	26.1	26.4
10	3	-8	14.0	12.7	10	8	-1	7.6	4.2
10	3	-9	32.9	33.9	10	8	0	8.5	10.6
10	3	-10	34.8	32.5	10	8	1	4.6	4.9
10	3	-11	21.6	18.5	10	9	0	16.8	15.1
10	4	-11	4.6	2.9	10	9	-1	43.9	42.8
10	4	-10	24.9	21.0	10	9	-2	11.6	13.3
10	4	-9	46.0	42.1	10	9	-3	16.1	16.5
10	4	-8	54.9	51.7	10	9	-4	68.6	66.1
10	4	-7	43.7	45.4	10	9	-5	41.7	39.3
10	4	-6	43.4	41.0	10	9	-6	6.6	7.9
10	4	-5	6.2	9.7	10	9	-7	10.3	12.9
10	4	-4	25.1	24.8	10	9	-8	11.7	10.7
10	4	-3	77.1	76.4	10	10	-6	24.6	24.6
10	4	-2	11.8	9.4	10	10	-5	12.4	7.7
10	4	-1	19.1	18.3	10	10	-4	4.7	9.3
10	4	0	24.0	27.2	10	10	-3	9.4	16.3
10	4	1	13.4	11.3	10	10	-2	32.4	32.1
10	4	2	35.8	35.0	10	10	-1	19.2	18.7
10	4	3	56.2	57.4	11	9	-6	10.1	13.8
10	5	2	25.1	26.9	11	9	-5	13.2	12.7
10	5	1	35.7	35.3	11	9	-4	9.7	12.2
10	5	0	5.7	4.0	11	9	-3	4.5	4.5
					11	9	-2	12.3	14.9
					11	8	-1	8.1	8.4

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11	8	-2	6.5	4.9	11	3	-10	4.5	3.5
11	8	-3	12.9	10.4	11	3	-9	10.9	6.5
11	8	-4	16.6	12.3	11	3	-8	32.2	31.2
11	8	-5	4.5	3.8	11	3	-7	20.9	18.8
11	8	-6	30.8	29.7	11	3	-6	39.8	38.0
11	8	-7	17.5	15.7	11	3	-5	22.2	23.1
11	8	-8	18.7	18.3	11	3	-4	31.0	31.1
11	7	-9	12.6	10.2	11	3	-3	23.8	24.5
11	7	-8	56.0	54.1	11	3	-2	54.6	56.3
11	7	-7	38.9	35.4	11	3	-1	17.1	17.5
11	7	-6	33.4	33.1	11	3	0	4.4	8.5
11	7	-5	12.0	12.4	11	3	1	18.1	16.6
11	7	-4	27.5	27.5	11	3	2	17.5	11.5
11	7	-3	9.9	1.4	11	2	2	10.9	12.8
11	7	-2	36.2	35.4	11	2	1	11.1	9.2
11	7	-1	4.5	5.2	11	2	0	62.4	62.8
11	7	0	6.3	7.2	11	2	-1	7.8	1.4
11	6	1	4.6	12.4	11	2	-2	4.0	5.0
11	6	0	61.9	63.5	11	2	-3	54.1	56.2
11	6	-1	18.4	17.9	11	2	-4	38.3	39.4
					11	2	-5	35.9	36.0
					11	2	-6	53.5	52.0
					11	2	-7	8.7	9.7
11	6	-2	4.4	2.3	11	2	-8	27.6	27.7
11	6	-3	56.2	54.7	11	2	-9	78.9	75.9
11	6	-4	4.2	1.2	11	2	-10	18.5	18.8
11	6	-5	4.3	2.0	11	2	-11	4.6	6.2
11	6	-6	25.3	22.8	11	1	-11	7.5	12.0
11	6	-7	7.5	3.7	11	1	-10	4.5	3.5
11	6	-8	19.6	19.8	11	1	-9	12.6	11.5
11	6	-9	65.6	64.5	11	1	-8	39.8	38.2
11	5	-10	13.8	14.2	11	1	-7	18.1	18.2
11	5	-9	16.6	19.6	11	1	-6	23.8	24.3
11	5	-8	24.8	25.4	11	1	-5	49.2	50.4
11	5	-7	12.3	9.7	11	1	-4	3.8	4.6
11	5	-6	14.8	13.9	11	1	-3	27.7	26.6
11	5	-5	44.2	40.7	11	1	-2	65.8	66.9
11	5	-4	8.5	14.2	11	1	-1	26.2	28.8
11	5	-3	9.7	7.8	11	1	0	4.1	1.5
11	5	-2	47.0	47.6	11	1	1	9.4	2.7
11	5	-1	54.1	53.6	11	1	2	10.9	15.7
11	5	0	14.9	9.1	12	0	-10	34.1	35.5
11	5	1	7.5	6.6	12	0	-9	18.5	18.3
11	4	1	9.8	6.2	12	0	-8	16.7	14.7
11	4	0	4.3	5.9	12	0	-7	73.1	71.0
11	4	-1	20.7	21.6	12	0	-6	48.4	47.3
11	4	-2	4.1	4.2	12	0	-5	6.0	4.5
11	4	-3	30.9	31.9	12	0	-4	18.2	19.6
11	4	-4	4.1	2.7	12	0	-3	5.2	6.5
11	4	-5	11.9	10.9	12	0	-2	9.5	2.8
11	4	-6	21.7	19.6	12	0	-1	55.8	56.2
11	4	-7	4.3	3.0	12	0	0	20.1	22.8
11	4	-8	36.5	36.6	12	0	1	49.6	46.9
11	4	-9	15.5	15.8	12	1	1	30.9	29.8
11	4	-10	4.6	6.0	12	1	0	15.7	20.3
					12	1	-1	11.1	7.8
					12	1	-2	21.2	20.9
					12	1	-3	4.2	6.0
					12	1	-4	4.1	1.6
					12	1	-5	45.3	42.1
					12	1	-6	7.3	19.3
					12	1	-7	11.8	11.9
					12	1	-8	51.4	47.4
					12	1	-9	50.7	28.6
					12	1	-10	11.4	9.7

12	2	-10	4.4	5.7
12	2	-9	7.8	2.3
12	2	-8	14.8	14.4
12	2	-7	4.5	2.9
12	2	-6	4.2	2.6
12	2	-5	4.1	0.5
12	2	-4	7.7	4.6
12	2	-3	15.0	11.6
12	2	-2	8.4	9.9
12	2	-1	4.3	1.1
12	2	0	24.0	22.9
12	3	0	10.8	11.8
12	3	-1	25.8	23.5
12	3	-2	23.8	23.9
12	3	-3	22.3	21.3
12	3	-4	7.6	4.4
12	3	-5	59.7	58.0
12	3	-6	27.2	27.1
12	3	-7	18.3	18.5
12	3	-8	46.0	44.1
12	3	-9	26.5	25.6
12	3	-10	20.4	18.2
12	4	-9	7.8	9.3
12	4	-8	4.4	2.5
12	4	-7	75.3	73.4
12	4	-6	24.8	23.9
12	4	-5	26.1	23.7
12	4	-4	7.6	5.6
12	4	-3	28.0	25.9
12	4	-2	7.1	6.3
12	4	-1	42.8	42.6
12	4	0	41.7	42.3
12	5	-1	4.4	2.3
12	5	-2	49.6	47.6
12	5	-3	4.3	7.8
12	5	-4	6.0	10.0
12	5	-5	30.2	31.0
12	5	-6	4.3	6.1
12	5	-7	4.5	9.6
12	5	-8	37.8	35.6
12	5	-9	11.3	7.0
12	6	-8	15.0	17.5
12	6	-7	18.7	16.0
12	6	-6	9.2	13.6
12	6	-5	35.3	33.9
12	6	-4	4.3	1.2
12	6	-3	36.0	32.9
12	6	-2	13.2	11.4
12	6	-1	10.9	4.9
12	7	-2	12.4	16.2
12	7	-3	19.8	16.6
12	7	-4	4.4	4.7
12	7	-5	42.4	38.0

12	7	-6	19.0	18.0
12	7	-7	41.2	39.8
12	8	-6	40.9	40.6
12	8	-5	45.2	43.9
12	8	-4	11.6	16.3
13	6	-4	55.8	55.4
13	6	-5	13.8	14.8
13	6	-6	24.1	19.8
13	5	-7	25.4	24.7
13	5	-6	16.6	14.9
13	5	-5	11.9	12.6
13	5	-4	23.2	21.5
13	5	-3	7.4	1.5
13	4	-2	4.4	8.7
13	4	-3	20.0	31.0
13	4	-4	20.4	19.1
13	4	-5	23.7	24.0
13	4	-6	9.6	6.1
13	4	-7	4.3	0.5
13	4	-8	23.2	22.1
13	3	-9	11.0	11.1
13	3	-8	14.3	8.4
13	3	-7	9.8	11.7
13	3	-6	23.8	22.7
13	3	-5	49.8	49.4
13	3	-4	45.6	44.5
13	3	-3	11.2	6.7
13	3	-2	20.6	19.6
13	2	-1	50.3	48.7
13	2	-2	28.2	28.0
13	2	-3	4.2	5.5
13	2	-4	27.0	24.6
13	2	-5	18.8	18.1
13	2	-6	16.6	13.3
13	2	-7	28.6	26.8
13	2	-8	12.8	15.6
13	2	-9	9.2	6.1
13	1	-9	8.3	1.7
13	1	-8	11.5	11.1
13	1	-7	4.3	2.9
13	1	-6	4.2	3.7
13	1	-5	26.2	24.2
13	1	-4	34.3	32.1
13	1	-3	4.3	1.3
13	1	-2	11.0	9.4
13	1	-1	20.1	18.8
14	0	-7	21.7	17.3
14	0	-6	4.4	2.4
14	0	-5	60.4	59.4
14	0	-4	45.0	41.2
14	1	-4	11.9	12.4
14	1	-5	22.4	23.3
14	1	-6	41.2	38.8
14	1	-7	18.6	20.9
14	2	-7	15.3	15.2
14	2	-6	6.6	0.6
14	2	-5	4.3	5.5

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End of supplemental material.

Palermoite, $\text{SrLi}_2[\text{Al}_2(\text{OH})_2(\text{PO}_4)_2]$: Its Atomic Arrangement and Relationship to Carminite, $\text{Pb}_2[\text{Fe}_2(\text{OH})_2(\text{AsO}_4)_2]$

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Abstract

Palermoite, $\text{SrLi}_2[\text{Al}_2(\text{OH})_2(\text{PO}_4)_2]$, space group *Imcb*, a 11.556(5), b 15.847(7), c 7.315(4) Å, $Z = 4$, is structurally related to carminite, $\text{Pb}_2[\text{Fe}_2(\text{OH})_2(\text{AsO}_4)_2]$, $R(hkl) = 0.090$ for 1471 non-equivalent reflections. Both contain the same $[\text{M}^{2+}(\text{OH})_2(\text{TO}_4)_2]^{2+}$ octahedral and tetrahedral slabs oriented parallel to [010]. They are distinguished by the link to symmetry-equivalent slabs across the glides at $b = 1/4$. The space group *Amca* for carminite shares the same subgroup (*Fmca*) with palermoite. In both structures, the octahedra form chains of edge-linked dimers which are corner-linked to symmetry-equivalent dimers resulting in the composition $\text{M}^{2+}_2(\text{O})_2(\text{OH})_2$. One-eighth of the tetrahedral oxygens are not bonded to the octahedra.

Polyhedral interatomic averages are $^{87}\text{Sr}-\text{O}$ 2.62 Å, $^{27}\text{Al}-\text{O}$ 1.91 Å, $^{7}\text{Li}-\text{O}$ 2.13 Å, $^{31}\text{P}(1)-\text{O}$ 1.53 Å and $^{31}\text{P}(2)-\text{O}$ 1.54 Å. Local isomorphism of all atoms excepting Li and Pb(2) occurs: the Li atoms are split into twice the equipoint rank number as Pb(2) and possess lower point symmetry.

Introduction

Palermoite occurs locally in moderate abundance as small striated prismatic colorless crystals at its type locality, the Palermo No. 1 pegmatite, near North Groton, New Hampshire. It was originally described by Mrose (1953), who proposed the formula $(\text{Li}, \text{Na})_2\text{SrAl}_2(\text{PO}_4)_2(\text{OH})_2$, $Z = 2$, and the unit cell parameters a 7.31 Å, b 15.79 Å, c 11.53 Å with the space group *Immm*. Another chemical analysis by Frondel and Ito (1965) led to the proposed formula $(\text{Li}, \text{Na})_2(\text{Sr}, \text{Ca})\text{Al}_2(\text{PO}_4)_2(\text{OH})_2$, $Z = 4$, with the refined cell parameters a 7.315(4), b 15.849(9), c 11.556(6) Å. Meanwhile, Strunz (1960) proposed an isotopic relationship between palermoite and carminite, $\text{PbFe}^{2+}_2(\text{AsO}_4)_2(\text{OH})_2$. To reconcile the rather complex formula of Mrose and the similarity in the crystal cell parameters between palermoite and carminite, he proposed the formula $\text{SrAl}_2(\text{PO}_4)_2(\text{OH})_2$.

Despite similarities in the cell dimensions, we were puzzled by the difference between the body-centered cell for palermoite and the end-centered cell for carminite. Atomic positions based on the crystal structure analysis of carminite by Finney (1963) could not be isomorphically transformed into the palermoite

cell since the space groups are neither isomorphic nor is one a subgroup of the other.

Experimental

Palermoite single crystals collected at the type locality by P.B.M. were submitted to single crystal X-ray study. In addition, a qualitative electron probe scan detected Sr, Al, P, and only minor Ca (< 1%). The extinction criteria, from films and single crystal diffractometer, suggested the space groups *I2cb* or *Imcb*, in disagreement with *Immm* proposed by Mrose (1953). Doubly terminated crystals and the three-dimensional crystal structure analysis support the centrosymmetric space group *Imcb*.

Refinement of the cell parameters on a PICKER automated diffractometer afforded a 11.556(5), b 15.847(7), c 7.315(4) Å. We selected the standard axial convention for the orthorhombic system to which the space group *Imcb* conforms and accepted the cell contents $4[\text{SrLi}_2\text{Al}_2(\text{OH})_2(\text{PO}_4)_2]$. Other salient details: graphite monochromatized $\text{MoK}\alpha$ radiation ($\lambda = 0.7093$ Å); maximum $\sin \theta/\lambda = 0.80$; twenty second background counting times; scan rate $1.0^\circ/\text{minute}$; half angle scan 1.8° . The thick prismatic crystal, of maximum dimension 0.12 mm, was not corrected for absorption. The equivalent reflec-

TABLE 1. Palermoite: Atomic Coordinate and Isotropic Thermal Vibration Parameters*

Atom	Point group	Mult.	x	y	z	$B(\text{Å}^2)$	Atom	Point group	Mult.	x	y	z	$B(\text{Å}^2)$
Sr	222	4	0.2500	0.5000	0.5000	0.40(2)	P(2)	m	2	0.0000	0.526(1)	0.771(2)	0.10(2)
Po(1)	222	4	0.2500	0.5000	0.5000	0.50(2)	P(2)	m	2	0.0000	0.527	0.760	0.10(2)
Li	m	8	0.5000	0.285(11)	0.272(21)	2.00(24)	O(1)	m	4	0.0000	0.493(3)	0.610(5)	0.6(3)
PO(2)	2/m	4	0.5000	0.2700	0.2100	0.21(2)	O(2)	m	4	0.0000	0.494	0.606	0.6(3)
Al	1	16	0.3307(1)	0.3727(1)	0.4176(2)	0.50(2)	O(3)	m	4	0.0000	0.416(2)	0.562(3)	0.76(4)
Fe	1	16	0.336	0.378	0.411	0.50(2)	O(4)	m	4	0.0000	0.416	0.562	0.76(4)
V(1)	2	8	0.2900	0.3222(1)	0.3000	0.45(2)	O(5)	1	16	0.3000(3)	0.657(2)	0.277(4)	0.9(4)
As(2)	2	8	0.2900	0.322	0.3000	0.50(2)	O(6)	1	16	0.3000	0.657	0.277	0.9(4)
O(1)	1	16	0.1875(3)	0.2132(2)	0.6197(4)	0.75(3)	OH(1)	m	8	0.0000	0.336(3)	0.608(6)	0.27(6)
O(2)	1	16	0.185	0.212	0.619	0.75(3)	OH(1)	m	8	0.0000	0.336	0.608	0.27(6)
O(3)	1	16	0.2757(3)	0.355(2)	0.333(5)	0.51(4)	OH(2)	2	8	0.2500	0.417(3)	0.690	0.2(1)
O(4)	1	16	0.281	0.378	0.336	0.51(4)	OH(2)	2	8	0.2500	0.417	0.690	0.2(1)

* Estimated standard errors refer to the last digit; the atomic parameters of carminite in (Finney 1963), appropriately corrected, are shown for comparison.

tions (hkl) and (hkl) were averaged, yielding 1471 independent F (obs), which were obtained through standard computational procedures.

Determination and Refinement of the Structure

Three-dimensional Patterson synthesis indicated strong vector densities at $0\ 0\ 0$, $1/2\ 0\ 0$, $0\ 0\ 1/2$; and $1/4\ 0\ 1/4$. Symmetry restrictions led to rapid determination of the Sr, Al, P(1), and P(2) positions. The β - and γ -syntheses of Ramachandran and Srinivasan (1970) led to unambiguous resolution of all non-hydrogen atoms.

Four cycles of full-matrix, least-squares refinement based on isotropic thermal vibration parameters, full site occupancies, secondary extinction correction with $c_e = 0.428 \times 10^{-8}$ (Zachariasen, 1968) and anomalous dispersion correction for Sr, Al, and P led to

$$R(hkl) = \frac{\sum ||F(obs) - |F(calc)||}{\sum |F(obs)|} = 0.090$$

for all 1471 reflections. The final atomic coordinates and the isotropic thermal vibration parameters are presented in Table 1. Table 2 lists the structure factor data.

Description of the Structures

The formula $SrLi_3[Al_2(OH)_2(PO_4)_4]$ (here idealized) proposed by Frondel and Ito (1965) is confirmed. Although the structures of palermoite and carminite are closely related, the two crystals do not exhibit an isotopic relation. Figure 1 features the symmetry

¹ To obtain a copy of Table 2, order document number AM-75-003-B from the Business Office, Mineralogical Society of America, 1909 K Street, N.W., Washington, D. C. 20006. Please remit \$1.00 for the microfiche.

diagrams of the space groups $Imcb$ (palermoite) and $Pmaa$ (carminite) down the c axis in the conventional $b > a > c$ orthorhombic setting. The essential difference between the two is a c glide at $b = 1/4$ in

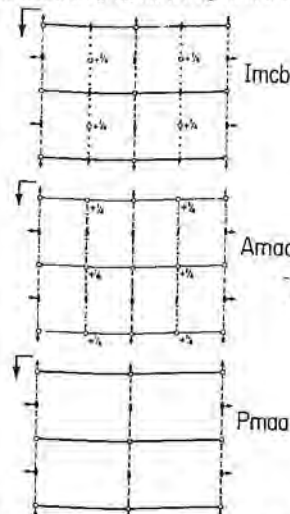


FIG. 1. Symmetry diagrams of the space groups $Imcb$, $Pmaa$, and $Pmaa$ in standard cell orientation (down the c axis). The first two groups apply to palermoite and carminite respectively. The third group is the subgroup common to the first two.

palermoite which is replaced by a n glide at $b = 1/4$ in carminite. Accordingly, the screw axis at $(0\ 1/4\ z)$ and the inversion at $(1/4\ 1/4\ 1/4)$ in $Im\bar{c}b$ is translated by $(1/4\ 0\ 0)$ to create $Amaa$. The two-fold rotations at $(1/4\ y\ 0)$; $(1/4\ 0\ z)$; $(x\ 0\ 0)$, the a -glide at $c = 0$; the a -glide at $b = 0$; the mirror plane at $a = 0$; and the inversion at (000) remain invariant in the two space groups. This corresponds to the mutual subgroup $Pnca$ (D_{2h}^{12}), shown at the bottom in Figure 1.

The palermoite and carminite structures (Fig. 2) both contain the same $[M^2(OH)(TO)_4]^{2-}$ octahedral (M) and tetrahedral (T) slab oriented parallel to (010) . The structures are distinguished by the links to symmetry equivalent slabs across the c glide at $b = 1/4$ in the former and the n glide at $b = 1/4$ in the latter. In fact, taking the symmetry operations which are invariant in the two space groups, the pairs of linked slabs between $1/4 < b < 3/4$ are isomorphous in the two structures. For this reason, the atomic coordinates for palermoite and carminite in Table I are compared within this bound. It is seen that all the parameters and their equipoint rank numbers and point symmetries are similar, with the exception of Li in palermoite and Pb(2) in carminite. The Li atom possesses an equipoint rank number of 8, point symmetry m , and two degrees of

freedom in the atomic coordinates. Pb(2) possesses rank number 4, point symmetry $2/m$, and no degrees of freedom.

Palermoite and carminite contain the same type of $M-O$ octahedral chain. In palermoite it consists of an edge-linked dimer which is corner-linked at the same level to symmetry equivalent dimers (see Fig. 2). The chains, which run parallel to the a axis, have composition $Al_2(O_p)(OH)_2$, where O_p are oxygens that belong to PO_4 tetrahedra. One-eighth of the tetrahedral oxygens, namely O(3) in both structures, do not bond to the trivalent octahedrally coordinated cations. The points of condensation of the octahedral chains include OH(1), OH(2), and O(4) in palermoite, each of equipoint rank number 8.

Remaining in the structures are pockets at $(1/4\ 1/2\ 1/2)$; and $(1/2\ 1/4\ 1/4)$, each of equipoint rank number 4. Both non-equivalent polyhedra are distorted cubes and accommodate Pb(1) and Pb(2) in carminite. Although Sr in palermoite is isomorphic to Pb(1) in carminite, the Li atoms in palermoite are split into two equivalences, the coordination polyhedron being a distorted tetrahedron. The polyhedral environments about Pb(2) and Li are shown as projections down the a axis in Figure 3. These regions are non-isomorphic as they do not

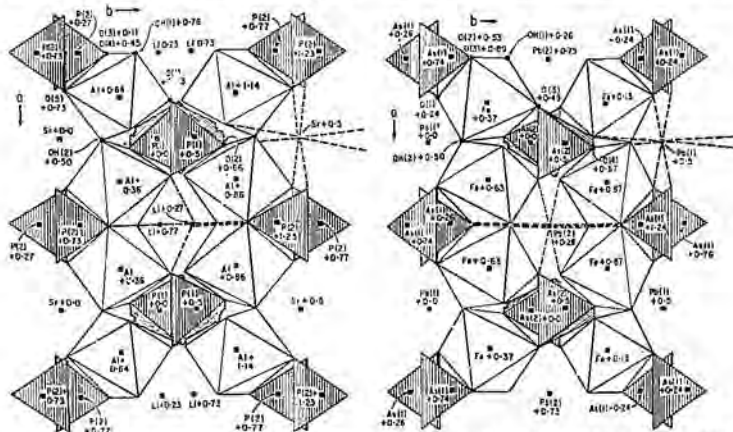


FIG. 2. Polyhedral diagrams of palermoite (left) and carminite (right) structures down the c axis. The outline $a \times b/2$ is shown. Heights are given as fractional coordinates in z . The Pb-Sr, and Li-O bonds are dashed in.

possess the same point symmetry in the two structures.

One of the curious features of the two structures is the observation that the "X" position at $(1/2, 1/4, 1/4)$ in palermito possesses a coordination polyhedron similar to that in carminite, both being distorted cubes. Figure 4 provides the bond distances for "X" in palermito and Pb(2) in carminite. The position "X", however, still has equipoint rank number 9 since its point symmetry remains m and to afford a carminite-like composition would require disordered half-occupied sites over the Pb(2) positions. Since the environments about the X and Pb(2) sites are non-isomorphic, the energetic relationships between the two structures are probably dictated by the charges and ionic radii of the cations competing for the X and Pb(2) environments, as the distinctions in the bonding over the rest of the structures are small.

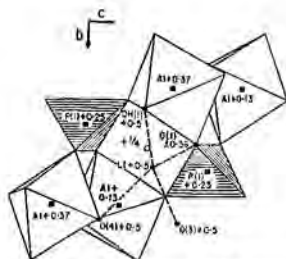
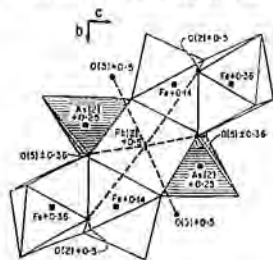


FIG. 3. The polyhedral environments of Pb(2) in carminite (top) and Li in palermito (bottom) down the a axis. The Pb(2) atom resides at $(1/2, 1/4, 1/4)$. In palermito, the locus at $(1/4, 1/4, 1/4)$ is drawn as a circle.

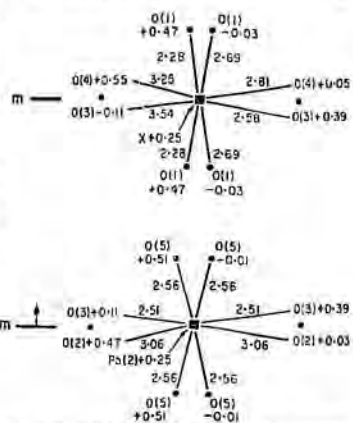


FIG. 4. The "X"-O bonds and Pb(2)-O bonds in palermito (top) and carminite (bottom). The symmetry elements m and $2/m$ respectively are shown on the left and apply to the loci of "X" and Pb(2). Bond distances are specified.

We propose that palermito and carminite structure ideals with compositions $X(1)X(2)M_2(OH)_2(TO)_2$ are *combinatorial polymorphs* in the sense defined by Moore (1975).

Bond Distances

Table 3 lists the anions and the coordinating cations in rows and columns. In this manner, the valence bond strengths can be conveniently tabulated and deviations from bond distance averages can be related to deviations in bond strength sums.

One problem immediately arises regarding the coordination of lithium. Although its nearest neighborhood defines a distorted trigonal bipyramid, the valence balances suggest that the true coordination is distorted tetrahedral, the polyhedral vertices including one OH(1), one O(3), and two O(1) atoms.

Interatomic distances are given in Table 4. The Li-O tetrahedral distances range from 1.94 to 2.29 Å, the fifth distance Li-O(4) = 2.46 Å suggesting that the tetrahedral coordination is more likely. We note in addition that a distorted trigonal bipyramid would require that the O(3)-O(4) edge be shared between Li and P(2). The additional distances which obtain from the distorted trigonal bipyramidal model are listed

TABLE 3. Palermito: Electrostatic Bond Strengths and Their Sums about the Anions*

Anion	Sr ²⁺	Li ¹⁺	Al ³⁺	P ⁵⁺	R(O)	R(O)	Σ	Me-O		
								Sr	Li	Al P
O(1)		1/4	3/6	5/4			2.00		+	- 0
O(2)	2/8		3/6	5/4			2.00		+	- 0
O(3)		1/4		5/4		1/6	1.67		-	-
O(4)			3/6+3/6	5/4			2.25		+	+
O(5)	2/8		3/6	5/4		1/6	2.08	0	+	0
OH(1)		1/4	3/6+3/6		5/6		2.08		-	-
OH(2)			3/6+3/6		5/6		1.83		-	-

*1/6-0 refers to distances which are greater than (+), less than (-), or within (0) 2σ of the interatomic error referred to the polyhedral average. R(O) = hydrogen donor, H(O) = hydrogen bond acceptor.

parenthetically in Table 4. The Sr-O polyhedron is a distorted cube with distances between 2.59 and 2.65 Å. The remaining polyhedral distance averages are typical, with the 1.91 Å average for Al-O and 1.53

and 1.54 Å averages for P(1)-O and P(2)-O respectively.

Table 4 also reveals the effects of polyhedral edge-sharing. The SrO₆ cube, for example, shares two

TABLE 4. Palermito: Interatomic Distances

Al		P(1)		Sr	
Al	-OH(2)	2 P(1)	-O(2)	4 Sr	- O(5) ¹
	-OH(1)	2	-O(1)		- O(2)
	-O(2) ¹				
	-O(1)	average		average	
	-O(5)				
	-O(4)	1 O(2)	-O(2) ⁱⁱⁱ	2 O(2)	- O(2) ⁱⁱⁱ
average	1.906	2 O(2)	-O(1) ⁱⁱⁱ	4 O(2)	- O(5) ^{iv}
		1 O(1)	-O(1) ⁱⁱⁱ	4 O(5) ⁱⁱ	- O(2) ^{iv}
		2 O(1)	-O(2)	2 O(5) ⁱ	- O(5) ^{vii}
		average		average	
OH(1) - O(4)	2.494(7) ⁺				
OH(1) - O(1)	2.535(6) ⁺⁺				
OH(2) - O(5)	2.651(6) ^v				
O(2) - O(5)	2.669(6)				
O(2) - O(1)	2.671(6)				
O(2) - OH(2)	2.681(6)	1 P(2)	-O(3)	1 Li	-OH(1) ^{ix}
OH(1) - O(5)	2.688(6)	2	-O(5) ^{iv}	1	- O(3)
O(4) - O(5)	2.732(6)	1	-O(4)	2	- O(1) ^{ix}
O(4) - O(1)	2.771(6)	average		1	- O(1) ^{ix}
O(2) - O(4)	2.825(6)			average	
OH(2) - O(4)	2.916(7)	1 O(3)	-O(4) ^v		
average	2.692	1 O(5)	iv-O(5) ^v		
		2 O(3)	-O(5) ^{iv}		
		2 O(4)	-O(5) ^{iv}		
		average			
Hydrogen Bonds					
OH(1)...O(3)	2.749(7)				
OH(2)...O(5)	2.645(6)				

⁺Edge sharing between Al-Al octahedra; ⁺⁺between Sr-P polyhedra; ^vbetween Sr-Al polyhedra; ^{ix}between Li-P polyhedra; ⁺between Li-Al polyhedra. ⁱ = 1/2 -x, 1/2 -y, 1/2 -z; ⁱⁱ = x, 1/2 -y, 1/2 +z; ⁱⁱⁱ = 1/2 -x, y, -z; ^{iv} = x, -y, -z; ^v = -x, -y, -z; ^{vi} = 1/2 -x, -y, z; ^{vii} = 1/2 -x, 1/2 +y, 1/2 +z; ^{viii} = x, 1/2 +y, 1/2 -z; ^{ix} = -x, 1/2 -y, 1/2 +z. These equivalences refer to the designated atoms in Fig. 2.

edges with the $P(1)O_4$ tetrahedron and four edges with the AlO_6 octahedra. These smaller more tightly bound polyhedra geometrically restrict the O-O' shared edges such that the shortest SiO_4 edge distances are associated with $P(1)O_4$ and AlO_6 respectively. The OH(1)-O(4) shared edge between AlO_6 octahedra is 2.49 Å and can be compared with the O(9)-O(9') shared edge distances (= 2.40 Å) in the structurally related bjarebyite (Moore and Araki, 1974).

Finney (1963) noted a short OH(2)-OH(2) = 2.44 ± 0.13 distance although that distance does not correspond to any cation-oxygen polyhedral edge. In palermoite, the OH(2)-OH(2)' = 2.80 Å distance is considerably longer.

The proposed hydrogen bonds involve OH(1) . . . O(3) = 2.75 Å and OH(2)-O(5) = 2.84 Å distances. Since O(5) resides in a general position, the hydrogen bond to it is on the average half-occupied. Deviations from average bond lengths can be roughly correlated with degree of undersaturation or oversaturation of cations about anions (Table 3). Thus, O(3), with $\Sigma = 2.25$, are all longer than average, OH(1), with $\Sigma = 2.08$, has shorter than average bonds, however. At present, we cannot offer a satisfactory explanation for this discrepancy.

Acknowledgments

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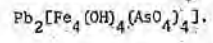
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The following material did not appear in the original publication.

AM-75-003-B

PAUL BRIAN MCORE and TAKAHARU ARAKI: Palermoite, $\text{SrLi}_2[\text{Al}_4(\text{OH})_4(\text{PO}_4)_4]$:

Its atomic arrangement and relationship to carminite,



Published in *The American Mineralogist*, Volume 60 (May-June, 1975).

TABLE 2. Palermoite. Observed and Calculated Structure Factors

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H	K	L	FD	FC	H	K	L	FD	FC	H	K	L	FD	FC
0	24	0	101.8	97.0	10	8	0	78.8	84.4	18	0	0	21.1	20.4
2	24	0	40.5	30.0	12	8	0	77.7	66.4	0	25	1	27.9	14.3
4	24	0	59.7	53.3	14	8	0	11.4	11.8	2	25	1	34.0	32.1
0	22	0	61.7	56.0	16	8	0	25.1	27.6	1	24	1	12.2	3.2
2	22	0	11.6	11.6	0	6	0	106.9	118.0	3	24	1	12.3	20.6
4	22	0	31.7	29.6	2	6	0	125.6	132.2	5	24	1	38.0	33.5
6	22	0	24.2	22.3	4	6	0	69.5	72.6	0	23	1	11.9	12.8
8	22	0	48.7	46.3	6	6	0	169.1	166.6	2	23	1	21.9	32.2
0	20	0	69.2	68.5	8	6	0	61.5	62.6	4	23	1	37.7	29.2
2	20	0	45.6	45.8	10	6	0	17.9	16.1	6	23	1	34.2	26.2
4	20	0	173.4	175.7	12	6	0	22.0	20.0	1	22	1	11.5	3.1
6	20	0	49.5	45.8	14	6	0	61.7	68.6	3	22	1	11.7	7.6
8	20	0	43.3	49.2	16	6	0	12.0	15.6	5	22	1	20.1	13.0
10	20	0	12.3	11.4	0	4	0	26.3	40.6	7	22	1	32.9	33.4
0	18	0	28.3	31.2	2	4	0	96.1	102.6	9	22	1	12.6	16.1
2	18	0	10.3	9.9	4	4	0	18.6	17.5	0	21	1	11.3	12.6
4	18	0	68.1	70.3	6	4	0	124.7	126.2	2	21	1	30.4	25.9
6	18	0	18.5	13.7	8	4	0	16.7	19.3	4	21	1	11.5	14.2
8	18	0	30.9	33.1	10	4	0	56.3	60.5	6	21	1	31.0	32.6
10	18	0	11.8	9.7	12	4	0	121.9	125.2	8	21	1	12.1	10.8
12	18	0	42.5	51.8	14	4	0	95.4	102.0	10	21	1	12.6	8.4
0	16	0	23.5	31.5	16	4	0	11.9	13.6	1	20	1	31.0	42.8
2	16	0	73.0	69.9	18	4	0	12.7	32.0	3	20	1	40.7	44.2
4	16	0	131.0	130.6	2	2	0	87.4	107.7	5	20	1	20.0	22.1
6	16	0	45.8	46.8	4	2	0	103.0	109.6	7	20	1	24.9	24.0
8	16	0	28.1	30.0	6	2	0	78.3	68.2	9	20	1	41.1	42.1
10	16	0	77.1	77.6	8	2	0	78.2	83.8	11	20	1	43.7	47.9
12	16	0	69.1	59.2	10	2	0	89.4	81.2	0	19	1	153.0	153.0
14	16	0	29.8	30.9	12	2	0	52.1	61.1	2	19	1	104.5	104.2
0	14	0	95.5	92.8	14	2	0	39.0	37.2	4	19	1	41.7	37.6
2	14	0	191.7	208.2	16	2	0	39.1	48.8	6	19	1	66.1	66.3
4	14	0	54.8	51.0	18	2	0	47.0	37.8	8	19	1	110.7	111.3
6	14	0	174.5	186.6	2	0	0	120.0	125.0	10	19	1	97.3	91.5
8	14	0	59.8	57.0	4	0	0	275.1	259.3	12	19	1	36.2	34.5
10	14	0	114.2	119.7	6	0	0	20.2	25.8	1	18	1	103.6	103.4
12	14	0	11.6	13.9	8	0	0	534.8	504.7	3	18	1	10.4	4.0
14	14	0	85.5	95.6	10	0	0	56.6	62.0	5	18	1	20.3	15.4
0	12	0	31.2	38.1	12	0	0	114.3	121.6	7	18	1	99.2	97.7
2	12	0	70.5	68.2	14	0	0	32.5	22.5	9	18	1	57.4	56.7
4	12	0	67.0	70.8	16	0	0	159.0	160.5	11	18	1	20.3	21.9
6	12	0	81.9	77.4						0	17	1	30.5	37.8
8	12	0	58.6	54.5						2	17	1	16.7	10.9
10	12	0	10.4	24.8						4	17	1	60.8	59.3
12	12	0	29.4	40.0						6	17	1	25.5	28.3
14	12	0	45.9	49.0						8	17	1	11.1	15.0
16	12	0	47.8	41.3						10	17	1	11.7	14.0
0	10	0	74.0	73.2						12	17	1	38.0	34.0
2	10	0	98.6	106.8						1	16	1	62.8	68.7
4	10	0	113.4	111.4						3	16	1	9.8	11.2
6	10	0	162.5	166.4						5	16	1	10.1	14.7
8	10	0	75.2	77.7						7	16	1	32.5	24.6
10	10	0	84.6	88.0						9	16	1	67.7	70.0
12	10	0	79.5	84.7						11	16	1	11.7	16.6
14	10	0	130.8	133.7						13	16	1	23.6	13.4
16	10	0	51.3	60.7						0	15	1	99.8	99.6
0	8	0	275.1	290.7						2	15	1	101.5	104.5
2	8	0	116.6	119.2						4	15	1	126.4	128.6
4	8	0	172.4	167.4						6	15	1	78.4	80.4
6	8	0	55.5	56.0						8	15	1	73.7	70.6
8	8	0	136.8	142.1						10	15	1	75.8	78.2

		H	K	L	FO	FC								
12	15	1	92.3	91.0	11	10	1	74.6	76.2					
14	15	1	44.0	46.1	13	10	1	50.9	49.2					
1	14	1	20.5	24.3	15	10	1	12.0	0.5	4	3	1	76.1	67.0
3	14	1	55.5	57.6	0	9	1	28.1	22.7	6	3	1	13.3	14.1
5	14	1	42.5	46.3	2	9	1	89.8	96.3	8	3	1	72.0	74.9
7	14	1	18.4	18.5	4	9	1	186.9	189.8	10	3	1	62.6	64.2
9	14	1	33.7	38.0	6	9	1	120.3	122.7	12	3	1	29.8	13.3
11	14	1	61.1	55.9	8	9	1	40.7	48.1	14	3	1	11.0	12.1
13	14	1	31.7	27.2	10	9	1	48.0	57.3	16	3	1	26.8	38.3
15	14	1	22.9	22.9	12	9	1	100.1	103.0	18	3	1	33.0	39.4
0	13	1	69.0	69.0	14	9	1	79.9	84.3	3	2	1	197.0	189.0
2	13	1	45.5	49.5	16	9	1	49.1	46.9	5	2	1	76.7	71.4
4	13	1	59.5	59.0	1	8	1	68.6	60.6	7	2	1	7.8	2.8
6	13	1	46.3	51.4	3	8	1	17.7	30.3	9	2	1	43.3	44.5
8	13	1	52.8	55.0	5	8	1	8.1	4.4	11	2	1	113.5	110.1
10	13	1	10.6	17.6	7	8	1	24.7	28.5	13	2	1	29.0	21.0
12	13	1	22.3	15.5	9	8	1	52.1	47.3	15	2	1	11.4	5.9
14	13	1	12.1	19.8	11	8	1	22.3	26.7	17	2	1	12.3	0.5
1	12	1	15.8	8.6	13	8	1	10.9	8.0	2	1	1	150.8	156.5
3	12	1	14.3	0.8	15	8	1	11.9	26.2	4	1	1	193.0	185.3
5	12	1	55.8	58.9	17	8	1	12.6	9.3	6	1	1	123.2	123.3
7	12	1	9.5	3.2	0	7	1	73.2	74.3	8	1	1	20.6	18.4
9	12	1	10.1	12.9	2	7	1	92.9	92.6	10	1	1	60.6	64.7
11	12	1	30.0	30.1	4	7	1	121.3	123.5	12	1	1	76.1	79.1
13	12	1	40.5	39.2	6	7	1	39.5	43.5	14	1	1	57.3	63.3
15	12	1	12.3	13.6	8	7	1	9.0	12.2	16	1	1	11.8	13.6
0	11	1	113.9	120.3	10	7	1	26.2	27.3	18	1	1	12.6	23.5
2	11	1	37.7	38.3	12	7	1	44.0	50.3	0	24	2	36.9	30.7
4	11	1	53.0	50.7	14	7	1	11.3	10.3	2	24	2	110.8	107.6
6	11	1	9.1	11.5	16	7	1	22.6	16.4	4	24	2	41.1	33.0
8	11	1	85.4	87.2	1	6	1	113.1	111.7	1	23	2	22.1	4.1
10	11	1	62.4	61.3	3	6	1	6.8	3.8	3	23	2	24.4	17.1
12	11	1	18.1	9.2	5	6	1	74.8	64.5	5	23	2	12.2	3.1
14	11	1	24.1	9.5	7	6	1	104.4	97.4	7	23	2	12.4	0.2
16	11	1	31.5	37.9	9	6	1	87.8	84.2	0	22	2	11.7	13.3
1	10	1	35.1	42.4	11	6	1	29.5	28.5	2	22	2	36.5	32.5
3	10	1	144.4	147.6	13	6	1	47.2	43.2	4	22	2	11.9	9.7
5	10	1	125.5	125.1	15	6	1	69.9	65.4	6	22	2	31.5	31.3
7	10	1	18.0	21.4	17	6	1	27.9	32.9	8	22	2	12.4	8.5
9	10	1	17.3	13.9	0	5	1	250.5	264.8	1	21	2	11.4	20.2
					2	5	1	210.8	222.7	3	21	2	41.9	46.9
					4	5	1	196.8	192.9	5	21	2	11.7	18.4
					6	5	1	173.0	171.6					
					8	5	1	186.8	183.9					
					10	5	1	126.8	130.7					
					12	5	1	86.3	87.7					
					14	5	1	77.3	84.1					
					16	5	1	95.3	96.9					
					18	5	1	63.6	66.8					
					1	4	1	119.4	131.9					
					3	4	1	101.7	108.6					
					5	4	1	150.9	145.6					
					7	4	1	69.1	69.5					
					9	4	1	78.0	76.5					
					11	4	1	31.3	34.7					
					13	4	1	71.1	69.3					
					15	4	1	37.2	43.1					
					17	4	1	33.7	36.0					
					0	3	1	74.0	73.5					
					2	3	1	37.8	36.7					

H	K	L	FO	FC
7	21	2	22.1	15.7
9	21	2	12.4	14.0
0	20	2	58.7	59.2
2	20	2	58.9	61.7
4	20	2	42.8	37.2
6	20	2	59.8	61.2
8	20	2	47.5	52.1
10	20	2	49.2	50.6
1	19	2	26.6	36.2
3	19	2	28.9	23.5
5	19	2	11.1	0.8
7	19	2	11.5	13.3
9	19	2	34.3	36.9
11	19	2	30.5	23.0
0	18	2	26.7	31.3
2	18	2	54.6	56.9
4	18	2	23.2	25.4
6	18	2	51.5	50.7
8	18	2	19.0	23.2
10	18	2	42.4	37.0
12	18	2	23.5	13.4
1	17	2	53.1	56.3
3	17	2	41.3	43.2
5	17	2	27.1	27.3
7	17	2	48.9	48.7
9	17	2	40.9	34.4
11	17	2	22.1	30.1
13	17	2	12.5	5.1
0	16	2	47.2	46.8
2	16	2	16.2	15.6
4	16	2	54.9	59.4
6	16	2	10.3	10.0
8	16	2	33.4	32.1
10	16	2	11.4	9.8
12	16	2	21.3	32.3
1	15	2	9.4	20.5
3	15	2	55.5	53.0
5	15	2	9.8	5.5
7	15	2	10.2	4.9
9	15	2	21.6	20.2
11	15	2	49.7	52.9
13	15	2	12.1	9.1
0	14	2	91.1	98.0
2	14	2	70.5	67.7
4	14	2	132.7	140.6
6	14	2	64.9	66.0
8	14	2	91.9	95.7
10	14	2	53.4	53.4
12	14	2	91.3	93.3
14	14	2	46.2	45.6
1	13	2	31.3	30.2
3	13	2	42.8	46.6
5	13	2	40.9	46.5
7	13	2	49.6	50.4
9	13	2	20.2	4.3
11	13	2	38.6	35.6
13	13	2	21.2	21.4
15	13	2	21.0	33.7
0	12	2	95.1	95.3
2	12	2	8.7	11.8

H	K	L	FO	FC
1	7	2	99.2	102.1
3	7	2	47.7	50.0
5	7	2	8.0	2.1
7	7	2	88.7	87.1
9	7	2	45.2	44.0
11	7	2	35.4	40.2
13	7	2	10.9	17.8
15	7	2	52.3	44.3
17	7	2	12.5	9.3
0	6	2	160.5	156.2
2	6	2	99.1	103.3
4	6	2	60.1	85.3
6	6	2	90.5	91.4
8	6	2	29.8	29.1
10	6	2	68.1	73.0
12	6	2	33.5	32.5
14	6	2	50.0	55.4
16	6	2	12.1	24.0
1	5	2	39.5	46.3
3	5	2	6.7	1.9
5	5	2	69.0	63.3
7	5	2	99.9	100.5
9	5	2	9.0	9.8
11	5	2	5.8	5.0
13	5	2	37.9	29.9
15	5	2	54.9	55.8
17	5	2	12.3	9.2
0	4	2	110.5	119.5
2	4	2	239.3	243.1
4	4	2	70.0	72.4
6	4	2	87.7	91.4
8	4	2	61.2	70.7
10	4	2	164.8	166.0
12	4	2	29.6	35.0
14	4	2	22.4	31.7
16	4	2	23.8	28.5
1	3	2	32.9	36.5
3	3	2	32.2	32.5
5	3	2	74.4	66.7
7	3	2	45.6	49.3
9	3	2	8.9	18.0
11	3	2	43.2	32.4
13	3	2	42.9	35.1
15	3	2	32.4	27.3
17	3	2	12.3	5.9
2	2	2	52.7	55.8
4	2	2	192.0	173.7
6	2	2	70.8	73.9
8	2	2	44.9	39.0
10	2	2	43.4	53.8
12	2	2	10.0	13.4
14	2	2	28.1	34.4
16	2	2	11.8	7.9
18	2	2	12.6	26.2
3	1	2	91.8	86.7
5	1	2	100.0	95.4
7	1	2	137.0	130.2
9	1	2	8.8	2.7
11	1	2	48.1	42.8
13	1	2	18.0	25.7

		H	K	L	FD	FC								
		7	18	3	28.0	22.8								
		9	18	3	27.3	23.7								
		11	18	3	48.6	42.2								
		0	17	3	62.3	60.4								
15	1	2	53.4	51.3	2	17	3	37.4	42.6	9	10	3	29.2	26.1
17	1	2	12.2	10.4	4	17	3	29.8	31.5	11	10	3	28.6	17.6
2	0	2	388.5	356.0	6	17	3	42.6	37.5	13	10	3	38.4	34.4
4	0	2	140.5	137.4	8	17	3	36.8	38.2	15	10	3	57.5	54.3
6	0	2	186.5	180.3	0	17	3	11.9	11.3	0	9	3	144.0	150.9
8	0	2	62.5	66.9	1	17	3	12.4	9.2	2	9	3	166.3	171.4
10	0	2	246.0	243.9	1	16	3	38.2	36.7	4	9	3	48.2	49.6
12	0	2	78.5	85.0	3	16	3	10.0	5.6	6	9	3	150.0	151.3
14	0	2	97.4	103.3	5	16	3	18.5	8.9	8	9	3	104.6	106.2
16	0	2	34.8	44.0	7	16	3	10.8	22.8	10	9	3	94.0	96.9
18	0	2	119.2	121.1	9	16	3	21.5	21.6	12	9	3	10.9	20.7
1	24	3	12.5	11.8	11	16	3	11.9	12.5	14	9	3	86.4	72.3
3	24	3	12.5	8.5	13	16	3	12.5	3.4	16	9	3	51.0	46.9
0	23	3	95.6	100.3	0	15	3	174.3	178.8	1	8	3	20.9	24.7
2	23	3	50.5	38.7	2	15	3	94.7	97.1	3	8	3	75.1	80.4
4	23	3	21.1	18.9	4	15	3	27.5	25.7	5	8	3	79.7	79.5
6	23	3	22.2	11.9	6	15	3	62.7	61.5	7	8	3	31.6	32.2
1	22	3	37.0	39.8	8	15	3	132.5	132.7	9	8	3	29.1	31.8
3	22	3	11.9	7.3	10	15	3	92.5	92.2	11	8	3	27.6	33.2
5	22	3	12.1	6.3	12	15	3	24.0	34.2	13	8	3	34.4	37.1
7	22	3	12.5	25.5	14	15	3	32.9	30.1	15	8	3	23.0	31.7
0	21	3	33.0	35.4	1	14	3	86.5	93.4	0	7	3	116.7	117.8
2	21	3	11.6	14.8	3	14	3	9.3	27.4	2	7	3	7.2	12.1
4	21	3	40.6	35.5	5	14	3	9.7	6.9	4	7	3	102.4	106.4
6	21	3	12.1	10.6	7	14	3	48.7	61.6	6	7	3	18.2	14.3
8	21	3	20.5	16.9	9	14	3	78.6	76.3	8	7	3	87.4	88.5
1	20	3	61.1	61.9	11	14	3	21.2	30.3	10	7	3	41.0	42.5
3	20	3	11.3	6.2	13	14	3	12.1	3.8	12	7	3	29.2	20.3
5	20	3	11.6	8.2	0	13	3	68.0	71.2	14	7	3	11.5	12.1
7	20	3	46.7	47.7	2	13	3	27.8	20.8	16	7	3	39.2	44.1
9	20	3	38.3	42.3	4	13	3	45.0	48.2	1	6	3	48.4	50.0
0	19	3	42.9	42.1	6	13	3	61.1	58.0	3	6	3	145.2	145.8
2	19	3	84.4	81.5	8	13	3	27.9	30.8	5	6	3	139.4	139.2
4	19	3	95.1	94.2	10	13	3	10.9	16.8	7	6	3	50.0	48.0
6	18	3	73.6	73.4	12	13	3	43.3	38.8	9	6	3	17.0	26.8
8	19	3	31.9	37.4	14	13	3	79.6	61.8	11	6	3	81.5	80.3
10	19	3	67.3	68.1	1	12	3	70.3	73.6	13	6	3	67.8	69.2
1	18	3	10.5	2.1	3	12	3	18.9	11.1	15	6	3	11.9	26.7
3	18	3	42.1	41.4	5	12	3	9.1	5.3	17	6	3	21.5	19.8
5	18	3	11.0	15.2	7	12	3	41.7	43.0	0	5	3	167.9	175.5
					9	12	3	44.1	40.9					
					11	12	3	11.1	5.2					
					13	12	3	11.8	8.6					
					15	12	3	12.5	9.3					
					0	11	3	8.7	13.1					
					2	11	3	97.9	105.0					
					4	11	3	57.4	58.3					
					6	11	3	82.9	88.2					
					8	11	3	25.9	28.7					
					10	11	3	40.1	49.8					
					12	11	3	27.9	28.8					
					14	11	3	37.9	42.5					
					1	10	3	72.0	73.5					
					3	10	3	8.6	0.3					
					5	10	3	38.0	37.1					
					7	10	3	88.9	88.6					

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H	K	L	F0	FC
2	5	3	142.1	146.2
4	5	3	274.2	274.0
6	5	3	169.6	165.0
8	5	3	107.8	113.7
10	5	3	65.4	68.7
12	5	3	141.9	147.8
14	5	3	103.0	101.0
16	5	3	60.0	62.3
1	4	3	9.3	11.3
3	4	3	68.8	70.0
5	4	3	57.0	59.0
7	4	3	24.7	26.3
9	4	3	9.0	21.9
11	4	3	41.4	36.9
13	4	3	29.4	29.6
15	4	3	25.0	25.3
17	4	3	25.5	19.8
0	3	3	137.9	137.9
2	3	3	65.9	67.4
4	3	3	187.1	181.1
6	3	3	54.0	58.4
8	3	3	33.8	32.8
10	3	3	25.5	21.5
12	3	3	66.4	71.2
14	3	3	11.2	14.1
16	3	3	21.3	13.8
3	2	3	116.3	111.5
5	2	3	66.0	62.9
7	2	3	28.4	21.8
9	2	3	8.8	0.5
11	2	3	58.4	56.5
13	2	3	10.7	12.2
15	2	3	11.7	19.4
17	2	3	12.4	5.5
2	1	3	54.8	52.9
4	1	3	62.2	52.8
6	1	3	62.0	61.4
8	1	3	131.1	130.7
10	1	3	60.7	61.6
12	1	3	21.0	24.0
14	1	3	30.3	43.0
16	1	3	64.8	71.6
1	23	4	12.3	8.7
3	23	4	12.4	16.9
0	22	4	12.0	15.8
2	22	4	12.1	7.6
4	22	4	46.5	44.5
6	22	4	12.5	7.2
1	21	4	23.6	10.4
3	21	4	11.9	18.7
5	21	4	12.0	1.2
7	21	4	12.4	11.9
0	20	4	96.7	95.0
2	20	4	37.9	41.7
4	20	4	19.8	18.5
6	20	4	24.1	28.5
8	20	4	87.5	83.7
1	19	4	34.3	27.8
3	19	4	11.2	6.4
5	19	4	11.5	6.6

7	19	4	11.9	3.6
9	19	4	36.0	33.0
0	18	4	65.7	65.4
2	18	4	34.5	30.8
4	18	4	27.2	36.9
6	18	4	28.8	22.5
8	18	4	47.3	49.2
10	18	4	12.4	20.7
1	17	4	28.0	36.4
3	17	4	10.5	0.2
5	17	4	10.8	1.7
7	17	4	19.5	22.0
9	17	4	33.5	31.8
11	17	4	12.3	5.4
0	16	4	43.3	45.2
2	16	4	50.6	50.6
4	16	4	61.6	60.0
6	16	4	53.9	56.0
8	16	4	45.9	41.3
10	16	4	11.9	18.6
12	16	4	35.6	28.8
1	15	4	26.4	25.3
3	15	4	17.2	26.0
5	15	4	10.2	2.5
7	15	4	32.3	32.2
9	15	4	11.3	4.8
11	15	4	32.8	35.1
13	15	4	12.5	2.9
0	14	4	44.4	43.7
2	14	4	101.9	101.9
4	14	4	69.4	69.6
6	14	4	109.8	111.2
8	14	4	40.9	43.6
10	14	4	76.5	77.2
12	14	4	49.4	53.7
14	14	4	84.8	84.1
1	13	4	8.9	4.5
3	13	4	26.7	26.9
5	13	4	18.7	17.6
7	13	4	21.1	20.5

H	K	L	F0	FC
9	13	4	23.3	24.4
11	13	4	23.7	23.9
13	13	4	21.7	5.2
0	12	4	93.7	97.7
2	12	4	61.0	60.7
4	12	4	98.4	102.6
6	12	4	34.5	36.5
8	12	4	60.7	62.9
10	12	4	52.7	56.5
12	12	4	55.2	49.8
14	12	4	12.3	14.3
1	11	4	40.7	44.5
3	11	4	33.9	38.9
5	11	4	9.0	7.2
7	11	4	9.6	14.8
9	11	4	26.8	30.4
11	11	4	29.1	25.3
13	11	4	11.8	9.5
15	11	4	12.6	0.2
0	10	4	117.5	117.4
2	10	4	198.1	208.6
4	10	4	68.7	60.6
6	10	4	187.6	195.5
8	10	4	77.6	76.5
10	10	4	115.6	118.4
12	10	4	24.7	31.3
14	10	4	103.5	106.1
1	9	4	26.2	23.4
3	9	4	24.7	22.7
5	9	4	65.2	68.2
7	9	4	16.2	8.5
9	9	4	20.6	19.3
11	9	4	10.7	2.3
13	9	4	50.4	48.6
15	9	4	12.3	6.3
0	8	4	63.4	63.2
2	8	4	65.5	62.1
4	8	4	41.6	44.7
6	8	4	84.1	84.6
8	8	4	58.8	54.2
10	8	4	27.0	27.8
12	8	4	38.8	43.5
14	8	4	62.2	65.2
16	8	4	44.1	33.3
1	7	4	30.1	33.6
3	7	4	63.8	64.1
5	7	4	57.3	57.1
7	7	4	30.8	24.4
9	7	4	45.6	43.8
11	7	4	22.1	26.1
13	7	4	22.4	22.9
15	7	4	29.0	25.1
0	6	4	69.9	71.8
2	6	4	20.3	18.3
4	6	4	66.6	67.1
6	6	4	44.3	47.8
8	6	4	62.8	63.5
10	6	4	16.7	13.0
12	6	4	49.3	56.0
14	6	4	46.9	49.7

H	K	L	FO	FC	H	K	L	FO	FC
11	8	5	38.4	36.7	1	21	6	33.7	33.1
13	8	5	30.9	33.4	3	21	6	22.1	22.9
15	8	5	12.3	6.5	0	20	6	37.7	37.8
0	7	5	76.6	79.0	2	20	6	82.6	80.0
2	7	5	37.3	39.2	4	20	6	66.6	62.1
4	7	5	39.0	39.8	6	20	6	78.5	74.0
6	7	5	22.3	10.0	1	19	6	26.7	26.7
8	7	5	53.8	52.5	3	19	6	35.6	38.4
10	7	5	34.5	30.6	5	19	6	21.3	22.3
12	7	5	10.9	14.0	7	19	6	19.9	15.3
14	7	5	21.0	21.2	0	18	6	10.8	8.7
1	6	5	49.6	50.2	2	18	6	26.3	32.9
3	6	5	139.9	146.3	4	18	6	11.2	14.6
5	6	5	87.2	88.2	6	18	6	36.8	34.3
7	6	5	29.0	25.8	8	18	6	11.9	9.1
9	6	5	18.1	20.4	1	17	6	24.1	31.2
11	6	5	100.1	98.2	3	17	6	58.9	63.2
13	6	5	28.4	27.2	5	17	6	44.5	46.6
15	6	5	24.4	7.6	7	17	6	25.3	14.1
0	5	5	110.6	114.3	9	17	6	35.3	33.2
2	5	5	131.9	135.1	0	16	6	50.2	50.7
4	5	5	210.6	210.0	2	16	6	24.0	22.2
6	5	5	113.9	113.7	4	16	6	26.6	11.5
8	5	5	92.4	95.7	6	16	6	11.0	23.4
10	5	5	98.7	97.3	8	16	6	50.1	48.1
12	5	5	112.2	112.9	10	16	6	12.0	7.7
14	5	5	59.7	68.1	1	15	6	47.2	49.1
16	5	5	59.3	61.8	3	15	6	10.0	2.9
1	4	5	54.4	54.2	5	15	6	10.4	4.9
3	4	5	69.4	68.5	7	15	6	23.6	28.5
5	4	5	56.0	52.1	9	15	6	46.0	43.8
7	4	5	70.2	71.4	11	15	6	21.5	3.1
9	4	5	19.7	17.8	0	14	6	133.6	133.3
11	4	5	47.7	46.6	2	14	6	73.2	74.1
13	4	5	39.2	33.3	4	14	6	122.1	122.7
15	4	5	46.2	40.7	6	14	6	54.2	56.1
0	3	5	62.2	68.6	8	14	6	100.6	98.9
2	3	5	60.1	60.8	10	14	6	44.9	43.1
4	3	5	48.7	44.8	12	14	6	69.7	66.6
6	3	5	39.3	42.5	1	13	6	38.2	36.5
8	3	5	43.3	36.6					
10	3	5	52.7	54.8					
12	3	5	22.6	22.4					
14	3	5	11.5	28.9					
16	3	5	20.2	9.2					
3	2	5	69.9	66.2					
5	2	5	12.7	0.2					
7	2	5	55.7	53.4					
9	2	5	74.0	70.8					
11	2	5	64.3	61.5					
13	2	5	11.0	14.6					
15	2	5	32.1	35.6					
2	1	5	149.8	146.3					
4	1	5	32.8	33.1					
6	1	5	101.0	97.5					
8	1	5	33.8	32.4					
10	1	5	107.3	110.1					
12	1	5	18.8	10.9					
14	1	5	40.8	44.8					
16	1	5	24.1	20.0					

4	3	7	36.1	34.5	3	9	8	9.0	13.8	8	0	8	162.5	155.9
6	3	7	23.5	18.8	5	9	8	26.0	14.9	10	0	8	58.4	59.2
8	3	7	100.2	98.9	7	9	8	74.1	76.7	12	0	8	59.5	58.4
10	3	7	9.9	13.3	9	9	8	18.1	4.5	1	15	9	11.2	4.9
12	3	7	20.1	9.8	11	9	8	11.6	8.0	0	15	9	46.2	36.1
14	3	7	11.8	7.1	0	8	8	61.8	60.9	2	15	9	61.1	53.1
3	2	7	5.9	5.0	2	8	8	32.4	34.7	4	15	9	65.6	62.1
5	2	7	26.4	29.1	4	8	8	39.0	38.7	1	14	9	10.4	5.5
7	2	7	28.0	22.8						3	14	9	19.9	24.8
9	2	7	9.2	9.2						5	14	9	29.8	24.9
11	2	7	17.8	5.2	6	8	8	30.0	30.2	0	13	9	26.4	35.5
13	2	7	19.2	19.8	8	8	8	49.9	47.2	2	13	9	21.5	19.5
2	1	7	24.3	22.3	10	8	8	18.5	28.6	4	13	9	37.3	29.2
4	1	7	146.8	141.3	12	8	8	23.0	22.8	6	13	9	21.6	25.6
6	1	7	43.7	46.4	1	7	8	18.6	15.6	1	12	9	9.7	13.8
8	1	7	62.8	63.3	3	7	8	91.0	95.2	3	12	9	25.0	14.0
10	1	7	17.5	18.9	5	7	8	73.5	73.1					
12	1	7	87.6	88.9	7	7	8	17.4	17.9					
14	1	7	28.4	31.0	9	7	8	19.1	23.7	5	12	9	18.4	5.2
0	18	8	38.9	26.4	11	7	8	60.7	63.8	7	12	9	11.1	15.1
2	18	8	31.0	16.3	0	6	8	70.3	69.1	0	11	9	71.9	63.7
1	17	8	11.3	15.6	2	6	8	26.2	24.9	2	11	9	19.4	13.3
3	17	8	36.9	30.6	4	6	8	32.4	27.3	4	11	9	88.5	86.4
5	17	8	11.7	13.3	6	6	8	29.4	23.0	6	11	9	10.5	17.2
0	16	8	35.6	40.5	8	6	8	53.8	53.2	8	11	9	50.5	51.1
2	16	8	32.9	28.7	10	6	8	21.5	21.1	1	10	9	33.5	32.9
4	16	8	22.3	26.1	12	6	8	22.3	29.1	3	10	9	60.0	58.9
6	16	8	32.0	18.8	1	5	8	22.1	18.9	5	10	9	36.3	40.6
1	15	8	44.2	49.5	3	5	8	24.4	25.7	7	10	9	32.7	35.5
3	15	8	20.2	9.9	5	5	8	66.5	64.6	9	10	9	11.3	9.5
5	15	8	11.3	8.9	7	5	8	18.8	3.2	0	9	9	95.7	97.9
7	15	8	11.6	15.1	9	5	8	28.2	21.4	2	9	9	50.6	41.5
0	14	8	68.7	63.5	11	5	8	11.1	4.8	4	9	9	107.7	106.4
2	14	8	77.4	73.7	0	4	8	27.9	23.1	6	9	9	19.9	20.2
4	14	8	35.1	36.6	2	4	8	62.7	59.4	8	9	9	76.3	75.6
6	14	8	68.8	65.8	4	4	8	123.3	120.1	1	8	9	15.2	6.3
8	14	8	53.2	52.4	6	4	8	81.4	79.5	3	8	9	16.3	3.9
1	13	8	42.3	37.9	8	4	8	9.4	20.1	5	8	9	9.1	2.9
3	13	8	10.0	0.6	10	4	8	26.7	21.2	7	8	9	10.0	5.3
5	13	8	10.4	17.6	12	4	8	66.2	71.1	9	8	9	10.9	16.2
7	13	8	32.3	30.9	1	3	8	5.1	13.7	0	7	9	25.7	28.4
9	13	8	33.2	28.9	3	3	8	17.9	22.7	2	7	9	14.1	11.8
0	12	8	24.8	35.5	5	3	8	13.5	5.1	4	7	9	32.0	27.6
2	12	8	9.5	18.1	7	3	8	18.3	20.0	6	7	9	17.0	11.3
4	12	8	46.0	45.8	9	3	8	9.8	14.7	8	7	9	10.2	9.4
6	12	8	27.4	31.5	11	3	8	10.9	13.6	10	7	9	11.2	12.4
8	12	8	22.9	26.8	13	3	8	11.8	7.0	1	6	9	37.2	39.7
10	12	8	11.8	7.5	2	2	8	20.2	17.8	3	6	9	23.7	25.2
1	11	8	9.0	12.2	4	2	8	20.6	15.3	5	6	9	20.1	12.4
3	11	8	9.3	10.1	6	2	8	20.2	15.7	7	6	9	32.1	36.7
5	11	8	5.8	11.2	8	2	8	35.4	33.0	9	6	9	31.6	28.4
7	11	8	10.5	16.4	10	2	8	22.1	10.5	0	5	9	50.9	57.2
9	11	8	11.3	3.5	12	2	8	11.4	15.8	2	5	9	122.4	119.3
0	10	8	75.4	76.0	3	1	8	23.4	29.9	4	5	9	71.4	73.9
2	10	8	109.1	109.7	5	1	8	22.3	27.5	6	5	9	96.6	89.1
4	10	8	65.9	63.7	7	1	8	64.8	61.6	8	5	9	47.5	48.9
6	10	8	101.6	59.4	9	1	8	9.7	9.6	10	5	9	106.3	101.6
8	10	8	55.2	55.7	11	1	8	24.4	13.2	1	4	9	19.0	22.6
10	10	8	76.7	76.9	13	1	8	11.7	2.6	3	4	9	13.0	8.9
1	9	8	43.4	47.5	2	0	8	75.2	74.1	5	4	9	26.9	18.5
					4	0	8	75.9	73.6					
					6	0	8	71.3	70.3					

7	4	9	16.0	19.9	2	10	10	74.8	75.4	4	3	11	56.4	49.9
9	4	9	24.0	15.6	4	10	10	71.9	67.9	1	2	11	13.6	14.9
11	4	9	11.2	3.6	6	10	10	57.9	55.1	3	2	11	7.0	1.8
0	3	9	10.6	22.1	1	9	10	9.3	9.4	5	2	11	23.0	20.3
2	3	9	82.8	82.6	3	9	10	54.2	59.0	2	1	11	11.5	8.2
4	3	9	21.3	16.6	5	9	10	42.2	41.1	4	1	11	36.0	22.0
6	3	9	60.9	54.4	7	9	10	10.6	3.2	6	1	11	9.5	9.2
8	3	9	20.5	23.6	0	8	10	29.1	28.9					
10	3	9	61.7	55.9	2	8	10	14.9	8.5					
3	2	9	49.2	50.4	4	8	10	60.0	56.3					
5	2	9	28.8	27.3	6	8	10	17.0	19.8					
7	2	9	42.7	39.4	1	7	10	47.1	49.5					
9	2	9	23.3	25.7	3	7	10	21.3	19.8					
11	2	9	42.1	41.7	5	7	10	36.4	31.5					
2	1	9	55.3	53.5	7	7	10	63.4	59.2					
4	1	9	47.7	42.5	0	6	10	28.6	20.8					
6	1	9	44.2	37.2	2	6	10	33.3	26.8					
8	1	9	20.4	11.4	4	6	10	15.7	11.6					
10	1	9	59.4	59.4	6	6	10	17.3	17.3					
1	13	10	10.4	6.0	8	6	10	21.2	19.5					
0	12	10	34.5	22.3	1	5	10	32.5	30.3					
2	12	10	10.1	15.2	3	5	10	17.1	12.6					
1	11	10	19.6	19.8	5	5	10	21.4	27.5					
3	11	10	17.7	5.9	7	5	10	18.7	19.3					
5	11	10	21.1	23.0	0	4	10	88.3	84.3					
0	10	10	98.8	95.4	2	4	10	62.3	56.8					
					4	4	10	47.3	44.5					
					6	4	10	54.8	47.7					
					8	4	10	72.5	66.0					
					1	3	10	9.2	6.9					
					3	3	10	29.3	30.6					
					5	3	10	19.5	30.3					
					7	3	10	9.3	14.2					
					9	3	10	10.5	3.0					
					0	2	10	33.3	31.9					
					2	2	10	23.8	24.3					
					4	2	10	13.5	10.0					
					6	2	10	15.0	9.3					
					8	2	10	27.7	19.6					
					3	1	10	46.6	44.8					
					5	1	10	23.7	18.8					
					7	1	10	9.8	12.7					
					9	1	10	16.9	8.1					
					2	0	10	79.3	76.6					
					4	0	10	102.7	99.6					
					6	0	10	98.1	92.7					
					8	0	10	17.7	16.1					
					1	8	11	9.2	8.0					
					0	7	11	34.1	34.8					
					2	7	11	33.6	23.7					
					1	6	11	16.5	8.7					
					3	6	11	8.7	7.1					
					0	5	11	54.5	55.8					
					2	5	11	72.1	68.3					
					4	5	11	72.3	63.0					
					1	4	11	6.6	2.3					
					3	4	11	16.0	0.0					
					5	4	11	15.6	9.3					
					0	3	11	22.1	18.7					
					2	3	11	12.0	20.9					

End of supplemental material.