$\Sigma\,|F_o - |F_c||/\Sigma\,F_o$, was 11 % after six cycles of least squares, anisotropic temperature factors being used in the final three cycles.

Inspection of observed and calculated F values showed that strong reflections were significantly affected by extinction. To minimize the extinction effects, the single crystal F_o's for strong reflections ($F_o \geq 100$) except for 020 and 040 peaks were replaced by the corresponding powder structure factors. Both single-crystal and powder data were placed on a common scale by comparing observed structure factors with those calculated in the preceding refinement. The 020 and 040 reflections, together with unobserved reflections, were given zero weight in the least-squares cycles, although included in the final calculation of the R index. The refinement of these combined single-crystal and powder data was complete after three cycles, giving $R = 6{\cdot}7$ %. Table 1 gives the values of the positional and thermal parameters. Observed and calculated structure factors (final refinement) are listed in Table 2. Table 3 lists interionic distances and angles computed from the structural parameters determined in the present work, and Fig. 1 shows that part of the unit cell which is relevant to the values listed in Table 3.

Table 2. *Observed and calculated structure factors*

For unobserved reflections the values are $(10/\sqrt{3})F_{\min}$, where $F_{\min}$ is the minimum F observed in the corresponding region of reciprocal space; those values are marked with an asterisk.

hkl	$10F_o$	$10F_c$	hkl	$10F_o$	$10F_c$	hkl	$10F_o$	$10F_c$
004	1091	1209	127	317	285	273	169	141
008	535	559	132	1636	1627	280	615	561
011	387	398	134	248	272	332	1517	1576
013	734	753	136	803	786	336	585	573
015	*40	95	141	258	218	341	565	502
017	119	144	143	337	341	343	159	160
020	1715	2118	145	248	259	345	238	230
022	654	632	147	228	215	352	991	1023
024	1239	1275	152	1061	996	354	248	228
026	*50	52	154	79	73	356	644	642
031	882	891	156	813	852	361	426	410
033	367	380	161	268	251	363	268	239
035	89	76	163	426	380	365	119	109
040	1685	1774	165	159	120	372	813	820
042	297	249	172	863	814	374	59	64
044	1061	1013	181	149	156	381	218	259
046	*30	31	183	129	150	440	1041	1099
051	218	183	220	1110	1132	444	912	874
053	555	531	224	1358	1327	451	129	144
055	*89	99	231	565	601	453	288	306
060	1110	1348	233	*40	28	455	208	218
062	*59	30	235	327	346	460	932	928
064	872	735	237	208	205	462	79	80
071	327	319	240	1130	1176	464	714	657
073	337	306	242	149	122	471	238	242
080	843	737	244	1100	1065	473	149	182
082	198	167	251	*69	87	480	535	541
091	248	257	253	278	270	552	714	711
112	1705	1579	255	307	318	561	149	169
116	1011	1049	260	991	1013	563	278	317
121	129	117	262	188	180	572	506	596
123	228	247	264	843	781			
125	367	393	271	238	248			

Table 3. *Interionic distances and angles*

Distances		Angles	
Y–O(1)	2·299 ± 0·008 Å	O(1)–Y–O(2)	155·6 ± 0·4°
		O(1)–Y–O(3)	92·6 ± 0·4
Y–O(5)	2·443 ± 0·008	O(5)–Y–O(6)	65·1 ± 0·4
		O(5)–Y–O(7)	135·3 ± 0·4
V–O	1·706 ± 0·008	O(5)–V–O(6)	100·9 ± 0·4
		O(5)–V–O(9)	113·9 ± 0·4

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On versions of a procedure for scaling X-ray photographs.

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Two modifications of a method for placing batches of X-ray data on a common scale have been proposed. One of these is an iteration which converges very slowly, and hence yields results with computing errors which are difficult to estimate reliably. This note describes an alternative which gives better convergence and suggests circumstances in which particular methods will be quickest.

The scaling method devised by Hamilton, Rollett & Sparks (1965) (HRS) has been modified by Fox & Holmes (1966) (FH), who found a more appropriate, but slightly more difficult, method of solving the singular set of simultaneous equations for the scale-factor changes. Monahan, Schiffer & Schiffer (1967) (MSS) have proposed a modification which gives a set of independent equations for the scale factors. In this note we show that the MSS method converges very slowly on the test case used by HRS and FH so that any convergence criterion based on the size of the shifts may allow large errors in the results. We therefore describe an approximation to HRS which yields faster convergence than the MSS method. Convergence rates are given in Table 1 and we indicate circumstances in which particular methods are likely to be useful.

Table 1. *Numbers of iterations required to reduce the maximum indicated shift in a scale-factor to various levels*

	Maximum shift in any scale factor				
Method	0·5	0·05	0·005	0·0005	0·00005
FH	3	4	5	6	7
HRS	4	5	6	7	8
FR	6	7	9	12	16
MSS	3	14	55	> 126	

The 14 parameter problem used as a test was that employed by HRS, FH. The final G_p varied from 0·7884 to 6·0622 and the initial G_p were unity. The value of G_1 was kept at unity throughout.

These methods minimize $\sum_h \sum_p w_{hp}(F_{hp}^2 - G_p F_h^2)^2$ with respect to G_p.

The MSS method calculates the scale factor $G_{p,r}$ for the pth of the n batches at iteration r and the scaled structure factors $F^2_{h,r}$ for reflection h at iteration r from:

$$F^2_{h,r} = \sum_p (G_{p,r-1}F^2_{hp}w_{hp}) / \sum_p (G^2_{p,r-1}w_{hp}) \qquad (1)$$

$$G_{p,r} = \sum_h (F^2_{h,r}F^2_{hp}w_{hp}) / \sum_h [(F^2_{h,r})^2 w_{hp}] , \qquad (2)$$

where w_{hp} is the weight given to the observational equation for reflexion h in batch p. Usually $w_{hp} = 1/\sigma^2_{hp}$ and σ_{hp} is the standard deviation of reflection h in batch p.

The iterations terminate when $|(F^2_{h,r} - F^2_{h,r-1})/F^2_{h,r-1}| \le \varepsilon$ for all h, and MSS use $\varepsilon = 0{\cdot}003$. It can be seen from Table 1 that we require many iterations to get stable values of G_p. This is because MSS yields changes in $G_{p,r}$ which are as small as 1/30 of the errors in $G_{p,r}$. Error estimates based on the shifts can therefore underestimate the errors by this factor. This behaviour can be explained by formulating the MSS equation to give shifts in $G_{p,r}$. The MSS equations then have the same right-hand sides as the HRS equations but the matrix of the HRS equations is replaced by a diagonal matrix with larger elements.

We have used a method in which equation (2) is replaced by

$$A_p = \sum_h \{w_{hp}(F^2_{h,r})^2 + w^2_{hp}F^2_{hp}(F^2_{hp} - 2F^2_{h,r}G_{p,r-1}) / (\sum_j w_{hj}G^2_{j,r-1})\} \qquad (3)$$

$$G_{p,r} = G_{p,r-1} + \sum_h (w_{hp}F^2_{h,r}F^2_{hp})/A_p - G_{p,r-1} \sum_h [(w_{hp}(F^2_{h,r})^2]/A_p . \qquad (4)$$

This is a correct diagonal approximation to the HRS equations. It can be unstable because the shifts can be too large. We have dealt with this in the method called FR in Table 1 by limiting the shifts, normalizing to make $G_{1,r} = 1$ for all r and then applying a simple acceleration device. The procedure is to replace equation (4) by

$$C_{p,r} = G_{p,r-1} + \sum_h (w_{hp}F^2_{h,r}F^2_{hp})/A_p - G_{p,r-1} \sum_h [w_{hp}(F^2_{h,r})^2]/A_p \qquad (5)$$

$$D_{p,r} = \max(C_{p,r},\ 0{\cdot}5\ G_{p,r-1}) \qquad (6)$$

$$E_{p,r} = D_{p,r}/D_{1,r} \qquad (7)$$

$$\mathbf{i}_r = \mathbf{E}_r - \mathbf{G}_{r-1}, \text{ where } \mathbf{G}_r = (G_{1,r}, \ldots, G_{n,r}) \textit{ etc.} \qquad (8)$$

$$\mathbf{G}_r = \mathbf{G}_{r-1} + \mathbf{a}_r \text{ where} \qquad (9)$$

$$\mathbf{a}_r = \mathbf{i}_r/(1-K) \text{ and} \qquad (10)$$

$$K = \mathbf{a}_{r-1} . \mathbf{i}_r / \mathbf{a}_{r-1} . \mathbf{a}_{r-1} . \qquad (11)$$

K is set equal to 0 in cycle 1 and is limited so that $K \le 0{\cdot}3$ to avoid excessive extrapolation. Note that similar acceleration of the MSS process would have little effect unless dangerously large values of $1/(1-K)$ were used.

We conclude that the FR method is likely to be the quickest if the number of scale factors is greater than 4 and the whole of the calculation can be performed in a rapid-access store. If, on the other hand, the data must be fetched from a slow peripheral device such as magnetic tape then the FH method has fewest cycles and the original HRS method should only be used if an efficient latent roots and vectors routine is not available. The MSS method is relatively slow and does not provide a reliable estimate of the computing error.

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Misuse of the 'riding' model in correcting bond lengths for effects of ther malmotion*.

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Some examples are cited of misuse of the 'riding' model of Busing and Levy. The appropriateness of the model for a particular bond should be assessed by consideration of the physical situation. Meaningful use of the model can lead only to positive bond-length corrections.

In recent reports of crystal-structure analyses several authors have incorrectly used the 'riding' model of Busing & Levy (1964) as embodied in the computer program *ORFFE* of Busing, Martin & Levy (1962), with the result that 'corrections' to bond lengths for the effects of thermal motion have been reported which are totally devoid of meaning. Instances of misuse of the riding model have been noted in oral presentations, in manuscripts prepared for publication, and, surprisingly, in at least six published papers. The occurrence of such errors may result in part from the fact that the program *ORFFE* was widely distributed before the appearance of the paper (Busing & Levy, 1964) which presented the theory of the riding-model correction.

One misconception evidenced in the published papers (Enrione, Boer & Lipscomb, 1964; Boer, Streib & Lipscomb, 1964; Hall, Perloff, Mauer & Block, 1965; Boer, 1966; Voet & Lipscomb, 1967; Friedman & Lipscomb, 1966) is the notion that the mean interatomic separation $\bar{S}$ as calculated by Busing & Levy can be less than the separation S_0 of the mean positions of the two atoms or, in other words, that corrections for thermal motion can be negative. Busing & Levy (1964) show that $\bar{S}$ is never less than S_0. The program *ORFFE*, however, will allow the unwary user to compute a value of $\bar{S}$ less than S_0. The

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